Chemical Name: High Benzene Naphthas Category
Submitter: ACC

Chemicals in Category:

CHEMICAL NAME	CASRN
Extracts, petroleum, light naphtha solvent	64741-99-7
Naphtha, petroleum, hydrotreated light	64742-49-0
Naphtha, petroleum, hydrodesulfurized light	64742-73-0
Naphtha, petroleum, light steam-cracked	64742-83-2
Distillates, petroleum, steam-cracked	64742-91-2
Distillates, petroleum, heavy arom.	67891-79-6
Distillates, petroleum, light arom.	67891-80-9
Distillates, petroleum, light distillate hydrotreating process, low-boiling	68410-97-9
Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived	68475-70-7
Hydrocarbons, C5-10 arom. conc., ethylene-manuf.-by-product	68476-45-9
Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum	68526-77-2
Gasoline, pyrolysis, debutanizer bottoms	68606-10-0
Hydrocarbons, C5 and C10-aliph. and C6-8-arom.	68606-28-0
Hydrocarbons, ethylene-manuf.-by-product distn. residues	68921-67-5
Distillates, petroleum, light thermal cracked, debutanized arom.	68955-29-3
Hydrocarbons, C4-8	68956-52-5
Petroleum products, C5-12, reclaimed, wastewater treatment	68956-70-7
Fuel oil, pyrolysis	69013-21-4
Naphtha	8030-30-6

As the Agency received data from High Production Challenge Program participants, it posted notice of and links to those data here for public review and comment. Companies and consortia were requested to defer any proposed new testing on their chemicals for a period of 120 days from when their Test Plans and Robust Summaries were posted to the Internet, in order to allow for technical public comment regarding the possible provision of additional existing data or other technical information which might address or eliminate the need for some new testing.

Some sponsors of chemicals submitted revised test plans and robust summaries to the Agency and referred to them as "final" submissions. EPA previously referred to the most recent submission as "revised" and has made no distinction or judgment whether a submission is final. Lastly, technical public comments on test plans and robust summaries were also provided for several chemicals/categories.

TABLE OF CONTENTS

The pdf contains the following documents:

December 12, 2001

Christine Todd Whitman, Administrator
U.S. Environmental Protection Agency
P. O. Box 1473
Merrifield, VA 22116

RE: Olefins Panel Test Plan for High Benzene Naphthas Category, HPV Registration No. 1101064

Dear Ms. Whitman:

The Olefins Panel of the American Chemistry Council submits its test plan for the High Benzene Naphthas Category under the High Production Volume (HPV) Challenge Program. This CAS numbers included in this category are listed in the attached table.

In preparing this test plan, the Panel has given careful consideration to the principles contained in the letter EPA sent to all HPV Challenge Program participants on October 14, 1999. As requested by EPA in that letter, the Panel has sought to maximize the use of scientifically appropriate categories of related chemicals and of structure activity relationships. The Panel has coordinated with other industry groups covering related chemicals. Additionally, and also as requested in EPA's letter, in analyzing the adequacy of existing data, the Panel has conducted a thoughtful, qualitative analysis rather than use a rote checklist approach. The Panel has taken the same thoughtful approach when developing this test plan and believes it conforms to those principles.

If you have any questions, please contact Elizabeth Moran, Manager of the Olefins Panel at (301) 924-2006 or Elizabeth_Moran@americanchemistry.com.

Courtney M. Price
Vice President, CHEMSTAR

cc: C. Auer, EPA
B. Leczynski, EPA
S. Russell, ACC
J. Keith, ACC

CAS Numbers and Descriptions Associated with Streams in the High Benzene Naphthas Category

CAS Number	CAS Number Description
64741-99-7	Extracts, petroleum, light naphtha solvent
64742-49-0	Naphtha, petroleum, hydrotreated light
64742-73-0	Naphtha, petroleum, hydrodesulfurized light
64742-83-2	Naphtha, petroleum, light steam-cracked
64742-91-2	Distillates, petroleum, steam-cracked
67891-79-6	Distillates, petroleum, heavy arom.
67891-80-9	Distillates, petroleum, light arom.
68410-97-9	Distillates, petroleum, light distillate hydrotreating process, low-boiling
68475-70-7	Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived
68476-45-9	Hydrocarbons, C5-10 arom. conc., ethylene-manuf.-by-product
68526-77-2	Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum
68606-10-0	Gasoline, pyrolysis, debutanizer bottoms
68606-28-0	Hydrocarbons, C5 and C10-aliph. and C6-8-arom.
68921-67-5	Hydrocarbons, ethylene-manuf.-by-product distn. residues
68955-29-3	Distillates, petroleum, light thermal cracked, debutanized arom.
68956-52-5	Hydrocarbons, C4-8
68956-70-7	Petroleum products, C5-12, reclaimed, wastewater treatment
69013-21-4	Fuel oil, pyrolysis
8030-30-6	Naphtha

Note: The definitions, found in the TSCA Chemical Substance Inventory, for the CAS numbers included in this group are vague with respect to composition. Therefore, it is not uncommon to find that the same CAS number is correctly used to describe different streams (compositions) or that two or more different CAS numbers are used to describe the same stream (composition).

HIGH PRODUCTION VOLUME (HPV)

CHEMICAL CHALLENGE PROGRAM

TEST PLAN

For The

High Benzene Naphthas Category

Prepared by:

American Chemistry Council
Olefins Panel
HPV Implementation Task Group

December 18, 2001

PLAIN ENGLISH SUMMARY

The High Benzene Naphthas Category was developed for the HPV Program by grouping ethylene manufacturing streams (products) that exhibit commonalities from both manufacturing process and compositional perspectives. The 19 CAS Numbers in the category are associated with ten streams. These 10 streams, which are commercial products or isolated intermediates, contain significant levels of benzene (generally greater than 10% and averaging about 55%).

All streams in this category are subject to the Occupational Safety and Health Administration (OSHA) Benzene Standard (29 CFR 1910.1028). Those streams containing 1,3-butadiene are subject to the OSHA Butadiene Standard (29 CFR 1910.1051). OSHA Permissible Exposure Limits exist for all major components. Benzene, as the predominant component in most streams, is expected to be the key driver with respect to health effects endpoints within the SIDS battery of tests. However, as the concentration of benzene is decreased and the concentrations of other components are increased, the observed effects of benzene are expected to diminish and the effects of other components are expected to increase. The major chemical components of the streams in the High Benzene Naphthas Category have been extensively tested for human health toxicity endpoints and some data are available for other components and for two streams. Additional supporting data for components of the High Benzene Naphthas streams, tested either individually or as components of other streams or mixtures, will be collected for other test plans within the Olefins Panel's HPV program, by other consortia participating in the HPV or ICCA programs, or for chemicals sponsored in the OECD SIDS program. Hence, the basic strategy of this screening level test plan for characterizing the human health hazards of this category is to evaluate data for the components of the streams, as well as data for mixtures of category components and analogous mixtures (existing data and data being developed by other test programs). These data are expected to provide sufficient information to develop scientific judgment-based characterizations of the human health effects of streams in this category for purposes of satisfying HPV program requirements. Therefore, no additional human health toxicity testing is proposed.

Data will be developed and/or identified to adequately characterize relevant physicochemical endpoints in the HPV Chemical Challenge Program.

Existing data provide sufficient information to adequately characterize the biodegradability and aquatic toxicity of products in this category. Therefore, no additional biodegradation or aquatic toxicity testing is proposed.

Information or data will be developed on the potential of products in the High Benzene Naphthas Category to photodegrade, hydrolyze, and partition within the environment.

EXECUTIVE SUMMARY

The Olefins Panel (Panel) of the American Chemistry Council and the Panel's member companies hereby submit for review and public comment the test plan for the "High Benzene Naphthas" Category under the Environmental Protection Agency (EPA) High Production Volume (HPV) Chemical Challenge Program (Program). It is the intent of the Panel and its member companies to use new information in conjunction with a variety of existing data and scientific judgment/analyses to adequately characterize the SIDS (Screening Information Data Set) human health, environmental fate and effects, and physicochemical endpoints for this category in satisfaction of HPV Program requirements.

The High Benzene Naphthas Category was developed for the HPV Program by grouping ethylene manufacturing streams that exhibit commonalities from both manufacturing process and compositional perspectives. The 19 CAS Numbers in the High Benzene Naphthas Category are associated with ten streams. The ten streams are commercial products or isolated intermediates. The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%. This grouping of CAS numbers represents hydrocarbon streams with a carbon number distribution that is predominantly C5 – C11, through components boiling at 650°F or higher.

Human Health Effects

All streams in this category are subject to the Occupational Safety and Health Administration (OSHA) Benzene Standard (29 CFR 1910.1028). Those streams containing 1,3-butadiene are subject to the OSHA Butadiene Standard (29 CFR 1910.1051). OSHA Permissible Exposure Limits exist for all major components. Benzene, as the predominant component in most streams, is expected to be the key driver with respect to health effects endpoints within the SIDS battery of tests, with genotoxicity and hematotoxicity the effects most likely to be seen. However, as the concentration of benzene is decreased and the concentrations of other components are increased, the observed effects of benzene are expected to diminish and the effects of other components are expected to increase.

Benzene has a robust toxicity dataset and has completed the OECD SIDS program. No further testing of benzene is needed for the HPV Chemical Challenge Program. The other major chemical components of streams in the High Benzene Naphthas Category have been extensively tested for human health toxicity endpoints, and all components present in the streams at concentrations greater than 5% have been tested in at least one toxicity study. Those components having only limited data lack structural alerts for mammalian toxicity and data exist for structural analogs. Some data are available for one High Benzene Naphthas stream [Hydrotreated C6-C8 Fraction] and a stream similar to the Pyrolysis Gasoline streams. Some data are also available regarding interactions between certain components that impact metabolism and toxicity. Additional supporting data for components of the High Benzene Naphthas streams, tested either individually or as components of other streams or mixtures, will be collected for other test plans within the Olefins Panel's HPV program, by other consortia participating in the HPV or ICCA programs, or for chemicals sponsored in the OECD SIDS program.

Hence, the basic strategy of this screening level test plan for characterizing the human health hazards of this category is to evaluate data for the components of the streams, as well as data for mixtures of category components and analogous mixtures (using existing data and data being developed by other test programs). These data are expected to provide sufficient information to develop scientific judgment-based characterizations of the human health effects of streams in this category in satisfaction of HPV program requirements. Based upon examinations of stream compositions and existing toxicity data, there is minimal likelihood for the appearance of unexpected or remarkable biological findings in testing of these streams. Therefore, no additional human health toxicity testing is proposed.

Physicochemical Properties, Environmental Fate, and Aquatic Toxicity

Existing measured data will be identified to adequately characterize physicochemical endpoints in the HPV Chemical Challenge Program. In addition, calculated data will be developed to characterize the physicochemical endpoints for selected chemicals in products from this category and compared with the existing measured data.

The strategy for characterizing the biodegradability and aquatic toxicity of products in this category is to evaluate data on component chemicals contained by products in this category and similar complex products. Read across biodegradation data show that products in the High Benzene Naphthas Category have the potential to exhibit a high extent of biodegradability. Read across aquatic toxicity data show that products in the High Benzene Naphthas Category have the potential to produce a moderate level of toxicity in freshwater algae and acute toxicity in freshwater fish and invertebrates. Existing data provide sufficient information to adequately characterize the biodegradability and aquatic toxicity of products in this category. Therefore, no additional biodegradation or aquatic toxicity testing is proposed.

The chemical components in these products are relatively volatile, and if released they would be expected to partition to the air phase to a significant extent. In the air, they are subject to rapid physical degradation through hydroxyl radical attack. Therefore, as a result of both biological and physical degradation processes, these products are not expected to persist in the environment. Information has not been developed on the potential of products in this category to photodegrade, hydrolyze, and partition within the environment. Therefore, information or data will be developed to characterize these endpoints in satisfaction of HPV program requirements.

LIST OF MEMBER COMPANIES
THE OLEFINS PANEL

The Olefins Panel includes the following member companies:

ATOFINA Petrochemicals, Inc.*
BP Chemical Company
Chevron Phillips Chemical Company
The Dow Chemical Company
E. I. du Pont de Nemours and Company
Eastman Chemical Company
Equistar Chemicals, LP
ExxonMobil Chemical Company
Formosa Plastics Corporation, U.S.A.
The Goodyear Tire & Rubber Company*
Huntsman Corporation
Koch Industries
NOVA Chemicals Inc.
Noveon, Inc*
Sasol America, Inc.
Shell Chemical Company
Sunoco, Inc.
Texas Petrochemicals Corporation*
Westlake Chemical Corporation
Williams Olefins, LLC

* These companies are part of the Olefins Panel but do not produce streams in the High Benzene Naphthas Category.

TABLE OF CONTENTS
TEST PLAN FOR THE HIGH BENZENE NAPHTHAS CATEGORY

TEST PLAN FOR THE HIGH BENZENE NAPHTHAS CATEGORY

I. INTRODUCTION

The Olefins Panel (Panel) of the American Chemistry Council and the Panel's member companies have committed to develop screening level human health effects, environmental effects and fate, and physicochemical data for the High Benzene Naphthas Category under the Environmental Protection Agency (EPA) High Production Volume (HPV) Chemical Challenge Program (Program).

In preparing this test plan, the Panel has given careful consideration to the principles contained in the letter EPA sent to all HPV Challenge Program participants on October 14, 1999. As directed by EPA in that letter, the Panel has sought to maximize the use of scientifically appropriate categories of related chemicals and structure activity relationships. Additionally, and also as directed in EPA's letter, in analyzing the adequacy of existing data, the Panel has conducted a thoughtful, qualitative analysis rather than use a rote checklist approach. The Panel has taken the same thoughtful approach when developing its test plan. The Panel believes its test plan conforms to the principles articulated in EPA's letter.

This plan identifies CAS numbers used to describe process streams in the category, identifies existing data of adequate quality for substances included in the category, and outlines activities to develop screening level data for this category under the Program. The objective of this effort is to identify and/or develop sufficient test data and/or other information to adequately characterize the human health effects and environmental effects and fate for the category in accordance with the EPA HPV Program. Physicochemical data that are requested in this program will be calculated as described in EPA guidance documents. In addition, measured data will be provided for selected products in this category where readily available.

II. DESCRIPTION OF THE HIGH BENZENE NAPHTHAS CATEGORY

A. The Category

The High Benzene Naphthas Category was developed for the HPV program by grouping ethylene manufacturing streams that exhibit commonalities from both manufacturing process and compositional perspectives. The 19 CAS numbers listed in Table 1 describe 10 streams which are complex products containing many components. Certain single streams are correctly represented by more than one CAS number, and a CAS number may be applicable to more than one stream. A description of the ethylene and associated stream production processes is included in Appendix I. A list of the other ethylene manufacturing stream categories being sponsored by the American Chemistry Council Olefins Panel is shown in Table 11.

The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about

55%. In some cases, petroleum refinery streams may be combined with intermediate streams from the ethylene unit and coprocessed to produce these products. This grouping of CAS numbers represents hydrocarbon streams with a carbon number distribution that is predominantly C5-C11, through components boiling at 650°F or higher. Pyrolysis gasoline is included in this category. The typical compositions of streams in this category are listed in Table 2.

The CAS Numbers in the High Benzene Naphthas Category are associated with the following streams, which are commercial products or isolated intermediates:

Pyrolysis Gasoline
Pyrolysis C6 Fraction
Pyrolysis C6-C8 Fraction
Pyrolysis C5-C6 Fraction
Hydrotreated C6 Fraction
Hydrotreated C6-C7 Fraction
Hydrotreated C6-C8 Fraction
Quench Loop Pyrolysis Oil and Compressor Oil
Recovered Oil from waste water treatment
Extract from Benzene Extraction

Descriptions of the ten streams associated with the High Benzene Naphthas Category are presented below:

1. Pyrolysis Gasoline

Pyrolysis Gasoline (Pygas) consists predominantly of C5+ hydrocarbons produced by the ethylene cracking furnaces. Typically the stream is derived from (1) the bottoms product from the debutanizer, (2) oils separated from furnace effluent quench systems, and (3) "drips" or condensate resulting from compression of the cracked gas. The oils from the quench systems and the "drips" may be stabilized to remove lights before blending with Pygas from the other sources. Depending on the plant configuration, Pygas may contain all of these intermediate streams, or the quench oils and stabilized drips may be transferred as separate streams. Low concentrations (e.g. 3% total) of C4 and lighter hydrocarbons may be present in the stream. A detailed analysis of Pygas may identify 60 or more hydrocarbon components or component groups, primarily unsaturated hydrocarbons and aromatics. Benzene, toluene, and dicyclopentadiene together may account for more than 50% of a Pygas stream and typically no other single component is present at a level greater than about 5%. The benzene concentration of Pygas is typically about 40% and the reported values range from 15 to 62%. The concentrations of individual hydrocarbon components in Pygas vary depending on the type of feedstock used by the ethylene plant, the mode of operation of the cracking furnaces (i.e. severity) and the ethylene process configuration. One non-typical Pygas stream is reported to contain vinylacetate at a concentration of up to about 10%. Vinylacetate is not typically found in ethylene process streams.

2. Pyrolysis Gasoline Fractions (Pyrolysis C6, C6-C8, and C5-C6 Fractions)

Pyrolysis gasoline is separated by distillation into various boiling-point-range fractions as intermediates in preparation for further processing. In some cases, petroleum refinery streams such as a C6 reformate fraction are combined with the pyrolysis gasoline prior to this separation. Similar to the situation for Pygas, the compositions of these fractions vary depending on the ethylene process feedstock and the other operating variables.

(a) Pyrolysis C5-C6 Fraction

The carbon number distribution for this stream is predominantly C5 to C6. One typical composition for this stream is reported as 70% benzene and 10% pentenes.

(b) Pyrolysis C6 Fraction

The carbon number distribution for this stream is predominantly C6. Reported compositions vary from 35 to 77% benzene, 0.5 to 5% toluene with the balance primarily C6 non-aromatics, which are expected to be largely unsaturates.

(c) Pyrolysis C6-C8 Fraction

This stream has a carbon number distribution that is predominantly C6 to C8. The reported compositions range from 30 to 80% benzene, 15 to 25% toluene and 3 to 23% C8 aromatics.

3. Hydrotreated Pyrolysis Fractions (C6, C6-C7 and C6-C8 Fractions)

Pyrolysis gasoline or distillate fractions of pyrolysis gasoline are sometimes treated with hydrogen over catalyst to saturate or partially saturate diolefins and/or olefins. In some cases, petroleum refinery streams such as a C6 reformate fraction are combined with the pyrolysis gasoline prior to this step. The hydrogenation process may be either one-stage or two-stage. The one-stage process is typically a liquid-phase process where the primary objective is to selectively convert diolefins to mono-olefins and to convert vinyl aromatics, for example, styrene to ethylbenzene. The second stage in a two-stage hydrogenation process is typically a vapor-phase, more severe hydrogenation that converts essentially all of the contained olefins to saturated hydrocarbons. A pygas fraction that will be processed by extraction or extractive distillation to produce high purity aromatics (benzene, toluene or xylenes) is subjected to two-stage hydrogenation. Pygas fractions may be forwarded to hydrodealkylation units (less common) for benzene production after one-stage of hydrogenation. Hydrotreated Pyrolysis fractions may be the result of either one- or two-stage hydrogenation.

(a) Hydrotreated C6 Fraction

This stream is very similar in composition to the Pyrolysis C6 fraction except that the non-

aromatics present in the hydrotreated stream are essentially all saturates. The reported composition for the Hydotreated C6 stream indicates typical benzene content of 75%.

(b) Hydrotreated C6-C7 Fraction

The carbon number distribution for this stream is predominantly C6 -C7 and the reported values indicate 40 to 70% benzene, and 3 to 15% toluene.

(c) Hydrotreated C6-C8 Fraction

The reported typical compositions for this stream are 40 to 60% benzene, 10 to 25% toluene and 3 to 10% C8 aromatics.

4. Quench Loop Pyrolysis Oil and Compressor Oil

Quench Loop Pyrolysis Oil (Pyoil) represents higher boiling hydrocarbons that condense in the water quench system of an ethylene plant, typically at an ethylene unit cracking ethane, propane or butane. The stream can also include liquids collected at the cracked gas compressor knock out drums, which may include compressor injection oil. The carbon number distribution for Pyoil is C4 (or even lower) through heavier hydrocarbons such as naphthalene or even heavier. The reported typical composition includes 10 to 22% benzene and 5 to11% toluene.

5. Recovered Oil from Wastewater Treatment

This stream can be expected to be of variable composition and made up largely of the components found in Pygas. No composition data or process specific information has been reported. Typically, water streams at ethylene units are processed to separate hydrocarbons from the water so that the water can be reused to generate steam for process-contact use (dilution steam for the cracking furnaces) or so that excess water can be forwarded to treatment prior to discharge or reuse. Water processing typically includes mechanical and gravity separation and steam or gas stripping. Hydrocarbons separated from the water in these systems are not usually isolated from the process. However, at least in one case, the Recovered Oil from Wastewater Treatment has been reported as an isolated intermediate.

6. Extract from Benzene Extraction

Hydrotreated pyrolysis fractions containing aromatics (most commonly benzene or benzene and toluene) are typically charged to extraction or extractive distillation units where the mixed aromatics are recovered as the Extract from Benzene Extraction. The carbon number distribution

for this steam is predominantly C6 to C8. A reported typical concentration indicates 60 to 75% benzene, 25 to 40% toluene and 0 to 1% xylenes.

III. TEST PLAN RATIONALE

A. Human Health Effects

The High Benzene Naphthas Category comprises 10 streams (complex products containing high levels of benzene [10-80%] plus many other components). All streams in this category are subject to the Occupational Safety and Health Administration (OSHA) Benzene Standard (29 CFR 1910.1028). Those streams containing 1,3-butadiene are subject to the OSHA Butadiene Standard (29 CFR 1910.1051). OSHA Permissible Exposure Limits exist for all major components. Benzene, as the predominant component in most streams, is expected to be the key driver with respect to health effects endpoints within the SIDS battery of tests, with genotoxicity and hematotoxicity the effects most likely to be seen. However, as the concentration of benzene is decreased and the concentrations of other components are increased, the observed effects of benzene are expected to diminish and the effects of other components are expected to increase.

Benzene has a robust toxicity dataset, including data on human experience, and has completed the OECD SIDS program. No further testing of benzene is needed for the HPV Chemical Challenge Program. The existing epidemiology and toxicology database for the components other than benzene and for mixtures containing the components is extensive. All components present in the streams at concentrations greater than 5% have been tested in at least one toxicity study. Those components having only limited data lack structural alerts for mammalian toxicity and data exist for their structural analogs. The C5 and C6 alkanes and alkenes present in the streams are not expected to significantly contribute to the toxicity profile as these substances are present in the streams at low concentrations and, with the exception of hexane, generally have a low level of toxicity. The toxic effects of hexane (present at $\leq$ 15%) are unlikely to be observed due to the presence of the other components, as noted below in Section III.A.1. Some data are available for one High Benzene Naphthas stream (Hydrotreated C6-C8 Fraction) and for a stream similar to the Pyrolysis Gasoline streams.

Additional data for the components, or for structural analogs of components, are under development by the American Chemistry Council Olefins Panel for other categories under the HPV program, by other HPV consortia, and by the OECD SIDS program (see Table 3). Furthermore, some of the materials being distilled out of Pyrolysis Gasoline are being tested in other Panel HPV Test Plans (Non-Cyclic C5s and Resin Oils and Cyclodiene Dimer Concentrates categories); and the High Benzene Naphthas Category shares many of the same components with the gasoline blending streams referenced in the API Petroleum HPV Gasoline Test Plan. These gasoline stream data can contribute to the hazard evaluation for the members of this category by showing effects, or lack thereof, due to mixtures containing components of this category when the benzene content is very low (~ 2%).

Hence, the basic strategy of this screening level test plan for characterizing the human health hazards of this category is to evaluate data for the components of the streams, as well as data for mixtures of

category components and analogous mixtures (existing data and data being developed by other test programs). For the HPV program, the Panel believes that the human health hazards of the category can be adequately characterized, using scientific judgment, without conducting additional toxicology tests. The Panel further believes that additional testing on streams is unlikely to demonstrate any adverse effects that have not been shown for components, and would provide little useful data for regulatory, industrial hygiene, emergency response or hazard communication purposes. Thus, no additional testing is proposed in this test plan.

Assessments of the hazards of the category members will be developed after all new data from other testing programs become available.

A discussion of chemical component interactions, specific strategies and rationales for each of the SIDS human health toxicity endpoints, and robust summaries is presented below:

1. Chemical Component Interactions

When tested as pure substances, some of the components other than benzene have caused genetic damage and adverse target organ effects in repeated-dose animal studies, as shown in Table 3. However, since the biologically active components of the High Benzene Naphthas streams are metabolized through a common P450 metabolic pathway, it is anticipated that multiple components will compete for the same active enzyme sites. Component toxicities, which are dependent on the formation of biologically active metabolites, may be reduced as less metabolite(s) will be produced through competition for these sites. Direct support for reduction or elimination of toxicities of individual components is provided by results of an existing mouse bone marrow micronucleus test with one of the High Benzene Naphthas streams, Hydrotreated C6-8 Fraction. This stream, containing approximately 55% benzene, was negative in a mouse bone marrow micronucleus test when administered by oral gavage at 5000 mg/kg to male and female CD-1 mice (see robust summary). Several studies have shown that benzene administered orally to CD-1 mice induces high frequencies of micronuclei in bone marrow erythrocytes at doses as low as 110 mg/kg (Ciranni et al., 1988; Suzuki et al., 1989; Hite et al., 1980; Gad-El Karim et al., 1986; Meyne and Legator, 1980). The presence in the Hydrotreated C6-8 Fraction of other components (approximately 25% toluene, 10% xylene, 7% pentane, 7% ethylbenzene, 3% cyclohexane, and 2% hexane) apparently inhibited the expected clastogenicity of benzene. Other similar interactions between components of the category have also been reported, as noted below.

Medinsky et al. (1994) and Bond et al. (1998) reviewed the metabolism of benzene and the effects of interactions with other organic chemicals on benzene toxicity and metabolism. Reports of interactions between other components of the High Benzene Naphthas Category have also been noted in the literature. Examples of these interactions and the effect on the formation of benzene metabolites and resultant hematotoxicity or genotoxicity are shown below:

- When benzene (440 mg/kg) and toluene (430, 860, or 1720 mg/kg) were coadministered orally to

mice, the clastogenic effect of benzene was reduced (Gad-El-Karim et al., 1984, 1986).

- Coadministration of toluene (1720 mg/kg), i.p., with benzene (440 and 880 mg/kg) to mice resulted in a reduction in the quantity of benzene metabolites measured in the urine (Andrews et al., 1977). Coexposure to toluene also protected against benzene-induced depression in ^{59}Fe utilization by red blood cells, which is used as a measure of hematotoxicity.
- Coexposure to 2000 ppm fully vaporized or light gasoline components reduced the incidence of genetic damage (micronuclei in bone marrow) resulting from a single 6-hr exposure to 40 ppm benzene (Bond et al., 1998). The major components of the fully vaporized gasoline and light gasoline mixtures, respectively, were n-butane (6.1%, 23.9%), n-pentane (3.7%, 8.4%), isopentane (12.3%, 33.5%), n-heptane (1.2%, 0.3%), toluene (8.2%, 1.1%), ethylbenzene (2.3%, 0.1%), and xylenes (8.4%, 0.2%). In these experiments, the fully vaporized gasoline mixture, which contained a higher fraction of aromatic hydrocarbons, was a more effective inhibitor of benzene metabolism than was the light fraction, which was composed primarily of aliphatic hydrocarbons.
- Results of studies with styrene-butadiene mixtures showed a decrease in the rate of metabolism of each chemical but an increase in the concentration of the circulating epoxide metabolites (Bond et al., 1998). The frequency of micronuclei seen in mice exposed by inhalation to butadiene was not altered by simultaneous exposure to styrene.
- Synergistic losses of auditory sensitivity occurred following combined exposure of rats to vapors of toluene plus n-hexane and xylene plus n-hexane (Nylen, 1996). These combined exposures, however, produced antagonistic effects in nerve conduction or action potential amplitudes in the auditory pathway, visual pathway, and peripheral nerve.
- Exposure of male rats to 1000 ppm n-hexane for 61 days caused testicular atrophy and loss of germ cell line (Nylen, 1989). Simultaneous administration of 1000 ppm toluene or xylene did not cause germ cell line alterations or testicular atrophy.
- Neurological effects have been observed in many intermediate-duration inhalation experiments in rats exposed to n-hexane (ATSDR, 1999). No neurotoxic effects were observed in a 2-year chronic study in rats and mice with commercial hexane containing 52.2% n-hexane, 16.0% 3-methylpentane, 15.6% methylchclopentane, 11.6% 2-methylpentane, 3.2% cyclohexane (Daughtrey et al., 1999). In a separate 13-week inhalation study of commercial hexane, a detailed neurobehavioral/neuropathological evaluation revealed no n-hexane-induced neuropathy (Soiefer et al., 1991).

2. Specific Strategies/Rationales for Each Endpoint

Specific strategies and rationales for each of the SIDS human health toxicity endpoints are presented below:

Acute Toxicity

There is an abundance of acute toxicity data for components present in the streams from this category at concentrations greater than 5% (see Table 3). Data is also available for one of the category streams (Hydrotreated C6-C8 Fraction) and a stream similar to the Pyrolysis Gasoline streams. Except for

dicyclopentadiene, the components have demonstrated low acute toxicity. High concentrations were needed to produce lethality via oral gavage and inhalation routes of exposure. In several studies with rats, dicyclopentadiene produced lethality at much lower doses (ranges: oral LD_{50} = 347 to 820 mg/kg, inhalation LC_{50} = 359 to >500 but < 1000 ppm). The oral LD_{50} for cyclopentadiene was 1.66 g/kg and the LD_{50}s for the other components were greater than 2 g/kg. The inhalation LC_{50}s for the components other than dicyclopentadiene ranged from 3680 to 120,000 ppm. The two streams that were tested had oral LD_{50}s greater than 2 g/kg and the one stream tested for acute inhalation toxicity had an LC_{50} greater than 12,408 ppm. Most components also have acute data for other species and routes of exposure. Thus, for purposes of the HPV Challenge Program, the available data is adequate to characterize the acute toxicity of the category members. Therefore, no additional testing for acute toxicity is proposed.

Genetic Toxicity – Gene Mutation

Of the identified category components present at concentrations greater than 5%, only 1,3-butadiene and benzene have consistently caused gene mutations in genetic toxicity tests (see Table 10). 1,3-Butadiene was positive in several *in vivo* and *in vitro* tests. Benzene was negative in several standard tests but was positive in an *in vivo* HPRT gene mutation test in mouse spleenocytes. Based on the data for components, the streams in the category are predicted to be negative in the HPV gene mutation test (Ames Test). Negative Ames Tests conducted with two streams (one from this category and one similar to category streams) support this prediction. Thus, no additional Ames Tests are proposed.

Genetic Toxicity – Chromosome Aberration

Benzene has caused chromosome aberrations in *in vitro* and *in vivo* tests. The other most prevalent component in streams in this category, toluene, is negative in both *in vitro* and *in vivo* tests. Of the remaining identified category components present at concentrations greater than 5%, only vinyl acetate, 1,3-butadiene, isoprene, hexane, and naphthalene have been reported to cause chromosome aberrations (see Table 3). As discussed above, coadministration of benzene with other hydrocarbons that are substrates for the cytochrome P450 enzymes can reduce clastogenicity, as was seen with benzene-toluene and benzene-gasoline mixtures. Further evidence for inhibition of clastogenicity is provided by results from a mouse micronucleus test with one the streams from this category, Hydrotreated C6-8 Fraction. Although the tested Hydrotreated C6-8 Fraction contained approximately 55% benzene, and benzene is positive in the mouse micronucleus test, this stream was negative. Additional information that may be useful will become available from mouse micronucleus testing that will be conducted with streams distilled from Pyrolysis Gasoline that are members of the Panel's C5 Non-Cyclics and Resin Oils and Cyclodiene Dimer Concentrates categories. Thus, based on the composition and available data for components and mixtures of components, sufficient data exist, or will become available, to allow use of scientific judgment to characterize the potential of streams in the category to cause chromosome aberrations. Thus, no additional testing for chromosome aberrations is proposed.

Subchronic Toxicity

Most of the components of the category have extensive epidemiology and toxicology databases, and most major components have been tested for chronic toxicity and carcinogenicity. In addition to the data for components, two streams were tested in repeated-dose studies. A mouse skin painting study was conducted with a stream similar to the Pyrolysis Gasoline fractions (feedstock for pyrolysis gasoline containing C5+ materials) (ExxonMobil, 1982), and a 5-day rat inhalation study was conducted with a Hydrotreated C6-8 stream. See Table 3 for a description of available data.

Repeated oral or inhalation exposures to many of the components of the streams in the category have been shown to cause adverse health effects in a variety of organs. However, existing data also show that antagonistic and synergistic interactions occur between some components comprising the streams, as noted above in Section III.A.1. The target organs affected by exposure to the mixtures, and the severity of the effects, will depend upon the relative concentrations of the components within each stream and the nature of the interactions between components.

Many of the C5 components of the High Benzene Naphthas Category are also components of the Pyrolysis C5s and Hydrotreated C5s streams (C5 Non-Cyclics Category) that will be tested for repeated-dose toxicity by the Panel, as part of the HPV Program. Based on structural similarity, pentenes are likely to have a toxicity profile similar to hexenes. The American Chemistry Council's Higher Olefins Panel will address hexenes as part of the HPV Program. Also, the International Hydrocarbon Solvents Consortium will cover the C5 aliphatic components in its C5 Aliphatics Category. Pentane will be addressed in the American Petroleum Institute's Petroleum Gases Test Plan. Other components are shared with the Panel's Resin Oils and Cyclodiene Dimer Concentrates Category streams.

Several components are sponsored in the OECD SIDS or ICCA programs (see Table 3). Additional studies with these components may be found or conducted within those programs.

Results of available data and relevant data resulting from other programs are expected to be sufficient to adequately characterize the repeated-dose human health hazard endpoints for the substances included in this category. Therefore, no additional repeated-dose testing is proposed.

Developmental Toxicity

Developmental toxicity data exist for most components present in this category at concentrations greater than 5% (see Table 3). In these studies, no convincing evidence was seen for teratogenicity in the absence of maternal toxicity. Fetotoxicity has been reported for some components, but mostly in the presence of maternal toxicity (see Table 3). Only five components (pentenes, cyclopentene, 3-methylpentane, methylcyclopentane, 1,3-cyclopentadiene) lack developmental toxicity tests. However, these components do not have structural alerts for developmental toxicity, and data being generated by other test plans within the HPV Program will provide additional information about the potential of these

substances to cause developmental effects. Three of the five materials are also components of the Pyrolysis C5s and Hydrotreated C5s streams (C5 Non-Cyclics Category) that will be tested for developmental toxicity by the Panel, as part of the HPV Program. Pentenes will be addressed by the International Hydrocarbon Solvents Consortium (C5 Aliphatics Test Plan). Also, based on structural similarity, pentenes are likely to have a developmental toxicity profile similar to hexenes. The American Chemistry Council's Higher Olefins Panel will address hexenes as part of the HPV Program. 3-Methylpentane and methylcyclopentane were components (16.0% and 15.6%, respectively) of a commercial hexane stream that was negative in a rat inhalation developmental toxicity study. A Pyrolysis Gasoline Fraction stream similar to the Pyrolysis Gasoline streams in the High Benzene Naphthas Category has been tested in an oral developmental toxicity study in rabbits. No developmental effects were seen. Additional developmental toxicity information will become available from testing conducted by the Panel for the Resin Oils and Cyclodiene Dimer Concentrates Category with streams distilled from Pyrolysis Gasoline. Thus, existing data and data that will be generated by other test programs are expected to be adequate to characterize the potential of the streams in the category to cause developmental toxicity. No further developmental toxicity tests are proposed for this endpoint.

Reproductive Toxicity

Reproductive toxicity data exist for most components present in this category at concentrations greater than 5% (see Table 3). In its review of benzene, ATSDR (1997) concluded that, although there are some data indicating adverse gonadal effects (e.g., atrophy/degeneration, decrease in spermatozoa, moderate increases in abnormal sperm forms), data on reproductive outcomes are either inconclusive or conflicting. However, most studies indicate no effects on reproductive indices, even at high doses. Reproductive organ effects were seen after inhalation exposure to isoprene and hexane. 1,3-Butadiene is sponsored in the OECD SIDS program and will be tested for reproductive toxicity. Some reproductive toxicity information exists for most major components. Many components have been tested in standard reproductive toxicity studies. Others have data from standard developmental toxicity studies. In addition, most components have data for reproductive organ toxicity, collected in repeated-dose studies. Those components lacking reproductive toxicity information do not have structural alerts for reproductive toxicity, and data being generated by other test plans within the HPV Program will provide additional information about the potential of these substances to cause reproductive effects. Some of these materials are also components of the Pyrolysis C5s and Hydrotreated C5s streams (C5 Non-Cyclics Category) that will be tested for reproductive toxicity by the Panel, as part of the HPV Program. Also, based on structural similarity, pentenes are likely to have a developmental toxicity profile similar to hexenes, which will be addressed by the American Chemistry Council's Higher Olefins Panel as part of the HPV Program. Pentenes will also be covered by the American Chemistry Council's Hydrocarbon Solvents Panel (C5 Aliphatics Test Plan). Additional reproductive toxicity information will become available from testing conducted by the Panel for the Resin Oils and Cyclodiene Dimer Concentrates Category with streams distilled from Pyrolysis Gasoline. 3-Methylpentane and methylcyclopentane were components (16.0% and 15.6%, respectively) of a commercial hexane stream that was negative in a rat inhalation two generation reproductive toxicity study. Thus, existing data and data that will be generated by other test programs are expected to be sufficient to adequately

characterize the potential for reproductive toxicity of the streams in this Category. No further reproductive toxicity tests are proposed.

3. Robust Summaries

Robust summaries for existing data for one stream from the category, Hydrotreated C6-8 Fraction, and for a stream similar to the Pyrolysis Gasoline streams (Pyrolysis Gasoline Fractions [generally C5-C10 but primarily C5-C7: Pyrolysis Gasoline, Rerun Tower Overheads]), are provided with this test plan. Robust summaries for data being developed by other groups for HPV, OECD SIDS, and ICCA high production volume testing programs will be provided when they become available through those programs. Most existing data for components of the category have been extensively reviewed in the literature as noted in Table 3, obviating the need for robust summaries.

B. Physical-Chemical Properties

The physicochemical (PC) endpoints in the HPV Chemical Program include:

- Melting Point
- Boiling Point
- Vapor Pressure
- Water Solubility
- Octanol/Water Partition Coefficient (K_{ow})

Calculated PC data for selected component chemicals in this category will be developed using a computer model to provide a consistent, representative data set. In addition, measured PC data will be identified for selected products in this category and will be summarized together with the calculated data to provide comparisons between the two data sets. The selection of component chemicals to be modeled will be made once an appropriate measured data set is identified.

Calculated PC data for selected component chemicals in the High Benzene Naphthas Category will be developed using the EPIWIN© computer model (EPIWIN, 1999), as discussed in the US EPA document entitled *The Use of Structure-Activity Relationships (SAR) in the High Production Volume Chemicals Challenge Program* (USEPA, 1999a). The use of computer modeling for the development of these data is appropriate since components of the streams in this category are all chemically related and are expected to exhibit relatively similar environmental properties. In addition, for all the chemicals selected to represent products in this category, a calculated dataset provides a common method in the development of these values.

Boiling point, melting point, and vapor pressure ranges will be determined using the MPBPVP subroutine in EPIWIN. K_{ow} and water solubility will be calculated using KOWIN and WSKOW subroutines, respectively. There is more information on calculating data for the HPV chemical program in the EPA document titled '*The Use of Structure-Activity Relationships (SAR) in the High*

Production Volume Chemicals Challenge Program" (U.S. EPA, 1999a).

Because the HPV substances covered under the High Benzene Naphthas Category testing plan are mixtures containing differing compositions, it is not possible to develop or calculate a single numerical value for each of the physicochemical properties. For example, a product that is a mixture of chemicals does not have boiling point, but rather a boiling range. Calculated values for physicochemical properties will be represented as a range of values according to the product's component composition and based on the results of computer modeling. Robust summaries characterizing the PC endpoints will be prepared upon completion of a review of available measured data, and will include the calculated and measured data.

C. Environmental Fate

The environmental fate endpoints in the HPV Chemical Challenge Program include:

- Biodegradation
- Photodegradation
- Hydrolysis
- Fugacity

Although biodegradation data are not available for products in the High Benzene Naphthas Category, there are data for selected component chemicals of those products, as well as for complex products, that can be used to characterize the potential biodegradability of products in this category. The complex product values are for substances composed of a range of chemicals with regard to carbon numbers and chemical classes (i.e., paraffins, alkenes or alkylbenzenes). As suggested by the experimental data, products in this category will exhibit a high extent of biodegradation.

Data or information for the fate endpoints, photodegradation and hydrolysis, will be developed and either will be calculated and/or discussed in technical summaries. Chemicals in this category are not subject to hydrolysis at measurable rates, therefore information for this endpoint will be summarized in a technical review document.

Equilibrium models are used to calculate chemical fugacity, which can provide information on where a chemical is likely to partition in the environment. These data are useful in identifying environmental compartments that could potentially receive a released chemical. Fugacity data can be calculated only for individual chemicals. For the HPV Chemical Challenge Program, environmental partitioning data will be developed for selected component chemicals of the products in this category.

A preliminary evaluation of chemicals in the High Benzene Naphthas Category suggests that they will partition largely to the air, and therefore their fate in air is of environmental interest. Because the air phase may be a compartment that could potentially receive many of the component chemicals in this category, data characterizing their potential for physical degradation in the atmosphere will be

developed (this is discussed below under photodegradation).

1. Biodegradation

There are sufficient data to characterize the potential biodegradability of products in this category. Data for constituent chemicals of products in this category (as well as for complex products not in this category that contain chemicals found in products from this category) suggest that high benzene naphthas products have the potential to biodegrade to a great extent (Table 4). The carbon number of products in this category ranges primarily between C5 to C11. Results for several chemicals, including benzene, with carbon numbers in this range that are contained by these products have been shown to biodegrade from 63 to 100% after 14 or 28 days, while results for several comparable, complex products containing several components range from 21 to 96% after 28 days. As seen by the data in Table 4, there is a relatively large biodegradation database for single chemicals and complex products that can be used to characterize this endpoint for high benzene naphthas products. Because products in this category are compositionally more comparable to the products identified in Table 4 as gasoline streams, these data best describe the potential biodegradability of the high benzene naphtha products. Gasoline stream compositions are provided in Table 5.

The data from the majority of tests in Table 4 were developed using a manometric respirometry test procedure. This procedure uses continuously stirred, closed systems, which is recommended when assessing the potential biodegradability of chemically complex, poorly water soluble, and volatile materials like those in this category. Stirring is recommended when evaluating products containing several chemicals, some of which may have limited water solubility.

2. Photodegradation – Photolysis

Direct photochemical degradation occurs through the absorbance of solar radiation by a chemical substance. If the absorbed energy is high enough, then the resultant excited state of the chemical may lead to its transformation. Simple chemical structures can be examined to determine whether a chemical has the potential for direct photolysis in water. First order reaction rates can be calculated for some chemicals that have a potential for direct photolysis using the procedures of Zepp and Cline (1977).

To develop information or data that will characterize the potential of products in this category to undergo direct photochemical degradation, the existing product chemical composition data will be evaluated to select a subset of chemicals that adequately represents products in this category. The selection process will consider chemical carbon number range, hydrocarbon type, and chemical structure. The UV light absorption of selected chemicals in products in the High Benzene Naphthas Category will be evaluated to identify those chemicals with a potential to degrade in solution. When possible, first order reaction rates will be calculated for chemicals identified to have a potential for direct photolysis in water. The results of the calculations will be summarized in a technical discussion for this endpoint. If instead, a low potential for direct photolysis is suggested by the evaluation, a technical discussion will be prepared to summarize the findings.

3. Photodegradation – Atmospheric Oxidation

Photodegradation can be measured (U.S. EPA, 1999b) (the US EPA identifies OECD test guideline 113 as a test method) or estimated using models accepted by the US EPA (U.S. EPA, 1999a). An estimation method accepted by the US EPA includes the calculation of atmospheric oxidation potential (AOP). Atmospheric oxidation as a result of hydroxyl radical attack is not direct photochemical degradation, but rather indirect degradation. AOPs can be calculated using a computer model. Hydrocarbons, such as those in the High Benzene Naphthas Category, have the potential to volatilize to air where they can react with hydroxyl radicals (OH-).

The computer program AOPWIN (atmospheric oxidation program for Microsoft Windows) (EPIWIN, 1999) is used by the US EPA OPPTS (Office of Pollution Prevention and Toxic Substances). This program calculates a chemical half-life based on an overall OH- reaction rate constant, a 12-hr day, and a given OH- concentration. This calculation will be performed for representative chemical components of products in the High Benzene Naphthas Category. The existing product chemical composition data will be evaluated to select a subset of chemicals that adequately represents products in this category. The selection process will consider chemical carbon number range, hydrocarbon type, and chemical structure. The resulting calculations will be summarized in a robust summary for this endpoint.

4. Hydrolysis

Hydrolysis of an organic chemical is the transformation process in which a water molecule or hydroxide ion reacts to form a new carbon-oxygen bond. Chemicals that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (Neely, 1985).

Chemical stability in water can be measured (EPA identifies OECD test guideline 111 as a test method) or estimated using models accepted by the EPA (U.S. EPA, 1999b). An estimation method accepted by the EPA includes a model that can calculate hydrolysis rate constants for esters, carbamates, epoxides, halomethanes, and selected alkylhalides. The computer program HYDROWIN (aqueous hydrolysis rate program for Microsoft windows) (EPIWIN, 1999) is used for this purpose by OPPTS.

However, all of the chemical structures included in the High Benzene Naphthas Category are hydrocarbons. That is, they consist entirely of carbon and hydrogen. As such they are not expected to hydrolyze at a measurable rate. A technical document will be prepared that discusses the potential hydrolysis rates of these substances, the nature of the chemical bonds present, and the potential reactivity of this class of chemicals with water.

5. Chemical Transport and Distribution in the Environment - Fugacity Modeling

Fugacity based multimedia modeling can provide basic information on the relative distribution of chemicals between selected environmental compartments (i.e., air, soil, sediment, suspended sediment, water, biota). The US EPA has acknowledged that computer modeling techniques are an appropriate approach to estimating chemical partitioning (fugacity is a calculated endpoint and is not measured). A widely used fugacity model is the EQC (Equilibrium Criterion) model (Mackay et al., 1996). The U.S. EPA cites the use of this model in its document titled "*Determining the Adequacy of Existing Data*" U.S. EPA, 1999b), which was prepared as guidance for the HPV Chemical Program.

In its document, U.S. EPA states that it accepts Level I fugacity data as an estimate of chemical distribution values. The input data required to run a Level I model include basic physicochemical parameters; distribution is calculated as percent of chemical partitioned to 6 compartments described above within a defined unit world. Level I data are basic partitioning data that allow for comparisons between chemicals and indicate the compartment(s) to which a chemical is likely to partition.

The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, melting point, vapor pressure, and water solubility to calculate distribution within a unit world. This model will be used to calculate distribution values for representative chemical components identified in products from this category. Existing product chemical composition data will be evaluated to select a subset of chemicals that adequately represents products in this category. The selection process will consider chemical carbon number range, hydrocarbon type, and chemical structure. A computer model, EPIWIN version 3.04 (EPIWIN, 1999), will be used to calculate the physicochemical properties needed to run the Level I EQC model.

D. Aquatic Toxicity

The aquatic toxicity endpoints for the HPV Chemical Program include:

- Acute Toxicity to a Freshwater Fish
- Acute Toxicity to a Freshwater Invertebrate
- Toxicity to a Freshwater Alga

Although aquatic toxicity data are not available for products in the High Benzene Naphthas Category, there are sufficient read across data from both constituent chemicals of those products and complex products to fully characterize the toxicity of this category. The use of data from selected read across materials to products in this category can be justified for the following reasons:

- Individual chemicals and complex products used for read across purposes contain a chemical class or combinations of chemical classes (i.e., olefins, aromatics, paraffins) that are found in products from this category.
- Individual chemicals and complex products used for read across purposes have a carbon

number or carbon number range that falls within the range of carbon numbers found in products from this category.

- Individual chemicals and complex products used for read across purposes as well as the products in this category are composed of chemicals that act by a similar mode of toxic action.

The data in Table 6 provides a comparison of the range of product compositions (i.e., carbon number, chemical class, weight percent) in the High Benzene Naphthas Category to materials used to characterize the aquatic toxicity of this category. This comparison illustrates the similarity in carbon number ranges between products in this category and the selected products with read across data. The data in Tables 7, 8, and 9 establish the range of toxicity that products in this category are expected to demonstrate, based on the read across data.

The aquatic toxicity data presented in this test plan fall within a narrow range of values regardless of their varying chemical class content and carbon number range. This is not unexpected, because the constituent chemicals of products in this category are neutral organic hydrocarbons whose toxic mode of action is non-polar narcosis. The mechanism of short-term toxicity for these chemicals is disruption of biological membrane function (Van Wezel and Opperhuizen, 1995), and the differences between measured toxicities (i.e., LC/LL50, EC/EL50) can be explained by the differences between the target tissue-partitioning behavior of the individual chemicals (Verbruggen et al., 2000).

The existing fish toxicity database for narcotic chemicals supports a critical body residue (CBR, the internal concentration that causes mortality) of between approximately 2-8 mmol/kg fish (wet weight) (McCarty and Mackay, 1993; McCarty et al., 1991), supporting the assessment that these chemicals have equal potencies. When normalized to lipid content, the CBR is approximately 50 umol of hydrocarbon/g of lipid for most organisms (Di Toro et al., 2000). Because the products in this category are all complex mixtures containing relatively similar series of homologous chemicals, their short-term toxicities are expected to fall within the range of toxicity demonstrated by the individual chemicals, as well as comparable products summarized in this test plan. Therefore, the existing data are believed to form a sufficiently robust dataset to fully characterize the aquatic toxicity endpoints in the HPV Chemical Program for this category.

The fish and invertebrate acute and alga toxicity values for individual chemicals and complex products similar to those in this category (Tables 7, 8, 9) fall within a range of approximately 1-64 mg/L and overlap between the three trophic levels. Because the products in the High Benzene Naphthas Category will range in paraffin, alkene, and/or aromatic carbon number content within approximately C5 to C11, a range in toxicity for products in this category will be comparable to the range of data summarized in Tables 7, 8, and 9.

As suggested by the experimental data, this category will exhibit a moderate range of acute toxicity to fish and invertebrates and a moderate range of toxicity to algae. For representative chemicals and products, experimental acute fish toxicity values range between 2.5 to 46 mg/L for two species (Table

7), while acute invertebrate toxicity values range between 0.9 to 32 mg/L for one species (Table 8). In comparison, alga toxicity values for one species range between 1.0 to 64 mg/L (for biomass and growth rate endpoints), while alga NOELR values range between 1.0 to 51 mg/L (for biomass or growth rate endpoints) (Table 9).

IV. TEST PLAN SUMMARY

Based upon examinations of stream compositions and existing toxicity data for components of streams in the category, there is minimal likelihood for the appearance of unexpected or remarkable biological findings in testing of these streams. All streams in this category are subject to the Occupational Safety and Health Administration (OSHA) Benzene Standard (29 CFR 1910.1028). Those streams containing 1,3-butadiene are subject to the OSHA Butadiene Standard (29 CFR 1910.1051). OSHA Permissible Exposure Limits exist for all major components. Hence, the basic strategy of this screening level test plan for characterizing the human health hazards of this category is to evaluate data for the components of the streams, as well as data for mixtures of category components and analogous mixtures (existing data and data being developed by other test programs). Benzene, as the predominant component in most streams, is expected to be the key driver with respect to health effects that would be observed in the SIDS battery of tests, with genotoxicity and hematotoxicity the effects most likely to be seen. However, as the concentration of benzene is decreased and the concentrations of other components are increased, the observed effects of benzene are expected to diminish and the effects of other components are expected to increase. Benzene has a robust toxicity dataset and has completed the OECD SIDS program. No further testing of benzene is needed for the HPV Chemical Challenge Program. The other major chemical components of streams in the High Benzene Naphthas Category have been extensively and comprehensively tested for human health toxicity endpoints, and all components present in the streams at concentrations greater than 5% have been tested in at least one toxicity study. Those components having only limited data lack structural alerts for mammalian toxicity and data exist for structural analogs. Some data are available for one High Benzene Naphthas stream [Hydrotreated C6-C8 Fraction] and a stream similar to the Pyrolysis Gasoline streams. Some data are also available regarding interactions between certain components that impact metabolism and toxicity. Additional supporting data for components of the High Benzene Naphthas streams, tested either individually or as components of other streams or mixtures, will be collected by other test plans within the Olefins Panel's HPV program, by other consortia participating in the HPV or ICCA programs, or from chemicals sponsored in the OECD SIDS program. These data are expected to provide sufficient information to develop scientific judgment-based characterizations of the human health effects of streams in this category. Therefore, no additional human health toxicity testing is proposed.

Data will be developed and/or identified to adequately characterize relevant physicochemical endpoints in the HPV Chemical Challenge Program.

Biodegradation data identified as read across data to the High Benzene Naphthas Category show that products in this category have the potential to exhibit a high extent of biodegradability. The existing read

across data provide sufficient information to adequately characterize the biodegradability of products in this category. Therefore, no additional biodegradation testing is proposed.

The chemical components in these products are relatively volatile, and if released they would be expected to partition to the air phase to a significant extent. In the air, they are subject to rapid physical degradation through hydroxyl radical attack. Therefore, as a result of both biological and physical degradation processes, these products are not expected to persist in the environment.

Sufficient information has not been developed on the potential of products in this category to photodegrade, hydrolyze, and partition within the environment. Therefore, information or data will be developed to adequately characterize these endpoints.

Read across aquatic toxicity data show that products in the High Benzene Naphthas Category have the potential to produce a moderate level of toxicity in freshwater algae and acute toxicity in freshwater fish and invertebrates. The existing read across data provide sufficient information to adequately characterize the aquatic toxicity of products in this category. Therefore, no additional toxicity testing is proposed.

The evaluations, modeling, and technical discussions that will be developed for the High Benzene Naphthas Category are summarized in Table 10.

REFERENCES

ACGIH (American Conference of Governmental Industrial Hygienists). 1986. Documentation of the TLV Values and Biological Exposure Indices, 5th ed., Cincinnati, IH, p. 163.

Andrews, L.S., E.W. Lee, C.M. Witmer, J.J. Kocsis, and R. Snyder. 1977. Effects of toluene on the metabolism, disposition and hemopoietic toxicity of [^{3}H]benzene. Biochem. Pharmacol. 26:293-300.

ATSDR (Agency for Toxic Substances and Disease Registry). 1997. Toxicological Profile for Benzene. Prepared by Research Triangle Institute for U.S. Department of Health & Human Services, Public Health Service, ATSDR [available on the internet].

ATSDR (Agency for Toxic Substances and Disease Registry). 1993. Toxicological Profile for 1,3-Butadiene. Prepared by Syracuse Research Corporation for U.S. Department of Health & Human Services, Public Health Service, ATSDR [available on the internet].

ATSDR (Agency for Toxic Substances and Disease Registry). 1999. Toxicological Profile for Ethylbenzene. Prepared by Research Triangle Institute for U.S. Department of Health & Human Services, Public Health Service, ATSDR [available on the internet].

ATSDR (Agency for Toxic Substances and Disease Registry). 1999. Toxicological Profile for n-Hexane. Prepared by Research Triangle Institute for U.S. Department of Health & Human Services, Public Health Service, ATSDR [available on the internet].

ATSDR (Agency for Toxic Substances and Disease Registry). 1995. Toxicological Profile for Naphthalene. Prepared by Sciences International, Inc. under contract to Research Triangle Institute for U.S. Department of Health & Human Services, Public Health Service, ATSDR [available on the internet].

ATSDR (Agency for Toxic Substances and Disease Registry). 1992. Toxicological Profile for Styrene. Prepared by Life Systems, Inc. under contract to Clement International Corporation for U.S. Department of Health & Human Services, Public Health Service, ATSDR [available on the internet].

ATSDR (Agency for Toxic Substances and Disease Registry). 2000. Toxicological Profile for Toluene. Prepared by Syracuse Research Corporation for U.S. Department of Health & Human Services, Public Health Service, ATSDR [available on the internet].

ATSDR (Agency for Toxic Substances and Disease Registry). 1995. Toxicological Profile for Xylenes. Prepared by Sciences International under contract to Research Triangle Institute for U.S. Department of Health & Human Services, Public Health Service, ATSDR [available on the internet].

Bamberger, J.R. 1996. 90-Day inhalation toxicity study with cyclohexane in mice. Haskell Laboratory

for Toxicology and Industrial Medicine, DuPont, Report No. HLR 17-96.

Beals, S.M., R.A. Jacobson, J.P. Robinson, H.T.Appleton, P.A. Howard, and J. Santodonato. 1986. Technical Support Document, Cyclohexane. Doc. No. SRC TR-86-030 [draft final]. Syracuse Research Corporation, Syracuse, NY. Prepared for Test Rules Development Branch Existing Chemical Assessment Division, Office of Toxic Substances, Washington, DC.

Bond, J.A, T.L. Leavens, M.J. Seaton, and M.A. Medinsky. 1998. Predicting the toxicity of chemical mixtures. CHEMTECH, July.

Brown, N.A. 1991. Reproductive and developmental toxicity of styrene. Reproductive Tox. 5:3-29.

Brown, N.A. 1993. Developmental and reproductive toxicity of styrene: A review update. International Symposium on Health Hazards of Butadiene and Styrene. Abstract reprinted in The SIRC Review 3(1):44-45.

Chemicals Inspection and Testing Institute, Japan. 1992. Biodegradation and Bioaccumulation Data of Existing Chemicals Based on the CSCL Japan. Japan Chemical Industry Ecology-Toxicology and Information Center. ISBN 4-89074-101-1.

Ciranni R, Barale R, Ghelardini G, & Loprieno N (1988) Benzene and the genotoxicity of its metabolites. II. The effect of the route of administration on the micronuclei and bone marrow depression in mouse bone marrow cells. Mutat Res, 209: 23-28.

Daughtrey, W.C., D.L. Putman, J. Duffy, A.I. Soiefer, C.J. Kirwin, L.N. Curcio, and T.H. Keenan. 1994a. Cytogenetic studies on commercial hexane solvent.

Daughtrey, W.C., T. Neeper-Bradley, J. Duffy, L. Haddock, T. Keenan, C. Kirwin, and A. Soiefer. 1994b. Two-generation reproduction study on commercial hexane solvent. J. Applied Toxicology 14(5):387-393.

Daughtrey, W.C., P. Newton, R. Rhoden, C. Kirwin, L. Haddock, J. Duffy, T. Keenan, W. Richter, and M. Nicolich. 1999. Chronic inhalation carcinogenicity study of commercial hexane solvent in F-344 rats and B6C3F1 mice. Toxicological Sciences 48:21-29.

Di Toro, D.M., J.A. McGrath, and D.J. Hansen. 2000. Technical Basis for Narcotic Chemicals and Polycyclic Aromatic Hydrocarbon Criteria. I. Water and Tissue. Environmental Toxicology and Chemistry, 19:1951-1970.

ECETOC (European Centre for Ecotoxicology and Toxicology of Chemicals) Special Report No. 12. 1,3-Butadiene OEL Criteria Document (Second Edition). 1997. Programme for the Joint Assessment of Commodity Chemicals. Jacc Report No. 19. Brussels, Belgium.

ECETOC (European Centre for Ecotoxicology and Toxicology of Chemicals) report on Dicyclopentadiene. 1991. Programme for the Joint Assessment of Commodity Chemicals. Jacc Report No. 19. Brussels, Belgium.

ECETOC (European Centre for Ecotoxicology and Toxicology of Chemicals) report on Xylenes. 1986. Programme for the Joint Assessment of Commodity Chemicals. Jacc Report No. 6. Brussels, Belgium.

EPA/OTS Doc.8690000024: Test for oral toxicity in rats with cyclopentadiene with cover letter dated 09/28/95.

EPA/OTS Doc.8690000121S: Subacute inhalation exposure of cyclopentadiene with cover letter dated 09/28/95.

EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. SyracuseResearchCorporation, Syracuse, NY, USA.

EU Risk Assessment. 2001. Benzene. Draft Risk Assessment Document [in Risk Assessment Review]. Available on internet at http://ecb.jrc.it/existing-chemicals.

EU Risk Assessment. 2000. Cyclohexane. ECB# 031. Draft Risk Assessment Document [in Risk Assessment Review]. Available on internet at http://ecb.jrc.it/existing-chemicals.

EU Risk Assessment. 2001. Naphthalene. Draft Risk Assessment Document [in Risk Assessment Review]. Available on internet at http://ecb.jrc.it/existing-chemicals.

EU Risk Assessment. 2001. Toluene. Draft Risk Assessment Document [in Risk Assessment Review]. Available on internet at http://ecb.jrc.it/existing-chemicals.

ExxonMobil. 1982. Unpublished reports for Rerun Tower Overheads: Mouse Lymphoma [M1252-78], DNA Repair [M1251-78], Drosophila [M1253-78], Mouse Skin Painting [M0417-77].

Frontali, N. M.D. Amantini, A. Spagnolo, A.M. Guarcini, and M.C. Saltari. 1981. Experimental neurotoxicity and urinary metabolites of the C5-C7 aliphatic hydrocarbons used as glue solvents in shoe manufacture. Clin. Tox. 18:1357-1367.

Gad-El-Karim, M.M., B.L. Harper and M.S. Legator. 1984. Modifications in the myeloclastogenic effect of benzene in mice with toluene, phenobarbital, 3-methylcholanthrene, Aroclor 1254 and SKF-525A. Mutation Res. 135:225-243.

Gad-El-Karim, M.M., V.M.S. Ramanujam and M.S. Legator. 1986. Correlation between the induction of micronuclei in bone marrow by benzene exposure and the excretion of metabolites in urine of CD-1

mice. Toxicol. Appl. Pharmacol. 85:464-477.

Galassi, S., M. Mingazzini, L. Viagano, D. Cesareo, and M.L. Tosato. 1988. Aproaches to Modeling Toxic Responses of Aquatic Organisms to Aromatic Hydrocarbons. Ecotox. Environ. Safety. 16:158-169.

Galvin, J.B. and F. Marashi. 1999. n-Pentane. J. Toxicology and Env. Health. Pt. A,58:35-36.

Halder, C.A., C.E. Holdsworth, B.Y. Cockrell, and V.J. Piccirillo. 1985. Hydrocarbon nephropathy in male rats: Identification of the nephrotoxic components of unleaded gasoline. Tox. and Industrial Health 1(3):67-87.

Hite, M., M. Pecharo, I. Smith and S. Thornton. 1980. The effect of benzene in the micronucleus test. Mut. Res. 77:149-155.

IARC (International Agency for Research on Cancer). 1999. Isoprene. Monographs on the Evaluation of Carcinogenic Risks to Humans. Vol. 71, Part 3, Lyon, France, pp. 1015-1024.

IARC (International Agency for Research on Cancer). 1994. Styrene. Monographs on the Evaluation of Carcinogenic Risks to Humans. Vol. 60, Lyon, France, pp. 233-320.

IARC (International Agency for Research on Cancer). 1999. Toluene. Monographs on the Evaluation of Carcinogenic Risks to Humans. Vol. 71, Part 2, Lyon, France, pp. 829-864.

IRIS (Integrated Risk Information System). 1990. Vinyl Acetate. Developed by the U.S. EPA.

HSDB: TOMES CPS™ System, MICROMEDEX, Englewood, Colorado, Vol. 38. CD-ROM.

JETOC (Japanese Chemical Industry Ecology – Toxicology and Information Center. 1998. Special Issue #3, No. 32 (March, 1998), Tokyo, Japan. In: Handbook of Existing and New Chemical Substances, 8th Ed. 1999. Supervised by Chemical Products Safety Division, Basic Industries Bureau, The Ministry of International Trade and Industry.

Kirwin, C. , R. San, J. Harbell, A. Soiefer, W. Daughtrey and T. Keenan.1991. Salmonella and CHO/HGPRT mutation assays of commercial hexane. The Toxicologist 11(1):315.

Kreckman, K.H. 1997. Inhalation developmental toxicity study of cyclohexane in rats. Haskell Laboratory for Toxicology and Industrial Medicine, DuPont, Report No. HLR 881-96.

Mackay, D., A. Di Guardo, S. Paterson, and C. E. Cowan. 1996. Evaluating the Environmental Fate of a Variety of Types of Chemicals Using the EQC Model. Environ.

Malley, L.A. 1996a. 90-Day inhalation toxicity study with cyclohexane in rats. Haskell Laboratory for Toxicology and Industrial Medicine, DuPont, Report No. HLR 298-96.

Malley, L.A. 1996b. 90-Day inhalation neurotoxicity study with cyclohexane in rats. Haskell Laboratory for Toxicology and Industrial Medicine, DuPont, Report No. HLR 752-95.

McCarty, L.S. and D. Mackay. 1993. Enhancing Ecotoxicological Modeling and Assessment. Environmental Science and Technology, 27:1719-1728.

McCarty, L.S., D. Mackay A.D. Smith, G.W. Ozburn, and D.G. Dixon. 1991. Interpreting Aquatic Toxicity QSARs: The Significance of Toxicant Body Residues at the Pharmacologic Endpoint. In: WSAR in Environmental Toxicology - IV. J.L.M. Hermens and A. Opperhuizen, eds. Elsevier.

McGregor, D. 1994. The genetic toxicology of toluene. Mut Res. 317:2134-228.

McKee, R., E. Frank, J. Heath, D. Owen, R. Przygoda, G. Trimmer, and F. Whitman. 1998. Toxicology of n-pentane. J. Appl. Toxicol. 18:431-442.

Medinsky, A., P.M. Schlosser, and J.A. Bond. 1994. Critical issues in benzene toxicity and metabolism: the effect of interactions with other organic chemicals on risk assessment. Env. Health Perspectives 102(Supp. 9):119-124.

Meyne, J. and M.S. Legator. 1980. Sex-related differences in cytogenetic effects of benzene in the bone marrow of Swiss mice. Environ. Mutagenesis 2:43-50.

Neely, W. B. 1985. Hydrolysis. In: W. B. Neely and G. E. Blau, eds. Environmental Exposure from Chemicals. Vol I., pp. 157-173. CRC Press, Boca Raton, FL, USA.

Nylen, P. 1996. Differing non-additive alterations in different parts of the nervous system of the rat. Food and Che.. Tox. 34(11/12): 1121-1123.

Nylen, P. 1989. Testicular atrophy and loss of nerve growth factor-immunoreactive germ cell line in rats exposed to n-hexane and a protective effect of simultaneous exposure to toluene or xylene. Arch. Toxicol. 63:296-307.

OECD (Organization for Economic Co-operation and Development). 1999. Draft Guidance Document on Aquatic Toxicity Testing of Difficult Substances. OECD Environmental Health and Safety Publications, Series on Testing and Assessment. OECD, Paris, France.

RTECS (Registry of Toxic Effects of Chemical Substances): TOMES CPS™ System, MICROMEDEX, Englewood, Colorado, Vol. 38, CD-ROM.

Soiefer, A., K. Robinson, B. Broxup, J. Duffy, T. Keenan, and W. Daughtrey. 1991. A subchronic neurotoxicity study of commercial hexane vapor in the rat. The Toxicologist II, p. 315 (abstract).

Suzuki, S., H.Atai, Y. Hatakeyama, M. Hara, and S. Nakagawa. 1989. Administration-route-related differences in the micronucleus test with benzene. Mut. Res. 223:407-410.

Toxicol. Chem. 15:1627-1637.

U.S. EPA. 1999a. The Use of Structure-Activity Relationships (SAR) in the High Production Volume Chemicals Challenge Program. OPPT, EPA. Washington, DC, USA.

U.S. EPA. 1999b. Determining the Adequacy of Existing Data. OPPT, EPA., Washington, DC, USA.

Van Wezel, A.P. and A. Opperhuizen. 1995. Narcosis Due to Environmental Pollutants in Aquatic Organisms: Residue-Based Toxicity, Mechanisms, and Membrane Burdens. Critical Reviews in Toxicology, 25:255-279.

Verbruggen, E.M.J., W.J.J. Vaes, T.F. Parkerton, and J.L.M. Hermens. 2000. Polyacrylate-Coated SPME Fibers as a Tool to Simulate Body Residues and Target Concentrations of Complex Organic Mixtures for Estimation of Baseline Toxicity. Environmental Science and Technology, 34;324-331.

WHO EHC. 1997. World Health Organization, International Programme on Chemical Safety, Environmental Health Criteria for Xylenes. No. 190.

Zepp, R. G., and D. M. Cline. 1977. Rates of Direct Photolysis in the Aqueous Environment. Environ. Sci. Technol. 11:359.366.

Table 1.
CAS Numbers and Descriptions Associated with Streams in the High Benzene Naphthas Category

CAS Number	CAS Number Description
64741-99-7	Extracts, petroleum, light naphtha solvent
64742-49-0	Naphtha, petroleum, hydrotreated light
64742-73-0	Naphtha, petroleum, hydrodesulfurized light
64742-83-2	Naphtha, petroleum, light steam-cracked
64742-91-2	Distillates, petroleum, steam-cracked
67891-79-6	Distillates, petroleum, heavy arom.
67891-80-9	Distillates, petroleum, light arom.
68410-97-9	Distillates, petroleum, light distillate hydrotreating process, low-boiling
68475-70-7	Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived
68476-45-9	Hydrocarbons, C5-10 arom. conc., ethylene-manuf.-by-product
68526-77-2	Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum
68606-10-0	Gasoline, pyrolysis, debutanizer bottoms
68606-28-0	Hydrocarbons, C5 and C10-aliph. and C6-8-arom.
68921-67-5	Hydrocarbons, ethylene-manuf.-by-product distn. residues
68955-29-3	Distillates, petroleum, light thermal cracked, debutanized arom.
68956-52-5	Hydrocarbons, C4-8
68956-70-7	Petroleum products, C5-12, reclaimed, wastewater treatment
69013-21-4	Fuel oil, pyrolysis
8030-30-6	Naphtha

Note: The definitions, found in the TSCA Chemical Substance Inventory, for the CAS numbers included in this group are vague with respect to composition. Therefore, it is not uncommon to find that the same CAS number is correctly used to describe different streams (compositions) or that two or more different CAS numbers are used to describe the same stream (composition).

Table 2.
Typical Composition Ranges (Percent) for High Benzene Naphthas
(See notes 1-4 at the end of this table)

Component	Pyrolysis Gasoline	Quench Loop Pyrolysis Oil Wastewater Treatment (see Note 4)	Pyrolysis C6 Fraction	Pyrolysis C6-C8 Fraction	Pyrolysis C5-C6 Fraction	Hydrotreated C6-C7 Fraction	Hydrotreated C6-C8 Fraction	Hydrotreated C6 Fraction	Extract from Benzene Unit
Vinyl Acetate	9.9								
1,3-Butadiene	6.7		0.1 - 2						
C4's	0.5 -5		0.1 - 1.5						
1,4-Pentadiene	0.3 - 0.9		0.1 - 2						
Isopentane (2-methylbutane)	2.0		0.1 - 1						
1-Pentene (Amylene)	0.6 - 4		1 - 3						
2-Methyl-1-Butene	1.0								
Pentene-2 (isomer mix)	0.2 - 1.8		0.1 - 5						
Isoprene (2-methylbutadiene-1,3)	0.6 -10		2 - 6		6				
Pentenes					10				
Pentane	10					1			
2-Methyl-2-Butene	1.2		2						
Other C5's	0.3						2.0		
3-methyl-1,2-butadiene			1 - 3						
1,3-Cyclopentadiene	1 - 20		0.1 - 5	1					
1,3-Pentadiene (isomer mix)	0.7 - 4.4		0.3 - 4						
Cyclopentene	0.6 - 5				8				
Cyclopentane	2.3					1 - 5		4	
1,5-hexadiene	0.6								
2-methylpentane	4							4	
2-methyl-1-Pentene	0 - 2.2								
3-methylpentane (Isohexane)	1.3					10 - 20		4	
hexene-1	0 - 2.2								
hexenes						2			
Methylcyclopentadiene	5			1					
Hexane isomers				1 - 3		5 - 20			
Hexane	0 – 9			1 - 5		2 - 15		6	
Methylcyclopentane	4.9					5 - 15			
1-methylcyclopentene	0.1 -								

Component	Pyrolysis Gasoline	Quench Loop Pyrolysis Oil Wastewater Treatment (see Note 4)	Pyrolysis C6 Fraction	Pyrolysis C6-C8 Fraction	Pyrolysis C5-C6 Fraction	Hydrotreated C6-C7 Fraction	Hydrotreated C6-C8 Fraction	Hydrotreated C6 Fraction	Extract from Benzene Unit
	2.4								
C6 non-aromatics		0.9	30						
non-Aromatic Hydrocarbons							20 - 26		
Benzene	15 - 62	10 - 21.6	35 - 77	30 - 80	70	40 - 69	40 - 60	75 - 75.7	60 - 75
1,3-cyclohexadiene	0.5 - 2.0								
Cyclohexane	2					1 - 3		6	
Cyclohexene	0.6								
cyclohexadienes	0.1 - 2.3								
3-ethylpentene-1			1						
C6 olefin	0.2 - 1.9								
heptenes						2			
2-methylhexane						2			
heptane isomers						1 - 5			
Heptane	0.4 -2			1		1 - 5			
C7 Paraffins & Napththenes	0.3 - 1.1								
C7 Olefins	0 - 1.2								
Methylcyclohexane						1 - 3			
C7-Non-aromatics		2.2	3						
Toluene	17.4	5 – 10.9	0.5 - 5	15 - 25	5	3 - 15	10 - 25	0.3	25 - 40
4-Vinlyclohexene (Butadiene Dimer)	0.1 - 1								
C8 Nonaromatics		1.3							
Ethylbenzene	0.3 - 5.5	1 – 3	1	1 - 3					
C8 Aromatics							3 - 10		1
Xylenes, mixed	10	1.5		1 - 10					
Styrene	10	10 – 15		1 - 10					
C9 Aromatics	0.4 - 1.7								
Ethyltoluenes	0.1 – 2								
C9 Paraffins and Naphthenes	0.3 - 1.3								

Component	Pyrolysis Gasoline	Quench Loop Pyrolysis Oil Wastewater Treatment (see Note 4)	Pyrolysis C6 Fraction	Pyrolysis C6-C8 Fraction	Pyrolysis C5-C6 Fraction	Hydrotreated C6-C7 Fraction	Hydrotreated C6-C8 Fraction	Hydrotreated C6 Fraction	Extract from Benzene Unit
1,3,5-Trimethylbenzene (mesitylene)	3								
C10+		40.6							
1,2,4-Trimethylbenzene (pseudocumene)	0 - 3.3			1					
4-methylstyrene	0 - 3.3								
Cyclopentadiene/Methyl cyclopentadiene Codimers	0.9 - 4.4			1 - 3					
Dicyclopentadiene	20	3.7		1 - 5					
1-Decene	1.5								
Vinyl Toluene	0.1 - 1.1								
dihydrodicyclopentadiene	2								
Decane	0.1 - 5								
C10 Aromatics	1.6								
C10's		1.6 - 27							
Indene	0.6 - 5								
C11+		38.8 - 50							
Naphthalene	15.0	4.3 - 10							
Methylnaphthalene	2.9								
1-Methylnaphthalene	1								
1,1'-Biphenyl	0.1 - 0.9								
C10 Olefins	1.2								

Note 1: The composition data shown above are composites of reported values.
Note 2: The balance of these streams is expected to be other hydrocarbons that have boiling points in the range of the listed components.
Note 3: The listed highs and lows should not be considered absolute values for these limits. They are instead the highs and lows of the reported values.
Note 4: No specific composition data are available. This stream is expected to contain components of Pyrolysis Gasoline.

Table 3. Summary Results from Existing Human Health Effects Data for Chemical Components and Streams of High Benzene Naphthas Category

(Note: This table is the product of a good faith effort to briefly summarize results of toxicity studies that were available to the reviewer for SIDS endpoints. Results from non-SIDS endpoints are not included. Since all information for a particular chemical may not have been available to the reviewer, the results presented should not be considered as final assessments of the hazards of the listed chemicals. Component data were not reviewed for data adequacy. Robust summaries for the listed components will not be submitted with the Test Plan.)

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/ References
Vinyl Acetate	Oral LD50 = 2.9 g/kg; inhalation LC50 = 3680 ppm [4h]	Negative in Ames Test	Positive in mouse bone marrow micronucleus test by i.p. but negative in rats and mice by inhalation and oral; positive in in-vitro chrom ab	4 and 13-wk rat and mouse inhalation study: decrease in BW gain, respiratory tract effects; no clearly treatment related effects in 4 and 13-wk rat and mouse oral	In rat inhalation study, no embryolethality or teratogenicity seen; fetal growth retardation seen at maternally toxic doses. In rat oral study, no effects.	In an oral rat 2-gen repro study, no effects were seen except for reduction in BW gain in high-dose F1 pups.		Review: IRIS[1] – 1990; HSDB[2]; ATSDR – 1992[4]

[1] IRIS: EPA Integrated Risk Information System
[2] HSDB: Hazardous Substances Data Bank [TOMES, MICROMEDEX, Inc.]

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/ References
1,3-Butadiene	Rat inhalation LC50[4h] = 129,000 ppm	Negative in UDS in mouse and rat, Drosophila; negative and positive in mouse lymphoma; positive in Ames, CHO and in vivo mouse spleenocyte HPRT tests and mouse spot test	Positive in mouse dominant lethal but negative in rat; positive in mouse bone marrow micronucleus and chrom. ab.; negative in rat bone marrow micronucleus	Many studies: Toxicity to blood cells in mice; no effects in rats [inhalation]	Effects seen at maternally toxic doses	Will become available through OECD SIDS	Olefins Panel's Crude Butadiene C4 Category, OECD SIDS	Reviews: ECETOC Special Report No. 12 - 1997[3]; ATSDR[4] - 1993
Isoprene (2-methylbutadiene-1,3)	Rat oral LD50= 2.1 g/kg; inhalation LC50 [4h] = 64,500 ppm	Negative in Ames Test	Negative in in-vitro CHO chrom. ab., mouse bone marrow chrom. ab. and rat lung cell micronucleus [inhalation]; positive in mouse bone marrow micronucleus [inhalation]	Many studies: Effect on testes in rats seen at 26 wks but not at 13 wks; effects on blood cells, nasal epithelium, liver, stomach, and testes in mice [inhalation]	No effects in rats; fetotoxicity in mice	Limited repro tox data [sperm motility, vaginal cytology, histopath of repro organs]obtained as part of 13-wk inhalation study: [slight effect on testis in rats; effects on testes, epididymus, sperm, estrus cycle in mice]	Olefins Panel's C5 Non-Cyclics Category/ICCA	Review: IARC[5] - 1999

[3] ECETOC: European Centre for Ecotoxicology and Toxicology of Chemicals
[4] ATSDR: U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry
[5] IARC: International Agency for Research on Cancer

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/ References
Pentenes				2-pentene: 4 wk rat oral evaluating nephrotoxicity showed no kidney lesions at 2 g/kg/day w/60% mortality			International Hydrocarbon Solvents Consortium [C5 Aliphatics Category Test Plan]; also, pentenes are likely to have a toxicity profile similar to hexenes which will be addresed by the Higher Olefins Panel	Halder et al., 1985

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/ References
Pentane	Rat oral: LD50>2 g/kg; inhalation LC50[4h] >7000 ppm	Negative in Ames Test	Negative in rat bone marrow micronucleus [inhalation] and dominant lethal [i.p.]; positive [not reproducible] in in-vitro CHO chrom.ab.	90-day rat inhalation: no effect at ~ 7000ppm. 16 wk and 7-30 wk rat inhalation neurotox evaluations : negative With 50/50 blend of n-butane and n-pentane, in a 90-day rat inhalation study with scope limited to evaluation of nephrotoxicity: decrease in BW and male hydrocarbon nephropathy.	No effect in rat oral	No effect on repro organs in 90-day rat inhalation	API [addressed in Petroleum Gases Test Plan]; International Hydrocarbon Solvents Consortium [C5 Aliphatic Category Test Plan]; OECD SIDS	Review: McKee et al., 1998; Galvin and Marashi, 1999

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/ References
1,3-Cyclopentadiene	Rat oral: 4/5 died at 1 g/kg; inhalation LC50 [4h] = 39 mg/L			Mild liver and kidney effects in rats after 35 exp. of 500 ppm ; no effects in guinea pigs, rabbits, dogs after 135 exp. of 250 ppm, or in dogs after 39 additional exp of 400 ppm and 16 additional exp of 800 ppm [inhalation]				ACGIH[6], RTECS[7], EPA Documents [86960000024, 86960000121S
Cyclopentene	Rat oral LD50 = 1.66 g/kg; inhalation LCLo [4h] = 16,000 ppm							RTECS
3-methylpentane (Isohexane)				16 wk and 7-30 wk rat inhalation neurotox evaluations : negative				Frontali et al., 1981

[6] ACGIH: American Conference of Governmental Industrial Hygienists
[7] RTECS: Registry of Toxic Effects of Chemical Substances

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/ References
Hexane isomers [Commercial Hexane tested: 52.2% n-hexane, 16.0% 3-methylpentane, 15.6% methylcyclopentane, 11.6% 2-methylpentane, 3.2% cyclohexane]		Negative in Ames Test, CHO HPRT	Negative in in-vitro CHO chrom. ab. and rat bone marrow chrom. ab. [inhalation]	No neurotoxicity; male rat hydrocarbon nephropathy [inhalation]	No effects in rats via inhalation	No effect in rat 2-gen study via inhalation except decrease in weight gain in high dose offspring		Daughtrey et al., 1994 a,b; 1999; Kirwin et al., 1991
Hexane	Rat oral LD50=28.7 g/kg; inhalation LC50[4h] = 48,000 ppm	Negative in Ames Test and in vitro UDS	Negative in in-vitro CHO chrom. ab. , inhalation dominant lethal and mouse micronucleus [inhalation and IP]; positive in rat oral bone marrow chrom. ab.	Several studies: Effects on peripheral nervous system and testes	Negative in inhalation and oral developmental studies	No repro tox studies found; testicular atrophy seen in subchronic inhalation studies	OECD SIDS - ICCA	Review: ATSDR[8] – 1999; rat chrom. ab. report in HSDB[9]
Methylcyclopentane				4 wk rat oral evaluating nephrotoxicity showed no kidney lesions at 0.5 g/kg/day but lesions at 2g/kg w/40%mortality				Halder et al., 1985

[8] ATSDR: U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry
[9] HSDB: Hazardous Substances Data Bank [TOMES, MICROMEDEX, Inc]

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/ References
Benzene	Rat oral LD50=810 mg/kg; inhalation LC50 [4h] = 13,700 ppm	Negative in Ames Test, mouse lymphoma, CHO HPRT, in-vitro UDS, Drosophila; positive in mouse spleen HPRT	Positive in vitro/in vivo in numerous studies and species [oral, inhalation]: in-vitro human lymphocytes; chrom. ab. and micronucleus in mouse bone marrow and spleen lymphocytes; rat bone marrow chrom. ab. and micronucleus	Many studies: Primary effect toxicity to blood cells	Several studies: fetotoxic at maternally toxic doses; not tetratogenic	No standard repro studies; most inhalation studies with repro parameters indicate no effect on reproductive indices, even at high doses	OECD SIDS	Review: ATSDR – 1997; EU Risk Assessment – 2001 [Draft]
Cyclohexane	Rat oral LD50 > 5 g/kg; inhalation LC50[4h] = 4044 ppm	Negative in Ames Test, mouse lymphoma, human lymphocyte UDS	Negative in rat bone marrow chrom. ab. [inhalation]	Effects on liver in mice and rats; on liver and kidney in rabbits [inhalation]	No effects seen in rats or rabbits [inhalation]	No effects in rat 2-gen inhalationrepro at doses not maternally toxic	OECD SIDS	Review: SRC Technical Support Document #TR-86-030 [Beals et al.,1986, draft][10]; EU Risk Assessment – 2000 [Draft] Bamberger, 1996; Kreckman, 1997; Malley, 1996 a,b

[10] SRC: Syracuse Research Corporation Center for Chemical Hazard Assessment, prepared for Test Rules Development Branch, Existing Chemical Assessment Division, Office of Toxic Substances

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/ References
Toluene	Rat oral LD50 = 5.5 – 7.53 g/kg; inhalation LC50[4h] = 8000 - 8800 ppm	Negative in Ames Test, SHE transformation, and Drosophila SLRL; equivocal in mouse lymphoma	Negative in in-vitro human lymphocyte and CHO chrom. ab., dominant lethal [oral], chrom. ab. in mice [oral] and rats [inhalation], and mouse micronucleus [oral]	Many studies: Effects on central nervous system; hearing loss in rats	In rats and mice: lower birth weight, delayed postnatal development and behavioral effects [inhalation]	No effects in mouse 2-gen inhalation repro study; in rats, effect on sperm count and epididymal weight at 2000 ppm, but no effect on fertility	OECD SIDS	Review: ATSDR[11] – 2000; IARC[12] – 1999; EU Risk Assessment - 2001 Genetic toxicity review: McGregor, 1994.
Ethylbenzene	Rat oral LD50> 3.5 g/kg; inhalation LC50[4h] LC50 = 4000 ppm	Negative in Ames Test, Drosophila SLRL, and in-vivo UDS in mouse hepatocytes; equivocal in mouse lymphoma	Negative in in-vitro CHO and RL4 cells chrom. ab. and in inhalation/i.p. mouse micronucleus	Several studies: Effects seen in liver, kidney, and lung in rats and mice; hearing loss in rats via inhalation	No effects in rabbits; only supernumerary ribs seen in rats	No repro study; in subchronic rat and mouse studies, no effects seen in gonads sperm, extrus cycle	OECD SIDS	Review: ATSDR[13] - 1999
Xylenes, mixed	Rat oral LD50 = 3.5-8.6 g/kg;Rat inhalation [4h]LC50 = 6,350 - 6,700 ppm	Negative Ames Test and mouse lymphoma	Negative in human lymphocytes [only w/o S9 tested] and CHO chrom. ab.	Many studies: liver, and nervous system effects via inhalation; hearing loss in rats via inhalation; nervous system effects via oral exposure	Fetotoxic effects seen in rat and mouse [oral,inhalation], mostly secondary to maternal toxicity	Negative in rat repro [exposed by inhalation 131 days prior to mating, during mating, gestation, day 5-20 of lactation]; no effect on repro organs in rat and mouse	ACC Toluene Xylene Panel/OECD SIDS/ICCA	Review: ATSDR – 1995; WHO EHC - 1997[14]; ECETOC - 1986

[11] ATSDR: U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry
[12] IARC: International Agency for Research on Cancer
[13] ATSDR: U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry
[14] WHO EHC: World Health Organization, International Programme on Chemical Safety. Environmental Health Criteria

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/ References
Styrene	Rat oral LD50 $\geq$ 5 g/kg; inhalation LC50 [4h] = 4940 ppm	Inconsistent results in Ames Test	Inconsistent results in in-vitro chrom. ab. tests; negative in chrom. ab. and micronucleus tests in mice and rats by oral and inhalation exposure	Many studies: Effects on liver in rats [oral, inhalation] and mice [inhalation]; hearing loss in rats [inhalation]; respiratory tract in rats [inhalation]; lungs in mice [oral]	No birth defects in rats [oral, inhalation] or in mice, rabbits and hamsters [inhalation]; other effects seen only at maternally toxic doses	Negative in rat 3 gen repro study [oral]	OECD SIDS	Reviews: ATSDR – 1992; IARC[15] – 1994 Brown, 1991, 1993 [repro/devel]
Dicyclopentadiene	Rat oral LD50 ranged from 347 – 820 mg/kg; inhalation LC50[4h] ranged from 359 to 500-1000 ppm	Negative in Ames Test	Negative in in-vitro CHO and CHL chrom. ab.	Many studies: Most studies showed no effects in rats or mice in dietary or inhalation studies except male rat hydrocarbon nephropathy in inhalation studies	No effect in rats in oral [diet] studies	Effects only at maternally toxic doses in rat 3-gen repro study [in diet]	OECD SIDS	Review: ECETOC[16] – 1991 JETOC[17] Issue 3 No. 32, 1998 [CHL chrom. ab and OECD 422 studies]; NTP[18] [CHO chrom. ab.]

[15] IARC: International Agency for Research on Cancer
[16] ECETOC: European Centre for Ecotoxicology and Toxicology of Chemicals
[17] JETOC: Japanese Chemical Industry Ecology – Toxicology and Information Center
[18] NTP: National Toxicology Program – personal communication

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/ References
Naphthalene	Rat oral LD50 ranged from 2200 to 2600 mg/kg; no effect at 78 ppm [4h] inhalation	Negative in Ames Test, transformation, in-vivo UDS in rat liver	Negative in mouse micronucleus; positive in in-vitro CHO chrom. ab.	Many studies: Toxicity to blood cells in dogs [hemolytic anemia][oral]but not rats or mice; cataracts in rabbits, rats, mice, guinea pigs [oral]; local irritative effects after inhalation in rats and mice	No birth defects in rabbits, rats, and mice [oral]; reduced litter size in mice at maternally toxic doses [oral on gestation day 7-14]; no effect in rabbits exposed orally on gestation days 6-18		OECD SIDS	Reviews: ATSDR[19] – 1995; EU Risk Assessment Document – Draft 2001

[19] ATSDR: U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/ References
Streams								
Pyrolysis Gasoline [C5-10 Fraction; Rerun Tower Overheads; approx. 40% benzene, 13% toluene, 26% C5, 20% other]	Rat oral LD50 > 2 g/kg;	Negative Ames Test, Drosophila; positive in mouse lymphoma , E.coli DNA repair , and transformation			No effects in rabbits in oral teratology study			Robust Summaries for acute oral, Ames, transformation, developmental; mouse lymphoma, DNA repair, Drosophila: Exxon Mobil, 1982
Pyrolysis Gasoline plus Rerun Tower Bottoms [Dripolene: C5+]	Rat oral LD50 > 2 g/kg							Robust Summary
Hydrogenated Pyrolysis Gasoline [Hydrotreated C6-8 Fraction] [55% benzene, 25% toluene, 10% xylene, 7% pentane, 7% ethylbenzene, 2% hexane, 3% cyclohexane]	Rat Oral LD50 = 5.17 g/kg; inhalation 4h LC50>12,408 ppm	Negative in Ames Test, in-vitro UDS; positive in transformation	Negative in micronucleus [mouse oral]	Rat 5 day inhalation: NOAEL 4869 ppm [deaths, bodyweight]				Robust Summaries

Table 4.
Read Across Data used to Characterize the Biodegradability of the High Benzene Naphtha Category from Chemicals Contained by Products in this Category and Chemically Complex Products not in this Category, but that Contain Like-Chemicals.

CHEMICAL / PRODUCT	CARBON NUMBER	PERCENT BIODEGRADATION(a) (28 days)	REFERENCE
n-Pentane	5	87	IHSC*
Isopentane	5	71	IHSC*
Cyclohexane	6	77	IHSC*
Alkenes, C6 Rich	6(b)	21	HOP**
1-Hexene (linear)	6	67-98(c)	****
Benzene	6	63	Robust Summary Provided with this test plan
Alkenes, C7-C9, C8 Rich	7-9	29	HOP**
p-Xylene	8	89	IHSC*
Styrene	8	100 (14 days)(c)	*****
Naphtha (Petroleum), light alkylate (gasoline stream)	5-8	42(d)	API***
Naphtha (Petroleum), Light Catalytically Cracked (gasoline stream)	5-8	74(d)	API***
Naphtha (Petroleum), Light Catalytically Reformed (gasoline stream)	5-9	96(d)	API***
C8-C10 Aromatics, Predominantly C9 Alkylbenzenes	9(b)	78	IHSC*
C8-C14 Aromatics, Predominantly Alkyl Naphthalenes and Naphthalene	10-12(b)	61	IHSC*

a OECD 301F, manometric respirometry test
b Predominant carbon number or range
c BOD test
d Test method for determining the inherent aerobic biodegradability of oil products and modification of ISO/DIS 14593
* Robust summary from the International Hydrocarbon Solvents Consortium: Contained in selected SIAR (to be submitted)
** Robust summary from the Higher Olefins Panel HPV Test Plan (submitted)
*** Robust summary from the American Petroleum Institute: Gasoline Test Plan (to be submitted)
**** Chemicals Inspection and Testing Institute, Japan. 1992. These chemicals are in the OECD SIDS program.
**** Styrene is in the OECD SIDS program.

Table 5.
Composition (Weight Percent) of Three Gasoline Streams with Biodegradation Data Used to Read Across to Products in the High Benzene Naphthas Category.

Naphtha, (Pet.) Light Alkylate		**Naphtha, (Pet.) Light Catalytically Cracked**		**Naphtha, (Pet.) Light Catalytically Reformed**	
CAS# 64741-66-8	Weight %	CAS# 64741-55-5	Weight %	CAS# 64741-55-5	Weight %
Isopentane	12.61	n-hexane	1.69	n-heptane	3.59
2,3 dimethyl butane	4.74	n-pentane	1.71	n-hexane	4.69
2,4 dimethyl pentane	4.09	isopentane	4.7	n-pentane	8.05
2,3 dimethyl pentane	2.25	2,3 dimethyl pentane	1.12	Isopentane	11.39
2,2,4 trimethyl pentane	23.92	2 methyl hexane	1.58	2,2 dimethyl butane	1.26
2,2,3 trimethyl pentane	1.76	3 methyl hexane	1.45	2,3 dimethyl butane	1.11
2,3,3 trimethyl pentane	8.99	2 methyl pentane	3.64	2,3 dimethyl pentane	1.70
2,3,4 trimethyl pentane	11.56	3 methyl pentane	2.20	2 methyl hexane	4.30
2,3,5 trimethyl hexane	1.25	methyl cyclopentane	1.87	3 methyl hexane	5.18
2,5 dimethyl hexane	4.34	methyl cyclohexane	1.19	2 methyl pentane	5.17
2,4 dimethyl hexane	3.60	1-pentene	1.25	3 methyl pentane	4.00
2,3 dimethyl hexane	2.60	2-methyl-1-butene	2.31	benzene	8.37
1methyl-1ethyl cyclopentane	9.44	2-methyl-2-butene	5.35	toluene	29.77
		trans-2-pentene	3.33		
		cis-2-pentene	1.94		
		2-methyl-1-pentene	2.31		
		cis-3-hexene	1.67		
		trans-2-hexene	1.97		
		2-methyl-2-pentene	1.83		
		1-methyl cyclopentene	1.85		
		ethylbenzene	1.47		
		m-xylene	3.05		
		p-xylene	1.34		
		o-xylene	1.83		
		benzene	1.48		

	toluene	6.73	

Table 6.
Approximate Weight Percent and Carbon Number Comparison of Hydrocarbons in High Benzene Naphtha Category and Comparable Products (a).

Substance Name	Olefins		Aromatics		Paraffins	
	% (wt.)	C # (b)	% (wt.)	C # (b)	% (wt.)	C # (b)
Products in High Benzene Naphtha Category	1-34	5-9	>40-100	6-11	>4-75	5-10
Alkenes, C6 Rich	100	5-7	0	-	0	-
Alkenes, C7-9, C8 Rich	100	7-9	0	-	0	-
C8-C10 Aromatics, Predominantly C9 Aromatics	0	-	>97	8-10	<3	-
C8-C14 Aromatics, Predominantly Alkyl Naphthalenes and Naphthalene	0	-	>94	10-14	<6	-
Naphtha (petroleum), Light Alkylate (gasoline stream)	0	-	0	-	92	5-8
Naphtha (petroleum), Light Catalytically Cracked (gasoline stream)	24	5-6	16	6-8	21	5-7
Naphtha (petroleum), Light Catalytically Reformed (gasoline stream)	0	-	38	6-7	50	5-7

a Approximate weight percent and carbon number ranges of the predominant chemical components by chemical class[olefins/aromatics/paraffins] for selected products contained by this category and for comparable products not in this category that have aquatic toxicity data that can be used as read across data for this category; % compositions may not total 100%.

b Predominant carbon number range

Table 7.
Acute Fish Toxicity Data for Selected Chemicals and Complex Products used to Characterize the Toxicity of Products in the High Benzene Naphtha Category.

CHEMICAL / PRODUCT	CARBON NUMBER	ORGANISM	AQUATIC TOXICITY (a) (96-hr, mg/L)	REFERENCE
n-Pentane	5	*Oncorhynchus mykiss*	LC50 = 4.3	IHSC*
n-Hexane	6	*Pimephales promelas*	LC50 = 2.5	IHSC*
Benzene	6	*Oncorhynchus mykiss*	LC50 = 5.9	****
Alkenes, C6 Rich	5-7(b)	*Oncorhynchus mykiss*	LL50 = 12.8	HOP**
Mixed Cycloparaffins, C7-8, C7 Rich	7	*Oncorhynchus mykiss*	LC50 = 5.4(c)	IHSC*
Toluene	7	*Pimephales promelas*	LC50 = 14.6	IHSC*
Alkenes, C7-9, C8 Rich	7-9(b)	*Oncorhynchus mykiss*	LL50 = 8.9	HOP**
o-Xylene	8	*Pimephales promelas*	LC50 = 16.4	IHSC*
p-Xylene	8	*Oncorhynchus mykiss*	LC50 = 2.6	IHSC*
p-Xylene	8	*Pimephales promelas*	LC50 = 8.9	IHSC*
Ethylbenzene	8	*Pimephales promelas*	LC50 = 12.1	IHSC*
Naphtha (Petroleum), Light Alkylate (gasoline stream)	5-8(b)	*Pimephales promelas*	LL50 = 8.2	API***
Naphtha (petroleum), Light Catalytically Cracked (gasoline stream)	5-8(b)	*Pimephales promelas*	LL50 = 46	API***
Naphtha (petroleum), Light Catalytically Reformed (gasoline stream)	5-7(b)	*Pimephales promelas*	LL50 = 34	API***
1,2,4-Trimethyl-benzene	9	*Pimephales promelas*	LC50 = 7.7	IHSC*
C8-C10 Aromatics, Predominantly C9 Aromatics	8-10(b)	*Oncorhynchus mykiss*	LL50 = 18.0	IHSC*
C8-C14 Aromatics, Predominantly alkyl Naphthalenes and Naphthalene	10-12(b)	*Oncorhynchus mykiss*	LL50 = 3.0	IHSC*

a Endpoint is mortality; LC = Lethal Concentration; LL = Lethal Loading; NOELR = No Observed Effect Loading Rate; values cited as "concentration" are based on measured values

b Predominant carbon number or range

c 93-hour value

* Robust summary from the International Hydrocarbon Solvents Consortium: Contained in selected

SIAR (to be submitted)

** Robust summary from the Higher Olefins Panel HPV Test Plan (submitted)

*** Robust summary from the American Petroleum Institute: Gasoline Test Plan (to be submitted)

**** Galassi, S., M. Mingazzini, L. Viagano, D. Cesareo, and M.L. Tosato, 1988. Benzene is in the OECD SIDS Program.

Table 8.
Acute Invertebrate Toxicity Data for Selected Chemicals and Complex Products used to Characterize the Toxicity of Products in the High Benzene Naphtha Category.

CHEMICAL / PRODUCT	CARBON NUMBER	ORGANISM	AQUATIC TOXICITY (a) (48-hr, mg/L)	REFERENCE
n-Pentane	5	*Daphnia magna*	EC50 = 2.7	IHSC*
n-Hexane	6	*Daphnia magna*	EC50 = 2.1	IHSC*
Cyclohexane	6	*Daphnia magna*	EC50 = 0.9	IHSC*
Benzene	6	*Daphnia magna*	EC50 = 18(b)	***
o-Xylene	8	*Daphnia magna*	EC50 = 1.0	IHSC*
m-Xylene	8	*Daphnia magna*	EC50 = 4.7	IHSC*
Naphtha (Petroleum), Light Catalytically Reformed (gasoline stream)	5-7(c)	*Daphnia magna*	EL50 = 10	API**
Naphtha (Petroleum), Light Alkylate (gasoline stream)	5-8(c)	*Daphnia magna*	EL50 = 32	API**
Naphtha (Petroleum), Light Catalytically Cracked (gasoline stream)	5-8(c)	*Daphnia magna*	EL50 = 18	API**
C8-C10 Aromatics, Predominantly C9 Aromatics	8-10(c)	*Daphnia magna*	EL50 = 21.3	IHSC*
Naphthalene	10	*Daphnia magna*	EL50 = 16.7(d)	IHSC*
C8-C14 Aromatics, Predominantly Alkyl Naphthalenes and Naphthalene	10-12(c)	*Daphnia magna*	EL50 = 3.0	IHSC*

a Endpoint is immobility; EC = Effect Concentration; EL = Effect Loading; NOELR = No Observed Effect Loading Rate; values cited as “concentration” are based on measured values

b 24-hour study

c Predominant carbon number or range

d Based on nominal values

* Robust summary from the International Hydrocarbon Solvents Consortium: Contained in selected

SIAR (to be submitted)

** Robust summary from the American Petroleum Institute: Gasoline Test Plan (to be submitted)

*** Galassi, S., M. Mingazzini, L. Viagano, D. Cesareo, and M.L. Tosato, 1988. Benzene is in the OECD SIDS program.

Table 9.
Alga Toxicity Data for Selected Chemicals and Complex Products Used to Characterize the Toxicity of Products in the High Benzene Naphtha Category.

CHEMICAL / PRODUCT	CARBON NUMBER	ORGANISM	AQUATIC TOXICITY (a) (72-hr, mg/L)	REFERENCE
n-Pentane	5	*Pseudokirchneriella subcapitata(b)*	EbC50 = 10.7 ErC50 = 7.5 NOECb = 1.3 NOECr = 2.0	IHSC*
Benzene	6	*Pseudokirchneriella subcapitata*	EbL50 = 29	***
Naphtha (Petroleum), Light Catalytically reformed (gasoline stream)	5-7(c)	*Pseudokirchneriella subcapitata*	EbL50 = 8.5 NOELRb = 5.0	API**
Naphtha (Petroleum), Light alkylate (gasoline stream)	5-8(c)	*Pseudokirchneriella subcapitata*	EbL50 = 45 NOELRb = 18	API**
Naphtha (Petroleum), Light Catalytically Cracked (gasoline stream)	5-8(c)	*Pseudokirchneriella subcapitata*	EbL50 = 64 NOELRb = 51	API**
C8-C10 Aromatics, Predominantly C9 Aromatics	8-10(c)	*Pseudokirchneriella subcapitata*	EbL50 = 2.6 ErL50 = 2.9 NOELRb = 1.0 NOELRr = 1.0	IHSC*
C8-C14 Aromatics, Predominantly Alkyl Naphthalenes and Naphthalene	10-12(c)	*Pseudokirchneriella subcapitata*	EbL50 = 1-3 ErL50 = 1-3 NOELRb = 1.0 NOELRr = 1.0	IHSC*

a Endpoint is growth inhibition; EbC = Effect Concentration for biomass); ErC = Effect Concentration for growth rate; EbL = Effect Loading for biomass; ErL = Effect Loading for growth rate; NOEC(b) = No Observed Effect Concentration for biomass; NOEC(r) = No Observed Effect Concentration for growth rate; NOELR(b) = No Observed Effect Loading Rate for biomass; NOELR(r) = No Observed Effect Loading Rate for growth rate; values cited as "concentration" are based on measured values

b Formerly known as *Selenastrum capricornutum*

c Predominant carbon number or range

* Robust summary from the International Hydrocarbon Solvents Consortium: Contained in selected SIAR (to be submitted)

** Robust summary from the American Petroleum Institute: Gasoline Test Plan (to be submitted)

*** Galassi, S., M. Mingazzini, L. Viagano, D. Cesareo, and M.L. Tosato, 1988. Benzene is in the OECD SIDS Program.

Table 10. Assessment Plan for High Benzene Naphthas Category Under the Program. (Robust summaries for existing studies are submitted separately.)

Stream Description	Human Health Effects						Ecotoxicity			Physical Chem.[1]	Environmental Fate			
	Acute Toxicity	Genetic Point Mut.	Genetic Chrom.	Sub-chronic	Develop-mental	Reproduc-tion	Acute Fish	Acute Invert.	Algal Toxicity		Photo-deg.	Hydro-lysis	Fugacity	Biodeg.
Pyrolysis Gasoline [15-67% benzene]	A	A	ACD	ACD	A	ACD	RA	RA	RA	CM	CM/TD	TD	CM	RA
Pyrolysis C6 Fraction [35-77% benzene]	ACD	ACD	ACD	ACD	ACD	ACD	RA	RA	RA	CM	CM/TD	TD	CM	RA
Pyrolysis C6-C8 Fraction [30-80% benzene]	ACD	ACD	ACD	ACD	ACD	ACD	RA	RA	RA	CM	CM/TD	TD	CM	RA
Pyrolysis C5-6 Fraction [70% benzene]	ACD	ACD	ACD	ACD	ACD	ACD	RA	RA	RA	CM	CM/TD	TD	CM	RA
Hydrotreated C6 Fraction [75-76% benzene]	ACD	ACD	ACD	ACD	ACD	ACD	RA	RA	RA	CM	CM/TD	TD	CM	RA
Hydrotreated C6-C7 Fraction [40-69% benzene]	ACD	ACD	ACD	ACD	ACD	ACD	RA	RA	RA	CM	CM/TD	TD	CM	RA
Hydrotreated C6-C8 Fraction [40-60% benzene]	A	A	A	ACD	ACD	ACD	RA	RA	RA	CM	CM/TD	TD	CM	RA
Quench Loop Pyrolysis Oil [10-22% benzene]	ACD	ACD	ACD	ACD	ACD	ACD	RA	RA	RA	CM	CM/TD	TD	CM	RA
Recovered Oil from Waste Water Treatment [NDA]	ACD	ACD	ACD	ACD	ACD	ACD	RA	RA	RA	CM	CM/TD	TD	CM	RA
Extract from Benzene Extraction [60-75% benzene]	ACD	ACD	ACD	ACD	ACD	ACD	RA	RA	RA	CM	CM/TD	TD	CM	RA
Benzene [OECD SIDS; not member of category]	A	A	A	A	A	A	A	A	A	CM	CM/TD	TD	CM	A

1 Measured data for selected physicochemical endpoints will be identified in conjunction with calculated data to characterize this category.

A Adequate existing data available

ACD Adequate existing component data for read across (see Sec. III.A.)

TD Technical Discussion proposed

CM Computer Modeling proposed

RA Read Across (see Sec. III.C. and D.)

Table 11.
American Chemistry Council Olefins Panel Sponsored HPV Test Categories

Category Number	Category Description
1	Crude Butadiene C4
2	Low Butadiene C4
3	C5 Non-Cyclics
4	Propylene Streams (C3) - Propylene sponsored through ICCA
5	High Benzene Naphthas
6	Low Benzene Naphthas
7, 8, 9	Resin Oils and Cyclodiene Dimer Concentrates
10	Fuel Oils

Appendix I

ETHYLENE PROCESS DESCRIPTION

A. The Ethylene Process

1. Steam Cracking

Steam cracking is the predominant process used to produce ethylene. Various hydrocarbon feedstocks are used in the production of ethylene by steam cracking, including ethane, propane, butane, and liquid petroleum fractions such as condensate, naphtha, and gas oils. The feedstocks are normally saturated hydrocarbons but may contain minor amounts of unsaturates. These feedstocks are charged to the coils of a cracking furnace. Heat is transferred through the metal walls of the coils to the feedstock from hot flue gas, which is generated by combustion of fuels in the furnace firebox. The outlet of the cracking coil is usually maintained at relatively low pressure in order to obtain good yields to the desired products. Steam is also added to the coil and serves as a diluent to improve yields and to control coke formation. This step of the ethylene process is commonly referred to as "steam cracking" or simply "cracking" and the furnaces are frequently referred to as "crackers."

Subjecting the feedstocks to high temperatures results in the partial conversion of the feedstock to olefins. In the simplest example, feedstock ethane is partially converted to ethylene and hydrogen. Similarly, propane, butane, or the liquid feedstocks are also converted to ethylene. While the predominant products produced are ethylene and propylene, a wide range of additional products are also formed. These products range from methane (C1) through fuel oil (C12 and higher) and include other olefins, diolefins, aromatics and saturates (naphthenes and paraffins).

2. Refinery Gas Separation

Ethylene and propylene are also produced by separation of these olefins from refinery gas streams, such as from the light ends product of a catalytic cracking process or from coker offgas. This separation is similar to that used in steam crackers, and in some cases both refinery gas streams and steam cracking furnace effluents are combined and processed in a single finishing section. These refinery gas streams differ from cracked gas in that the refinery streams have a much narrower carbon number distribution, predominantly C2 and/or C3. Thus the finishing of these refinery gas streams yields primary ethylene and ethane, and/or propylene and propane.

B. Products of the Ethylene Process

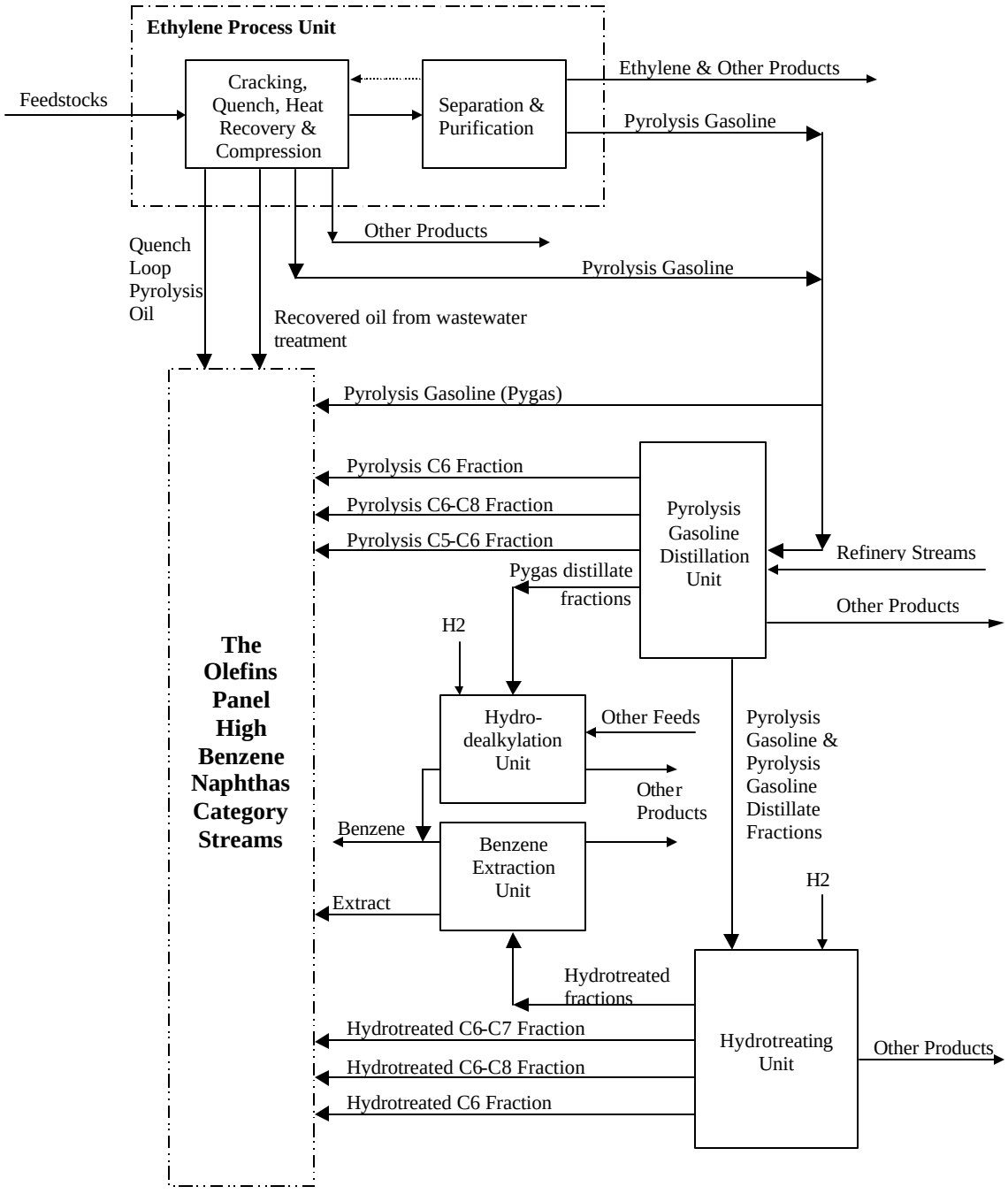
The intermediate stream that exits the cracking furnaces (i.e., the furnace effluent) is forwarded to the finishing section of the ethylene plant. The furnace effluent is commonly referred to as "cracked gas" and consists of a mixture of hydrogen, methane, and various hydrocarbon compounds with two

or more carbon atoms per molecule (C2+). The relative amount of each component in the cracked gas varies depending on what feedstocks are cracked and cracking process variables. Cracked gas may also contain relatively small concentrations of organic sulfur compounds that were present as impurities in the feedstock or were added to the feedstock to control coke formation. The cracked gas stream is cooled, compressed and then separated into the individual streams of the ethylene process. These streams can be sold commercially and/or put into further steps of the process to produce additional materials. In some ethylene processes, a liquid fuel oil product is produced when the cracked gas is initially cooled. The ethylene process is a closed process and the products are contained in pressure systems.

The final products of the ethylene process include hydrogen, methane (frequently used as fuel), and the high purity products ethylene and propylene. Other products of the ethylene process are typically mixed streams that are isolated by distillation according to boiling point ranges. It is a subset of these mixed streams that make up the constituents of the High Benzene Naphthas Category.

The chemical process operations that are associated with the process streams in the High Benzene Naphthas Category are shown in Figure 1.

Figure 1. Chemical Processing Operations Associated with Process Streams in the High Benzene Naphthas Category



AR201-13436B

CAS No.: 71-43-2
Robust Summary No.: OP E-002

Biodegradation

Test Substance:	CAS No. 71-43-2; Benzene
Method/Guideline:	OECD 301F
Year (guideline):	1993
Type (test type):	Ready Biodegradability, Manometric Respirometry Test
GLP:	Yes
Year (study performed):	2000
Inoculum:	Domestic activated sludge
Exposure Period:	28 days
Test Conditions: (FT - TC) • **Note: Concentration prep., vessel type, replication, test conditions.**	Activated sludge and test medium were combined prior to test material addition. Test medium consisted of glass distilled water and mineral salts (Phosphate buffer, Ferric chloride, Magnesium sulfate, Calcium chloride, EDTA). Test vessels were 500 mL dark glass bottles placed on a magnetic stirrer and electronically monitored for oxygen consumption. Test material and blanks were tested in triplicate, controls were tested in duplicate. Test material (benzene) concentration was 17mg/L. Sodium benzoate (positive control) concentration was 30mg/L. Toxicity control with benzene and Na Benzoate concentrations at 17 and 30 mg/L, respectively. Test temperature was 22 +/- 2 Deg C. All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.
Results: (FT - RS) **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Test material was readily biodegradable. Half-life was <2 weeks. By day 28, 63.0% degradation of the test material was observed. 10% biodegradation was achieved in less than 5 days, 50% biodegradation on approximately day 5. By day 5, >60% biodegradation of positive control was observed, which meets the guideline requirement. No excursions from the protocol were noted. Biodegradation was based on oxygen consumption and the theoretical oxygen demand of the test material as calculated using results of an elemental analysis of the test material.

Sample	% Degradation* (day 28)	Mean % Degradation (day 28)
Benzene	54, 72, 63	63
Na Benzoate	65, 75	70
Toxicity Control	59, 65	62

* replicate data

Conclusion: (FT - CL)

CAS No.: 71-43-2
Robust Summary No.: OP E-002

Biodegradation

Reliability: (FT - RL)	(1) Reliable without restriction
Reference: (FT - RE)	Brixham Environmental Laboratory. 2001. OECD 301F, Ready biodegradability: Manometric respirometry. Study # AH0378/A.
Other (source): (FT - SO)	Olefins Panel, American Chemistry Council

* IUCLID field abbreviations include:
FT - Freetext
TC - Test Conditions
RS - Results
CL - Conclusion
RL - Reliability
RE - Reference
SO - Source

Robust Summary - Group 5: High Benzene Naphthas

Acute Toxicity

Test Substance	Dripolene. Yellow, homogeneous liquid, stable for 5 years at ambient temperature. (CRU #93329)
Method	
Method/guideline followed	Not specified
Type (test type)	Acute, limit test
GLP	Yes
Year	1994
Species/Strain	Rat, Sprague-Dawley
Sex	Males and females
No. of animals per sex per dose	5
Vehicle	None
Route of administration	Oral gavage
Test Conditions	Sprague Dawley rats (180-350g) were individually housed in stainless steel suspended cages and fasted overnight prior to administration of 2g/kg neat dripolene. The study room was maintained at 68-72^{0}F with a relative humidity of 35-63% and a 12 hr light-dark cycle. Water and chow diet were available ad lib after dosing. Test article was administered once on day 1 by oral gavage through a blunted needle. Rats were observed for clinical signs approx. 30 min, 1hr, and 4hr, after dosing, and daily thereafter until sacrifice on day 15. Rats were checked once a day for mortality and moribundity. Observations were not made on weekends. Body wts were recorded prior to fasting and on days 1, 8 and 15.
Results	
LD_{50} with confidence limits.	The LD_{50} was not reached at 2g/kg. There were no deaths and all rats gained some weight during the study. Clinical signs noted in one or more rats were salivation, decreased activity, rales, lacrimation, chromodacryorrhea, ataxia, head shaking, chromorhinorrhea, miosis, slight tremors, mydriasis, hyperactivity, hypothermia, urogenital discharge, nasal discharge, decreased food consumption, decreased fecal output, vocalization, and decreased stool size. No gross pathological findings were noted at necropsy.
Remarks	
Conclusions (study author)	The LD_{50} was not reached at 2g/kg.
Data Quality	
Reliability	**1.** Reliable without restriction.
References	Rodriguez, S.C. and Dalbey, W.E. 1994. Acute oral toxicity of dripolene in Sprague Dawley Rats. Study #65642. Stonybrook Laboratories, Princeton, NJ. for Mobil Chemical Co., Edison, NJ.
Other	
Last changed	10/23/2001 (Prepared by a contractor to the Olefins Panel)

Robust Summary - Group 5: High Benzene Naphthas

Acute Toxicity

Test Substance	Dripolene. Yellow, homogeneous liquid, stable for 5 years at ambient temperature. (CRU #93329)
Method	
Method/guideline followed	Not specified
Type (test type)	Acute, limit test
GLP	Yes
Year	1994
Species/Strain	Rabbit, New Zealand White
Sex	Males and females
No. of animals per sex per dose	3
Vehicle	None
Route of administration	dermal
Test Conditions	Rabbits, weighing at least 2kg, were individually housed in stainless steel suspended cages in a study room maintained at 69-72^{0}F with a relative humidity of 40-85% and a 12 hr light-dark cycle. Water and chow diet were available ad lib. The dorsal skin surface extending down from the front to rear legs and from left to right lower flanks was clipped free of hair the day prior to test article administration. Test article was spread evenly over the clipped area (approx. 10% of body surface area) at a dose of 2g/kg. A layer of 8-ply gauze was placed on the dorsal site, and a rubber dam sleeve was fitted snugly over the gauze pad and around the trunk. Edges of the dam were taped in place. An Elizabethan collar was affixed to the neck to prevent oral ingestion of test article and mechanical irritation of the test site. After 24 hrs, the collar and wrappings were removed and residual test article was wiped off. Body wts were recorded on days 1, 8 and 15. Rabbits were observed for toxicity at about 1 and 2 hr post-dose and daily thereafter on weekdays, through day 14. Observations for mortality/moribundity were made daily. Rabbits were sacrificed on day 15 and necropsies were performed.
Results	
LD_{50} with confidence limits.	The LD_{50} was not reached at 2g/kg. There were no deaths during the study and rabbits either gained some weight or remained at day 1 body wt. Signs that might have resulted from treatment in one or more rabbits were: decreased fecal output, decreased fecal pellet size, soft stool, and decreased food consumption. No gross pathological findings were noted at necropsy.
Remarks	
Conclusions	
(study author)	The LD_{50} was not reached at 2g/kg.
Data Quality	
Reliability	**1.** Reliable without restriction.
References	Rodriguez, S.C. and Dalbey, W.E. 1994. Dermal toxicity of dripolene in the New Zealand White rabbit. Study #65643. Stonybrook Laboratories, Princeton, NJ. for Mobil Chemical Co., Edison, NJ.
Other	
Last changed	10/23/2001 (Prepared by a contractor to the Olefins Panel)

Robust Summary - Group 5: High Benzene Naphthas

Acute Toxicity

Test Substance	Dripolene. Yellow, homogeneous liquid. Stable for 5 years at ambient temperature (CRU #93329)
Method	
Method/guideline followed	Not specified.
Type (test type)	Acute irritation
GLP	Yes
Year	1994
Species/Strain	Rabbit, New Zealand White
Sex	Males and females
No. of animals per sex per dose	3
Vehicle	None
Route of administration	Dermal
Test Conditions	Three males and 3 female rabbits, weighing at least 2kg, were individually housed in stainless steel suspended cages in a room maintained at 69-72^{0}F with relative humidity of 38-85% and 12hr light-dark cycle. Water and chow diet were available ad lib. One 1sq. inch test site was selected on the right anterior flank of 4 animals and the left anterior flank of 2 animals. The sites were designated as anterior flank (1-hr occlusion) test sites. A second 1 sq. inch test site was selected on the right posterior flank of 4 animals and the left posterior flank of 2 animals. The sites were designated as posterior flank (4-hr occlusion) test sites. The test sites were not abraded. 0.5ml of test substance was applied to the posterior test site under 1 sq. inch Webril patch. The patch was secured to the skin with an occlusive rubber dam followed by surgical tape. 0.5ml of test substance was applied to the anterior test site under a 1 sq. inch patch and similarly secured. Following 1hr exposure, the anterior patch was removed and the site evaluated for DOT corrosion. This site was reevaluated at 48hrs post-dosing. After the initial evaluation, residual test substance was removed by gently wiping the site with saline dampened cotton. Following a 4hr exposure, the posterior patch was removed and the site evaluated for DOT corrosion and OSHA Primary Irritation Index (PII). This site was reevaluated at 48hrs post-dosing. After the initial evaluation, the residual test substance was removed by gently wiping the site with saline dampened cotton. The posterior test site was also evaluated for dermal irritation according to the Draize method at 4.5, 28, 52, and 76hrs and at 7, 10 and 14 days post-dosing. Clinical observations were recorded at approx. 1hr and 4hr post-dosing and daily thereafter. The condition of each animal was checked once daily in the morning. The rabbits in this study were concurrently evaluated for ocular irritation to reduce the number of animals used. (Study 65644, see separate summary)
Results	The test material was negative for DOT corrosion after 1hr and 4hr occlusions and 48hr post-dose. After the 4hr occlusion, rabbits showed well-defined erythema (Draize score 2.2) and slight edema (Draize score 2.2) that cleared almost completely after 14 days (Draize scores<1.0). The OSHA PII score was 3.9, corresponding to a rating of "non-irritant". Skin flaking in 4 rabbits and skin cracking in 2 rabbits were observed on day 7.
Remarks	
Conclusions (study author)	The test article was rated non-corrosive by DOT criteria after 1hr and 4hr occlusions, and non-irritating by OSHA PII criteria.
Data Quality	
Reliability	**1.** Reliable without restrictions.
References	Rodriguez, S.C. and Dalbey, W.E. 1994. Acute dermal irritation/corrosion of dripolene in the New Zeakand White rabbit. Study #65644. Stonybrook Laboratories, Inc., Princeton, NJ. for Mobil Chemical Co., Edison, NJ
Other	
Last changed	10/23/2001 (Prepared by a contractor to the Olefins Panel)

Robust Summary - Group 5: High Benzene Naphthas

Acute Toxicity

Test Substance	Dripolene. Yellow, homogeneous liquid, stable for 5 years at ambient temperature. (CRU #93329)
Method	
Method/guideline followed	Not specified
Type (test type)	Acute irritation
GLP	Yes
Year	1994
Species/Strain	Rabbit, New Zealand White
Sex	Males and females
No. of animals per sex per dose	3
Vehicle	None
Route of admin istration	Instillation into conjunctival sac
Test Conditions	Rabbits, weighing at least 2kg, were individually housed in stainless steel suspended cages in a study room maintained at 69-72^{0}F with relative humidity of 40-85% and a 12 hr light-dark cycle. Water and chow diet were available ad lib. The left eye was designated as the test eye and the right eye served as untreated control; 0.1ml of test article was instilled into the left conjunctival sac of 3 males and 3 females. Both eyes were grossly examined and the test eye was scored according to the Draize method at 1, 24, 48 and 72 hrs post-dose. The rabbits tested in this study were also concurrently evaluated for dermal irritation/corrosion to reduce the number of animals used (Study #65645 - see separate summary).
Results	
Remarks	Slight irritation of the iris was seen at 1 hr., which gradually resolved over 10 days; conjunctivae and cornea were irritated to a much greater extent but the effect also resolved over the 10-day post-dose period. One hour Draize scores were cornea, 16.7; iris, 2.5 and conjunctivae, 15.3. Total scores were: 1 hr. 34.5; 24 hr. 15.3; 48 hr, 10.7; 72 hr 9.9; 7 days, 4.5; 10 days, 1.7. Four rabbits had corneal ulceration; conjunctival redness and swelling; two of these rabbits had corneal opacity and iritis.
Conclusions	
(study author)	Total Draize scores were: 1 hr. 34.5; 24 hr. 15.3; 48 hr, 10.7; 72 hr 9.9; 7 days, 4.5; 10 days, 1.7. Four rabbits had corneal ulceration; conjunctival redness and swelling; two of these rabbits had corneal opacity and iritis.
Data Quality	
Reliability	**1.** Reliable without restriction.
References	Rodriguez, S.C. and Dalbey, W.E. 1994. Ocular irritation of dripolene in the New Zealand White rabbit. Study #65644. Stonybrook Laboratories, Princeton, NJ. for Mobil Chemical Co., Edison, NJ. Rodriguez, S.C. and Dalbey, W.E. 1994. Acute dermal irritation/corrosion of dripolene in the New Zealand White rabbit. Study #65645. Stonybrook Laboratories, Princeton, NJ. for Mobil Chemical Co., Edison, NJ.
Other	
Last changed	10/23/2001 (Prepared by a contractor to the Olefins Panel)

Robust Summary - Group 5: High Benzene Naphthas

Acute Toxicity

Test Substance	Hydrogenated Pyrolysis Gasoline CAS# 68410-97-9. Clear liquid, aromatic odor
Method	
Method/guideline followed	Standard method (not referenced) with doses based on a limit test and range-finding study
Type (test type)	Acute LD50
GLP	Yes
Year	1984
Species/Strain	Rat, Fischer 344
Sex	Males and females
No. of animals per sex per dose	5
Vehicle	None
Route of administration	Oral
Test Conditions	Rats (99.9-134.0 g; 57 days old) were individually housed in screen-bottomed cages in a room with 70.6^{0}F temperature, relative humidity of 59% and a 12 hr light/dark cycle. Chow diet and tap water from an automatic watering system were available ad lib. Rats were fasted for 24 hours prior to dosing at 4.2, 4.6, 5.0, and 5.4g/kg and observed at 1 and 4 hrs after dosing on day 1, and daily thereafter, over 14 days for clinical signs, morbidity and mortality. Gross necropsies were performed on all rats. LD50 was calculated by Probit analysis.
Results	
LD_{50} with confidence limits.	LD50 = 5.17g/kg (95% confidence limits: 5.02-5.45g/kg)
Remarks	On day 1, males and females showed dose responsive increases in ataxia, harsh respiratory sounds, and a non-dose responsive increase in red ocular discharge. Soft feces were observed in treated males and females on day 2. Frequency of clinical signs decreased by day 3 and signs were absent by day 5. There were no changes in body weight gain among the groups. Male and female mortalities were combined to calculate an LD50. Mortality from a previously performed limit test, conducted at 5.0g/kg was combined with results from the 5.0g/kg dose in this definitive study, raising that group number to 20. Mortalities were: 0/10 at 4.2, and 4.6g/kg, 7/20 at 5.0g/kg, 7/10 at 5.4g/kg. Gross necropsies revealed red lungs, gas-filled stomach and intestine, mottled liver, discoloration of kidney, and opaque eyes in rats that died during the study. These observations, with the exception of opacity in the left eye of one 5.4g/kg female, were absent in rats sacrificed at study termination (day 15).
Conclusions (study author)	The acute median lethal dose (LD50) for Hydrogenated Pyrolysis Gasoline in male and female rats was 5.17g/kg. A descriptive classification of Practically Non-toxic for acute oral exposure was assigned.
Data Quality	
Reliability	**1.** Reliable without restrictions.
References	Rausina, G.A. 1984. Acute oral toxicity study in rats of hydrogenated pyrolysis gasoline. Proj. #2091. Gulf Life Sciences Center, Pittsburgh, PA
Other	
Last change	5/7/2001 (Prepared by a contractor to the Olefins Panel)

Robust Summary - Group 5: High Benzene Naphthas

Acute Toxicity

Test Substance	Hydrogenated Pyrolysis Gasoline CAS# 68410-97-9. Clear liquid, aromatic odor
Method	
Method/guideline followed	Standard method (not referenced)
Type (test type)	Acute LC50
GLP	Yes
Year	1984
Species/Strain	Rat, Fischer 344
Sex	Males and females
No. of animals per sex /dose	5
Vehicle	Filtered air
Route of administration	Inhalation
Test Conditions	Rats (8 wks. old, 100-172g at initiation) were individually housed in stainless steel, screen-bottomed cages in a room maintained at 73.0^0F (75.5^0F during exposure) temperature, relative humidity of 51% (40% during exposure) and a 12 hr light/dark cycle. Rats received chow diet and tap water ad lib, except during exposure. One group of 10 rats was exposed to aerosolized test article generated by a ball jet nebulizer for 4 hrs. A condensing flask was used to prevent large particles from entering the chamber. Actual average chamber concentration was 12,408ppm (range 8,642-17,371ppm) determined by gas chromatography. Particulate phase was negligible. Rats were observed for clinical signs at 1 and 4 hrs after dosing on day 1 and daily thereafter over 14 days, and for morbidity and mortality twice daily on weekdays, once daily on weekends. Body wt. was determined at initiation and on days 8 and 15. Gross necropsies were performed on all rats at termination on day 15.
Results	
LC_{50} with confidence limits.	LC50>12,408ppm
Remarks	There were no deaths during the study, no effects on body wt gain, and no gross alterations were seen at necropsy. Immediately after exposure, all rats exhibited lethargy, increased and labored respiration, and ocular discharge; most animals showed twitching and dry red material around nose/mouth. There were a few instances of harsh respiratory sounds, trembling, and perianal soiling. These clinical signs decreased in frequency by 4 hr post-exposure and disappeared by day 2.
Conclusions (study author)	No deaths occurred at the dose of 12,408ppm of test article, indicating a descriptive classification of Practically Non-toxic for acute inhalation exposure. Clinical signs noted immediately after exposure (increased/labored respiration, twitching, trembling, lethargy, ocular discharge) were not observed by day 2 and thereafter.
Data Quality Reliability	**1.** Reliable without restrictions.
References	Rausina, G.A. 1984. Acute inhalation toxicity study in rats of hydrogenated pyrolysis gasoline. Proj. #2092. Gulf Life Sciences Center, Pittsburgh, PA
Other	
Last change	Revised 7/27/2001 (Prepared by a contractor to the Olefins Panel)

Robust Summary - Group 5: High Benzene Naphthas

Genetic Toxicity - in Vitro

Test Substance	Hydrogenated Pyrolysis Gasoline, CAS #68410-97-9. clear liquid with aromatic odor, negligible solubility in water, contains <55.0% benzene, <25% toluene, <10% dimethyl benzene/xylene, <7% pentane, <7% ethylbenzene, <3% cyclohexane, <2% hexane
Test substance	
Method	
Method/guideline followed	Standard method per Ames et al
Type	Reverse mutation bacterial assay
System of testing	Salmonella typhimurium, Escherichia coli with and without metabolic activation
GLP	Yes
Year	1991
Species/Strain	S. typh. TA1535, TA1537, TA98, TA100; E. coli WP2(uvrA)
Metabolic activation	Yes
Species and cell type	Male Sprague Dawley rat liver (S9 fraction), Molecular Toxicology, Inc., Annapolis, MD
Quantity	20% S9 fraction in 0.5ml S9 mix/plate
Induced or not induced	Aroclor 1254induced, rats given a single 500mg/kg ip dose
Concentrations tested	0, 33, 100, 333, 1000, 3333, 10,000µg/plate ± S9. All diluted in acetone (200mg/ml)
Statistical Methods	None specified. Test article considered mutagenic when it induces a reproductive, dose-related increase in number of revertants in one or more strains at 3 consecutive dose levels. A non-mutagen does not induce a dose-related increase in at least 2 independent tests.
Remarks for Test Conditions	Hydrogenated pyrolysis gasoline (HPG) was prepared in acetone immediately prior to use. At end of the study, an aliquot of the stock dilution was sent to PTRL West, Richmond, CA to confirm concentration. Salmonella (approx. 10^8cells/ml) were exposed to either test material or acetone in 3 plates/dose ± S9 by the plate incorporation method. Six dose levels from 33-10,000µg/plate were employed in both the range-finding trial using TA100 and the mutagenicity test with all strains of Salmonella and E. coli. Optimum level of S9 for the mutagenicity assay was determined by testing the highest non-toxic dose, 10,000µg per plate with metabolic activation systems containing 4, 20 or 80% S9 fraction. No noteworthy increases in revertants or cytotoxicity was observed at any S9 concentration; 20% S9 was used in the mutagenicity test. All plates were incubated at 37^0C for 48 hrs then revertant colonies were counted. Positive control compounds were: cultures-S9, sodium azide (5µg/plate) for TA1535, TA100; 9-aminoacridine (50µg/plate) for TA1537; 2-nitrofluorene (5µg/plate) for TA98; N-ethyl-N'-Nitro-N-Nitrosoguanidene (5ug/plate) for E. coli WP2, and cultures+S9, 2-anthramine (4µg/plate) for TA1535, TA1537, (2µg/plate) for TA98, TA100, and (20µg/plate) for E. coli WP2. Two independent assays were performed.
Results	HPG did not induce increases in number of revertant colonies and no toxicity was observed in any Salmonella strain or E. coli WP2 with or without 20% S9 metabolic activation in both studies. Positive control compounds performed appropriately.
Genotoxic effects	
Conclusions	Hydrogenated pyrolysis gasoline is not mutagenic to bacteria under conditions of this assay.
(contractor)	
Data Quality	
Reliabilities	**1**. Reliable without restriction
Reference	Riccio, E.S. and Stewart, K.R. 1991. Salmonella-Escherichia coli/microsome plate incorporation assay of Hydrogenated Pyrolysis Gasoline. SRI Study #2545-A03-91, Sponsor study #91-66. SRI International, Menlo Park, CA for Chevron Environmental Health Center, Richmond, CA
Other	
Last changed	5/7/2001 (Prepared by a contractor to the Olefins Panel)

Robust Summary - Group 5: High Benzene Naphthas

Genetic Toxicity - in Vitro

Test Substance	Hydrogenated Pyrolysis Gasoline, CAS #68410-97-9. clear liquid with aromatic odor.
Test substance	Composition, purity and stability referred to sponsor.
Method	
Method/guideline followed	Standard method based on Cortesi et al (1983), Dunkel et al (1981), Reznikoff et al (1973)
Type	In vitro cell transformation
System of testing	Mouse embryo cells
GLP	Yes
Year	1984
Species/Strain	BALB/3T3-A31-1-1 from T. Kakunaga, National Cancer Inst., 1983
Metabolic activation	No
Species and cell type	NA
Quantity	NA
Induced or not induced	NA
Concentrations tested	Cytotoxicity: 8, 16, 32, 64, 128, 256, 512, 1024, 2048, and 5000µg/ml; Transformation: 100, 250, 500, 1500µg/ml, all diluted in 10% Pluronic® polyol F68 (prepared in deionized water, mol. wt. 8350, 80% hydrophilic).
Exposure period	2 days
Statistical Methods	None employed. Criteria for positive response were a two-fold increase in type III foci at the highest dose over vehicle control (at least 2 type III foci if vehicle control had none) with or without a dose related response, or a two-fold increase at two or more consecutive doses. Test is equivocal if two-fold increase occurred at any one level other than the highest acceptable dose.
Remarks for Test Conditions	Sufficient Hydrogenated Pyrolysis Gasoline (HPG) was weighed separately for each dose level, 0.40ml of 10% F68 added per ml of final volume and medium (Eagles MEM with 10% heat-inactivated fetal calf serum) added as required to achieve final volume for testing. Test preparations were mixed just prior to addition to cultures at 50µl to each 5 ml culture. All cultures were incubated at 37^0C in 5% CO_2 enriched humidified atmosphere. For cytotoxicity, 2 cultures/dose group, 2 cultures for vehicle F68 or medium negative control were seeded with $1x10^4$ cells/plate in day 1, exposed on days 2-3, trypsinized and counted with a Coulter Model ZB on day 4 for at least 20% survival. For transformation, 15 cultures ($1x10^4$ cells/flask/dose group)) and two colony-forming cultures (100 cells/plate/dose group) were seeded on day 1, exposed on days 2-3 and culture medium changed on day 4. For transformation cultures, medium continued to be changed weekly to day 29. Positive control was 3-methylcholanthrene (1µg/ml). Colony forming cultures were fixed, stained, and counted visually on day 10 to determine cloning efficiency (avg. number colonies/plate ÷ 100 cells seeded). Transformation cultures were fixed and stained on day 29 for focus counting and evaluation. Transformation frequency = total type III foci ÷ total flasks/dose group.
Results	
Genotoxic effects	HPG induced toxicity in BALB/3T3 cells after two days exposure beginning at 128 µg/ml (45.4% relative survival) with relative survivals of 26.7, 25.6, 3.2 and 0% at 512, 1024, 2048 and 5000µg/ml, respectively. In the transformation assay, toxicity was seen at all dose levels (relative cloning efficiencies of 53.7, 67.8, 78.5 and 0% at 100, 250, 500 and 1500µg/ml). At 1500µg/ml, the highest dose level, HPG induced 5 Type III foci; no other dose levels produced a positive response. Transformation frequencies were 0.13, 0, 0, 0.07 and 0.36 for medium control, vehicle control, 100, 250, 500 and 1500µg/ml, respectively. Positive and negative controls gave appropriate responses.
Conclusions	
(contractor)	Hydrogenated Pyrolysis Gasoline induced transformation in BALB/3T3 cells under conditions of this assay. Cytotoxicity and impairment of cloning efficiency were also observed. The positive response was observed only at the highest dose level, a level that appeared to be too toxic for cells to recover and form colonies (0% relative colony forming efficiency)

Data Quality	
Reliabilities	**1.** Reliable without restriction
Reference	Brecher, S. 1984. Transformation test of Hydrogenated Pyrolysis Gasoline. Proj. #2098. Gulf Life Sciences Center, Pittsburgh, PA for Gulf Oil Chemicals Co, Houston, TX Cortesi, E. et al. 1983. Teratogenesis, Carcinogenesis, Mutagenesis 3: 101-110. Dunkel, V.A. et al. 1981. J. Nat'l Cancer Inst. 67: 1303-1315. Reznikoff, C.A. et al. 1973. Cancer Res. 3239-3249.
Other	
Last changed	Revised 8/27/2001 (Prepared by a contractor to the Olefins Panel).

Robust Summary - Group 5: High Benzene Naphthas

Genetic Toxicity - in Vitro

Test Substance	Hydrogenated Pyrolysis Gasoline, CAS #68410-97-9. clear liquid with aromatic odor.
Test substance	Composition, purity and stability referred to sponsor.
Method	
Method/guideline followed	Standard method based on Williams et al (1977, 1982)
Type	In vitro mammalian DNA repair assay
System of testing	Unscheduled DNA synthesis (UDS) in primary hepatocyte cultures
GLP	Yes
Year	1984
Species/Strain	Fischer 344 male rat (10 wks old)
Metabolic activation	No
Species and cell type	NA
Quantity	NA
Induced or not induced	NA
Concentrations tested	8, 16, 32, 64, 128, 256, 512, 1024µg/ml diluted in 10% Pluronic F68 (prepared in deionized water, mol. wt 8350, 80% hydrophilic)
Exposure period	18 hrs.
Statistical Methods	None specified. Criteria for positive response are incorporation of radioactive precursor (^{3}H-thymidine) in cells that are not normally synthesizing DNA, indicating repair of damage. A positive response is defined as a mean net nuclear grain count at any treatment level that exceeds concurrent negative control by at least 6 grains/nucleus; negative control value must not exceed 5 grains. If this criterion is not met, a positive response can be identified if there is a significant difference ($p<0.01$) in % cells in repair at any dose level and negative control value. This indicator defines whether a small fraction of cells is undergoing repair (Casciano & Gaylor, 1983). A positive response need not be dose related.
Remarks for Test Conditions	Sufficient Hydrogenated Pyrolysis Gasoline (HPG) was weighed separately for each dose level, 0.40ml of 10% F68 added per ml of final volume and sufficient medium (Williams Medium E with 10% fetal bovine serum and insulin) added to achieve final volume. Test preparations were mixed just prior to addition at 20µl to each 2ml culture. The conc. of ^{3}H-thymidine (½ life 12.4 yrs.) used in these assays was 1mCi/ml. All cultures were incubated at 37^0C in 5% CO_2 enriched humidified atmosphere. No range finding assay was performed. In the UDS assay, $2x10^5$ cells/ml were seeded into coverslip cultures, exposed to ^{3}H-thymidine and test substance for 18 hours (3 cultures/dose level, 8 dose levels), untreated controls, vehicle F68 control and positive control, 2-acetyl aminofluorene (0.01µg/ml). Cells growing on coverslips were rinsed, fixed and glued to microscope slides on day 2. On day 3, slides were dipped in autoradiographic emulsion and stored in the dark at 2-8^0C. Autoradiographs were developed, stained and coverslipped on day 10. Numbers of grains overlying 50 randomly selected nuclei/slide were counted. The highest of 3 cytoplasmic grain counts/cell were subtracted and this number was divided by a conversion factor (unspecified) to obtain net nuclear grain count. Avg. net nuclear grain count/slide (sum of net nuclear grain count ÷ 50) and mean net nuclear grain count (avg. net nuclear grain count/slide ÷3) were calculated. In addition, % cells in repair were determined for each dose level.
Results	
Genotoxic effects	HPG induced toxicity in primary hepatocytes following 18 hr exposure that left too few cells for UDS analysis at doses of 512 and 1024µg/ml. HPG did not induce unscheduled DNA synthesis at any dose level with sufficient cells to be analyzed. Positive and negative controls gave appropriate responses.
Conclusions	
(contractor)	Hydrogenated Pyrolysis Gasoline did not induce unscheduled DNA synthesis in primary cultures of rat hepatocytes under conditions of this assay.

Data Quality *Reliabilities*	**2.** Reliable with restrictions. No table of cell counts/viability. No individual data to verify calculations and identify conversion factor. Statistical criteria are mentioned but method is not cited.
Reference	Brecher, S. 1984. Hepatocyte primary culture/DNA repair test of Hydrogenated Pyrolysis Gasoline. Proj. # 2097. Gulf Life Sciences Center, Pittsburgh, PA for Gulf Oil Chemicals Co., Houston, TX Williams, G.M. 1977. Cancer Res. 37: 1845-1851 Williams et al. 1977. In Vitro 13: 809-817 Williams et al. 1982. Mut. Res. 97:359-370 Casciano, D.A. and Gaylor, D.W. 1983. Mut. Res. 122:81-86
Other *Last changed*	5/7/2001 (Prepared by a contractor to the Olefins Panel)

Robust Summary - Group 5: High Benzene Naphthas

Genetic Toxicity - in Vivo

Test Substance	
Remarks	Hydrogenated Pyrolysis Gasoline, CAS #68410-97-9. Clear liquid with aromatic odor. Compositional analysis, purity and stability referred to sponsor.
Method	
Method/guideline followed	None specified. Comparable to standard assay.
Type	Mammalian bone marrow erythrocyte micronucleus assay
GLP	Yes
Year	1984
Species	Mice
Strain	Crl:CD-1(ICR)BR Swiss
Sex	Male and female. Range-finding 2M, 2F (10 wks old)/group; 3 groups; Micronucleus test 10M, 10F (11 wks old)/group in 4 groups, 15M, 15F in one group.
Route of administration	Oral gavage
Doses/concentration levels	0, 0.5, 1.0, 2.0g/kg (2doses), 2.0g/kg (1 dose) undiluted
Exposure period	1 dose/day for 2 days: one group- 1 dose, 1 day only
Statistical methods	Values from treated groups for daily mean body weights, group means and std. dev. for polychromatic erythrocytes (PCEs) with micronuclei (MN) , and group mean ratios of PCE to normochromatic erythrocytes (NORMs) were calculated and compared with vehicle control values by Student's t-test. Positive response was indicated by statistically significant ($p<0.05$) increases in micronucleated PCE at any dose level with a dose related response evident. Results were considered equivocal if only one of these criteria was met.
Remarks for Test Conditions.	Animals in the range-finding study (2M, 2F/group), 3 treated groups (no control group) were given 1.25, 2.5, and 5.0g/kg neat hydrogenated pyrolysis gasoline (HPG) by gavage once each day for two days. Eighty percent of the dose level that produced =50% mortality was selected for the maximum dose in the micronucleus study. In the micronucleus study, three groups of mice were given undiluted HPG by oral gavage daily for two days at doses of 0.5, 1.0, 2.0g/kg, negative control mice were given corn oil (5g/kg). One-half of each treated group and negative control (5M, 5F) was killed on day 3 and the remainder on day 4. One group (15M, 15F), given 2.0 g/kg by gavage in a single dose for 1 day only, was killed on days 2, 3, 4 (5/sex/day). Positive control mice (4M, 4F) given cyclophosphamide (75 mg/kg) ip daily for 2 days were killed on day 3. Survival, body wt, and clinical signs were observed and recorded daily. Slides of femoral bone marrow smears were prepared, stained with May-Grunewald/Giemsa stain and examined microscopically. For each mouse, 1000 PCE and all associated mature erythrocytes (NORMs) were counted. Data collected included group mean body weights for each day, total PCEs, total NORMs, PCEs with MN, and NORMs with MN.
Results	
Genotoxic effects	NOAELmortality = 1.0g/kg; NOELgenetics > 2.0g/kg (Assigned by reviewer)
NOAEL (NOEL)	In the range-finding study, half of the animals given HPG at conc of 5.0g/kg died on or before day 2. Gross necropsy of dead mice was unremarkable. In the micronucleus test, 1/10 males given 2.0g/kg (2 doses) died on day 2. No other mortality or significant wt changes were observed. Lethargy was observed among high dose mice. Surviving mice treated with HPG did not show any significant increase in micronucleus formation in PCE and no significant changes in ratio of PCE/NORM compared to negative controls. Negative and positive controls gave appropriate results.
LOAEL (LOEL)	
Conclusions	
(study authors)	Oral treatment of mice with Hydrogenated Pyrolysis Gasoline for 1-2 days at doses up to 2.0g/kg/day had no effect on frequency of micronucleated polychromatic erythrocytes in bone marrow under these test conditions. HPG did not induce cytogenetic damage.

Data Quality	
Reliabilities	**1.** Reliable without restriction
References	Khan, S.H. 1984. Micronucleus test of Hydrogenated Pyrolysis Gasoline. Proj. #2096. Gulf Life Sciences Center, Pittsburgh, PA for Gulf Oil Chemicals Co., Houston, TX
Other	
Last changed	5/7/2001 (Prepared by a contractor to the Olefins Panel)

Robust Summary - Group 5: High Benzene Naphthas

Repeated Dose Toxicity

Test Substance	Hydrogenated Pyrolysis Gasoline CAS #68410-97-9, Clear liquid with aromatic odor.
Remarks	
Method	
Method/guideline followed	Standard method, method not referenced
Test type	Subacute
GLP	Yes
Year	1984
Species	Rat
Strain	Fischer 344
Route of administration	Inhalation
Duration of test	8 days
Doses/concentration levels	0, 4869±470, 9137±917ppm±SD, actual exposure conc.
Sex	Males and females (5/sex/group)
Exposure period	6 hrs.
Frequency of treatment	once daily for 5 days (d1-5)
Control group and treatment	5M, 5F; filtered air
Post exposure observation period	2 days
Statistical methods	Body wt variance compared by Bartlett's test and one way analysis of variance. Group mean body wt compared either with Dunnett's test or a modified t-test to assess significance.
Test Conditions	Rats (9 wks old, 113-195g at initiation) were housed individually in stainless steel, screen-bottomed cages. Rooms were maintained at 72.2^0F (exposure chamber 75^0F) with relative humidity of 54% (exposure chamber 50%), and 12 hr light/dark cycle. Rats received chow diet and tap water ad lib throughout the study, except during exposure. Three groups of 10 rats (5M, 5F/group) each, were exposed to test article or air. Test article was aerosolized with a ball jet nebulizer; an in-line condensing flask was used to prevent large particles from entering the exposure chamber. Chamber concentration of test article was measured by gas chromatography. Rats were observed twice daily on weekdays and once daily on weekends for morbidity/mortality, and once daily for clinical signs immediately after exposure on days 1-5. Surviving rats were sacrificed on day 8. Gross necropsies were performed on all rats.
Results	
NOAEL (NOEL)	NOAEL< 4869ppm (estimated by reviewer)
LOAEL (LOEL)	LOAEL= 4869ppm (estimated by reviewer) based on clinical observations, reduced wt gain.
Remarks	Two rats (1M, 1F) from group 3 (9137ppm) died on day 2; one female from group 3 died during exposure on day 1. Rats in groups 2 and 3 showed ocular discharge throughout d1-5. Rats in group 2 showed increased respiratory rate and dry red material around nose and mouth. All rats in group 2 were lethargic and showed labored respiration. Many rats in group 3 were lethargic and exhibited twitching and harsh respiratory sounds during days 1-5. All rats in group 2 and all but one survivor in group 3 appeared normal on day 8. Group mean body wt was significantly decreased in a dose related manner. No test article related effects were seen at gross necropsy on day 8; the male rat that died during the study showed gas in the G.I. tract and red-tinged fluid in the stomach.
Conclusions (study authors)	Exposure to test article caused a significant decrease in group mean body wt of male and female rats of low and high dose groups that was correlated with exposure level. Three deaths occurred in the high dose group during exposure. Major clinical signs were lethargy, twitching, harsh respiratory sounds and ocular discharge. No gross alterations were found in rats surviving to sacrifice.
Quality Reliabilities	**1.** Reliable without restrictions
References	Rausina, G.A. 1984. Five-day repeated dose inhalation toxicity study in rats of Hydrogenated Pyrolysis Gasoline. Proj. #2099. Gulf Life Sciences Center, Pittsburgh, PA
Other	
Last changed	Revised 7/27/2001 (Prepared by a contractor to the Olefins Panel)

Robust Summary – Group 5: High Benzene Naphthas

Fish Acute Toxicity

Test Substance	Hydrogenated Pyrolysis Gasoline, CAS #68410-97-9. 100% pure, colorless liquid.. Composition and stability referred to sponsor.
Method	
Method/guideline followed	OECD Guideline #203, US EPA 40CFR, Part 797.1400
Year (guideline)	1992
Type (test type)	Static Fish Acute Toxicity- Water Accommodated Fraction (WAF)
GLP	Yes
Year (study performed)	1993
Species	Rainbow trout (Oncorhynchus mykiss) from Westacre Trout Farm, Norfolk, UK
Analytical Monitoring	Total carbon analysis using Ionics TC/TOC Model 555 with infra-red gas analyzer to verify concentrations of 0,32, and 320mg/L(WAF)
Exposure Period	96 hrs
Statistical Methods	LC50 and 95% confidence limits were calculated by method of Thompson and Weil (1952, Biometrics 8: 51-54).
Test Conditions Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, supplier of organisms, age, size, weight, loading	Individual test material exposure solutions were prepared as WAFs by adding ratios of test material to dilution water equivalent to 32, 56, 100, 180, and 320mg/L, stirring with a propeller stirrer for 24 hr at 14^0C. After settling for approx. 1hr, WAFs were withdrawn via a siphon into 2 replicate 20liter test vessels/dose group. Ten juvenile fish were introduced into each vessel containing 19cm of either test media or diluent water, an initial loading rate of 0.46g body wt/liter. Animals were exposed for 96 hrs without renewal. Fish were not fed for 48 hrs prior to or during exposure; supplementary aeration was not provided. Average size of fish was determined by measuring control fish at end of exposure: mean std. length= 4.3±0.23cm, mean wt.= 0.92±0.14g. Exposure temperature was 14 ± 1^0C, photoperiod was 16hr light/8hr dark (light intensity not specified); pH increased from 7.5 to 7.9 with increasing dose; mg dissolved O_2/liter was 7.8-8.2 in controls and doses up to 180mg/L, and 9.6-9.8 at 320mg/L (WAF). TC/TOC analysis was not performed at 96 hr since values obtained at 0 hr indicated that TC(dissolved) analysis was not appropriate for verification of HPG(WAF) concentrations; exposure media results were similar to control levels. Criteria for death were absence of respiratory movement and absence of response to physical stimulation of caudal peduncle.
Results	
Units/Value: Note: Deviations from protocol or guideline, analytical method, biological observations, control survival	24 hr LC_{50} = 230mg/L; 48 hr and 72 hr LC_{50} = 180mg/L 96 hr LC_{50} = 170mg/L. 100% mortality occurred at 320mg/L by 24 hrs. Other marked reactions to exposure at 180 and 320mg/L were lethargy, loss of equilibrium and moribundity.
Conclusions (study author)	The 96 hr LC_{50} for Hydrogenated Pyrolysis Gasoline WAF in rainbow trout is 170mg/L (95% CL= 150-200) based on nominal values. The no observed effect level (NOEL) is 100 mg/L (WAF)
Data Quality *Reliabilities*	**2.** Reliable with restriction. Analytical method was inappropriate.
Reference	Douglas, M.T. 1993. Hydrogenated pyrolysis gasoline (Water accommodate fraction) Acute toxicity to Rainbow trout (Oncorrhynchus mykiss). CRTC Ref. #92-79. Huntingdon Research Centre, Ltd., Cambridgeshire, England, for Chevron Research and Technology Co., Richmond, CA
Other *Last changed*	Revised 7/27/2001 (Prepared by a contractor to the Olefins Panel)

Robust Summary – Group 5: High Benzene Naphthas

Algal Toxicity

Test Substance	Hydrogenated Pyrolysis Gasoline, CAS #68410-97-9. 100% pure, colorless liquid.. Composition and stability referred to sponsor.
Method	
Method/guideline followed	OECD Guideline #201, US EPA 40CFR 797.1050
Year (guideline)	1992
Type (test type)	Algae acute toxicity- Water accommodated fraction (WAF)
GLP	Yes
Year (study performed)	1993
Species	Fresh water green algae (Selenastrum capricornutum), strain # CCAP278/4 from Freshwater Biological Assoc. Cumbria, UK
Analytical Monitoring	Yes. Total carbon analysis using Ionics TC/TOC Model 555 with infrared gas analyzer to verify test conc. at 0, 62.5 and 1000mg/L (WAF) at 0 and 96 hrs.
Exposure Period	96 hrs
Statistical Methods	None specified
Test Conditions Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, age.	Individual test material solutions were prepared as WAF by adding ratios of test material to dilution water equivalent to 62.5, 125, 250, 500 and 1000mg/L, stirred on a magnetic stirrer for 24 hr at 24^0C. After settling for approx. 1hr, WAFs were withdrawn by siphon and 100ml measured into 250 ml conical flasks. Two ml of algal suspension in log phase (0.802 absorbance at 665nm) were added to each of 3 flasks/dose level. Cultures were incubated without media renewal for 96 hrs under continuous illumination of approx. 7000 lux, provided by 7x30W "warm white " 1 meter fluorescent tubes in a Gallenkamp Illuminated Orbital Incubator at 24 ± 1^0C and oscillation of 120 cycles/min. Samples were taken at 0, 24, 48, 72 and 96 hr and absorbance measured in a spectrophotometer at 665nm wavelength. Cell densities of control cultures were counted with a haemocytometer at initiation and study termination. pH values ranged from 7.8-8.0 at initiation and 7.6-8.4 at 96 hrs. Index of growth was calculated from the area under the growth curve; percent inhibition of growth at each dose was calculated by comparing the area under test curve with control. Median effective conc. for inhibition of growth (EbC_{50}) is based on comparison of areas under growth curves after 72 and 96 hrs. Avg. max growth rate is calculated from the log phase of growth curve for each culture. ErC_{50} is the median effective conc. for inhibition of growth based on comparison of max growth (24-48 hrs).
Results Units/Value: Measurement (cells/growth) Note: Deviations from protocol or guideline, analytical method, biological observations, control survival	Mean cell densities of control cultures at initiation (0 hr)= $8.91x10^4$ cells/ml and at termination (96 hrs) = $2.41x10^6$ cells/ml. No cultures were contaminated and no abnormalities were seen in any culture upon microscopic examination at 96 hrs. Total dissolved carbon was 7.1, 7.0, 17.2 mg/L at initiation and 9.7, 7.9 and 13.0mg/L at 96hrs for 0(control), 62.5 and 1000 mg/L (WAF) respectively. Biomass: EbC_{50} (72 hr) >1000 mg/L (WAF); EbC_{50} (96 hr) >1000 mg/L (WAF) Growth rate: ErC_{50} (24-48hr) >1000mg/L (WAF) NOAEL = 125mg/L
Conclusions (study author)	Hydrogenated pyrolysis gasoline is not inhibitory to the growth of Selenastrum capricornutum at conc of 125mg/L (WAF). EbC_{50} (96hr) and ErC_{50} (24-48hrs) are both >1000mg/L (WAF).
Data Quality *Reliabilities*	**1.** Reliable without restriction
Reference	Douglas, M.T. 1993. Hydrogenated pyrolysis gasoline (Water accommodated fraction) Algal Growth Inhibition. CRTC Ref. #92-81. Huntingdon Research Centre, Ltd, Cambridgeshire, England, for Chevron Research and Technology Co, Richmond, CA
Other *Last changed*	5/10/2001 (Prepared by a contractor to the Olefins Panel)

Robust Summary – Group 5: High Benzene Naphthas

Biodegradation

Test Substance	Hydrogenated Pyrolysis Gasoline, CAS #68410-97-9 100% pure, colorless liquid.. Composition and stability referred to sponsor.
Method	
Method/guideline followed	OECD guideline 301D; EEC directive 67/548 Annex V part C.6 (84/449/EEC)
Year (guideline)	1984
Type (test type)	Aerobic Aquatic Biodegradation (Closed Bottle Test)
GLP	Yes
Year (study performed)	1993
Inoculum	Domestic activated sewage sludge bacteria from Huntingdon Research Centre sewage treatment plant.
Exposure Period	28 days
Test Conditions Note: Concentration prep., vessel type, replication, test conditions.	Hydrogenated pyrolysis gasoline (HPG, 2mg/L) was added, via a Hamilton microliter syringe to reduce loss of volatile constituents, to culture bottles containing inorganic nutrient medium with or without activated sewage sludge bacteria. The nutrient medium consisted of aerated reverse osmosis purified, deionized water, phosphate buffer, magnesium sulfate, calcium chloride and ferric chloride. Activated sewage sludge filtrate was added at a rate of 1 drop of inoculum/liter. Glass 500ml culture bottles covered in foil, fitted with plastic screw caps and PTFE faced sealing discs of ethylene propylene, were filled by siphon and tightened to exclude all air bubbles. Duplicate bottles were prepared in each test and control series to allow single oxygen determination/bottle at 0, 5, 15, and 28 days. Sodium benzoate (3mg/L), the standard substance, was dispensed directly into sludge-inoculated nutrient medium, or added to a sludge-inoculated medium containing 2mg/L HPG. The bottles containing HPG+sodium benzoate were sampled on day 0 and 28 only to examine inhibitory effects. All bottles were incubated in a water bath at 20 ± 1^0C; measurements of dissolved oxygen conc. were made with a Yellow Springs BOD meter. Concentrations of HPG or sodium benzoate as mg carbon/L were not provided.
Results Units/Value: Note: Deviations from protocol or guideline, analytical method.	Percent biodegradation values were calculated as % of Theoretical Oxygen Demand (NO_3); $TOD_{(NO3)}$ was $3.15mgO_2/mg$ for HPG and $1.67mgO_2/mg$ for sodium benzoate. Hydrogenated pyrolysis gasoline attained 68% biodegradation within 28 days but did not degrade 60% within 10 days of exceeding the 10% degradation level. HPG is thus not readily biodegradable. Sodium benzoate degraded 86% within 28 days. Cultures containing both HPG and sodium benzoate showed an oxygen depletion value 5% lower than separate cultures. HPG is not considered to have an inhibitory effect on sewage bacteria.
Conclusions (study author)	Hydrogenated pyrolysis gasoline is not readily biodegradable but is considered ultimately biodegradable. No inhibitory effects on sewage bacteria were observed in this assay.
Data Quality *Reliabilities*	**1.** Reliable without restriction
Reference	Douglas, M.T. 1993. Hydrogenated Pyrolysis Gasoline Ready Biodegradability (Closed Bottle Test). CRTC Ref. #92-82. Huntingdon Research Centre Ltd. Cambridgeshire England for Chevron Research and Technology Co., Richmond, CA
Other *Last changed*	5/10/2001 (Prepared by a contractor to the Olefins Panel)

Robust Summary - Group 5: High Benzene Naphthas

Acute Toxicity

Test Substance	Pyrolysis gasoline (Rerun Tower Overheads) Yellow, homogeneous liquid, stable for 5 years at ambient temperature.
Method	
Method/guideline followed	Not specified
Type (test type)	Acute, limit test
GLP	Yes
Year	1994
Species/Strain	Rat, Sprague-Dawley
Sex	Males and females
No. of animals per sex per dose	5
Vehicle	None
Route of administration	Oral gavage
Test Conditions	Sprague Dawley rats (180-350g) were individually housed in stainless steel suspended cages and fasted overnight prior to administration of 2g/kg neat pyrolysis gasoline. The study room was maintained at 68-72^{0}F with a relative humidity of 35-63% and a 12 hr light-dark cycle. Water and chow diet were available ad lib after dosing. Test article was administered once on day 1 by oral gavage through a blunted needle. Rats were observed for clinical signs approx. 30 min, 1hr and 4hr, after dosing, and daily thereafter until sacrifice on day 15. Rats were checked once a day for mortality and moribundity. Observations were not made on weekends. Body wts were recorded prior to fasting and on days 1, 8 and 15.
Results	
LD_{50} with confidence limits.	The LD_{50} was not reached at 2g/kg. There were no deaths and all rats gained some weight during the study. Clinical signs noted in one or more rats were salivation, decreased activity, rales, lacrimation, chromodacryorrhea, ataxia, chromorhinorrhea, miosis, slight tremors, mydriasis, hyperactivity, hypothermia, urogenital discharge, nasal discharge, decreased food consumption, decreased fecal output, vocalization, and penile discharge. No gross pathological findings were noted at necropsy.
Remarks	
Conclusions (study author)	The LD_{50} was not reached at 2g/kg.
Data Quality	
Reliability	**1.** Reliable without restriction.
References	Rodriguez, S.C. and Dalbey, W.E. 1994. Acute oral toxicity of pyrolysis gasoline in Sprague Dawley Rats. Study #65636. Stonybrook Laboratories, Princeton, NJ. for Mobil Chemical Co., Edison, NJ.
Other	
Last changed	10/16/2001 (Prepared by a contractor to the Olefins Panel)

Robust Summary - Group 5: High Benzene Naphthas

Acute Toxicity

Test Substance	Pyrolysis gasoline (Rerun Tower Overheads). Yellow, homogeneous liquid, stable for 5 years at ambient temperature. (CRU #93328)
Method	
Method/guideline followed	Not specified
Type (test type)	Acute, limit test
GLP	Yes
Year	1994
Species/Strain	Rabbit, New Zealand White
Sex	Males and females
No. of animals per sex per dose	3
Vehicle	None
Route of administration	dermal
Test Conditions	Rabbits, weighing at least 2kg, were individually housed in stainless steel suspended cages in a study room maintained at 69-72^{0}F with a relative humidity of 38-85% and a 12 hr light-dark cycle. Water and chow diet were available ad lib. The dorsal skin surface extending down from the front to rear legs and from left to right lower flanks was clipped free of hair the day prior to test article administration. Test article was spread evenly over the clipped area (approx. 10% of body surface area) at a dose of 2g/kg. A layer of 8-ply gauze was placed on the dorsal site, and a rubber dam sleeve was fitted snugly over the gauze pad and around the trunk. Edges of the dam were taped in place. An Elizabethan collar was affixed to the neck to prevent oral ingestion of test article and mechanical irritation of the test site. After 24 hrs, the collar and wrappings were removed and residual test article was wiped off. Body wts were recorded on days 1, 8 and 15. Rabbits were observed for toxicity at about 1 and 2 hr post-dose and daily thereafter on weekdays through day 14. Observations for mortality/moribundity were made daily. Rabbits were sacrificed on day 15 and necropsies were performed.
Results	
LD_{50} with confidence limits.	The LD_{50} was not reached at 2g/kg. There were no deaths during the study and rabbits either gained some weight or remained at day 1 body wt. Signs that might have resulted from treatment in one or more rabbits were: soft stool, decreased fecal pellet size, nasal discharge, and test site erythema. No gross pathological findings were noted at necropsy.
Remarks	
Conclusions (study author)	The LD_{50} was not reached at 2g/kg.
Data Quality	**1.** Reliable without restriction.
Reliability	
References	Rodriguez, S.C. and Dalbey, W.E. 1994. Dermal toxicity of pyrolysis gasoline in the New Zealand White rabbit. Study #65637. Stonybrook Laboratories, Princeton, NJ. for Mobil Chemical Co., Edison, NJ.
Other	
Last changed	10/16/2001 (Prepared by a contractor to the Olefins Panel)

Robust Summary - Group 5: High Benzene Naphthas

Acute Toxicity

Test Substance	Pyrolysis gasoline (rerun tower overhead). Yellow, homogeneous liquid. Stable for 5 years at ambient temperature. (CRU #93328)
Method	
Method/guideline followed	Not specified.
Type (test type)	Acute irritation
GLP	Yes
Year	1994
Species/Strain	Rabbit, New Zealand White
Sex	Males and females
No. of animals per sex per dose	3
Vehicle	None
Route of administration	Dermal
Test Conditions	Three males and 3 female rabbits, weighing at least 2kg, were individually housed in stainless steel suspended cages in a room maintained at 69-72^{0}F with relative humidity of 38-85% and 12hr light-dark cycle. Water and chow diet were available ad lib. One 1sq. inch test site was selected on the right anterior flank of 4 animals and the left anterior flank of 2 animals. The sites were designated as anterior flank (1-hr occlusion) test sites. A second 1 sq. inch test site was selected on the right posterior flank of 4 animals and the left posterior flank of 2 animals. The sites were designated as posterior flank (4-hr occlusion) test sites. The test sites were not abraded. 0.5ml of test substance was applied to the posterior test site under 1 sq. inch Webril patch. The patch was secured to the skin with an occlusive rubber dam followed by surgical tape. 0.5ml of test substance was applied to the anterior test site under a 1 sq. inch patch and similarly secured. Following 1hr exposure, the anterior patch was removed and the site evaluated for DOT corrosion. This site was reevaluated at 48hrs post-dosing. After the initial evaluation, residual test substance was removed by gently wiping the site with saline dampened cotton. Following a 4hr exposure, the posterior patch was removed and the site evaluated for DOT corrosion and OSHA Primary Irritation Index (PII). This site was reevaluated at 48hrs post-dosing. After the initial evaluation, the residual test substance was removed by gently wiping the site with saline dampened cotton. The posterior test site was also evaluated for dermal irritation according to the Draize method at 4.5, 28, 52, and 76hrs and at 7, 10 and 14 days post-dosing. Clinical observations were recorded at approx. 1hr and 4hr post-dosing and daily thereafter. The condition of each animal was checked once daily in the morning. The rabbits in this study were concurrently evaluated for ocular irritation to reduce the number of animals used. (Study 65638, see separate summary)
Results	The test material was negative for DOT corrosion after 1hr and 4hr occlusions, and 48hr post-dose. After the 4hr occlusion, the 4.5hr to 14day post-dose Draize scores for erythema and edema varied between 2.2 and 3.2, and 1.5 to 3.3, respectively, with no trend over time. The OSHA PII score was 4.7, corresponding to a rating of "non-irritant".
Remarks	Diarrhea, soft stool, decreased fecal pellet size and nasal discharge were observed during the study.
Conclusions (study author)	The test article was rated non-corrosive by DOT criteria after 1hr and 4hr occlusions, and non-irritating by OSHA PII criteria.
Data Quality	
Reliability	**1.** Reliable without restrictions.
References	Rodriguez, S.C. and Dalbey, W.E. 1994. Acute dermal irritation/corrosion of pyrolysis gasoline in the New Zealand White rabbit. Study #65639. Stonybrook Laboratories, Inc., Princeton, NJ. for Mobil Chemical Co., Edison, NJ
Other	
Last changed	10/23/2001 (Prepared by a contractor to the Olefins Panel)

Robust Summary - Group 5: High Benzene Naphthas

Acute Toxicity

Test Substance	Pyrolysis gasoline (Rerun Tower Overheads). Yellow, homogeneous liquid, stable for 5 years at ambient temperature. (CRU #93328)
Method	
Method/guideline followed	Not specified
Type (test type)	Acute irritation
GLP	Yes
Year	1994
Species/Strain	Rabbit, New Zealand White
Sex	Males and females
No. of animals per sex per dose	3
Vehicle	None
Route of administration	Instillation into conjunctival sac
Test Conditions	Rabbits, weighing at least 2kg, were individually housed in stainless steel suspended cages in a study room maintained at 69-72^{0}F with relative humidity of 38-85% and a 12 hr light-dark cycle. Water and chow diet were available ad lib. The left eye was designated as the test eye and the right eye served as untreated control; 0.1ml of test article was instilled into the left conjunctival sac of 3 males and 3 females. Both eyes were grossly examined and the test eye was scored according to the Draize method at 1, 24, 48 and 72 hrs post-dose. The rabbits tested in this study were also concurrently evaluated for dermal irritation/corrosion to reduce the number of animals used (Study #65639 - see separate summary).
Results	
Remarks	Cornea and iris were not affected by treatment, however conjunctivae yielded Draize scores of 13.7 (1hr); 3.7 (24hr); 2.3 (48hr) and 0.7 (72hr).
Conclusions	
(study author)	Pyrolysis gasoline produced conjunctival irritation shortly after instillation that cleared almost completely by 72 hrs.
Data Quality	
Reliability	**1.** Reliable without restriction.
References	Rodriguez, S.C. and Dalbey, W.E. 1994. Ocular irritation of pyrolysis gasoline in the New Zealand White rabbit. Study #65638. Stonybrook Laboratories, Princeton, NJ. for Mobil Chemical Co., Edison, NJ. Rodriguez, S.C. and Dalbey, W.E. 1994. Acute dermal irritation/corrosion of pyrolysis gasoline in the New Zealand White rabbit. Study #65639. Stonybrook Laboratories, Princeton, NJ. for Mobil Chemical Co., Edison, NJ.
Other	
Last changed	10/16/2001 (Prepared by a contractor to the Olefins Panel)

Robust Summary - Group 5: High Benzene Naphthas

Genetic Toxicity - in Vitro

Test Substance	Rerun Tower Overheads from Olefins/Aromatics Plant (light thermal cracked naphtha)
Test substance	CAS # 64741-74-8. Straw colored liquid; 40% benzene, 26% C5, 13% toluene, 20% C4, C6-C8 and xylene.
Method	
Method/guideline followed	Standard method based on Ames et al, 1975
Type	Reverse mutation bacterial assay
System of testing	Salmonella typhimurium with and without metabolic activation
GLP	Yes
Year	1981
Species/Strain	S. typhimurium TA 98, TA100, TA1535, TA1537, and TA1538.
Metabolic activation	Yes
Species and cell type	Sprague Dawley male rat liver (S9 fraction) from Litton Bionetics, Kensington, MD
Quantity	50ul S9 fraction in 0.5ml S9 mix/plate
Induced or not induced	Aroclor 1254-induced, rats were given a single ip 500mg/kg dose, 5 days prior to sacrifice.
Concentrations tested	0, 0.029, 0.094, 0.30, 0.97µl/plate –S9, and 0.094, 0.30, 0.97, and 3.1µl/plate + S9; samples diluted in dimethyl sulfoxide (DMSO). Negative control 50µl DMSO
Statistical Method	None. Criteria for a positive response were an increase in revertant colonies at least two-fold that of negative control at the lowest active dose, and a dose response curve. Positive results must be reproducible in an independent repeat assay.
Remarks for Test Conditions	Rerun tower overheads test solutions were prepared in DMSO immediately prior to use. Salmonella (Approx. 1.4-2x10^8 cells/ml) were exposed to either test solution or DMSO ±S9 by the preincubation method. Doses of 0.029-0.97µl/plate-S9 and 0.094-3.1µl/plate +S9 were determined by a pretest toxicity test in TA 100 and TA1537±S9 using incremental doses from 0.01-10µl/plate. Culture tubes containing 50µl test solution or DMSO, 0.1ml Salmonella and 0.5 ml phosphate buffer or S9 mix were combined and incubated with shaking (150 rpm) for 20 minutes at 37^0C. At the end of the preincubation period, top agar was added, mixed and cultures were overlaid on minimal agar plates, 3 plates/dose/strain. Plates were incubated at 37^0C for 48 hrs, then counted automatically (Biotran II) and background lawn evaluated by stereomicroscope. Positive control compounds were: -S9, 2-nitrofluorene (2-NF, 20µg/plate) for TA98 and TA1538; N-methyl-N'-nitro-N-nitrosoguanidine (MNNG, 2.0µg/plate) for TA100 and TA1535; 9-aminoacridine (9-AA, 25µg/plate) for TA1537; +S9 2-aminoanthracene (2µg/plate) for all strains except TA1537.
Results	
Genotoxic effects	The preliminary toxicity test exhibited severe toxicity at 10µl/plate with activation and at 3.1 and 10µl/plate without activation (individual data not shown). In the mutagenicity test, none of the 5 strains of Salmonella exhibited revertant frequencies substantially different from the solvent or spontaneous controls at any dose level with or without metabolic activation (e.g. TA98-S9: 16, 15, 12, 12, and 0 average revertants/plate and TA100-S9: 111, 115, 107, 94, and 0 at 0[DMSO], 0.029, 0.094, 0.30, and 0.97µl/plate, respectively: TA98+S9: 33, 26, 26, 22, and 0 revertants/plate, and TA100+S9: 128, 161, 128, 118, and 0 revertants/plate at 0[DMSO], 0.094, 0.30, 0.97 and 3.1µl/plate, respectively). Clearing of background lawn and microcolonies were observed at the maximum doses (0.97µl/plate-S9; 3.1µl/plate+S9). Positive control compounds (2 plates/strain) performed appropriately (-S9: MNNG 1906, 1883 revertants/plate in TA 100 and TA1535, respectively; 9-AA 586 revertants/plate in TA1537; 2-NF 2114, 1214 revertants/plate in TA98 and TA1538, respectively; and +S9 2-aminoanthracene 406-2307 revertants/plate for all strains except TA1537). The results of this assay indicate that rerun tower overheads had no mutagenic activity in this test system. (Reviewer's note: Due to toxicity, tests were performed over a low dose range; 3 of 4 doses were non-toxic and showed sufficient growth to evaluate mutagenicity. Testing at any lower doses was impractical).
Conclusions	Rerun Tower Overheads did not induce an increase in revertant colonies in any Salmonella

(contractor)	strain, tested at any dose level with or without metabolic activation in this single Ames test.
Data Quality	
Reliabilities	**1.** Reliable without restriction
Reference	Blackburn, G.R. 1981. An Ames Salmonella/mammalian microsome mutagenesis assay for the determination of potential mutagenicity of Rerun Tower Overheads from an olefins/aromatics plant. Study No. 1781-80. Mobil Environmental and Health Sciences Laboratory, Princeton, NJ. Ames B. N. et al. 1975. Mutat. Res. 31: 347-364.
Other	
Last changed	10/02/2001 (Prepared by a contractor for the Olefins Panel)

Robust Summary - Group 5: High Benzene Naphthas

Genetic Toxicity - in Vitro

Test Substance	Rerun tower overheads (RT0, 0818805). Compositional analysis, stability and purity
Test substance	referred to sponsor
Method	
Method/guideline followed	Standard method, no guideline specified
Type	Cell transformation
System of testing	Mouse embryo cells
GLP	Yes
Year	1981
Species/Strain	BALB-c/3T3 mouse cell line
Metabolic activation	No
Species and cell type	NA
Quantity	NA
Induced or not induced	NA
Concentrations tested	Initial cytotoxicity: 0, 0.01, 0.1, 1.0, 10.0, 100.0µg/ml medium; Transformation: 0. 0.8, 4.0, 20.0 and 100µg/ml, diluted in dimethyl sulfoxide. Negative control was DMSO at 2.5% vol. concentration.
Statistical Method	T-test specified. Standard criteria for positive response is a two fold increase in type III foci at highest dose over vehicle control with or without a dose related response or a 2 fold increase at 2 or more consecutive doses.
Remarks for Test Conditions	Routine procedures were referred to Appendix 1 Standard Operating Procedures, which was not included with this report. Only specifics unique to this assay are presented. Due to the volatile nature of test material, the cytotoxicity assay and transformation assays were conducted in tightly capped T-25 flasks in sealed plastic bags. The pH of medium during the 72hr exposure period was maintained at 7.4 by 0.02M Hepes buffer in flasks. RTO was prepared as a 1% stock solution in DMSO, which, when added to culture medium at a 2.5% vol. conc. was a suspension. Despite limited solubility, RTO produced a dose-dependent cytotoxic effect after a 3-day exposure period. In the initial toxicity assay, RTO was added to flasks, seeded with BALB-c/3T3 cells, at concentrations of 0, 0.01, 0.1, 1.0, 10.0 and 100.0µg/ml, incubated for 3 days at 37^0C in a CO_2 in air incubator, after which cells were counted for survival. In the transformation assay, RTO was tested at 0, 0.8, 4.0, 20.0 and 100µg/ml. In a standard BALB-c/3T3 transformation assay, colony formation cultures (approx. 100 cells/culture) and transformation cultures (approx. 10^4 cells/culture, 20 cultures/dose) were seeded on day 1, exposed to test material for 2-3 days, and culture medium was changed on day 4. For transformation cultures, medium continued to be changed weekly to day 29. Colony formation cultures were fixed, stained and counted visually on day 8 to determine cloning efficiency; transformation cultures were fixed and stained on day 29 for focus counting and evaluation. Transformation frequency = total type III foci ÷ total cultures/dose. Positive control compound was 3-methyl cholanthrene (2µg/ml).
Results	
Genotoxic effects	RTO induced toxicity in BALB-c/3T3 cells after 3 days exposure at concentrations of 10µg/ml (59% viability) and at 100µg/ml (18% viability). In the transformation assay, inhibition of cloning efficiency (CE, clones/100 cells) occurred at 4.0µg/ml (89% CE), 20.0µg/ml (81% CE) and 100µg/ml (65% C.E.); cell toxicity was somewhat less than in the initial cytotoxicity assay [40% viability at 100µg/ml]. RTO did not induce statistically significant increased incidence of transformed foci compared to negative controls at any dose level. Values were 0.10 foci/flask, 2/20 flasks with foci at 100µg/ml, 0.0 foci/flask, 0/20 flasks with foci at 20.0µg/ml, 0.15 foci/flask, 3/20 flasks with foci at 4.0µg/ml, 0.10 foci /flask, 2/20 flasks with foci at 0.8µg/ml compared to 0.05 foci/flask, 1/20 flasks with foci in negative control group. [Reviewer's note: Negative control value of 1 focus/20 flasks was lower than control values in other concurrent studies on 2 other compounds in this series where negative controls had 4 foci in 20 flasks (0.20 foci/flask)]. Positive control compound, 3 methyl cholanthrene, induced 56 foci/19 flasks (2.95 foci/flask),

	18/19 flasks with foci.
Conclusions (contractor)	Rerun tower overheads did not induce neoplastic transformation in BALB-c/3T3 cells and was not active in this test system.
Data Quality *Reliabilities*	**2.** Reliable with restrictions. Complete details of assay methods are not included in the report. Specifics of statistics are not supplied.
Reference	Tu, A.S. and Sivak, A. 1981. BALB-c/3T3 Neoplastic transformation assay on 0818802, 08188003 and 08188005 (Rerun tower overheads). ALD Ref. #86374. Arthur D. Little, Inc. Cambridge, MA for Mobil Oil Corp, Study #1771-80, Princeton, NJ Roy, T.A., 1981. Analysis of rerun tower bottom oil by combined capillary gas chromatography/mass spectrometry. Study #1272-81-. Toxicology division, Mobil Oil Co., Princeton, NJ
Other *Last changed*	12/07/01 (Prepared by a contractor to the Olefins Panel)

Robust Summary – Group 5: High Benzene Naphthas

Developmental Toxicity/Teratogenicity

Test Substance	
Remarks	Rerun Tower Overheads, light thermal cracked naphtha, CAS #64741-74-8. Unsaturated hydrocarbons in C4-C8 range; boiling over 20-120^{0}C (68^0-248^{0}F); approximately 40% benzene, 26% C5, 13% toluene, 20% C4, C6-C8 and xylene.
Method	
Method/guideline followed	Standard method, no guidelines specified
Test type	Teratology
GLP	Yes
Year	1981
Species	Rabbit
Strain	New Zealand white
Route of administration	Oral gavage
Concentration levels	0,10, 25 and 50mg/kg/day in Mazola® corn oil
Sex	Female; 16 pregnant rabbits/group
Exposure period	Days 6-28 of gestation
Frequency of treatment	Once/day
Control group and treatment	16 pregnant rabbits; 0.5ml corn oil/kg/day
Duration of test	32 days (from artificial insemination to Caesarean section on day 29 of gestation)
Statistical methods	Chi-square test with Yates's correction for 2x2 contingency tables and/or Fisher's exact probability test used for male/female sex distribution and number of litters with malformations. Mann-Whitney U test to compare number of early and late resorptions, and postimplantation losses. Analysis of variance (one-way), Bartlett's test and T-test (for equal and unequal variance) with Dunnett's multiple comparison tables used to compare mean number of viable fetuses, total implantations, corpora lutea and mean fetal body weights. All comparisons at $p<0.05$.
Remarks for Test Conditions.	Sixty-four sexually mature, virgin NZW female rabbits (7 months old, 3.4 - 4.2kg) were ear-tagged and individually housed in suspended wire cages in a room with temperature and humidity control (data not presented), a 12 hr light-dark cycle and special ventilation due to volatility of test sample. Purina Certified Rabbit Chow® and tap water were available ad lib. Sperm was collected from each of 6 proven NZW breeder males, using an artificial vagina. Semen was immediately evaluated for motility and used for insemination only if motility was =55%. Useable ejaculate was diluted with 0.9%NaCl at 35^{0}C; 0.25-0.50ml of dilute semen introduced into the anterior vagina. Ovulation was induced by injection of 100 units of chorionic gonadotropin (Ayerst, NY) in the marginal ear vein of the female immediately after insemination. Semen from each male was used to inseminate an equal number of females in each group. Insemination was performed over 2 days; day of insemination was designated day 0 of gestation. Rerun tower overhead test solutions were prepared daily in corn oil and shaken by hand to ensure proper mixing. No analysis of dosing solution compositions was provided. Dosage levels of 0, 10, 25 and 50mg/kg/day were administered at a constant volume of 0.5ml/kg by oral gavage once daily from day 6-28 of gestation. Individual doses were determined from body wt recorded on gestation day 6. Dams were observed daily for mortality, overt changes in appearance and behavior, and clinical signs of toxicity during treatment. Maternal body wts were recorded on gestation days 0, 6, 12, 18, 24 and 29. On gestation day 29, all females were sacrificed by an overdose of sodium pentobarbital in the marginal ear vein; the uterus was excised and weighed prior to removal of fetuses. Number and location of viable and non-viable fetuses, early and late resorptions, total implantations and corpora lutea were recorded. Abdominal and thoracic cavities and organs of dams were examined grossly and the carcasses discarded. Uteri from females that appeared non-gravid were opened and placed in 10% ammonium sulfide solution to confirm pregnancy status. All fetuses were weighed individually and examined for external malformations and variations. Each fetus was dissected, internally sexed and examined for visceral malformations and variations, including brain by a mid-coronal slice and heart by Staples technique (Staples, 1974). Eviscerated, skinned fetuses were

	numbered and tagged for identification, fixed, mascerated and stained with Alizarin Red S for skeletal evaluation..
Results	
NOAEL maternal toxicity	NOAEL maternal= 25mg/kg (based on one female aborting on gestation day 19)
NOAEL developmental toxic ity	NOAEL developmental = 50mg/kg (based on 2 malformations) Assigned by reviewer. In a preliminary study, rerun tower overheads was administered undiluted to 16 mated female rabbits/group at 0, 10, 25 and 50mg/kg/day. Forty-two rabbits died between day 8-29 of gestation, of which 6 aborted prior to death and 6 aborted and were sacrificed. Total dead or aborted and sacrificed animals were 14/16, 11/16, 10/16, and 13/16 in 0(untreated control), 10, 25, and 50mg/kg/day, respectively. Intubation errors or respiratory disorders were determined to be probable cause of deaths; extremely high mortality in control group negated any meaningful comparisons of any parameters with treated groups. Study was repeated at same doses of rerun tower overheads diluted in corn oil.
Maternal effects	Maternal survival was 100% in all groups. Slight increase in occurrence of matted hair coat (nasal region) and slight reduction in fecal material was noted in 50mg/kg group only. One rabbit (50mg/kg) aborted on gestation day 19 and remained on study until scheduled sacrifice; aborted material was discarded. At Caesarean section, congested consolidated or emphysematous lungs and hydrocele(s) on the oviduct(s) were noted with similar frequency in all groups including controls. There were no biologically meaningful differences in mean maternal body wt, body wt gain or adjusted mean body wt (body wt exclusive of uterus and contents) in any treated group compared to controls. [Reviewer's comment: Maternal body wt data did not appear to be statistically analyzed.]
Embryo/fetal effects	There were no biologically meaningful or statistically significant differences in mean number of corpora lutea, total imp lants, early and late resorptions, postimplantation loss, viable fetuses, fetal sex distribution or mean fetal body wts in any treated group compared to controls. No significant differences were present in number of litters with malformations or genetic or developmental variations in treated groups compared with controls. In the 50mg/kg./day group, 1 pup in 1 litter had an atlas-occipital anomaly of the skeleton and one pup in 1 litter had an enlarged heart with an interventricular spetal defect, interrupted aortic arch and retroesophophageal left subclavian vessel (sexes not specified). Scoliosis was observed in all groups including controls. All malformations were within historical ranges for the laboratory.
Conclusions (study authors)	Rerun Tower Overheads did not induce significant maternal or fetal toxicity or significant malformations/variations in offspring of New Zealand White rabbits treated with oral doses of 10, 25, and 50mg/kg/day in corn oil from day 6-28 of gestations.
Data Quality	
Reliabilities	**2.** Reliable with restrictions. No analysis of dosing solution to verify correct test material volume was performed.
References	Miller, L.G. and Schardein, J.L. 1981. Rerun Tower Overheads: Teratology study in rabbits (MCTR-171-79). IRDC study #450-011a. International Research and Development Corp., Mattawan, Mich. for Mobil Oil Corp., Princeton, NJ Staples, R.E. 1974. Teratology 9: A37-A38.
Other	
Las*t changed*	10/09/2001 (Prepared by a contractor to the Olefins Panel)

High Benzene Naphthas - Comments of Environmental Defense

(Submitted via Internet 6/14/02)

Environmental Defense appreciates this opportunity to submit comments on the robust summary/test plan for high benzene naphthas.

The American Chemistry Council's Olefins Panel has prepared the test plan and robust summaries for the high benzene naphthas. The sponsor proposes a vast category which would include a grouping of 10 ethylene manufacturing streams comprising 19 CAS numbers and more than 100 individual chemicals based on information presented in Table 2. Individual chemicals include benzene, 1,3-butadiene, vinyl acetate, toluene, isoprene, hexane, styrene, naphthalene and at least 10 others found at a concentration of at least 5% in at least one of the streams.

The sponsor concludes that although some data are needed to characterize the streams for physiochemical endpoints, biodegradation and hydrolysis, no additional health effects studies are needed. While we did not review the ecological components of the test plan, we do have major concerns over the health effects section. We do recognize the complexity of the test plan and the difficulty in preparing it but we disagree with the sponsor's conclusion that no additional health effects studies are needed. The chemicals found in the 10 high benzene naphtha streams are structurally divergent and possess qualitatively different toxicological properties. While benzene is clearly the driver for cancer causing effects, other chemicals present in the steams are likely more significant for other effects such as reproductive, developmental and neurotoxic effects.

The test plan clearly summarized an abundance of data for most of the chemicals present in the streams in excess of 5% (i.e. benzene, 1,3-butadiene, toluene etc.), but the mammalian toxicity data on the streams themselves is very limited. For example, there is only one repeat dose study on the streams and this was a 5-day inhalation study on hydrotreated gasoline; no reproductive studies and only one developmental study using pyrolysis gasoline were reported. Moreover, some of the chemicals present at 5% or greater in some of the 10 streams covered in this test plan do not have adequate toxicity data (i.e. cyclopentadiene, cyclopentene and methylcyclopentane). The sponsor states on page 19 of the test plan that the many chemicals present in the high benzene naphtha streams could have antagonistic or synergistic interactions.

Based on the above considerations, we recommend that some of the mixtures themselves be subjected to toxicological evaluation. This approach was undertaken in a very credible way by the American Petroleum Institute in its test plan on gasoline blending streams. After reviewing the composition data presented in Table 2, we recommend that repeat dose, genotoxicity, reproductive and developmental studies be conducted on pyrolysis gasoline and quench loop pyrolysis oil. Data from these two streams should be usable to extrapolate to the other 8 streams.

Thank you for this opportunity to comment.

George Lucier, Ph.D.
Consulting Toxicologist, Environmental Defense

Karen Florini
Senior Attorney, Environmental Defense

August 21, 2002

Elizabeth J. Moran, Ph.D.
American Chemistry Council Olefins Panel
Panel Manager
1300 Wilson Boulevard
Arlington, VA 22209

Dear Dr. Moran:

We have conducted a review of the High Benzene Naphtha category submitted by the Olefins Panel as part of their commitment made under the HPV Challenge Program. Our analysis focused initially on the category justification and implementation strategy with the aim of determining the feasibility of achieving the stated objective of characterizing members of this group with the proposed design.

Our analysis concluded that, while the category proposal appears to be a reasonable approach to characterization of process streams from the ethylene process unit, the implementation strategy was difficult to grasp. The proposed strategy describes different approaches to characterization of this category ranging from a lead chemical component (benzene; other?), data on other components in the various streams, and analog data (both for individual components and analogous streams). The proposal, however, does not articulate how the desired characterization of component streams will be achieved. In addition, the organization and presentation of data in the document should be improved to increase clarity and facilitate analysis. There is no explicit relationship between the CAS numbers comprising the category and the different streams. For example, for which stream is the “Dripolene” acute toxicity data to be used for?

I encourage the Olefins Panel to take the necessary steps to make this category viable. We are prepared to proceed to data adequacy determinations as soon as we get your response.

If you have any questions about this response, please contact Richard Hefter, Chief of the HPV Chemicals Branch, at 202-564-7649. Submit questions about the HPV Challenge Program through the HPV Challenge Program Web site “Submit Technical Questions” button or through the TSCA Assistance Information Service (TSCA Hotline) at (202) 554-1404. The TSCA Hotline can also be reached by e-mail at tsca-hotline@epa.gov.

Sincerely,

-S-

Oscar Hernandez, Director
Risk Assessment Division

American Chemistry Council Good Chemistry Makes It Possible

August 7, 2003

Oscar Hernandez, Director
Risk Assessment Division
Office of Pollution Prevention and Toxics
U.S. Environmental Protection Agency
1201 Constitution Avenue N.W.
Washington, DC 20460-0001

RE: Response to EPA Comments on the Olefins Panel Test Plan for High Benzene Naphthas Category, HPV Registration No. 1101064

On December 12, 2001, the American Chemistry Council Olefins Panel (Panel) submitted a test plan on the High Benzene Naphthas Category under the HPV Chemical Challenge Program. In a letter dated August 21, 2002, you noted several questions about the Panel's test plan. Subsequently, several Panel scientists met with Mr. Richard Hefter, Chief of the HPV Chemicals Branch, and other EPA staff members to discuss the issues raised in your letter. The focus of EPA's comments, as the Panel understands them, is on the presentation and clarity in the test plan, rather than on the plan itself. The Panel is submitting the attached Revised Test Plan, which addresses these issues of presentation and clarity. In addition, we are submitting Robust Summaries, which have been revised to address your comments. In preparing these revised documents, the Panel also reviewed comments filed by Environmental Defense on June 14, 2002.

The Panel believes that this letter and the revised Test Plan and Robust Summaries address the issues raised in your letter. However, if you have additional questions, please contact me at 301 924 2006 or Elizabeth_Moran@americanchemistry.com.

Yours truly,

Elizabeth J. Moran, Ph.D.
Manager, Olefins Panel

Attachments

cc: Richard Hefter

HIGH PRODUCTION VOLUME (HPV)

CHEMICAL CHALLENGE PROGRAM

REVISED TEST PLAN

For The

High Benzene Naphthas Category

Prepared by:

American Chemistry Council
Olefins Panel
HPV Implementation Task Group

REVISED
August 7, 2003

PLAIN ENGLISH SUMMARY

The High Benzene Naphthas Category was developed for the HPV Program by grouping ethylene manufacturing streams (products) that exhibit commonalities from both manufacturing process and compositional perspectives. The 19 CAS Numbers in the category are associated with 10 streams, which are commercial products or isolated intermediates containing significant levels of benzene (generally greater than 10% and averaging about 55%).

Pyrolysis gasoline is the major stream in this category and essentially all of the other category streams are derived from it, either as simple distillate fractions or hydrogenated distillate fractions. These streams all contain significant concentrations of benzene. They are the Industry's intermediate streams that are processed to high purity benzene and other byproducts. Pyrolysis gasoline and these fractions account for 99.8% of the category production. The remaining 0.2% of the category production consists of similar benzene-containing industry streams. Some test data exist for two streams in the category.

The basic strategy of this test plan for characterizing the human health hazards of this category is to evaluate data for the components of the streams, as well as data for mixtures of category components and analogous mixtures (existing data and data being developed by other test programs). The major chemical components of the streams in the High Benzene Naphthas Category have been extensively tested for human health toxicity endpoints and some data are available for other components and for two streams. Additional supporting data for components of the High Benzene Naphtha streams, tested either individually or as components of other streams or mixtures, will be collected for other testing programs. These data are expected to provide sufficient information to allow use of component analysis to develop scientific judgment-based characterizations of the human health effects of streams in this category for purposes of satisfying HPV program requirements. Therefore, no additional human health toxicity testing is proposed. The hazard characterization for each stream will include the hazards of benzene (cancer, genetic toxicity, hematotoxicity) plus any reproductive or developmental toxicity or target organ effects of the other components, unless there is clear evidence that specific component interactions eliminate toxicity.

Data will be developed and/or identified to adequately characterize relevant physicochemical endpoints in the HPV Chemical Challenge Program.

Existing data provide sufficient information to adequately characterize the biodegradability and aquatic toxicity of products in this category. Therefore, no additional biodegradation or aquatic toxicity testing is proposed.

Information or data will be developed on the potential of products in the High Benzene Naphthas Category to photodegrade, hydrolyze, and partition within the environment.

EXECUTIVE SUMMARY

The Olefins Panel (Panel) of the American Chemistry Council and the Panel's member companies hereby submits a revised test plan for the "High Benzene Naphthas" Category under the Environmental Protection Agency (EPA) High Production Volume (HPV) Chemical Challenge Program (Program). The Panel has reviewed comments on the original posted version of this test plan and where appropriate, has made revisions in response to those comments. It is the intent of the Panel and its member companies to use new information in conjunction with a variety of existing data and scientific judgment/analyses to characterize the SIDS (Screening Information Data Set) human health, environmental fate and effects, and physicochemical endpoints for this category in accordance with participation in the HPV Program.

The High Benzene Naphthas Category was developed for the HPV Program by grouping ethylene manufacturing streams that exhibit commonalities from both manufacturing process and compositional perspectives. The 19 CAS Numbers in the High Benzene Naphthas Category are associated with 10 streams. The 10 streams are commercial products or isolated intermediates. The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%. This grouping of CAS numbers represents hydrocarbon streams with a carbon number distribution that is predominantly C5 – C11, through components boiling at 650°F or higher.

Pyrolysis gasoline is the major stream in this category and essentially all of the other category streams are derived from it, either as simple distillate fractions or hydrogenated distillate fractions. These streams all contain significant concentrations of benzene. They are the Industry's intermediate streams that are processed to high purity benzene and other byproducts. Pyrolysis gasoline and these fractions account for 99.8% of the category production. The remaining 0.2% of the category production consists of similar benzene-containing industry streams.

Human Health Effects

The basic strategy of this screening level test plan for characterizing the human health hazards of this category is to evaluate data for the components of the streams, as well as data for mixtures of category components and analogous mixtures (using existing data and data being developed by other test programs). Benzene, as the predominant component in most streams, is expected to be the key driver with respect to health effects endpoints within the SIDS battery of tests, with genotoxicity and hematotoxicity the effects most likely to be seen. However, the effects of other components may also contribute to the toxicity of the streams.

Benzene has a robust toxicity dataset and has completed the OECD SIDS program. No further testing of benzene is needed for the HPV Chemical Challenge Program. The other major chemical components of streams in the High Benzene Naphthas Category have been extensively tested for human health toxicity endpoints, and all components present in the streams at concentrations greater than 5% have been tested in at least one toxicity study. Those components having only limited data lack structural alerts for mammalian toxicity and data exist for structural analogs. Some data are available for Pyrolysis Gasoline [Dripolene] and Rerun Tower Overheads, a C5-C10 distillate fraction of a Pyrolysis Gasoline stream that is similar to the category stream. The Hydrotreated C6-C8 Fraction has also been tested.

Some data are also available regarding interactions between certain components that impact metabolism and toxicity. Additional supporting data for components of the High Benzene Naphtha streams, tested either individually or as components of other streams or mixtures, will be collected for other test plans within the Olefins Panel's HPV program, by other consortia participating in the HPV or ICCA programs, or for chemicals sponsored in the OECD SIDS program. These data are expected to provide sufficient information to allow the use of component data to develop scientific judgment-based characterizations of the human health effects of streams in this category in satisfaction of HPV program requirements. Based upon examinations of stream compositions and existing toxicity data, there is minimal likelihood for the appearance of unexpected or remarkable biological findings in testing of these streams. Therefore, no additional human health toxicity testing is proposed. The hazard characterization for each stream will include the hazards of benzene (cancer, genetic toxicity, hematotoxicity) plus any reproductive or developmental toxicity or target organ effects of the other components, unless there is clear evidence that specific component interactions eliminate toxicity.

Physicochemical Properties, Environmental Fate, and Aquatic Toxicity

Existing measured data will be identified to adequately characterize physicochemical endpoints in the HPV Chemical Challenge Program. In addition, calculated data will be developed to characterize the physicochemical endpoints for selected chemicals in products from this category and compared with the existing measured data.

The strategy for characterizing the biodegradability and aquatic toxicity of products in this category is to evaluate data on component chemicals contained by products in this category and similar complex products. Read across biodegradation data show that products in the High Benzene Naphthas Category have the potential to exhibit a high extent of biodegradability. Read across aquatic toxicity data show that products in the High Benzene Naphthas Category have the potential to produce a moderate level of toxicity in freshwater algae and acute toxicity in freshwater fish and invertebrates. Existing data provide sufficient information to adequately characterize the biodegradability and aquatic toxicity of products in this category. Therefore, no additional biodegradation or aquatic toxicity testing is proposed.

The chemical components in these products are relatively volatile, and if released they would be expected to partition to the air phase to a significant extent. In the air, they are subject to rapid physical degradation through hydroxyl radical attack. Therefore, as a result of both biological and physical degradation processes, these products are not expected to persist in the environment. Information has not been developed on the potential of products in this category to photodegrade, hydrolyze, and partition within the environment. Therefore, information or data will be developed to characterize these endpoints in.

LIST OF MEMBER COMPANIES
THE OLEFINS PANEL

The Olefins Panel includes the following member companies:

ATOFINA Petrochemicals, Inc.*
BP Chemical Company
Chevron Phillips Chemical Company
The Dow Chemical Company
E. I. du Pont de Nemours and Company
Eastman Chemical Company
Equistar Chemicals, LP
ExxonMobil Chemical Company
Formosa Plastics Corporation, U.S.A.
The Goodyear Tire & Rubber Company*
Huntsman Corporation
Koch Industries
NOVA Chemicals Inc.
Noveon, Inc*
Sasol America, Inc.
Shell Chemical Company
Sunoco, Inc.
Texas Petrochemicals Corporation*
Westlake Chemical Corporation
Williams Olefins, LLC

* These companies are part of the Olefins Panel but do not produce streams in the High Benzene Naphthas Category.

TABLE OF CONTENTS
TEST PLAN FOR THE HIGH BENZENE NAPHTHAS CATEGORY

TABLES AND FIGURES

TEST PLAN FOR THE HIGH BENZENE NAPHTHAS CATEGORY

I. INTRODUCTION

The Olefins Panel (Panel) of the American Chemistry Council and the Panel's member companies have committed to develop screening level human health effects, environmental effects and fate, and physicochemical data for the High Benzene Naphthas Category under the Environmental Protection Agency (EPA) High Production Volume (HPV) Chemical Challenge Program (Program).

In preparing this test plan, the Panel has given careful consideration to the principles contained in the letter EPA sent to all HPV Challenge Program participants on October 14, 1999. As directed by EPA in that letter, the Panel has sought to maximize the use of scientifically appropriate categories of related chemicals and structure activity relationships. Additionally, and also as directed in EPA's letter, in analyzing the adequacy of existing data, the Panel has conducted a thoughtful, qualitative analysis rather than use a rote checklist approach. The Panel has taken the same thoughtful approach when developing its test plan. The Panel believes its test plan conforms to the principles articulated in EPA's letter. In addition, the Panel has reviewed comments on the original posted version of this test plan and where appropriate, has made revisions in response to those comments.

This plan identifies CAS numbers used to describe process streams in the category, identifies existing data of adequate quality for substances included in the category, and outlines activities to develop screening level data for this category under the Program. The objective of this effort is to identify and/or develop sufficient test data and/or other information to adequately characterize the human health effects and environmental effects and fate for the category in accordance with the EPA HPV Program. Physicochemical data that are requested in this program will be calculated as described in EPA guidance documents. In addition, measured data will be provided for selected products in this category where readily available.

II. DESCRIPTION OF THE HIGH BENZENE NAPHTHAS CATEGORY

A. The Category

The High Benzene Naphthas Category was developed for the HPV program by grouping ethylene manufacturing streams that exhibit commonalities from both manufacturing process and compositional perspectives. The 19 CAS numbers listed in Table 1 describe 10 streams which are complex products containing many components. Certain single streams are correctly represented by more than one CAS number, and a CAS number may be applicable to more than one stream. A description of the ethylene and associated stream production processes is included in Appendix I. A list of the other ethylene manufacturing stream categories being sponsored by the American Chemistry Council Olefins Panel is shown in Table 13.

The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%. In some cases, petroleum refinery streams may be combined with intermediate streams from the ethylene unit and coprocessed to produce these products. This grouping of CAS numbers represents hydrocarbon streams with a carbon number distribution that is predominantly C5-C11, through components boiling at 650°F or higher. Pyrolysis gasoline is included in this category. The typical compositions of streams in this category are listed in Table 2 and Figures 1 and 2.

The CAS Numbers in the High Benzene Naphthas Category are associated with the following streams, which are commercial products or isolated intermediates:

Pyrolysis Gasoline
Pyrolysis C6 Fraction
Pyrolysis C6-C8 Fraction
Pyrolysis C5-C6 Fraction
Hydrotreated C6 Fraction
Hydrotreated C6-C7 Fraction
Hydrotreated C6-C8 Fraction
Quench Loop Pyrolysis Oil and Compressor Oil
Recovered Oil from waste water treatment
Extract from Benzene Extraction

Pyrolysis gasoline, is the major product in this category. Pyrolysis gasoline and its 3 distillate fractions together make up about 66% of the production capacity in the category. Test data exists for one of these 4 streams (pyrolysis gasoline) and for a fraction of pyrolysis gasoline. Three hydrotreated pyrolysis gasoline fractions make up approximately 33% of the production capacity in the category and test data exist for one of these 3 streams. The remaining 3 streams are included in this category because they are similar benzene-containing intermediate streams produced by the Industry. Figure 3 provides information on the production volume of the streams in the category.

Descriptions of the 10 streams associated with the High Benzene Naphthas Category are presented below:

1. Pyrolysis Gasoline

Pyrolysis Gasoline (Pygas) consists predominantly of C5+ hydrocarbons produced by ethylene cracking furnaces. Typically the stream is derived from (1) the bottoms product from the debutanizer, (2) oils separated from furnace effluent quench systems, and (3) “drips” or condensate resulting from compression of the cracked gas. The oils from the quench systems and the “drips” may be stabilized to remove lights before blending with Pygas from the other sources. Depending on the plant configuration, Pygas may contain all of these intermediate streams, or the quench oils and stabilized drips may be transferred as separate streams. Low concentrations (e.g. 3% total) of C4 and lighter hydrocarbons

may be present in the stream. A detailed analysis of Pygas may identify 60 or more hydrocarbon components or component groups, primarily unsaturated hydrocarbons and aromatics. Benzene, toluene, and dicyclopentadiene together may account for more than 50% of a Pygas stream and typically no other single component is present at a level greater than about 5%. The benzene concentration of Pygas is typically about 40% and the reported values range from 15 to 62%. The concentrations of individual hydrocarbon components in Pygas vary depending on the type of feedstock used by the ethylene plant, the mode of operation of the cracking furnaces (i.e. severity) and the ethylene process configuration. One non-typical Pygas stream is reported to contain vinylacetate at a concentration of up to about 10%. Vinylacetate is not typically found in ethylene process streams.

2. Pyrolysis Gasoline Fractions

Pyrolysis gasoline is separated by distillation into various boiling-point-range fractions as intermediates in preparation for further processing. In some cases, petroleum refinery streams such as a C6 reformate fraction are combined with the pyrolysis gasoline prior to this separation. Similar to the situation for Pygas, the compositions of these fractions vary depending on the ethylene process feedstock and the other operating variables.

(a) Pyrolysis C5-C6 Fraction

The carbon number distribution for this stream is predominantly C5 to C6. One typical composition for this stream is reported as 70% benzene and 10% pentenes.

(b) Pyrolysis C6 Fraction

The carbon number distribution for this stream is predominantly C6. Reported compositions vary from 35 to 77% benzene, 0.5 to 5% toluene with the balance primarily C6 non-aromatics, which are expected to be largely unsaturates.

(c) Pyrolysis C6-C8 Fraction

This stream has a carbon number distribution that is predominantly C6 to C8. The reported compositions range from 30 to 80% benzene, 15 to 25% toluene and 3 to 23% C8 aromatics.

3. Hydrotreated Pyrolysis Fractions

Pyrolysis gasoline or distillate fractions of pyrolysis gasoline are sometimes treated with hydrogen over catalyst to saturate or partially saturate diolefins and/or olefins. In some cases, petroleum refinery streams such as a C6 reformate fraction are combined with the pyrolysis gasoline prior to this step. The hydrogenation process may be either one-stage or two-stage. The one-stage process is typically a liquid-phase process where the primary objective is to selectively convert diolefins to mono-olefins and to convert vinyl aromatics into alkyl aromatics, for example, styrene to ethylbenzene. The second stage

in a two-stage hydrogenation process is typically a vapor-phase, more severe hydrogenation that converts essentially all of the contained olefins to saturated hydrocarbons. A pygas fraction that will be processed by extraction or extractive distillation to produce high purity aromatics (benzene, toluene or xylenes) is subjected to two-stage hydrogenation. Pygas fractions may be forwarded to hydrodealkylation units (less common) for benzene production after one-stage of hydrogenation. Hydrotreated Pyrolysis fractions may be the result of either one- or two-stage hydrogenation.

(a) Hydrotreated C6 Fraction

This stream is very similar in composition to the Pyrolysis C6 fraction except that the non-aromatics present in the hydrotreated stream are essentially all saturates. The reported composition for the Hydotreated C6 stream indicates typical benzene content of 75%.

(b) Hydrotreated C6-C7 Fraction

The carbon number distribution for this stream is predominantly C6 -C7 and the reported values indicate 40 to 70% benzene, and 3 to 15% toluene.

(c) Hydrotreated C6-C8 Fraction

The reported typical compositions for this stream are 40 to 60% benzene, 10 to 25% toluene and 3 to 10% C8 aromatics.

4. Quench Loop Pyrolysis Oil and Compressor Oil

Quench Loop Pyrolysis Oil (Pyoil) represents higher boiling hydrocarbons that condense in the water quench system of an ethylene plant, typically at an ethylene unit cracking ethane, propane or butane. The stream can also include liquids collected at the cracked gas compressor knock out drums, which may include compressor injection oil. The carbon number distribution for Pyoil is C4 (or even lower) through heavier hydrocarbons such as naphthalene or even heavier. The reported typical composition includes 10 to 22% benzene and 5 to11% toluene.

5. Recovered Oil from Wastewater Treatment

This stream can be expected to be of variable composition and made up largely of the components found in Pygas. No composition data or process specific information has been reported. Typically, water streams at ethylene units are processed to separate hydrocarbons from the water so that the water can be reused to generate steam for process-contact use (dilution steam for the cracking furnaces) or so that excess water can be forwarded to treatment prior to discharge or reuse. Water processing typically includes mechanical and gravity separation and steam or gas stripping. Hydrocarbons separated from the water in these systems are not usually isolated from the process. However, at least in one case, the Recovered Oil from Wastewater Treatment has been reported as an

isolated intermediate.

6. Extract from Benzene Extraction

Hydrotreated pyrolysis fractions containing aromatics (most commonly benzene or benzene and toluene) are typically charged to extraction or extractive distillation units where the mixed aromatics are recovered as the Extract from Benzene Extraction. The carbon number distribution for this stream is predominantly C6 to C8. A reported typical concentration indicates 60 to 75% benzene, 25 to 40% toluene and 0 to 1% xylenes.

III. TEST PLAN RATIONALE

A. Human Health Effects

The basic strategy of this screening level test plan for characterizing the human health hazards of this category is to evaluate data for the components of the streams, as well as data for mixtures of category components and analogous mixtures (existing data and data being developed by other test programs).

The High Benzene Naphthas Category comprises 10 streams, which are complex products containing high levels of benzene (10-80%) plus many other components (predominantly C5-C11), many of which are shared across streams. All streams in this category are subject to the Occupational Safety and Health Administration (OSHA) Benzene Standard (29 CFR 1910.1028). Those streams containing 1,3-butadiene are subject to the OSHA Butadiene Standard (29 CFR 1910.1051). OSHA Permissible Exposure Limits exist for all major components. Benzene, as the predominant component in most streams, is expected to be the key driver with respect to health effects endpoints within the SIDS battery of tests, with genotoxicity and hematotoxicity the effects most likely to be seen. However, the other components may also contribute to the toxicity of the streams.

Benzene has a robust toxicity dataset, including data on human experience, and has completed the OECD SIDS program. No further testing of benzene is needed for the HPV Chemical Challenge Program. The existing epidemiology and toxicology database for the components other than benzene and for mixtures containing the components is extensive. All components present in the streams at concentrations greater than 5% have been tested in at least one toxicity study. Those components having only limited data lack structural alerts for mammalian toxicity and data exist for their structural analogs. The C5 and C6 alkanes and alkenes present in the streams are not expected to significantly contribute to the toxicity profile as these substances are present in the streams at low concentrations and, with the exception of hexane, generally have a low level of toxicity. The toxic effects of hexane (present at $\leq$ 15%) are unlikely to be observed due to the presence of the other components, as noted below in Section III.A.1. Some data are available for Pyrolysis Gasoline [Dripolene] and for a C5-C10 distillate fraction of a Pyrolysis Gasoline stream [Rerun Tower Overheads], that is similar to Pyrolysis Gasoline. Data also exist for the Hydrotreated C6-C8 Fraction.

Additional data for the components, or for structural analogs of components, are under development by the American Chemistry Council Olefins Panel for other categories under the HPV program, by other HPV consortia, and by the OECD SIDS program (see Table 5). Furthermore, some of the materials being distilled out of Pyrolysis Gasoline are being tested in other Panel HPV Test Plans (Non-Cyclic C5s and Resin Oils and Cyclodiene Dimer Concentrates categories); and the High Benzene Naphthas Category shares many of the same components with the gasoline blending streams referenced in the API Petroleum HPV Gasoline Blending Streams Test Plan. These gasoline stream data can contribute to the hazard evaluation for the members of this category by showing effects, or lack thereof, due to mixtures containing components of this category when the benzene content is very low (~ 2%).

For the HPV program, the Panel believes that the human health hazards of the category can be adequately characterized by using scientific judgment to analyze component data (existing data and data being developed by other testing programs), without conducting additional toxicology tests. The Panel further believes that additional testing on streams is unlikely to demonstrate any adverse effects that have not been shown for components, and would provide little useful data for regulatory, industrial hygiene, emergency response or hazard communication purposes. Thus, no additional testing is proposed in this test plan.

Assessments of the hazards of the category members will be developed after new data from other testing programs become available. As shown in Table 3, the hazard characterization for each stream will include the hazards of benzene (cancer, genetic toxicity, hematotoxicity) plus any reproductive or developmental toxicity or target organ effects of the other components, unless there is clear evidence that specific component interactions eliminate toxicity. Sources of data for hazard evaluations for mammalian toxicity for each stream are summarized in Table 4.

A discussion of chemical component interactions, specific strategies and rationales for each of the SIDS human health toxicity endpoints, and robust summaries is presented below:

1. Chemical Component Interactions

When tested as pure substances, some of the components other than benzene have caused genetic damage and adverse target organ effects in repeated-dose animal studies, as shown in Table 5. However, since the biologically active components of the High Benzene Naphtha streams are metabolized through a common P450 metabolic pathway, it is anticipated that multiple components will compete for the same active enzyme sites. Component toxicities, which are dependent on the formation of biologically active metabolites, may be reduced as less metabolite(s) will be produced through competition for these sites. Direct support for reduction or elimination of toxicities of individual components is provided by results of an existing mouse bone marrow micronucleus test with one of the High Benzene Naphtha streams, Hydrotreated C6-8 Fraction. This stream, containing approximately 55% benzene, was negative in a mouse bone marrow micronucleus test when administered by oral gavage at 2000 mg/kg to male and female CD-1 mice (see robust summary). Several studies have shown that benzene administered orally to CD-1 mice induces high frequencies of micronuclei in bone

marrow erythrocytes at doses as low as 110 mg/kg (Ciranni et al., 1988; Suzuki et al., 1989; Hite et al., 1980; Gad-El Karim et al., 1986; Meyne and Legator, 1980). The presence in the Hydrotreated C6-8 Fraction of other components (approximately 25% toluene, 10% xylene, 7% pentane, 7% ethylbenzene, 3% cyclohexane, and 2% hexane) apparently inhibited the expected clastogenicity of benzene. Other similar interactions between components of the category have also been reported, as noted below.

Medinsky et al. (1994) and Bond et al. (1998) reviewed the metabolism of benzene and the effects of interactions with other organic chemicals on benzene toxicity and metabolism. Reports of interactions between other components of the High Benzene Naphthas Category have also been noted in the literature. Examples of these interactions and the effect on the formation of benzene metabolites and resultant hematotoxicity or genotoxicity are shown below:

- When benzene (440 mg/kg) and toluene (430, 860, or 1720 mg/kg) were coadministered orally to mice, the clastogenic effect of benzene was reduced (Gad-El-Karim et al., 1984, 1986).
- Coadministration of toluene (1720 mg/kg), i.p., with benzene (440 and 880 mg/kg) to mice resulted in a reduction in the quantity of benzene metabolites measured in the urine (Andrews et al., 1977). Coexposure to toluene also protected against benzene-induced depression in ^{59}Fe utilization by red blood cells, which is used as a measure of hematotoxicity.
- Coexposure to 2000 ppm fully vaporized or light gasoline components reduced the incidence of genetic damage (micronuclei in bone marrow) resulting from a single 6-hr exposure to 40 ppm benzene (Bond et al., 1998). The major components of the fully vaporized gasoline and light gasoline mixtures, respectively, were n-butane (6.1%, 23.9%), n-pentane (3.7%, 8.4%), isopentane (12.3%, 33.5%), n-heptane (1.2%, 0.3%), toluene (8.2%, 1.1%), ethylbenzene (2.3%, 0.1%), and xylenes (8.4%, 0.2%). In these experiments, the fully vaporized gasoline mixture, which contained a higher fraction of aromatic hydrocarbons, was a more effective inhibitor of benzene metabolism than was the light fraction, which was composed primarily of aliphatic hydrocarbons.
- Results of studies with styrene-butadiene mixtures showed a decrease in the rate of metabolism of each chemical but an increase in the concentration of the circulating epoxide metabolites (Bond et al., 1998). The frequency of micronuclei seen in mice exposed by inhalation to butadiene was not altered by simultaneous exposure to styrene.
- Synergistic losses of auditory sensitivity occurred following combined exposure of rats to vapors of toluene plus n-hexane and xylene plus n-hexane (Nylen, 1996). These combined exposures, however, produced antagonistic effects in nerve conduction or action potential amplitudes in the auditory pathway, visual pathway, and peripheral nerve.
- Exposure of male rats to 1000 ppm n-hexane for 61 days caused testicular atrophy and loss of germ cell line (Nylen, 1989). Simultaneous administration of 1000 ppm toluene or xylene did not cause germ cell line alterations or testicular atrophy.
- Neurological effects have been observed in many intermediate-duration inhalation experiments in rats exposed to n-hexane (ATSDR, 1999). No neurotoxic effects were observed in a 2-year chronic study in rats and mice with commercial hexane containing 52.2% n-hexane, 16.0% 3-

methylpentane, 15.6% methylchclopentane, 11.6% 2-methylpentane, 3.2% cyclohexane (Daughtrey et al., 1999). In a separate 13-week inhalation study of commercial hexane, a detailed neurobehavioral/neuropathological evaluation revealed no n-hexane-induced neuropathy (Soiefer et al., 1991).

2. Specific Strategies/Rationales for Each Endpoint

Specific strategies and rationales for each of the SIDS human health toxicity endpoints are presented below:

Acute Toxicity

There is an abundance of acute toxicity data for components present in the streams from this category at concentrations greater than 5% (see Table 5). Data are also available for Pyrolysis Gasoline [Dripolene] and a C5-C10 distillate fraction of a Pyrolysis Gasoline stream [Rerun Tower Overheads] and data are available for the Hydrotreated C6-C8 Fraction. Except for dicyclopentadiene, the components have demonstrated low acute toxicity. High concentrations were needed to produce lethality via oral gavage and inhalation routes of exposure. In several studies with rats, dicyclopentadiene produced lethality at much lower doses (ranges: oral LD_{50} = 347 to 820 mg/kg, inhalation LC_{50} = 359 to >500 but < 1000 ppm). The oral LD_{50} for cyclopentene was 1.66 g/kg and the LD_{50}s for the other components were greater than 2 g/kg. The inhalation LC_{50}s for the components other than dicyclopentadiene ranged from 3680 to 120,000 ppm. The two streams that were tested had oral LD_{50}s greater than 2 g/kg and the one stream tested for acute inhalation toxicity had an LC_{50} greater than 12,408 ppm. Most components also have acute data for other species and routes of exposure. Thus, for purposes of the HPV Challenge Program, the available component data is adequate to characterize the acute toxicity of the category members. Therefore, no additional testing for acute toxicity is proposed.

Genetic Toxicity – Gene Mutation

Of the identified category components present at concentrations greater than 5%, only 1,3-butadiene and benzene have consistently caused gene mutations in genetic toxicity tests (see Table 5). 1,3-Butadiene was positive in several *in vivo* and *in vitro* tests. Benzene was negative in several standard tests but was positive in an *in vivo* HPRT gene mutation test in mouse splenocytes. Based on the data for components, the streams in the category are predicted to be negative in the HPV gene mutation test (Ames Test). Negative Ames Tests conducted with two streams (one from this category [Hydrotreated C6-8 Fraction] and one with a C5-C10 distillate fraction of the Pyrolysis Gasoline category stream) support this prediction. Thus, no additional Ames Tests are proposed.

Genetic Toxicity – Chromosome Aberration

Benzene has caused chromosome aberrations in *in vitro* and *in vivo* tests. The other most prevalent component in streams in this category, toluene, is negative in both *in vitro* and *in vivo* tests. Of the

remaining identified category components present at concentrations greater than 5%, only vinyl acetate, 1,3-butadiene, isoprene, hexane, and naphthalene have been reported to cause chromosome aberrations (see Table 5). As discussed above, coadministration of benzene with other hydrocarbons that are substrates for the cytochrome P450 enzymes can reduce clastogenicity, as was seen with benzene-toluene and benzene-gasoline mixtures. Further evidence for inhibition of clastogenicity is provided by results from a mouse micronucleus test with one the streams from this category, Hydrotreated C6-8 Fraction. Although the tested Hydrotreated C6-8 Fraction contained approximately 55% benzene, and benzene is positive in the mouse micronucleus test, this stream was negative. Additional information that may be useful will become available from mouse micronucleus testing that will be conducted with streams distilled from Pyrolysis Gasoline that are members of the Panel's C5 Non-Cyclics and Resin Oils and Cyclodiene Dimer Concentrates categories. Thus, based on the composition and available data for components and mixtures of components, sufficient component data exist, or will become available, to allow use of scientific judgment to characterize the potential of streams in the category to cause chromosome aberrations. Thus, no additional testing for chromosome aberrations is proposed.

Subchronic Toxicity

Most of the components of the category have extensive epidemiology and toxicology databases, and most major components have been tested for chronic toxicity and carcinogenicity. In addition to the data for components, two streams were tested in repeated-dose studies. A 5-day rat inhalation study was conducted with a Hydrotreated C6-8 stream (Hydrogenated Pyrolysis Gasoline), and a 21-day rabbit dermal irritation study, which included evaluations for systemic effects, was conducted with a C5-C10 fraction of Pyrolysis Gasoline (Rerun Tower Overheads). See Table 5 for a description of available data.

Repeated oral or inhalation exposures to many of the components of the streams in the category have been shown to cause adverse health effects in a variety of organs. However, existing data also show that antagonistic and synergistic interactions occur between some components comprising the streams, as noted above in Section III.A.1. The target organs affected by exposure to the mixtures, and the severity of the effects, will depend upon the relative concentrations of the components within each stream and the nature of the interactions between components.

Many of the C5 components of the High Benzene Naphthas Category are also components of the Pyrolysis C5s and Hydrotreated C5s streams (C5 Non-Cyclics Category) that will be tested for repeated-dose toxicity by the Panel, as part of the HPV Program. Based on structural similarity, pentenes are likely to have a toxicity profile similar to hexenes. The American Chemistry Council's Higher Olefins Panel will address hexenes as part of the HPV Program. Also, the International Hydrocarbon Solvents Consortium will cover the C5 aliphatic components in its C5 Aliphatics Category. Pentane will be addressed in the American Petroleum Institute's Petroleum Gases Test Plan. Other components are shared with the Panel's Resin Oils and Cyclodiene Dimer Concentrates Category streams.

Several components are sponsored in the OECD SIDS or ICCA programs (see Table 5). Additional studies with these components may be found or conducted within those programs.

Results of available data and relevant data resulting from other programs are expected to be sufficient to adequately characterize the repeated-dose human health hazard endpoints for the substances included in this category. Therefore, no additional repeated-dose testing is proposed.

Developmental Toxicity

Developmental toxicity data exist for most components present in this category at concentrations greater than 5% (see Table 5). In these studies, no convincing evidence was seen for teratogenicity in the absence of maternal toxicity. Fetotoxicity has been reported for some components, but mostly in the presence of maternal toxicity (see Table 5). Only five components (pentenes, cyclopentene, 3-methylpentane, methylcyclopentane, 1,3-cyclopentadiene) lack developmental toxicity tests. However, these components do not have structural alerts for developmental toxicity, and data being generated by other test plans within the HPV Program will provide additional information about the potential of these substances to cause developmental effects. Three of the five materials are also components of the Pyrolysis C5s and Hydrotreated C5s streams (C5 Non-Cyclics Category) that will be tested for developmental toxicity by the Panel, as part of the HPV Program. Pentenes will be addressed by the International Hydrocarbon Solvents Consortium (C5 Aliphatics Test Plan). Also, based on structural similarity, pentenes are likely to have a developmental toxicity profile similar to hexenes. The American Chemistry Council's Higher Olefins Panel will address hexenes as part of the HPV Program. 3-Methylpentane and methylcyclopentane were components (16.0% and 15.6%, respectively) of a commercial hexane stream that was negative in a rat inhalation developmental toxicity study. A C5-C10 fraction of a Pyrolysis Gasoline stream has been tested in an oral developmental toxicity study in rabbits. No developmental effects were seen. Additional developmental toxicity information will become available from testing conducted by the Panel for the Resin Oils and Cyclodiene Dimer Concentrates Category with streams distilled from Pyrolysis Gasoline. Thus, existing data and data that will be generated by other test programs are expected to be adequate to characterize the potential of the streams in the category to cause developmental toxicity. No further developmental toxicity tests are proposed for this endpoint.

Reproductive Toxicity

Reproductive toxicity data exist for most components present in this category at concentrations greater than 5% (see Table 5). In its review of benzene, ATSDR (1997) concluded that, although there are some data indicating adverse gonadal effects (e.g., atrophy/degeneration, decrease in spermatozoa, moderate increases in abnormal sperm forms), data on reproductive outcomes are either inconclusive or conflicting. However, most studies indicate no effects on reproductive indices, even at high doses. Reproductive organ effects were seen after inhalation exposure to isoprene and hexane. 1,3-Butadiene is sponsored in the OECD SIDS program and will be tested for reproductive toxicity. Some reproductive toxicity information exists for most major components. Many components have been

tested in standard reproductive toxicity studies. Others have data from standard developmental toxicity studies. In addition, most components have data for reproductive organ toxicity, collected in repeated-dose studies. Those components lacking reproductive toxicity information do not have structural alerts for reproductive toxicity, and data being generated by other test plans within the HPV Program will provide additional information about the potential of these substances to cause reproductive effects. Some of these materials are also components of the Pyrolysis C5s and Hydrotreated C5s streams (C5 Non-Cyclics Category) that will be tested for reproductive toxicity by the Panel, as part of the HPV Program. Also, based on structural similarity, pentenes are likely to have a developmental toxicity profile similar to hexenes, which will be addressed by the American Chemistry Council's Higher Olefins Panel as part of the HPV Program. Pentenes will also be covered by the American Chemistry Council's Hydrocarbon Solvents Panel (C5 Aliphatics Test Plan). Additional reproductive toxicity information will become available from testing conducted by the Panel for the Resin Oils and Cyclodiene Dimer Concentrates Category with streams distilled from Pyrolysis Gasoline. 3-Methylpentane and methylcyclopentane were components (16.0% and 15.6%, respectively) of a commercial hexane stream that was negative in a rat inhalation two generation reproductive toxicity study. Thus, existing data and data that will be generated by other test programs are expected to be sufficient to adequately characterize the potential for reproductive toxicity of the streams in this Category. No further reproductive toxicity tests are proposed.

3. Robust Summaries

Robust summaries for existing data for two streams from the category (Pyrolysis Gasoline [Dripolene] and Hydrotreated C6-8 Fraction) and for a C5-C10 distillate fraction of a Pyrolysis Gasoline stream (Rerun Tower Overheads) are provided with this test plan. Robust summaries for data being developed by other groups for HPV, OECD SIDS, and ICCA high production volume testing programs will be provided when they become available through those programs. Most existing data for components of the category have been extensively reviewed in the literature as noted in Table 5, obviating the need for robust summaries.

B. Physical-Chemical Properties

The physicochemical (PC) endpoints in the HPV Chemical Program include:

- Melting Point
- Boiling Point
- Vapor Pressure
- Water Solubility
- Octanol/Water Partition Coefficient (K_{ow})

Calculated PC data for selected component chemicals in this category will be developed using a computer model to provide a consistent, representative data set. In addition, measured PC data will be identified for selected products in this category and will be summarized together with the calculated data to provide comparisons between the two data sets. The selection of component chemicals to be modeled will be made once an appropriate measured data set is identified.

Calculated PC data for selected component chemicals in the High Benzene Naphthas Category will be developed using the EPIWIN© computer model (EPIWIN, 1999), as discussed in the US EPA document entitled *The Use of Structure-Activity Relationships (SAR) in the High Production Volume Chemicals Challenge Program* (US EPA, 1999a). The use of computer modeling for the development of these data is appropriate since components of the streams in this category are all chemically related and are expected to exhibit relatively similar environmental properties. In addition, for all the chemicals selected to represent products in this category, a calculated dataset provides a common method in the development of these values.

Boiling point, melting point, and vapor pressure ranges will be determined using the MPBPVP subroutine in EPIWIN. K_{ow} and water solubility will be calculated using KOWIN and WSKOW subroutines, respectively. There is more information on calculating data for the HPV chemical program in the EPA document titled '*The Use of Structure-Activity Relationships (SAR) in the High Production Volume Chemicals Challenge Program*" (US EPA, 1999a).

Because the HPV substances covered under the High Benzene Naphthas Category testing plan are mixtures containing differing compositions, it is not possible to develop or calculate a single numerical value for each of the physicochemical properties. For example, a product that is a mixture of chemicals does not have boiling point, but rather a boiling range. Calculated values for physicochemical properties will be represented as a range of values according to the product's component composition and based on the results of computer modeling. Robust summaries characterizing the PC endpoints will be prepared upon completion of a review of available measured data, and will include the calculated and measured data.

C. Environmental Fate

The environmental fate endpoints in the HPV Chemical Challenge Program include:

- Biodegradation
- Photodegradation
- Hydrolysis
- Fugacity

Although biodegradation data are not available for products in the High Benzene Naphthas Category, there are data for selected component chemicals of those products, as well as for complex products, that can be used to characterize the potential biodegradability of products in this category. The complex product values are for substances composed of a range of chemicals with regard to carbon numbers and chemical classes (i.e., paraffins, alkenes or alkylbenzenes). As suggested by the experimental data, products in this category will exhibit a high extent of biodegradation.

Data or information for the fate endpoints, photodegradation and hydrolysis, will be developed and either will be calculated and/or discussed in technical summaries. Chemicals in this category are not

subject to hydrolysis at measurable rates, therefore information for this endpoint will be summarized in a technical review document.

Equilibrium models are used to calculate chemical fugacity, which can provide information on where a chemical is likely to partition in the environment. These data are useful in identifying environmental compartments that could potentially receive a released chemical. Fugacity data can be calculated only for individual chemicals. For the HPV Chemical Challenge Program, environmental partitioning data will be developed for selected component chemicals of the products in this category.

A preliminary evaluation of chemicals in the High Benzene Naphthas Category suggests that they will partition largely to the air, and therefore their fate in air is of environmental interest. Because the air phase may be a compartment that could potentially receive many of the component chemicals in this category, data characterizing their potential for physical degradation in the atmosphere will be developed (this is discussed below under photodegradation).

1. Biodegradation

There are sufficient data to characterize the potential biodegradability of products in this category. Data for constituent chemicals of products in this category (as well as for complex products not in this category that contain chemicals found in products from this category) suggest that high benzene naphtha products have the potential to biodegrade to a great extent (Table 6). The carbon number of products in this category ranges primarily between C5 to C11. Results for several chemicals, including benzene, with carbon numbers in this range that are contained by these products have been shown to biodegrade from 63 to 100% after 14 or 28 days, while results for several comparable, complex products containing several components range from 21 to 96% after 28 days. As seen by the data in Table 6, there is a relatively large biodegradation database for single chemicals and complex products that can be used to characterize this endpoint for high benzene naphtha products. Because products in this category are compositionally more comparable to the products identified in Table 6 as gasoline streams, these data best describe the potential biodegradability of the high benzene naphtha products. Gasoline stream compositions are provided in Table 7.

The data from the majority of tests in Table 6 were developed using a manometric respirometry test procedure. This procedure uses continuously stirred, closed systems, which is recommended when assessing the potential biodegradability of chemically complex, poorly water soluble, and volatile materials like those in this category. Stirring is recommended when evaluating products containing several chemicals, some of which may have limited water solubility.

2. Photodegradation – Photolysis

Direct photochemical degradation occurs through the absorbance of solar radiation by a chemical substance. If the absorbed energy is high enough, then the resultant excited state of the chemical may lead to its transformation. Simple chemical structures can be examined to determine whether a chemical

has the potential for direct photolysis in water. First order reaction rates can be calculated for some chemicals that have a potential for direct photolysis using the procedures of Zepp and Cline (1977).

To develop information or data that will characterize the potential of products in this category to undergo direct photochemical degradation, the existing product chemical composition data will be evaluated to select a subset of chemicals that adequately represents products in this category. The selection process will consider chemical carbon number range, hydrocarbon type, and chemical structure. The UV light absorption of selected chemicals in products in the High Benzene Naphthas Category will be evaluated to identify those chemicals with a potential to degrade in solution. When possible, first order reaction rates will be calculated for chemicals identified to have a potential for direct photolysis in water. The results of the calculations will be summarized in a technical discussion for this endpoint. If instead, a low potential for direct photolysis is suggested by the evaluation, a technical discussion will be prepared to summarize the findings.

3. Photodegradation – Atmospheric Oxidation

Photodegradation can be measured (US EPA, 1999b) (the US EPA identifies OECD test guideline 113 as a test method) or estimated using models accepted by the US EPA (US EPA, 1999a). An estimation method accepted by the US EPA includes the calculation of atmospheric oxidation potential (AOP). Atmospheric oxidation as a result of hydroxyl radical attack is not direct photochemical degradation, but rather indirect degradation. AOPs can be calculated using a computer model. Hydrocarbons, such as those in the High Benzene Naphthas Category, have the potential to volatilize to air where they can react with hydroxyl radicals (OH-).

The computer program AOPWIN (atmospheric oxidation program for Microsoft Windows) (EPIWIN, 1999) is used by the US EPA OPPTS (Office of Pollution Prevention and Toxic Substances). This program calculates a chemical half-life based on an overall OH- reaction rate constant, a 12-hr day, and a given OH- concentration. This calculation will be performed for representative chemical components of products in the High Benzene Naphthas Category. The existing product chemical composition data will be evaluated to select a subset of chemicals that adequately represents products in this category. The selection process will consider chemical carbon number range, hydrocarbon type, and chemical structure. The resulting calculations will be summarized in a robust summary for this endpoint.

4. Hydrolysis

Hydrolysis of an organic chemical is the transformation process in which a water molecule or hydroxide ion reacts to form a new carbon-oxygen bond. Chemicals that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (Neely, 1985).

Chemical stability in water can be measured (EPA identifies OECD test guideline 111 as a test method) or estimated using models accepted by the EPA (US EPA, 1999b). An estimation method accepted by

the EPA includes a model that can calculate hydrolysis rate constants for esters, carbamates, epoxides, halomethanes, and selected alkylhalides. The computer program HYDROWIN (aqueous hydrolysis rate program for Microsoft windows) (EPIWIN, 1999) is used for this purpose by OPPTS.

However, all of the chemical structures included in the High Benzene Naphthas Category are hydrocarbons. That is, they consist entirely of carbon and hydrogen. As such they are not expected to hydrolyze at a measurable rate. A technical document will be prepared that discusses the potential hydrolysis rates of these substances, the nature of the chemical bonds present, and the potential reactivity of this class of chemicals with water.

5. Chemical Transport and Distribution in the Environment - Fugacity Modeling

Fugacity based multimedia modeling can provide basic information on the relative distribution of chemicals between selected environmental compartments (i.e., air, soil, sediment, suspended sediment, water, biota). The US EPA has acknowledged that computer modeling techniques are an appropriate approach to estimating chemical partitioning (fugacity is a calculated endpoint and is not measured). A widely used fugacity model is the EQC (Equilibrium Criterion) model (Mackay et al., 1996). The US EPA cites the use of this model in its document titled "*Determining the Adequacy of Existing Data*" (US EPA, 1999b), which was prepared as guidance for the HPV Chemical Program.

In its document, US EPA states that it accepts Level I fugacity data as an estimate of chemical distribution values. The input data required to run a Level I model include basic physicochemical parameters; distribution is calculated as percent of chemical partitioned to 6 compartments described above within a defined unit world. Level I data are basic partitioning data that allow for comparisons between chemicals and indicate the compartment(s) to which a chemical is likely to partition.

The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, melting point, vapor pressure, and water solubility to calculate distribution within a unit world. This model will be used to calculate distribution values for representative chemical components identified in products from this category. Existing product chemical composition data will be evaluated to select a subset of chemicals that adequately represents products in this category. The selection process will consider chemical carbon number range, hydrocarbon type, and chemical structure. A computer model, EPIWIN version 3.04 (EPIWIN, 1999), will be used to calculate the physicochemical properties needed to run the Level I EQC model.

D. Aquatic Toxicity

The aquatic toxicity endpoints for the HPV Chemical Program include:

- Acute Toxicity to a Freshwater Fish
- Acute Toxicity to a Freshwater Invertebrate
- Toxicity to a Freshwater Alga

Although aquatic toxicity data are not available for products in the High Benzene Naphthas Category, there are sufficient read across data from both constituent chemicals of those products and complex products to fully characterize the toxicity of this category. The use of data from selected read across materials to products in this category can be justified for the following reasons:

- Individual chemicals and complex products used for read across purposes contain a chemical class or combinations of chemical classes (i.e., olefins, aromatics, paraffins) that are found in products from this category.
- Individual chemicals and complex products used for read across purposes have a carbon number or carbon number range that falls within the range of carbon numbers found in products from this category.
- Individual chemicals and complex products used for read across purposes as well as the products in this category are composed of chemicals that act by a similar mode of toxic action.

The data in Table 8 provides a comparison of the range of product compositions (i.e., carbon number, chemical class, weight percent) in the High Benzene Naphthas Category to materials used to characterize the aquatic toxicity of this category. This comparison illustrates the similarity in carbon number ranges between products in this category and the selected products with read across data. The data in Tables 9, 10, and 11 establish the range of toxicity that products in this category are expected to demonstrate, based on the read across data.

The aquatic toxicity data presented in this test plan fall within a narrow range of values regardless of their varying chemical class content and carbon number range. This is not unexpected, because the constituent chemicals of products in this category are neutral organic hydrocarbons whose toxic mode of action is non-polar narcosis. The mechanism of short-term toxicity for these chemicals is disruption of biological membrane function (Van Wezel and Opperhuizen, 1995), and the differences between measured toxicities (i.e., LC/LL50, EC/EL50) can be explained by the differences between the target tissue-partitioning behavior of the individual chemicals (Verbruggen et al., 2000).

The existing fish toxicity database for narcotic chemicals supports a critical body residue (CBR, the internal concentration that causes mortality) of between approximately 2-8 mmol/kg fish (wet weight) (McCarty and Mackay, 1993; McCarty et al., 1991), supporting the assessment that these chemicals have equal potencies. When normalized to lipid content, the CBR is approximately 50 umol of

hydrocarbon/g of lipid for most organisms (Di Toro et al., 2000). Because the products in this category are all complex mixtures containing relatively similar series of homologous chemicals, their short-term toxicities are expected to fall within the range of toxicity demonstrated by the individual chemicals, as well as comparable products summarized in this test plan. Therefore, the existing data are believed to form a sufficiently robust dataset to fully characterize the aquatic toxicity endpoints in the HPV Chemical Program for this category.

The fish and invertebrate acute and alga toxicity values for individual chemicals and complex products similar to those in this category (Tables 9, 10, 11) fall within a range of approximately 1-64 mg/L and overlap between the three trophic levels. Because the products in the High Benzene Naphthas Category will range in paraffin, alkene, and/or aromatic carbon number content within approximately C5 to C11, a range in toxicity for products in this category will be comparable to the range of data summarized in Tables 9, 10, and 11.

As suggested by the experimental data, this category will exhibit a moderate range of acute toxicity to fish and invertebrates and a moderate range of toxicity to algae. For representative chemicals and products, experimental acute fish toxicity values range between 2.5 to 46 mg/L for two species (Table 9), while acute invertebrate toxicity values range between 0.9 to 32 mg/L for one species (Table 10). In comparison, alga toxicity values for one species range between 1.0 to 64 mg/L (for biomass and growth rate endpoints), while alga NOELR values range between 1.0 to 51 mg/L (for biomass or growth rate endpoints) (Table 11).

IV. TEST PLAN SUMMARY

The basic strategy of this screening level test plan for characterizing the human health hazards of this category is to evaluate data for the components of the streams, as well as data for mixtures of category components and analogous mixtures (existing data and data being developed by other test programs). Based upon examinations of stream compositions and existing toxicity data for components of streams in the category, there is minimal likelihood for the appearance of unexpected or remarkable biological findings in testing of these streams. All streams in this category are subject to the Occupational Safety and Health Administration (OSHA) Benzene Standard (29 CFR 1910.1028). Those streams containing 1,3-butadiene are subject to the OSHA Butadiene Standard (29 CFR 1910.1051). OSHA Permissible Exposure Limits exist for all major components. Benzene, as the predominant component in most streams, is expected to be the key driver with respect to health effects that would be observed in the SIDS battery of tests, with genotoxicity and hematotoxicity the effects most likely to be seen. However, the effects of other components may also contribute to the toxicity of the streams. Benzene has a robust toxicity dataset and has completed the OECD SIDS program. No further testing of benzene is needed for the HPV Chemical Challenge Program. The other major chemical components of streams in the High Benzene Naphthas Category have been extensively and comprehensively tested for human health toxicity endpoints, and all components present in the streams at concentrations greater than 5% have been tested in at least one toxicity study. Those components having only limited data lack

structural alerts for mammalian toxicity and data exist for structural analogs. Some data are available for two High Benzene Naphtha streams (Pyrolysis Gasoline [Dripolene] and Hydrotreated C6-C8 Fraction) and for a C5-C10 distillate fraction of a Pyrolysis Gasoline stream (Rerun Tower Overheads). Some data are also available regarding interactions between certain components that impact metabolism and toxicity. Additional supporting data for components of the High Benzene Naphtha streams, tested either individually or as components of other streams or mixtures, will be collected by other test plans within the Olefins Panel's HPV program, by other consortia participating in the HPV or ICCA programs, or from chemicals sponsored in the OECD SIDS program. These data are expected to provide sufficient information to allow use of component data to develop scientific judgment-based characterizations of the human health effects of streams in this category. Therefore, no additional human health toxicity testing is proposed. The hazard characterization for each stream will include the hazards of benzene (cancer, genetic toxicity, hematotoxicity) plus any reproductive or developmental toxicity or target organ effects of the other components, unless there is clear evidence that specific component interactions eliminate toxicity.

Data will be developed and/or identified to characterize relevant physicochemical endpoints in the HPV Chemical Challenge Program.

Biodegradation data identified as read across data to the High Benzene Naphthas Category show that products in this category have the potential to exhibit a high extent of biodegradability. The existing read across data provide sufficient information to adequately characterize the biodegradability of products in this category. Therefore, no additional biodegradation testing is proposed.

The chemical components in these products are relatively volatile, and if released they would be expected to partition to the air phase to a significant extent. In the air, they are subject to rapid physical degradation through hydroxyl radical attack. Therefore, as a result of both biological and physical degradation processes, these products are not expected to persist in the environment.

Sufficient information has not been developed on the potential of products in this category to photodegrade, hydrolyze, and partition within the environment. Therefore, information or data will be developed to adequately characterize these endpoints.

Read across aquatic toxicity data show that products in the High Benzene Naphthas Category have the potential to produce a moderate level of toxicity in freshwater algae and acute toxicity in freshwater fish and invertebrates. The existing read across data provide sufficient information to adequately characterize the aquatic toxicity of products in this category. Therefore, no additional toxicity testing is proposed.

The evaluations, modeling, and technical discussions that will be developed for the High Benzene Naphthas Category are summarized in Table 12.

REFERENCES

ACGIH (American Conference of Governmental Industrial Hygienists). 1986. Documentation of the TLV Values and Biological Exposure Indices, 5th ed., Cincinnati, IH, p. 163.

Andrews, L.S., E.W. Lee, C.M. Witmer, J.J. Kocsis, and R. Snyder. 1977. Effects of toluene on the metabolism, disposition and hemopoietic toxicity of [^{3}H]benzene. Biochem. Pharmacol. 26:293-300.

ATSDR (Agency for Toxic Substances and Disease Registry). 1997. Toxicological Profile for Benzene. Prepared by Research Triangle Institute for U.S. Department of Health & Human Services, Public Health Service, ATSDR [available on the internet].

ATSDR (Agency for Toxic Substances and Disease Registry). 1993. Toxicological Profile for 1,3-Butadiene. Prepared by Syracuse Research Corporation for U.S. Department of Health & Human Services, Public Health Service, ATSDR [available on the internet].

ATSDR (Agency for Toxic Substances and Disease Registry). 1999. Toxicological Profile for Ethylbenzene. Prepared by Research Triangle Institute for U.S. Department of Health & Human Services, Public Health Service, ATSDR [available on the internet].

ATSDR (Agency for Toxic Substances and Disease Registry). 1999. Toxicological Profile for n-Hexane. Prepared by Research Triangle Institute for U.S. Department of Health & Human Services, Public Health Service, ATSDR [available on the internet].

ATSDR (Agency for Toxic Substances and Disease Registry). 1995. Toxicological Profile for Naphthalene. Prepared by Sciences International, Inc. under contract to Research Triangle Institute for U.S. Department of Health & Human Services, Public Health Service, ATSDR [available on the internet].

ATSDR (Agency for Toxic Substances and Disease Registry). 1992. Toxicological Profile for Styrene. Prepared by Life Systems, Inc. under contract to Clement International Corporation for U.S. Department of Health & Human Services, Public Health Service, ATSDR [available on the internet].

ATSDR (Agency for Toxic Substances and Disease Registry). 2000. Toxicological Profile for Toluene. Prepared by Syracuse Research Corporation for U.S. Department of Health & Human Services, Public Health Service, ATSDR [available on the internet].

ATSDR (Agency for Toxic Substances and Disease Registry). 1995. Toxicological Profile for Xylenes. Prepared by Sciences International under contract to Research Triangle Institute for U.S. Department of Health & Human Services, Public Health Service, ATSDR [available on the internet].

Bamberger, J.R. 1996. 90-Day inhalation toxicity study with cyclohexane in mice. Haskell Laboratory for Toxicology and Industrial Medicine, DuPont, Report No. HLR 17-96.

Beals, S.M., R.A. Jacobson, J.P. Robinson, H.T.Appleton, P.A. Howard, and J. Santodonato. 1986. Technical Support Document, Cyclohexane. Doc. No. SRC TR-86-030 [draft final]. Syracuse Research Corporation, Syracuse, NY. Prepared for Test Rules Development Branch Existing Chemical Assessment Division, Office of Toxic Substances, Washington, DC.

Bond, J.A, T.L. Leavens, M.J. Seaton, and M.A. Medinsky. 1998. Predicting the toxicity of chemical mixtures. CHEMTECH, July.

Brown, N.A. 1991. Reproductive and developmental toxicity of styrene. Reproductive Tox. 5:3-29.

Brown, N.A. 1993. Developmental and reproductive toxicity of styrene: A review update. International Symposium on Health Hazards of Butadiene and Styrene. Abstract reprinted in The SIRC Review 3(1):44-45.

Chemicals Inspection and Testing Institute, Japan. 1992. Biodegradation and Bioaccumulation Data of Existing Chemicals Based on the CSCL Japan. Japan Chemical Industry Ecology-Toxicology and Information Center. ISBN 4-89074-101-1.

Ciranni R, Barale R, Ghelardini G, & Loprieno N (1988) Benzene and the genotoxicity of its metabolites. II. The effect of the route of administration on the micronuclei and bone marrow depression in mouse bone marrow cells. Mutat Res, 209: 23-28.

Daughtrey, W.C., D.L. Putman, J. Duffy, A.I. Soiefer, C.J. Kirwin, L.N. Curcio, and T.H. Keenan. 1994a. Cytogenetic studies on commercial hexane solvent.

Daughtrey, W.C., T. Neeper-Bradley, J. Duffy, L. Haddock, T. Keenan, C. Kirwin, and A. Soiefer. 1994b. Two-generation reproduction study on commercial hexane solvent. J. Applied Toxicology 14(5):387-393.

Daughtrey, W.C., P. Newton, R. Rhoden, C. Kirwin, L. Haddock, J. Duffy, T. Keenan, W. Richter, and M. Nicolich. 1999. Chronic inhalation carcinogenicity study of commercial hexane solvent in F-344 rats and B6C3F1 mice. Toxicological Sciences 48:21-29.

Di Toro, D.M., J.A. McGrath, and D.J. Hansen. 2000. Technical Basis for Narcotic Chemicals and Polycyclic Aromatic Hydrocarbon Criteria. I. Water and Tissue. Environmental Toxicology and Chemistry, 19:1951-1970.

ECETOC (European Centre for Ecotoxicology and Toxicology of Chemicals) Special Report No. 12. 1,3-Butadiene OEL Criteria Document (Second Edition). 1997. Programme for the Joint Assessment of Commodity Chemicals. Jacc Report No. 19. Brussels, Belgium.

ECETOC (European Centre for Ecotoxicology and Toxicology of Chemicals) report on Dicyclopentadiene. 1991. Programme for the Joint Assessment of Commodity Chemicals. Jacc Report No. 19. Brussels, Belgium.

ECETOC (European Centre for Ecotoxicology and Toxicology of Chemicals) report on Xylenes. 1986. Programme for the Joint Assessment of Commodity Chemicals. Jacc Report No. 6. Brussels, Belgium.

EPA/OTS Doc.8690000024: Test for oral toxicity in rats with cyclopentadiene with cover letter dated 09/28/95.

EPA/OTS Doc.8690000121S: Subacute inhalation exposure of cyclopentadiene with cover letter dated 09/28/95.

EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. SyracuseResearchCorporation, Syracuse, NY, USA.

EU Risk Assessment. 2001. Benzene. Draft Risk Assessment Document [in Risk Assessment Review]. Available on internet at http://ecb.jrc.it/existing-chemicals.

EU Risk Assessment. 2000. Cyclohexane. ECB# 031. Draft Risk Assessment Document [in Risk Assessment Review]. Available on internet at http://ecb.jrc.it/existing-chemicals.

EU Risk Assessment. 2001. Naphthalene. Draft Risk Assessment Document [in Risk Assessment Review]. Available on internet at http://ecb.jrc.it/existing-chemicals.

EU Risk Assessment. 2001. Toluene. Draft Risk Assessment Document [in Risk Assessment Review]. Available on internet at http://ecb.jrc.it/existing-chemicals.

ExxonMobil. 1982. Unpublished reports for Rerun Tower Overheads: Mouse Lymphoma [M1252-78], DNA Repair [M1251-78], Drosophila [M1253-78], Mouse Skin Painting [M0417-77].

Frontali, N. M.D. Amantini, A. Spagnolo, A.M. Guarcini, and M.C. Saltari. 1981. Experimental neurotoxicity and urinary metabolites of the C5-C7 aliphatic hydrocarbons used as glue solvents in shoe manufacture. Clin. Tox. 18:1357-1367.

Gad-El-Karim, M.M., B.L. Harper and M.S. Legator. 1984. Modifications in the myeloclastogenic effect of benzene in mice with toluene, phenobarbital, 3-methylcholanthrene, Aroclor 1254 and SKF-525A. Mutation Res. 135:225-243.

Gad-El-Karim, M.M., V.M.S. Ramanujam and M.S. Legator. 1986. Correlation between the induction of micronuclei in bone marrow by benzene exposure and the excretion of metabolites in urine of CD-1 mice. Toxicol. Appl. Pharmacol. 85:464-477.

Galassi, S., M. Mingazzini, L. Viagano, D. Cesareo, and M.L. Tosato. 1988. Aproaches to Modeling Toxic Responses of Aquatic Organisms to Aromatic Hydrocarbons. Ecotox. Environ. Safety. 16:158-169.

Galvin, J.B. and F. Marashi. 1999. n-Pentane. J. Toxicology and Env. Health. Pt. A,58:35-36.

Halder, C.A., C.E. Holdsworth, B.Y. Cockrell, and V.J. Piccirillo. 1985. Hydrocarbon nephropathy in male rats: Identification of the nephrotoxic components of unleaded gasoline. Tox. and Industrial Health 1(3):67-87.

Hite, M., M. Pecharo, I. Smith and S. Thornton. 1980. The effect of benzene in the micronucleus test. Mut. Res. 77:149-155.

IARC (International Agency for Research on Cancer). 1999. Isoprene. Monographs on the Evaluation of Carcinogenic Risks to Humans. Vol. 71, Part 3, Lyon, France, pp. 1015-1024.

IARC (International Agency for Research on Cancer). 1994. Styrene. Monographs on the Evaluation of Carcinogenic Risks to Humans. Vol. 60, Lyon, France, pp. 233-320.

IARC (International Agency for Research on Cancer). 1999. Toluene. Monographs on the Evaluation of Carcinogenic Risks to Humans. Vol. 71, Part 2, Lyon, France, pp. 829-864.

IRIS (Integrated Risk Information System). 1990. Vinyl Acetate. Developed by the U.S. EPA.

HSDB: TOMES CPS™ System, MICROMEDEX, Englewood, Colorado, Vol. 38. CD-ROM.

JETOC (Japanese Chemical Industry Ecology – Toxicology and Information Center. 1998. Special Issue #3, No. 32 (March, 1998), Tokyo, Japan. In: Handbook of Existing and New Chemical Substances, 8th Ed. 1999. Supervised by Chemical Products Safety Division, Basic Industries Bureau, The Ministry of International Trade and Industry.

Kirwin, C. , R. San, J. Harbell, A. Soiefer, W. Daughtrey and T. Keenan.1991. Salmonella and CHO/HGPRT mutation assays of commercial hexane. The Toxicologist 11(1):315.

Kreckman, K.H. 1997. Inhalation developmental toxicity study of cyclohexane in rats. Haskell Laboratory for Toxicology and Industrial Medicine, DuPont, Report No. HLR 881-96.

Mackay, D., A. Di Guardo, S. Paterson, and C. E. Cowan. 1996. Evaluating the Environmental Fate of a Variety of Types of Chemicals Using the EQC Model. Environ.

Malley, L.A. 1996a. 90-Day inhalation toxicity study with cyclohexane in rats. Haskell Laboratory for Toxicology and Industrial Medicine, DuPont, Report No. HLR 298-96.

Malley, L.A. 1996b. 90-Day inhalation neurotoxicity study with cyclohexane in rats. Haskell Laboratory for Toxicology and Industrial Medicine, DuPont, Report No. HLR 752-95.

McCarty, L.S. and D. Mackay. 1993. Enhancing Ecotoxicological Modeling and Assessment. Environmental Science and Technology, 27:1719-1728.

McCarty, L.S., D. Mackay A.D. Smith, G.W. Ozburn, and D.G. Dixon. 1991. Interpreting Aquatic Toxicity QSARs: The Significance of Toxicant Body Residues at the Pharmacologic Endpoint. In: WSAR in Environmental Toxicology - IV. J.L.M. Hermens and A. Opperhuizen, eds. Elsevier.

McGregor, D. 1994. The genetic toxicology of toluene. Mut Res. 317:2134-228.

McKee, R., E. Frank, J. Heath, D. Owen, R. Przygoda, G. Trimmer, and F. Whitman. 1998. Toxicology of n-pentane. J. Appl. Toxicol. 18:431-442.

Medinsky, A., P.M. Schlosser, and J.A. Bond. 1994. Critical issues in benzene toxicity and metabolism: the effect of interactions with other organic chemicals on risk assessment. Env. Health Perspectives 102(Supp. 9):119-124.

Meyne, J. and M.S. Legator. 1980. Sex-related differences in cytogenetic effects of benzene in the bone marrow of Swiss mice. Environ. Mutagenesis 2:43-50.

Neely, W. B. 1985. Hydrolysis. In: W. B. Neely and G. E. Blau, eds. Environmental Exposure from Chemicals. Vol I., pp. 157-173. CRC Press, Boca Raton, FL, USA.

Nylen, P. 1996. Differing non-additive alterations in different parts of the nervous system of the rat. Food and Che.. Tox. 34(11/12): 1121-1123.

Nylen, P. 1989. Testicular atrophy and loss of nerve growth factor-immunoreactive germ cell line in rats exposed to n-hexane and a protective effect of simultaneous exposure to toluene or xylene. Arch. Toxicol. 63:296-307.

OECD (Organization for Economic Co-operation and Development). 1999. Draft Guidance Document on Aquatic Toxicity Testing of Difficult Substances. OECD Environmental Health and Safety Publications, Series on Testing and Assessment. OECD, Paris, France.

RTECS (Registry of Toxic Effects of Chemical Substances): TOMES CPS™ System, MICROMEDEX, Englewood, Colorado, Vol. 38, CD-ROM.

Soiefer, A., K. Robinson, B. Broxup, J. Duffy, T. Keenan, and W. Daughtrey. 1991. A subchronic neurotoxicity study of commercial hexane vapor in the rat. The Toxicologist II, p. 315 (abstract).

Suzuki, S., H.Atai, Y. Hatakeyama, M. Hara, and S. Nakagawa. 1989. Administration-route-related differences in the micronucleus test with benzene. Mut. Res. 223:407-410.

Toxicol. Chem. 15:1627-1637.

U.S. EPA. 1999a. The Use of Structure-Activity Relationships (SAR) in the High Production Volume Chemicals Challenge Program. OPPT, EPA. Washington, DC, USA.

U.S. EPA. 1999b. Determining the Adequacy of Existing Data. OPPT, EPA., Washington, DC, USA.

Van Wezel, A.P. and A. Opperhuizen. 1995. Narcosis Due to Environmental Pollutants in Aquatic Organisms: Residue-Based Toxicity, Mechanisms, and Membrane Burdens. Critical Reviews in Toxicology, 25:255-279.

Verbruggen, E.M.J., W.J.J. Vaes, T.F. Parkerton, and J.L.M. Hermens. 2000. Polyacrylate-Coated SPME Fibers as a Tool to Simulate Body Residues and Target Concentrations of Complex Organic Mixtures for Estimation of Baseline Toxicity. Environmental Science and Technology, 34;324-331.

WHO EHC. 1997. World Health Organization, International Programme on Chemical Safety, Environmental Health Criteria for Xylenes. No. 190.

Zepp, R. G., and D. M. Cline. 1977. Rates of Direct Photolysis in the Aqueous Environment. Environ. Sci. Technol. 11:359.366.

Table 1.
CAS Numbers and Descriptions Associated with Streams in the High Benzene Naphthas Category

CAS Number	CAS Number Description
64741-99-7	Extracts, petroleum, light naphtha solvent
64742-49-0	Naphtha, petroleum, hydrotreated light
64742-73-0	Naphtha, petroleum, hydrodesulfurized light
64742-83-2	Naphtha, petroleum, light steam-cracked
64742-91-2	Distillates, petroleum, steam-cracked
67891-79-6	Distillates, petroleum, heavy arom.
67891-80-9	Distillates, petroleum, light arom.
68410-97-9	Distillates, petroleum, light distillate hydrotreating process, low-boiling
68475-70-7	Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived
68476-45-9	Hydrocarbons, C5-10 arom. conc., ethylene-manuf.-by-product
68526-77-2	Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum
68606-10-0	Gasoline, pyrolysis, debutanizer bottoms
68606-28-0	Hydrocarbons, C5 and C10-aliph. and C6-8-arom.
68921-67-5	Hydrocarbons, ethylene-manuf.-by-product distn. residues
68955-29-3	Distillates, petroleum, light thermal cracked, debutanized arom.
68956-52-5	Hydrocarbons, C4-8
68956-70-7	Petroleum products, C5-12, reclaimed, wastewater treatment
69013-21-4	Fuel oil, pyrolysis
8030-30-6	Naphtha

Note: The definitions, found in the TSCA Chemical Substance Inventory, for the CAS numbers included in this group are vague with respect to composition. Therefore, it is not uncommon to find that the same CAS number is correctly used to describe different streams (compositions) or that two or more different CAS numbers are used to describe the same stream (composition).

Table 2.
Typical Composition Ranges (Percent) for High Benzene Naphthas
(See notes 1-4 at the end of this table)

Component	Pyrolysis Gasoline	Pyrolysis C6 Fraction	Pyrolysis C6-C8 Fraction	Pyrolysis C5-C6 Fraction	Hydrotreated C6 Fraction	Hydrotreated C6-C7 Fraction	Hydrotreated C6-C8 Fraction	Quench Loop Pyrolysis Oil	Wastewater Treatment (see Note 4)	Extract from Benzene Unit
Vinyl Acetate	9.9									
1,3-Butadiene	6.7	0.1 - 2								
C4's	0.5 -5	0.1 - 1.5								
1,4-Pentadiene	0.3 - 0.9	0.1 - 2								
Isopentane (2-methylbutane)	2.0	0.1 - 1								
1-Pentene (Amylene)	0.6 - 4	1 - 3								
2-Methyl-1-Butene	1.0									
Pentene-2 (isomer mix)	0.2 - 1.8	0.1 - 5								
Isoprene (2-methylbutadiene-1,3)	0.6 - 10	2 - 6		6						
Pentenes				10						
Pentane	10					1				
2-Methyl-2-Butene	1.2	2								
Other C5's	0.3						2.0			
3-methyl-1,2-butadiene		1 - 3								
1,3-Cyclopentadiene	1 - 20	0.1 - 5	1							
1,3-Pentadiene (isomer mix)	0.7 - 4.4	0.3 - 4								
Cyclopentene	0.6 - 5			8						
Cyclopentane	2.3				4	1 - 5				
1,5-hexadiene	0.6									
2-methylpentane	4				4					
2-methyl-1-Pentene	0 - 2.2									
3-methylpentane (Isohexane)	1.3				4	10 - 20				
hexene-1	0 - 2.2									
hexenes						2				
Methylcyclopentadiene	5		1							
Hexane isomers			1 - 3			5 - 20				

Component	Pyrolysis Gasoline	Pyrolysis C6 Fraction	Pyrolysis C6-C8 Fraction	Pyrolysis C5-C6 Fraction	Hydrotreated C6 Fraction	Hydrotreated C6-C7 Fraction	Hydrotreated C6-C8 Fraction	Quench Loop Pyrolysis Oil Wastewater Treatment (see Note 4)	Extract from Benzene Unit
Hexane	0 – 9		1 - 5		6	2 - 15			
Methylcyclopentane	4.9					5 - 15			
1-methylcyclopentene	0.1 - 2.4								
C6 non-aromatics		30						0.9	
non-Aromatic Hydrocarbons							20 - 26		
Benzene	15 - 62	35 - 77	30 - 80	70	75 - 75.7	40 - 69	40 - 60	10 - 21.6	60 - 75
1,3-cyclohexadiene	0.5 - 2.0								
Cyclohexane	2				6	1 - 3			
Cyclohexene	0.6								
cyclohexadienes	0.1 - 2.3								
3-ethylpentene-1		1							
C6 olefin	0.2 - 1.9								
heptenes						2			
2-methylhexane						2			
heptane isomers						1 - 5			
Heptane	0.4 -2		1			1 - 5			
C7 Paraffins & Napththenes	0.3 - 1.1								
C7 Olefins	0 - 1.2								
Methylcyclohexane						1 - 3			
C7-Non-aromatics		3						2.2	
Toluene	17.4	0.5 - 5	15 - 25	5	0.3	3 - 15	10 - 25	5 – 10.9	25 - 40
4-Vinlyclohexene (Butadiene Dimer)	0.1 - 1								
C8 Nonaromatics								1.3	
Ethylbenzene	0.3 - 5.5	1	1 - 3					1 – 3	
C8 Aromatics							3 - 10		1
Xylenes, mixed	10		1 - 10					1.5	
Styrene	10		1 - 10					10 – 15	
C9 Aromatics	0.4 - 1.7								

Component	Pyrolysis Gasoline	Pyrolysis C6 Fraction	Pyrolysis C6-C8 Fraction	Pyrolysis C5-C6 Fraction	Hydrotreated C6 Fraction	Hydrotreated C6-C7 Fraction	Hydrotreated C6-C8 Fraction	Quench Loop Pyrolysis Oil	Wastewater Treatment (see Note 4)	Extract from Benzene Unit
Ethyltoluenes	0.1 – 2									
C9 Paraffins and Naphthenes	0.3 - 1.3									
1,3,5-Trimethylbenzene (mesitylene)	3									
C10+								40.6		
1,2,4-Trimethylbenzene (pseudocumene)	0 - 3.3		1							
4-methylstyrene	0 - 3.3									
Cyclopentadiene/Methylcyclopentadiene Codimers	0.9 - 4.4		1 - 3							
Dicyclopentadiene	20		1 - 5					3.7		
1-Decene	1.5									
Vinyl Toluene	0.1 - 1.1									
dihydrodicyclopentadiene	2									
Decane	0.1 - 5									
C10 Aromatics	1.6									
C10's								1.6 - 27		
Indene	0.6 - 5									
C11+								38.8 - 50		
Naphthalene	15.0							4.3 - 10		
Methylnaphthalene	2.9									
1-Methylnaphthalene	1									
1,1'-Biphenyl	0.1 - 0.9									
C10 Olefins	1.2									

Note 1: The composition data shown above are composites of reported values.
Note 2: The balance of these streams is expected to be other hydrocarbons that have boiling points in the range of the listed components.
Note 3: The listed highs and lows should not be considered absolute values for these limits. They are instead the highs and lows of the reported values.
Note 4: No specific composition data are available. This stream is expected to contain components of Pyrolysis Gasoline.

Table 3.
Process For Hazard Evaluation For Mammalian Toxicity By Toxicity Endpoint

Toxicity Endpoint	**Hazard Evaluation for Streams**
Cancer	Since all streams contain >10% benzene, all streams are considered to be cancer hazards.
Genetic Toxicity	Since all streams contain >10% benzene, all streams are considered to cause genetic toxicity.
Acute Toxicity	Adequate acute toxicity data for the components are available to evaluate the acute toxicity hazards of the streams. Scientific judgment will be used for the evaluation, on a case-by-case basis.
Subchronic, Reproductive and Developmental Toxicity	Data are available for most components present at concentrations >5%; additional data for components and for mixtures of components will be developed by other test plans/programs. These data will be adequate to evaluate the target organ, reproductive and developmental toxicity of the streams. Per the OSHA Hazard Communication Standard, for these endpoints, hazards for components present at $\geq$1% in an untested mixture must be reported in the MSDS and on the label. Thus, hazards of the components will be considered to be hazards of the streams, unless there is sufficient data available to show that the specific combination of components does not present the hazard.

Table 4.
Sources of Data for Hazard Evaluations for mammalian toxicity

[All streams are subject to the OSHA Benzene Standard. For hazard communication, the final hazard characterization for each stream will include the hazards of benzene (cancer, genetic toxicity, hematotoxicity) plus any reproductive or developmental toxicity or target organ effects of the other components, unless there is clear evidence that specific component interactions eliminate toxicity.]

Stream	**Sources of Data for Hazard Evaluation** **[These data will be evaluated using scientific judgment and complying with the requirements of the OSHA Benzene, 1,3-Butadiene, and Hazard Communication Standards]**
Pyrolysis Gasoline	• Available data for components [benzene, 1,3-butadiene, cyclohexane, cyclopentadiene, cyclopentene, 3-methylpentane, dicyclopentadiene, ethylbenzene, hexane, isoprene, methylcyclopentane, naphthalene, pentadiene, pentane, pentenes, styrene, toluene, vinyl acetate, xylene] • Data for streams containing Pyrolysis Gasoline or fractions thereof [Pyrolysis Gasoline Fractions, Dripolene, Hydrogenated Pyrolysis Gasoline (robust summaries provided)] • Data for streams distilled out of Pyrolysis Gasoline that are being tested in other Panel HPV Test Plans [C5 Non-Cyclics and Resin Oils and Cyclodiene Dimer Concentrates categories] • Data for gasoline blending streams referenced in the API Petroleum HPV Gasoline Blending Streams Test Plan • Data for commercial hexane, which contains n-hexane, 3-methylpentane, methylcyclopentane, 2-methylpentane, cyclohexane • Data for hexenes being developed by the ACC Higher Olefins Panel, for C5 aliphatic components being addressed by the ACC Hydrocarbon Solvents Panel in its C5 Aliphatics Category, and for pentane which is addressed in the API Petroleum Gases Test Plan • Literature data regarding interactions between components present in these streams
Pyrolysis C6 Fraction	• Available data for components [benzene, 1,3-butadiene, cyclopentadiene, ethylbenzene, isoprene, pentenes, pentadiene, toluene] • Data for streams distilled out of Pyrolysis Gasoline that are being tested in other Panel HPV Test Plans [C5 Non-Cyclics Category] • Data for hexenes being developed by the ACC Higher Olefins Panel (as structurally similar to pentenes), for C5 aliphatic components being addressed by the ACC Hydrocarbon Solvents Panel in its C5 Aliphatics Category • Literature data regarding interactions between components present in these streams

Stream	**Sources of Data for Hazard Evaluation** **[These data will be evaluated using scientific judgment and complying with the requirements of the OSHA Benzene, 1,3-Butadiene, and Hazard Communication Standards]**
Pyrolysis C6-C8 Fraction	• Available data for components [benzene, dicyclopentadiene, ethylbenzene, hexane, styrene, toluene, xylene] • Literature data regarding interactions between components present in these streams
Pyrolysis C5-C6 Fraction	• Available data for components [benzene, cyclopentene, isoprene, pentenes , toluene] • Data for hexenes being developed by the ACC Higher Olefins Panel (as structurally similar to pentenes) • Literature data regarding interactions between components present in these streams
Hydrotreated C6 Fraction	• Available data for components [benzene, cyclohexane, hexane, 3-methylpentane] • Data for commercial hexane, which contains n-hexane, 3-methylpentane, methylcyclopentane, 2-methylpentane, cyclohexane • Literature data regarding interactions between components present in these streams
Hydrotreated C6-C7 Fraction	• Available data for components [benzene, cyclohexane, hexane, methylcyclopentane, 3-methylpentane, toluene] • Data for commercial hexane, which contains n-hexane, 3-methylpentane, methylcyclopentane, 2-methylpentane, cyclohexane • Literature data regarding interactions between components present in these streams
Hydrotreated C6-C8 Fraction	• Available data for components [benzene, toluene and other identified components] • Data for Hydrogenated Pyrolysis Gasoline (robust summaries provided) • Literature data regarding interactions between components present in these streams
Quench Loop Pyrolysis Oil and Compressor Oil	• Available data for components [benzene, dicyclopentadiene, ethylbenzene, naphthalene, styrene, toluene, xylene and other identified components] • Literature data regarding interactions between components present in these streams
Recovered Oil from Waste Water Treatment	• Available data for components, on a case-by-case basis
Extract from Benzene Extraction Unit	• Available data for components [benzene, toluene] • Literature data regarding interactions between components present in these streams

Table 5.
Summary Results from Existing Human Health Effects Data for Chemical Components and Streams of High Benzene Naphthas Category

(Note: This table is the product of a good faith effort to briefly summarize results of toxicity studies that were available to the reviewer for SIDS endpoints. Results from non-SIDS endpoints are not included. Since all information for a particular chemical may not have been available to the reviewer, the results presented should not be considered as final assessments of the hazards of the listed chemicals. Component data were not reviewed for data adequacy. Robust summaries for the listed components will not be submitted with the Test Plan.)

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/ References
Vinyl Acetate	Oral LD50 = 2.9 g/kg; inhalation LC50 = 3680 ppm [4h]	Negative in Ames Test	Positive in mouse bone marrow micronucleus test by i.p. but negative in rats and mice by inhalation and oral; positive in in-vitro chrom ab	4 and 13-wk rat and mouse inhalation study: decrease in BW gain, respiratory tract effects; no clearly treatment related effects in 4 and 13-wk rat and mouse oral	In rat inhalation study, no embryolethality or teratogenicity seen; fetal growth retardation seen at maternally toxic doses. In rat oral study, no effects.	In an oral rat 2-gen repro study, no effects were seen except for reduction in BW gain in high-dose F1 pups.		Review: IRIS[1] – 1990; HSDB[2]; ATSDR – 1992[4]
1,3-Butadiene	Rat inhalation LC50[4h] = 129,000 ppm	Negative in UDS in mouse and rat, Drosophila; negative and positive in mouse lymphoma; positive in Ames, CHO and in vivo mouse spleenocyte HPRT tests and mouse spot test	Positive in mouse dominant lethal but negative in rat; positive in mouse bone marrow micronucleus and chrom. ab.; negative in rat bone marrow micronucleus	Many studies: Toxicity to blood cells in mice; no effects in rats [inhalation]	Effects seen at maternally toxic doses	Will become available through OECD SIDS	Olefins Panel's Crude Butadiene C4 Category, OECD SIDS	Reviews: ECETOC Special Report No. 12 - 1997[3]; ATSDR[4] - 1993

[1] IRIS: EPA Integrated Risk Information System
[2] HSDB: Hazardous Substances Data Bank [TOMES, MICROMEDEX, Inc.]
[3] ECETOC: European Centre for Ecotoxicology and Toxicology of Chemicals

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/ References
Isoprene (2-methylbutadiene-1,3)	Rat oral LD50= 2.1 g/kg; inhalation LC50 [4h] = 64,500 ppm	Negative in Ames Test	Negative in in-vitro CHO chrom. ab., mouse bone marrow chrom. ab. and rat lung cell micronucleus [inhalation]; positive in mouse bone marrow micronucleus [inhalation]	Many studies: Effect on testes in rats seen at 26 wks but not at 13 wks; effects on blood cells, nasal epithelium, liver, stomach, and testes in mice [inhalation]	No effects in rats; fetotoxicity in mice	Limited repro tox data [sperm motility, vaginal cytology, histopath of repro organs]obtained as part of 13-wk inhalation study: [slight effect on testis in rats; effects on testes, epididymus, sperm, estrus cycle in mice]	Olefins Panel's C5 Non-Cyclics Category/ICCA	Review: IARC[5] - 1999
Pentenes				2-pentene: 4 wk rat oral evaluating nephrotoxicity showed no kidney lesions at 2 g/kg/day w/60% mortality			International Hydrocarbon Solvents Consortium [C5 Aliphatics Category Test Plan]; also, pentenes are likely to have a toxicity profile similar to hexenes which will be addresed by the Higher Olefins Panel	Halder et al., 1985

[4] ATSDR: U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry
[5] IARC: International Agency for Research on Cancer

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/ References
Pentane	Rat oral: LD50>2 g/kg; inhalation LC50[4h] >7000 ppm	Negative in Ames Test	Negative in rat bone marrow micronucleus [inhalation] and dominant lethal [i.p.]; positive [not reproducible] in in-vitro CHO chrom.ab.	90-day rat inhalation: no effect at ~ 7000ppm. 16 wk and 7-30 wk rat inhalation neurotox evaluations : negative With 50/50 blend of n-butane and n-pentane, in a 90-day rat inhalation study with scope limited to evaluation of nephrotoxicity: decrease in BW and male hydrocarbon nephropathy.	No effect in rat oral	No effect on repro organs in 90-day rat inhalation	API [addressed in Petroleum Gases Test Plan]; International Hydrocarbon Solvents Consortium [C5 Aliphatics Category Test Plan]; OECD SIDS	Review: McKee et al., 1998; Galvin and Marashi, 1999
1,3-Cyclopentadiene	Rat oral: 4/5 died at 1 g/kg; inhalation LC50 [4h] = 39 mg/L			Mild liver and kidney effects in rats after 35 exp. of 500 ppm ; no effects in guinea pigs, rabbits, dogs after 135 exp. of 250 ppm, or in dogs after 39 additional exp of 400 ppm and 16 additional exp of 800 ppm [inhalation]				ACGIH[6], RTECS[7], EPA Documents [86960000024, 86960000121S

[6] ACGIH: American Conference of Governmental Industrial Hygienists
[7] RTECS: Registry of Toxic Effects of Chemical Substances

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/ References
Cyclopentene	Rat oral LD50 = 1.66 g/kg; inhalation LCLo [4h] = 16,000 ppm							RTECS
3-methylpentane (Isohexane)				16 wk and 7-30 wk rat inhalation neurotox evaluations : negative				Frontali et al., 1981
Hexane isomers [Commercial Hexane tested: 52.2% n-hexane, 16.0% 3-methylpentane, 15.6% methylcyclopentane, 11.6% 2-methylpentane, 3.2% cyclohexane]		Negative in Ames Test, CHO HPRT	Negative in in-vitro CHO chrom. ab. and rat bone marrow chrom. ab. [inhalation]	No neurotoxicity; male rat hydrocarbon nephropathy [inhalation]	No effects in rats via inhalation	No effect in rat 2-gen study via inhalation except decrease in weight gain in high dose offspring		Daughtrey et al., 1994 a,b; 1999; Kirwin et al., 1991
Hexane	Rat oral LD50=28.7 g/kg; inhalation LC50[4h] = 48,000 ppm	Negative in Ames Test and in vitro UDS	Negative in in-vitro CHO chrom. ab. , inhalation dominant lethal and mouse micronucleus [inhalation and IP]; positive in rat oral bone marrow chrom. ab.	Several studies: Effects on peripheral nervous system and testes	Negative in inhalation and oral developmental studies	No repro tox studies found; testicular atrophy seen in subchronic inhalation studies	OECD SIDS - ICCA	Review: ATSDR[8] – 1999; rat chrom. ab. report in HSDB[9]
Methylcyclopentane				4 wk rat oral evaluating nephrotoxicity showed no kidney lesions at 0.5 g/kg/day but lesions at 2g/kg w/40%mortality				Halder et al., 1985

[8] ATSDR: U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry
[9] HSDB: Hazardous Substances Data Bank [TOMES, MICROMEDEX, Inc]

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/ References
Benzene	Rat oral LD50=810 mg/kg; inhalation LC50 [4h] = 13,700 ppm	Negative in Ames Test, mouse lymphoma, CHO HPRT, in-vitro UDS, Drosophila; positive in mouse spleen HPRT	Positive in vitro/in vivo in numerous studies and species [oral, inhalation]: in-vitro human lymphocytes; chrom. ab. and micronucleus in mouse bone marrow and spleen lymphocytes; rat bone marrow chrom. ab. and micronucleus	Many studies: Primary effect toxicity to blood cells	Several studies: fetotoxic at maternally toxic doses; not tetratogenic	No standard repro studies; most inhalation studies with repro parameters indicate no effect on reproductive indices, even at high doses	OECD SIDS	Review: ATSDR – 1997; EU Risk Assessment – 2001 [Draft]
Cyclohexane	Rat oral LD50 > 5 g/kg; inhalation LC50[4h] = 4044 ppm	Negative in Ames Test, mouse lymphoma, human lymphocyte UDS	Negative in rat bone marrow chrom. ab. [inhalation]	Effects on liver in mice and rats; on liver and kidney in rabbits [inhalation]	No effects seen in rats or rabbits [inhalation]	No effects in rat 2-gen inhalationrepro at doses not maternally toxic	OECD SIDS	Review: SRC Technical Support Document #TR-86-030 [Beals et al.,1986, draft][10]; EU Risk Assessment – 2000 [Draft] Bamberger, 1996; Kreckman, 1997; Malley, 1996 a,b

[10] SRC: Syracuse Research Corporation Center for Chemical Hazard Assessment, prepared for Test Rules Development Branch, Existing Chemical Assessment Division, Office of Toxic Substances

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/ References
Toluene	Rat oral LD50 = 5.5 – 7.53 g/kg; inhalation LC50[4h] = 8000 - 8800 ppm	Negative in Ames Test, SHE transformation, and Drosophila SLRL; equivocal in mouse lymphoma	Negative in in-vitro human lymphocyte and CHO chrom. ab., dominant lethal [oral], chrom. ab. in mice [oral] and rats [inhalation], and mouse micronucleus [oral]	Many studies: Effects on central nervous system; hearing loss in rats	In rats and mice: lower birth weight, delayed postnatal development and behavioral effects [inhalation]	No effects in mouse 2-gen inhalation repro study; in rats, effect on sperm count and epididymal weight at 2000 ppm, but no effect on fertility	OECD SIDS	Review: ATSDR[11] – 2000; IARC[12] – 1999; EU Risk Assessment - 2001 Genetic toxicity review: McGregor, 1994.
Ethylbenzene	Rat oral LD50> 3.5 g/kg; inhalation LC50[4h] LC50 = 4000 ppm	Negative in Ames Test, Drosophila SLRL, and in-vivo UDS in mouse hepatocytes; equivocal in mouse lymphoma	Negative in in-vitro CHO and RL4 cells chrom. ab. and in inhalation/i.p. mouse micronucleus	Several studies: Effects seen in liver, kidney, and lung in rats and mice; hearing loss in rats via inhalation	No effects in rabbits; only supernumerary ribs seen in rats	No repro study; in subchronic rat and mouse studies, no effects seen in gonads sperm, extrus cycle	OECD SIDS	Review: ATSDR[13] - 1999
Xylenes, mixed	Rat oral LD50 = 3.5-8.6 g/kg;Rat inhalation [4h]LC50 = 6,350 - 6,700 ppm	Negative Ames Test and mouse lymphoma	Negative in human lymphocytes [only w/o S9 tested] and CHO chrom. ab.	Many studies: liver, and nervous system effects via inhalation; hearing loss in rats via inhalation; nervous system effects via oral exposure	Fetotoxic effects seen in rat and mouse [oral,inhalation], mostly secondary to maternal toxicity	Negative in rat repro [exposed by inhalation 131 days prior to mating, during mating, gestation, day 5-20 of lactation]; no effect on repro organs in rat and mouse	ACC Toluene Xylene Panel/OECD SIDS/ICCA	Review: ATSDR – 1995; WHO EHC - 1997[14]; ECETOC - 1986

[11] ATSDR: U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry
[12] IARC: International Agency for Research on Cancer
[13] ATSDR: U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry
[14] WHO EHC: World Health Organization, International Programme on Chemical Safety. Environmental Health Criteria

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/ References
Styrene	Rat oral LD50 $\geq$ 5 g/kg; inhalation LC50 [4h] = 4940 ppm	Inconsistent results in Ames Test	Inconsistent results in in-vitro chrom. ab. tests; negative in chrom. ab. and micronucleus tests in mice and rats by oral and inhalation exposure	Many studies: Effects on liver in rats [oral, inhalation] and mice [inhalation]; hearing loss in rats [inhalation]; respiratory tract in rats [inhalation]; lungs in mice [oral]	No birth defects in rats [oral, inhalation] or in mice, rabbits and hamsters [inhalation]; other effects seen only at maternally toxic doses	Negative in rat 3 gen repro study [oral]	OECD SIDS	Reviews: ATSDR – 1992; IARC[15] – 1994 Brown, 1991, 1993 [repro/devel]
Dicyclopentadiene	Rat oral LD50 ranged from 347 – 820 mg/kg; inhalation LC50[4h] ranged from 359 to 500-1000 ppm	Negative in Ames Test	Negative in in-vitro CHO and CHL chrom. ab.	Many studies: Most studies showed no effects in rats or mice in dietary or inhalation studies except male rat hydrocarbon nephropathy in inhalation studies	No effect in rats in oral [diet] studies	Effects only at maternally toxic doses in rat 3-gen repro study [in diet]	OECD SIDS	Review: ECETOC[16] – 1991 JETOC[17] Issue 3 No. 32, 1998 [CHL chrom. ab and OECD 422 studies]; NTP[18] [CHO chrom. ab.]

[15] IARC: International Agency for Research on Cancer
[16] ECETOC: European Centre for Ecotoxicology and Toxicology of Chemicals
[17] JETOC: Japanese Chemical Industry Ecology – Toxicology and Information Center
[18] NTP: National Toxicology Program – personal communication

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/ References
Naphthalene	Rat oral LD50 ranged from 2200 to 2600 mg/kg; no effect at 78 ppm [4h] inhalation	Negative in Ames Test, transformation, in-vivo UDS in rat liver	Negative in mouse micronucleus; positive in in-vitro CHO chrom. ab.	Many studies: Toxicity to blood cells in dogs [hemolytic anemia][oral]but not rats or mice; cataracts in rabbits, rats, mice, guinea pigs [oral]; local irritative effects after inhalation in rats and mice	No birth defects in rabbits, rats, and mice [oral]; reduced litter size in mice at maternally toxic doses [oral on gestation day 7-14]; no effect in rabbits exposed orally on gestation days 6-18		OECD SIDS	Reviews: ATSDR[19] – 1995; EU Risk Assessment Document – Draft 2001
Streams								
Rerun Tower Overheads [approx. 40% benzene, 13% toluene, 26% C5, 20% other] [C5-10 Fraction of Pyrolysis Gasoline HPV stream]	Rat oral LD50 > 2 g/kg; rabbit dermal LD50>2g/kg	Negative Ames Test, Drosophila (point mutation), and transformation (BALB-c/3T3 and C3H 10T½); weakly positive in mouse lymphoma and bacterial DNA repair	Negative in Drosophila chromosome loss and chromosome aberration studies	Rabbit 21-day dermal irritation: NOAEL (systemic) = 1.0 ml/kg/day (top dose); NOAEL (irritation) = <0.10 ml/kg/day	No effects in rabbits in oral teratology pilot and main studies			Robust Summaries
Dripolene [HPV stream: Pyrolysis Gasoline]	Rat oral and dermal LD50 > 2 g/kg							Robust Summary
Hydrogenated Pyrolysis Gasoline [55% benzene, 25% toluene, 10% xylene, 7% pentane, 7% ethylbenzene, 2% hexane, 3% cyclohexane] [HPV stream: Hydrotreated C6-8 Fraction]	Rat Oral LD50 = 5.17 g/kg; inhalation 4h LC50>12,408 ppm	Negative in Ames Test, in-vitro UDS; positive in transformation	Negative in micronucleus [mouse oral]	Rat 5 day inhalation: NOAEL <4869 ppm [deaths, bodyweight]				Robust Summaries

[19] ATSDR: U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry

Table 6.
Read Across Data used to Characterize the Biodegradability of the High Benzene Naphthas Category from Chemicals Contained by Products in this Category and Chemically Complex Products not in this Category, but that Contain Like-Chemicals.

CHEMICAL / PRODUCT	CARBON NUMBER	PERCENT BIODEGRADATION[a] (28 days)	REFERENCE
n-Pentane	5	87	IHSC[e]
Isopentane	5	71	IHSC[e]
Cyclohexane	6	77	IHSC[e]
Alkenes, C6 Rich	6[b]	21	HOP[f]
1-Hexene (linear)	6	67-98 [c]	[g]
Benzene	6	63	Robust Summary Provided with this test plan
Alkenes, C7-C9, C8 Rich	7-9	29	HOP[f]
p-Xylene	8	89	XIC[h]
Styrene	8	100 (14 days) [c]	[i]
Naphtha (Petroleum), light alkylate (gasoline stream)	5-8	42 [d]	API[j]
Naphtha (Petroleum), Light Catalytically Cracked (gasoline stream)	5-8	74 [d]	API[j]
Naphtha (Petroleum), Light Catalytically Reformed (gasoline stream)	5-9	96 [d]	API[j]
C8-C10 Aromatics, Predominantly C9 Alkylbenzenes	9 [b]	78	IHSC[e]
C8-C14 Aromatics, Predominantly Alkyl Naphthalenes and Naphthalene	10-12 [b]	61	IHSC[e]

a OECD 301F, manometric respirometry test
b Predominant carbon number or range
c BOD test
d Test method for determining the inherent aerobic biodegradability of oil products and modification of ISO/DIS 14593
e Covered by the International Hydrocarbon Solvents Consortium: Contained in selected SIAR (expected to be submitted at SIAM 19)
f Robust summary from the Higher Olefins Panel: C6, C7, C8, C9, and C12 Internal Olefins and C16 and C18 Alpha Olefins Category Test Plan (submitted)
g These chemicals are in the OECD SIDS program (Chemicals Inspection & Testing Institute, Japan 1992)
h Robust summary submitted with High Benzene Naphthas test plan
i Part of the Xylene ICCA Consortium and were reviewed by OECD at SIAM 16
j Robust summary from the American Petroleum Institute: Gasoline Blending Streams Test Plan (submitted)

Table 7.
Composition (Weight Percent) of Three Gasoline Streams with Biodegradation Data Used to Read Across to Products in the High Benzene Naphthas Category.

Naphtha, (Pet.) Light Alkylate		**Naphtha, (Pet.) Light Catalytically Cracked**		**Naphtha, (Pet.) Light Catalytically Reformed**	
CAS# 64741-66-8	Weight %	CAS# 64741-55-5	Weight %	CAS# 64741-55-5	Weight %
Isopentane	12.61	n-hexane	1.69	n-heptane	3.59
2,3 dimethyl butane	4.74	n-pentane	1.71	n-hexane	4.69
2,4 dimethyl pentane	4.09	isopentane	4.7	n-pentane	8.05
2,3 dimethyl pentane	2.25	2,3 dimethyl pentane	1.12	Isopentane	11.39
2,2,4 trimethyl pentane	23.92	2 methyl hexane	1.58	2,2 dimethyl butane	1.26
2,2,3 trimethyl pentane	1.76	3 methyl hexane	1.45	2,3 dimethyl butane	1.11
2,3,3 trimethyl pentane	8.99	2 methyl pentane	3.64	2,3 dimethyl pentane	1.70
2,3,4 trimethyl pentane	11.56	3 methyl pentane	2.20	2 methyl hexane	4.30
2,3,5 trimethyl hexane	1.25	methyl cyclopentane	1.87	3 methyl hexane	5.18
2,5 dimethyl hexane	4.34	methyl cyclohexane	1.19	2 methyl pentane	5.17
2,4 dimethyl hexane	3.60	1-pentene	1.25	3 methyl pentane	4.00
2,3 dimethyl hexane	2.60	2-methyl-1-butene	2.31	benzene	8.37
1methyl-1ethyl cyclopentane	9.44	2-methyl-2-butene	5.35	toluene	29.77
		trans-2-pentene	3.33		
		cis-2-pentene	1.94		
		2-methyl-1-pentene	2.31		
		cis-3-hexene	1.67		
		trans-2-hexene	1.97		
		2-methyl-2-pentene	1.83		
		1-methyl cyclopentene	1.85		
		ethylbenzene	1.47		
		m-xylene	3.05		
		p-xylene	1.34		
		o-xylene	1.83		
		benzene	1.48		
		toluene	6.73		

Table 8.
Approximate Weight Percent and Carbon Number Comparison of Hydrocarbons in High Benzene Naphthas Category and Comparable Products[a].

Substance Name	Olefins		Aromatics		Paraffins	
	% (wt.)	C #[b]	% (wt.)	C #[b]	% (wt.)	C #[b]
Products in High Benzene Naphtha Category	**1-34**	**5-9**	**>40-100**	**6-11**	**>4-75**	**5-10**
Alkenes, C6 Rich	**100**	**5-7**	**0**	**-**	**0**	**-**
Alkenes, C7-9, C8 Rich	**100**	**7-9**	**0**	**-**	**0**	**-**
C8-C10 Aromatics, Predominantly C9 Aromatics	**0**	**-**	**>97**	**8-10**	**<3**	**-**
C8-C14 Aromatics, Predominantly Alkyl Naphthalenes and Naphthalene	**0**	**-**	**>94**	**10-14**	**<6**	**-**
Naphtha (petroleum), Light Alkylate (gasoline stream)	**0**	**-**	**0**	**-**	**92**	**5-8**
Naphtha (petroleum), Light Catalytically Cracked (gasoline stream)	**24**	**5-6**	**16**	**6-8**	**21**	**5-7**
Naphtha (petroleum), Light Catalytically Reformed (gasoline stream)	**0**	**-**	**38**	**6-7**	**50**	**5-7**

a Approximate weight percent and carbon number ranges of the predominant chemical components by chemical class[olefins/aromatics/paraffins] for selected products contained by this category and for comparable products not in this category that have aquatic toxicity data that can be used as read across data for this category; % compositions may not total 100%.

b Predominant carbon number range

Table 9.
Acute Fish Toxicity Data for Selected Chemicals and Complex Products (used to Characterize the Toxicity of Products in the High Benzene Naphthas Category).

CHEMICAL / PRODUCT	CARBON NUMBER	ORGANISM	AQUATIC TOXICITY[a] (96-hr, mg/L)	REFERENCE
n-Pentane	5	*Oncorhynchus mykiss*	LC50 = 4.3	IHSC [d]
n-Hexane	6	*Pimephales promelas*	LC50 = 2.5	IHSC [d]
Benzene	6	*Oncorhynchus mykiss*	LC50 = 5.9	[e]
Alkenes, C6 Rich	5-7[b]	*Oncorhynchus mykiss*	LL50 = 12.8	HOP [f]
Mixed Cycloparaffins, C7-8, C7 Rich	7	*Oncorhynchus mykiss*	LC50 = 5.4 [c]	IHSC [d]
Toluene	7	*Pimephales promelas*	LC50 = 14.6	IHSC [d]
Alkenes, C7-9, C8 Rich	7-9 [b]	*Oncorhynchus mykiss*	LL50 = 8.9	HOP [f]
o-Xylene	8	*Pimephales promelas*	LC50 = 16.4	XIC[g]
p-Xylene	8	*Oncorhynchus mykiss*	LC50 = 2.6	XIC[g]
p-Xylene	8	*Pimephales promelas*	LC50 = 8.9	XIC[g]
Ethylbenzene	8	*Pimephales promelas*	LC50 = 12.1	[h]
Naphtha (Petroleum), Light Alkylate (gasoline stream)	5-8 [b]	*Pimephales promelas*	LL50 = 8.2	API[i]
Naphtha (petroleum), Light Catalytically Cracked (gasoline stream)	5-8 [b]	*Pimephales promelas*	LL50 = 46	API[i]
Naphtha (petroleum), Light Catalytically Reformed (gasoline stream)	5-7 [b]	*Pimephales promelas*	LL50 = 34	API[i]
1,2,4-Trimethyl-benzene	9	*Pimephales promelas*	LC50 = 7.7	IHSC [d]
C8-C10 Aromatics, Predominantly C9 Aromatics	8-10 [b]	*Oncorhynchus mykiss*	LL50 = 18.0	IHSC [d]
C8-C14 Aromatics, Predominantly alkyl Naphthalenes and Naphthalene	10-12 [b]	*Oncorhynchus mykiss*	LL50 = 3.0	IHSC [d]

a Endpoint is mortality; LC = Lethal Concentration; LL = Lethal Loading; Loading Rate; values cited as "concentration" are based on measured values
b Predominant carbon number or range
c 93-hour value
d Covered by the International Hydrocarbon Solvents Consortium: Contained in selected SIAR (expected to be submitted at SIAM 19)
e Galassi, S., M. Mingazzini, L. Viagano, D. Cesareo, and M.L. Tosato, 1988. Benzene is in the OECD SIDS program
f Robust summary from the Higher Olefins Panel HPV Test Plan (submitted)
g Xylenes are part of the Xylene ICCA Consortium and were reviewed by OECD at SIAM 16
h Ethylbenzene is in the OECD program and was reviewed as part of SIAM 15
i Robust summary from the American Petroleum Institute: Gasoline Blending Streams Test Plan (submitted)

Table 10.
Acute Invertebrate Toxicity Data for Selected Chemicals and Complex Products (used to Characterize the Toxicity of Products in the High Benzene Naphthas Category).

CHEMICAL / PRODUCT	CARBON NUMBER	ORGANISM	AQUATIC TOXICITY [a] (48-hr, mg/L)	REFERENCE
n-Pentane	5	*Daphnia magna*	EC50 = 2.7	IHSC [e]
n-Hexane	6	*Daphnia magna*	EC50 = 2.1	IHSC [e]
Cyclohexane	6	*Daphnia magna*	EC50 = 0.9	IHSC [e]
Benzene	6	*Daphnia magna*	EC50 = 18 [b]	[f]
o-Xylene	8	*Daphnia magna*	EC50 = 1.0	XIC [g]
m-Xylene	8	*Daphnia magna*	EC50 = 4.7	XIC [g]
Naphtha (Petroleum), Light Catalytically Reformed (gasoline stream)	5-7 [c]	*Daphnia magna*	EL50 = 10	API [h]
Naphtha (Petroleum), Light Alkylate (gasoline stream)	5-8 [c]	*Daphnia magna*	EL50 = 32	API [h]
Naphtha (Petroleum), Light Catalytically Cracked (gasoline stream)	5-8 [c]	*Daphnia magna*	EL50 = 18	API [h]
C8-C10 Aromatics, Predominantly C9 Aromatics	8-10 [c]	*Daphnia magna*	EL50 = 21.3	IHSC [e]
Naphthalene	10	*Daphnia magna*	EL50 = 16.7 [d]	[i]
C8-C14 Aromatics, Predominantly Alkyl Naphthalenes and Naphthalene	10-12 [c]	*Daphnia magna*	EL50 = 3.0	IHSC [e]

a Endpoint is immobility; EC = Effect Concentration; EL = Effect Loading; Loading Rate; values cited as "concentration" are based on measured values
b 24-hour study
c Predominant carbon number or range
d Based on nominal values
e Covered by the International Hydrocarbon Solvents Consortium: Contained in selected SIAR (expected to be submitted at SIAM 19)
f Galassi, S., M. Mingazzini, L. Viagano, D. Cesareo, and M.L. Tosato, 1988. Benzene is in the OECD SIDS program
g Xylenes are part of the Xylene ICCA Consortium and were reviewed by OECD at SIAM 16
h Robust summary from the American Petroleum Institute: Gasoline Blending Streams Test Plan (submitted)
i Naphthalene is part of the OECD program and was reviewed in SIAM 13

Table 11.
Alga Toxicity Data for Selected Chemicals and Complex Products
(Used to Characterize the Toxicity of Products in the High Benzene Naphthas Category).

CHEMICAL / PRODUCT	CARBON NUMBER	ORGANISM	AQUATIC TOXICITY [a] (72-hr, mg/L)	REFERENCE
n-Pentane	5	*Pseudokirchneriella subcapitata* [b]	EbC50 = 10.7 ErC50 = 7.5 NOECb = 1.3 NOECr = 2.0	IHSC [d]
Benzene	6	*Pseudokirchneriella subcapitata*	EbL50 = 29	[e]
Naphtha (Petroleum), Light Catalytically reformed (gasoline stream)	5-7 [c]	*Pseudokirchneriella subcapitata*	EbL50 = 8.5 NOELRb = 5.0	API [f]
Naphtha (Petroleum), Light alkylate (gasoline stream)	5-8 [c]	*Pseudokirchneriella subcapitata*	EbL50 = 45 NOELRb = 18	API [f]
Naphtha (Petroleum), Light Catalytically Cracked (gasoline stream)	5-8 [c]	*Pseudokirchneriella subcapitata*	EbL50 = 64 NOELRb = 51	API [f]
C8-C10 Aromatics, Predominantly C9 Aromatics	8-10 [c]	*Pseudokirchneriella subcapitata*	EbL50 = 2.6 ErL50 = 2.9 NOELRb = 1.0 NOELRr = 1.0	IHS [d]
C8-C14 Aromatics, Predominantly Alkyl Naphthalenes and Naphthalene	10-12 [c]	*Pseudokirchneriella subcapitata*	EbL50 = 1-3 ErL50 = 1-3 NOELRb = 1.0 NOELRr = 1.0	IHS [d]

a Endpoint is growth inhibition; EbC = Effect Concentration for biomass; ErC = Effect Concentration for growth rate; EbL = Effect Loading for biomass; ErL = Effect Loading for growth rate; NOECb = No Observed Effect Concentration for biomass; NOECr = No Observed Effect Concentration for growth rate; NOELRb = No Observed Effect Loading Rate for biomass; NOELRr = No Observed Effect Loading Rate for growth rate; values cited as "concentration" are based on measured values

b Formerly known as *Selenastrum capricornutum*

c Predominant carbon number or range

d Covered by the International Hydrocarbon Solvents Consortium: Contained in selected SIAR (expected to be submitted at SIAM 19)

e Galassi, S., M. Mingazzini, L. Viagano, D. Cesareo, and M.L. Tosato, 1988. Benzene is in the OECD SIDS Program

f Robust summary from the American Petroleum Institute: Gasoline Blending Streams Test Plan (submitted)

Table 12. Assessment Plan for High Benzene Naphthas Category Under the Program. (Robust summaries for existing studies are submitted separately.)

Stream Description	Human Health Effects						Ecotoxicity			**Physical Chem.[1]**	Environmental Fate			
	Acute Toxicity	**Genetic Point Mut.**	**Genetic Chrom.**	**Sub-chronic**	**Develop-mental**	**Reproduc-tion**	**Acute Fish**	**Acute Invert.**	**Algal Toxicity**		**Photo-deg.**	**Hydro-lysis**	**Fugacity**	**Biodeg.**
Pyrolysis Gasoline [15-67% benzene]	A	A	ACD	ACD	A	ACD	ACD	ACD	ACD	CM	CM/TD	TD	CM	ACD
Pyrolysis C6 Fraction [35-77% benzene]	ACD	ACD	ACD	ACD	ACD	ACD	ACD	ACD	ACD	CM	CM/TD	TD	CM	ACD
Pyrolysis C6-C8 Fraction [30-80% benzene]	ACD	ACD	ACD	ACD	ACD	ACD	ACD	ACD	ACD	CM	CM/TD	TD	CM	ACD
Pyrolysis C5-6 Fraction [70% benzene]	ACD	ACD	ACD	ACD	ACD	ACD	ACD	ACD	ACD	CM	CM/TD	TD	CM	ACD
Hydrotreated C6 Fraction [75-76% benzene]	ACD	ACD	ACD	ACD	ACD	ACD	ACD	ACD	ACD	CM	CM/TD	TD	CM	ACD
Hydrotreated C6-C7 Fraction [40-69% benzene]	ACD	ACD	ACD	ACD	ACD	ACD	ACD	ACD	ACD	CM	CM/TD	TD	CM	ACD
Hydrotreated C6-C8 Fraction [40-60% benzene]	A	A	A	ACD	ACD	ACD	ACD	ACD	ACD	CM	CM/TD	TD	CM	ACD
Quench Loop Pyrolysis Oil [10-22% benzene]	ACD	ACD	ACD	ACD	ACD	ACD	ACD	ACD	ACD	CM	CM/TD	TD	CM	ACD
Recovered Oil from Waste Water Treatment [NDA]	ACD	ACD	ACD	ACD	ACD	ACD	ACD	ACD	ACD	CM	CM/TD	TD	CM	ACD
Extract from Benzene Extraction [60-75% benzene]	ACD	ACD	ACD	ACD	ACD	ACD	ACD	ACD	ACD	CM	CM/TD	TD	CM	ACD
Benzene [OECD SIDS; not member of category]	A	A	A	A	A	A	A	A	A	CM	CM/TD	TD	CM	A

1 Measured data for selected physicochemical endpoints will be identified in conjunction with calculated data to characterize this category.

A Adequate existing data available

ACD Adequate existing component data for read across (see Sec. III.A.)

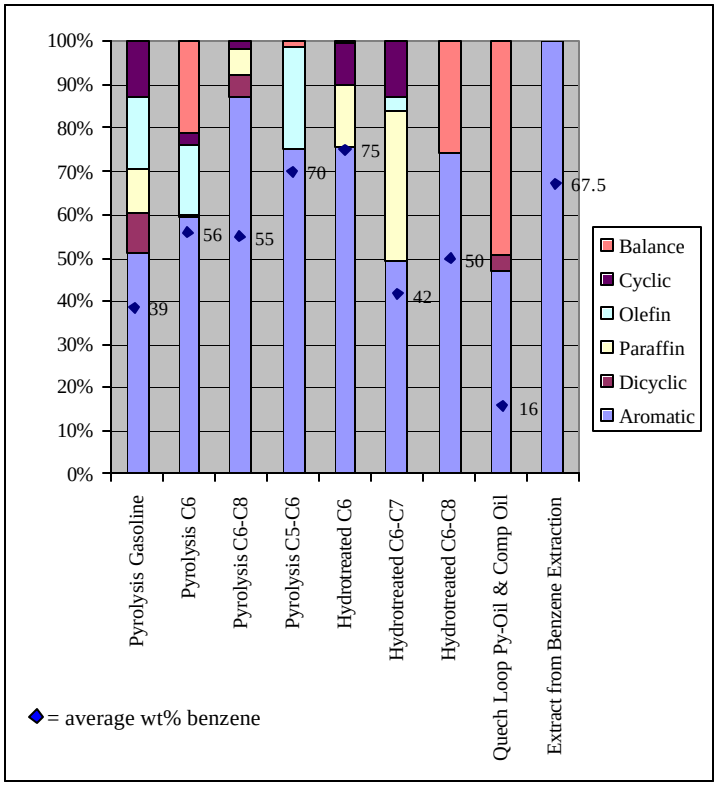
TD Technical Discussion proposed

CM Computer Modeling proposed

Table 13.
American Chemistry Council Olefins Panel Sponsored HPV Test Categories

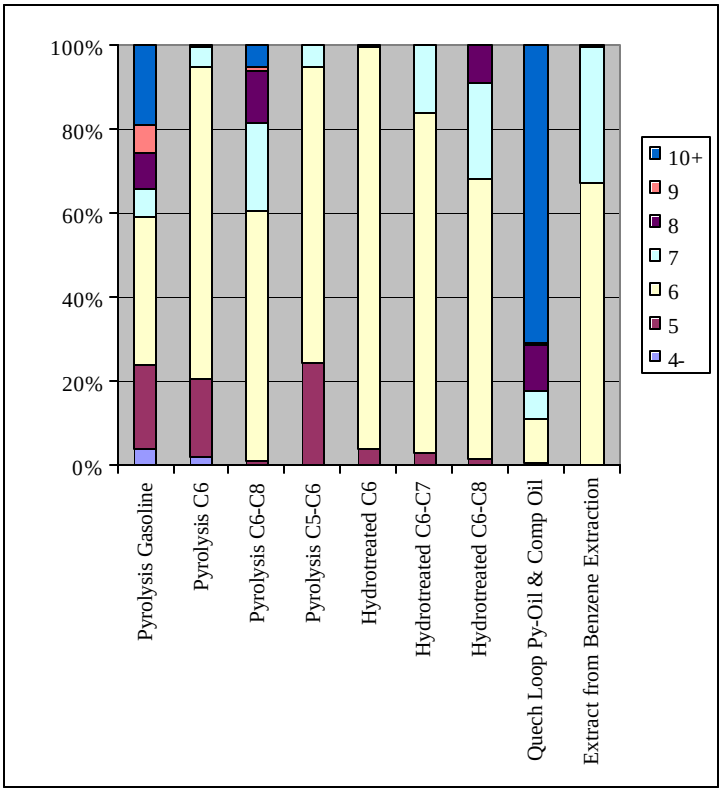
Category Number	Category Description
1	Crude Butadiene C4
2	Low Butadiene C4
3	C5 Non-Cyclics
4	Propylene Streams (C3) - Propylene sponsored through ICCA
5	High Benzene Naphthas
6	Low Benzene Naphthas
7, 8, 9	Resin Oils and Cyclodiene Dimer Concentrates
10	Fuel Oils

Figure 1
Stream Compositions
High Benzene Naphthas Category



Compositions are averages of the ranges reported for the complex, variable composition streams. In some cases, because of overlaps and variations in the way components were sometimes grouped in individual reports, the sum of the averages for the streams exceeded 100%. In those cases, compositions were normalized for plotting in Figure 1. When the total of the average of reported values was less than 100%, a "Balance" was added and included. Average wt% benzene content (actual average of reported values) of the streams is shown as diamonds with the average wt% given. Components grouped as "cyclic" include both paraffin and olefin cyclic hydrocarbons. The term "olefin" as used here does not include the cyclic olefins.

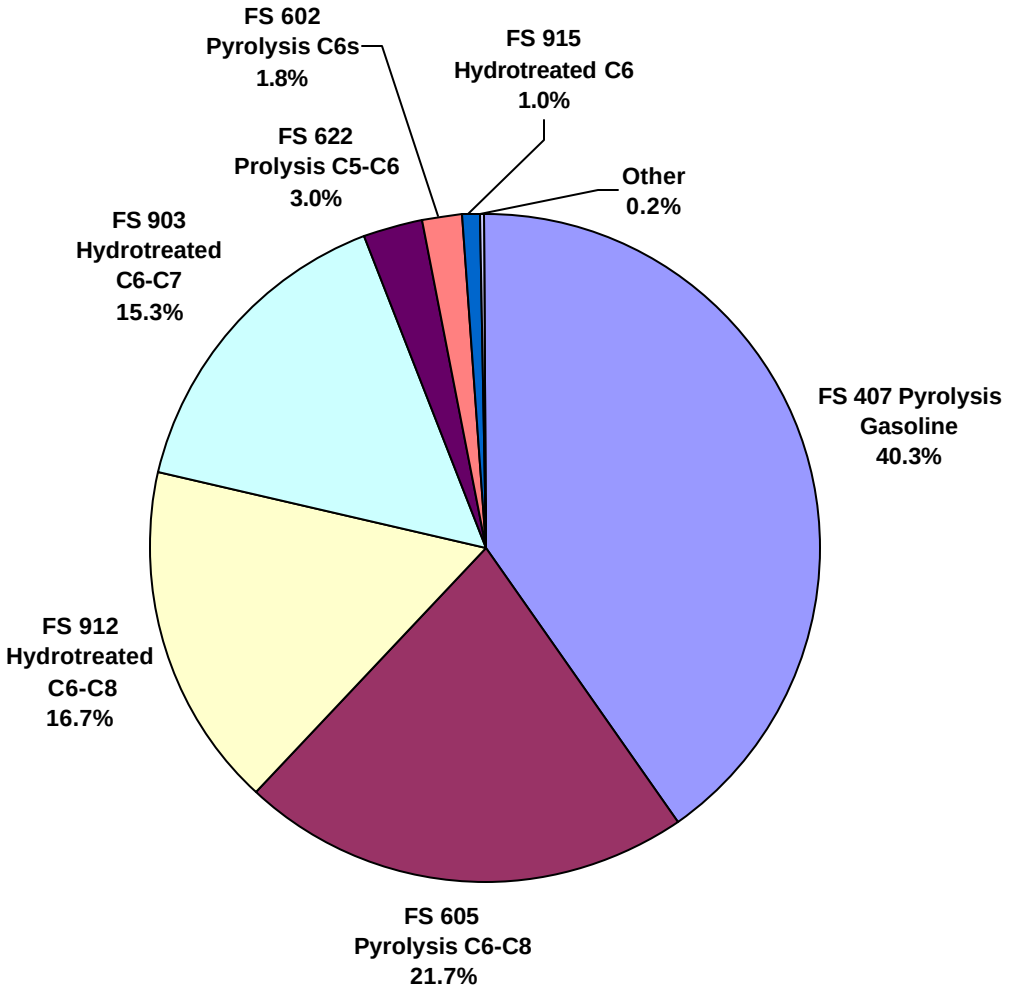
Figure 2
Stream Carbon Range Content
High Benzene Naphthas Category



Carbon range contents were normalized. Any apparent inconsistencies may exist between Figure 1 and Figure 2 are largely due to normalization of the data.

Figure 3

Production Volumes
High Benzene Naphthas Category



Pyrolysis Gasoline is the primary stream in the category, and all of the other category streams, except Quench Loop Pyoil and Recovered Oil from Wastewater Treatment, are derived from this stream. These two exceptions are relatively low-volume streams that are isolated in the Ethylene Process Unit, and together with the Extract from Benzene Extraction make up the 0.2% "Other" portion of the category production shown below. The category consists of the benzene-containing streams of the Olefins Industry

Appendix I

ETHYLENE PROCESS DESCRIPTION

A. The Ethylene Process

1. Steam Cracking

Steam cracking is the predominant process used to produce ethylene. Various hydrocarbon feedstocks are used in the production of ethylene by steam cracking, including ethane, propane, butane, and liquid petroleum fractions such as condensate, naphtha, and gas oils. The feedstocks are normally saturated hydrocarbons but may contain minor amounts of unsaturates. These feedstocks are charged to the coils of a cracking furnace. Heat is transferred through the metal walls of the coils to the feedstock from hot flue gas, which is generated by combustion of fuels in the furnace firebox. The outlet of the cracking coil is usually maintained at relatively low pressure in order to obtain good yields to the desired products. Steam is also added to the coil and serves as a diluent to improve yields and to control coke formation. This step of the ethylene process is commonly referred to as "steam cracking" or simply "cracking" and the furnaces are frequently referred to as "crackers."

Subjecting the feedstocks to high temperatures results in the partial conversion of the feedstock to olefins. In the simplest example, feedstock ethane is partially converted to ethylene and hydrogen. Similarly, propane, butane, or the liquid feedstocks are also converted to ethylene. While the predominant products produced are ethylene and propylene, a wide range of additional products are also formed. These products range from methane (C1) through fuel oil (C12 and higher) and include other olefins, diolefins, aromatics and saturates (naphthenes and paraffins).

2. Refinery Gas Separation

Ethylene and propylene are also produced by separation of these olefins from refinery gas streams, such as from the light ends product of a catalytic cracking process or from coker offgas. This separation is similar to that used in steam crackers, and in some cases both refinery gas streams and steam cracking furnace effluents are combined and processed in a single finishing section. These refinery gas streams differ from cracked gas in that the refinery streams have a much narrower carbon number distribution, predominantly C2 and/or C3. Thus the finishing of these refinery gas streams yields primarily ethylene and ethane, and/or propylene and propane.

B. Products of the Ethylene Process

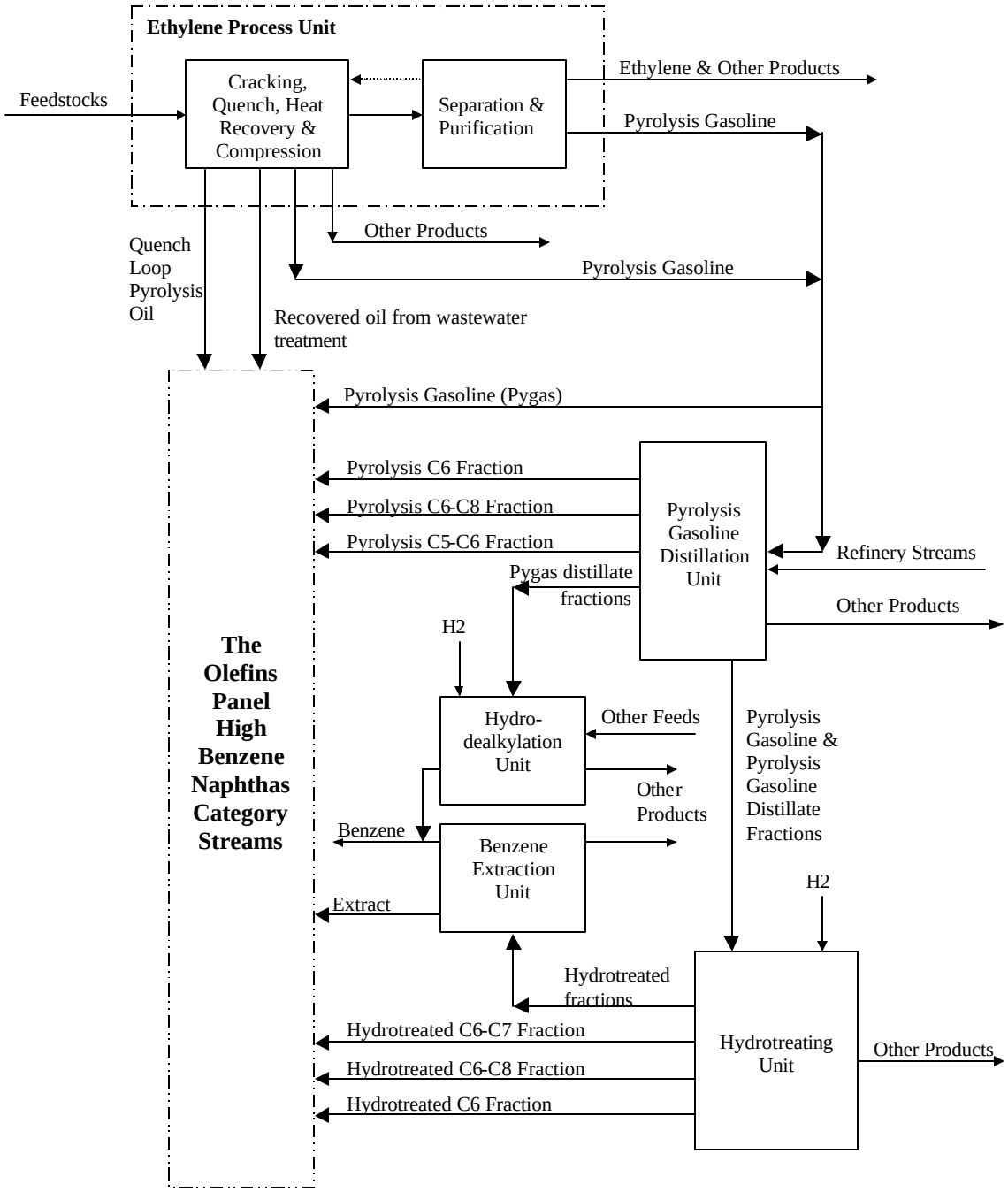
The intermediate stream that exits the cracking furnaces (i.e., the furnace effluent) is forwarded to the finishing section of the ethylene plant. The furnace effluent is commonly referred to as "cracked gas" and consists of a mixture of hydrogen, methane, and various hydrocarbon compounds with two

or more carbon atoms per molecule (C2+). The relative amount of each component in the cracked gas varies depending on what feedstocks are cracked and cracking process variables. Cracked gas may also contain relatively small concentrations of organic sulfur compounds that were present as impurities in the feedstock or were added to the feedstock to control coke formation. The cracked gas stream is cooled, compressed and then separated into the individual streams of the ethylene process. These streams can be sold commercially and/or put into further steps of the process to produce additional materials. In some ethylene processes, a liquid fuel oil product is produced when the cracked gas is initially cooled. The ethylene process is a closed process and the products are contained in pressure systems.

The final products of the ethylene process include hydrogen, methane (frequently used as fuel), and the high purity products ethylene and propylene. Other products of the ethylene process are typically mixed streams that are isolated by distillation according to boiling point ranges. It is a subset of these mixed streams that make up the constituents of the High Benzene Naphthas Category.

The chemical process operations that are associated with the process streams in the High Benzene Naphthas Category are shown in Figure 1.

Figure 1.
Chemical Processing Operations Associated with Process Streams in the High Benzene Naphthas Category



CAS No.: 71-43-2
Robust Summary No.: OP E-002

RECEIVED
OPPT CBIC

2003 AUG 12 PM 1:23

Biodegradation

Test Substance:	CAS No. 71-43-2; Benzene
Method/Guideline:	OECD 301F
Year (guideline):	1993
Type (test type):	Ready Biodegradability, Manometric Respirometry Test
GLP:	Yes
Year (study performed):	2000
Inoculum:	Domestic activated sludge
Exposure Period:	28 days

Test Conditions: (FT - TC)

- **Note: Concentration prep., vessel type, replication, test conditions.**

Activated sludge and test medium were combined prior to test material addition. Test medium consisted of glass distilled water and mineral salts (Phosphate buffer, Ferric chloride, Magnesium sulfate, Calcium chloride, EDTA).
Test vessels were 500 mL dark glass bottles placed on a magnetic stirrer and electronically monitored for oxygen consumption.
Test material and blanks were tested in triplicate, controls were tested in duplicate.
Test material (benzene) concentration was 17mg/L. Sodium benzoate (positive control) concentration was 30mg/L. Toxicity control with benzene and Na Benzoate concentrations at 17 and 30 mg/L, respectively.
Test temperature was 22 +/- 2 Deg C.
All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.

Results: (FT - RS)

Units/Value:

- **Note: Deviations from protocol or guideline, analytical method.**

Test material was readily biodegradable. Half-life was <2 weeks.
By day 28, 63.0% degradation of the test material was observed.
10% biodegradation was achieved in less than 5 days, 50% biodegradation on approximately day 5.
By day 5, >60% biodegradation of positive control was observed, which meets the guideline requirement. No excursions from the protocol were noted.
Biodegradation was based on oxygen consumption and the theoretical oxygen demand of the test material as calculated using results of an elemental analysis of the test material.

Sample	% Degradation* (day 28)	Mean % Degradation (day 28)
Benzene	54, 72, 63	63
Na Benzoate	65, 75	70
Toxicity Control	59, 65	62

* replicate data

Conclusion: (FT - CL)

CAS No.: 71-43-2
Robust Summary No.: OP E-002

Biodegradation

Reliability: (FT - RL)	(1) Reliable without restriction
Reference: (FT - RE)	Brixham Environmental Laboratory. 2001. OECD 301F, Ready biodegradability: Manometric respirometry. Study # AH0378/A.
Other (source): (FT - SO)	Olefins Panel, American Chemistry Council

* IUCLID field abbreviations include:
FT - Freetext
TC - Test Conditions
RS - Results
CL - Conclusion
RL - Reliability
RE - Reference
SO - Source

Robust Summary - Group 5: High Benzene Naphthas

Acute Toxicity

Test Substance	Dripolene. Yellow, homogeneous liquid, stable for 5 years at ambient temperature. (CRU #93329). Olefins Panel HVP Stream: Pyrolysis Gasoline. Typical composition ranges for Pyrolysis Gasoline are shown in Table 2 of the Test Plan.
Method	
Method/guideline followed	Not specified
Type (test type)	Acute, limit test
GLP	Yes
Year	1994
Species/Strain	Rat, Sprague-Dawley
Sex	Males and females
No. of animals per sex per dose	5
Vehicle	None
Route of administration	Oral gavage
Test Conditions	Sprague Dawley rats (180-350g) were individually housed in stainless steel suspended cages and fasted overnight prior to administration of 2g/kg neat dripolene. The study room was maintained at 68-72^{0}F with a relative humidity of 35-63% and a 12 hr light-dark cycle. Water and chow diet were available ad lib after dosing. Test article was administered once on day 1 by oral gavage through a blunted needle. Rats were observed for clinical signs approx. 30 min, 1hr, and 4hr, after dosing, and daily thereafter until sacrifice on day 15. Rats were checked once a day for mortality and moribundity. Observations were not made on weekends. Body wts were recorded prior to fasting and on days 1, 8 and 15.
Results	
LD_{50} with confidence limits.	The LD_{50} was not reached at 2g/kg. There were no deaths and all rats gained some weight during the study. Clinical signs noted in one or more rats were salivation, decreased activity, rales, lacrimation, chromodacryorrhea, ataxia, head shaking, chromorhinorrhea, miosis, slight tremors, mydriasis, hyperactivity, hypothermia, urogenital discharge, nasal discharge, decreased food consumption, decreased fecal output, vocalization, and decreased stool size. No gross pathological findings were noted at necropsy.
Remarks	
Conclusions (study author)	The LD_{50} was not reached at 2g/kg.
Data Quality Reliability	**1.** Reliable without restriction.
References	Rodriguez, S.C. and Dalbey, W.E. 1994. Acute oral toxicity of dripolene in Sprague Dawley Rats. Study #65642. Stonybrook Laboratories, Princeton, NJ. for Mobil Chemical Co., Edison, NJ.
Other *Last changed*	10/23/2001 (Prepared by a contractor to the Olefins Panel)

Robust Summary - Group 5: High Benzene Naphthas

Acute Toxicity

Test Substance	Dripolene. Yellow, homogeneous liquid, stable for 5 years at ambient temperature. (CRU #93329). Olefins Panel HVP Stream: Pyrolysis Gasoline. Typical composition ranges for Pyrolysis Gasoline are shown in Table 2 of the Test Plan.
Method	
Method/guideline followed	Not specified
Type (test type)	Acute, limit test
GLP	Yes
Year	1994
Species/Strain	Rabbit, New Zealand White
Sex	Males and females
No. of animals per sex per dose	3
Vehicle	None
Route of administration	dermal
Test Conditions	Rabbits, weighing at least 2kg, were individually housed in stainless steel suspended cages in a study room maintained at 69-72^{0}F with a relative humidity of 40-85% and a 12 hr light-dark cycle. Water and chow diet were available ad lib. The dorsal skin surface extending down from the front to rear legs and from left to right lower flanks was clipped free of hair the day prior to test article administration. Test article was spread evenly over the clipped area (approx. 10% of body surface area) at a dose of 2g/kg. A layer of 8-ply gauze was placed on the dorsal site, and a rubber dam sleeve was fitted snugly over the gauze pad and around the trunk. Edges of the dam were taped in place. An Elizabethan collar was affixed to the neck to prevent oral ingestion of test article and mechanical irritation of the test site. After 24 hrs, the collar and wrappings were removed and residual test article was wiped off. Body wts were recorded on days 1, 8 and 15. Rabbits were observed for toxicity at about 1 and 2 hr post-dose and daily thereafter on weekdays, through day 14. Observations for mortality/moribundity were made daily. Rabbits were sacrificed on day 15 and necropsies were performed.
Results	
LD_{50} with confidence limits.	The LD_{50} was not reached at 2g/kg. There were no deaths during the study and rabbits either gained some weight or remained at day 1 body wt. Signs that might have resulted from treatment in one or more rabbits were: decreased fecal output, decreased fecal pellet size, soft stool, and decreased food consumption. No gross pathological findings were noted at necropsy.
Remarks	
Conclusions	
(study author)	The LD_{50} was not reached at 2g/kg.
Data Quality	
Reliability	**1.** Reliable without restriction.
References	Rodriguez, S.C. and Dalbey, W.E. 1994. Dermal toxicity of dripolene in the New Zealand White rabbit. Study #65643. Stonybrook Laboratories, Princeton, NJ. for Mobil Chemical Co., Edison, NJ.
Other	
Last changed	10/23/2001 (Prepared by a contractor to the Olefins Panel)

Robust Summary - Group 5: High Benzene Naphthas

Acute Toxicity

Test Substance	Hydrogenated Pyrolysis Gasoline CAS# 68410-97-9. Clear liquid, aromatic odor. Olefins Panel HVP Stream: Hydrotreated C6-C8.
Method	
Method/guideline followed	Standard method (not referenced) with doses based on a limit test and range-finding study
Type (test type)	Acute LD50
GLP	Yes
Year	1984
Species/Strain	Rat, Fischer 344
Sex	Males and females
No. of animals per sex per dose	5
Vehicle	None
Route of administration	Oral
Test Conditions	Rats (99.9-134.0 g; 57 days old) were individually housed in screen-bottomed cages in a room with 70.6^{0}F temperature, relative humidity of 59% and a 12 hr light/dark cycle. Chow diet and tap water from an automatic watering system were available ad lib. Rats were fasted for 24 hours prior to dosing at 4.2, 4.6, 5.0, and 5.4g/kg and observed at 1 and 4 hrs after dosing on day 1, and daily thereafter, over 14 days for clinical signs, morbidity and mortality. Gross necropsies were performed on all rats. LD50 was calculated by Probit analysis.
Results	
LD_{50} with confidence limits.	LD50 = 5.17g/kg (95% confidence limits: 5.02-5.45g/kg)
Remarks	On day 1, males and females showed dose responsive increases in ataxia, harsh respiratory sounds, and a non-dose responsive increase in red ocular discharge. Soft feces were observed in treated males and females on day 2. Frequency of clinical signs decreased by day 3 and signs were absent by day 5. There were no changes in body weight gain among the groups. Male and female mortalities were combined to calculate an LD50. Mortality from a previously performed limit test, conducted at 5.0g/kg was combined with results from the 5.0g/kg dose in this definitive study, raising that group number to 20. Mortalities were: 0/10 at 4.2, and 4.6g/kg, 7/20 at 5.0g/kg, 7/10 at 5.4g/kg. Gross necropsies revealed red lungs, gas-filled stomach and intestine, mottled liver, discoloration of kidney, and opaque eyes in rats that died during the study. These observations, with the exception of opacity in the left eye of one 5.4g/kg female, were absent in rats sacrificed at study termination (day 15).
Conclusions (study author)	The acute median lethal dose (LD50) for Hydrogenated Pyrolysis Gasoline in male and female rats was 5.17g/kg. A descriptive classification of Practically Non-toxic for acute oral exposure was assigned.
Data Quality	
Reliability	**1.** Reliable without restrictions.
References	Rausina, G.A. 1984. Acute oral toxicity study in rats of hydrogenated pyrolysis gasoline. Proj. #2091. Gulf Life Sciences Center, Pittsburgh, PA
Other	
Last change	5/7/2001 (Prepared by a contractor to the Olefins Panel)

Robust Summary - Group 5: High Benzene Naphthas

Acute Toxicity

Test Substance	Hydrogenated Pyrolysis Gasoline CAS# 68410-97-9. Clear liquid, aromatic odor. Olefins Panel HVP Stream: Hydrotreated C6-C8.
Method	
Method/guideline followed	Standard method (not referenced)
Type (test type)	Acute LC50
GLP	Yes
Year	1984
Species/Strain	Rat, Fischer 344
Sex	Males and females
No. of animals per sex /dose	5
Vehicle	Filtered air
Route of administration	Inhalation
Test Conditions	Rats (8 wks. old, 100-172g at initiation) were individually housed in stainless steel, screen-bottomed cages in a room maintained at 73.0^0F (75.5^0F during exposure) temperature, relative humidity of 51% (40% during exposure) and a 12 hr light/dark cycle. Rats received chow diet and tap water ad lib, except during exposure. One group of 10 rats was exposed to aerosolized test article generated by a ball jet nebulizer for 4 hrs. A condensing flask was used to prevent large particles from entering the chamber. Actual average chamber concentration was 12,408ppm (range 8,642-17,371ppm) determined by gas chromatography. Particulate phase was negligible. Rats were observed for clinical signs at 1 and 4 hrs after dosing on day 1 and daily thereafter over 14 days, and for morbidity and mortality twice daily on weekdays, once daily on weekends. Body wt. was determined at initiation and on days 8 and 15. Gross necropsies were performed on all rats at termination on day 15.
Results	
LC_{50} with confidence limits.	LC50>12,408ppm
Remarks	There were no deaths during the study, no effects on body wt gain, and no gross alterations were seen at necropsy. Immediately after exposure, all rats exhibited lethargy, increased and labored respiration, and ocular discharge; most animals showed twitching and dry red material around nose/mouth. There were a few instances of harsh respiratory sounds, trembling, and perianal soiling. These clinical signs decreased in frequency by 4 hr post-exposure and disappeared by day 2.
Conclusions (study author)	No deaths occurred at the dose of 12,408ppm of test article, indicating a descriptive classification of Practically Non-toxic for acute inhalation exposure. Clinical signs noted immediately after exposure (increased/labored respiration, twitching, trembling, lethargy, ocular discharge) were not observed by day 2 and thereafter.
Data Quality Reliability	**1.** Reliable without restrictions.
References	Rausina, G.A. 1984. Acute inhalation toxicity study in rats of hydrogenated pyrolysis gasoline. Proj. #2092. Gulf Life Sciences Center, Pittsburgh, PA
Other	
Last change	Revised 7/27/2001 (Prepared by a contractor to the Olefins Panel)

Robust Summary - Group 5: High Benzene Naphthas

Genetic Toxicity - in Vitro

Test Substance	
Test substance	Hydrogenated Pyrolysis Gasoline, CAS #68410-97-9. clear liquid with aromatic odor, negligible solubility in water, contains <55.0% benzene, <25% toluene, <10% dimethyl benzene/xylene, <7% pentane, <7% ethylbenzene, <3% cyclohexane, <2% hexane. Olefins Panel HVP Stream: Hydrotreated C6-C8.
Method	
Method/guideline followed	Standard method per Ames et al
Type	Reverse mutation bacterial assay
System of testing	Salmonella typhimurium, Escherichia coli with and without metabolic activation
GLP	Yes
Year	1991
Species/Strain	S. typh. TA1535, TA1537, TA98, TA100; E. coli WP2(uvrA)
Metabolic activation	Yes
Species and cell type	Male Sprague Dawley rat liver (S9 fraction), Molecular Toxicology, Inc., Annapolis, MD
Quantity	20% S9 fraction in 0.5ml S9 mix/plate
Induced or not induced	Aroclor 1254induced, rats given a single 500mg/kg ip dose
Concentrations tested	0, 33, 100, 333, 1000, 3333, 10,000µg/plate ± S9. All diluted in acetone (200mg/ml)
Statistical Methods	None specified. Test article considered mutagenic when it induces a reproductive, dose-related increase in number of revertants in one or more strains at 3 consecutive dose levels. A non-mutagen does not induce a dose-related increase in at least 2 independent tests.
Remarks for Test Conditions	Hydrogenated pyrolysis gasoline (HPG) was prepared in acetone immediately prior to use. At end of the study, an aliquot of the stock dilution was sent to PTRL West, Richmond, CA to confirm concentration. Salmonella (approx. 10^8cells/ml) were exposed to either test material or acetone in 3 plates/dose ± S9 by the plate incorporation method. Six dose levels from 33-10,000µg/plate were employed in both the range-finding trial using TA100 and the mutagenicity test with all strains of Salmonella and E. coli. Optimum level of S9 for the mutagenicity assay was determined by testing the highest non-toxic dose, 10,000µg per plate with metabolic activation systems containing 4, 20 or 80% S9 fraction. No noteworthy increases in revertants or cytotoxicity was observed at any S9 concentration; 20% S9 was used in the mutagenicity test. All plates were incubated at 37^0C for 48 hrs then revertant colonies were counted. Positive control compounds were: cultures-S9, sodium azide (5µg/plate) for TA1535, TA100; 9-aminoacridine (50µg/plate) for TA1537; 2-nitrofluorene (5µg/plate) for TA98; N-ethyl-N'-Nitro-N-Nitrosoguanidene (5ug/plate) for E. coli WP2, and cultures+S9, 2-anthramine (4µg/plate) for TA1535, TA1537, (2µg/plate) for TA98, TA100, and (20µg/plate) for E. coli WP2. Two independent assays were performed.
Results	
Genotoxic effects	HPG did not induce increases in number of revertant colonies and no toxicity was observed in any Salmonella strain or E. coli WP2 with or without 20% S9 metabolic activation in both studies. Positive control compounds performed appropriately.
Conclusions	
(contractor)	Hydrogenated pyrolysis gasoline is not mutagenic to bacteria under conditions of this assay.
Data Quality	
Reliabilities	**1**. Reliable without restriction
Reference	Riccio, E.S. and Stewart, K.R. 1991. Salmonella-Escherichia coli/microsome plate incorporation assay of Hydrogenated Pyrolysis Gasoline. SRI Study #2545-A03-91, Sponsor study #91-66. SRI International, Menlo Park, CA for Chevron Environmental Health Center, Richmond, CA
Other	
Last changed	5/7/2001 (Prepared by a contractor to the Olefins Panel)

Robust Summary - Group 5: High Benzene Naphthas

Genetic Toxicity - in Vitro

Test Substance	Hydrogenated Pyrolysis Gasoline, CAS #68410-97-9. clear liquid with aromatic odor.
Test substance	Composition, purity and stability referred to sponsor. Olefins Panel HVP Stream: Hydrotreated C6-C8.
Method	
Method/guideline followed	Standard method based on Cortesi et al (1983), Dunkel et al (1981), Reznikoff et al (1973)
Type	In vitro cell transformation
System of testing	Mouse embryo cells
GLP	Yes
Year	1984
Species/Strain	BALB/3T3-A31-1-1 from T. Kakunaga, National Cancer Inst., 1983
Metabolic activation	No
Species and cell type	NA
Quantity	NA
Induced or not induced	NA
Concentrations tested	Cytotoxicity: 8, 16, 32, 64, 128, 256, 512, 1024, 2048, and 5000µg/ml; Transformation: 100, 250, 500, 1500µg/ml, all diluted in 10% Pluronic® polyol F68 (prepared in deionized water, mol. wt. 8350, 80% hydrophilic).
Exposure period	2 days
Statistical Methods	None employed. Criteria for positive response were a two-fold increase in type III foci at the highest dose over vehicle control (at least 2 type III foci if vehicle control had none) with or without a dose related response, or a two-fold increase at two or more consecutive doses. Test is equivocal if two-fold increase occurred at any one level other than the highest acceptable dose.
Remarks for Test Conditions	Sufficient Hydrogenated Pyrolysis Gasoline (HPG) was weighed separately for each dose level, 0.40ml of 10% F68 added per ml of final volume and medium (Eagles MEM with 10% heat-inactivated fetal calf serum) added as required to achieve final volume for testing. Test preparations were mixed just prior to addition to cultures at 50µl to each 5 ml culture. All cultures were incubated at 37^0C in 5% CO_2 enriched humidified atmosphere. For cytotoxicity, 2 cultures/dose group, 2 cultures for vehicle F68 or medium negative control were seeded with $1x10^4$ cells/plate in day 1, exposed on days 2-3, trypsinized and counted with a Coulter Model ZB on day 4 for at least 20% survival. For transformation, 15 cultures ($1x10^4$ cells/flask/dose group)) and two colony-forming cultures (100 cells/plate/dose group) were seeded on day 1, exposed on days 2-3 and culture medium changed on day 4. For transformation cultures, medium continued to be changed weekly to day 29. Positive control was 3-methylcholanthrene (1µg/ml). Colony forming cultures were fixed, stained, and counted visually on day 10 to determine cloning efficiency (avg. number colonies/plate ÷ 100 cells seeded). Transformation cultures were fixed and stained on day 29 for focus counting and evaluation. Transformation frequency = total type III foci ÷ total flasks/dose group.
Results	
Genotoxic effects	HPG induced toxicity in BALB/3T3 cells after two days exposure beginning at 128 µg/ml (45.4% relative survival) with relative survivals of 26.7, 25.6, 3.2 and 0% at 512, 1024, 2048 and 5000µg/ml, respectively. In the transformation assay, toxicity was seen at all dose levels (relative cloning efficiencies of 53.7, 67.8, 78.5 and 0% at 100, 250, 500 and 1500µg/ml). At 1500µg/ml, the highest dose level, HPG induced 5 Type III foci; no other dose levels produced a positive response. Transformation frequencies were 0.13, 0, 0, 0.07 and 0.36 for medium control, vehicle control, 100, 250, 500 and 1500µg/ml, respectively. Positive and negative controls gave appropriate responses.
Conclusions	
(contractor)	Hydrogenated Pyrolysis Gasoline induced transformation in BALB/3T3 cells under conditions of this assay. Cytotoxicity and impairment of cloning efficiency were also observed. The positive response was observed only at the highest dose level, a level that appeared to be too toxic for cells to recover and form colonies (0% relative colony forming efficiency)

Data Quality	
Reliabilities	**1.** Reliable without restriction
Reference	Brecher, S. 1984. Transformation test of Hydrogenated Pyrolysis Gasoline. Proj. #2098. Gulf Life Sciences Center, Pittsburgh, PA for Gulf Oil Chemicals Co, Houston, TX Cortesi, E. et al. 1983. Teratogenesis, Carcinogenesis, Mutagenesis 3: 101-110. Dunkel, V.A. et al. 1981. J. Nat'l Cancer Inst. 67: 1303-1315. Reznikoff, C.A. et al. 1973. Cancer Res. 3239-3249.
Other	
Last changed	Revised 8/27/2001 (Prepared by a contractor to the Olefins Panel).

Robust Summary - Group 5: High Benzene Naphthas

Genetic Toxicity - in Vitro

Test Substance	Hydrogenated Pyrolysis Gasoline, CAS #68410-97-9. clear liquid with aromatic odor.
Test substance	Composition, purity and stability referred to sponsor. Olefins Panel HVP Stream: Hydrotreated C6-C8.
Method	
Method/guideline followed	Standard method based on Williams et al (1977, 1982)
Type	In vitro mammalian DNA repair assay
System of testing	Unscheduled DNA synthesis (UDS) in primary hepatocyte cultures
GLP	Yes
Year	1984
Species/Strain	Fischer 344 male rat (10 wks old)
Metabolic activation	No
Species and cell type	NA
Quantity	NA
Induced or not induced	NA
Concentrations tested	8, 16, 32, 64, 128, 256, 512, 1024µg/ml diluted in 10% Pluronic F68 (prepared in deionized water, mol. wt 8350, 80% hydrophilic)
Exposure period	18 hrs.
Statistical Methods	None specified. Criteria for positive response are incorporation of radioactive precursor (^{3}H-thymidine) in cells that are not normally synthesizing DNA, indicating repair of damage. A positive response is defined as a mean net nuclear grain count at any treatment level that exceeds concurrent negative control by at least 6 grains/nucleus; negative control value must not exceed 5 grains. If this criterion is not met, a positive response can be identified if there is a significant difference ($p<0.01$) in % cells in repair at any dose level and negative control value. This indicator defines whether a small fraction of cells is undergoing repair (Casciano & Gaylor, 1983). A positive response need not be dose related.
Remarks for Test Conditions	Sufficient Hydrogenated Pyrolysis Gasoline (HPG) was weighed separately for each dose level, 0.40ml of 10% F68 added per ml of final volume and sufficient medium (Williams Medium E with 10% fetal bovine serum and insulin) added to achieve final volume. Test preparations were mixed just prior to addition at 20µl to each 2ml culture. The conc. of ^{3}H-thymidine (½ life 12.4 yrs.) used in these assays was 1mCi/ml. All cultures were incubated at 37^0C in 5% CO_2 enriched humidified atmosphere. No range finding assay was performed. In the UDS assay, $2x10^5$ cells/ml were seeded into coverslip cultures, exposed to ^{3}H-thymidine and test substance for 18 hours (3 cultures/dose level, 8 dose levels), untreated controls, vehicle F68 control and positive control, 2-acetyl aminofluorene (0.01µg/ml). Cells growing on coverslips were rinsed, fixed and glued to microscope slides on day 2. On day 3, slides were dipped in autoradiographic emulsion and stored in the dark at 2-8^0C. Autoradiographs were developed, stained and coverslipped on day 10. Numbers of grains overlying 50 randomly selected nuclei/slide were counted. The highest of 3 cytoplasmic grain counts/cell were subtracted and this number was divided by a conversion factor (unspecified) to obtain net nuclear grain count. Avg. net nuclear grain count/slide (sum of net nuclear grain count ÷ 50) and mean net nuclear grain count (avg. net nuclear grain count/slide ÷3) were calculated. In addition, % cells in repair were determined for each dose level.
Results	
Genotoxic effects	HPG induced toxicity in primary hepatocytes following 18 hr exposure that left too few cells for UDS analysis at doses of 512 and 1024µg/ml. HPG did not induce unscheduled DNA synthesis at any dose level with sufficient cells to be analyzed. Positive and negative controls gave appropriate responses.
Conclusions	
(contractor)	Hydrogenated Pyrolysis Gasoline did not induce unscheduled DNA synthesis in primary cultures of rat hepatocytes under conditions of this assay.

Data Quality *Reliabilities*	**2.** Reliable with restrictions. No table of cell counts/viability. No individual data to verify calculations and identify conversion factor. Statistical criteria are mentioned but method is not cited.
Reference	Brecher, S. 1984. Hepatocyte primary culture/DNA repair test of Hydrogenated Pyrolysis Gasoline. Proj. # 2097. Gulf Life Sciences Center, Pittsburgh, PA for Gulf Oil Chemicals Co., Houston, TX Williams, G.M. 1977. Cancer Res. 37: 1845-1851 Williams et al. 1977. In Vitro 13: 809-817 Williams et al. 1982. Mut. Res. 97:359-370 Casciano, D.A. and Gaylor, D.W. 1983. Mut. Res. 122:81-86
Other *Last changed*	5/7/2001 (Prepared by a contractor to the Olefins Panel)

Robust Summary - Group 5: High Benzene Naphthas

Genetic Toxicity - in Vivo

Test Substance	
Remarks	Hydrogenated Pyrolysis Gasoline, CAS #68410-97-9. Clear liquid with aromatic odor. Compositional analysis , purity and stability referred to sponsor. Olefins Panel HVP Stream: Hydrotreated C6-C8.
Method	
Method/guideline followed	None specified. Comparable to standard assay.
Type	Mammalian bone marrow erythrocyte micronucleus assay
GLP	Yes
Year	1984
Species	Mice
Strain	Crl:CD-1(ICR)BR Swiss
Sex	Male and female. Range-finding 2M, 2F (10 wks old)/group; 3 groups; Micronucleus test 10M, 10F (11 wks old)/group in 4 groups, 15M, 15F in one group.
Route of administration	Oral gavage
Doses/concentration levels	0, 0.5, 1.0, 2.0g/kg (2doses), 2.0g/kg (1 dose) undiluted
Exposure period	1 dose/day for 2 days: one group- 1 dose, 1 day only
Statistical methods	Values from treated groups for daily mean body weights, group means and std. dev. for polychromatic erythrocytes (PCEs) with micronuclei (MN) , and group mean ratios of PCE to normochromatic erythrocytes (NORMs) were calculated and compared with vehicle control values by Student's t-test. Positive response was indicated by statistically significant ($p<0.05$) increases in micronucleated PCE at any dose level with a dose related response evident. Results were considered equivocal if only one of these criteria was met.
Remarks for Test Conditions.	Animals in the range-finding study (2M, 2F/group), 3 treated groups (no control group) were given 1.25, 2.5, and 5.0g/kg neat hydrogenated pyrolysis gasoline (HPG) by gavage once each day for two days. Eighty percent of the dose level that produced =50% mortality was selected for the maximum dose in the micronucleus study. In the micronucleus study, three groups of mice were given undiluted HPG by oral gavage daily for two days at doses of 0.5, 1.0, 2.0g/kg, negative control mice were given corn oil (5g/kg). One-half of each treated group and negative control (5M, 5F) was killed on day 3 and the remainder on day 4. One group (15M, 15F), given 2.0 g/kg by gavage in a single dose for 1 day only, was killed on days 2, 3, 4 (5/sex/day). Positive control mice (4M, 4F) given cyclophosphamide (75 mg/kg) ip daily for 2 days were killed on day 3. Survival, body wt, and clinical signs were observed and recorded daily. Slides of femoral bone marrow smears were prepared, stained with May-Grunewald/Giemsa stain and examined microscopically. For each mouse, 1000 PCE and all associated mature erythrocytes (NORMs) were counted. Data collected included group mean body weights for each day, total PCEs, total NORMs, PCEs with MN, and NORMs with MN.
Results	
Genotoxic effects	NOAELmortality = 1.0g/kg; NOELgenetics > 2.0g/kg (Assigned by reviewer)
NOAEL (NOEL)	In the range-finding study, half of the animals given HPG at conc of 5.0g/kg died on or before day 2. Gross necropsy of dead mice was unremarkable. In the micronucleus test, 1/10 males given 2.0g/kg (2 doses) died on day 2. No other mortality or significant wt changes were observed. Lethargy was observed among high dose mice. Surviving mice treated with HPG did not show any significant increase in micronucleus formation in PCE and no significant changes in ratio of PCE/NORM compared to negative controls. Negative and positive controls gave appropriate results.
LOAEL (LOEL)	
Conclusions	
(study authors)	Oral treatment of mice with Hydrogenated Pyrolysis Gasoline for 1-2 days at doses up to 2.0g/kg/day had no effect on frequency of micronucleated polychromatic erythrocytes in bone marrow under these test conditions. HPG did not induce cytogenetic damage.

Data Quality	
Reliabilities	**1.** Reliable without restriction
References	Khan, S.H. 1984. Micronucleus test of Hydrogenated Pyrolysis Gasoline. Proj. #2096. Gulf Life Sciences Center, Pittsburgh, PA for Gulf Oil Chemicals Co., Houston, TX
Other	
Last changed	5/7/2001 (Prepared by a contractor to the Olefins Panel)

Robust Summary - Group 5: High Benzene Naphthas

Repeated Dose Toxicity

Test Substance	Hydrogenated Pyrolysis Gasoline CAS #68410-97-9, Clear liquid with aromatic odor.
Remarks	Olefins Panel HVP Stream: Hydrotreated C6-C8.
Method	
Method/guideline followed	Standard method, method not referenced
Test type	Subacute
GLP	Yes
Year	1984
Species	Rat
Strain	Fischer 344
Route of administration	Inhalation
Duration of test	8 days
Doses/concentration levels	0, 4869±470, 9137±917ppm±SD, actual exposure conc.
Sex	Males and females (5/sex/group)
Exposure period	6 hrs.
Frequency of treatment	once daily for 5 days (d1-5)
Control group and treatment	5M, 5F; filtered air
Post exposure observation period	2 days
Statistical methods	Body wt variance compared by Bartlett's test and one way analysis of variance. Group mean body wt compared either with Dunnett's test or a modified t-test to assess significance.
Test Conditions	Rats (9 wks old, 113-195g at initiation) were housed individually in stainless steel, screen-bottomed cages. Rooms were maintained at 72.2^0F (exposure chamber 75^0F) with relative humidity of 54% (exposure chamber 50%), and 12 hr light/dark cycle. Rats received chow diet and tap water ad lib throughout the study, except during exposure. Three groups of 10 rats (5M, 5F/group) each, were exposed to test article or air. Test article was aerosolized with a ball jet nebulizer; an in-line condensing flask was used to prevent large particles from entering the exposure chamber. Chamber concentration of test article was measured by gas chromatography. Rats were observed twice daily on weekdays and once daily on weekends for morbidity/mortality, and once daily for clinical signs immediately after exposure on days 1-5. Surviving rats were sacrificed on day 8. Gross necropsies were performed on all rats.
Results	
NOAEL (NOEL)	NOAEL< 4869ppm (estimated by reviewer)
LOAEL (LOEL)	LOAEL= 4869ppm (estimated by reviewer) based on clinical observations, reduced wt gain.
Remarks	Two rats (1M, 1F) from group 3 (9137ppm) died on day 2; one female from group 3 died during exposure on day 1. Rats in groups 2 and 3 showed ocular discharge throughout d1-5. Rats in group 2 showed increased respiratory rate and dry red material around nose and mouth. All rats in group 2 were lethargic and showed labored respiration. Many rats in group 3 were lethargic and exhibited twitching and harsh respiratory sounds during days 1-5. All rats in group 2 and all but one survivor in group 3 appeared normal on day 8. Group mean body wt was significantly decreased in a dose related manner. No test article related effects were seen at gross necropsy on day 8; the male rat that died during the study showed gas in the G.I. tract and red-tinged fluid in the stomach.
Conclusions (study authors)	Exposure to test article caused a significant decrease in group mean body wt of male and female rats of low and high dose groups that was correlated with exposure level. Three deaths occurred in the high dose group during exposure. Major clinical signs were lethargy, twitching, harsh respiratory sounds and ocular discharge. No gross alterations were found in rats surviving to sacrifice.
Quality Reliabilities	**1.** Reliable without restrictions
References	Rausina, G.A. 1984. Five-day repeated dose inhalation toxicity study in rats of Hydrogenated Pyrolysis Gasoline. Proj. #2099. Gulf Life Sciences Center, Pittsburgh, PA
Other	
Last changed	Revised 7/27/2001 (Prepared by a contractor to the Olefins Panel)

Robust Summary - Group 5: High Benzene Naphthas

Acute Toxicity

Test Substance	Pyrolysis gasoline (Rerun Tower Overheads). Yellow, homogeneous liquid; 40% benzene, 26% C5, 13% toluene, 20% other. Test substance is described as a sample of a Pyrolysis Gasoline distillate fraction and is similar to Pyrolysis gasoline, a stream included in the test plan.
Method	
Method/guideline followed	Not specified
Type (test type)	Acute, limit test
GLP	Yes
Year	1994
Species/Strain	Rat, Sprague-Dawley
Sex	Males and females
No. of animals per sex per dose	5
Vehicle	None
Route of administration	Oral gavage
Test Conditions	Sprague Dawley rats (180-350g) were individually housed in stainless steel suspended cages and fasted overnight prior to administration of 2g/kg neat pyrolysis gasoline. The study room was maintained at 68-72^{0}F with a relative humidity of 35-63% and a 12 hr light-dark cycle. Water and chow diet were available ad lib after dosing. Test article was administered once on day 1 by oral gavage through a blunted needle. Rats were observed for clinical signs approx. 30 min, 1hr and 4hr, after dosing, and daily thereafter until sacrifice on day 15. Rats were checked once a day for mortality and moribundity. Observations were not made on weekends. Body wts were recorded prior to fasting and on days 1, 8 and 15.
Results	
LD_{50} with confidence limits.	The LD_{50} was not reached at 2g/kg. There were no deaths and all rats gained some weight during the study. Clinical signs noted in one or more rats were salivation, decreased activity, rales, lacrimation, chromodacryorrhea, ataxia, chromorhinorrhea, miosis, slight tremors, mydriasis , hyperactivity, hypothermia, urogenital discharge, nasal discharge, decreased food consumption, decreased fecal output, vocalization, and penile discharge. No gross pathological findings were noted at necropsy.
Remarks	
Conclusions (study author)	The LD_{50} was not reached at 2g/kg.
Data Quality	
Reliability	**1.** Reliable without restriction.
References	Rodriguez, S.C. and Dalbey, W.E. 1994. Acute oral toxicity of pyrolysis gasoline in Sprague Dawley Rats. Study #65636. Stonybrook Laboratories, Princeton, NJ. for Mobil Chemical Co., Edison, NJ.
Other	
Last changed	10/16/2001 (Prepared by a contractor to the Olefins Panel)

Robust Summary - Group 5: High Benzene Naphthas

Acute Toxicity

Test Substance	Pyrolysis gasoline (Rerun Tower Overheads). Yellow, homogeneous liquid; 40% benzene, 26% C5, 13% toluene, 20% other. Test substance is described as a sample of a Pyrolysis Gasoline distillate fraction and is similar to Pyrolysis gasoline, a stream included in the test plan.
Method	
Method/guideline followed	Not specified
Type (test type)	Acute, limit test
GLP	Yes
Year	1994
Species/Strain	Rabbit, New Zealand White
Sex	Males and females
No. of animals per sex per dose	3
Vehicle	None
Route of administration	dermal
Test Conditions	Rabbits, weighing at least 2kg, were individually housed in stainless steel suspended cages in a study room maintained at 69-72^{0}F with a relative humidity of 38-85% and a 12 hr light-dark cycle. Water and chow diet were available ad lib. The dorsal skin surface extending down from the front to rear legs and from left to right lower flanks was clipped free of hair the day prior to test article administration. Test article was spread evenly over the clipped area (approx. 10% of body surface area) at a dose of 2g/kg. A layer of 8-ply gauze was placed on the dorsal site, and a rubber dam sleeve was fitted snugly over the gauze pad and around the trunk. Edges of the dam were taped in place. An Elizabethan collar was affixed to the neck to prevent oral ingestion of test article and mechanical irritation of the test site. After 24 hrs, the collar and wrappings were removed and residual test article was wiped off. Body wts were recorded on days 1, 8 and 15. Rabbits were observed for toxicity at about 1 and 2 hr post-dose and daily thereafter on weekdays through day 14. Observations for mortality/moribundity were made daily. Rabbits were sacrificed on day 15 and necropsies were performed.
Results	
LD_{50} with confidence limits.	The LD_{50} was not reached at 2g/kg. There were no deaths during the study and rabbits either gained some weight or remained at day 1 body wt. Signs that might have resulted from treatment in one or more rabbits were: soft stool, decreased fecal pellet size, nasal discharge, and test site erythema. No gross pathological findings were noted at necropsy.
Remarks	
Conclusions (study author)	The LD_{50} was not reached at 2g/kg.
Data Quality Reliability	**1.** Reliable without restriction.
References	Rodriguez, S.C. and Dalbey, W.E. 1994. Dermal toxicity of pyrolysis gasoline in the New Zealand White rabbit. Study #65637. Stonybrook Laboratories, Princeton, NJ. for Mobil Chemical Co., Edison, NJ.
Other	
Last changed	10/16/2001 (Prepared by a contractor to the Olefins Panel)

Robust Summary - Group 5: High Benzene Naphthas

Genetic Toxicity - in Vitro

Test Substance	Rerun Tower Overheads from Olefins/Aromatics Plant (light thermal cracked naphtha)
Test substance	CAS # 64741-74-8. Straw colored liquid; 40% benzene, 26% C5, 13% toluene, 20% other. Test substance is described as a sample of a Pyrolysis Gasoline distillate fraction and is similar to Pyrolysis gasoline, a stream included in the test plan.
Method	
Method/guideline followed	Standard method based on Ames et al, 1975
Type	Reverse mutation bacterial assay
System of testing	Salmonella typhimurium with and without metabolic activation
GLP	Yes
Year	1981
Species/Strain	S. typhimurium TA 98, TA100, TA1535, TA1537, and TA1538.
Metabolic activation	Yes
Species and cell type	Sprague Dawley male rat liver (S9 fraction) from Litton Bionetics, Kensington, MD
Quantity	50ul S9 fraction in 0.5ml S9 mix/plate
Induced or not induced	Aroclor 1254-induced, rats were given a single ip 500mg/kg dose, 5 days prior to sacrifice.
Concentrations tested	0, 0.029, 0.094, 0.30, 0.97µl/plate –S9, and 0.094, 0.30, 0.97, and 3.1µl/plate + S9; samples diluted in dimethyl sulfoxide (DMSO). Negative control 50µl DMSO
Statistical Method	None. Criteria for a positive response were an increase in revertant colonies at least two-fold that of negative control at the lowest active dose, and a dose response curve. Positive results must be reproducible in an independent repeat assay.
Remarks for Test Conditions	Rerun tower overheads test solutions were prepared in DMSO immediately prior to use. Salmonella (Approx. 1.4-2x10^8 cells/ml) were exposed to either test solution or DMSO ±S9 by the preincubation method. Doses of 0.029-0.97µl/plate-S9 and 0.094-3.1µl/plate +S9 were determined by a pretest toxicity test in TA 100 and TA1537±S9 using incremental doses from 0.01-10µl/plate. Culture tubes containing 50µl test solution or DMSO, 0.1ml Salmonella and 0.5 ml phosphate buffer or S9 mix were combined and incubated with shaking (150 rpm) for 20 minutes at 37^0C. At the end of the preincubation period, top agar was added, mixed and cultures were overlaid on minimal agar plates, 3 plates/dose/strain. Plates were incubated at 37^0C for 48 hrs, then counted automatically (Biotran II) and background lawn evaluated by stereomicroscope. Positive control compounds were: -S9, 2-nitrofluorene (2-NF, 20µg/plate) for TA98 and TA1538; N-methyl-N'-nitro-N-nitrosoguanidine (MNNG, 2.0µg/plate) for TA100 and TA1535; 9-aminoacridine (9-AA, 25µg/plate) for TA1537; +S9 2-aminoanthracene (2µg/plate) for all strains except TA1537.
Results	
Genotoxic effects	The preliminary toxicity test exhibited severe toxicity at 10µl/plate with activation and at 3.1 and 10µl/plate without activation (individual data not shown). In the mutagenicity test, none of the 5 strains of Salmonella exhibited revertant frequencies substantially different from the solvent or spontaneous controls at any dose level with or without metabolic activation (e.g. TA98-S9: 16, 15, 12, 12, and 0 average revertants/plate and TA100-S9: 111, 115, 107, 94, and 0 at 0[DMSO], 0.029, 0.094, 0.30, and 0.97µl/plate, respectively: TA98+S9: 33, 26, 26, 22, and 0 revertants/plate, and TA100+S9: 128, 161, 128, 118, and 0 revertants/plate at 0[DMSO], 0.094, 0.30, 0.97 and 3.1µl/plate, respectively). Clearing of background lawn and microcolonies were observed at the maximum doses (0.97µl/plate-S9; 3.1µl/plate+S9). Positive control compounds (2 plates/strain) performed appropriately (-S9: MNNG 1906, 1883 revertants/plate in TA 100 and TA1535, respectively; 9-AA 586 revertants/plate in TA1537; 2-NF 2114, 1214 revertants/plate in TA98 and TA1538, respectively; and +S9 2-aminoanthracene 406-2307 revertants/plate for all strains except TA1537). The results of this assay indicate that rerun tower overheads had no mutagenic activity in this test system. (Reviewer's note: Due to toxicity, tests were performed over a low dose range; 3 of 4 doses were non-toxic and showed sufficient growth to evaluate mutagenicity. Testing at any lower doses was impractical).

Conclusions	Rerun Tower Overheads did not induce an increase in revertant colonies in any Salmonella
(contractor)	strain, tested at any dose level with or without metabolic activation in this single Ames test.
Data Quality	
Reliabilities	**1.** Reliable without restriction
Reference	Blackburn, G.R. 1981. An Ames Salmonella/mammalian microsome mutagenesis assay for the determination of potential mutagenicity of Rerun Tower Overheads from an olefins/aromatics plant. Study No. 1781-80. Mobil Environmental and Health Sciences Laboratory, Princeton, NJ. Ames B. N. et al. 1975. Mutat. Res. 31: 347-364.
Other	
Last changed	10/02/2001 (Prepared by a contractor for the Olefins Panel)

Robust Summary - Group 5: High Benzene Naphthas

Genetic Toxicity - in Vitro

Test Substance	Rerun Tower Overheads from Olefins/Aromatics Plant (light thermal cracked naphtha)
Test substance	CAS # 64741-74-8. Straw colored liquid; 40% benzene, 26% C5, 13% toluene, 20% other. Test substance is described as a sample of a Pyrolysis Gasoline distillate fraction and is similar to Pyrolysis gasoline, a stream included in the test plan.
Method	
Method/guideline followed	None specified. Standard method based on Slater et al., 1971, Green and Muriel, 1976, and Ames et al., 1973.
Type	Bacterial DNA repair
System of testing	*Escherichia coil, Salmonella typhimurium*
GLP	Not specified
Year	1978
Species/Strain	*E. coli* WP2 uvrA$^+$ recA$^+$, WP100 uvrA$^-$ recA$^-$; *S. typh*. TA1978 uvrB$^+$, TA 1538 uvrB$^-$
Metabolic activation	Yes
Species and cell type	Sprague Dawley male rat liver (S9 fraction)
Quantity	50µl S9 fraction in 1.0ml S9 mix/plate
Induced or not induced	Aroclor 1254 induced (single ip injection of 500mg/kg, 5 days prior to sacrifice)
Concentrations tested	Spot test: 10µl/plate undiluted
Statistical Methods	None. Compounds that cause damage to DNA will more severely affect repair deficient strains than repair proficient stains. Toxic compounds that do not affect DNA will not induce differential toxicity.
Remarks for Test Conditions	Tester strains were stored in liquid nitrogen and fresh cultures were inoculated directly from frozen stock, grown overnight at 37^0C, re-diluted and grown to final cell concentration of $2x10^8$ cells/ml. Each test article -strain combination was plated in triplicate with and without metabolic activation. Log phase cultures (0.1ml) added to 2.5ml top agar were poured on Vogel-Bonner minimal medium plates. For plates without activation, a 6.5mm paper disc (antibiotic type) was placed in the center of each plate; 10µl test article is placed on disc. For plates with S9 activation, after top agar sets, a 9.5mm diameter hole was cut in agar in the center of the plate, the well was sealed with 0.1ml top agar, and 150µl of S9 mix/control or test article mix (14:1) added to the well. All inverted plates were incubated at 37^0C for 24hr. The diameter of any resulting zone of inhibition was measured in mm. Zone diameter of a repair deficient strain was divided by the zone diameter of the repair proficient parent strain. Positive control compounds were 4-nitro-quinoline-1-oxide (4-NQO; 30µg/plate) –S9, 2-aminofluorene (2-AF; 250µg/plate) +S9, and negative control was 25µg/plate penicillin. Tests were performed twice ± S9.
Results	
Genotoxic effects	In duplicate tests, average inhibition ratios induced by Rerun tower overheads –S9 were 1.4, 1.8 for *E. coli* WP100/WP2, and 1.3, 1.5 for *S. typh*. TA1538/TA1978 compared to negative control values of 1.0, 1.1, and 1.1, 1.2 in *E coli* strains and *S. typh*. strains, respectively, suggesting a weak differential killing of repair deficient strains without metabolic activation. Positive control ratios for 4-NQ –S9 were 2.3, 2.5 for *E coli* WP100/WP2, and 1.7, 1.6 for *S. typh*. TA1538/TA1978. In tests with metabolic activation (+S9), average inhibition ratios were 1.0, 1.0 for *E.coli* strains and 1.0, 1.0 for *S. typh*. strains in duplicate tests compared to negative control values of 1.1, 1.1, and 1.1, 1.1 in *E. coli* and *S. typh*. strains, respectively, indicating no test article induced toxicity. Positive control, 2-AF, inhibition ratios were 2.1, 2.1 for *E. coli* WP100/WP2, and 1.9, 1.4 for *S. typh*. TA1538/TA1978.
Conclusions (contractor)	Rerun tower overheads did cause weak differential killing in DNA repair deficient strains, *E. coli* WP100 and *S. typhimurium*. TA1538 in the absence of metabolic activation, suggesting that the test article can cause direct acting damage to bacterial DNA. No differential killing was observed in the presence of metabolic activation.
Data Quality	
Reliabilities	**1.** Reliable without restriction

Reference	Haworth, S.R. 1978. Bacterial DNA repair assay of Mobil Chemical Company Compound MCTR-125-78 (MRI #110). E. G. and G. Mason Research Institute, Rockville, MD. for Mobil Chemical Co, Edison, NJ Slater, E.E. et al. 1971. Cancer Res. 31: 970-973. Green, M.H.L. and Muriel, W.J. 1976. Mutat. Res. 38:3-32 Ames, B.N. et al. 1973. Proc. Natl. Acad. Sci., USA 70: 782-786.	
Other		
Last changed	2/28/2002 (Prepared by a contractor to the Olefins Panel)	

Robust Summary - Group 5: High Benzene Naphthas

Genetic Toxicity - in Vitro

Test Substance	Rerun Tower Overheads from Olefins/Aromatics Plant (light thermal cracked naphtha)
Test substance	CAS # 64741-74-8. Straw colored liquid; 40% benzene, 26% C5, 13% toluene, 20% other. Test substance is described as a sample of a Pyrolysis Gasoline distillate fraction and is similar to Pyrolysis gasoline, a stream included in the test plan.
Method	Standard method, no guideline specified
Method/guideline followed	Cell transformation
Type	Mouse embryo cells
System of testing	Yes
GLP	1981
Year	BALB-c/3T3 mouse cell line
Species/Strain	No
Metabolic activation	NA
Species and cell type	NA
Quantity	NA
Induced or not induced	Initial cytotoxicity: 0, 0.01, 0.1, 1.0, 10.0, 100.0µg/ml medium; Transformation: 0. 0.8, 4.0, 20.0 and 100µg/ml, diluted in dimethyl sulfoxide. Negative control was DMSO at 2.5% vol. concentration.
Concentrations tested	T-test specified. Standard criteria for positive response is a two fold increase in type III foci at highest dose over vehicle control with or without a dose related response or a 2 fold increase at 2 or more consecutive doses.
Statistical Method	Routine procedures were referred to Appendix 1 Standard Operating Procedures, which was not included with this report. Only specifics unique to this assay are presented. Due to the volatile nature of test material, the cytotoxicity assay and transformation assays were conducted in tightly capped T-25 flasks in sealed plastic bags. The pH of medium during the 72hr exposure period was maintained at 7.4 by 0.02M Hepes buffer in flasks. RTO was prepared as a 1% stock solution in DMSO, which, when added to culture medium at a 2.5% vol. conc. was a suspension. Despite limited solubility, RTO produced a dose-dependent cytotoxic effect after a 3-day exposure period. In the initial toxicity assay, RTO was added to flasks, seeded with BALB-c/3T3 cells, at concentrations of 0, 0.01, 0.1, 1.0, 10.0 and 100.0µg/ml, incubated for 3 days at 37^0C in a CO_2 in air incubator, after which cells were counted for survival. In the transformation assay, RTO was tested at 0, 0.8, 4.0, 20.0 and 100µg/ml. In a standard BALB-c/3T3 transformation assay, colony formation cultures (approx. 100 cells/culture) and transformation cultures (approx. 10^4 cells/culture, 20 cultures/dose) were seeded on day 1, exposed to test material for 2-3 days, and culture medium was changed on day 4. For transformation cultures, medium continued to be changed weekly to day 29. Colony formation cultures were fixed, stained and counted visually on day 8 to determine cloning efficiency; transformation cultures were fixed and stained on day 29 for focus counting and evaluation. Transformation frequency = total type III foci ÷ total cultures/dose. Positive control compound was 3-methyl cholanthrene (2µg/ml).
Remarks for Test Conditions	
Results	RTO induced toxicity in BALB-c/3T3 cells after 3 days exposure at concentrations of 10µg/ml (59% viability) and at 100µg/ml (18% viability). In the transformation assay, inhibition of cloning efficiency (CE, clones/100 cells) occurred at 4.0µg/ml (89% CE), 20.0µg/ml (81% CE) and 100µg/ml (65% C.E.); cell toxicity was somewhat less than in the initial cytotoxicity assay [40% viability at 100µg/ml]. RTO did not induce statistically significant increased incidence of transformed foci compared to negative controls at any dose level. Values were 0.10 foci/flask, 2/20 flasks with foci at 100µg/ml, 0.0 foci/flask, 0/20 flasks with foci at 20.0µg/ml, 0.15 foci/flask, 3/20 flasks with foci at 4.0µg/ml, 0.10 foci /flask, 2/20 flasks with foci at 0.8µg/ml compared to 0.05 foci/flask, 1/20 flasks with foci in negative control group. [Reviewer's note: Negative control value of 1 focus/20 flasks was lower than control values in other concurrent studies on 2 other compounds in this series where negative controls had 4 foci in 20 flasks (0.20 foci/flask)]. Positive
Genotoxic effects	

	control compound, 3 methyl cholanthrene, induced 56 foci/19 flasks (2.95 foci/flask), 18/19 flasks with foci.
Conclusions (contractor)	Rerun tower overheads did not induce neoplastic transformation in BALB-c/3T3 cells and was not active in this test system.
Data Quality *Reliabilities*	**2.** Reliable with restrictions. Complete details of assay methods are not included in the report. Specifics of statistics are not supplied.
Reference	Tu, A.S. and Sivak, A. 1981. BALB-c/3T3 Neoplastic transformation assay on 0818802, 08188003 and 08188005 (Rerun tower overheads). ALD Ref. #86374. Arthur D. Little, Inc. Cambridge, MA for Mobil Oil Corp, Study #1771-80, Princeton, NJ Roy, T.A., 1981. Analysis of rerun tower bottom oil by combined capillary gas chromatography/mass spectrometry. Study #1272-81-. Toxicology division, Mobil Oil Co., Princeton, NJ
Other *Last changed*	12/07/01 (Prepared by a contractor to the Olefins Panel)

Robust Summary - Group 5: High Benzene Naphthas

Genetic Toxicity - in Vitro

Test Substance	Rerun Tower Overheads from Olefins/Aromatics Plant (light thermal cracked naphtha)
Test substance	CAS # 64741-74-8. Straw colored liquid; 40% benzene, 26% C5, 13% toluene, 20% other. Test substance is described as a sample of a Pyrolysis Gasoline distillate fraction and is similar to Pyrolysis gasoline, a stream included in the test plan.
Method	
Method/guideline followed	None specified. Standard method based on Clive and Spector, 1975
Type	Mammalian cell mutation assay
System of testing	Mouse lymphoma cells
GLP	Not specified
Year	1979
Species/Strain	Mouse lymphoma L5178Y TK+/- cells
Metabolic activation	Yes
Species and cell type	Sprague Dawley males rat liver (S9 fraction)
Quantity	50µl S9 fraction/ml S9mix)
Induced or not induced	Aroclor 1254 induced (single ip injection of 500mg/kg, 5 days prior to sacrifice)
Concentrations tested	-S9 cloned doses: 0.0, 0.013, 0.018, 0.024, 0.032, 0.042, 0.056, 0.075, and 0.10µl/ml +S9 cloned doses: 0.0, 0.048, 0.063, 0.085, 0. 11, 0.15, 0.20, 0.27, and 0.36µl/ml. All doses diluted in acetone
Statistical Methods	None. Compound was designated as mutagenic if it induced a mutation frequency (mutant cells/10^4 surviving cells) greater than 3 times the standard error (S.E. [f]) calculated by formula from the viable counts and total mutant cells (trifluorothymidine resistant cells) at each dose level.
Remarks for Test Conditions	Freshly prepared actively growing cultures of L5178Y cells ($1x10^6$ cells/ml) were dispensed in 6ml aliquots into 44 polypropylene centrifuge tubes. Rerun tower overheads, solubilized in acetone, beginning at a concentration equal to LD90 from a preliminary toxicity test, was diluted over 15 serial 1/8 log dilutions, producing 16 dose levels decreasing approximately 100 fold from highest to lowest, and added to cells in the centrifuge tubes. Four ml of S9 activation mixture or 4ml culture medium was added, yielding a final cell suspension of $0.6x10^6$ cells/ml. Positive control compounds were ethyl methyl sulfonate (EMS, 1.0µl/ml) –S9 and 7,12-dimethylbenzanthracene (7,12-DMBA, 2.5µl/ml) +S9 cultures. All tubes were gassed with 5% CO2/air and placed on a roller drum for 4hrs at 37^0C in the dark. At the end of exposure, calls were washed with fresh medium, re-suspended, gassed, replaced on roller drum at 37^0C and incubated for 3 days with a cell population adjustment every 24 hrs to maintain a cell population density of $0.3x10^6$ cells/ml. After 3 days expression, 8 cultures ± S9, which exhibited toxicity from 10-90% growth inhibition during the expression period, were selected for cloning. At cloning, cells were placed in restrictive suspension medium containing trifluorothymidine (TFT, 1µg/ml) that allows only TK-/- cells to grow. Two Florence flasks/concentration ± S9, one for restrictive medium, on for viable cell counts, were filled with 100ml cloning medium and maintained at 37^0C. Six 100mm petri plates/concentration ± S9 were prepared, 3 for restrictive medium, 3 for viable cell counts. Cell counts were made from each centrifuge tube to determine the volume of cell population = $3x10^6$cells. This volume was retained, centrifuged and the supernatant discarded except for 2ml in which cells were re-suspended and placed in restrictive medium flask. A $5x10^{-4}$ dilution was prepared and added to the appropriate viable count flask containing 100ml cloning medium. After this dilution, 1 ml of TFT stock solution was added to the restrictive medium flask and incubated with shaking (125rpm) at 37^0C for 15min. Flasks were removed, 33ml of cell suspension was pipetted into each of 3 appropriately labeled plates and placed in the cold (4^0C) for 20 min to accelerate gelling. Plates were removed and incubated at 37^0C in humidified 5% CO2/air for 10 days. At the end of incubation, plates were scored for total number of colonies/plate, 3 counts/plate, on an automated colony counter. Mutation frequency (MF) = avg. number of colonies in 3 restrictive medium plates ÷ avg. number of colonies $x10^4$ in 3 corresponding viable count plates. Induced mutation frequency (IMF) = MF test article – MF solvent control.

Results Genotoxic effects	In cultures without metabolic activation, the two highest concentrations cloned, 0.10µl/ml (MF=1.4, IMF=0.8) and 0.075µl/ml (MF=1.0, IMF=0.4) exhibited slight dose related increases in IMF compared with acetone control (MF=0.6); only the 0.10µl/ml concentration caused a doubling of MF over controls. EMS positive control values were MF=27.1, IMF=26. The first activated assay was discarded due to loss of positive control cultures by contamination. In the repeat test with metabolic activation, 2 dose concentrations had MF 2 times greater than acetone controls: the highest dose cloned, 0.36µl/ml (MF=0.8, IMF=0.4) and 0.15µl/ml, the 4th highest dose cloned (MF=0.9, IMF=0.5) versus control (MF=0.4). However, intervening cloned doses of 0.20, and 0.27µl/ml did not show increased MF; the values for the positive doses were not dose related and were within the range of experimental error for the assay. Positive control values +S9 for 7,12- DMBA were MF=2.6, IMF=2.0.
Conclusions (contractor)	Without metabolic activation, Rerun tower overheads appears to induce a weak mutagenic response at the two highest doses only; a dose response trend was not observed in the 6 lower doses cloned. Test article did not induce significant mutagenic activity in cultures containing S9, suggesting that any mutagenic activity is suppressed or inactivated by the presence of the liver microsome metabolizing system.
Data Quality *Reliabilities*	**1.** Reliable without restriction.
Reference	Kirby, P.E. et al., 1979. An evaluation of mutagenic potential of MCTR-125-78 (MRI #110) employing the L5178Y TK+/- mouse lymphoma assay. E.G. and G. Mason Research Institute, Rockville, MD for Mobil Chemical Co., Edison, NJ Clive, D., and Spector, J.F.S. 1975. Mutat. Res. 31: 17-29
Other *Last changed*	2/28/2002 (Prepared by a contractor to the Olefins Panel)

Robust Summary - Group 5: High Benzene Naphthas

Genetic Toxicity - in Vitro

Test Substance	Rerun Tower Overheads from Olefins/Aromatics Plant (light thermal cracked naphtha)
Test substance	CAS # 64741-74-8. Straw colored liquid; 40% benzene, 26% C5, 13% toluene, 20% other. Test substance is described as a sample of a Pyrolysis Gasoline distillate fraction and is similar to Pyrolysis gasoline, a stream included in the test plan.
Method	
Method/guideline followed	None specified. Standard method based on Bertram, 1977
Type	Mammalian cell transformation assay
System of testing	Mouse C3H embryo cells
GLP	Not specified
Year	1978
Species/Strain	Mouse embryo cells/ C3H 10T½
Metabolic activation	No
Species and cell type	NA
Quantity	NA
Induced or not induced	NA
Concentrations tested	0, 0.625, 1.25, 2.5 and 5.0µl/ml, all diluted in acetone
Statistical Methods	None. A positive response is determined by the appearance of any type II foci (50% can be malignantly transformed) and type III foci (85% can be malignantly transformed) compared to negative controls. The C3H 10T½ cell line has no spontaneous transformation.
Remarks for Test Conditions	For the preliminary toxicity assay, cells (200/plate) were exposed to Rerun tower overheads diluted in acetone, over a range of concentrations from 0.0003-5.0µl/ml, at 2-fold dilutions for 18hrs; cells were then washed, re-fed with fresh Eagle's basal medium and incubated for 10 days in 5% CO2/air at 37^0C. After incubation, cells were washed, fixed with absolute methanol (20 min) and stained with Giemsa (30 min); number of cells/plate were counted and cloning efficiency (CE) determined=Avg. number colonies/plate ÷ number cells plated x100. In the transformation assay, cells in late log phase were plated at a concentration of $1x10^3$ cells/60mm petri dish. Cultures for concurrent toxicity determination were prepared at 200 cells/plate. After 24 hrs, cultures were treated with appropriate test article concentrations in 25µl volumes at 4 dose levels, 12 plates/dose, in decreasing 2-fold dilutions from concentrations which exhibit 25-75% relative CE. Positive control compound was 7, 12-dimethylbenzanthracene (7, 12-DMBA, 0.5µg/ml). After 18hr treatment, test article was removed, cultures were re-fed, and re-incubated. Toxicity plates were incubated for 10 days, stained and CE determined. Transformation cultures were re-fed weekly until 35 days after removal of test article had elapsed. All plate cultures were washed, fixed, stained and scored for the presence of type II and type III foci by macroscopic and microscopic examination. Type II foci show massive piling up in virtually opaque monolayers, cells are moderately polar. Type III foci are composed of highly polar, fibroblastic, multilayered, criss-crossed arrays of densely stained cells.
Results	
Genotoxic effects	Rerun tower overheads induced 71% relative cloning efficiency at 5.0µl/ml; transformation assay was performed at 2-fold dilutions from 5.0µl/ml. In the toxicity study conducted in parallel with the transformation assay, test article induced 100% cell death at 5.0µl/ml. In the transformation assay, sufficient cells survived to form a confluent layer in 8/12 plates at 5.0µl/ml dose level after 35 days. No indication of type II or type III foci were induced by rerun tower overheads at any dose level. Positive control, 7,12-DMBA induced 9 type II and 12 type III foci on 12 plates.
Conclusions (contractor)	Rerun tower overheads does not induce cell transformation in mouse embryo C3H 10T½ cells.
Data Quality	
Reliabilities	**1.** Reliable without restriction

Reference	Jensen, E.M., and Thilager, A.K. 1978. C3H 10T½ cell transformation assay, Mobil Chemical Co. Compound MCTR-125-78 (MRI #110). E.G. and G. Mason Research Institute, Rockville, MD Bertram, J.S. 1977. Cancer Res. 37: 514-523
Other *Last changed*	2/28/2002 (Prepared by a contractor to the Olefins Panel)

Robust Summary - Group 5: High Benzene Naphthas

Genetic Toxicity - in Vivo

Test Substance	
Remarks	Rerun Tower Overheads from Olefins/Aromatics Plant (light thermal cracked naphtha) CAS # 64741-74-8. Straw colored liquid; 40% benzene, 26% C5, 13% toluene, 20% other. Test substance is described as a sample of a Pyrolysis Gasoline distillate fraction and is similar to Pyrolysis gasoline, a stream included in the test plan.
Method	
Method/guideline followed	None specified. Standard method based on Bowman, 1969; Lewis, 1954; Mendelson, 1976
Type	*Drosophila* assays for point mutation, chromosome aberrations & chromosome loss
GLP	Not specified
Year	1979
Species	*Drosophila melanogaster*
Strain	Dominant lethal: Canton S; Y chromosome loss: males red/white eye; females white/ white eye; Somatic reversion: males white ivory ($\underline{w^i}$), yellow body ($\underline{y}$), echinus ($\underline{ec}$); females $\underline{w^i}/\underline{w^i}$; Bithrox test: males Ultrabithorax ($\underline{Ubx}$); females bithorax ($\underline{bx^{34e}}$); Sex-linked recessive lethal: males Canton S; females $\underline{Basc}/\underline{Basc}$
Sex	Males and females
Route of administration	Aerosol
Doses/concentration levels	0.3ml in 50ml air
Exposure period	10 min.
Statistical methods	Events in these tests have very low probabilities. Analysis based on Poisson distribution with fiducial limits computed according to Stevens, 1942.
Remarks for Test Conditions.	*Drosophila* stocks were maintained in agar/corn meal/sugar/yeast medium at 23^0C. One set of stocks was transferred each week to isolate virgin females for breeding. Four days are required for maturation of *Drosophila* sperm cells after meiosis. In all assays, treated males were mated for 3 days only to assure use of a uniform sample of treated sperm. In all assays, test article was administered as an aerosol, 0.3ml in 50ml volume of air.when administered for 1hr anesthesized flies and killed approximately 30%. Longer treatments reduced fertility. Exposure in all assays was 10 minutes in duration. Somatic reversion of white-ivory: Larvae from mating of males carrying 5 copies of white-ivory gene on the X chromosome ($\underline{w^i}$, $\underline{y}$, $\underline{ec}$) with $\underline{w^i}/\underline{w^i}$ females were treated with aerosolized test article for 10 min. Positive control compound was 0.04M mitomycin C. Larvae were washed and transferred to culture bottles to complete development. After eclosion, female offspring, genotype Qn(1)$\underline{w^i}$, $\underline{y}$, $\underline{ec}/\underline{w^i}$ were scored for red spots in the eye, which signals reversion of $\underline{w^i}$ to a pigment cell. Y chromosome loss: Males carrying a duplication of the gene for normal (red) eyes on Y chromosome and a mutant allele, white ($\underline{w}$) on the X chromosome were treated with aerosolized test article for 10 min and mated to white-eyed females ($\underline{w}/\underline{w}$). Positive control were males exposed to 3kr X-rays. Frequency of occurrence of white-eyed male progeny measured frequency of Y chromosome loss. Dominant lethal mutations: Defined as any genetic change that blocks development prior to hatching. Treated Canton S males were mated with untreated females in nylon net cages on Welch's grape juice solidified with 2% agar. After 12 hr, agar plates were removed and stored at room temp. (23^0C) for 30 hrs. Positive control was 0.04M ethyl methane sulfonate. Eggs were scored for hatching after 30hrs. Bithorax test of Lewis: Occurrence of rearrangements with one breakpoint between centromere and the locus of bithorax ($\underline{bx}$) was determined by scoring offspring of treated Ultrabithorax males and bithorax females. Males treated with 3kr X-rays were the positive controls. Distinctive phenotype was the presence of a mesonotum Sex-linked recessive lethals: Canton-S males, treated with test article, were mated with Basc (balancer X chromosome) females. Individual (F1) female progeny were mated with Basc males. Any single female culture containing at least 20 flies (F2), at least 8 of which are males, but no males are wild type, is scored as a lethal. Ethyl methane sulfonate (0.04M) treated males were the positive controls. A repeat study was performed due to loss of cultures to dessication.

Results Genotoxic effects NOAEL (NOEL) LOAEL (LOEL)	Rerun tower overheads did not induce genetic damage in *Drosophila melanogaster* under experimental conditions in any test employed. The repeated sex-linked recessive lethal test, performed due to technical problems in the initial assay, did not demonstrate any genetic damage in *Drosophila* from exposure to the test article
Conclusions (study authors)	Rerun tower overheads did not induce genetic damage in *Drosophila melanogaster*.
Data Quality *Reliabilities*	**1.** Reliable without restrictions.
References	Bowman, J.T. 1979. *Drosophila* mutagenicity assays of Mobil Chemical Compound MCTR-125-78. MRI #110. E.G. and G. Mason Research Institute, Rockville, MD, for Mobil Chemical Co., Edison, NJ. Bowman, J.T. 1969. Mutat. Res. 7: 409-415 Lewis, E.B. 1954. Am. Nat. 88: 225-239 Mendelson, D. 1976. Mutat. Res. 41: 269-276 Stevens, W.L. 1942. J. Genetics 43: 301-307
Other *Last changed*	2/28/2002 (Prepared by a contractor to the Olefins Panel)

Robust Summary – Group 5: High Benzene Naphthas

Repeated Dose Toxicity

Test Substance	Rerun Tower Overheads from Olefins/Aromatics Plant (light thermal cracked naphtha)
Remarks	CAS # 64741-74-8. Straw colored liquid; 40% benzene, 26% C5, 13% toluene, 20% other. Test substance is described as a sample of a Pyrolysis Gasoline distillate fraction and is similar to Pyrolysis gasoline, a stream included in the test plan.
Method	
Method/guideline followed	None specified, comparable to standard methods
Test type	Subacute
GLP	Not specified
Year	1980
Species	Rabbit (4/sex/group)
Strain	New Zealand White
Route of administration	Dermal
Duration of test	21 days
Doses/concentration levels	0, 0.1, 0.5, and 1.0ml/kg/day
Sex	Male and females
Exposure period	Continuous (no wipe-off)
Frequency of treatment	Once/day
Control group and treatment	Males and females (4M, 4F), saline (0.9%), 1ml/kg/day
Post exposure observation period	3 days
Statistical methods	Bartletts test, analysis of variance, Scheffe's multiple pair wise comparison, Gaines and Howell's multiple pair wise comparison
Test Conditions	Rabbits were housed individually in stainless steel cages and received water and rabbit chow diet, ad lib. Initial body wt ranged from 2455-3005g for males and 2455-3035g for females. Four rabbits of each sex were assigned to treatment groups of 0, 0.1, 0.5, and 1.0ml of neat test article/kg/day. Control rabbits received 1.0ml/kg/day of 0.9%NaCl. Prior to initiation, the dorsal dosing area was clipped free of hair and clipping was done periodically during the study. The exposure area was abraded with minor incisions deep enough to penetrate the stratum corneum but not deep enough to produce bleeding. Abrasions were made prior to the first application, and thereafter, on the first day of each week. Test article was applied to the skin once a day, starting on day 1, for 21 consecutive days; rabbits were sacrificed between day 22 and day 24. Each rabbit wore a plexiglass collar for the entire study to retard ingestion of test article. Rabbits were observed daily for mortality and moribundity, food/water intake, general appearance/behavior, toxic/pharmacological effects, and dermal reactions for 24 consecutive days. Dermal irritation was graded each morning prior to dosing. Food consumption was determined 3 times /wk and body weight on days1, 8, 15, and at termination. Prior to study initiation and during wk 3, hematocrit (Hct), hemoglobin (Hgb), erythrocyte count (RBC), total leukocyte count (WBC) and differential leukocyte count, mean cell volume (MCV), mean corpuscular hemoglobin (MCH), mean corpuscular hemoglobin conc. (MCHC), serum glutamate pyruvate transaminase (SGPT), serum glutamate oxaloacetate transaminase (SGOT), alkaline phosphatase (Alk Phos), fasting glucose, and blood urea nitrogen (BUN); urine (pH, specific gravity, glucose, ketones, total protein, bilirubin[BIH]), and microscopic examination of sediment were evaluated. Rabbits were sacrificed on day 24; necropsies were performed and gross observations recorded for all rabbits. Liver, kidney, thyroid, and adrenals were weighed and preserved for microscopic analysis along with brain, pituitary, lung, heart, spleen, pancreas, urinary bladder, testis/ovary, skin, and any unusual lesions.
Results	
NOAEL (NOEL)	NOAEL <0.10ml/kg/day both sexes (skin irr). LOAEL = 0.1ml/kg/day both sexes (skin irr)
LOAEL (LOEL)	NOAEL = 1.0ml/kg/day both sexes (systemic effects). LOAEL >1.0ml/kg/day both sexes (systemic effects).
Remarks	Two rabbits died during the study from cardiac puncture blood sampling. No test article induced effects were noted during clinical observations. Two 0.1ml/kg/day group males and one female showed erythema from day 10 to termination; 3 0.5ml/kg/day group males showed erythema from day 8 to termination; all 0.5ml/kg/day males and females, and

	1.0ml/kg/day males and females had well defined erythema from day 9 to termination. Edema was not present in any rabbits. Skin thickening was noted in all test article groups from wk 1 to termination. Fissuring was seen in 3 0.1ml/kg/day males, 3 0.5ml/kg/day males and all 1.0ml/kg/day males; all test article treated females showed fissuring. Necrosis was present in 2males and 3 females given 0.1ml/kg/day, 3males and all females given 0.5ml/kg/day, and all males and females given 1.0ml/kg/day. There were no significant changes in body wt or food consumption between controls and treatment groups. Terminal basophilic values were elevated in all male test article treated groups; all other hematology values were comparable to controls. Urinalysis findings were unremarkable. There were no significant differences in organ wt between control and any treatment group. Histological evaluation for the skin showed effects consistent with gross observations with no dose-related gradation of severity between doses, including hyperkeratosis, acanthosis, accumulation of heterophils, and cellular debris in stratum corneum, and hyperplasia of sebaceous glands. There were no abnormal microscopic findings attributable to test article administration in organs from the three treatment levels compared to controls.
Conclusions (study authors)	Daily epidermal application of test article resulted in skin irritation at the application site.
Quality Reliabilities	**2.** Reliable with restriction. There was no mention of GLP.
References	Fieser, S., Alsaker, R.D., Brown, H.R., and Wolfe, G.W. 1980. 21-Day dermal irritation study in rabbits. Proj. #230-213. Hazleton Laboratories America, Inc., Vienna, VA. For Mobil Chemical Co., Edison NJ (This study was actually for subacute toxicity, not only skin irritation)
Other Last changed	2/28/2002 (Prepared by a contractor to the Olefins Panel)

Developmental Toxicity/Teratogenicity

Test Substance	
Remarks	Rerun Tower Overheads from Olefins/Aromatics Plant (light thermal cracked naphtha) CAS # 64741-74-8. Straw colored liquid; 40% benzene, 26% C5, 13% toluene, 20% other. Test substance is described as a sample of a Pyrolysis Gasoline distillate fraction and is similar to Pyrolysis gasoline, a stream included in the test plan.
Method	
Method/guideline followed	None specified, conforms to standard method
Test type	Teratology
GLP	Yes
Year	1981
Species	Rabbit
Strain	New Zealand White
Route of administration	Oral gavage
Concentration levels	0, 10, 25, and 50mg/kg/day, diluted in corn oil
Sex	Pregnant females (16/group)
Exposure period	Day 6-28 of gestation
Frequency of treatment	Once/day
Control group and treatment	16 pregnant females received 0.5ml/kg/day corn oil
Duration of test	29 days
Statistical methods	Chi square with Yates' correction for 2x2 contingency table and /or Fisher's exact probability test; Mann-Whitney U test; analysis of variance (one-way), Bartlett's test and t-test using Dunnett's multiple comparison tables. Level of significance $p<0.05$.
Remarks for Test Conditions.	In an initial study, RTO was administered by oral gavage, undiluted to 16 pregnant rabbits/group at levels of 0 (distilled water), 10, 25 and 50 mg/kg/day. Forty-two rabbits died: 14, 11, 13, and 13 in the 0, 10, 25 and 50mg/kg/day groups respectively. Due to excess mortality in all treated groups and the controls, the study was terminated and repeated at the same concentrations diluted in corn oil. Sixty-four sexually mature virgin female rabbits (7 months old, 3.46-4.19kg at study initiation) were acclimated for 59 days, assigned a unique animal number and ear-tagged when placed on study. All rabbits were individually housed in suspended wire cages and maintained in a temperature, humidity, and light (12 hr light/dark cycle) controlled environment. Certified rabbit chow and tap water were available ad lib. Only coccidiosis-free rabbits were used in the study. Prior to insemination, females were randomly assigned to groups (16/group) according to body wt, by a computer-generated program. Sperm was collected from each of 6 proven breeder males of the same source and strain, using an artificial vagina. Semen was immediately evaluated for motility, and was used for insemination only if motility was=50%. Useable ejaculate was diluted in 0.9%NaCl at 35^0C; 0.25-0.50ml of dilute semen was introduced into the anterior vagina. Ovulation was induced by injection of 100 units chorionic gonadotropin (Ayerst, NY) in the marginal ear vein of the female immediately after insemination. Semen from one male was used to inseminate an equal number of females in each group. Inseminations were performed on two consecutive days; an equal number of females was inseminated in each group/day, designated as day 0 of gestation. RTO was mixed with corn oil daily at appropriate doses and shaken by hand. No analysis of dosing solution was reported. Negative control dams were given 0.5ml corn oil/kg/day, the volume equal to the highest treatment group. Individual doses were determined from individual body wt on day 6 of gestation. Females were observed daily for mortality, overt changes in appearance and behavior, and, from day 6-29 of gestation, for clinical signs of toxicity. One dam aborted on gest. day 19 and remained on study until scheduled sacrifice; aborted material was discarded. Body wt was recorded on gestation days 0, 6, 12, 18, 24, and 29. On gest. day 29, all females were sacrificed by overdose of sodium pentabarbitol, uteri were excised and weighed prior to removal of fetuses. Number and location of viable and non-viable fetuses, early and late resorptions, number of total implantations, and corpora lutea were recorded. Abdominal and thoracic cavity and organs of dams were examined grossly and discarded. Uteri from apparently non-gravid animals were opened and placed in 10% ammonium sulfide solution to confirm pregnancy status.

	All fetuses were individually weighed and examined for external malformations and variations. Each fetus was internally sexed and examined for internal malformations and variations, including the brain by mid-coronal slice. The heart was dissected using Staples' technique. Eviscerated, skinned fetuses were individually numbered and tagged, fixed in alcohol, macerated and stained with Alizarin Red S for skeletal examination. Fetal findings were classified as malformations or genetic or developmental variations.
Results	
NOAEL maternal toxicity	NOAEL maternal = 25mg/kg/day (based on 1 abortion at 50mg/kg/day)
NOAEL developmental toxicity	NOAEL developmental = 50mg/kg/day; both values assigned by reviewer
Maternal effects	Maternal survival was 100% in all groups. Slight increase in matted haircoat (primarily in nasal region) and slight reduction in fecal material beneath cages was noted in 50mg/kg/day rabbits. Occasional instances of nasal discharge, soft stool, hair loss and scabbing were noted in all groups during gestation. One 50mg/kg/day rabbit aborted on day 19 of gestation. Maternal body wt in treated rabbits at all doses were comparable to controls throughout treatment (gest. day 6-28) and gestation (day 0-29) periods. Mean maternal adjusted body wt (minus gravid uterus) at termination in all groups was comparable to controls. Pregnancy ratio was 87.5, 81.3, 81.3, 93.8 in 0, 10, 25 and 50mg/kg/day groups, respectively. Two control dams and one 50mg/kg/day dam had all resorptions. There were no biologically or statistically significant differences in mean number of corpora lutea, total implantations, early or late resorptions, postimplantation loss, viable fetuses, fetal sex index, or mean fetal body wt in any RTO treated group compared to controls.
Embryo/fetal effects	Average litter size was 6.1, 6.5, 6.4, and 5.9 and average fetal body wt (both sexes) was 38.9, 43.0, 42.5, and 42.4g in 0, 10, 25, and 50mg/kg/day groups, respectively. There were no biologically or statistically significant differences in number of litters with malformations (external, soft tissue, skeletal) in any treated group compared to controls: 5/12 litters (85 pups), 1/13 litters (84 pups), 3/13 litters (83 pups) and 5/13 litters (82 pups examined) in 0, 10, 25, and 50mg/kg/day, respectively. In the 50mg/kg/day group, one occurrence of atlas-occipital anomaly and one occurrence of enlarged heart with great vessel anomaly, were observed in 2 separate litters. Scoliosis was present in all groups including control, with slightly higher incidence in the 50mg/kg/day group., but incidences were within the range of historical control data for this laboratory. Fetuses and litters with genetic or developmental variations were comparable in all groups.
Conclusions (study authors)	Rerun tower overhead did not produce a teratogenic response in pregnant New Zealand White rabbits when administered orally in corn oil vehicle at dose levels of 10, 25 and 50mg/kg/day. With the exception of one 50mg/kg/day female that aborted, minimal maternal toxicity was observed at any dose level.
Data Quality *Reliabilities*	**2.** Reliable with restrictions. Analysis of test article concentration in corn oil vehicle was not performed.
References	Schardein, J.L. 1981. Teratology study in rabbits: Rerun tower overheads (MRTC-171-79) IRDC #450-011. International Research and Development Corp., Mattawan, MI. for Mobil Petrochemicals Division, Edison, NJ
Other	
Last *changed*	2/28/2002 (Prepared by a contractor to the Olefins Panel)

COURTNEY M. PRICE
VICE PRESIDENT
CHEMSTAR

January 12, 2004

American Chemistry Council

The Honorable Michael O. Leavitt
Administrator
U.S. Environmental Protection Agency
P. O. Box 1473
Merrifield, VA 22116

RE: Olefins Panel Robust Summaries for Testing and Modeling Conducted Under the HPV Challenge Program: High Benzene Naphthas Category
HPV Registration No. 1101064

Dear Administrator Leavitt:

On December 12, 2001, the American Chemistry Council Olefins Panel (Panel) submitted a Test Plan under the High Production Volume (HPV) Chemical Challenge Program pertaining to the High Benzene Naphthas Category. On August 7, 2003, the Panel submitted a revised test plan for this category. In the test plans, the Panel proposed to use predictive computer models to develop relevant physical chemical properties, and environmental fate data.

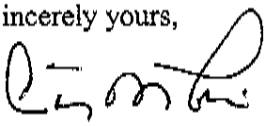
With this letter, the Panel submits robust summaries for modeling and calculations outlined in the test plan for the High Benzene Naphthas Category, as follows:

- Calculated Boiling Point Range
- Calculated Hydrolysis (Stability in Water)
- Calculated Melting Point Range
- Calculated Partition Coefficient
- Calculated Photodegradation (Direct)
- Calculated Photodegradation (indirect)
- Calculated Transport/Distribution (Fugacity)
- Calculated Vapor Pressure Range
- Calculated Water Solubility Range

The Panel plans to submit a report on the category in 2004.

If you have any questions, please contact Dr. Elizabeth Moran, Manager of the Olefins Panel at 301 924 2006 or Elizabeth_Moran@americanchemistry.com.

Sincerely yours,



Courtney M. Price
Vice President, CHEMSTAR

Attachments
cc: R. Hefter (EPA)

Boiling Point (Range)

201-14657A

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E560

HIGH BENZENE NAPHTHAS ROBUST SUMMARY

Boiling Point

Test Substance*:	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]
Method/Guideline:	Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Pressure:	760 mm Hg
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Boiling Point is calculated by the MPBPWIN subroutine, which is based on the calculation method of S. Stein and R. Brown in "Estimation of Normal Boiling Points from Group Contributions". 1994. J. Chem. Inf. Comput. Sci. 34: 581-587.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Calculated and measured boiling point data for representative constituents of the High Benzene Naphthas Category are listed below. The data identify a potential boiling point range for substances represented by the 19 CAS numbers under Test Substance. Substances in this category do not have a specific boiling point value. Actual boiling point ranges for substances in this category will vary dependent on their constituent composition. Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C11. The 12 chemicals selected to represent the boiling point range of this category are C5-C10 hydrocarbons that can be found in substances identified by the 19 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.

Boiling Point (Range)

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6
Robust Summary No.: OP E560

Results: (continued)

Units/Value:

Note: Deviations from protocol or guideline, analytical method.

Substance Constituent	Calculated BP (°C)	Measured* BP (°C)
Isoprene	34.95	34.0
n-pentane	46.01	36.0
1,3-cyclopentadiene	69.17	41.0
Isohexane	56.26	63.2
n-hexane	71.53	68.7
methylcyclopentane	80.34	71.8
benzene	102.24	80.0
toluene	125.72	110.6
m-xylene	148.29	139.1
styrene	146.65	145.0
dicyclopentadiene	176.78	170.0
naphthalene	231.64	217.9

* Experimental values from EPIWIN database.
The data represent a potential boiling point range for substances represented by the 19 CAS numbers under Test Substance.

Test Substance:

The High Benzene Naphthas Category includes the following CAS numbers:

64741-99-7	Extracts, petroleum, light naphtha solvent
64742-49-0	Naphtha, petroleum, hydrotreated light
64742-73-0	Naphtha, petroleum, hydrodesulfurized light
64742-83-2	Naphtha, petroleum, light steam-cracked
64742-91-2	Distillates, petroleum, steam-cracked
67891-79-6	Distillates, petroleum, heavy aromatic
67891-80-9	Distillates, petroleum, light aromatic
68410-97-9	Distillates, petroleum, light distillate hydrotreating process, low-boiling
68475-70-7	Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived
68476-45-9	Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product
68526-77-2	Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum
68606-10-0	Gasoline, pyrolysis, debutanizer bottoms
68606-28-0	Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic
68921-67-5	Hydrocarbons, ethylene-manufacture-by-product distillation residues
68955-29-3	Distillates, petroleum, light thermal cracked, debutanized aromatic
68956-52-5	Hydrocarbons, C4-8
68956-70-7	Petroleum products, C5-12, reclaimed, wastewater treatment
69013-21-4	Fuel oil, pyrolysis
8030-30-6	Naphtha

Boiling Point (Range)

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E560

	High Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 19 CAS numbers are used to describe the ten process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%. More information on the High Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	The calculated boiling points for some representative constituents that are present in the category streams vary from 34.95 to 231.64°C @ 760 mm Hg. The measured boiling points of these same constituents vary from 34.0 to 217.9°C @ 760 mm Hg. Although this does not define the actual boiling points of the category streams, it offers an indication of a range that might be expected to encompass the boiling points of these complex streams with variable compositions. Boiling points outside of these ranges may be possible for some category streams.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential boiling point range for substances represented by the 19 CAS numbers listed under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in High Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for boiling point range based on constituent data.
Reference:	EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Boiling point values were calculated by the MPBPWIN subroutine and measured data came from the database in the computer program.)
Other (source):	American Chemistry Council, Olefins Panel (Prepared 7/03)

Boiling Point (Range)

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E560

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Boiling Point. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E568

HIGH BENZENE NAPHTHAS ROBUST SUMMARY

Photodegradation (Direct)

Test Substance*:	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]
Method/Guideline:	Other: Technical discussion
Year (guideline):	Not applicable
GLP (Y/N):	Not applicable
Year (study performed):	Not applicable
Type (air, soil, water, other):	Water
Light Source:	Not applicable
Light Spectrum: • **Wave length value (upper/lower)**	Not applicable
Relative Intensity:	Not applicable
Test Substance Spectrum:	Not applicable
Test Conditions: • **Note: Concentration, temperature, test system type, replication, deviations from guideline or protocol**	Not applicable
Direct Photolysis:** • **Results: half-life, % degradation, quantum yield**	**Summary** In the environment, direct photolysis will not significantly contribute to the degradation of constituent chemicals in the High Benzene Naphthas Category. The High Benzene Naphthas Category includes ten process streams: • **Pyrolysis Gasoline** • **Pyrolysis C6 Fraction** • **Pyrolysis C6-C8 Fraction** • **Pyrolysis C5-C6 Fraction** • **Hydrotreated C6 Fraction**

- **Hydrotreated C6-C7 Fraction**
- **Hydrotreated C6-C8 Fraction**
- **Quench Loop Pyrolysis Oil and Compressor Oil**
- **Recovered Oil from Waste Water Treatment**
- **Extract from Benzene Extraction**

Nineteen CAS numbers (see Test Substance) identify products derived from these process streams. As discussed below, the reaction process involved in direct photolysis occurs when sufficient light energy excites a molecule to the degree that a structural transformation occurs. In general, substances in this category do not contain component chemicals that will undergo direct photolysis.

The High Benzene Naphthas Category

A process stream is a mixture of chemicals that arises from a chemical reaction or separation activity. The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%. In some cases, petroleum refinery streams may be combined with intermediate streams from the ethylene unit and co-processed to produce these products. This grouping of CAS numbers represents hydrocarbon streams with a carbon number distribution that is predominantly C5-C11, through components boiling at 650°F or higher. That is why this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated High Benzene Naphthas.

The definitions found in the TSCA Chemical Substance Inventory for the CAS numbers included in this group are vague with respect to composition. Therefore, it is possible to find that the same CAS number is correctly used to describe different streams (compositions) or that two or more different CAS numbers are used to describe the same stream (composition or process).

More information on the High Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). The plan is available on the U.S. Environmental Protection Agency website under the HPV Chemical Program. A brief description of the production and composition of the ten process streams in this category are:

- **Pyrolysis Gasoline** (Pygas) consists predominantly of C5+ hydrocarbons produced by the ethylene cracking furnaces. Typically the stream is derived from (1) the bottoms product from the debutanizer, (2) oils separated from furnace effluent quench systems, and (3) “drips” or condensate resulting from compression of the cracked gas. The oils from the quench systems and the “drips” may be stabilized to remove lights before blending with Pygas from the other sources. Depending on the plant configuration, Pygas may contain all of these intermediate streams, or the quench oils and stabilized drips may be

transferred as separate streams. Low concentrations (e.g. 3% total) of C4 and lighter hydrocarbons may be present in the stream. A detailed analysis of Pygas may identify 60 or more hydrocarbon components or component groups, primarily unsaturated hydrocarbons and aromatics. Benzene, toluene, and dicyclopentadiene together may account for more than 50% of a Pygas stream and typically no other single component is present at a level greater than about 5%. The benzene concentration of Pygas is typically about 40% and the reported values range from 15 to 62%. The concentrations of individual hydrocarbon components in Pygas vary depending on the type of feedstock used by the ethylene plant, the mode of operation of the cracking furnaces (i.e. severity) and the ethylene process configuration. One non-typical Pygas stream is reported to contain vinylacetate at a concentration of up to about 10%. Vinylacetate is not typically found in ethylene process streams.

- **Pyrolysis Gasoline Fractions (C5-C6, C6, and C6-C8 Fractions)** are separated by distillation into various boiling-point range fractions as intermediates in preparation for further processing. In some cases, petroleum refinery streams such as a C6 reformate fraction are combined with the pyrolysis gasoline prior to this separation. Similar to the situation for Pygas, the composition of these fractions vary depending on the ethylene process feedstock and the other operating variables.

  1. **Pyrolysis C5-C6 Fraction** has a carbon number distribution that is predominantly C5 to C6. One typical composition for this stream is reported as 70% benzene and 10% pentenes.

  2. **Pyrolysis C6 Fraction** has a carbon number distribution that is predominantly C6. Reported compositions vary from 35 to 77% benzene, 0.5 to 5% toluene with the balance primarily C6 non-aromatics, which are expected to be largely unsaturates.

  3. **Pyrolysis C6-C8 Fraction** has a carbon number distribution that is predominantly C6 to C8. The reported compositions range from 30 to 80% benzene, 15 to 25% toluene and 3 to 23% C8 aromatics.

- **Hydrotreated Pyrolysis Fractions (C6, C6-C7, and C6-C8 Fractions)** are Pyrolysis gasoline or distillate fractions of pyrolysis gasoline that are treated with hydrogen over catalyst to saturate or partially saturate diolefins and/or olefins. In some cases, petroleum refinery streams such as a C6 reformate fraction are combined with the pyrolysis gasoline prior to this step. The hydrogenation process may be either one-stage or two-stage. The one-stage process is typically a liquid-phase process where the primary objective is to selectively convert diolefins to mono-olefins and to convert vinyl aromatics, for

	example, styrene to ethylbenzene. The second stage in a two-stage hydrogenation process is typically a vapor-phase, more severe hydrogenation that converts essentially all of the contained olefins to saturated hydrocarbons. A pygas fraction that will be processed by extraction or extractive distillation to produce high purity aromatics (benzene, toluene, or xylenes) is subjected to two-stage hydrogenation. Pygas fractions may be forwarded to hydrodealkylation units (less common) for benzene production after one-stage of hydrogenation. Hydrotreated Pyrolysis fractions may be the result of either one- or two-stage hydrogenation. 1. **Hydrotreated C6 Fraction** is very similar to the Pyrolysis C6 fraction except that the non-aromatics present in the hydrotreated stream are essentially all saturates. The reported composition for the Hydrotreated C6 stream indicates typical benzene content of 75%. 2. **Hydrotreated C6-C7 Fraction** has a carbon number distribution that is predominantly C6-C7 and the reported values indicate 40 to 70% benzene, and 3 to 15% toluene. 3. **Hydrotreated C6-C8 Fraction** has a reported typical composition of 40 to 60% benzene, 10 to 25% toluene, and 3 to 10% C8 aromatics. • **Quench Loop Pyrolysis Oil and Compressor Oil** (Pyoil) represents higher boiling hydrocarbons that condense in the water quench system of an ethylene plant, typically at an ethylene unit cracking ethane, propane or butane. The stream can also include liquids collected at the cracked gas compressor knock out drums, which may include compressor injection oil. The carbon number distribution for Pyoil is C4 (or even lower) through heavier hydrocarbons such as naphthalene or even heavier. The reported typical composition includes 10 to 22% benzene and 5 to 11% toluene. • **Recovered Oil from Wastewater Treatment** can be expected to be of variable composition and made up largely of the components found in Pygas. No composition data or process specific information has been reported. Typically, water streams at ethylene units are processed to separate hydrocarbons from the water so that the water can be reused to generate steam for process-contact use (dilution steam for the cracking furnaces) or so that excess water can be forwarded to treatment prior to discharge or reuse. Water processing typically includes mechanical and gravity separation and steam or gas stripping. Hydrocarbons separated from the water in these systems are not usually isolated from the process. However, at least in one case, the Recovered Oil from Wastewater Treatment has been reported as an isolated intermediate.

- **Extract from Benzene Extraction** are hydrotreated pyrolysis fractions containing aromatics (most commonly benzene or benzene and toluene) which are typically charged to extraction or extractive distillation units where the mixed aromatics are recovered. The carbon number distribution for this stream is predominantly C6 to C8. A reported typical concentration indicates 60 to 75% benzene, 25 to 40% toluene and 0 to 1% xylenes.

Photolysis of Hydrocarbons

The direct photolysis of an organic molecule occurs when it absorbs sufficient light energy to result in a structural transformation (2). The reaction process is initiated when light energy in a specific wavelength range elevates a molecule to an electronically excited state. However, the excited state is competitive with various deactivation processes that can result in the return of the molecule to a non excited state.

The absorption of light in the ultra violet (UV)-visible range, 110-750 nm, can result in the electronic excitation of an organic molecule. Light in this range contains energy of the same order of magnitude as covalent bond dissociation energies (2). Higher wavelengths (e.g. infrared) result only in vibrational and rotational transitions, which do not tend to produce structural changes to a molecule.

The stratospheric ozone layer prevents UV light of less than 290 nm from reaching the earth's surface. Therefore, only light at wavelengths between 290 and 750 nm can result in photochemical transformations in the environment (2). Although the absorption of UV light in the 290-750 nm range is necessary, it is not always sufficient for a chemical to undergo photochemical degradation. Energy may be re-emitted from an excited molecule by mechanisms other than chemical transformation, resulting in no change to the parent molecule.

A conservative approach to estimating a photochemical degradation rate is to assume that degradation will occur in proportion to the amount of light wavelengths >290 nm absorbed by the molecule (3). Saturated hydrocarbons do not absorb light above 200 nm. Some characteristic absorbance maxima (λ_{max}) and associated molar absorptivities (ε) for selected unsaturated hydrocarbons are shown below (2):

	l below 290 nm		**l above 290 nm**	
Hydrocarbon	l_{max}	e	l_{max}	e
Ethylene	193	10,000	-	-
Benzene	255	215	-	-
Styrene	244	12,000	-	-
	282	450		
Naphthalene	221	100,000	311	250
	270	5,000		

Photodegradation (Direct)

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E568

	Olefins with one double bond, or two conjugated double bonds, which constitute the majority of the chemicals in the High Benzene Naphthas category, do not absorb appreciable light energy above 290 nm. The absorption of UV light to cause cis-trans isomerism about the double bond of an olefin occurs only if it is in conjugation with an aromatic ring (2). Products in the High Benzene Naphthas Category do not contain component molecules that will undergo direct photolysis. Therefore, this fate process will not contribute to a measurable degradative removal of chemical components in this category from the environment. **References** 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. Virginia, USA. 2. Harris, J. C. 1982. "Rate of Aqueous Photolysis," Chapter 8 in: W. J. Lyman, W. F. Reehl, and D. H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, USA. 3. Zepp, R. G. and D. M. Cline. 1977. Rates of Direct Photolysis in the Aqueous Environment, Environ. Sci. Technol., 11:359-366.
Indirect Photolysis:** • **Results: type of sensitizer, concentration of sensitizer, rate constant, % degradation, half-life**	Not applicable
Degradation Products:** • **Note: Identification, concentration**	Unknown

Photodegradation (Direct)

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E568

Test Substance:	The High Benzene Naphthas Category includes the following CAS numbers: 64741-99-7 Extracts, petroleum, light naphtha solvent 64742-49-0 Naphtha, petroleum, hydrotreated light 64742-73-0 Naphtha, petroleum, hydrodesulfurized light 64742-83-2 Naphtha, petroleum, light steam-cracked 64742-91-2 Distillates, petroleum, steam-cracked 67891-79-6 Distillates, petroleum, heavy aromatic 67891-80-9 Distillates, petroleum, light aromatic 68410-97-9 Distillates, petroleum, light distillate hydrotreating process, low-boiling 68475-70-7 Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived 68476-45-9 Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product 68526-77-2 Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum 68606-10-0 Gasoline, pyrolysis, debutanizer bottoms 68606-28-0 Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic 68921-67-5 Hydrocarbons, ethylene-manufacture-by-product distillation residues 68955-29-3 Distillates, petroleum, light thermal cracked, debutanized aromatic 68956-52-5 Hydrocarbons, C4-8 68956-70-7 Petroleum products, C5-12, reclaimed, wastewater treatment 69013-21-4 Fuel oil, pyrolysis 8030-30-6 Naphtha
Conclusion:	Not applicable
Reliability:	These data represent a key study for characterizing the potential of substances in the High Benzene Naphthas Category to undergo direct photodegradation.
Reference:	American Chemistry Council, Olefins Panel. 2003. Photodegradation (Direct): High Benzene Naphthas Category. Rosslyn, VA, USA.
Other (source):	American Chemistry Council, Olefins Panel (Prepared 7/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Photodegradation (Direct). Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E567

HIGH BENZENE NAPHTHAS ROBUST SUMMARY

Hydrolysis (Stability in Water)

Test Substance*:	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]
Method/Guideline:	Other: Technical discussion
Year (guideline):	Not applicable
Type (test type):	Not applicable
GLP (Y/N):	Not applicable
Year (study performed):	Not applicable
Analytical Monitoring:	Not applicable
Test Conditions: • **Note: Concentration preparation, vessel type, volume, replication, deviations from guideline or protocol**	Not applicable
Results: **Units/Value:** • **Note: Analytical method, observations, half-lives by pH, degradation products**	Not applicable
Test Substance:	The High Benzene Naphthas Category includes the following CAS numbers: 64741-99-7 Extracts, petroleum, light naphtha solvent 64742-49-0 Naphtha, petroleum, hydrotreated light 64742-73-0 Naphtha, petroleum, hydrodesulfurized light 64742-83-2 Naphtha, petroleum, light steam-cracked 64742-91-2 Distillates, petroleum, steam-cracked 67891-79-6 Distillates, petroleum, heavy aromatic 67891-80-9 Distillates, petroleum, light aromatic 68410-97-9 Distillates, petroleum, light distillate hydrotreating process, low-boiling

	68475-70-7 Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived 68476-45-9 Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product 68526-77-2 Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum 68606-10-0 Gasoline, pyrolysis, debutanizer bottoms 68606-28-0 Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic 68921-67-5 Hydrocarbons, ethylene-manufacture-by-product distillation residues 68955-29-3 Distillates, petroleum, light thermal cracked, debutanized aromatic 68956-52-5 Hydrocarbons, C4-8 68956-70-7 Petroleum products, C5-12, reclaimed, wastewater treatment 69013-21-4 Fuel oil, pyrolysis 8030-30-6 Naphtha High Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 19 CAS numbers are used to describe the ten process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%. More information on the High Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	**<u>Summary</u>** In the environment, hydrolysis will not contribute to the degradation of chemicals in the High Benzene Naphthas Category. The High Benzene Naphthas Category includes ten process streams: • **Pyrolysis Gasoline** • **Pyrolysis C6 Fraction** • **Pyrolysis C6-C8 Fraction** • **Pyrolysis C5-C6 Fraction** • **Hydrotreated C6 Fraction** • **Hydrotreated C6-C7 Fraction** • **Hydrotreated C6-C8 Fraction** • **Quench Loop Pyrolysis Oil and Compressor Oil** • **Recovered Oil from Waste Water Treatment** • **Extract from Benzene Extraction**

Nineteen CAS numbers (see Test Substance) identify substances derived from these process streams. As discussed below, the chemicals in these streams are composed of carbon and hydrogen and are not amenable to hydrolysis because of their molecular structure and the chemical reaction required for this type of transformation to occur.

The High Benzene Naphthas Category

A process stream is a mixture of chemicals that arises from a chemical reaction or separation activity. The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%. In some cases, petroleum refinery streams may be combined with intermediate streams from the ethylene unit and co-processed to produce these products. This grouping of CAS numbers represents hydrocarbon streams with a carbon number distribution that is predominantly C5-C11, through components boiling at 650°F or higher. That is why this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated High Benzene Naphthas.

The definitions found in the TSCA Chemical Substance Inventory for the CAS numbers included in this group are vague with respect to composition. Therefore, it is possible to find that the same CAS number is correctly used to describe different streams (compositions) or that two or more different CAS numbers are used to describe the same stream (composition or process).

More information on the High Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). The plan is available on the U.S. Environmental Protection Agency website under the HPV Chemical Program. A brief description of the production and composition of the ten process streams in this category are:

- **Pyrolysis Gasoline** (Pygas) consists predominantly of C5+ hydrocarbons produced by the ethylene cracking furnaces. Typically the stream is derived from (1) the bottoms product from the debutanizer, (2) oils separated from furnace effluent quench systems, and (3) “drips” or condensate resulting from compression of the cracked gas. The oils from the quench systems and the “drips” may be stabilized to remove lights before blending with Pygas from the other sources. Depending on the plant configuration, Pygas may contain all of these intermediate streams, or the quench oils and stabilized drips may be transferred as separate streams. Low concentrations (e.g. 3% total) of C4 and lighter hydrocarbons may be present in the stream. A detailed analysis of Pygas may identify 60 or more hydrocarbon components or component groups, primarily unsaturated hydrocarbons and aromatics. Benzene, toluene, and dicyclopentadiene together may account for more than 50% of a Pygas stream and typically no other single component is present

	at a level greater than about 5%. The benzene concentration of Pygas is typically about 40% and the reported values range from 15 to 62%. The concentrations of individual hydrocarbon components in Pygas vary depending on the type of feedstock used by the ethylene plant, the mode of operation of the cracking furnaces (i.e. severity) and the ethylene process configuration. One non-typical Pygas stream is reported to contain vinylacetate at a concentration of up to about 10%. Vinylacetate is not typically found in ethylene process streams. • **Pyrolysis Gasoline Fractions (C5-C6, C6, and C6-C8 Fractions)** are separated by distillation into various boiling-point range fractions as intermediates in preparation for further processing. In some cases, petroleum refinery streams such as a C6 reformate fraction are combined with the pyrolysis gasoline prior to this separation. Similar to the situation for Pygas, the composition of these fractions vary depending on the ethylene process feedstock and the other operating variables. 1. **Pyrolysis C5-C6 Fraction** has a carbon number distribution that is predominantly C5 to C6. One typical composition for this stream is reported as 70% benzene and 10% pentenes. 2. **Pyrolysis C6 Fraction** has a carbon number distribution that is predominantly C6. Reported compositions vary from 35 to 77% benzene, 0.5 to 5% toluene with the balance primarily C6 non-aromatics, which are expected to be largely unsaturates. 3. **Pyrolysis C6-C8 Fraction** has a carbon number distribution that is predominantly C6 to C8. The reported compositions range from 30 to 80% benzene, 15 to 25% toluene and 3 to 23% C8 aromatics. • **Hydrotreated Pyrolysis Fractions (C6, C6-C7, and C6-C8 Fractions)** are Pyrolysis gasoline or distillate fractions of pyrolysis gasoline that are treated with hydrogen over catalyst to saturate or partially saturate diolefins and/or olefins. In some cases, petroleum refinery streams such as a C6 reformate fraction are combined with the pyrolysis gasoline prior to this step. The hydrogenation process may be either one-stage or two-stage. The one-stage process is typically a liquid-phase process where the primary objective is to selectively convert diolefins to mono-olefins and to convert vinyl aromatics, for example, styrene to ethylbenzene. The second stage in a two-stage hydrogenation process is typically a vapor-phase, more severe hydrogenation that converts essentially all of the contained olefins to saturated hydrocarbons. A pygas fraction that will be processed by extraction or extractive distillation to produce high purity aromatics (benzene, toluene, or xylenes) is subjected to two-stage hydrogenation. Pygas fractions may be

	forwarded to hydrodealkylation units (less common) for benzene production after one-stage of hydrogenation. Hydrotreated Pyrolysis fractions may be the result of either one- or two-stage hydrogenation. 1. **Hydrotreated C6 Fraction** is very similar to the Pyrolysis C6 fraction except that the non-aromatics present in the hydrotreated stream are essentially all saturates. The reported composition for the Hydrotreated C6 stream indicates typical benzene content of 75%. 2. **Hydrotreated C6-C7 Fraction** has a carbon number distribution that is predominantly C6-C7 and the reported values indicate 40 to 70% benzene, and 3 to 15% toluene. 3. **Hydrotreated C6-C8 Fraction** has a reported typical composition of 40 to 60% benzene, 10 to 25% toluene, and 3 to 10% C8 aromatics. • **Quench Loop Pyrolysis Oil and Compressor Oil** (Pyoil) represents higher boiling hydrocarbons that condense in the water quench system of an ethylene plant, typically at an ethylene unit cracking ethane, propane or butane. The stream can also include liquids collected at the cracked gas compressor knock out drums, which may include compressor injection oil. The carbon number distribution for Pyoil is C4 (or even lower) through heavier hydrocarbons such as naphthalene or even heavier. The reported typical composition includes 10 to 22% benzene and 5 to 11% toluene. • **Recovered Oil from Wastewater Treatment** can be expected to be of variable composition and made up largely of the components found in Pygas. No composition data or process specific information has been reported. Typically, water streams at ethylene units are processed to separate hydrocarbons from the water so that the water can be reused to generate steam for process-contact use (dilution steam for the cracking furnaces) or so that excess water can be forwarded to treatment prior to discharge or reuse. Water processing typically includes mechanical and gravity separation and steam or gas stripping. Hydrocarbons separated from the water in these systems are not usually isolated from the process. However, at least in one case, the Recovered Oil from Wastewater Treatment has been reported as an isolated intermediate. • **Extract from Benzene Extraction** are hydrotreated pyrolysis fractions containing aromatics (most commonly benzene or benzene and toluene) which are typically charged to extraction or extractive distillation units where the mixed aromatics are recovered. The carbon number distribution for this stream is predominantly C6 to C8. A reported typical concentration indicates 60 to 75% benzene, 25 to 40% toluene and 0 to 1%

xylenes.

Hydrolysis of Hydrocarbons as a Function of Molecular Structure

Hydrolysis of an organic molecule occurs when a molecule (R-X) reacts with water (H_2O) to form a new carbon-oxygen bond after the carbon-X bond is cleaved (2,3). Mechanistically, this reaction is referred to as a nucleophilic substitution reaction, where X is the leaving group being replaced by the incoming nucleophilic oxygen from the water molecule. The leaving group, X, must be a molecule other than carbon because for hydrolysis to occur, the R-X bond cannot be a carbon-carbon bond.

The carbon atom lacks sufficient electronegativity to be a good leaving group and carbon-carbon bonds are too stable (high bond energy) to be cleaved by nucleophilic substitution. Thus, hydrocarbons, including alkenes, are not subject to hydrolysis (3) and this fate process will not contribute to the degradative loss of chemical components in this category from the environment.

Under strongly acidic conditions the carbon-carbon double bond found in alkenes, such as those in the High Benzene Naphthas Category, will react with water by an addition reaction mechanism (2). The reaction product is an alcohol. This reaction is not considered to be hydrolysis because the carbon-carbon linkage is not cleaved and because the reaction is freely reversible (3). Substances that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (4).

The substances in the High Benzene Naphthas Category are primarily olefins that contain at least one double bond (alkenes). The remaining chemicals are saturated hydrocarbons (alkanes). These two groups of chemicals contain only carbon and hydrogen. As such, their molecular structure is not subject to the hydrolytic mechanism discussed above. Therefore, chemicals in the High Benzene Naphthas Category have a very low potential to hydrolyze, and this degradative process will not contribute to their removal in the environment.

References

1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
2. Gould, E.S. (1959), Mechanism and Structure in Organic Chemistry, Holt, Reinhart and Winston, New York, NY, USA.
3. Harris, J.C. (1982), "Rate of Hydrolysis," Chapter 7 in: W.J. Lyman, W.F. Reehl, and D.H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, NY, USA.
4. Neely, W. B. 1985. Hydrolysis. In: W. B. Neely and G. E. Blau, eds.

Hydrolysis (Stability in Water)

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E567

	Environmental Exposure from Chemicals. Vol I., pp. 157-173. CRC Press, Boca Raton, FL, USA.
Reliability:	These data represent a key study for characterizing the potential of substances in the High Benzene Naphthas Category to undergo hydrolysis.
Reference:	American Chemistry Council, Olefins Panel. 2003. Hydrolysis High Benzene Naphthas Category. Rosslyn, VA, USA.
Other (source):	American Chemistry Council, Olefins Panel (Prepared 7/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Hydrolysis. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E570

HIGH BENZENE NAPHTHAS ROBUST SUMMARY

Photodegradation (Indirect)

Test Substance*:	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]
Method/Guideline:	Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
GLP (Y/N):	Not applicable
Year (study performed):	Not applicable
Type (air, soil, water, other):	Not applicable
Light Source:	Sunlight
Light Spectrum: • **Wave length value (upper/lower)**	Natural sunlight
Relative Intensity:	1
Test Substance Spectrum:	Not applicable
Test Conditions: • **Note: Concentration, temperature, test system type, replication, deviations from guideline or protocol**	Indirect photodegradation, or atmospheric oxidation potential, is based on the structure-activity relationship methods developed by R. Atkinson. Temperature: 25°C Sensitizer: OH radical Concentration of Sensitizer: 1.5 E^6 OH radicals/cm^3
Direct Photolysis:** **Results: half-life, % degradation, quantum yield**	Not applicable

Photodegradation (Indirect)

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E570

Indirect Photolysis:** • **Results: type of sensitizer, concentration of sensitizer, rate constant, % degradation, half-life**	**The High Benzene Naphthas Category** High Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 19 CAS numbers are used to describe the ten process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%. Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C11. That is why this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated High Benzene Naphthas. The 12 chemicals selected to represent the atmospheric oxidation potential of this category are C5-C10 hydrocarbons that can be found in substances identified by the 19 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge. **Atmospheric Oxidation of Hydrocarbons** In the environment, organic chemicals emitted into the troposphere are degraded by several important transformation processes. The dominant transformation process for most compounds is the daylight reaction with hydroxyl (OH-) radicals (Atkinson, 1988, 1989). The rate at which an organic compound reacts with OH-radicals is a direct measure of its atmospheric persistence (Meylan and Howard, 1993). AOPWIN estimates the rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. The rate constants estimated by the program are then used to calculate atmospheric half-lives for organic compounds based upon average atmospheric concentrations of hydroxyl radicals. Since the reactions only take place in the presence of sunlight, the atmospheric half-lives are normalized for a 12-hour day.

Photodegradation (Indirect)

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E570

Indirect Photolysis: (cont'd)** **Results: type of sensitizer, concentration of sensitizer, rate constant, % degradation, half-life**	<table><tr><th>Chemical</th><th>Calculated* half-life (hrs)</th><th>OH- Rate Constant (cm^3/molecule-sec)</th></tr><tr><td>Isoprene</td><td>1.2</td><td>105.1 E^{-12}</td></tr><tr><td>n-pentane</td><td>31.7</td><td>4.0 E^{-12}</td></tr><tr><td>1,3-cyclopentadiene</td><td>0.9</td><td>142.6 E^{-12}</td></tr><tr><td>Isohexane</td><td>22.4</td><td>5.7 E^{-12}</td></tr><tr><td>n-hexane</td><td>23.5</td><td>5.5 E^{-12}</td></tr><tr><td>methylcyclopentane</td><td>22.7</td><td>5.7 E^{-12}</td></tr><tr><td>benzene</td><td>65.8</td><td>1.9 E^{-12}</td></tr><tr><td>toluene</td><td>24.6</td><td>5.2 E^{-12}</td></tr><tr><td>m-xylene</td><td>9.5</td><td>13.6 E^{-12}</td></tr><tr><td>styrene</td><td>4.6</td><td>28.1 E^{-12}</td></tr><tr><td>dicyclopentadiene</td><td>1.1</td><td>119.2 E^{-12}</td></tr><tr><td>naphthalene</td><td>5.9</td><td>21.6 E^{-12}</td></tr></table> * Atmospheric half-life values are based on a 12-hr day. More information on the High Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (Olefins Panel, 2001). References: 1. Atkinson, R. 1988. Estimation of gas-phase hydroxyl radical rate constants for organic chemicals. *Environ. Toxicol. Chem*. **7**:435-442. 2. Atkinson, R. 1989. Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds. J. Phys. Chem. Ref. Data Monograph No. 1, Amer. Inst. Physics & Amer. Chem. Soc., NY. 3. Meylan, W.M. and P.H. Howard. 1993. Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. *Chemosphere* **12**:2293-2299. 4. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Degradation Products:** • **Note: Identification, concentration**	Unknown

Photodegradation (Indirect)

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E570

Test Substance:	The High Benzene Naphthas Category includes the following CAS numbers: 64741-99-7 Extracts, petroleum, light naphtha solvent 64742-49-0 Naphtha, petroleum, hydrotreated light 64742-73-0 Naphtha, petroleum, hydrodesulfurized light 64742-83-2 Naphtha, petroleum, light steam-cracked 64742-91-2 Distillates, petroleum, steam-cracked 67891-79-6 Distillates, petroleum, heavy aromatic 67891-80-9 Distillates, petroleum, light aromatic 68410-97-9 Distillates, petroleum, light distillate hydrotreating process, low-boiling 68475-70-7 Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived 68476-45-9 Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product 68526-77-2 Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum 68606-10-0 Gasoline, pyrolysis, debutanizer bottoms 68606-28-0 Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic 68921-67-5 Hydrocarbons, ethylene-manufacture-by-product distillation residues 68955-29-3 Distillates, petroleum, light thermal cracked, debutanized aromatic 68956-52-5 Hydrocarbons, C4-8 68956-70-7 Petroleum products, C5-12, reclaimed, wastewater treatment 69013-21-4 Fuel oil, pyrolysis 8030-30-6 Naphtha
Conclusion:	Atmospheric oxidation via hydroxyl radicals can be a significant route of degradation for products in this category. Based on calculated values, products in this category can have an atmospheric half-life range of 0.9 to 65.8 hours as a result of indirect photolysis by hydroxyl radical attack.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by AOPWIN. The data represent a potential atmospheric half-life range for substances represented by the 19 CAS numbers under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the High Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for atmospheric half-life range based on constituent data.

Photodegradation (Indirect)

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E570

Reference:	Meylan, M., SRC 1994-1999. AOPWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
Other (source):	American Chemistry Council, Olefins Panel (Prepared 10/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Photodegradation (Indirect). Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

** In IUCLID, provide additional discussion if needed in the results freetext

Partition Coefficient (Range)

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E563

HIGH BENZENE NAPHTHAS ROBUST SUMMARY

Partition Coefficient

Test Substance*:	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]
Method/Guideline:	Calculated values using KOWWIN version 1.65, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Octanol / Water Partition Coefficient is calculated by the KOWWIN subroutine, which is based on an atom/fragment contribution method of W. Meylan and P. Howard in "Atom/fragment contribution method for estimating octanol-water partition coefficients". 1995. *J. Pharm. Sci*. 84:83-92.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Calculated and measured log K_{ow} data for representative constituents of the High Benzene Naphthas Category are listed below. The data identify a potential log K_{ow} range for substances represented by the 19 CAS numbers under Test Substance. Substances in this category do not have a specific log K_{ow} value. Actual log K_{ow} ranges for substances in this category will vary dependent on their constituent composition. Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C11. The 12 chemicals selected to represent the log K_{ow} range of this category are C5-C10 hydrocarbons that can be found in substances identified by the 19 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.

Partition Coefficient (Range)

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E563

Results: (continued)

Units/Value:

Note: Deviations from protocol or guideline, analytical method.

Substance Constituent	Calculated log K_{ow} @ 25°C	Measured* log K_{ow} @ 25°C
Isoprene	2.58	2.42
n-pentane	2.80	3.39
1,3-cyclopentadiene	2.25	na
Isohexane	3.21	3.60
n-hexane	3.29	3.90
methylcyclopentane	3.10	3.37
benzene	1.99	2.13
toluene	2.54	2.73
m-xylene	3.09	3.20
styrene	2.89	2.95
dicyclopentadiene	3.16	na
naphthalene	3.17	3.30

* Experimental values from EPIWIN database.
na = not available
The data represent a potential log K_{ow} range for substances represented by the 19 CAS numbers under Test Substance.

Test Substance:

The High Benzene Naphthas Category includes the following CAS numbers:

64741-99-7	Extracts, petroleum, light naphtha solvent
64742-49-0	Naphtha, petroleum, hydrotreated light
64742-73-0	Naphtha, petroleum, hydrodesulfurized light
64742-83-2	Naphtha, petroleum, light steam-cracked
64742-91-2	Distillates, petroleum, steam-cracked
67891-79-6	Distillates, petroleum, heavy aromatic
67891-80-9	Distillates, petroleum, light aromatic
68410-97-9	Distillates, petroleum, light distillate hydrotreating process, low-boiling
68475-70-7	Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived
68476-45-9	Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product
68526-77-2	Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum
68606-10-0	Gasoline, pyrolysis, debutanizer bottoms
68606-28-0	Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic
68921-67-5	Hydrocarbons, ethylene-manufacture-by-product distillation residues
68955-29-3	Distillates, petroleum, light thermal cracked, debutanized aromatic
68956-52-5	Hydrocarbons, C4-8
68956-70-7	Petroleum products, C5-12, reclaimed, wastewater treatment
69013-21-4	Fuel oil, pyrolysis
8030-30-6	Naphtha

Partition Coefficient (Range)

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E563

	High Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 19 CAS numbers are used to describe the ten process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%. More information on the High Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	The calculated log K_{ow} for some representative constituents that are present in the category streams vary from 1.99 to 3.29 @ 25°C. The measured log K_{ow} of these same constituents vary from 2.13 to 3.90 @ 25°C. Although this does not define the actual log K_{ow} of the category streams, it offers an indication of a range that might be expected to encompass the log K_{ow} of these complex streams with variable compositions. Log K_{ow} values outside of these ranges may be possible for some category streams.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential log K_{ow} range for substances represented by the 19 CAS numbers under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the High Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for log K_{ow} range based on constituent data.
Reference:	EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Log K_{ow} values were calculated by the KOWWIN subroutine and measured data came from the database in the computer program.)
Other (source):	American Chemistry Council, Olefins Panel (Prepared 7/03)

Partition Coefficient (Range)

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E563

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Partition Coefficient. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

Melting Point (Range)

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6
Robust Summary No.: OP E561

HIGH BENZENE NAPHTHAS ROBUST SUMMARY

Melting Point

Test Substance*:	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]
Method/Guideline:	Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Melting Point is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of K. Joback and Gold and Ogle. Joback's Method is described in Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds. The Gold and Ogle Method simply uses the formula Tm = 0.5839Tb, where Tm is the melting point in Kelvin and Tb is the boiling point in Kelvin. The Gold and Ogle Method is described by Lyman, W.J., 1985, In: Environmental Exposure from Chemicals. Volume 1. Neely, W.B. and Blau, G.E. (eds), Boca Raton, FL, CRC Press, Inc., Chapter 2.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Calculated and measured melting point data for representative constituents of the High Benzene Naphthas Category are listed below. The data identify a potential melting point range for substances represented by the 19 CAS numbers under Test Substance. Substances in this category do not have a specific melting point value. Actual melting point ranges for substances in this category will vary dependent on their constituent composition. Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C11. The 12 chemicals selected to represent the melting point range of this category are C5-C10 hydrocarbons that can be found in substances identified by the 19 CAS numbers. Constituents representing category members were selected on the basis of

Melting Point (Range)

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6
Robust Summary No.: OP E561

Results: (continued)

Units/Value:

Note: Deviations from protocol or guideline, analytical method.

carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.

Substance Constituent	Calculated MP (°C)	Measured* MP (°C)
Isoprene	-118.89	-145.9
n-pentane	-106.92	-129.7
1,3-cyclopentadiene	-91.83	-85.0
Isohexane	-105.80	-162.9
n-hexane	-93.84	-95.3
methylcyclopentane	-85.82	-142.5
benzene	-77.92	5.5
toluene	-59.17	-94.9
m-xylene	-40.69	-47.8
styrene	-48.31	-31.0
dicyclopentadiene	-16.78	32.0
naphthalene	5.01	80.2

* Experimental values from EPIWIN database.
The data represent a potential melting point range for substances represented by the 19 CAS numbers under Test Substance.

Test Substance:

The High Benzene Naphthas Category includes the following CAS numbers:

64741-99-7	Extracts, petroleum, light naphtha solvent
64742-49-0	Naphtha, petroleum, hydrotreated light
64742-73-0	Naphtha, petroleum, hydrodesulfurized light
64742-83-2	Naphtha, petroleum, light steam-cracked
64742-91-2	Distillates, petroleum, steam-cracked
67891-79-6	Distillates, petroleum, heavy aromatic
67891-80-9	Distillates, petroleum, light aromatic
68410-97-9	Distillates, petroleum, light distillate hydrotreating process, low-boiling
68475-70-7	Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived
68476-45-9	Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product
68526-77-2	Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum
68606-10-0	Gasoline, pyrolysis, debutanizer bottoms
68606-28-0	Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic
68921-67-5	Hydrocarbons, ethylene-manufacture-by-product distillation residues
68955-29-3	Distillates, petroleum, light thermal cracked, debutanized aromatic
68956-52-5	Hydrocarbons, C4-8
68956-70-7	Petroleum products, C5-12, reclaimed, wastewater treatment
69013-21-4	Fuel oil, pyrolysis
8030-30-6	Naphtha

Melting Point (Range)

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6
Robust Summary No.: OP E561

Test Substance: (continued)	High Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 19 CAS numbers are used to describe the ten process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%. More information on the High Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	The calculated melting points for some representative constituents that are present in the category streams vary from -118.89 to 5.01 °C. The measured melting points of these same constituents vary from -162.9 to 80.2°C. Although this does not define the actual melting points of the category streams, it offers an indication of a range that might be expected to encompass the melting points of these complex streams with variable compositions. Melting points outside of these ranges may be possible for some category streams.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential melting point range for substances represented by the 19 CAS numbers listed under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the High Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for melting point range based on constituent data.
Reference:	EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Melting point values were calculated by the MPBPWIN subroutine and measured data came from the database in the computer program.)
Other (source):	American Chemistry Council, Olefins Panel (Prepared 7/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Melting Point. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6
Robust Summary No.: OP E569

HIGH BENZENE NAPHTHAS ROBUST SUMMARY

Transport / Distribution (Fugacity)

Test Substance*:	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]
Method/Guideline:	Calculated according to Mackay Level I, EQC Model version 1.01
Year (guideline):	1997
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment. Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.04 program (1). Measured input values were also used where available and obtained from the EPIWIN database (1). Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, sediment, suspended sediment, biota). 1. EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

Transport / Distribution (Fugacity)

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E569

Results:

Units/Value:

- **Note: Deviations from protocol or guideline, analytical method.**

Calculated partitioning data for representative constituents of the High Benzene Naphthas Category are listed below. The data identify a potential distribution for substances represented by the 19 CAS numbers under Test Substance. Actual distribution of substances in this category will vary dependent on their constituent composition.

Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C11. The 12 chemicals selected to represent the boiling point range of this category are C5-C10 hydrocarbons that can be found in substances identified by the 19 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.

The range of distribution data for constituent chemicals in each of the compartments can be used as an estimate of the partitioning behavior for category substances.

The following Mackay Level I model distribution values for representative constituents of substances in this category were determined using physicochemical input data calculated using the EPIWIN program:

	Calculated* Percent Distribution			
Chemical	Air	Water	Soil	Sediment
Isoprene	99.97	0.02	0.01	-
n-pentane	99.97	0.02	0.01	-
1,3-cyclopentadiene	99.93	0.06	0.01	-
Isohexane	99.96	0.02	0.02	-
n-hexane	99.95	0.02	0.02	-
methylcyclopentane	99.94	0.03	0.03	-
benzene	98.46	1.42	0.12	-
toluene	98.17	1.40	0.43	-
m-xylene	97.19	1.33	1.45	0.03
styrene	95.55	2.61	1.80	0.04
dicyclopentadiene	98.00	0.87	1.11	0.02
naphthalene	24.47	32.28	42.28	0.94

* Distribution values determined using calculated input data from EPIWIN program

Transport / Distribution (Fugacity)

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E569

Results: (cont'd)

Units/Value:

- **Note: Deviations from protocol or guideline, analytical method.**

	Measured** Percent Distribution			
Chemical	Air	Water	Soil	Sediment
Isoprene	99.96	0.03	0.01	-
n-pentane	99.99	0.01	-	-
1,3-cyclopentadiene	99.93	0.06	0.01	-
Isohexane	99.97	0.01	0.02	-
n-hexane	99.96	-	0.04	-
methylcyclopentane	99.95	0.02	0.03	-
benzene	98.89	1.00	0.11	-
toluene	98.80	0.81	0.39	-
m-xylene	97.91	0.86	1.20	0.03
styrene	96.65	1.85	1.46	0.04
dicyclopentadiene	98.55	0.63	0.80	0.02
naphthalene	42.27	20.56	36.33	0.81

** Distribution values determined using input data from the EPIWIN program experimental database

Test Substance:

The High Benzene Naphthas Category includes the following CAS numbers:

64741-99-7	Extracts, petroleum, light naphtha solvent
64742-49-0	Naphtha, petroleum, hydrotreated light
64742-73-0	Naphtha, petroleum, hydrodesulfurized light
64742-83-2	Naphtha, petroleum, light steam-cracked
64742-91-2	Distillates, petroleum, steam-cracked
67891-79-6	Distillates, petroleum, heavy aromatic
67891-80-9	Distillates, petroleum, light aromatic
68410-97-9	Distillates, petroleum, light distillate hydrotreating process, low-boiling
68475-70-7	Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived
68476-45-9	Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product
68526-77-2	Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum
68606-10-0	Gasoline, pyrolysis, debutanizer bottoms
68606-28-0	Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic
68921-67-5	Hydrocarbons, ethylene-manufacture-by-product distillation residues
68955-29-3	Distillates, petroleum, light thermal cracked, debutanized aromatic
68956-52-5	Hydrocarbons, C4-8
68956-70-7	Petroleum products, C5-12, reclaimed, wastewater treatment
69013-21-4	Fuel oil, pyrolysis
8030-30-6	Naphtha

Transport / Distribution (Fugacity)

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E569

	High Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 19 CAS numbers are used to describe the ten process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%. More information on the High Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	The partitioning data represent a potential distribution range for substances in the 19 CAS numbers listed under Test Substance. Substances in the High Benzene Naphthas Category are calculated to partition primarily to air with a small percentage partitioning to water, soil, and sediment. Relatively high vapor pressure and high water solubility largely control the partitioning behavior of constituent chemicals in substances from this category. The input data used to run the EQC Level I model included estimated values calculated by the EPIWIN program based on chemical structure and measured data from the EPIWIN database. A comparison of the distribution data developed using either all calculated input values or measured values where data were available indicate a similar partitioning behavior and support the use of the dataset for chemicals without any measured data.
Reliability:	(2) Reliable with restrictions The input data used to run the EQC Level I model include calculated and experimental values available through the EPIWIN program. The data represent a potential environmental distribution range for substances with the 19 CAS numbers listed under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the High Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for distribution range based on constituent data.

Transport / Distribution (Fugacity)

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E569

Reference:	Mackay, D.A. DiGuardo, S. Paterson, and C. Cowan. EQC Model Version 1.01. 1997. Available from the Environmental Modeling Centre, Trent University, Canada.
Other (source):	American Chemistry Council, Olefins Panel (Prepared 7/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Transport-Distribution. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

Vapor Pressure (Range)

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E562

HIGH BENZENE NAPHTHAS ROBUST SUMMARY

Vapor Pressure

Test Substance*:	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]
Method/Guideline:	Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Vapor Pressure is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of Antoine and Grain. Both methods use boiling point for the calculation. The Antoine Method is described in the Handbook of Chemical Property Estimation. Chapter 14. W.J. Lyman, W.F. Reehl and D.H. Rosenblatt, Eds. Washington, D.C.: American Chemical Society. 1990. A modified Grain Method is described on page 31 of Neely and Blau's Environmental Exposure from Chemicals, Volume 1, CRC Press. 1985.

Vapor Pressure (Range)

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E562

Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Calculated and measured vapor pressure data for representative constituents of the High Benzene Naphthas Category are listed below. The data identify a potential vapor pressure range for substances represented by the 19 CAS numbers under Test Substance. Substances in this category do not have a specific vapor pressure value. Actual vapor pressure ranges for substances in this category will vary dependent on their constituent composition. Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C11. The 12 chemicals selected to represent the vapor pressure range of this category are C5-C10 hydrocarbons that can be found in substances identified by the 19 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.

Substance Constituent	Calculated VP (hPa @ 25°C)	Measured* VP (hPa @ 25°C)
Isoprene	7.35 E^2	7.33 E^2
n-pentane	6.84 E^2	6.85 E^2
1,3-cyclopentadiene	5.69 E^2	5.80 E^2
Isohexane	2.48 E^2	2.53 E^2
n-hexane	2.00 E^2	2.01 E^2
methylcyclopentane	1.77 E^2	1.84 E^2
benzene	1.16 E^2	1.26 E^2
toluene	31.60	37.86
m-xylene	8.83	11.05
styrene	6.73	8.53
dicyclopentadiene	2.20	3.05
naphthalene	0.05	0.11

* Experimental values from EPIWIN database.
The data represent a potential vapor pressure range for substances represented by the 19 CAS numbers under Test Substance.

Vapor Pressure (Range)

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E562

Test Substance:	The High Benzene Naphthas Category includes the following CAS numbers: 64741-99-7 Extracts, petroleum, light naphtha solvent 64742-49-0 Naphtha, petroleum, hydrotreated light 64742-73-0 Naphtha, petroleum, hydrodesulfurized light 64742-83-2 Naphtha, petroleum, light steam-cracked 64742-91-2 Distillates, petroleum, steam-cracked 67891-79-6 Distillates, petroleum, heavy aromatic 67891-80-9 Distillates, petroleum, light aromatic 68410-97-9 Distillates, petroleum, light distillate hydrotreating process, low-boiling 68475-70-7 Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived 68476-45-9 Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product 68526-77-2 Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum 68606-10-0 Gasoline, pyrolysis, debutanizer bottoms 68606-28-0 Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic 68921-67-5 Hydrocarbons, ethylene-manufacture-by-product distillation residues 68955-29-3 Distillates, petroleum, light thermal cracked, debutanized aromatic 68956-52-5 Hydrocarbons, C4-8 68956-70-7 Petroleum products, C5-12, reclaimed, wastewater treatment 69013-21-4 Fuel oil, pyrolysis 8030-30-6 Naphtha High Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 19 CAS numbers are used to describe the ten process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%. More information on the High Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.

Vapor Pressure (Range)

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E562

Conclusion:	The calculated vapor pressures for some representative constituents that are present in the category streams vary from 0.05 to 7.35 E^2 hPa @ 25°C. The measured vapor pressures of these same constituents vary from 0.11 to 7.33 E^2 hPa @ 25°C. Although this does not define the actual vapor pressures of the category streams, it offers an indication of a range that might be expected to encompass the vapor pressures of these complex streams with variable compositions. Vapor pressure outside of these ranges may be possible for some category streams.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential vapor pressure range for substances represented by the 19 CAS numbers under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the High Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for vapor pressure range based on constituent data.
Reference:	EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Vapor pressure values were calculated by the MPBPWIN subroutine and measured data came from the database in the computer program.)
Other (source):	American Chemistry Council, Olefins Panel (Prepared 7/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Vapor Pressure. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

Water Solubility (Range)

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E564

HIGH BENZENE NAPHTHAS ROBUST SUMMARY

Water Solubility

Test Substance*:	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]
Method/Guideline:	Calculated values using WSKOWWIN version 1.36, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Water Solubility is calculated by the WSKOWWIN subroutine, which is based on a Kow correlation method described by W. Meylan, P. Howard and R. Boethling in "Improved method for estimating water solubility from octanol/water partition coefficient". *Environ. Toxicol. Chem*. 15:100-106. 1995.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Calculated and measured water solubility data for representative constituents of the High Benzene Naphthas Category are listed below. The data identify a potential water solubility range for substances represented by the 19 CAS numbers under Test Substance. Substances in this category do not have a specific water solubility value. Actual water solubility ranges for substances in this category will vary dependent on their loading rate (i.e., weight of test material added to a volume of water). Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C11. The 12 chemicals selected to represent the water solubility range of this category are C5-C10 hydrocarbons that can be found in substances identified by the 19 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.

Water Solubility (Range)

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E564

Results: (continued) **Units/Value:** **Note: Deviations from protocol or guideline, analytical method.**	Substance Constituent / Calculated WS (mg/L @ 25°C) / Measured WS* (mg/L @ 25°C) Isoprene 247.2 338.6 n-pentane 159.70 49.8 1,3-cyclopentadiene 470.6 na Isohexane 66.94 31.1 n-hexane 57.42 17.2 methylcyclopentane 83.95 49.4 benzene 2634.0 2000.0 toluene 832.7 573.1 m-xylene 258.4 207.2 styrene 386.7 343.7 dicyclopentadiene 51.9 na naphthalene 183.8 142.1 * Experimental values from EPIWIN database. na = not available The data represent a potential water solubility range for substances represented by the 19 CAS numbers under Test Substance.
Test Substance:	The High Benzene Naphthas Category includes the following CAS numbers: 64741-99-7 Extracts, petroleum, light naphtha solvent 64742-49-0 Naphtha, petroleum, hydrotreated light 64742-73-0 Naphtha, petroleum, hydrodesulfurized light 64742-83-2 Naphtha, petroleum, light steam-cracked 64742-91-2 Distillates, petroleum, steam-cracked 67891-79-6 Distillates, petroleum, heavy aromatic 67891-80-9 Distillates, petroleum, light aromatic 68410-97-9 Distillates, petroleum, light distillate hydrotreating process, low-boiling 68475-70-7 Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived 68476-45-9 Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product 68526-77-2 Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum 68606-10-0 Gasoline, pyrolysis, debutanizer bottoms 68606-28-0 Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic 68921-67-5 Hydrocarbons, ethylene-manufacture-by-product distillation residues 68955-29-3 Distillates, petroleum, light thermal cracked, debutanized aromatic 68956-52-5 Hydrocarbons, C4-8 68956-70-7 Petroleum products, C5-12, reclaimed, wastewater treatment 69013-21-4 Fuel oil, pyrolysis 8030-30-6 Naphtha

Water Solubility (Range)

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6
Robust Summary No.: OP E564

Test Substance: (cont'd)	High Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 19 CAS numbers are used to describe the ten process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%. More information on the High Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	The calculated water solubility for some representative constituents that are present in the category streams vary from 51.9 to 2634.0 mg/L @ 25°C. The measured water solubility of these same constituents vary from 17.2 to 2000.0 mg/L @ 25°C. Although this does not define the actual water solubility of the category streams, it offers an indication of a range that might be expected to encompass the water solubility of these complex streams with variable compositions. Water solubilities outside of these ranges may be possible for some category streams.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential water solubility range for substances represented by the 19 CAS numbers under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the High Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for water solubility range based on constituent data.
Reference:	EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Water solubility values were calculated by the WSKOWWIN subroutine and measured data came from the database in the computer program.)
Other (source):	American Chemistry Council, Olefins Panel (Prepared 7/03)

Water Solubility (Range)

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E564

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Water Solubility. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

COURTNEY M. PRICE
VICE PRESIDENT
CHEMSTAR

December 10, 2004

American Chemistry Council *Good Chemistry Makes It Possible*

The Honorable Michael O. Leavitt
Administrator
U.S. Environmental Protection Agency
P. O. Box 1473
Merrifield, VA 22116

RE: Olefins Panel Category Report for the High Benzene Naphthas Category Under the HPV Challenge Program: HPV Registration No. 1101064

Dear Administrator Leavitt:

On December 18, 2001, the American Chemistry Council Olefins Panel (Panel) submitted a Test Plan under the High Production Volume (HPV) Chemical Challenge Program pertaining to the High Benzene Naphthas Category. On August 7, 2003, the Panel submitted a revised Test Plan for this category. Robust summaries for modeling studies conducted for this category were submitted to EPA on January 11, 2004. With this letter, the Panel submits the Category Summary Report for the High Benzene Naphthas Category.

With the submission of this category report, the Panel has completed its commitment under the HPV Challenge Program for the High Benzene Naphthas category.

If you have any questions, please contact Elizabeth Moran, Manager of the Olefins Panel, at 301 924 2006 or Elizabeth_Moran@americanchemistry.com.

Sincerely Yours,

Attachment

US High Production Volume Chemical Program

Category Summary
For
High Benzene Naphthas Category

Prepared by:

Olefins Panel of the American Chemistry Council

December 10, 2004

EXECUTIVE SUMMARY

The Olefins Panel of the American Chemistry Council (ACC) hereby submits the category summary report for the High Benzene Naphthas Category under the U.S. Environmental Protection Agency's High Production Volume (HPV) Chemical Challenge Program. The purpose of this report is to:

- Present results of an assessment to determine whether the 19 CAS numbers which represent 10 production streams are adequately characterized with the existing data from hydrocarbon constituents of the production streams and analogous mixtures as described in the High Benzene Naphthas Category test plan.

- Summarize the SIDS (Screening Information Data Set) physicochemical, environmental fate and effects, and human health HPV program endpoints for the High Benzene Naphthas Category.

- Provide a description of manufacturing processes, potential exposure sources, and uses for High Benzene Naphtha streams.

- Demonstrate that the extensive body of data available for mammalian and environmental endpoints on representative constituents of products in this category, and streams of similar complex hydrocarbon composition, as well as some data on representative streams within the category are sufficient to fully define the High Benzene Naphthas Category.

The High Benzene Naphthas Category is composed of 10 ethylene manufacturing streams that exhibit commonalities of manufacturing process and composition. The 19 CAS numbers in this category each represent at least one of the category production streams. In some cases, a single CAS number represents more than one stream. The production streams consist of complex hydrocarbon reaction products, predominantly C5 through C11, through components boiling at 650^0F or higher, and may be correctly represented by more than one CAS number.

Pyrolysis gasoline is the major stream in this category and essentially all of the other category streams are derived from it, either as simple distillate fractions or hydrogenated distillate fractions. These streams all contain significant concentrations of benzene, generally greater than 10% and averaging 55%. They are the industry's intermediate streams that are processed to high purity benzene and other by-products. Pyrolysis gasoline and these fractions account for 99.9% of the category production. The remaining 0.1% of the category production consists of similar benzene-containing industry streams.

Exposure

The primary use of streams in the High Benzene Naphthas Category is the isolation of high purity benzene. There are no known consumer uses for these category streams. The streams are either used on the site where they were produced or shipped to other industrial sites for additional processing. Production is performed in closed systems and products are transported in bulk in closed systems by pipeline, barge, tank car or tank truck. The streams are typically inventoried in bulk storage tanks, either floating roof or fixed roof with vents routed to a control device in order to reduce emissions. Environmental exposure can occur through accidental spills, fugitive emissions, leakage or release of vapors into the atmosphere during tankage, delivery, or transfer for storage.

Exposure of workers is expected to be minimal because high benzene naphtha streams are isolated in production or used in closed system process units. Exposure could occur by inhalation of low-level concentrations of fugitive emissions from process units or storage tanks, from sampling, or by displaced emissions during loading of bulk transportation vessels, from emissions from control devices such as flares, or dermally by accidental spillage. The general population is not usually exposed to high benzene naphthas unless situated near industrial facilities that use or produce the category streams, but may be exposed to benzene through inhalation of contaminated ambient air, particularly in heavy traffic areas and around filling stations or in cigarette smoke-filled environments. The OSHA Benzene Standard applies to streams in the High Benzene Naphthas Category and limits occupational exposure. OSHA and ACGIH have established guidelines for other components (e.g. toluene, pentane, naphthalene, styrene) found in the category streams.

Human Health

Evaluation of data on representative streams and read-across from chemical components indicate that High Benzene Naphtha streams are not acutely toxic by the oral, dermal or inhalation routes of exposure. Data suggests that it is unlikely that most streams in this category would cause significant genetic toxicity. Tested streams did not cause mutational events in bacteria, and a weak direct effect in mammalian cells from treatment with a C5-C10 fraction of Pyrolysis gasoline was not confirmed *in vivo* by any expression of gene mutation in *Drosophila*. Although these streams contain substantial concentrations of benzene, a known clastogen, no cytogenetic damage was induced by oral treatment of rats with the Hydrogenated C6-C8 stream [55% benzene], demonstrating the inhibitory effects of other components in the stream, probably from competition for metabolic sites.

Benzene, as a predominant component in most streams is considered a key driver in establishing health effects within the SIDS battery of tests. To provide a conservative estimate of health hazard, results of benzene-induced systemic toxicity must be addressed – hazards from components should be considered hazards for the streams until sufficient data become available to show the specific combination of components does not present a hazard. However, as it has been demonstrated in the area of cytogenetics, the presence of biologically active components blended together can inhibit toxicity inducible by individual components. Repeated dose studies from 2 representative streams in the category reported skin irritation and concomitant effect on dermal tissue histologically [NOAEL<0.10ml/kg] but no other systemic toxicity in rabbits, and lethargy and labored respiration in rats from inhalation exposure at high doses [NOAEL<4869ppm]. Results were similar to effects reported in the API Gasoline Blending Streams test plan, effects from which animals recovered after 4 weeks without exposure. Such data suggest that toxicity of the blended streams may be less severe than that of individual components due to lower individual component concentrations, component interaction and competitive inhibition. No significant reproductive effects were reported in multi-generation studies of stream components. Developmental effects from components present in High Benzene Naphtha streams occurred primarily at doses that were maternally toxic as well. A developmental study in rabbits with a representative high benzene naphtha stream did not result in adverse effects on any developmental parameters except for 1 high dose rabbit that aborted, and no malformations were induced [NOAEL = 50mg/kg].

Environmental

For environmental endpoints, measured data on components present in the products of the High Benzene Naphthas Category, and on other complex products that contain a similar range of chemical classes and carbon numbers were used. These data demonstrate that the hydrocarbons that comprise this category have a very low potential to hydrolyze and do not photodegrade directly due to a minimal capacity to absorb appreciable light energy above 290nm. However, atmospheric

oxidation constitutes a significant route of degradation. Calculation of atmospheric half-lives of representative constituent chemicals identified a range of 0.9 - 65.8 hours as a result of indirect hydrolysis by hydroxyl radical attack. Fugacity modeling demonstrated that members of this category partition primarily into the air, with slight partitioning into water and soil, and minimal partitioning into sediment. Read-across data show that these products are likely to biodegrade significantly and have the potential to produce a moderate level of toxicity in freshwater algae and a moderate level of acute toxicity in freshwater fish and invertebrates. Aquatic toxicity for products in this category can be predicted based on carbon number, measured or calculated toxicities of constituent hydrocarbons and constituent composition.

Conclusions

The data available for mammalian and environmental endpoints on representative constituents of products in this category, and streams of similar complex hydrocarbon composition and on some data from representative streams, are sufficient to characterize the potential toxicity for streams in this category and demonstrate the integrity of the category, itself, for purposes of the HPV Program.

New data on hydrocarbons present in High Benzene Naphtha streams that are developed in other HPV programs will be evaluated when they become available in the context of the present completed assessment. This category summary document will be amended should the new data result in substantial changes to the conclusions.

AMERICAN CHEMISTRY COUNCIL

OLEFINS PANEL

Member Companies

BP
Chevron Phillips Chemical Company LP
The Dow Chemical Company
E. I. du Pont de Nemours and Company
Eastman Chemical Company
Equistar Chemicals, LP
ExxonMobil Chemical Company
Flint Hill Resources, Inc.
Formosa Plastics Corporation, U.S.A.
The Goodyear Tire & Rubber Company*
Huntsman Corporation
NOVA Chemicals Inc.
Noveon, Inc.*
Sasol North America, Inc.
Shell Chemical Company LP
Sunoco, Inc.
Texas Petrochemicals Corporation*
TOTAL Petrochemicals U.S.A., Inc *
Westlake Chemical Corporation
Williams Olefins, LLC

*Companies that are part of the Panel but do not produce products in the High Benzene Naphthas Category

Table of Contents

TABLES

FIGURES

APPENDICES

1 CATEGORY DESCRIPTION AND JUSTIFICATION

1.1 Category Identification

The High Benzene Naphthas Category was developed for the HPV program by grouping ethylene manufacturing streams that exhibit commonalities from both manufacturing process and compositional perspectives. The 19 CAS numbers listed in Table 1 describe 10 streams which are complex products containing many components. Certain single streams are correctly represented by more than one CAS number, and a CAS number may be applicable to more than one stream. A description of the ethylene and associated stream production processes is included in Appendix 1.

The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%. In some cases, petroleum refinery streams may be combined with intermediate streams from the ethylene unit and co-processed to produce these products. This grouping of CAS numbers represents hydrocarbon streams with a carbon number distribution that is predominantly C5-C11, through components boiling at 650°F or higher.

The CAS Numbers in the High Benzene Naphthas Category are associated with the following streams, which are commercial products or isolated intermediates:

Pyrolysis Gasoline
Pyrolysis C6 Fraction
Pyrolysis C6-C8 Fraction
Pyrolysis C5-C6 Fraction
Hydrotreated C6 Fraction
Hydrotreated C6-C7 Fraction
Hydrotreated C6-C8 Fraction
Quench Loop Pyrolysis Oil and Compressor Oil
Recovered Oil from wastewater treatment
Aromatic Extract from Benzene Extraction

Pyrolysis gasoline, is the major product in this category. Pyrolysis gasoline and its 3 distillate fractions together make up about 66% of the production capacity in the category. Test data exists for one of these 4 streams (pyrolysis gasoline) and for a fraction of pyrolysis gasoline. Three hydrotreated pyrolysis gasoline fractions make up approximately 33% of the production capacity in the category and test data exist for one of these 3 streams. The remaining 3 streams are included in this category because they are similar benzene-containing intermediate streams produced by industry.

Table 1. CAS Numbers[1] and CAS Names Associated with Streams in the High Benzene Naphthas HPV Category

Production Streams	CAS RN	CAS RN Name
Pyrolysis Gasoline	68606-10-0	Gasoline, pyrolysis, debutanizer bottoms
	68921-67-5	Hydrocarbons, ethylene-manuf.-by-product distn. residues
	64742-83-2	Naphtha, petroleum, light steam-cracked
	64742-91-2	Distillates, petroleum, steam-cracked
	67891-79-6	Distillates, petroleum, heavy arom.
	67891-80-9	Distillates, petroleum, light arom.
	68476-45-9	Hydrocarbons, C5-10 arom. conc., ethylene-manuf.-by-product
	68526-77-2	Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum
	68606-28-0	Hydrocarbons, C5 and C10-aliph. and C6-8-arom.
	68955-29-3	Distillates, petroleum, light thermal cracked, debutanized arom.
Pyrolysis C5-C6 Fraction	68955-29-3	Distillates, petroleum, light thermal cracked, debutanized arom.
	64742-83-2	Naphtha, petroleum, light steam-cracked
	68956-52-5	Hydrocarbons, C4-8
Pyrolysis C6 Fraction	68955-29-3	Distillates, petroleum, light thermal cracked, debutanized arom.
	64742-83-2	Naphtha, petroleum, light steam-cracked
	68606-10-0	Gasoline, pyrolysis, debutanizer bottoms
Pyrolysis C6-C8 Fraction	68475-70-7	Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived
	68955-29-3	Distillates, petroleum, light thermal cracked, debutanized arom.
	64742-83-2	Naphtha, petroleum, light steam-cracked
	68476-45-9	Hydrocarbons, C5-10 arom. conc., ethylene-manuf.-by-product
Hydrotreated C6 Fraction	68410-97-9	Distillates, petroleum, light distillate hydrotreating process, low-boiling
	8030-30-6	Naphtha
Hydrotreated C6-C7 Fraction	68410-97-9	Distillates, petroleum, light distillate hydrotreating process, low-boiling
	64742-49-0	Naphtha, petroleum, hydrotreated light
	64742-73-0	Naphtha, petroleum, hydrodesulfurized light
	68955-29-3	Distillates, petroleum, light thermal cracked, debutanized arom.
Hydrotreated C6-C8 Fraction	68410-97-9	Distillates, petroleum, light distillate hydrotreating process, low-boiling
Quench Loop Pyrolysis Oil and Compressor Oil	69013-21-4	Fuel oil, pyrolysis
Recovered Oil from Wastewater Treatment	68956-70-7	Petroleum products, C5-12, reclaimed, wastewater treatment
Aromatic Extract from Benzene Extraction	64741-99-7	Extracts, petroleum, light naphtha solvent

Note 1: The CAS numbers associated with the corresponding production streams are shown in the above table. In some cases, more than one CAS number is used to represent a specific stream and in other cases a single CAS number may be used to represent more than one stream. The Olefins Industry or others may use these same CAS numbers to represent substances that may, in various degrees, be dissimilar to the category streams. CAS numbers, other than those shown in this table may be used to describe these streams in future reporting.

Descriptions of the 10 streams associated with the High Benzene Naphthas Category are presented below:

1. Pyrolysis Gasoline

Pyrolysis Gasoline (Pygas) consists predominantly of C5+ hydrocarbons produced by ethylene cracking furnaces. Typically the stream is derived from (1) the bottoms product from the

debutanizer, (2) oils separated from furnace effluent quench systems, and (3) "drips" or condensate resulting from compression of the cracked gas. The oils from the quench systems and the "drips" may be stabilized to remove lights before blending with Pygas from the other sources. Depending on the plant configuration, Pygas may contain all of these intermediate streams, or the quench oils and stabilized drips may be transferred as separate streams. Low concentrations (e.g. 3% total) of C4 and lighter hydrocarbons may be present in the stream. A detailed analysis of Pygas may identify 60 or more hydrocarbon components or component groups, primarily unsaturated hydrocarbons and aromatics. Benzene, toluene, and dicyclopentadiene together may account for more than 50% of a Pygas stream and typically no other single component is present at a level greater than about 5%. The benzene concentration of Pygas is typically about 40% and the reported values range from 15 to 62%. The concentrations of individual hydrocarbon components in Pygas vary depending on the type of feedstock used by the ethylene plant, the mode of operation of the cracking furnaces (i.e. severity) and the ethylene process configuration. One non-typical Pygas stream is reported to contain vinyl acetate at a concentration of up to about 10%. Vinyl acetate is not typically found in ethylene process streams.

2. Pyrolysis Gasoline Fractions

Pyrolysis gasoline is separated by distillation into various boiling-point-range fractions as intermediates in preparation for further processing. In some cases, petroleum refinery streams such as a C6 reformate fraction are combined with the pyrolysis gasoline prior to this separation.

(a) Pyrolysis C5-C6 Fraction
The carbon number distribution for this stream is predominantly C5 to C6. One typical composition for this stream is reported as 70% benzene and 10% pentenes.

(b) Pyrolysis C6 Fraction
The carbon number distribution for this stream is predominantly C6. Reported compositions vary from 35 to 77% benzene, 0.5 to 5% toluene with the balance primarily C6 non-aromatics, which are expected to be largely unsaturates.

(c) Pyrolysis C6-C8 Fraction
This stream has a carbon number distribution that is predominantly C6 to C8. The reported compositions range from 30 to 80% benzene, 15 to 25% toluene and 3 to 23% C8 aromatics.

3. Hydrotreated Pyrolysis Fractions

Pyrolysis gasoline or distillate fractions of pyrolysis gasoline are sometimes treated with hydrogen over catalyst to saturate or partially saturate diolefins and/or olefins. In some cases, petroleum refinery streams such as a C6 reformate fraction are combined with the pyrolysis gasoline prior to this step. The hydrogenation process may be either one-stage or two-stage. The one-stage process is typically a liquid-phase process where the primary objective is to selectively convert diolefins to mono-olefins and to convert vinyl aromatics into alkyl aromatics, for example, styrene to ethylbenzene. The second stage in a two-stage hydrogenation process is typically a vapor-phase, more severe hydrogenation that converts essentially all of the contained

olefins to saturated hydrocarbons. A pygas fraction that will be processed by extraction or extractive distillation to produce high purity aromatics (benzene, toluene or xylenes) is subjected to two-stage hydrogenation. Pygas fractions may be forwarded to hydrodealkylation units (less common) for benzene production after one-stage of hydrogenation. Hydrotreated Pyrolysis fractions may be the result of either one- or two-stage hydrogenation.

(a) Hydrotreated C6 Fraction
This stream is very similar in composition to the Pyrolysis C6 fraction except that the non-aromatics present in the hydrotreated stream are essentially all saturates. The reported composition for the Hydotreated C6 stream indicates typical benzene content of 75%.

(b) Hydrotreated C6-C7 Fraction
The carbon number distribution for this stream is predominantly C6 -C7 and the reported values indicate 40 to 70% benzene, and 3 to 15% toluene.

(c) Hydrotreated C6-C8 Fraction
The reported typical compositions for this stream are 40 to 60% benzene, 10 to 25% toluene and 3 to 10% C8 aromatics.

4. Quench Loop Pyrolysis Oil and Compressor Oil

Quench Loop Pyrolysis Oil (Pyoil) represents higher boiling hydrocarbons that condense in the water quench system of an ethylene plant, typically at an ethylene unit cracking ethane, propane or butane. The stream can also include liquids collected at the cracked gas compressor knock out drums, which may include compressor injection oil. The carbon number distribution for Pyoil is C4 (or even lower) through heavier hydrocarbons such as naphthalene or even heavier. The reported typical composition includes 10 to 22% benzene and 5 to11% toluene.

5. Recovered Oil from Wastewater Treatment

This stream can be expected to be of variable composition and made up largely of the components found in Pygas. No composition data or process specific information have been reported. Typically, water streams at ethylene units are processed to separate hydrocarbons from the water so that the water can be reused to generate steam for process-contact use (dilution steam for the cracking furnaces) or so that excess water can be forwarded to treatment prior to discharge or reuse. Water processing typically includes mechanical and gravity separation and steam or gas stripping. Hydrocarbons separated from the water in these systems are not usually isolated from the process. However, at least in one case, the Recovered Oil from Wastewater Treatment has been reported as an isolated intermediate.

6. Aromatic Extract from Benzene Extraction

Hydrotreated pyrolysis fractions containing aromatics (most commonly benzene or benzene and toluene) are typically charged to extraction or extractive distillation units where the mixed aromatics are recovered as the Aromatic Extract from Benzene Extraction. The carbon number

distribution for this stream is predominantly C6 to C8. A reported typical concentration indicates 60 to 75% benzene, 25 to 40% toluene and 0 to 1% xylenes.

1.2 Purity/Impurities/Additives

CAS numbers in this category are used to represent extremely complex mixture of hydrocarbons in the C5 – C11carbon range. Typically there are no impurities in the streams in this category. The typical compositions of streams in this category are listed in Appendix 2 Table A2-1 and Figures 4 and 5.

1.3 Physico-Chemical Properties

Properties for the High Benzene Naphthas category have been estimated from calculated and measured values for representative constituents of the category. Substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C11. The 12 chemicals selected to represent physico-chemical properties of the category are C5 –C10 hydrocarbons that can be found in substances identified by the 19 CAS numbers. Calculated data have been derived using subroutines of the EPIWIN© version 3.04 computer model (EPIWIN, 1999) described in the US EPA document "The Use of Structure-Activity Relations (SAR) in the High Production Volume Chemical Challenge Program (US EPA, 1999)." Robust summaries for Physico-Chemical property studies are provided as Attachment 1a.

Table 2. Summary of Calculated Physico-Chemical Properties for Selected Chemicals Contained by Streams in the High Benzene Naphthas Category

Substance Constituent	Melting Point (°C)	Boiling Point (°C@760mm Hg)	Vapor Pressure (hPa@ 25°C)	Log K_{ow} (@ 25^0C)	Water Solubility (mg/L@25^0C)
Isoprene	-118.89	34.95	7.35 E^2	2.58	247.2
n-pentane	-106.92	46.01	6.84 E^2	2.80	159.7
1,3-cyclo-pentadiene	-91.83	69.17	5.69 E^2	2.25	470.6
Isohexane	-105.80	56.26	2.48 E^2	3.21	66.94
n-hexane	-93.84	71.53	2.00 E^2	3.29	57.42
Methylcyclo-pentane	-85.82	80.34	1.77 E^2	3.10	83.95
Benzene	-77.92	102.24	1.16 E^2	1.99	2634.0
Toluene	-59.17	125.72	31.60	2.54	832.7
m-Xylene	-40.69	148.29	8.83	3.09	258.4
Styrene	-48.31	146.65	6.73	2.89	386.7
Dicyclo-pentadiene	-16.78	176.78	2.20	3.16	na
Naphthalene	5.01	231.64	0.05	3.17	142.1

na =not available.
Calculated values determined by EPIWIN [EPIWIN 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.].

Table 3. Summary of Measured Physico-Chemical Properties for Selected Chemicals Contained by Streams in the High Benzene Naphthas Category

Substance Constituent	Melting Point (°C)	Boiling Point (°C@760mm Hg)	Vapor Pressure (hPa@ 25°C)	Log K_{ow} (@ 25^0C)	Water Solubility (mg/L@25^0C)
Isoprene	-145.9	34.0	7.33 E^2	2.42	338.6
n-pentane	-129.7	36.0	6.85 E^2	3.39	49.8
1,3-cyclo-pentadiene	- 85.0	41.0	5.80 E^2	na	na
Isohexane	-162.9	63.2	2.53 E^2	3.60	31.1
n-hexane	- 95.3	68.7	2.01 E^2	3.90	17.2
Methylcyclo-pentane	-142.5	71.8	1.84 E^2	3.37	49.4
Benzene	5.5	80.0	1.26 E^2	2.13	2000.0
Toluene	- 94.9	110.6	37.86	2.73	573.1
m-Xylene	- 47.8	139.1	11.05	3.20	207.2
Styrene	- 31.0	145.0	8.53	2.95	343.7
Dicyclo-pentadiene	32.0	170.0	3.05	na	na
Naphthalene	80.2	217.9	0.11	3.30	142.1

na = not available
Measured values from the experimental database in EPIWIN [EPIWIN, 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.].

The following ranges can be used to define the five physico-chemical endpoints of substances in this category. The calculated and measured ranges overall compare favorably with each other.

1.3.1 Melting Point (Range)

The calculated melting points (by subroutine MPBPWIN, version 1.40) for representative constituents that are present in the category streams vary from –118.89 to 5.01^{0}C. The measured melting points of these same constituents vary from –162.9 to 80.2°C. Although this does not define the actual melting points of the category streams, it offers an indication of a range that might be expected to encompass the melting points of these complex streams with variable compositions. Melting points outside these ranges may be possible for some category streams.

1.3.2 Boiling Point (Range)

The calculated boiling points (by subroutine MPBPWIN, version 1.40) for representative constituents that are present in the category streams vary from 34.95 to 231.64°C @ 760 mm Hg. The measured boiling points of these same constituents vary from 34.0 to 217.9°C @ 760 mm Hg. Although this does not define the actual boiling points of the category streams, it offers an indication of a range that might be expected to encompass the boiling points of these complex streams with variable compositions. Boiling points outside these ranges may be possible for some category streams.

1.3.3 Vapor Pressure (Range)

The calculated vapor pressures (by subroutine MPBPWIN, version 1.40) for representative constituents that are present in the category streams vary from 0.05 to 7.35 E^2 hPa @ 25°C. The measured vapor pressures of these same constituents vary from 0.11 to 7.33 E^2 hPa @ 25°C. Although this does not define the actual vapor pressures of the category streams, it offers an indication of a range that might be expected to encompass the vapor pressures of these complex streams with variable compositions. Vapor pressure outside these ranges may be possible for some category streams.

1.3.4 Partition Coefficient: Log K_{ow} (Range)

The calculated log K_{ow} (by subroutine KOWWIN, version 1.65) for some representative constituents that are present in the category streams vary from 1.99 to 3.29 @ 25°C. The measured log K_{ow} of these same constituents vary from 2.13 to 3.90 @ 25°C. Although this does not define the actual log K_{ow} of the category streams, it offers an indication of a range that might be expected to encompass the log K_{ow} of these complex streams with variable compositions. Log K_{ow} values outside these ranges may be possible for some category streams.

1.3.5 Water Solubility (Range)

The calculated water solubility (by subroutine WSKOWWIN, version 1.36) for some representative constituents that are present in the category streams vary from 57.42 to 2634.0 mg/L @ 25°C. The measured water solubility of these same constituents vary from 17.2 to 2000.0 mg/L @ 25°C. Although this does not define the actual water solubility of the category streams, it offers an indication of a range that might be expected to encompass the water solubility of these complex streams with variable compositions. Water solubilities outside these ranges may be possible for some category streams.

1.4 Category Justification

The High Benzene Naphthas Category is comprised of 10 streams associated with 19 CAS numbers, which are complex products containing high levels of benzene (10-80%) plus many other components (predominantly C5-C11), many of which are shared across streams. The average benzene content is 55%. All streams in this category are subject to the Occupational Safety and Health Administration (OSHA) Benzene Standard (29 CFR 1910.1028). Those streams containing 1,3-butadiene are subject to the OSHA Butadiene Standard (29 CFR 1910.1051). OSHA Permissible Exposure Limits exist for most major components. Benzene, as the predominant component in most streams, is expected to be the key driver with respect to health effects endpoints within the SIDS battery of tests, with genotoxicity and hematotoxicity the effects most likely to be seen. However, the other components may also contribute to the toxicity of the streams. Pyrolysis gasoline is the major stream in this category and essentially all of the other category streams are derived from it, either as simple distillate fractions or hydrogenated distillate fractions. They are the Olefins Industry's intermediate streams that are processed to high purity benzene and other byproducts. Pyrolysis gasoline and these fractions account for 99.9% of the category production. The remaining 0.1% of the category production consists of similar benzene-containing industry streams.

The basic strategy of this screening level test plan for characterizing the human health hazards of this category is to evaluate data for representative streams in the category, for the components of the streams, as well as data for mixtures of category components and analogous mixtures.

Benzene has a robust toxicity dataset, including data on human experience, and has completed the OECD SIDS program. The existing epidemiology and toxicology database for the components other than benzene and for mixtures containing the components is extensive. All components present in the streams at concentrations greater than 5% have been tested in at least one toxicity study. Those components having only limited data lack structural alerts for mammalian toxicity and data exist for their structural analogs.

Additional data for the components, or for structural analogs of components, are under development by the American Chemistry Council Olefins Panel for other categories under the HPV program (Appendix 7), by other HPV consortia, and by the OECD SIDS program (Appendix 3, Table A3-1). Furthermore, some of the materials obtained by distillation from Pyrolysis Gasoline are being tested in other Panel HPV Test Plans (Non-Cyclic C5s and Resin Oils and Cyclodiene Dimer Concentrates categories); and the High Benzene Naphthas Category shares many of the same components with the gasoline blending streams referenced in the API Petroleum HPV Gasoline Blending Streams Test Plan. These gasoline stream data can contribute to the hazard evaluation for the members of this category by showing effects, or lack thereof, due to mixtures containing components of this category when the benzene content is very low (~ 2%).

For the HPV program, the Panel believes that the human health hazards of the category can be adequately characterized by using scientific judgment to analyze component data (existing data and data being developed by other testing programs), without conducting additional toxicology tests. The Panel further believes that additional testing on streams is unlikely to demonstrate any adverse effects that have not been shown for components, and would provide little useful data for regulatory, industrial hygiene, emergency response or hazard communication purposes.

Assessment of human health hazards for category members has been developed using data from testing of representative streams, and data from the sources listed in Appendix 4 Assessments will be supplemented and revised, if needed, as data becomes available for other cited testing programs now in progress.

The strategy for characterizing the physical-chemical properties, and environmental hazards of products in the High Benzene Naphthas Category also employs a constituent approach, evaluating measured data on high purity hydrocarbons and components of reaction products in the High Benzene Naphthas Category. Where measured data do not exist, calculated data for selected constituents of these naphthas have been developed using the Epiwin© computer models described by EPA. For biodegradability and aquatic toxicity, data on component chemicals contained in streams in this category and similar complex products were evaluated and read-across assessments developed.

2 EXPOSURE AND USE

The Category and HPV Stream Production:

The High Benzene Naphthas Category includes ten product streams produced by the Olefins Processes. The category streams are complex mixtures with variable compositions and all contain significant concentrations of benzene. Benzene is separated from the category streams, or from streams obtained from the category streams, in downstream processing units. The category streams are isolated intermediates that are used on site where they are manufactured or transferred under controlled conditions to a limited number of locations within the same company or to second parties that use the streams in a controlled way as an intermediate with well-known technology.

Pyrolysis gasoline is the primary stream in the category. This stream is produced by the ethylene production process and consists of a complex mixture of hydrocarbons, primarily carbon number 5 and higher. Typically, Pyrolysis Gasoline contains about 40% benzene, although the content reported for this program varied from 15% to 62%. Pyrolysis gasoline is separated by distillation into various boiling-point-range streams. Some of these streams are included in this HPV category, and some in other categories of the Olefins Panel's HPV program. Typically, the Pyrolysis Gasoline-derived streams include a C5 fraction (Olefins Panel HPV C5 non-Cyclics); various benzene-containing fractions (streams in this HPV category); non-benzene, gasoline-like streams (Olefins Panel HPV Low Benzene Naphthas); aromatic or aromatic/cyclodiene dimer streams (Olefins Panel HPV Resin Oils & Cyclodiene Dimer Concentrates); and fuel oil streams (Olefins Panel HPV Fuel Oils). Pyrolysis Gasoline, or intermediate streams derived from pyrolysis gasoline are typically hydrogenated, which is a necessary processing step prior to isolation of benzene by extraction or extractive distillation. The hydrogenation step produces the hydrogenated streams in this HPV category as well as in the hydrogenated streams in the Olefins Panels HPV C5 non-Cyclics and HPV Low Benzene Naphthas categories. Distribution of the 24 billion pounds/year[1] of category production among the category streams is shown in Figure 1.

Combustion processes and other industrial processes also produce the individual hydrocarbon components present in the complex streams of the category. Potential exposures to these individual components from other manufacturing processes, from combustion, or from natural sources are considered to be out of scope for this assessment. This assessment is limited to potential exposures to the streams in the category. Some data are presented for specific components of the category streams, which is intended to help clarify the potential for exposure to the streams. There are nineteen CAS numbers that are used by the Olefins Industry to represent the ten category streams. This assessment addresses the use of these CAS numbers for the High Benzene Naphtha Category streams. Some of the CAS numbers in this category may be used by the Olefins Industry or others to represent other substances that are not included in the High Benzene Naphthas Category, and may be included in other HPV categories.

This screening level exposure assessment is based on information received from fourteen of the sixteen original sponsors of the category and upon other available information.

[1] 24 Billion pounds per year is the approximate total annual commercial production of category streams reported by the sponsors of the category and based on their 1998 TSCA IUR.

Figure 1

High Benzene Naphthas
Category Production (1998 Data)

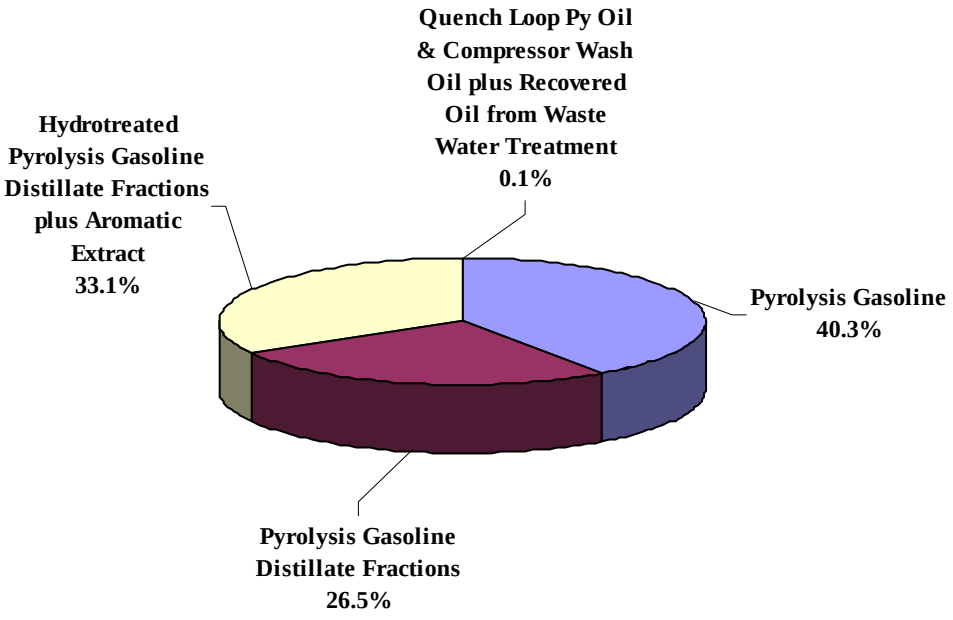


Table 4. High Benzene Naphthas Category Streams

Pyrolysis Gasoline & Distillate Fractions	Hydrotreated Fractions & Aromatic Extract	Other Category Streams
Pyrolysis Gasoline	Hydrotreated C6-C7	Recovered Oil from Waste Water Treatment
Pyrolysis C6	Hydrotreated C6-C8	Quench Loop Pyrolysis Oil & Compressor Wash Oil
Pyrolysis C6-C8	Hydrotreated C6	
Pyrolysis C5-C6	Aromatic Extract from Benzene Extraction	

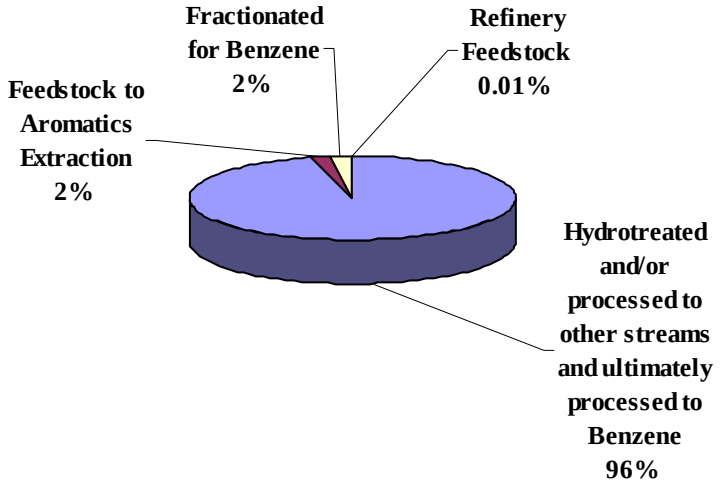
Storage and Transportation of Category Streams: The High Benzene Naphtha streams are either used on-site where they were produced, or shipped to other industrial sites for additional processing. When shipped between industrial sites, the category streams are transported in bulk in closed systems by pipeline, barge, tank car or tank truck. The streams are typically inventoried in bulk storage tanks, either floating roof or fixed roof with vents routed to a control device in order to reduce emissions.

Use: There are no known consumer uses for these category streams. Uses of the category streams are shown in Figure 2. Pyrolysis Gasoline and other category intermediates streams are processed to produce other streams in this category or streams in other of the Olefins Panel's

HPV categories, as discussed above. Figure 2 illustrates that 96% of the category volume is processed to benzene and other intermediate streams, most of which are not isolated intermediates in this HPV category. Only 4% of the category volume is isolated from the process prior to being transferred to the aromatic extraction unit (for benzene production) or transferred to the Benzene fractionation unit. Virtually all of the benzene contained in the category streams is ultimately isolated as high purity benzene product, which is the primary use of the category streams. Some of the non-benzene components of the streams are isolated as other streams. Figure 2 does not include use data for the following three category streams – Recovered Oil from waste water treatment and Hydrotreated C6 (producers of these two streams indicated that the streams were not isolated in the year that the use data were collected), and Pyrolysis C6s (specific use data were not available from the producers of this stream).

FIGURE 2

USE OF THE HIGH BENZENE NAPHTHA CATEGORY STREAMS (2001 DATA) [2]



Route of Potential Exposure: The category streams are liquids at ambient conditions, with volatility similar to gasoline. Inhalation is a likely route of potential exposure due to the volatility of the streams. There is also a potential for dermal exposure as a result of accidental contact. The streams or components in the streams are slightly soluble in water and therefore groundwater contamination is possible in the event of spills or leaks from processing,

[2] The percentage uses of the category streams are based on data received from 14 of the original 16 category sponsors. Although similar information was not available from the other sponsor at the time this report was written, the uses shown in Figure 2 are expected to be representative of the industry. Uses of 3 of the category streams are not included in Figure 2, because the streams were either not isolated during the reporting year, or the specific use information was not available from the sponsors of the streams at the time this report was written.

transportation or storage equipment. All of these streams contain significant concentrations of benzene.

Sources of Potential Exposure: Exposure to the category streams for workers in the Olefins Industry process units where the category streams are isolated or used is expected to be low because that equipment and those processes are closed systems. Emissions from storage and loading equipment are typically controlled by using floating roof storage tanks or by routing vents from fixed roof storage tanks and loading equipment to control or recovery systems, or back to the process. For the industrial workers at these facilities, the most likely exposure potential occurs through inhalation of low-level concentrations in air of vapors that escape from the closed process, such as fugitive emissions from valve packing and from pump seals. There is also potential for exposure during operations such as sampling, loading of bulk transportation vessels (tank cars and barges), from emissions at floating roof storage tanks, during infrequent opening of equipment for maintenance, or from emissions from control devices, such as flares.

The above-described sources of emissions of the category streams may present a potential for exposure to the public and to the environment adjacent to the industrial facilities that use or produce the category streams.

All of the category streams contain significant concentrations of benzene. "Emissions of benzene to the atmosphere result from gasoline vapors, auto exhaust, and chemical production and user facilities."[3] "Occupational exposure to benzene may occur through inhalation and dermal contact with this compound at workplaces where benzene is produced or used. The general population may be exposed to benzene via inhalation of ambient air, ingestion of drinking water, and dermal contact with gasoline products containing benzene.."[4] EPA's Total Exposure Assessment Monitoring (TEAM) studies carried out between 1980 and 1990 indicate that for chemicals such as benzene, "the most important sources of pollution are small and close to the person, and that exposures are not clearly correlated with emissions. For example, the TEAM study findings indicated that, although nearly 85% of atmospheric benzene in outdoor air is produced by cars burning petroleum products and the remaining 15% is produced by industry, about half of the total national exposure to benzene comes from cigarette smoke."[3]

Controls that Limit Exposure: The OSHA Benzene Standard applies to the streams in the High Benzene Naphthas category and thus limits occupational exposure to the streams. The Standard requires controls and work practices that limit benzene occupational exposure to less than 1 ppm, 8-hour TWA and a short-term level of 5 ppm (15 minute)[5]. In addition, the OSHA Standard establishes an action level of 0.5 ppm (8-hour TWA). Since benzene is a primary component of all the category streams, these limits on benzene occupational exposure effectively limits occupational exposure to the category streams.

---

[3] http://atsdr1.atsdr.cdc.gov/toxprofiles/tp3-c5.pdf (ATSDR Toxicological Profile for Benzene), September 1997 updates

[4] http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB (HSBD references 1986 to 1997 sources for at least a portion or this information.) (HSBD references 1986 to 1997 sources for at least a portion or this information.)

[5] OSHA Standard for Benzene: 29 CFR 1910.1028.
http://www.osha.gov/pls/oshaweb/owadisp.show_document?p_table=STANDARDS&p_id=10042

In addition OSHA and ACGIH have established guidelines for some components in the category streams. For example, the OSHA PEL for Toluene (a component in most of the category streams) is 200 ppm; and the ACGIH TLV is 50 ppm. Eleven of the original sixteen sponsors of the category streams reported that they have programs that assess exposure to the category streams, including specific measurements for benzene. Industrial hygiene programs for a specific production site are typically unique to the site and address the specific chemical exposure issues. Some of the components typically present in the category streams and that have OSHA PELs or ACGIH TLVs are shown in Table 5.

Table 5. Components Typically Present in Some Streams in the High Benzene Naphthas Category & That Have OSHA PELs or ACGIH TLVs

Component	OSHA PEL	ACGIH TLV	Component	OSHA PEL	ACGIH TLV	Component	OSHA PEL	ACGIH TLV
Benzene[a]	1	0.5	Ethylbenzene	100	100	Styrene	100	20
Biphenyl	0.2	0.2	Heptane	500	400	Toluene	200	50
Cumene	50	50	Indene	-	10	Vinyltoluene	100	50
CPD[b]	75	75	Naphthalene	10	10	Mixed Xylenes (o-, m-, p - Isomers)	100	100
Cyclo-pentane	--	600	Octane isomer	500	300			
DCPD[c]	-	5	Pentane Isomers	1000	600			

[a] Benzene OSHA Action Limit is 0.5 ppm [b] CPD: Cyclopentadiene [c] DCPD: Dicyclopentadiene

Among other reasons, the release of the category streams from process, storage and transportation equipment at industrial facilities is avoided because the streams are flammable liquids, similar in flammability and volatility characteristics to gasoline.

The category streams are mixtures of volatile organic compounds (VOC) and are therefore subject to multiple US EPA and state environmental regulations that limit VOC emissions. Limits on emissions of the components of the category streams effectively limits exposures to the category streams. The US EPA new source performance standards (NSPS) of 40 CFR Part 60 may be applicable and limit emissions of VOC at new or modified Olefins process units where the streams in the category are produced and used. Subpart VV of NSPS limits emission from equipment leaks, subpart NNN limits emissions from distillation operations, subpart RRR limits emissions from reactor systems and subpart Kb limits emissions from VOC storage tanks. The category streams contain benzene and are typically subject the National Emissions Standard for Hazardous Air Pollutants (NESHAPs) of 40 CFR Part 61. NESHAP subpart J and V limit emissions of benzene from equipment leaks, subpart FF limits emissions from benzene wastes, subpart Y limits emissions from benzene storage tanks, and subpart BB limits emissions from benzene transfer operations. In addition, facilities that produce or use these streams and that are major sources may be subject to the National Emission Standards for Hazardous Air Pollutants for Source Categories: Generic Maximum Achievable Control Technology Standards, which includes ethylene manufacturing processes and may be subject to the Hazardous Organic

NESHAP (HON), 40 CFR Part 63, subpart F, G and H. Facilities that produce and use the category streams are also typically subject to state operating permits and state regulations that further limit VOC emissions. These emissions control requirements effectively limit exposure potentials for the category streams for both workers at the facilities and the neighboring public and environment.

Ambient Air Concentration Data: Ambient air concentration data for the complex category streams are not available. However, all of the category streams contain significant concentrations of benzene.

"Atmospheric benzene concentrations were studied throughout the USA between 1977-1980 in which out of 487 samples taken, benzene was found at an average concentration of 3.0 ppb. The concentration of benzene near USA chemical factories where benzene is used ranged from 0.6-34 ppb, near service stations 0.0003-3.2 ppm, and in cigarette smoke 57-64 ppm."[4] Ambient air concentrations (1994 through 1997) for benzene at selected industrial sites in Texas are available from the Texas Community Air Toxics Monitoring Network[6]. Calculated values from that data indicate an average annual mean value of 0.96 ppb, with a range of from 0.22 to 7.0 ppb, and an average of the 24-hour annual high values of 5.03 ppb, with a range of from 0.34 to 63.63 ppb.

Estimates of Potentially Exposed Workers: NIOSH (NOES Survey 1981-1983) has statistically estimated that 272,275 workers (143,066 of these are female) are potentially exposed to benzene in the US[4]. A number of limitations to this survey have been identified over the years, and the estimates of the number of workers potentially exposed to various substances are generally thought to be high.

Category emissions: Emissions quantities of the mixed streams are not available. Benzene is a component found at significant concentrations in all of the category streams. Emissions of benzene in these category streams are included in the industrial emissions of benzene that are reported to the EPA and made available to the public in the Toxics Release Inventory (TRI) [7]. This inventory was established under the Emergency Planning and Community Right-to-Know Act of 1986 (EPCRA) and expanded by the Pollution Prevention Act of 1990.

The TRI data indicate that emissions of benzene have significantly decreased since 1988 (Figure 3). The TRI data from 2002 indicate that emissions and disposal quantities of benzene reported in the TRI for the chemical sector (SIC 28) have declined by 81% since 1988, and the number is down 79.7% for all US industries. However the relevance of individual component emissions values with regard to the category streams is uncertain, because the category streams likely account for a minor portion of the total emissions for specific components.

[6] http://www.tnrcc.state.tx.us/air/monops/cat97/cat97.html

[7] EPA website for TRI: http://www.epa.gov/tri/

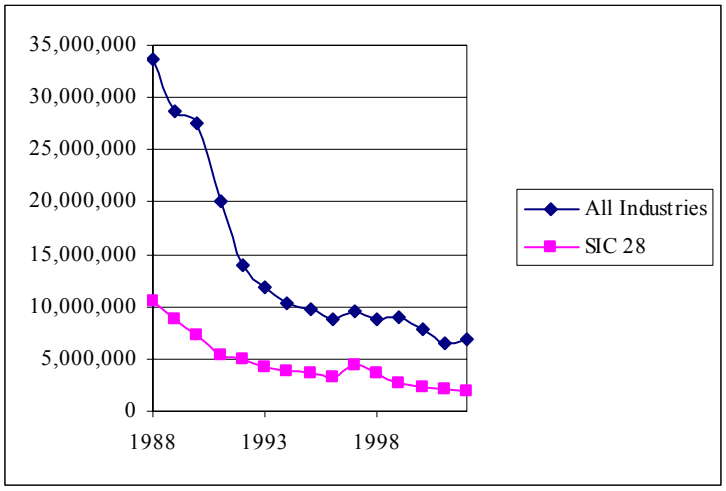


Figure 3
TRI Benzene Total Disposal & Emissions (lbs/year) for All Industries and for the Chemical Sector (SIC 28) 1988 - 2002

2.1 Summary of Exposure Assessment

The HPV High Benzene Naphthas Category includes the ten isolated product streams from the Olefins Industry that contain significant concentrations of benzene. Nineteen CAS numbers are used to represent these streams. The category streams are complex mixtures of variable composition. Benzene is separated from the category streams, or from other intermediate streams derived from the category streams, in downstream process units.

There are no expected consumer applications for these materials.

The category streams are typically used at the same location where they are produced or transported to other industrial facilities in bulk by pipeline, barge, tank car or tank truck.

Inhalation is a likely route of potential exposure due to the volatility of the hydrocarbon components that make up the streams. Other possible exposure routes include dermal (from spills) and oral (from contaminated ground water).

Occupational exposure is limited because production and use of these streams is in closed systems, and the requirements of the OSHA Benzene Standard limits occupational exposure to benzene. Benzene is a common, primary component of all these streams. OSHA and ACGIH exposure limits also exist for several of the other components of the category streams.

Environmental exposure is limited since emissions from production and use are limited and controlled by a number of volatile organic compound and hazardous air pollutant environmental regulations at both the federal and state level. The category streams are produced, transported and used in closed systems. The subsequent processing of the process streams in this HPV Category ultimately result in the production of other products (e.g. benzene and other non-benzene containing products) and the consumption of the original category streams.

3. ENVIRONMENTAL FATE

3.1 Photodegradation

3.1.1 Direct Photodegradation:

The absorption of light in the ultraviolet (UV) visible range (110-750nm) can induce electronic excitation of an organic molecule. The stratospheric ozone layer allows only light in wavelengths in the 290-750nm range to reach earth's surface with the potential to result in photochemical transformation in the environment. To estimate photochemical degradation, it is assumed that degradation will occur in proportion to the amount of light wavelengths greater than 290nm absorbed by the molecule. Saturated hydrocarbons do not absorb appreciable light energy above 200nm. Olefins with one double bond or two conjugated double bonds, which constitute the majority of chemicals in the High Benzene Naphthas category, do not absorb appreciable light energy above 290nm. The absorption of UV light to cause cis-trans isomerism about the double bond of an olefin occurs only if it is in conjunction with an aromatic ring [Harris et al., 1982]. Examples of absorbance maxima (λ max) and associated molar absorptivities (ϵ) for representative hydrocarbons are shown below.

Table 6. Characteristic Absorbance Maxima (λ_{max}) and Associated Molar Absorptivities (ε) for Representative Hydrocarbons of the High Benzene Naphthas Category

Hydrocarbon	λ below 290 nm		λ above 290 nm	
	λ_{max}	ε	λ_{max}	ε
Ethylene	193	10,000	--	--
Benzene	255	215	--	--
Styrene	244 282	12,000 450	--	--
Naphthalene	221 270	100,000 5,000	311	250

Only naphthalene demonstrated some photochemical degradation at wavelengths above 290nm.

Products in the High Benzene Naphthas category do not contain component molecules that will undergo direct photolysis, with the exception of naphthalene. This process will not contribute a measurable degradative removal of chemical components in this category from the environment.

3.1.2 Indirect Photodegradation (Atmospheric Oxidation):

Atmospheric oxidation as a result of hydroxyl radical attack is not direct photochemical degradation but an indirect degradation process. Hydrocarbons such as those in the High Benzene Naphthas Category have the potential to volatilize to air where they can react with hydroxyl radicals (OH-). The rate at which an organic compound reacts with OH- radicals is a direct measure of its atmospheric persistence. The AOPWIN version 1.89 computer program (subroutine of EPIWIN 3.04) was used here to estimate the rate constants for OH- radical reactions of representative organic constituents of the products in the High Benzene Naphthas

category, which are then used to calculate atmospheric half-lives for these constituents as shown below:

Table 7. Hydroxy Radical Photodegradation Half-lives of Representative Hydrocarbons of the High Benzene Naphthas Category

Chemical	Calculated* half-life (hrs)	OH- Rate Constant (cm^3/molecule-sec)
Isopentane	1.2	105.1 E^{-12}
n-pentane	31.7	4.0 E^{-12}
1,3-cyclopentadiene	0.9	142.6 E^{-12}
Isohexane	22.4	5.7 E^{-12}
n-hexane	23.5	5.5 E^{-12}
Methylcyclopentane	22.7	5.7 E^{-12}
Benzene	65.8	1.9 E^{-12}
Toluene	24.6	5.2 E^{-12}
m-xylene	9.5	13.6 E^{-12}
Styrene	4.6	28.1 E^{-12}
Dicyclopentadiene	1.1	119.2 E^{-12}
Naphthalene	5.9	21.6 E^{-12}

* Atmospheric half-life values are based on a 12-hr day.

Based on these calculated values, for representative stream constituents, products in the High Benzene Naphthas category can have an atmospheric half-life range of 0.9 –65.8 hours, indicating that atmospheric oxidation can be a significant route of degradation for products in this category.

3.2 Stability in Water

Hydrolysis is unlikely for product streams in the High Benzene Naphthas category. Hydrolysis is a nucleophilic substitution reaction in which a water molecule or hydroxide ion reacts with an organic molecule to form a new carbon-oxygen bond. Carbon to carbon double bonds are too stable to be cleaved by nucleophilic substitution and the carbon atom lacks sufficient electronegativity to be a good "leaving group". Chemicals that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters and sulfonic acid esters. The chemical components of the High Benzene Naphthas are hydrocarbons that are not included in these groups and have very low potential to hydrolyze. This degradative process will not contribute to removal of these hydrocarbons in the environment.

3.3 Distribution in the Environment

Substances in the High Benzene Naphthas category are calculated to partition primarily into air with negligible percentages partitioning in water, soil and sediment. Relatively high vapor pressure and low water solubility largely control the partitioning behavior of constituent chemicals in substances from this category.

The EQC level 1 fugacity model (Mackay et al., 1996) recommended by U.S. EPA (1999b) was used to determine partitioning of representative chemical constituents into different environmental compartments under steady state conditions, in order to estimate the partitioning behavior for the category substances. Mackay level 1 distribution values, calculated and measured, for 12 representative constituents of products in this category are presented below:

Table 8. Environmental Distribution as Calculated by EQC Level I Fugacity Model for Representative Hydrocarbons of the High Benzene Naphthas Category

Chemical	Percent Distribution: Calculated[a] [Measured][b]			
	Air	Water	Soil	Sediment
Isoprene	99.97 [99.96]	0.02 [0.03]	0.01 [0.01]	-
n-pentane	99.97 [99.99]	0.02 [0.01]	0.01 [-]	-
1,3-cyclo-pentadiene	99.93 [99.93]	0.06 [0.06]	0.01 [0.01]	-
Isohexane	99.96 [99.97]	0.02 [0.01]	0.02 [0.02]	-
n-hexane	99.95 [99.96]	0.02 [-]	0.02 [0.04]	-
Methylcyclo-pentane	99.94 [99.95]	0.03 [0.02]	0.03 [0.03]	-
Benzene	98.46 [98.89]	1.42 [1.00]	0.12 [0.11]	-
Toluene	98.17 [98.80]	1.40 [0.81]	0.43 [0.39]	-
m-Xylene	97.19 [97.91]	1.33 [0.86]	1.45 [1.20]	0.03 [0.03]
Styrene	95.55 [96.65]	2.61 [1.85]	1.80 [1.46]	0.04 [0.04]
Dicyclo-pentadiene	98.00 [98.55]	0.87 [0.63]	1.11 [0.80]	0.02 [0.02]
Naphthalene	24.47 [42.27]	32.28 [20.56]	42.28 [36.33]	0.94 [0.81]

a- Values determined using calculated input data from EPIWIN program
b- Values determined using input data from the EPIWIN program experimental database.

With the exception of naphthalene, the representative components partition into air at >95%; water 0.01 – 2.61%; soil 0.01 – 1.8% and sediment <1.0%.

3.4 Biodegradation

There are sufficient data to characterize the potential biodegradability of products in this category. Data for constituent chemicals of products in this category (as well as for complex products not in this category that contain chemicals found in products from this category) suggest that high benzene naphtha products have the potential to biodegrade to a great extent (Appendix 5, Table A5-1). The carbon number of products in this category ranges primarily

between C5 to C11. Results for several chemicals, including benzene, with carbon numbers in this range that are contained by these products have been shown to biodegrade from 63 to 100% after 14 or 28 days, while results for several comparable, complex streams containing several components range from 21 to 96% after 28 days. As seen by the data in Table A5-1, there is a relatively large biodegradation database for single chemicals and complex streams that can be used to characterize this endpoint for high benzene naphtha products. Because products in this category are compositionally more comparable to the products identified in Table A5-1 as gasoline streams (although gasoline streams contain less benzene), these data best describe the potential biodegradability of the high benzene naphtha streams. Gasoline stream compositions are provided in Table A5-2.

The data from the majority of tests in Table A5-1 were developed using a manometric respirometry test procedure. This procedure uses continuously stirred, closed systems, which is recommended when assessing the potential biodegradability of chemically complex, poorly water soluble, and volatile materials like those in this category. Stirring is recommended when evaluating products containing several chemicals, some of which may have limited water solubility. The manometric respirometry test of benzene [Robust summary in Attachment 1b] indicates that benzene is readily biodegradable with a half-life of less than 2 weeks. By day 28, 63% degradation had occurred; 10% biodegradation was achieved in less than 5 days with 50% biodegradation by approximately day 5.

4. HUMAN HEALTH HAZARDS

4.1 Effects on Human Health

The 10 streams in the High Benzene Naphthas Category are commercial hydrocarbon products or isolated intermediates derived from Ethylene manufacturing and contain significant levels of benzene, averaging 55% [range of 10-80%]. The toxicity and epidemiology databases for benzene and other components of this category as well as mixtures containing the components, are extensive. Health effects data on components present in the streams is summarized in Appendix 3, Table A3-1.

Pyrolysis gasoline is the major stream in this category and data are available for 3 streams: Data for Pyrolysis gasoline [Dripolene], a C5-C10 distillate fraction of a pyrolysis gasoline [Rerun Tower Overheads] and the hydrotreated C6-C8 fraction [Hydrogenated Pyrolysis Gasoline] are summarized below and presented in Robust Summaries in Attachment 1c.

Benzene is the likely key driver for health effects, primarily in genotoxicity and hematotoxicity for HPV endpoints. All components present in the streams at concentrations greater than 5% have been tested in at least one toxicity study. Those components having only limited data lack structural alerts for mammalian toxicity and data exist for their structural analogs. The C5 and C6 alkanes and alkenes present in the streams are not expected to significantly contribute to the toxicity profile as these substances are present in the streams at low concentrations and, with the exception of hexane, generally have a low level of toxicity. The toxic effects of hexane (present at $\leq$ 15%) are unlikely to be observed due to the presence of and interaction with other components.

Chemical Component Interactions

When tested as pure substances, some of the components in the High Benzene Naphthas streams other than benzene have caused genetic damage and adverse target organ effects in repeated-dose animal studies. However, since the biologically active components of the High Benzene Naphtha streams are metabolized through a common P450 metabolic pathway, it is anticipated that multiple components will compete for the same active enzyme sites. Component toxicities, which are dependent on the formation of biologically active metabolites, may be reduced as less metabolite(s) will be produced through competition for these sites. Direct support for reduction or elimination of toxicities of individual components is provided by results of an existing mouse bone marrow micronucleus test with one of the High Benzene Naphtha streams, Hydrotreated C6-8 Fraction described in the summary of *in vivo* mutagenicity data below. This stream, containing approximately 55% benzene, was negative in a mouse bone marrow micronucleus test when administered by oral gavage at 2000 mg/kg to male and female CD-1 mice (see robust summary). Several studies have shown that benzene administered orally to CD-1 mice induces high frequencies of micronuclei in bone marrow erythrocytes at doses as low as 110 mg/kg (Ciranni et al., 1988; Suzuki et al., 1989; Hite et al., 1980; Gad-El Karim et al., 1986; Meyne and Legator, 1980). The presence in the Hydrotreated C6-8 Fraction of other components (approximately 25% toluene, 10% xylene, 7% pentane, 7% ethylbenzene, 3% cyclohexane, and 2% hexane) apparently inhibited the expected clastogenicity of benzene. Other similar interactions between components of the category have also been reported, as noted below.

Medinsky et al. (1994) and Bond et al. (1998) reviewed the metabolism of benzene and the effects of interactions with other organic chemicals on benzene toxicity and metabolism. Reports of interactions between other components of the High Benzene Naphthas Category have also been noted in the literature. Examples of these interactions and the effect on the formation of benzene metabolites and resultant hematotoxicity or genotoxicity are shown below:

- When benzene (440 mg/kg) and toluene (430, 860, or 1720 mg/kg) were coadministered orally to mice, the clastogenic effect of benzene was reduced (Gad-El-Karim et al., 1984, 1986).
- Coadministration of toluene (1720 mg/kg), i.p., with benzene (440 and 880 mg/kg) to mice resulted in a reduction in the quantity of benzene metabolites measured in the urine (Andrews et al., 1977). Coexposure to toluene also protected against benzene-induced depression in ^{59}Fe utilization by red blood cells, which is used as a measure of hematotoxicity.
- Coexposure to 2000 ppm fully vaporized or light gasoline components reduced the incidence of genetic damage (micronuclei in bone marrow) resulting from a single 6-hr exposure to 40 ppm benzene (Bond et al., 1998). The major components of the fully vaporized gasoline and light gasoline mixtures, respectively, were n-butane (6.1%, 23.9%), n-pentane (3.7%, 8.4%), isopentane (12.3%, 33.5%), n-heptane (1.2%, 0.3%), toluene (8.2%, 1.1%), ethylbenzene (2.3%, 0.1%), and xylenes (8.4%, 0.2%). In these experiments, the fully vaporized gasoline mixture, which contained a higher fraction of aromatic hydrocarbons, was a more effective inhibitor of benzene metabolism than was the light fraction, which was composed primarily of aliphatic hydrocarbons.
- Results of studies with styrene-butadiene mixtures showed a decrease in the rate of metabolism of each chemical but an increase in the concentration of the circulating epoxide

metabolites (Bond et al., 1998). The frequency of micronuclei seen in mice exposed by inhalation to butadiene was not altered by simultaneous exposure to styrene.

- Synergistic losses of auditory sensitivity occurred following combined exposure of rats to vapors of toluene plus n-hexane and xylene plus n-hexane (Nylen, 1996). These combined exposures, however, produced antagonistic effects in nerve conduction or action potential amplitudes in the auditory pathway, visual pathway, and peripheral nerve.
- Exposure of male rats to 1000 ppm n-hexane for 61 days caused testicular atrophy and loss of germ cell line (Nylen, 1989). Simultaneous administration of 1000 ppm toluene or xylene did not cause germ cell line alterations or testicular atrophy.
- Neurological effects have been observed in many intermediate-duration inhalation experiments in rats exposed to n-hexane (ATSDR, 1999). No neurotoxic effects were observed in a 2-year chronic study in rats and mice with commercial hexane containing 52.2% n-hexane, 16.0% 3-methylpentane, 15.6% methylcyclopentane, 11.6% 2-methylpentane, 3.2% cyclohexane (Daughtrey et al., 1999). In a separate 13-week inhalation study of commercial hexane, a detailed neurobehavioral/neuropathological evaluation revealed no n-hexane-induced neuropathy (Soiefer et al., 1991).

4.1.1 Acute Toxicity

Studies in Animals

Table 9. Summary of Acute Toxicity Data for Representative Streams and Components in the High Benzene Naphthas Category

Route	Dripolene	Hydrotreated C6-8 stream (Hydrogenated Pyrolysis Gasoline)	C5-C10 fraction of Pyrolysis Gasoline (Rerun Tower Overheads)	Benzene[a]	Toluene[a]
Oral LD50	>2.0g/kg	5.17g/kg	>2.0g/kg	0.81-1.0g/kg	5.5g/kg
Dermal LD50	> 2.0g/kg	---	>2.0g/kg	---	12.4g/kg
Inhalation LC50 [4hr exposure]	---	>12,408ppm	---	13,700ppm	8000-8800ppm

a- data from Table A3-1

Conclusion

High benzene naphtha streams demonstrate minimal toxicity by oral, dermal or inhalation routes of exposure. With the exception of dicyclopentadiene (see Table A3-1) the components of these streams demonstrate overall low levels of acute toxicity as well.

4.1.2 Repeated Dose Toxicity

Studies in Animals

Two streams were tested in repeated-dose studies. A 5-day rat inhalation study was conducted with a Hydrotreated C6-8 stream (Hydrogenated Pyrolysis Gasoline), and a 21-day rabbit dermal

irritation study, which included evaluations for systemic effects, was conducted with a C5-C10 fraction of Pyrolysis Gasoline (Rerun Tower Overheads).

Inhalation

Hydrotreated C6-C8 stream (Hydrogenated Pyrolysis gasoline) was evaluated for toxicity in a 5 day inhalation study using F344 rats. Animals (5/sex/group) were exposed at concentrations of 0, 4869 and 9137ppm daily for 5 days and sacrificed on day 8 after a 2-day post-exposure observation period. Three rats (1M, 2F) from the high dose group died on day 1-2 of exposure. Rats were lethargic and showed labored respiration on days 1-5 of treatment but all but one high dose rat recovered fully by day 8. Group mean body weights were significantly decreased in a dose-related manner but no test material-related effects were reported at gross necropsy.
NOAEL <4869ppm

Dermal

C5-C10 fraction of Pyrolysis Gasoline (Rerun Tower Overheads) was evaluated for skin irritation and systemic toxicity in a 21-day dermal study using New Zealand White rabbits. Test material [undiluted] was applied to the shaved abraded back of 4M and 4F rabbits per group at concentrations of 0, 0.1, 0.5, and 1.0ml once a day for 21 consecutive days. Exposed sites were unoccluded and each rabbit wore a Plexiglas collar to retard ingestion of test material. Skin irritation and erythema were observed in a dose-related manner. No significant effects were seen on body or organ weight, feed consumption, hematology or serum chemistries. No abnormal microscopic changes were observed in any organ system with the exception of damage to dermal layers consistent with gross observations of irritation.
NOAEL (irritation) <0.10ml/kg; NOAEL (systemic) =1.0ml/kg.

Oral

No studies are available for these streams.

Conclusion

Inhalation exposure to Hydrotreated C6-C8 stream produced lethargy and labored respiration, effects from which most rats recovered after 2 days without exposure. Dermal exposure to the C5-C10 fraction of Pyrolysis gasoline induced skin irritation in rabbits but no other systemic toxicity.

The effects reported for these representatives of the High Benzene Naphthas category are similar to those observed for gasoline blending streams (API HPV test plan, 2003) in which dermal treatment induced primarily skin irritation and concomitant systemic effects and inhalation exposure-induced effects on lung, liver, kidney and blood occurred at high doses and were no longer observed after 4 weeks of recovery in most studies.

Repeated oral or inhalation exposures to many of the components of the streams in the category have been shown to cause adverse health effects in a variety of organs. Of the components summarized in Table A3-1, benzene demonstrated toxicity primarily in the hematopoietic system, toluene affected the central nervous system and induced loss of auditory sensitivity, and light hydrocarbon nephropathy was seen with exposure to hexane isomers, a 50/50 blend of n-butane and n-pentane, or with dicyclopentadiene. However, existing data also show that

antagonistic and synergistic interactions occur between some components comprising the streams, as noted above in the Chemical Component Interaction section of the Introduction to Section 4.1, which alter the effects of individual hydrocarbons. The target organs affected by exposure to the mixtures, and the severity of the effects, depend upon the relative concentrations of the components within each stream and the nature of the interactions between components.

Many of the C5 components of the High Benzene Naphthas Category are also components of the Pyrolysis C5s and Hydrotreated C5s streams (C5 Non-Cyclics Category) being tested for repeated-dose toxicity by the Panel, as part of the HPV Program. Based on structural similarity, pentenes are likely to have a toxicity profile similar to hexenes. The American Chemistry Council's Higher Olefins Panel addresses hexenes as part of the HPV Program. Also, the International Hydrocarbon Solvents Consortium covers the C5 aliphatic components in its C5 Aliphatics Category. Pentane is being addressed in the American Petroleum Institute's Petroleum Gases Test Plan. Other components are shared with the Panel's Resin Oils and Cyclodiene Dimer Concentrates Category streams. Several components are sponsored in the OECD SIDS or ICCA programs (see Table A3-1). Results of these studies will supplement the current assessment as data become available.

The most conservative assessment for repeated-dose human health hazards would be based on toxicity results for individual components (e.g. benzene). However data from testing of similar streams suggest the actual toxicity may be somewhat less in these blended streams due to lower concentrations, component interaction and competitive inhibition of biologically active hydrocarbon constituents.

4.1.3 Mutagenicity

In vivo Studies

Hydrotreated C6-C8 stream (Hydrogenated Pyrolysis Gasoline) was evaluated for cytogenetic damage in the mammalian bone marrow erythrocyte micronucleus assay using male and female Swiss mice. Mice were given oral doses of 0, 0.5, 1.0, or 2.0g/kg/day for 2 days or 1 dose of 2.0g/kg for one day. Treatment did not increase the frequency of micronucleated polychromatic erythrocytes in mouse bone marrow.

C5-C10 fraction of Pyrolysis gasoline (Rerun tower overheads) was tested in *Drosophila melanogaster* for gene (point) mutations and cytogenetic damage (chromosome loss or aberrations). The stream did not induce gene mutation or chromosome damage in this fruit fly system

In vitro Studies

Hydrotreated C6-C8 stream (Hydrogenated Pyrolysis Gasoline) did not induce mutagenic events in 4 strains of *Salmonella typhimurium* or one strain of *Escherichia coli* with or without metabolic activation from rat liver S9. This stream also did not induce unscheduled DNA synthesis in primary rat hepatocytes.

C5-C10 fraction of Pyrolysis gasoline (Rerun tower overheads) did not induce mutagenic events in 5 strains of *Salmonella typhimurium* with or without metabolic activation from rat liver S9.

However, this stream did cause weak differential killing in DNA repair-deficient strains of *E. coli* and *S. typhimurium*. In mammalian cells, a weak positive response in mouse lymphoma cells without metabolic activation was induced but no increase in revertant colonies with metabolic activation was seen.

Conclusion

Chromosome aberrations: The representative streams tested did not induce cytogenetic damage in animals. Indeed, Hydrotreated C6-C8 demonstrated how interaction and competition for metabolic sites can block toxicity of individual components. Although containing 55% benzene, the presence in the Hydrotreated C6-8 Fraction of other components (approximately 25% toluene, 10% xylene, 7% pentane, 7% ethylbenzene, 3% cyclohexane, and 2% hexane) apparently inhibited the expected clastogenicity of benzene.

Although benzene has caused chromosome aberrations *in vivo* and *in vitro*, toluene, the other most prevalent component in this category, is not clastogenic. Of the remaining identified category components present at concentrations greater than 5%, only vinyl acetate, 1,3-butadiene, isoprene, hexane, and naphthalene have been reported to cause chromosome aberrations (see Table A3-1). As discussed above and in the introduction to Sect.4.1, coadministration of benzene with other hydrocarbons that are substrates for the cytochrome P450 enzymes can reduce clastogenicity. Additional information that may be useful will become available from mouse micronucleus testing conducted with streams distilled from Pyrolysis Gasoline that are members of the Panel's C5 Non-Cyclics and Resin Oils and Cyclodiene Dimer Concentrates categories.

Gene mutation*:* Neither stream induced gene mutation in bacterial systems. Although the C5-C10 fraction of Pyrolysis gasoline did cause a direct weak positive response in mammalian cells, inclusion of metabolic activation in the test system did not cause mutation, indicating that detoxification of the test material had occurred. The suggestion of genetic toxicity posed by this weak mutational activity and weak differential killing in repair-deficient strains of bacteria was not confirmed *in vivo*. No gene mutation or clastogenic events were observed in the sensitive *Drosophila* test system. Most of the stream components (Table A3-1) with the exception of 1,3-butadiene did not induce mutation in bacteria and are not considered gene mutagens.

Thus, based on composition and available data for representative streams, components and mixtures of components, it is unlikely that most streams in the High Benzene Naphthas category are gene mutagens or are significantly clastogenic.

4.1.4 Carcinogenicity [Non-HPV SIDS Endpoint]

In vivo Studies

No studies are available on high benzene naphtha streams. Of significant components, benzene is a demonstrated leukemogen in humans (acute mylogenous leukemia) and induces solid tumors in laboratory animals. However, toluene, also a major constituent of the High Benzene Naphthas Category streams, and a competitor with benzene for metabolic sites did not induce tumors at concentrations as high as 1200ppm in a 2-year inhalation study in rats and mice (NTP, 1990). In a 2-year inhalation study of wholly vaporized gasoline (MacFarland et al., 1984), the principal

tumorigenic effect occurred in kidneys of male rats and was later demonstrated to be a species and sex specific event unrelated to health hazards for man (US EPA, 1991).

In vitro Studies

Hydrotreated C6-C8 stream (Hydrogenated Pyrolysis Gasoline) caused cell transformation in BALB-c/3T3 cells at a high concentration of 5000ug/ml, a level that was too toxic for cells to recover and form colonies.

C5-C10 fraction of Pyrolysis gasoline (Rerun tower overheads) did not induce cell transformation in two test systems; the mouse embryo C3H 10T1/2 cell line or the BALB-c/3T3 cell line

Conclusions

Cell transformation assays on representative streams demonstrated minimal if any carcinogenic potential. Transformation induced by the Hydrotreated C6-C8 stream occurred at a high dose from which cells are unlikely to survive and produce potentially tumorigenic colonies, and the C5-C10 fraction did not induce cell transformation.

Although no carcinogenesis studies were available on high benzene naphtha streams, extrapolation from 2-year cancer bioassays on gasoline and toluene, and the apparent competitive detoxifying effects of toluene when co-administered with benzene seen in other studies, suggest that carcinogensis is unlikely to be a significant endpoint of toxicity for this naptha category.

4.1.5 Toxicity for Reproduction

Effects on Fertility

No reproductive toxicity studies are available on high benzene naphtha streams. However, data are available on many components in reproductive studies and/or pathological evaluations of reproductive organs in systemic toxicity studies (see Table A3-1). In its review of benzene, ATSDR (1997) concluded that, although there are some data indicating adverse gonadal effects (e.g., atrophy/degeneration, decrease in spermatozoa, moderate increases in abnormal sperm forms), data on reproductive outcomes are either inconclusive or conflicting. However, most studies indicate no effects on reproductive indices, even at high doses. Reproductive organ effects were seen after inhalation exposure to isoprene and hexane in subchronic toxicity studies but such effects may not affect reproductive capabilities in practice. However, for hydrocarbons tested in multi-generation reproductive studies – toluene, cyclohexane, pentane, commercial hexane (isomers), mixed xylenes, and styrene, no effects on fertility or other reproductive parameters were reported. 3-Methylpentane and methylcyclopentane were components (16.0% and 15.6%, respectively) of a commercial hexane stream that was negative in a rat inhalation two-generation reproductive toxicity study. Dicyclopentadiene demonstrated reproductive effects in a 3-generation reproductive study only at maternally toxic doses.

For other chemical components present in High Benzene Naphtha streams, data generated by other test plans within the HPV Program will provide additional information about the potential of these substances to cause reproductive effects. Some of these materials are also components of the Pyrolysis C5s and Hydrotreated C5s streams (C5 Non-Cyclics Category) that being tested for

reproductive toxicity by the Panel, as part of the HPV Program. Also, based on structural similarity, pentenes are likely to have a developmental toxicity profile similar to hexenes, which will be addressed by the American Chemistry Council's Higher Olefins Panel as part of the HPV Program. Pentenes are also covered by the American Chemistry Council's Hydrocarbon Solvents Panel (C5 Aliphatics Test Plan). Additional reproductive toxicity information will become available from testing conducted by the Panel for the Resin Oils and Cyclodiene Dimer Concentrates Category with streams distilled from Pyrolysis Gasoline. 1,3-Butadiene is being tested for reproductive effects in the OECD SIDS program.

Developmental Toxicity

C5-C10 fraction of Pyrolysis gasoline (Rerun tower overheads) was tested for developmental toxicity in New Zealand White rabbits at oral gavage doses of 0, 10, 25 and 50mg/kg/day from days 6-28 of gestation. One rabbit given 50mg/kg/day aborted on day 19 but all other animals completed gestation. Maternal body weights were comparable to controls throughout gestation. There were no biologically or statistically significant differences in pregnancy ratios, number of corpora lutea, total implantations, resorptions, postimplanation loss, viable fetuses, litter size, fetal sex index, or mean fetal body weights. No statistically significant differences in number of litters with malformations were reported. C5-C10 fraction did not produce a teratogenic response in New Zealand White rabbits. Maternal NOAEL = 25mg/kg/day. Developmental NOAEL = 50mg/kg/day.

In addition to this study on a representative stream of the High Benzene Naphthas Category, developmental toxicity data exist for most components present in this category at concentrations greater than 5% (see Table A3-1). In these studies, no convincing evidence was seen for teratogenicity in the absence of maternal toxicity. Fetotoxicity has been reported for some components, but mostly in the presence of maternal toxicity (see Table A3-1). Only five components (pentenes, cyclopentene, 3-methylpentane, methylcyclopentane, 1,3-cyclopentadiene) lack developmental toxicity tests. However, these components do not have structural alerts for developmental toxicity, and data being generated by other test plans within the HPV Program will provide additional information about the potential of these substances to cause developmental effects. Three of the five chemicals are also components of the Pyrolysis C5s and Hydrotreated C5s streams (C5 Non-Cyclics Category) that are being tested for developmental toxicity by the Panel, as part of the HPV Program. Pentenes are addressed by the International Hydrocarbon Solvents Consortium (C5 Aliphatics Test Plan). Also, based on structural similarity, pentenes are likely to have a developmental toxicity profile similar to hexenes. The American Chemistry Council's Higher Olefins Panel address hexenes as part of the HPV Program. 3-Methylpentane and methylcyclopentane were components (16.0% and 15.6%, respectively) of a commercial hexane stream that was negative in a rat inhalation developmental toxicity study. Additional developmental toxicity information will become available from testing conducted by the Panel for the Resin Oils and Cyclodiene Dimer Concentrates Category with streams distilled from Pyrolysis Gasoline.

Conclusion

On the basis of available data, High Benzene Naphtha streams seem unlikely to cause significant reproductive or developmental toxicity. Reproductive studies on components present in these streams overall gave negative results. The C5-C10 fraction of Pyrolysis gasoline, a

representative high benzene naphtha stream did not induce developmental effects in rabbits and stream components that induced developmental toxicity did so primarily at doses that were also toxic to the dam. Additional data from the ongoing programs cited above will provide further supplementary data.

4.2 Assessment Summary for Human Health

Existing data are sufficient to characterize human health hazards of substances included in the High Benzene Naphthas Category and thus, satisfy HPV testing requirements. From data on representative streams, and read-across from chemical components and analogous streams, it can be concluded that High Benzene Naphthas are not acutely toxic by the oral, dermal or inhalation routes of exposure.

Although these streams contain substantial concentrations of benzene, they are unlikely to induce genetic damage *in vivo*, as demonstrated by the absence of clastogenicity induced by oral exposure to the Hydrotreated C6-C8 stream and the absence of gene mutation or chromosome damage in *Drosophila* exposed to the C5-C10 fraction of Pyrolysis gasoline. Mixtures of benzene with other hydrocarbons such as toluene and gasoline have resulted in inhibition of benzene chromosome damage potential. In addition, most stream components did not induce mutation in bacteria.

Repeated dose toxicity studies of two representative streams of the High Benzene Naphthas category showed results similar to those observed for analogous gasoline blending streams. Dermal exposure produced primarily skin irritation and concomitant systemic effects. Lethargy and labored respiration induced by limited duration inhalation exposure at high doses were resolved after treatment was terminated. The high content of benzene in these streams dictates that, from a conservative perspective, the systemic hazards from components be considered hazards for the streams until sufficient data becomes available to show the specific combination of components does not present the hazard. However, it is probable that any systemic toxicity demonstrated in laboratory animals would occur at doses well in excess of established workplace standards.

Based on available data, no significant reproductive or developmental toxicity is likely to result from exposure to streams in the High Benzene Naphthas category. Reproductive studies on components present in these streams overall gave negative results. The C5-C10 fraction of Pyrolysis gasoline did not induce developmental toxicity in rabbits and stream components that were biologically active caused effects primarily at high doses that were maternally toxic. Again, established workplace standards for components are sufficient to protect against human health hazards from exposure to member streams of the High Benzene Naphthas category.

The compositional similarities of these streams and consistency of data from mammalian studies using representative streams and components of these streams, along with published toxicity data from other naphtha streams in this boiling range, justifies the designation of the High Benzene Naphthas as a category for HPV.

5. HAZARDS TO THE ENVIRONMENT

5.1 Aquatic Effects

Acute Toxicity

The aquatic toxicity endpoints for the HPV Chemical Program include:

- Acute Toxicity to a Freshwater Fish
- Acute Toxicity to a Freshwater Invertebrate
- Toxicity to a Freshwater Alga

Although aquatic toxicity data are not available for products in the High Benzene Naphthas Category, there are sufficient read across data from constituent chemicals of those products and comparably complex products to fully characterize the toxicity of this category. Study specifics and robust summaries for analogous streams are available in the API Gasoline Blending Streams test plan on the US EPA HPV website. The use of data from selected read across materials to products in this category can be justified for the following reasons:

- Individual chemicals and complex products used for read across purposes contain a chemical class or combinations of chemical classes (i.e., olefins, aromatics, paraffins) that are found in streams from this category.
- Individual chemicals and complex products used for read across purposes have a carbon number or carbon number range that falls within the range of carbon numbers found in streams from this category.
- Individual chemicals and complex products used for read across purposes as well as the streams in this category are composed of chemicals that all act by a similar mode of toxic action.

The data in Appendix 6, Table A6-1 provides a comparison of the range of product compositions (i.e., carbon number, chemical class, weight percent) in the High Benzene Naphthas Category to products that have been used to characterize the aquatic toxicity of this category. This comparison illustrates the similarity in carbon number ranges between products in this category and the selected products with read across data.

The data in Appendix 6, Tables A6-2 (Fish), A6-3 (Daphnia), and A6-4 (Algae) establish the range of toxicity for products in this category, based on the read across data. Generally, the fish, invertebrate, and alga studies followed the OECD Guidelines 203, 202, and 201, respectively. For complex products, the test procedures used to develop the test material exposure solutions also applied the OECD guidance described in "Guidance Document on Aquatic Toxicity Testing of Difficult Substances and Mixtures" (OECD, 1999). For these studies, the results are represented as lethal loading (LL) endpoints, a designation used to define results for multi-hydrocarbon mixtures, tested as water accommodated fractions [WAF], compared to the data developed for pure chemicals, which represent results as lethal concentration endpoints where test material is analytically verified. High benzene naphthas are likely to exhibit a moderate range of acute toxicity in freshwater fish and invertebrates and a moderate level of toxicity in freshwater algae.

For representative chemicals and products, experimental acute fish toxicity values range between 2.5 to 46.0 mg/L for two species (Table A6-2), while acute invertebrate (*Daphnia*) toxicity

values range between 0.9 to 32 mg/L for one species (Table A6-3). In comparison, alga toxicity values for one species range between 1.0 to 64 mg/L (for biomass or growth rate endpoints), while alga loading rate NOELR values range between 1.0 to 51 mg/L (for biomass and growth rate endpoints) (Table A6-4). Although not an HPV SIDS endpoint, chronic toxicity data from a representative high aromatic gasoline blending stream (API Gasoline Blending Streams Test Plan, 2003)gave similar results for fish and invertebrate toxicity:

Daphnia Reproductive EL50 = 14mg/L; NOEL <0.30mg/L
Fathead Minnow LL50 [survival] = 5.2mg/L;
NOEL[growth and survival] = 2.6mg/L

The fairly narrow range of effect is expected because the chemical constituents of products in this category are neutral organic hydrocarbons whose toxic mode of action is non-polar narcosis. The mechanism of short-term toxicity for these chemicals is disruption of biological membrane function (Van Wezel and Opperhuizan, 1995), and the differences between measured toxicities (i.e., LC/LL50, EC/EL50) can be explained by the differences between the target tissue-partitioning behavior of the individual chemicals (Verbruggen, et al., 2000).

The existing fish toxicity database for narcotic chemicals supports a critical body residue (CBR, the internal concentration that causes mortality) of between approximately 2-8 mmol/kg fish (wet weight (McCarty and MacKay, 1993; McCarty et al., 1991), supporting the assessment that these chemicals have equal potencies. When normalized to lipid content, the CBR is approximately 50 µmol of hydrocarbon/g of lipid for most organisms (Di Toro et al., 2000). Because the products in this category are all complex mixtures containing relatively similar series of homologous chemicals [paraffin, olefins and/or aromatic carbon number content within approximately C5-C11], their short-term toxicities are expected to fall within the range of toxicity demonstrated by the individual chemicals, as well as comparable products. The existing data are believed to form a sufficiently robust dataset to fully characterize the aquatic toxicity endpoints in the HPV Chemical Program for this category.

5.2 Assessment Summary for the Environment

The environmental impact of products in the High Benzene Naphthas Category has been determined by evaluating data developed for chemical components found in the products in this category and for similar complex products. The hydrocarbons that comprise this category have a very low potential to hydrolyze and do not photodegrade directly due to a minimal capacity to absorb appreciable light energy above 290nm. However, atmospheric oxidation constitutes a significant route of degradation. Calculation of atmospheric half-lives of representative constituent chemicals identified a range of 0.9 - 65.8hours as a result of indirect hydrolysis by hydroxyl radical attack. Fugacity modelling demonstrated that members of this category partition primarily into the air, with slight partitioning into water and soil, and minimal partitioning into sediment. Read-across data shows that these products are likely to biodegrade significantly and have the potential to produce a moderate level of toxicity in freshwater algae and a moderate level of acute toxicity in freshwater fish and invertebrates. Aquatic toxicity for products in this category can be predicted based on carbon number, measured or calculated toxicities of constituent hydrocarbons and constituent composition.

Extensive data on chemical components of the products in this category and on streams containing similar mixtures of complex hydrocarbons have demonstrated that, based on biological and physical degradation processes, products in the High Benzene Naphthas Category, although moderately toxic to aquatic species at exposure, are not expected to persist in the environment. The consistency of results in environmental studies for these materials justifies the designation of High Benzene Naphthas as a category for HPV.

6. PROGRAM SUMMARY AND RECOMMENDATIONS

The High Benzene Naphthas Test Plan has addressed petrochemical streams (products) derived from ethylene manufacturing processes. The category is comprised of 19 CAS numbers and 10 petrochemical streams. The category includes complex hydrocarbon mixtures containing primarily C5 through C11 olefins, paraffins, and aromatic molecules. The average benzene content of these streams is 55% but ranges from 10 –80%; toluene content ranges from 0.3 -40% depending on the stream. Virtually all of the benzene contained in the category streams is ultimately isolated as high purity benzene product, which is the primary use of the category streams. There are no known consumer uses for these category products. All of these products are produced and used on-site and/or transferred in closed systems so that occupational and public exposure to High Benzene Naphtha streams is very low.

Human Health Effects: Data on representative streams and read-across from chemical components indicate that High Benzene Naphtha streams are not acutely toxic by the oral, dermal or inhalation routes of exposure. It is unlikely that most streams in this category would cause significant genetic toxicity. Tested streams did not cause mutational events in bacteria, and a weak direct effect in mammalian cells from treatment with a C5-C10 fraction of Pyrolysis gasoline, was not confirmed *in vivo* by any expression of gene mutation in *Drosophila*. Although these streams contain substantial concentrations of benzene, a known clastogen, no cytogenetic damage was induced by oral treatment of rats with the Hydrogenated C6-C8 stream [55% benzene], demonstrating the inhibitory effects of other components in the stream, probably from competition for metabolic sites.

Benzene, as a predominant component in most streams is considered a key driver in establishing health effects within the SIDS battery of tests. To provide a conservative estimate of health hazard, results of benzene-induced systemic toxicity must be addressed – hazards from components should be considered hazards for the streams until sufficient data become available to show the specific combination of components does not present a hazard. However, as it has been demonstrated in the area of cytogenetics, the presence of biologically active components blended together can inhibit toxicity inducible by individual components. Limited repeat dose studies from representative streams in the High Benzene Naphthas Category demonstrated skin irritation and concomitant systemic effects from dermal exposure, and lethargy and labored respiration inducde by inhalation at high doses. Results were similar to effects reported in the API Gasoline Blending Streams test plan (2003), effects from which animals recovered after 4 weeks without exposure. Such data suggest that toxicity of the blended streams may be less severe than that of individual components due to lower individual component concentrations, component interaction and competitive inhibition. No significant reproductive effects were reported in multigeneration studies of stream components. Developmental effects from components present in High Benzene Naphtha streams occurred primarily at doses that were maternally toxic as well. A developmental study in rabbits with a representative high benzene

naphtha stream did not result in adverse effects on any developmental parameters except for 1 high dose rabbit who aborted, and no malformations were induced.

Physicochemical, Environmental and Aquatic Endpoints: For environmental endpoints, measured data on components present in the products of the High Benzene Naphthas category, and on other complex products that contain a similar range of chemical classes and carbon numbers were used. Where measured data do not exist, calculated data for selected constituents of these naphthas have been developed using the EPIWIN© computer models described by EPA. The hydrocarbons that comprise this category have a very low potential to hydrolyze and do not photodegrade directly due to a minimal capacity to absorb appreciable light energy above 290nm. However, atmospheric oxidation constitutes a significant route of degradation. Calculation of atmospheric half-lives of representative constituent chemicals identified a range of 0.9 – 65.8 hours as a result of indirect hydrolysis by hydroxyl radical attack. Fugacity modeling demonstrated that members of this category partition primarily into the air, with slight partitioning into water and soil, and minimal partitioning into sediment. Read-across data shows that these products have the potential to produce a moderate level of toxicity in freshwater algae and a moderate level of acute toxicity in freshwater fish and invertebrates but are likely to biodegrade significantly and are not expected to persist in the environment.

The extensive body of data available for mammalian and environmental endpoints on representative constituents of products in this category, on streams of similar complex hydrocarbon composition and some data from representative streams, are sufficient to fully characterize the potential toxicity for materials in this category and demonstrate the integrity of the category, itself. No additional testing is needed to meet the requirements of the HPV program.

New data on hydrocarbons present in High Benzene Naphtha streams that are developed in other HPV programs will be evaluated when available in the context of the present assessment. This category summary document will be amended should the new data result in substantial changes to the conclusions.

7. REFERENCES

ACGIH (American Conference of Governmental Industrial Hygienists). 1986. Documentation of the TLV Values and Biological Exposure Indices, 5th ed., Cincinnati, IH, p. 163.

Andrews, L.S., E.W. Lee, C.M. Witmer, J.J. Kocsis, and R. Snyder. 1977. Effects of toluene on the metabolism, disposition and hemopoietic toxicity of [^{3}H]benzene. Biochem. Pharmacol. 26:293-300.

ATSDR (Agency for Toxic Substances and Disease Registry). 1997. Toxicological Profile for Benzene. Prepared by Research Triangle Institute for U.S. Department of Health & Human Services, Public Health Service, ATSDR [available on the internet].

ATSDR (Agency for Toxic Substances and Disease Registry). 1993. Toxicological Profile for 1,3-Butadiene. Prepared by Syracuse Research Corporation for U.S. Department of Health & Human Services, Public Health Service, ATSDR [available on the internet].

ATSDR (Agency for Toxic Substances and Disease Registry). 1999. Toxicological Profile for Ethylbenzene. Prepared by Research Triangle Institute for U.S. Department of Health & Human Services, Public Health Service, ATSDR [available on the internet].

ATSDR (Agency for Toxic Substances and Disease Registry). 1999. Toxicological Profile for n-Hexane. Prepared by Research Triangle Institute for U.S. Department of Health & Human Services, Public Health Service, ATSDR [available on the internet].

ATSDR (Agency for Toxic Substances and Disease Registry). 1995. Toxicological Profile for Naphthalene. Prepared by Sciences International, Inc. under contract to Research Triangle Institute for U.S. Department of Health & Human Services, Public Health Service, ATSDR [available on the internet].

ATSDR (Agency for Toxic Substances and Disease Registry). 1992. Toxicological Profile for Styrene. Prepared by Life Systems, Inc. under contract to Clement International Corporation for U.S. Department of Health & Human Services, Public Health Service, ATSDR [available on the internet].

ATSDR (Agency for Toxic Substances and Disease Registry). 2000. Toxicological Profile for Toluene. Prepared by Syracuse Research Corporation for U.S. Department of Health & Human Services, Public Health Service, ATSDR [available on the internet].

ATSDR (Agency for Toxic Substances and Disease Registry). 1995. Toxicological Profile for Xylenes. Prepared by Sciences International under contract to Research Triangle Institute for U.S. Department of Health & Human Services, Public Health Service, ATSDR [available on the internet].

API Petroleum HPV Testing Group. 2003. Gasoline Blending Streams Test Plan and Robust SummariesAPI, Washington, D.C. EPA website for HPV Chemical Challenge test plans: http://www.epa.gov/chemrtk/viewsrch.htm.

Bamberger, J.R. 1996. 90-Day inhalation toxicity study with cyclohexane in mice. Haskell Laboratory for Toxicology and Industrial Medicine, DuPont, Report No. HLR 17-96.

Beals, S.M., R.A. Jacobson, J.P. Robinson, H.T.Appleton, P.A. Howard, and J. Santodonato. 1986. Technical Support Document, Cyclohexane. Doc. No. SRC TR-86-030 [draft final]. Syracuse Research Corporation, Syracuse, NY. Prepared for Test Rules Development Branch Existing Chemical Assessment Division, Office of Toxic Substances, Washington, DC.

Bond, J.A, T.L. Leavens, M.J. Seaton, and M.A. Medinsky. 1998. Predicting the toxicity of chemical mixtures. CHEMTECH, July.

Brown, N.A. 1991. Reproductive and developmental toxicity of styrene. Reproductive Tox. 5:3-29.

Brown, N.A. 1993. Developmental and reproductive toxicity of styrene: A review update. International Symposium on Health Hazards of Butadiene and Styrene. Abstract reprinted in The SIRC Review 3(1):44-45.

Chemicals Inspection and Testing Institute, Japan. 1992. Biodegradation and Bioaccumulation Data of Existing Chemicals Based on the CSCL Japan. Japan Chemical Industry Ecology-Toxicology and Information Center. ISBN 4-89074-101-1.

Ciranni R, Barale R, Ghelardini G, & Loprieno N (1988) Benzene and the genotoxicity of its metabolites. II. The effect of the route of administration on the micronuclei and bone marrow depression in mouse bone marrow cells. Mutat Res, 209: 23-28.

Daughtrey, W.C., D.L. Putman, J. Duffy, A.I. Soiefer, C.J. Kirwin, L.N. Curcio, and T.H. Keenan. 1994a. Cytogenetic studies on commercial hexane solvent.

Daughtrey, W.C., T. Neeper-Bradley, J. Duffy, L. Haddock, T. Keenan, C. Kirwin, and A. Soiefer. 1994b. Two-generation reproduction study on commercial hexane solvent. J. Applied Toxicology 14(5):387-393.

Daughtrey, W.C., P. Newton, R. Rhoden, C. Kirwin, L. Haddock, J. Duffy, T. Keenan, W. Richter, and M. Nicolich. 1999. Chronic inhalation carcinogenicity study of commercial hexane solvent in F-344 rats and B6C3F1 mice. Toxicological Sciences 48:21-29.

Di Toro, D.M., J.A. McGrath, and D.J. Hansen. 2000. Technical Basis for Narcotic Chemicals and Polycyclic Aromatic Hydrocarbon Criteria. I. Water and Tissue. Environmental Toxicology and Chemistry, 19:1951-1970.

ECETOC (European Centre for Ecotoxicology and Toxicology of Chemicals) Special Report No. 12. 1,3-Butadiene OEL Criteria Document (Second Edition). 1997. Programme for the Joint Assessment of Commodity Chemicals. Jacc Report No. 19. Brussels, Belgium.

ECETOC (European Centre for Ecotoxicology and Toxicology of Chemicals) report on Dicyclopentadiene. 1991. Programme for the Joint Assessment of Commodity Chemicals. Jacc Report No. 19. Brussels, Belgium.

ECETOC (European Centre for Ecotoxicology and Toxicology of Chemicals) report on Xylenes. 1986. Programme for the Joint Assessment of Commodity Chemicals. Jacc Report No. 6. Brussels, Belgium.

EPA/OTS Doc.8690000024: Test for oral toxicity in rats with cyclopentadiene with cover letter dated 09/28/95.

EPA/OTS Doc.8690000121S: Subacute inhalation exposure of cyclopentadiene with cover letter dated 09/28/95.

EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. SyracuseResearchCorporation, Syracuse, NY, USA.

EU Risk Assessment. 2001. Benzene. Draft Risk Assessment Document [in Risk Assessment Review]. Available on internet at http://ecb.jrc.it/existing-chemicals.

EU Risk Assessment. 2000. Cyclohexane. ECB# 031. Draft Risk Assessment Document [in Risk Assessment Review]. Available on internet at http://ecb.jrc.it/existing-chemicals.

EU Risk Assessment. 2001. Naphthalene. Draft Risk Assessment Document [in Risk Assessment Review]. Available on internet at http://ecb.jrc.it/existing-chemicals.

EU Risk Assessment. 2001. Toluene. Draft Risk Assessment Document [in Risk Assessment Review]. Available on internet at http://ecb.jrc.it/existing-chemicals.

ExxonMobil. 1982. Unpublished reports for Rerun Tower Overheads: Mouse Lymphoma [M1252-78], DNA Repair [M1251-78], Drosophila [M1253-78], Mouse Skin Painting [M0417-77].

Frontali, N. M.D. Amantini, A. Spagnolo, A.M. Guarcini, and M.C. Saltari. 1981. Experimental neurotoxicity and urinary metabolites of the C5-C7 aliphatic hydrocarbons used as glue solvents in shoe manufacture. Clin. Tox. 18:1357-1367.

Gad-El-Karim, M.M., B.L. Harper and M.S. Legator. 1984. Modifications in the myeloclastogenic effect of benzene in mice with toluene, phenobarbital, 3-methylcholanthrene, Aroclor 1254 and SKF-525A. Mutation Res. 135:225-243.

Gad-El-Karim, M.M., V.M.S. Ramanujam and M.S. Legator. 1986. Correlation between the induction of micronuclei in bone marrow by benzene exposure and the excretion of metabolites in urine of CD-1 mice. Toxicol. Appl. Pharmacol. 85:464-477.

Galassi, S., M. Mingazzini, L. Viagano, D. Cesareo, and M.L. Tosato. 1988. Aproaches to Modeling Toxic Responses of Aquatic Organisms to Aromatic Hydrocarbons. Ecotox. Environ. Safety. 16:158-169.

Galvin, J.B. and F. Marashi. 1999. n-Pentane. J. Toxicology and Env. Health. Pt. A,58:35-36.

Halder, C.A., C.E. Holdsworth, B.Y. Cockrell, and V.J. Piccirillo. 1985. Hydrocarbon nephropathy in male rats: Identification of the nephrotoxic components of unleaded gasoline. Tox. and Industrial Health 1(3):67-87.

Harris, J.C. 1982. Rate of Aqueous Photolysis. Chapter 8 in Lyman.W.J., Reehl, W.F., and Rosenblatt, D.H., eds. Handbook of Chemical Property Estimation Methods. McGraw-Hill., New York, NY.

Hite, M., M. Pecharo, I. Smith and S. Thornton. 1980. The effect of benzene in the micronucleus test. Mut. Res. 77:149-155.

IARC (International Agency for Research on Cancer). 1999. Isoprene. Monographs on the Evaluation of Carcinogenic Risks to Humans. Vol. 71, Part 3, Lyon, France, pp. 1015-1024.

IARC (International Agency for Research on Cancer). 1994. Styrene. Monographs on the Evaluation of Carcinogenic Risks to Humans. Vol. 60, Lyon, France, pp. 233-320.

IARC (International Agency for Research on Cancer). 1999. Toluene. Monographs on the Evaluation of Carcinogenic Risks to Humans. Vol. 71, Part 2, Lyon, France, pp. 829-864.

IRIS (Integrated Risk Information System). 1990. Vinyl Acetate. Developed by the U.S. EPA.

HSDB: TOMES CPS™ System, MICROMEDEX, Englewood, Colorado, Vol. 38. CD-ROM.

JETOC (Japanese Chemical Industry Ecology – Toxicology and Information Center. 1998. Special Issue #3, No. 32 (March, 1998), Tokyo, Japan. In: Handbook of Existing and New Chemical Substances, 8th Ed. 1999. Supervised by Chemical Products Safety Division, Basic Industries Bureau, The Ministry of International Trade and Industry.

Kirwin, C. , R. San, J. Harbell, A. Soiefer, W. Daughtrey and T. Keenan.1991. Salmonella and CHO/HGPRT mutation assays of commercial hexane. The Toxicologist 11(1):315.

Kreckman, K.H. 1997. Inhalation developmental toxicity study of cyclohexane in rats. Haskell Laboratory for Toxicology and Industrial Medicine, DuPont, Report No. HLR 881-96.

MacFarland, H.N., Ulrich, C.E., Holdsworth, C.E., et al. 1984. A chronic inhalation study with unleaded gasoline vapor. J Amer College of Toxicol 3: 231-248.

Mackay, D., A. Di Guardo, S. Paterson, and C. E. Cowan. 1996. Evaluating the Environmental Fate of a Variety of Types of Chemicals Using the EQC Model. Environ.

Malley, L.A. 1996a. 90-Day inhalation toxicity study with cyclohexane in rats. Haskell Laboratory for Toxicology and Industrial Medicine, DuPont, Report No. HLR 298-96.

Malley, L.A. 1996b. 90-Day inhalation neurotoxicity study with cyclohexane in rats. Haskell Laboratory for Toxicology and Industrial Medicine, DuPont, Report No. HLR 752-95.

McCarty, L.S. and D. Mackay. 1993. Enhancing Ecotoxicological Modeling and Assessment. Environmental Science and Technology, 27:1719-1728.

McCarty, L.S., D. Mackay A.D. Smith, G.W. Ozburn, and D.G. Dixon. 1991. Interpreting Aquatic Toxicity QSARs: The Significance of Toxicant Body Residues at the Pharmacologic Endpoint. In: WSAR in Environmental Toxicology - IV. J.L.M. Hermens and A. Opperhuizen, eds. Elsevier.

McGregor, D. 1994. The genetic toxicology of toluene. Mut Res. 317:2134-228.

McKee, R., E. Frank, J. Heath, D. Owen, R. Przygoda, G. Trimmer, and F. Whitman. 1998. Toxicology of n-pentane. J. Appl. Toxicol. 18:431-442.

Medinsky, A., P.M. Schlosser, and J.A. Bond. 1994. Critical issues in benzene toxicity and metabolism: the effect of interactions with other organic chemicals on risk assessment. Env. Health Perspectives 102(Supp. 9):119-124.

Meyne, J. and M.S. Legator. 1980. Sex-related differences in cytogenetic effects of benzene in the bone marrow of Swiss mice. Environ. Mutagenesis 2:43-50.

National Toxicology Program 1990. Toxicology and carcinogenesis studies of toluene CAS #108-88-3) in F344/N rats and B6C3F1 mice (inhalation studies). NTP Technical Report Series No. 371. U.S. Dept. of Health and Human Services.

Neely, W. B. 1985. Hydrolysis. In: W. B. Neely and G. E. Blau, eds. Environmental Exposure from Chemicals. Vol I., pp. 157-173. CRC Press, Boca Raton, FL, USA.

Nylen, P. 1996. Differing non-additive alterations in different parts of the nervous system of the rat. Food and Che.. Tox. 34(11/12): 1121-1123.

Nylen, P. 1989. Testicular atrophy and loss of nerve growth factor-immunoreactive germ cell line in rats exposed to n-hexane and a protective effect of simultaneous exposure to toluene or xylene. Arch. Toxicol. 63:296-307.

OECD (Organization for Economic Co-operation and Development). 1999. Draft Guidance Document on Aquatic Toxicity Testing of Difficult Substances. OECD Environmental Health and Safety Publications, Series on Testing and Assessment. OECD, Paris, France.

RTECS (Registry of Toxic Effects of Chemical Substances): TOMES CPS™ System, MICROMEDEX, Englewood, Colorado, Vol. 38, CD-ROM.

Soiefer, A., K. Robinson, B. Broxup, J. Duffy, T. Keenan, and W. Daughtrey. 1991. A subchronic neurotoxicity study of commercial hexane vapor in the rat. The Toxicologist II, p. 315 (abstract).

Suzuki, S., H.Atai, Y. Hatakeyama, M. Hara, and S. Nakagawa. 1989. Administration-route-related differences in the micronucleus test with benzene. Mut. Res. 223:407-410.

U.S. Environmental Protection Agency (U.S. EPA). 1991. Alpha 2 microglobulin: association with chemically induced renal toxicity and neoplasia in the male rat. In Risk Assessment Forum. US Government Printing Office, Washington, DC: EPA:85

U.S. EPA. 1999a. The Use of Structure-Activity Relationships (SAR) in the High Production Volume Chemicals Challenge Program. OPPT, EPA. Washington, DC, USA.

U.S. EPA. 1999b. Determining the Adequacy of Existing Data. OPPT, EPA., Washington, DC, USA.

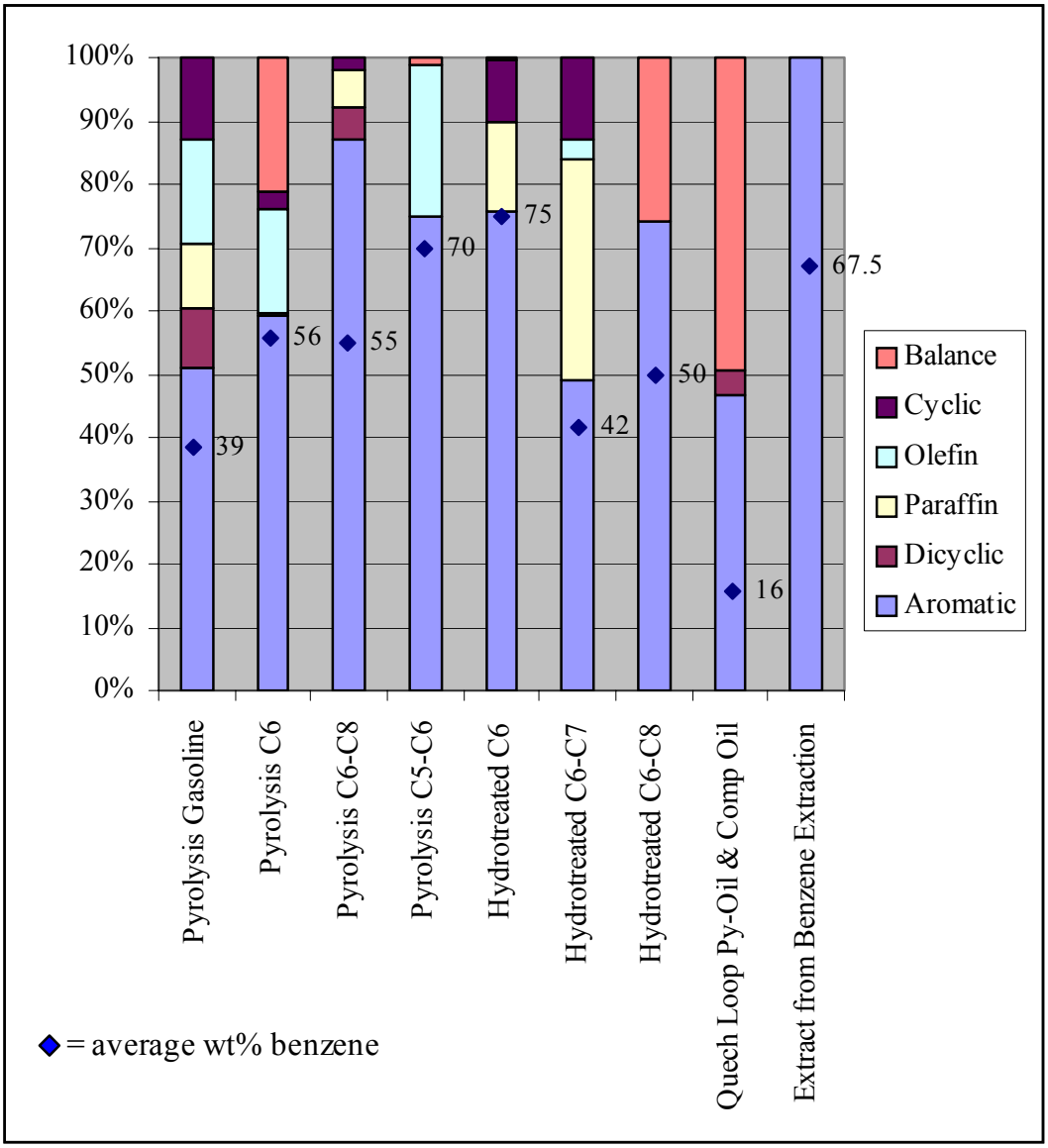
Van Wezel, A.P. and A. Opperhuizen. 1995. Narcosis Due to Environmental Pollutants in Aquatic Organisms: Residue-Based Toxicity, Mechanisms, and Membrane Burdens. Critical Reviews in Toxicology, 25:255-279.

Verbruggen, E.M.J., W.J.J. Vaes, T.F. Parkerton, and J.L.M. Hermens. 2000. Polyacrylate-Coated SPME Fibers as a Tool to Simulate Body Residues and Target Concentrations of Complex Organic Mixtures for Estimation of Baseline Toxicity. Environmental Science and Technology, 34;324-331.

WHO EHC. 1997. World Health Organization, International Programme on Chemical Safety, Environmental Health Criteria for Xylenes. No. 190.

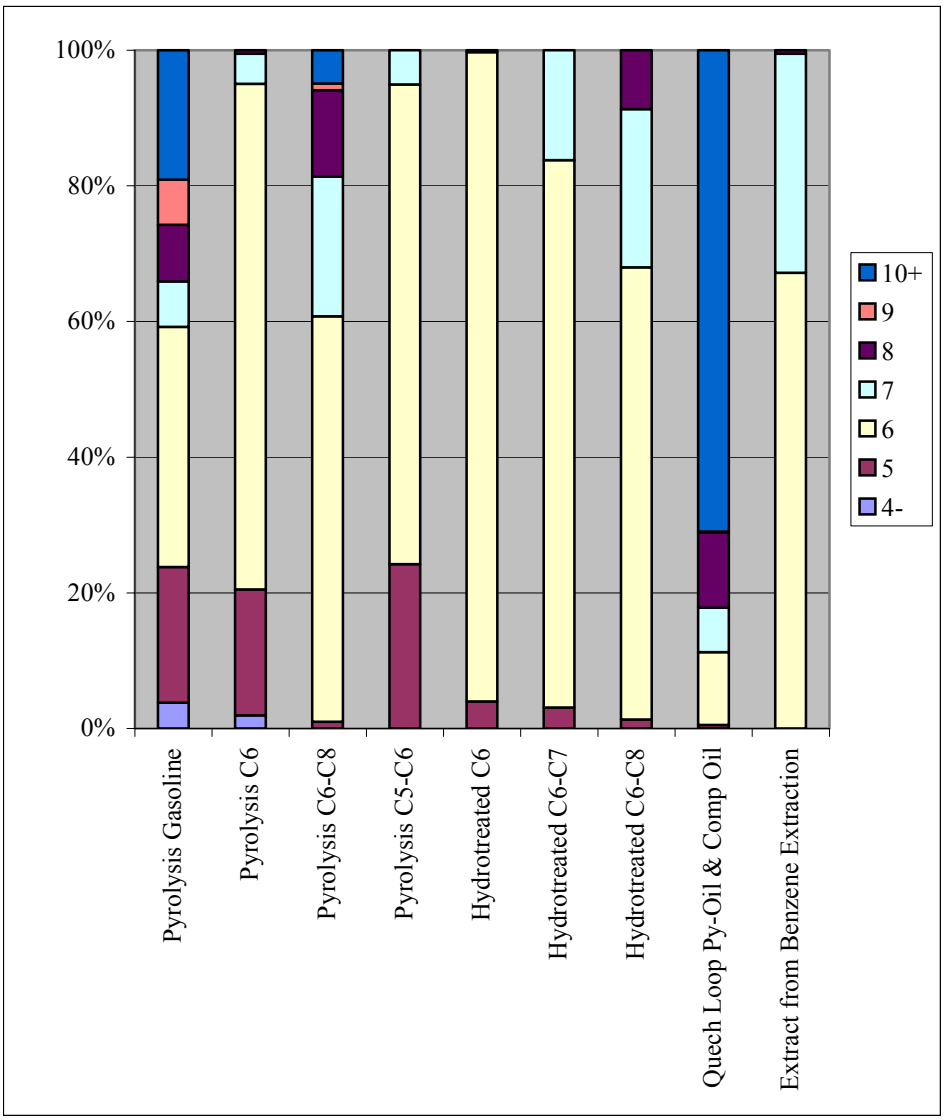
Zepp, R. G., and D. M. Cline. 1977. Rates of Direct Photolysis in the Aqueous Environment. Environ. Sci. Technol. 11:359.366.

Figure 4.
Stream Compositions: High Benzene Naphthas Category



Compositions are averages of the ranges reported for the complex, variable composition streams. In some cases, because of overlaps and variations in the way components were sometimes grouped in individual reports, the sum of the averages for the streams exceeded 100%. In those cases, compositions were normalized for plotting in Figure 4. When the total of the average of reported values was less than 100%, a "Balance" was added and included. Average wt% benzene content (actual average of reported values) of the streams is shown as diamonds with the average wt% given. Components grouped as "cyclic" include both paraffin and olefin cyclic hydrocarbons. The term "olefin" as used here does not include the cyclic olefins.

Figure 5
Stream Carbon Range Content - High Benzene Naphthas Category



Carbon range contents were normalized. Any apparent inconsistencies that may exist between Figure 4 and Figure 5 are largely due to normalization of the data.

Appendix 1: Ethylene Process Description

A. The Ethylene Process

1. Steam Cracking

Steam cracking is the predominant process used to produce ethylene. Various hydrocarbon feedstocks are used in the production of ethylene by steam cracking, including ethane, propane, butane, and liquid petroleum fractions such as condensate, naphtha, and gas oils. The feedstocks are normally saturated hydrocarbons but may contain minor amounts of unsaturates. These feedstocks are charged to the coils of a cracking furnace. Heat is transferred through the metal walls of the coils to the feedstock from hot flue gas, which is generated by combustion of fuels in the furnace firebox. The outlet of the cracking coil is usually maintained at relatively low pressure in order to obtain good yields to the desired products. Steam is also added to the coil and serves as a diluent to improve yields and to control coke formation. This step of the ethylene process is commonly referred to as "steam cracking" or simply "cracking" and the furnaces are frequently referred to as "crackers."

Subjecting the feedstocks to high temperatures results in the partial conversion of the feedstock to olefins. In the simplest example, feedstock ethane is partially converted to ethylene and hydrogen. Similarly, propane, butane, or the liquid feedstocks are also converted to ethylene. While the predominant products produced are ethylene and propylene, a wide range of additional products are also formed. These products range from methane (C1) through fuel oil (C12 and higher) and include other olefins, diolefins, aromatics and saturates (naphthenes and paraffins).

2. Refinery Gas Separation

Ethylene and propylene are also produced by separation of these olefins from refinery gas streams, such as from the light ends product of a catalytic cracking process or from coker offgas. This separation is similar to that used in steam crackers, and in some cases both refinery gas streams and steam cracking furnace effluents are combined and processed in a single finishing section. These refinery gas streams differ from cracked gas in that the refinery streams have a much narrower carbon number distribution, predominantly C2 and/or C3. Thus the finishing of these refinery gas streams yields primarily ethylene and ethane, and/or propylene and propane.

B. Products of the Ethylene Process

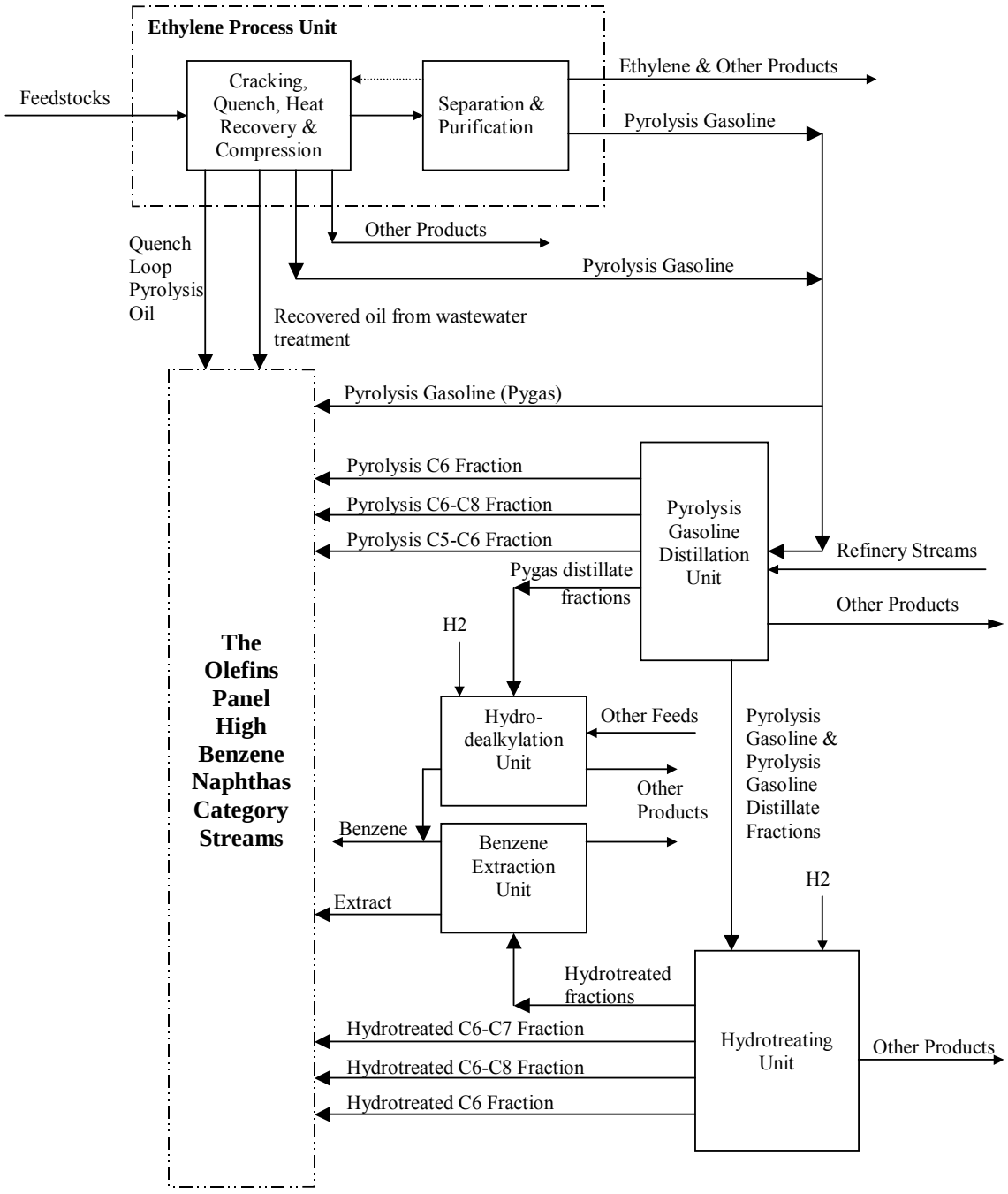
The intermediate stream that exits the cracking furnaces (i.e., the furnace effluent) is forwarded to the finishing section of the ethylene plant. The furnace effluent is commonly referred to as "cracked gas" and consists of a mixture of hydrogen, methane, and various hydrocarbon compounds with two or more carbon atoms per molecule (C2+). The relative amount of each component in the cracked gas varies depending on what feedstocks are cracked and cracking process variables. Cracked gas may also contain relatively small concentrations of organic sulfur compounds that were present as impurities in the feedstock or were added to the feedstock to control coke formation. The cracked gas stream is cooled, compressed and then separated into the individual streams of the ethylene process. These streams can be sold commercially and/or put into further steps of the process to produce additional materials. In some ethylene processes,

a liquid fuel oil product is produced when the cracked gas is initially cooled. The ethylene process is a closed process and the products are contained in pressure systems.

The final products of the ethylene process include hydrogen, methane (frequently used as fuel), and the high purity products ethylene and propylene. Other products of the ethylene process are typically mixed streams that are isolated by distillation according to boiling point ranges and in some cases further processed. It is a subset of these mixed streams that make up the constituents of the Low Benzene Naphthas Category.

The chemical process operations that are associated with the process streams in the Low Benzene Naphthas Category are shown in Figure 1.

Figure A1-1. Chemical Process Operations Associated with Process Streams in the High Benzene Naphthas Category.



Appendix 2: Composition

Table A2-1 Typical Stream Compositions (wt. %) for the High Benzene Naphthas Category.

(See notes 1-4 at the end of this table)

Component Name	Pyrolysis Gasoline	Pyrolysis C6 fraction	Pyrolysis C6-C8 fraction	Pyrolysis C5-C6 fraction	Hydro-treated C6 fraction	Hydro-treated C6-C7 fraction	Hydro-treated C6-C8 fraction	Quench Loop Pyrol. Oil & Compressor Wash Oil	Recovered Oil from Waste Water treatment [see note 4]	Aromatic Extract from Benzene Extract-ion
Vinyl Acetate	9.9									
1,3-Butadiene	6.7	0.1-2.0								
C4's	0.5-5.0	0.1-1.5								
1,4-Pentadiene	0.3-0.9	0.1-2.0								
Isopentane (2-methylbutane)	2.0	0.1-1.0								
1-Pentene (Amylene)	0.6-4.0	1.0-3.0								
2-Methyl-1-Butene	1.0									
Pentene-2 (isomer mix)	0.2-1.8	0.1-5.0								
Isoprene (2-methylbutadiene-1,3)	0.6-10.0	2.0-6.0		6.0						
Pentenes				10.0						
Pentane	10.0					1.0				
2-Methyl-2-Butene	1.2	2.0								
Other C5's	0.3						2.0			
3-methly-1,2-butadiene		1.0-3.0								
1,3-Cyclopentadiene	1.0-20.0	0.1-5.0	1.0							
1,3-Pentadiene (isomer mix)	0.7-4.4	0.3-4.0								
Cyclopentene	0.6-5.0			8.0						
Cyclopentane	2.3				4.0	1.0-5.0				
1,5-Hexadiene	0.6									
2-Methylpentane	4.0				4.0					
2-Methyl-1-Pentene	0.0-2.2									
3-Methlypentane (Isohexane)	1.3				4.0	10.0-20.0				
Hexene-1	0.0-2.2									
Hexenes						2.0				
Methylcyclopentadiene	5.0		1.0							
Hexane Isomers			1.0-3.0			5.0-20.0				

Table A2-1 Typical Stream Compositions (wt. %) for the High Benzene Naphthas Category (cont).

Component Name	Pyrolysis Gasoline	Pyrolysis C6 fraction	Pyrolysis C6-C8 fraction	Pyrolysis C5-C6 fraction	Hydro-treated C6 fraction	Hydro-treated C6-C7 fraction	Hydro-treated C6-C8 fraction	Quench Loop Pyrol. Oil & Compressor Wash Oil	Recovered Oil from Waste Water treatment [see note 4]]	Aromatic Extract from Benzene Extract-ion
Hexane	0.0-9.0		1.0-5.0		6.0	2.0-15.0				
Methylcyclopentane	4.9					5.0-15.0				
1-Methylcyclopentene	0.1-2.4									
C6 non-aromatics		30.0						0.9		
Non-Aromatic hydrocarbons							20.0-26.0			
Benzene	15.0-62.0	35.0-77.0	30.0-80.0	70.0	75.0-75.7	40.0-69.0	40.0-60.0	10.0-21.6		60.0-75.0
1,3-Cyclohexadiene	0.5-2.0									
Cyclohexane	2.0				6.0	1.0-3.0				
Cyclohexene	0.6									
Cyclohexadienes	0.1-2.3									
3-Ethylpentene-1		1.0								
C6 olefin	0.2-1.9									
Heptenes						2.0				
2-Methylhexane						2.0				
Heptane Isomers						1.0-5.0				
Heptane	0.4-2.0		1.0			1.0-5.0				
C7 Paraffins & Naphthenes	0.3-1.1									
C7 Olefins	0.0-1.2									
Methylcyclohexane						1.0-3.0				
C7 Non-aromatics		3.0						2.2		
Toluene	17.4	0.5-5.0	15.0-25.0	5.0	0.3	3.0-15.0	10.0-25.0	5.0-10.9		25.0-40.0
4-Vinylcyclohexene [Butadiene dimer]	0.1-1.0									
C8 Nonaromatics								1.3		
Ethylbenzene	0.3-5.5	1.0	1.0-3.0					1.0-3.0		
C8 Aromatics							3.0-10.0			1.0
Xylenes, mixed	10.0		1.0-10.0					1.5		
Styrene	10.0		1.0-10.0					10.0-15.0		
C9 Aromatics	0.4-1.7									

Table A2-1 Typical Stream Compositions (wt. %) for the High Benzene Naphthas Category. (cont.)

Component Name	Pyrolysis Gasoline	Pyrolysis C6 fraction	Pyrolysis C6-C8 fraction	Pyrolysis C5-C6 fraction	Hydro-treated C6 fraction	Hydro-treated C6-C7 fraction	Hydro-treated C6-C8 fraction	Quench Loop Pyrol. Oil & Compressor Wash Oil	Recovered Oil from Waste Water treatment [see note 4]]	Aromatic Extract from Benzene Extract-ion
Ethyltoluenes	0.1-2.0									
C9 Paraffins & Naphthenes	0.3-1.3									
1,3,5-Trimethylbenzene (mesitylene)	3.0									
C10+								40.6		
1,2,4-Trimethylbenzene (Pseudocumene)	0.0-3.3		1.0							
4-Methylstyrene	0.0-3.3									
Cyclopentadiene/ Methylcyclopentadiene Codimers	0.9-4.4		1.0-3.0							
Dicyclopentadiene	20.0		1.0-5.0					3.7		
1-Decene	1.5									
Vinyl Toluene	0.1-1.1									
Dihydro-dicyclopentadiene	2.0									
Decane	0.1-5.0									
C10 Aromatics	1.6									
C10's								1.6-27.0		
Indene	0.6-5.0									
C11+								38.8-50.0		
Naphthalene	15.0							4.3-10.0		
Methylnaphthalene	2.9									
1-Methylnaphthalene	1.0									
1,1"-Biphenyl	0.1-0.9									
C10 Olefins	1.2									

Note 1: The composition data shown above are composites of reported values..
Note 2: The balance of these streams is expected to be other hydrocarbons that have boiling points in the range of the listed components.
Note 3: The listed highs and lows should not be considered absolute values for these limits. They are instead highs and lows of reported values.
Note 4: No specific composition data are available. This stream is expected to contain components of Pyrolysis Gasoline

Appendix 3.

Summary Results from Existing Human Health Effects Data for Chemical Components and Streams of High Benzene Naphthas Category

(Note: This table is the product of a good faith effort to briefly summarize results of toxicity studies that were available to the reviewer for SIDS endpoints. Results from non-SIDS endpoints are not included. Since all information for a particular chemical may not have been available to the reviewer, the results presented should not be considered as final assessments of the hazards of the listed chemicals. Component data were not reviewed for data adequacy. Robust summaries for the listed components will not be submitted with the Test Plan.)

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/ References
Vinyl Acetate	Oral LD50 = 2.9 g/kg; inhalation LC50 = 3680 ppm [4h]	Negative in Ames Test	Positive in mouse bone marrow micronucleus test by i.p. but negative in rats and mice by inhalation and oral; positive in in-vitro chrom ab	4 and 13-wk rat and mouse inhalation study: decrease in BW gain, respiratory tract effects; no clearly treatment related effects in 4 and 13-wk rat and mouse oral	In rat inhalation study, no embryolethality or teratogenicity seen; fetal growth retardation seen at maternally toxic doses. In rat oral study, no effects.	In an oral rat 2-gen repro study, no effects were seen except for reduction in BW gain in high-dose F1 pups.		Review: IRIS[8] – 1990; HSDB[9]; ATSDR – 1992[4]
1,3-Butadiene	Rat inhalation LC50[4h] = 129,000 ppm	Negative in UDS in mouse and rat, Drosophila; negative and positive in mouse lymphoma; positive in Ames, CHO and in vivo mouse spleenocyte HPRT tests and mouse spot test	Positive in mouse dominant lethal but negative in rat; positive in mouse bone marrow micronucleus and chrom. ab.; negative in rat bone marrow micronucleus	Many studies: Toxicity to blood cells in mice; no effects in rats [inhalation]	Effects seen at maternally toxic doses	Will become available through OECD SIDS	Olefins Panel's Crude Butadiene C4 Category, OECD SIDS	Reviews: ECETOC Special Report No. 12 - 1997[10]; ATSDR[11] - 1993

[8] IRIS: EPA Integrated Risk Information System

[9] HSDB: Hazardous Substances Data Bank [TOMES, MICROMEDEX, Inc.]

[10] ECETOC: European Centre for Ecotoxicology and Toxicology of Chemicals

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/ References
Isoprene (2-methylbutadiene-1,3)	Rat oral LD50= 2.1 g/kg; inhalation LC50 [4h] = 64,500 ppm	Negative in Ames Test	Negative in in-vitro CHO chrom. ab., mouse bone marrow chrom. ab. and rat lung cell micronucleus [inhalation]; positive in mouse bone marrow micronucleus [inhalation]	Many studies: Effect on testes in rats seen at 26 wks but not at 13 wks; effects on blood cells, nasal epithelium, liver, stomach, and testes in mice [inhalation]	No effects in rats; fetotoxicity in mice	Limited repro tox data [sperm motility, vaginal cytology, histopath of repro organs]obtained as part of 13-wk inhalation study: [slight effect on testis in rats; effects on testes, epididymus, sperm, estrus cycle in mice]	Olefins Panel's C5 Non-Cyclics Category/ICCA	Review: IARC[12] - 1999
Pentenes				2-pentene: 4 wk rat oral evaluating nephrotoxicity showed no kidney lesions at 2 g/kg/day w/60% mortality			International Hydrocarbon Solvents Consortium [C5 Aliphatics Category Test Plan]; also, pentenes are likely to have a toxicity profile similar to hexenes which will be addresed by the Higher Olefins Panel	Halder et al., 1985

[11] ATSDR: U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry

[12] IARC: International Agency for Research on Cancer

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/ References
Pentane	Rat oral: LD50>2 g/kg; inhalation LC50[4h] >7000 ppm	Negative in Ames Test	Negative in rat bone marrow micronucleus [inhalation] and dominant lethal [i.p.]; positive [not reproducible] in in-vitro CHO chrom.ab.	90-day rat inhalation: no effect at ~ 7000ppm. 16 wk and 7-30 wk rat inhalation neurotox evaluations : negative With 50/50 blend of n-butane and n-pentane, in a 90-day rat inhalation study with scope limited to evaluation of nephrotoxicity: decrease in BW and male hydrocarbon nephropathy.	No effect in rat oral	No effect on repro organs in 90-day rat inhalation	API [addressed in Petroleum Gases Test Plan]; International Hydrocarbon Solvents Consortium [C5 Aliphatics Category Test Plan]; OECD SIDS	Review: McKee et al., 1998; Galvin and Marashi, 1999
1,3-Cyclopentadiene	Rat oral: 4/5 died at 1 g/kg; inhalation LC50 [4h] = 39 mg/L			Mild liver and kidney effects in rats after 35 exp. of 500 ppm ; no effects in guinea pigs, rabbits, dogs after 135 exp. of 250 ppm, or in dogs after 39 additional exp of 400 ppm and 16 additional exp of 800 ppm [inhalation]				ACGIH[13], RTECS[14], EPA Documents [86960000024, 86960000121S
Cyclopentene	Rat oral LD50 = 1.66 g/kg; inhalation LCLo [4h] = 16,000 ppm							RTECS

[13] ACGIH: American Conference of Governmental Industrial Hygienists

[14] RTECS: Registry of Toxic Effects of Chemical Substances

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/ References
3-methylpentane (Isohexane)				16 wk and 7-30 wk rat inhalation neurotox evaluations : negative				Frontali et al., 1981
Hexane isomers [Commercial Hexane tested: 52.2% n-hexane, 16.0% 3-methylpentane, 15.6% methylcyclopentane, 11.6% 2-methylpentane, 3.2% cyclohexane]		Negative in Ames Test, CHO HPRT	Negative in in-vitro CHO chrom. ab. and rat bone marrow chrom. ab. [inhalation]	No neurotoxicity; male rat hydrocarbon nephropathy [inhalation]	No effects in rats via inhalation	No effect in rat 2-gen study via inhalation except decrease in weight gain in high dose offspring		Daughtrey et al., 1994 a,b; 1999; Kirwin et al., 1991
Hexane	Rat oral LD50=28.7 g/kg; inhalation LC50[4h] = 48,000 ppm	Negative in Ames Test and in vitro UDS	Negative in in-vitro CHO chrom. ab. , inhalation dominant lethal and mouse micronucleus [inhalation and IP]; positive in rat oral bone marrow chrom. ab.	Several studies: Effects on peripheral nervous system and testes	Negative in inhalation and oral developmental studies	No repro tox studies found; testicular atrophy seen in subchronic inhalation studies	OECD SIDS - ICCA	Review: ATSDR[15] – 1999; rat chrom. ab. report in HSDB[16]
Methylcyclopentane				4 wk rat oral evaluating nephrotoxicity showed no kidney lesions at 0.5 g/kg/day but lesions at 2g/kg w/40%mortality				Halder et al., 1985

[15] ATSDR: U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry

[16] HSDB: Hazardous Substances Data Bank [TOMES, MICROMEDEX, Inc]

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/ References
Benzene	Rat oral LD50=810 mg/kg: Rat oral LD50= 1000mg/kg [Smyth et al., 1962] Inhalation LC50 [4h] = 13,700 ppm	Negative in Ames Test, mouse lymphoma, CHO HPRT, in-vitro UDS, Drosophila; positive in mouse spleen HPRT	Positive in vitro/in vivo in numerous studies and species [oral, inhalation]: in-vitro human lymphocytes; chrom. ab. and micronucleus in mouse bone marrow and spleen lymphocytes; rat bone marrow chrom. ab. and micronucleus	Many studies: Primary effect toxicity to blood cells	Several studies: fetotoxic at maternally toxic doses; not tetratogenic	No standard repro studies; most inhalation studies with repro parameters indicate no effect on reproductive indices, even at high doses	OECD SIDS	Review: ATSDR – 1997; EU Risk Assessment – 2001 [Draft]
Cyclohexane	Rat oral LD50 > 5 g/kg; inhalation LC50[4h] = 4044 ppm	Negative in Ames Test, mouse lymphoma, human lymphocyte UDS	Negative in rat bone marrow chrom. ab. [inhalation]	Effects on liver in mice and rats; on liver and kidney in rabbits [inhalation]	No effects seen in rats or rabbits [inhalation]	No effects in rat 2-gen inhalationrepro at doses not maternally toxic	OECD SIDS	Review: SRC Technical Support Document #TR-86-030 [Beals et al.,1986, draft][17]; EU Risk Assessment – 2000 [Draft] Bamberger, 1996; Kreckman, 1997; Malley, 1996 a,b

[17] SRC: Syracuse Research Corporation Center for Chemical Hazard Assessment, prepared for Test Rules Development Branch, Existing Chemical Assessment Division, Office of Toxic Substances

Smyth, H.F. Carpenter, C.P., Weil, C.S. et al., 1962. Range-finding toxicity data. List VI. Ind. Hyg. J 23: 95-107.

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/ References
Toluene	Rat oral LD50 = 5.5 – 7.53 g/kg; inhalation LC50[4h] = 8000 - 8800 ppm	Negative in Ames Test, SHE transformation, and Drosophila SLRL; equivocal in mouse lymphoma	Negative in in-vitro human lymphocyte and CHO chrom. ab., dominant lethal [oral], chrom. ab. in mice [oral] and rats [inhalation], and mouse micronucleus [oral]	Many studies: Effects on central nervous system; hearing loss in rats	In rats and mice: lower birth weight, delayed postnatal development and behavioral effects [inhalation]	No effects in mouse 2-gen inhalation repro study; in rats, effect on sperm count and epidydymal weight at 2000 ppm, but no effect on fertility	OECD SIDS	Review: ATSDR[18] – 2000; IARC[19] – 1999; EU Risk Assessment - 2001 Genetic toxicity review: McGregor, 1994.
Ethylbenzene	Rat oral LD50> 3.5 g/kg; inhalation LC50[4h] LC50 = 4000 ppm	Negative in Ames Test, Drosophila SLRL, and in-vivo UDS in mouse hepatocytes; equivocal in mouse lymphoma	Negative in in-vitro CHO and RL4 cells chrom. ab. and in inhalation/i.p. mouse micronucleus	Several studies: Effects seen in liver, kidney, and lung in rats and mice; hearing loss in rats via inhalation	No effects in rabbits; only supernumerary ribs seen in rats	No repro study; in subchronic rat and mouse studies, no effects seen in gonads sperm, extrus cycle	OECD SIDS	Review: ATSDR[20] - 1999
Xylenes, mixed	Rat oral LD50 = 3.5-8.6 g/kg;Rat inhalation [4h]LC50 = 6,350 - 6,700 ppm	Negative Ames Test and mouse lymphoma	Negative in human lymphocytes [only w/o S9 tested] and CHO chrom. ab.	Many studies: liver, and nervous system effects via inhalation; hearing loss in rats via inhalation; nervous system effects via oral exposure	Fetotoxic effects seen in rat and mouse [oral,inhalation], mostly secondary to maternal toxicity	Negative in rat repro [exposed by inhalation 131 days prior to mating, during mating, gestation, day 5-20 of lactation]; no effect on repro organs in rat and mouse	ACC Toluene Xylene Panel/OECD SIDS/ICCA	Review: ATSDR – 1995; WHO EHC - 1997[21]; ECETOC - 1986

[18] ATSDR: U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry

[19] IARC: International Agency for Research on Cancer

[20] ATSDR: U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry

[21] WHO EHC: World Health Organization, International Programme on Chemical Safety. Environmental Health Criteria

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/ References
Styrene	Rat oral LD50 $\geq$ 5 g/kg; inhalation LC50 [4h] = 4940 ppm	Inconsistent results in Ames Test	Inconsistent results in in-vitro chrom. ab. tests; negative in chrom. ab. and micronucleus tests in mice and rats by oral and inhalation exposure	Many studies: Effects on liver in rats [oral, inhalation] and mice [inhalation]; hearing loss in rats [inhalation]; respiratory tract in rats [inhalation]; lungs in mice [oral]	No birth defects in rats [oral, inhalation] or in mice, rabbits and hamsters [inhalation]; other effects seen only at maternally toxic doses	Negative in rat 3 gen repro study [oral]	OECD SIDS	Reviews: ATSDR – 1992; IARC[22] – 1994 Brown, 1991, 1993 [repro/devel]
Dicyclopentadiene	Rat oral LD50 ranged from 347 – 820 mg/kg; inhalation LC50[4h] ranged from 359 to 500-1000 ppm	Negative in Ames Test	Negative in in-vitro CHO and CHL chrom. ab.	Many studies: Most studies showed no effects in rats or mice in dietary or inhalation studies except male rat hydrocarbon nephropathy in inhalation studies	No effect in rats in oral [diet] studies	Effects only at maternally toxic doses in rat 3-gen repro study [in diet]	OECD SIDS	Review: ECETOC[23] – 1991 JETOC[24] Issue 3 No. 32, 1998 [CHL chrom. ab and OECD 422 studies]; NTP[25] [CHO chrom. ab.]

[22] IARC: International Agency for Research on Cancer

[23] ECETOC: European Centre for Ecotoxicology and Toxicology of Chemicals

[24] JETOC: Japanese Chemical Industry Ecology – Toxicology and Information Center

[25] NTP: National Toxicology Program – personal communication

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/ References
Naphthalene	Rat oral LD50 ranged from 2200 to 2600 mg/kg; no effect at 78 ppm [4h] inhalation	Negative in Ames Test, transformation, in-vivo UDS in rat liver	Negative in mouse micronucleus; positive in in-vitro CHO chrom. ab.	Many studies: Toxicity to blood cells in dogs [hemolytic anemia][oral]but not rats or mice; cataracts in rabbits, rats, mice, guinea pigs [oral]; local irritative effects after inhalation in rats and mice	No birth defects in rabbits, rats, and mice [oral]; reduced litter size in mice at maternally toxic doses [oral on gestation day 7-14]; no effect in rabbits exposed orally on gestation days 6-18		OECD SIDS	Reviews: ATSDR[26] – 1995; EU Risk Assessment Document – Draft 2001

[26] ATSDR: U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/ References
STREAMS								
Rerun Tower Overheads [approx. 40% benzene, 13% toluene, 26% C5, 20% other] [C5-10 Fraction of Pyrolysis Gasoline HPV stream]	Rat oral LD50 > 2 g/kg; rabbit dermal LD50>2g/kg	Negative Ames Test, Drosophila (point mutation), and transformation (BALB-c/3T3 and C3H 10T½); weakly positive in mouse lymphoma and bacterial DNA repair	Negative in Drosophila chromosome loss and chromosome aberration studies	Rabbit 21-day dermal irritation: NOAEL (systemic) = 1.0 ml/kg/day (top dose); NOAEL (irritation) = <0.10 ml/kg/day	No effects in rabbits in oral teratology pilot and main studies			Robust Summaries
Dripolene [HPV stream: Pyrolysis Gasoline]	Rat oral and dermal LD50 > 2 g/kg							Robust Summary
Hydrogenated Pyrolysis Gasoline [55% benzene, 25% toluene, 10% xylene, 7% pentane, 7% ethylbenzene, 2% hexane, 3% cyclohexane] [HPV stream: Hydrotreated C6-8 Fraction]	Rat Oral LD50 = 5.17 g/kg; inhalation 4h LC50>12,408 ppm	Negative in Ames Test, in-vitro UDS; positive in transformation	Negative in micronucleus [mouse oral]	Rat 5 day inhalation: NOAEL <4869 ppm [deaths, bodyweight]				Robust Summaries

Appendix 4.

Sources of Data for Hazard Evaluations for Mammalian Toxicity

[All streams are subject to the OSHA Benzene Standard. For hazard communication, the final hazard characterization for each stream will include the hazards of benzene (cancer, genetic toxicity, hematotoxicity) plus any reproductive or developmental toxicity or target organ effects of the other components, unless there is clear evidence that specific component interactions eliminate toxicity.]

STREAM	SOURCES OF DATA FOR HAZARD EVALUATION **[These data will be evaluated using scientific judgment and complying with the requirements of the OSHA benzene, 1,3-butadiene, and hazard communication standards]**
Pyrolysis Gasoline	• Available data for components [benzene, 1,3-butadiene, cyclohexane, cyclopentadiene, cyclopentene, 3-methylpentane, dicyclopentadiene, ethylbenzene, hexane, isoprene, methylcyclopentane, naphthalene, pentadiene, pentane, pentenes, styrene, toluene, vinyl acetate, xylene] • Data for streams containing Pyrolysis Gasoline or fractions thereof [Pyrolysis Gasoline Fractions, Dripolene, Hydrogenated Pyrolysis Gasoline (robust summaries provided)] • Data for streams distilled out of Pyrolysis Gasoline that are being tested in other Panel HPV Test Plans [C5 Non-Cyclics and Resin Oils and Cyclodiene Dimer Concentrates categories] • Data for gasoline blending streams referenced in the API Petroleum HPV Gasoline Blending Streams Test Plan • Data for commercial hexane, which contains n-hexane, 3-methylpentane, methylcyclopentane, 2-methylpentane, cyclohexane • Data for hexenes being developed by the ACC Higher Olefins Panel, for C5 aliphatic components being addressed by the ACC Hydrocarbon Solvents Panel in its C5 Aliphatics Category, and for pentane which is addressed in the API Petroleum Gases Test Plan • Literature data regarding interactions between components present in these streams
Pyrolysis C6 Fraction	• Available data for components [benzene, 1,3-butadiene, cyclopentadiene, ethylbenzene, isoprene, pentenes, pentadiene, toluene] • Data for streams distilled out of Pyrolysis Gasoline that are being tested in other Panel HPV Test Plans [C5 Non-Cyclics Category] • Data for hexenes being developed by the ACC Higher Olefins Panel (as structurally similar to pentenes), for C5 aliphatic components being addressed by the ACC Hydrocarbon Solvents Panel in its C5 Aliphatics Category • Literature data regarding interactions between components present in these streams

STREAM	SOURCES OF DATA FOR HAZARD EVALUATION **[These data will be evaluated using scientific judgment and complying with the requirements of the OSHA benzene, 1,3-butadiene, and hazard communication standards]**
Pyrolysis C6-C8 Fraction	• Available data for components [benzene, dicyclopentadiene, ethylbenzene, hexane, styrene, toluene, xylene] • Literature data regarding interactions between components present in these streams
Pyrolysis C5-C6 Fraction	• Available data for components [benzene, cyclopentene, isoprene, pentenes , toluene] • Data for hexenes being developed by the ACC Higher Olefins Panel (as structurally similar to pentenes) • Literature data regarding interactions between components present in these streams
Hydrotreated C6 Fraction	• Available data for components [benzene, cyclohexane, hexane, 3-methylpentane] • Data for commercial hexane, which contains n-hexane, 3-methylpentane, methylcyclopentane, 2-methylpentane, cyclohexane • Literature data regarding interactions between components present in these streams
Hydrotreated C6-C8 Fraction	• Available data for components [benzene, toluene and other identified components] • Data for Hydrogenated Pyrolysis Gasoline (robust summaries provided) • Literature data regarding interactions between components present in these streams
Quench Loop Pyrolysis Oil and Compressor Oil	• Available data for components [benzene, dicyclopentadiene, ethylbenzene, naphthalene, styrene, toluene, xylene and other identified components] • Literature data regarding interactions between components present in these streams
Recovered Oil from Waste Water Treatment	• Available data for components, on a case-by-case basis
Aromatic Extract from Benzene Extraction Unit	• Available data for components [benzene, toluene] • Literature data regarding interactions between components present in these streams

Appendix 5. Biodegradation

Table A5-1.
Read Across Data used to Characterize the Biodegradability of the High Benzene Naphthas Category from Chemicals Contained by Products in this Category and Chemically Complex Products not in this Category, but that Contain Like-Chemicals.

CHEMICAL / PRODUCT	CARBON NUMBER	PERCENT BIODEGRADATION[a] (28 days)	REFERENCE
n-Pentane	5	87	IHSC[e]
Isopentane	5	71	IHSC[e]
Cyclohexane	6	77	IHSC[e]
Alkenes, C6 Rich	6[b]	21	HOP[f]
1-Hexene (linear)	6	67-98[c]	[g]
Benzene	6	63	Robust Summary Provided with this test plan
Alkenes, C7-C9, C8 Rich	7-9	29	HOP[f]
p-Xylene	8	89	XIC[h]
Styrene	8	100 (14 days)[c]	[i]
Naphtha (Petroleum), light alkylate (gasoline stream)	5-8	42[d]	API[j]
Naphtha (Petroleum), Light Catalytically Cracked (gasoline stream)	5-8	74[d]	API[j]
Naphtha (Petroleum), Light Catalytically Reformed (gasoline stream)	5-9	96[d]	API[j]
C8-C10 Aromatics, Predominantly C9 Alkylbenzenes	9[b]	78	IHSC[e]
C8-C14 Aromatics, Predominantly Alkyl Naphthalenes and Naphthalene	10-12[b]	61	IHSC[e]

a OECD 301F, manometric respirometry test
b Predominant carbon number or range
c BOD test
d Test method for determining the inherent aerobic biodegradability of oil products and modification of ISO/DIS 14593
e Covered by the International Hydrocarbon Solvents Consortium: Contained in selected SIAR (expected to be submitted at SIAM 19)
f Robust summary from the Higher Olefins Panel: C6, C7, C8, C9, and C12 Internal Olefins and C16 and C18 Alpha Olefins Category Test Plan (submitted)
g These chemicals are in the OECD SIDS program (Chemicals Inspection & Testing Institute, Japan 1992)
h Robust summary submitted with High Benzene Naphthas test plan
i Part of the Xylene ICCA Consortium and were reviewed by OECD at SIAM 16
j Robust summary from the American Petroleum Institute: Gasoline Blending Streams Test Plan (submitted)

Table A5-2
Composition (Weight Percent) of Three Gasoline Streams with Biodegradation Data Used to Read Across to Products in the High Benzene Naphthas Category.

Naphtha, (Pet.) Light Alkylate		**Naphtha, (Pet.) Light Catalytically Cracked**		**Naphtha, (Pet.) Light Catalytically Reformed**	
CAS# 64741-66-8	Weight %	CAS# 64741-55-5	Weight %	CAS# 64741-63-5	Weight %
Isopentane	12.61	n-hexane	1.69	n-heptane	3.59
2,3 dimethyl butane	4.74	n-pentane	1.71	n-hexane	4.69
2,4 dimethyl pentane	4.09	isopentane	4.7	n-pentane	8.05
2,3 dimethyl pentane	2.25	2,3 dimethyl pentane	1.12	Isopentane	11.39
2,2,4 trimethyl pentane	23.92	2 methyl hexane	1.58	2,2 dimethyl butane	1.26
2,2,3 trimethyl pentane	1.76	3 methyl hexane	1.45	2,3 dimethyl butane	1.11
2,3,3 trimethyl pentane	8.99	2 methyl pentane	3.64	2,3 dimethyl pentane	1.70
2,3,4 trimethyl pentane	11.56	3 methyl pentane	2.20	2 methyl hexane	4.30
2,3,5 trimethyl hexane	1.25	methyl cyclopentane	1.87	3 methyl hexane	5.18
2,5 dimethyl hexane	4.34	methyl cyclohexane	1.19	2 methyl pentane	5.17
2,4 dimethyl hexane	3.60	1-pentene	1.25	3 methyl pentane	4.00
2,3 dimethyl hexane	2.60	2-methyl-1-butene	2.31	benzene	8.37
1methyl-1ethyl cyclopentane	9.44	2-methyl-2-butene	5.35	toluene	29.77
		trans-2-pentene	3.33		
		cis-2-pentene	1.94		
		2-methyl-1-pentene	2.31		
		cis-3-hexene	1.67		
		trans-2-hexene	1.97		
		2-methyl-2-pentene	1.83		
		1-methyl cyclopentene	1.85		
		ethylbenzene	1.47		
		m-xylene	3.05		
		p-xylene	1.34		
		o-xylene	1.83		
		benzene	1.48		
		toluene	6.73		

Appendix 6. Aquatic Toxicity

Table A6-1

Approximate Weight Percent and Carbon Number Comparison of Hydrocarbons in High Benzene Naphthas Category and Comparable Products[a].

Substance Name	Olefins		Aromatics		Paraffins	
	% (wt.)	C #[b]	% (wt.)	C #[b]	% (wt.)	C #[b]
Products in High Benzene Naphtha Category	**1-34**	**5-9**	**>40-100**	**6-11**	**>4-75**	**5-10**
Alkenes, C6 Rich	**100**	**5-7**	**0**	**-**	**0**	**-**
Alkenes, C7-9, C8 Rich	**100**	**7-9**	**0**	**-**	**0**	**-**
C8-C10 Aromatics, Predominantly C9 Aromatics	**0**	**-**	**>97**	**8-10**	**<3**	**-**
C8-C14 Aromatics, Predominantly Alkyl Naphthalenes and Naphthalene	**0**	**-**	**>94**	**10-14**	**<6**	**-**
Naphtha (petroleum), Light Alkylate (gasoline stream)	**0**	**-**	**0**	**-**	**92**	**5-8**
Naphtha (petroleum), Light Catalytically Cracked (gasoline stream)	**24**	**5-6**	**16**	**6-8**	**21**	**5-7**
Naphtha (petroleum), Light Catalytically Reformed (gasoline stream)	**0**	**-**	**38**	**6-7**	**50**	**5-7**

a Approximate weight percent and carbon number ranges of the predominant chemical components by chemical class [olefins/aromatics/paraffins] for selected products contained by this category and for comparable products not in this category that have aquatic toxicity data that can be used as read across data for this category; % compositions may not total 100%.

b Predominant carbon number range

Table A6-2

Acute Fish Toxicity Data for Selected Chemicals and Complex Products used to Characterize the Toxicity of Products in the High Benzene Naphthas Category

CHEMICAL / PRODUCT	CARBON NUMBER	ORGANISM	AQUATIC TOXICITY[a] (96-hr, mg/L)	REFERENCE
n-Pentane	5	*Oncorhynchus mykiss*	LC50 = 4.3	IHSC [d]
n-Hexane	6	*Pimephales promelas*	LC50 = 2.5	IHSC [d]
Benzene	6	*Oncorhynchus mykiss*	LC50 = 5.9	[e]
Alkenes, C6 Rich	5-7[b]	*Oncorhynchus mykiss*	LL50 = 12.8	HOP [f]
Mixed Cycloparaffins, C7-8, C7 Rich	7	*Oncorhynchus mykiss*	LC50 = 5.4 [c]	IHSC [d]
Toluene	7	*Pimephales promelas*	LC50 = 14.6	IHSC [d]
Alkenes, C7-9, C8 Rich	7-9 [b]	*Oncorhynchus mykiss*	LL50 = 8.9	HOP [f]
o-Xylene	8	*Pimephales promelas*	LC50 = 16.4	XIC[g]
p-Xylene	8	*Oncorhynchus mykiss*	LC50 = 2.6	XIC[g]
p-Xylene	8	*Pimephales promelas*	LC50 = 8.9	XIC[g]
Ethylbenzene	8	*Pimephales promelas*	LC50 = 12.1	[h]
Naphtha (Petroleum), Light Alkylate (gasoline stream)	5-8 [b]	*Pimephales promelas*	LL50 = 8.2	API[i]
Naphtha (petroleum), Light Catalytically Cracked (gasoline stream)	5-8 [b]	*Pimephales promelas*	LL50 = 46	API[i]
Naphtha (petroleum), Light Catalytically Reformed (gasoline stream)	5-7 [b]	*Pimephales promelas*	LL50 = 34	API[i]
1,2,4-Trimethyl-benzene	9	*Pimephales promelas*	LC50 = 7.7	IHSC [d]
C8-C10 Aromatics, Predominantly C9 Aromatics	8-10 [b]	*Oncorhynchus mykiss*	LL50 = 18.0	IHSC [d]
C8-C14 Aromatics, Predominantly alkyl Naphthalenes and Naphthalene	10-12 [b]	*Oncorhynchus mykiss*	LL50 = 3.0	IHSC [d]

a Endpoint is mortality; LC = Lethal Concentration; LL = Lethal Loading; values cited as "concentration" are based on measured values
b Predominant carbon number or range
c 93-hour value
d Covered by the International Hydrocarbon Solvents Consortium: Contained in selected SIAR (expected to be submitted at SIAM 19)
e Galassi, S., M. Mingazzini, L. Viagano, D. Cesareo, and M.L. Tosato, 1988. Benzene is in the OECD SIDS program
f Robust summary from the Higher Olefins Panel HPV Test Plan (submitted)
g Xylenes are part of the Xylene ICCA Consortium and were reviewed by OECD at SIAM 16
h Ethylbenzene is in the OECD program and was reviewed as part of SIAM 15
i Robust summary from the American Petroleum Institute: Gasoline Blending Streams Test Plan (submitted)

Table A6-3

Acute Invertebrate Toxicity Data for Selected Chemicals and Complex Products used to Characterize the Toxicity of Products in the High Benzene Naphthas Category.

CHEMICAL / PRODUCT	CARBON NUMBER	ORGANISM	AQUATIC TOXICITY [a] (48-hr, mg/L)	REFERENCE
n-Pentane	5	*Daphnia magna*	EC50 = 2.7	IHSC[e]
n-Hexane	6	*Daphnia magna*	EC50 = 2.1	IHSC[e]
Cyclohexane	6	*Daphnia magna*	EC50 = 0.9	IHSC[e]
Benzene	6	*Daphnia magna*	EC50 = 18[b]	[f]
Toluene	7	*Daphnia magna*	EC50 = 14.9	Hermens et al[J]
o-Xylene	8	*Daphnia magna*	EC50 = 1.0	XIC[g]
m-Xylene	8	*Daphnia magna*	EC50 = 4.7	XIC[g]
Naphtha (Petroleum), Light Catalytically Reformed (gasoline stream)	5-7[c]	*Daphnia magna*	EL50 = 10	API[h]
Naphtha (Petroleum), Light Alkylate (gasoline stream)	5-8 [c]	*Daphnia magna*	EL50 = 32	API[h]
Naphtha (Petroleum), Light Catalytically Cracked (gasoline stream)	5-8 [c]	*Daphnia magna*	EL50 = 18	API[h]
C8-C10 Aromatics, Predominantly C9 Aromatics	8-10 [c]	*Daphnia magna*	EL50 = 21.3	IHSC[e]
Naphthalene	10	*Daphnia magna*	EL50 = 16.7 [d]	[i]
C8-C14 Aromatics, Predominantly Alkyl Naphthalenes and Naphthalene	10-12 [c]	*Daphnia magna*	EL50 = 3.0	IHSC[e]

a Endpoint is immobility; EC = Effect Concentration; EL = Effect Loading; values cited as "concentration" are based on measured values
b 24-hour study
c Predominant carbon number or range
d Based on nominal values
e Covered by the International Hydrocarbon Solvents Consortium: Contained in selected SIAR (expected to be submitted at SIAM 19)
f Benzene is in the OECD program and was reviewed as part of SIAM 15 (Galassi, et. al., 1988)
g Xylenes are part of the Xylene ICCA Consortium and were reviewed by OECD at SIAM 16
h Robust summary from the American Petroleum Institute: Gasoline Blending Streams Test Plan (2003)
i Naphthalene is part of the OECD program and was reviewed in SIAM 13
j Hermens, J., Canton, H., Janssen, P., and deJong, R. (1984). Quantitative structure-activity relationships and toxicity studies of mixtures of chemicals with anesthetic potency: acute lethal and sublethal toxicity to *Daphnia magna*. Aquat Toxicol 5: 143 –154. In EU Toluene SIAR 10888

Table A6-4

Alga Toxicity Data for Selected Chemicals and Complex Products Used to Characterize the Toxicity of Products in the High Benzene Naphthas Category

CHEMICAL / PRODUCT	CARBON NUMBER	ORGANISM	AQUATIC TOXICITY [a] (72-hr, mg/L)	REFERENCE
n-Pentane	5	*Pseudokirchneriella subcapitata*[b]	EbC50 = 10.7 ErC50 = 7.5 NOECb = 1.3 NOECr = 2.0	IHSC[d]
Benzene	6	*Pseudokirchneriella subcapitata*	EbL50 = 29	[e]
Naphtha (Petroleum), Light Catalytically reformed (gasoline stream)	5-7[c]	*Pseudokirchneriella subcapitata*	EbL50 = 8.5 NOELRb = 5.0	API[f]
Naphtha (Petroleum), Light alkylate (gasoline stream)	5-8 [c]	*Pseudokirchneriella subcapitata*	EbL50 = 45 NOELRb = 18	API[f]
Naphtha (Petroleum), Light Catalytically Cracked (gasoline stream)	5-8 [c]	*Pseudokirchneriella subcapitata*	EbL50 = 64 NOELRb = 51	API[f]
C8-C10 Aromatics, Predominantly C9 Aromatics	8-10 [c]	*Pseudokirchneriella subcapitata*	EbL50 = 2.6 ErL50 = 2.9 NOELRb = 1.0 NOELRr = 1.0	IHSC[d]
C8-C14 Aromatics, Predominantly Alkyl Naphthalenes and Naphthalene	10-12 [c]	*Pseudokirchneriella subcapitata*	EbL50 = 1-3 ErL50 = 1-3 NOELRb = 1.0 NOELRr = 1.0	IHSC[d]

a Endpoint is growth inhibition; EbC = Effect Concentration for biomass; ErC = Effect Concentration for growth rate; EbL = Effect Loading for biomass; ErL = Effect Loading for growth rate; NOECb = No Observed Effect Concentration for biomass; NOECr = No Observed Effect Concentration for growth rate; NOELRb = No Observed Effect Loading Rate for biomass; NOELRr = No Observed Effect Loading Rate for growth rate; values cited as "concentration" are based on measured values

b Formally known as *Selenastrum capricornutum*

c Predominant carbon number or range

d Covered by the International Hydrocarbon Solvents Consortium: Contained in selected SIAR (expected to be submitted at SIAM 19)

e Benzene is in the OECD program and was reviewed as part of SIAM 15 (Galassi, et. al., 1988)

f Robust summary from the American Petroleum Institute: Gasoline Blending Streams Test Plan (2003)

Appendix 7.

American Chemistry Council

Olefins Panel Sponsored HPV Test Categories.

Category Number	Category Description
1	Crude Butadiene C4
2	Low Butadiene C4
3	C5 Non-Cyclics
4	Propylene Streams (C3) - Propylene sponsored through ICCA
5	High Benzene Naphthas
6	Low Benzene Naphthas
7, 8, & 9	Resin Oil & Cyclodiene Dimer Concentrates
10	Fuel Oils
11	Pyrolysis C3+ and Pyrolysis C4+

Attachments [Separate documents]

Attachment 1a. Robust Summaries: PhysicoChemical and Environmental Fate

Attachment 1b. Robust Summary: Biodegradation Study Benzene

Attachment 1c. Robust Summaries: Mammalian Toxicology

201-14657A

ATTACHMENT 1A

HIGH BENZENE NAPHTHAS ROBUST SUMMARIES:

PHYSICAL-CHEMICAL PROPERTIES AND ENVIRONMENTAL FATE

HIGH BENZENE NAPHTHAS ROBUST SUMMARY

Boiling Point

Test Substance*:	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]
Method/Guideline:	Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Pressure:	760 mm Hg
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Boiling Point is calculated by the MPBPWIN subroutine, which is based on the calculation method of S. Stein and R. Brown in "Estimation of Normal Boiling Points from Group Contributions". 1994. J. Chem. Inf. Comput. Sci. 34: 581-587.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Calculated and measured boiling point data for representative constituents of the High Benzene Naphthas Category are listed below. The data identify a potential boiling point range for substances represented by the 19 CAS numbers under Test Substance. Substances in this category do not have a specific boiling point value. Actual boiling point ranges for substances in this category will vary dependent on their constituent composition. Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C11. The 12 chemicals selected to represent the boiling point range of this category are C5-C10 hydrocarbons that can be found in substances identified by the 19 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.
Results: (continued) **Units/Value:** **Note: Deviations from protocol or guideline, analytical method.**	Substance Constituent / Calculated BP (°C) / Measured* BP (°C) Isoprene: 34.95 / 34.0 n-pentane: 46.01 / 36.0

	1,3-cyclopentadiene 69.17 41.0 Isohexane 56.26 63.2 n-hexane 71.53 68.7 methylcyclopentane 80.34 71.8 benzene 102.24 80.0 toluene 125.72 110.6 m-xylene 148.29 139.1 styrene 146.65 145.0 dicyclopentadiene 176.78 170.0 naphthalene 231.64 217.9 * Experimental values from EPIWIN database. The data represent a potential boiling point range for substances represented by the 19 CAS numbers under Test Substance.
Test Substance:	The High Benzene Naphthas Category includes the following CAS numbers: 64741-99-7 Extracts, petroleum, light naphtha solvent 64742-49-0 Naphtha, petroleum, hydrotreated light 64742-73-0 Naphtha, petroleum, hydrodesulfurized light 64742-83-2 Naphtha, petroleum, light steam-cracked 64742-91-2 Distillates, petroleum, steam-cracked 67891-79-6 Distillates, petroleum, heavy aromatic 67891-80-9 Distillates, petroleum, light aromatic 68410-97-9 Distillates, petroleum, light distillate hydrotreating process, low-boiling 68475-70-7 Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived 68476-45-9 Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product 68526-77-2 Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum 68606-10-0 Gasoline, pyrolysis, debutanizer bottoms 68606-28-0 Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic 68921-67-5 Hydrocarbons, ethylene-manufacture-by-product distillation residues 68955-29-3 Distillates, petroleum, light thermal cracked, debutanized aromatic 68956-52-5 Hydrocarbons, C4-8 68956-70-7 Petroleum products, C5-12, reclaimed, wastewater treatment 69013-21-4 Fuel oil, pyrolysis 8030-30-6 Naphtha High Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 19 CAS numbers are used to describe the ten process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%. More information on the High Benzene Naphthas Category can be

	found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	The calculated boiling points for some representative constituents that are present in the category streams vary from 34.95 to 231.64°C @ 760 mm Hg. The measured boiling points of these same constituents vary from 34.0 to 217.9°C @ 760 mm Hg. Although this does not define the actual boiling points of the category streams, it offers an indication of a range that might be expected to encompass the boiling points of these complex streams with variable compositions. Boiling points outside of these ranges may be possible for some category streams.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential boiling point range for substances represented by the 19 CAS numbers listed under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in High Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for boiling point range based on constituent data.
Reference:	EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Boiling point values were calculated by the MPBPWIN subroutine and measured data came from the database in the computer program.)
Other (source):	American Chemistry Council, Olefins Panel (Prepared 7/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Boiling Point. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

HIGH BENZENE NAPHTHAS ROBUST SUMMARY

Melting Point

Test Substance*:	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]
Method/Guideline:	Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Melting Point is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of K. Joback and Gold and Ogle. Joback's Method is described in Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds. The Gold and Ogle Method simply uses the formula Tm = 0.5839Tb, where Tm is the melting point in Kelvin and Tb is the boiling point in Kelvin. The Gold and Ogle Method is described by Lyman, W.J., 1985, In: Environmental Exposure from Chemicals. Volume 1. Neely, W.B. and Blau, G.E. (eds), Boca Raton, FL, CRC Press, Inc., Chapter 2.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Calculated and measured melting point data for representative constituents of the High Benzene Naphthas Category are listed below. The data identify a potential melting point range for substances represented by the 19 CAS numbers under Test Substance. Substances in this category do not have a specific melting point value. Actual melting point ranges for substances in this category will vary dependent on their constituent composition. Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C11. The 12 chemicals selected to represent the melting point range of this category are C5-C10 hydrocarbons that can be found in substances identified by the 19 CAS numbers. Constituents representing category members were selected on the basis of
Results: (continued)	carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category

Units/Value: **Note: Deviations from protocol or guideline, analytical method.**	substances, and olefinic process (distillation) knowledge. Substance Constituent / Calculated MP (°C) / Measured* MP (°C) Isoprene -118.89 -145.9 n-pentane -106.92 -129.7 1,3-cyclopentadiene -91.83 -85.0 Isohexane -105.80 -162.9 n-hexane -93.84 -95.3 methylcyclopentane -85.82 -142.5 benzene -77.92 5.5 toluene -59.17 -94.9 m-xylene -40.69 -47.8 styrene -48.31 -31.0 dicyclopentadiene -16.78 32.0 naphthalene 5.01 80.2 * Experimental values from EPIWIN database. The data represent a potential melting point range for substances represented by the 19 CAS numbers under Test Substance.
Test Substance:	The High Benzene Naphthas Category includes the following CAS numbers: 64741-99-7 Extracts, petroleum, light naphtha solvent 64742-49-0 Naphtha, petroleum, hydrotreated light 64742-73-0 Naphtha, petroleum, hydrodesulfurized light 64742-83-2 Naphtha, petroleum, light steam-cracked 64742-91-2 Distillates, petroleum, steam-cracked 67891-79-6 Distillates, petroleum, heavy aromatic 67891-80-9 Distillates, petroleum, light aromatic 68410-97-9 Distillates, petroleum, light distillate hydrotreating process, low-boiling 68475-70-7 Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived 68476-45-9 Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product 68526-77-2 Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum 68606-10-0 Gasoline, pyrolysis, debutanizer bottoms 68606-28-0 Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic 68921-67-5 Hydrocarbons, ethylene-manufacture-by-product distillation residues 68955-29-3 Distillates, petroleum, light thermal cracked, debutanized aromatic 68956-52-5 Hydrocarbons, C4-8 68956-70-7 Petroleum products, C5-12, reclaimed, wastewater treatment 69013-21-4 Fuel oil, pyrolysis 8030-30-6 Naphtha
Test Substance: (continued)	High Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 19 CAS numbers are used to describe the ten process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon

	product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%. More information on the High Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	The calculated melting points for some representative constituents that are present in the category streams vary from -118.89 to 5.01 °C. The measured melting points of these same constituents vary from -162.9 to 80.2°C. Although this does not define the actual melting points of the category streams, it offers an indication of a range that might be expected to encompass the melting points of these complex streams with variable compositions. Melting points outside of these ranges may be possible for some category streams.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential melting point range for substances represented by the 19 CAS numbers listed under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the High Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for melting point range based on constituent data.
Reference:	EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Melting point values were calculated by the MPBPWIN subroutine and measured data came from the database in the computer program.)
Other (source):	American Chemistry Council, Olefins Panel (Prepared 7/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Melting Point. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

HIGH BENZENE NAPHTHAS ROBUST SUMMARY

Vapor Pressure

Test Substance*:	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]
Method/Guideline:	Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Vapor Pressure is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of Antoine and Grain. Both methods use boiling point for the calculation. The Antoine Method is described in the Handbook of Chemical Property Estimation. Chapter 14. W.J. Lyman, W.F. Reehl and D.H. Rosenblatt, Eds. Washington, D.C.: American Chemical Society. 1990. A modified Grain Method is described on page 31 of Neely and Blau's Environmental Exposure from Chemicals, Volume 1, CRC Press. 1985.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Calculated and measured vapor pressure data for representative constituents of the High Benzene Naphthas Category are listed below. The data identify a potential vapor pressure range for substances represented by the 19 CAS numbers under Test Substance. Substances in this category do not have a specific vapor pressure value. Actual vapor pressure ranges for substances in this category will vary dependent on their constituent composition. Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C11. The 12 chemicals selected to represent the vapor pressure range of this category are C5-C10 hydrocarbons that can be found in substances identified by the 19 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.

	Substance Constituent / Calculated VP (hPa @ 25°C) / Measured* VP (hPa @ 25°C) Isoprene 7.35 E^2 7.33 E^2 n-pentane 6.84 E^2 6.85 E^2 1,3-cyclopentadiene 5.69 E^2 5.80 E^2 Isohexane 2.48 E^2 2.53 E^2 n-hexane 2.00 E^2 2.01 E^2 methylcyclopentane 1.77 E^2 1.84 E^2 benzene 1.16 E^2 1.26 E^2 toluene 31.60 37.86 m-xylene 8.83 11.05 styrene 6.73 8.53 dicyclopentadiene 2.20 3.05 naphthalene 0.05 0.11 * Experimental values from EPIWIN database. The data represent a potential vapor pressure range for substances represented by the 19 CAS numbers under Test Substance.
Test Substance:	The High Benzene Naphthas Category includes the following CAS numbers: 64741-99-7 Extracts, petroleum, light naphtha solvent 64742-49-0 Naphtha, petroleum, hydrotreated light 64742-73-0 Naphtha, petroleum, hydrodesulfurized light 64742-83-2 Naphtha, petroleum, light steam-cracked 64742-91-2 Distillates, petroleum, steam-cracked 67891-79-6 Distillates, petroleum, heavy aromatic 67891-80-9 Distillates, petroleum, light aromatic 68410-97-9 Distillates, petroleum, light distillate hydrotreating process, low-boiling 68475-70-7 Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived 68476-45-9 Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product 68526-77-2 Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum 68606-10-0 Gasoline, pyrolysis, debutanizer bottoms 68606-28-0 Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic 68921-67-5 Hydrocarbons, ethylene-manufacture-by-product distillation residues 68955-29-3 Distillates, petroleum, light thermal cracked, debutanized aromatic 68956-52-5 Hydrocarbons, C4-8 68956-70-7 Petroleum products, C5-12, reclaimed, wastewater treatment 69013-21-4 Fuel oil, pyrolysis 8030-30-6 Naphtha High Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing.

	The 19 CAS numbers are used to describe the ten process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%. More information on the High Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	The calculated vapor pressures for some representative constituents that are present in the category streams vary from 0.05 to 7.35 E^2 hPa @ 25°C. The measured vapor pressures of these same constituents vary from 0.11 to 7.33 E^2 hPa @ 25°C. Although this does not define the actual vapor pressures of the category streams, it offers an indication of a range that might be expected to encompass the vapor pressures of these complex streams with variable compositions. Vapor pressure outside of these ranges may be possible for some category streams.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential vapor pressure range for substances represented by the 19 CAS numbers under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the High Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for vapor pressure range based on constituent data.
Reference:	EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Vapor pressure values were calculated by the MPBPWIN subroutine and measured data came from the database in the computer program.)
Other (source):	American Chemistry Council, Olefins Panel (Prepared 7/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Vapor Pressure. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

HIGH BENZENE NAPHTHAS ROBUST SUMMARY

Water Solubility

Test Substance*:	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]
Method/Guideline:	Calculated values using WSKOWWIN version 1.36, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Water Solubility is calculated by the WSKOWWIN subroutine, which is based on a Kow correlation method described by W. Meylan, P. Howard and R. Boethling in "Improved method for estimating water solubility from octanol/water partition coefficient". *Environ. Toxicol. Chem*. 15:100-106. 1995.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Calculated and measured water solubility data for representative constituents of the High Benzene Naphthas Category are listed below. The data identify a potential water solubility range for substances represented by the 19 CAS numbers under Test Substance. Substances in this category do not have a specific water solubility value. Actual water solubility ranges for substances in this category will vary dependent on their loading rate (i.e., weight of test material added to a volume of water). Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C11. The 12 chemicals selected to represent the water solubility range of this category are C5-C10 hydrocarbons that can be found in substances identified by the 19 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.
Results: (continued) **Units/Value:** **Note: Deviations from protocol or**	Substance Constituent / Calculated WS (mg/L @ 25°C) / Measured WS* (mg/L @ 25°C) Isoprene — 247.2 — 338.6

guideline, analytical method.	n-pentane 159.70 49.8 1,3-cyclopentadiene 470.6 na Isohexane 66.94 31.1 n-hexane 57.42 17.2 methylcyclopentane 83.95 49.4 benzene 2634.0 2000.0 toluene 832.7 573.1 m-xylene 258.4 207.2 styrene 386.7 343.7 dicyclopentadiene 51.9 na naphthalene 183.8 142.1 * Experimental values from EPIWIN database. na = not available The data represent a potential water solubility range for substances represented by the 19 CAS numbers under Test Substance.
Test Substance:	The High Benzene Naphthas Category includes the following CAS numbers: 64741-99-7 Extracts, petroleum, light naphtha solvent 64742-49-0 Naphtha, petroleum, hydrotreated light 64742-73-0 Naphtha, petroleum, hydrodesulfurized light 64742-83-2 Naphtha, petroleum, light steam-cracked 64742-91-2 Distillates, petroleum, steam-cracked 67891-79-6 Distillates, petroleum, heavy aromatic 67891-80-9 Distillates, petroleum, light aromatic 68410-97-9 Distillates, petroleum, light distillate hydrotreating process, low-boiling 68475-70-7 Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived 68476-45-9 Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product 68526-77-2 Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum 68606-10-0 Gasoline, pyrolysis, debutanizer bottoms 68606-28-0 Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic 68921-67-5 Hydrocarbons, ethylene-manufacture-by-product distillation residues 68955-29-3 Distillates, petroleum, light thermal cracked, debutanized aromatic 68956-52-5 Hydrocarbons, C4-8 68956-70-7 Petroleum products, C5-12, reclaimed, wastewater treatment 69013-21-4 Fuel oil, pyrolysis 8030-30-6 Naphtha
Test Substance: (cont'd)	High Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 19 CAS numbers are used to describe the ten process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%.

	More information on the High Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	The calculated water solubility for some representative constituents that are present in the category streams vary from 51.9 to 2634.0 mg/L @ 25°C. The measured water solubility of these same constituents vary from 17.2 to 2000.0 mg/L @ 25°C. Although this does not define the actual water solubility of the category streams, it offers an indication of a range that might be expected to encompass the water solubility of these complex streams with variable compositions. Water solubilities outside of these ranges may be possible for some category streams.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential water solubility range for substances represented by the 19 CAS numbers under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the High Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for water solubility range based on constituent data.
Reference:	EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Water solubility values were calculated by the WSKOWWIN subroutine and measured data came from the database in the computer program.)
Other (source):	American Chemistry Council, Olefins Panel (Prepared 7/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Water Solubility. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

HIGH BENZENE NAPHTHAS ROBUST SUMMARY

Hydrolysis (Stability in Water)

Test Substance*:	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]
Method/Guideline:	Other: Technical discussion
Year (guideline):	Not applicable
Type (test type):	Not applicable
GLP (Y/N):	Not applicable
Year (study performed):	Not applicable
Analytical Monitoring:	Not applicable
Test Conditions: • **Note: Concentration preparation, vessel type, volume, replication, deviations from guideline or protocol**	Not applicable
Results: **Units/Value:** • **Note: Analytical method, observations, half-lives by pH, degradation products**	Not applicable
Test Substance:	The High Benzene Naphthas Category includes the following CAS numbers: 64741-99-7 Extracts, petroleum, light naphtha solvent 64742-49-0 Naphtha, petroleum, hydrotreated light 64742-73-0 Naphtha, petroleum, hydrodesulfurized light 64742-83-2 Naphtha, petroleum, light steam-cracked 64742-91-2 Distillates, petroleum, steam-cracked 67891-79-6 Distillates, petroleum, heavy aromatic 67891-80-9 Distillates, petroleum, light aromatic 68410-97-9 Distillates, petroleum, light distillate hydrotreating process, low-boiling 68475-70-7 Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived 68476-45-9 Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product

	68526-77-2 Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum 68606-10-0 Gasoline, pyrolysis, debutanizer bottoms 68606-28-0 Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic 68921-67-5 Hydrocarbons, ethylene-manufacture-by-product distillation residues 68955-29-3 Distillates, petroleum, light thermal cracked, debutanized aromatic 68956-52-5 Hydrocarbons, C4-8 68956-70-7 Petroleum products, C5-12, reclaimed, wastewater treatment 69013-21-4 Fuel oil, pyrolysis 8030-30-6 Naphtha High Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 19 CAS numbers are used to describe the ten process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%. More information on the High Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	**Summary** In the environment, hydrolysis will not contribute to the degradation of chemicals in the High Benzene Naphthas Category. The High Benzene Naphthas Category includes ten process streams: • **Pyrolysis Gasoline** • **Pyrolysis C6 Fraction** • **Pyrolysis C6-C8 Fraction** • **Pyrolysis C5-C6 Fraction** • **Hydrotreated C6 Fraction** • **Hydrotreated C6-C7 Fraction** • **Hydrotreated C6-C8 Fraction** • **Quench Loop Pyrolysis Oil and Compressor Oil** • **Recovered Oil from Waste Water Treatment** • **Extract from Benzene Extraction** Nineteen CAS numbers (see Test Substance) identify substances derived from these process streams. As discussed below, the chemicals in these streams are composed of carbon and hydrogen and are not amenable to hydrolysis because of their molecular structure and the chemical reaction required for this type of transformation to occur.

	The High Benzene Naphthas Category A process stream is a mixture of chemicals that arises from a chemical reaction or separation activity. The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%. In some cases, petroleum refinery streams may be combined with intermediate streams from the ethylene unit and co-processed to produce these products. This grouping of CAS numbers represents hydrocarbon streams with a carbon number distribution that is predominantly C5-C11, through components boiling at 650°F or higher. That is why this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated High Benzene Naphthas. The definitions found in the TSCA Chemical Substance Inventory for the CAS numbers included in this group are vague with respect to composition. Therefore, it is possible to find that the same CAS number is correctly used to describe different streams (compositions) or that two or more different CAS numbers are used to describe the same stream (composition or process). More information on the High Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). The plan is available on the U.S. Environmental Protection Agency website under the HPV Chemical Program. A brief description of the production and composition of the ten process streams in this category are: • **Pyrolysis Gasoline** (Pygas) consists predominantly of C5+ hydrocarbons produced by the ethylene cracking furnaces. Typically the stream is derived from (1) the bottoms product from the debutanizer, (2) oils separated from furnace effluent quench systems, and (3) “drips” or condensate resulting from compression of the cracked gas. The oils from the quench systems and the “drips” may be stabilized to remove lights before blending with Pygas from the other sources. Depending on the plant configuration, Pygas may contain all of these intermediate streams, or the quench oils and stabilized drips may be transferred as separate streams. Low concentrations (e.g. 3% total) of C4 and lighter hydrocarbons may be present in the stream. A detailed analysis of Pygas may identify 60 or more hydrocarbon components or component groups, primarily unsaturated hydrocarbons and aromatics. Benzene, toluene, and dicyclopentadiene together may account for more than 50% of a Pygas stream and typically no other single component is present at a level greater than about 5%. The benzene concentration of Pygas is typically about 40% and the reported values range from 15 to 62%. The concentrations of individual hydrocarbon components in Pygas vary depending on the type of feedstock used by the ethylene plant, the mode of operation of the cracking furnaces (i.e. severity) and the ethylene process configuration. One non-typical Pygas stream is reported to contain vinylacetate at a concentration of up to about 10%. Vinylacetate is not typically found in ethylene process streams.

	• **Pyrolysis Gasoline Fractions (C5-C6, C6, and C6-C8 Fractions)** are separated by distillation into various boiling-point range fractions as intermediates in preparation for further processing. In some cases, petroleum refinery streams such as a C6 reformate fraction are combined with the pyrolysis gasoline prior to this separation. Similar to the situation for Pygas, the composition of these fractions vary depending on the ethylene process feedstock and the other operating variables. **1. Pyrolysis C5-C6 Fraction** has a carbon number distribution that is predominantly C5 to C6. One typical composition for this stream is reported as 70% benzene and 10% pentenes. **2. Pyrolysis C6 Fraction** has a carbon number distribution that is predominantly C6. Reported compositions vary from 35 to 77% benzene, 0.5 to 5% toluene with the balance primarily C6 non-aromatics, which are expected to be largely unsaturates. **3. Pyrolysis C6-C8 Fraction** has a carbon number distribution that is predominantly C6 to C8. The reported compositions range from 30 to 80% benzene, 15 to 25% toluene and 3 to 23% C8 aromatics. • **Hydrotreated Pyrolysis Fractions (C6, C6-C7, and C6-C8 Fractions)** are Pyrolysis gasoline or distillate fractions of pyrolysis gasoline that are treated with hydrogen over catalyst to saturate or partially saturate diolefins and/or olefins. In some cases, petroleum refinery streams such as a C6 reformate fraction are combined with the pyrolysis gasoline prior to this step. The hydrogenation process may be either one-stage or two-stage. The one-stage process is typically a liquid-phase process where the primary objective is to selectively convert diolefins to mono-olefins and to convert vinyl aromatics, for example, styrene to ethylbenzene. The second stage in a two-stage hydrogenation process is typically a vapor-phase, more severe hydrogenation that converts essentially all of the contained olefins to saturated hydrocarbons. A pygas fraction that will be processed by extraction or extractive distillation to produce high purity aromatics (benzene, toluene, or xylenes) is subjected to two-stage hydrogenation. Pygas fractions may be forwarded to hydrodealkylation units (less common) for benzene production after one-stage of hydrogenation. Hydrotreated Pyrolysis fractions may be the result of either one- or two-stage hydrogenation. 1. **Hydrotreated C6 Fraction** is very similar to the Pyrolysis C6 fraction except that the non-aromatics present in the hydrotreated stream are essentially all saturates. The reported composition for the Hydrotreated C6 stream indicates typical benzene content of 75%. 2. **Hydrotreated C6-C7 Fraction** has a carbon number distribution that is predominantly C6-C7 and the reported values indicate 40 to 70% benzene, and 3 to 15% toluene. 3. **Hydrotreated C6-C8 Fraction** has a reported typical composition of 40 to 60% benzene, 10 to 25% toluene, and 3 to 10% C8

aromatics.

- **Quench Loop Pyrolysis Oil and Compressor Oil** (Pyoil) represents higher boiling hydrocarbons that condense in the water quench system of an ethylene plant, typically at an ethylene unit cracking ethane, propane or butane. The stream can also include liquids collected at the cracked gas compressor knock out drums, which may include compressor injection oil. The carbon number distribution for Pyoil is C4 (or even lower) through heavier hydrocarbons such as naphthalene or even heavier. The reported typical composition includes 10 to 22% benzene and 5 to 11% toluene.

- **Recovered Oil from Wastewater Treatment** can be expected to be of variable composition and made up largely of the components found in Pygas. No composition data or process specific information has been reported. Typically, water streams at ethylene units are processed to separate hydrocarbons from the water so that the water can be reused to generate steam for process-contact use (dilution steam for the cracking furnaces) or so that excess water can be forwarded to treatment prior to discharge or reuse. Water processing typically includes mechanical and gravity separation and steam or gas stripping. Hydrocarbons separated from the water in these systems are not usually isolated from the process. However, at least in one case, the Recovered Oil from Wastewater Treatment has been reported as an isolated intermediate.

- **Extract from Benzene Extraction** are hydrotreated pyrolysis fractions containing aromatics (most commonly benzene or benzene and toluene) which are typically charged to extraction or extractive distillation units where the mixed aromatics are recovered. The carbon number distribution for this stream is predominantly C6 to C8. A reported typical concentration indicates 60 to 75% benzene, 25 to 40% toluene and 0 to 1% xylenes.

Hydrolysis of Hydrocarbons as a Function of Molecular Structure

Hydrolysis of an organic molecule occurs when a molecule (R-X) reacts with water (H_2O) to form a new carbon-oxygen bond after the carbon-X bond is cleaved (2,3). Mechanistically, this reaction is referred to as a nucleophilic substitution reaction, where X is the leaving group being replaced by the incoming nucleophilic oxygen from the water molecule. The leaving group, X, must be a molecule other than carbon because for hydrolysis to occur, the R-X bond cannot be a carbon-carbon bond.

The carbon atom lacks sufficient electronegativity to be a good leaving group and carbon-carbon bonds are too stable (high bond energy) to be cleaved by nucleophilic substitution. Thus, hydrocarbons, including alkenes, are not subject to hydrolysis (3) and this fate process will not contribute to the degradative loss of chemical components in this category from the environment.

Under strongly acidic conditions the carbon-carbon double bond found

	in alkenes, such as those in the High Benzene Naphthas Category, will react with water by an addition reaction mechanism (2). The reaction product is an alcohol. This reaction is not considered to be hydrolysis because the carbon-carbon linkage is not cleaved and because the reaction is freely reversible (3). Substances that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (4). The substances in the High Benzene Naphthas Category are primarily olefins that contain at least one double bond (alkenes). The remaining chemicals are saturated hydrocarbons (alkanes). These two groups of chemicals contain only carbon and hydrogen. As such, their molecular structure is not subject to the hydrolytic mechanism discussed above. Therefore, chemicals in the High Benzene Naphthas Category have a very low potential to hydrolyze, and this degradative process will not contribute to their removal in the environment. **References** 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA. 2. Gould, E.S. (1959), Mechanism and Structure in Organic Chemistry, Holt, Reinhart and Winston, New York, NY, USA. 3. Harris, J.C. (1982), "Rate of Hydrolysis," Chapter 7 in: W.J. Lyman, W.F. Reehl, and D.H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, NY, USA. 4. Neely, W. B. 1985. Hydrolysis. In: W. B. Neely and G. E. Blau, eds. Environmental Exposure from Chemicals. Vol I., pp. 157-173. CRC Press, Boca Raton, FL, USA.
Reliability:	These data represent a key study for characterizing the potential of substances in the High Benzene Naphthas Category to undergo hydrolysis.
Reference:	American Chemistry Council, Olefins Panel. 2003. Hydrolysis High Benzene Naphthas Category. Rosslyn, VA, USA.
Other (source):	American Chemistry Council, Olefins Panel (Prepared 7/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Hydrolysis. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

HIGH BENZENE NAPHTHAS ROBUST SUMMARY

Photodegradation (Direct)

Test Substance*:	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]
Method/Guideline:	Other: Technical discussion
Year (guideline):	Not applicable
GLP (Y/N):	Not applicable
Year (study performed):	Not applicable
Type (air, soil, water, other):	Water
Light Source:	Not applicable
Light Spectrum: • **Wave length value (upper/lower)**	Not applicable
Relative Intensity:	Not applicable
Test Substance Spectrum:	Not applicable
Test Conditions: • **Note: Concentration, temperature, test system type, replication, deviations from guideline or protocol**	Not applicable
Direct Photolysis:** • **Results: half-life, % degradation, quantum yield**	**Summary** In the environment, direct photolysis will not significantly contribute to the degradation of constituent chemicals in the High Benzene Naphthas Category. The High Benzene Naphthas Category includes ten process streams: • **Pyrolysis Gasoline** • **Pyrolysis C6 Fraction** • **Pyrolysis C6-C8 Fraction** • **Pyrolysis C5-C6 Fraction** • **Hydrotreated C6 Fraction** • **Hydrotreated C6-C7 Fraction** • **Hydrotreated C6-C8 Fraction** • **Quench Loop Pyrolysis Oil and Compressor Oil** • **Recovered Oil from Waste Water Treatment**

	• **Extract from Benzene Extraction** Nineteen CAS numbers (see Test Substance) identify products derived from these process streams. As discussed below, the reaction process involved in direct photolysis occurs when sufficient light energy excites a molecule to the degree that a structural transformation occurs. In general, substances in this category do not contain component chemicals that will undergo direct photolysis. **The High Benzene Naphthas Category** A process stream is a mixture of chemicals that arises from a chemical reaction or separation activity. The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%. In some cases, petroleum refinery streams may be combined with intermediate streams from the ethylene unit and co-processed to produce these products. This grouping of CAS numbers represents hydrocarbon streams with a carbon number distribution that is predominantly C5-C11, through components boiling at 650°F or higher. That is why this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated High Benzene Naphthas. The definitions found in the TSCA Chemical Substance Inventory for the CAS numbers included in this group are vague with respect to composition. Therefore, it is possible to find that the same CAS number is correctly used to describe different streams (compositions) or that two or more different CAS numbers are used to describe the same stream (composition or process). More information on the High Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). The plan is available on the U.S. Environmental Protection Agency website under the HPV Chemical Program. A brief description of the production and composition of the ten process streams in this category are: • **Pyrolysis Gasoline** (Pygas) consists predominantly of C5+ hydrocarbons produced by the ethylene cracking furnaces. Typically the stream is derived from (1) the bottoms product from the debutanizer, (2) oils separated from furnace effluent quench systems, and (3) “drips” or condensate resulting from compression of the cracked gas. The oils from the quench systems and the “drips” may be stabilized to remove lights before blending with Pygas from the other sources. Depending on the plant configuration, Pygas may contain all of these intermediate streams, or the quench oils and stabilized drips may be transferred as separate streams. Low concentrations (e.g. 3% total) of C4 and lighter hydrocarbons may be present in the stream. A detailed analysis of Pygas may identify 60 or more hydrocarbon components or component groups, primarily unsaturated hydrocarbons and aromatics. Benzene, toluene, and dicyclopentadiene together may account for more than 50% of a Pygas stream and typically no other single component is present at a level greater than about 5%. The benzene concentration of

	Pygas is typically about 40% and the reported values range from 15 to 62%. The concentrations of individual hydrocarbon components in Pygas vary depending on the type of feedstock used by the ethylene plant, the mode of operation of the cracking furnaces (i.e. severity) and the ethylene process configuration. One non-typical Pygas stream is reported to contain vinylacetate at a concentration of up to about 10%. Vinylacetate is not typically found in ethylene process streams. • **Pyrolysis Gasoline Fractions (C5-C6, C6, and C6-C8 Fractions)** are separated by distillation into various boiling-point range fractions as intermediates in preparation for further processing. In some cases, petroleum refinery streams such as a C6 reformate fraction are combined with the pyrolysis gasoline prior to this separation. Similar to the situation for Pygas, the composition of these fractions vary depending on the ethylene process feedstock and the other operating variables. **4.** **Pyrolysis C5-C6 Fraction** has a carbon number distribution that is predominantly C5 to C6. One typical composition for this stream is reported as 70% benzene and 10% pentenes. **5.** **Pyrolysis C6 Fraction** has a carbon number distribution that is predominantly C6. Reported compositions vary from 35 to 77% benzene, 0.5 to 5% toluene with the balance primarily C6 non-aromatics, which are expected to be largely unsaturates. **6.** **Pyrolysis C6-C8 Fraction** has a carbon number distribution that is predominantly C6 to C8. The reported compositions range from 30 to 80% benzene, 15 to 25% toluene and 3 to 23% C8 aromatics. • **Hydrotreated Pyrolysis Fractions (C6, C6-C7, and C6-C8 Fractions)** are Pyrolysis gasoline or distillate fractions of pyrolysis gasoline that are treated with hydrogen over catalyst to saturate or partially saturate diolefins and/or olefins. In some cases, petroleum refinery streams such as a C6 reformate fraction are combined with the pyrolysis gasoline prior to this step. The hydrogenation process may be either one-stage or two-stage. The one-stage process is typically a liquid-phase process where the primary objective is to selectively convert diolefins to mono-olefins and to convert vinyl aromatics, for example, styrene to ethylbenzene. The second stage in a two-stage hydrogenation process is typically a vapor-phase, more severe hydrogenation that converts essentially all of the contained olefins to saturated hydrocarbons. A pygas fraction that will be processed by extraction or extractive distillation to produce high purity aromatics (benzene, toluene, or xylenes) is subjected to two-stage hydrogenation. Pygas fractions may be forwarded to hydrodealkylation units (less common) for benzene production after one-stage of hydrogenation. Hydrotreated Pyrolysis fractions may be the result of either one- or two-stage hydrogenation. 4. **Hydrotreated C6 Fraction** is very similar to the Pyrolysis C6 fraction except that the non-aromatics present in the hydrotreated stream are essentially all saturates. The reported composition for the Hydrotreated C6 stream indicates typical benzene content of

	75%. 5. **Hydrotreated C6-C7 Fraction** has a carbon number distribution that is predominantly C6-C7 and the reported values indicate 40 to 70% benzene, and 3 to 15% toluene. 6. **Hydrotreated C6-C8 Fraction** has a reported typical composition of 40 to 60% benzene, 10 to 25% toluene, and 3 to 10% C8 aromatics. • **Quench Loop Pyrolysis Oil and Compressor Oil** (Pyoil) represents higher boiling hydrocarbons that condense in the water quench system of an ethylene plant, typically at an ethylene unit cracking ethane, propane or butane. The stream can also include liquids collected at the cracked gas compressor knock out drums, which may include compressor injection oil. The carbon number distribution for Pyoil is C4 (or even lower) through heavier hydrocarbons such as naphthalene or even heavier. The reported typical composition includes 10 to 22% benzene and 5 to 11% toluene. • **Recovered Oil from Wastewater Treatment** can be expected to be of variable composition and made up largely of the components found in Pygas. No composition data or process specific information has been reported. Typically, water streams at ethylene units are processed to separate hydrocarbons from the water so that the water can be reused to generate steam for process-contact use (dilution steam for the cracking furnaces) or so that excess water can be forwarded to treatment prior to discharge or reuse. Water processing typically includes mechanical and gravity separation and steam or gas stripping. Hydrocarbons separated from the water in these systems are not usually isolated from the process. However, at least in one case, the Recovered Oil from Wastewater Treatment has been reported as an isolated intermediate. • **Extract from Benzene Extraction** are hydrotreated pyrolysis fractions containing aromatics (most commonly benzene or benzene and toluene) which are typically charged to extraction or extractive distillation units where the mixed aromatics are recovered. The carbon number distribution for this stream is predominantly C6 to C8. A reported typical concentration indicates 60 to 75% benzene, 25 to 40% toluene and 0 to 1% xylenes. **<u>Photolysis of Hydrocarbons</u>** The direct photolysis of an organic molecule occurs when it absorbs sufficient light energy to result in a structural transformation (2). The reaction process is initiated when light energy in a specific wavelength range elevates a molecule to an electronically excited state. However, the excited state is competitive with various deactivation processes that can result in the return of the molecule to a non excited state. The absorption of light in the ultra violet (UV)-visible range, 110-750 nm, can result in the electronic excitation of an organic molecule. Light in this range contains energy of the same order of magnitude as

covalent bond dissociation energies (2). Higher wavelengths (e.g. infrared) result only in vibrational and rotational transitions, which do not tend to produce structural changes to a molecule.

The stratospheric ozone layer prevents UV light of less than 290 nm from reaching the earth's surface. Therefore, only light at wavelengths between 290 and 750 nm can result in photochemical transformations in the environment (2). Although the absorption of UV light in the 290-750 nm range is necessary, it is not always sufficient for a chemical to undergo photochemical degradation. Energy may be re-emitted from an excited molecule by mechanisms other than chemical transformation, resulting in no change to the parent molecule.

A conservative approach to estimating a photochemical degradation rate is to assume that degradation will occur in proportion to the amount of light wavelengths >290 nm absorbed by the molecule (3). Saturated hydrocarbons do not absorb light above 200 nm. Some characteristic absorbance maxima (λ_{max}) and associated molar absorptivities (ε) for selected unsaturated hydrocarbons are shown below (2):

	λ below 290 nm		**λ above 290 nm**	
Hydrocarbon	λ_{max}	ε	λ_{max}	ε
Ethylene	193	10,000	-	-
Benzene	255	215	-	-
Styrene	244	12,000	-	-
	282	450		
Naphthalene	221	100,000	311	250
	270	5,000		

Olefins with one double bond, or two conjugated double bonds, which constitute the majority of the chemicals in the High Benzene Naphthas category, do not absorb appreciable light energy above 290 nm. The absorption of UV light to cause cis-trans isomerism about the double bond of an olefin occurs only if it is in conjugation with an aromatic ring (2).

Products in the High Benzene Naphthas Category do not contain component molecules that will undergo direct photolysis. Therefore, this fate process will not contribute to a measurable degradative removal of chemical components in this category from the environment.

References

1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. Virginia, USA.

2. Harris, J. C. 1982. "Rate of Aqueous Photolysis," Chapter 8 in: W. J. Lyman, W. F. Reehl, and D. H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, USA.

3. Zepp, R. G. and D. M. Cline. 1977. Rates of Direct Photolysis in the Aqueous Environment, Environ. Sci. Technol., 11:359-366.

Indirect Photolysis:** • **Results: type of sensitizer, concentration of sensitizer, rate constant, % degradation, half-life**	Not applicable
Degradation Products:** • **Note: Identification, concentration**	Unknown
Test Substance:	The High Benzene Naphthas Category includes the following CAS numbers: 64741-99-7 Extracts, petroleum, light naphtha solvent 64742-49-0 Naphtha, petroleum, hydrotreated light 64742-73-0 Naphtha, petroleum, hydrodesulfurized light 64742-83-2 Naphtha, petroleum, light steam-cracked 64742-91-2 Distillates, petroleum, steam-cracked 67891-79-6 Distillates, petroleum, heavy aromatic 67891-80-9 Distillates, petroleum, light aromatic 68410-97-9 Distillates, petroleum, light distillate hydrotreating process, low-boiling 68475-70-7 Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived 68476-45-9 Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product 68526-77-2 Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum 68606-10-0 Gasoline, pyrolysis, debutanizer bottoms 68606-28-0 Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic 68921-67-5 Hydrocarbons, ethylene-manufacture-by-product distillation residues 68955-29-3 Distillates, petroleum, light thermal cracked, debutanized aromatic 68956-52-5 Hydrocarbons, C4-8 68956-70-7 Petroleum products, C5-12, reclaimed, wastewater treatment 69013-21-4 Fuel oil, pyrolysis 8030-30-6 Naphtha
Conclusion:	Not applicable
Reliability:	These data represent a key study for characterizing the potential of substances in the High Benzene Naphthas Category to undergo direct photodegradation.
Reference:	American Chemistry Council, Olefins Panel. 2003. Photodegradation (Direct): High Benzene Naphthas Category. Rosslyn, VA, USA.
Other (source):	American Chemistry Council, Olefins Panel (Prepared 7/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Photodegradation (Direct). Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

HIGH BENZENE NAPHTHAS ROBUST SUMMARY

Photodegradation (Indirect)

Test Substance*:	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]
Method/Guideline:	Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
GLP (Y/N):	Not applicable
Year (study performed):	Not applicable
Type (air, soil, water, other):	Not applicable
Light Source:	Sunlight
Light Spectrum: • **Wave length value (upper/lower)**	Natural sunlight
Relative Intensity:	1
Test Substance Spectrum:	Not applicable
Test Conditions: • **Note: Concentration, temperature, test system type, replication, deviations from guideline or protocol**	Indirect photodegradation, or atmospheric oxidation potential, is based on the structure-activity relationship methods developed by R. Atkinson. Temperature: 25°C Sensitizer: OH radical Concentration of Sensitizer: 1.5 E^6 OH radicals/cm^3
Direct Photolysis:** **Results: half-life, % degradation, quantum yield**	Not applicable

Indirect Photolysis:** • **Results: type of sensitizer, concentration of sensitizer, rate constant, % degradation, half-life**	**The High Benzene Naphthas Category** High Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 19 CAS numbers are used to describe the ten process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%. Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C11. That is why this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated High Benzene Naphthas. The 12 chemicals selected to represent the atmospheric oxidation potential of this category are C5-C10 hydrocarbons that can be found in substances identified by the 19 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge. **Atmospheric Oxidation of Hydrocarbons** In the environment, organic chemicals emitted into the troposphere are degraded by several important transformation processes. The dominant transformation process for most compounds is the daylight reaction with hydroxyl (OH-) radicals (Atkinson, 1988, 1989). The rate at which an organic compound reacts with OH-radicals is a direct measure of its atmospheric persistence (Meylan and Howard, 1993). AOPWIN estimates the rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. The rate constants estimated by the program are then used to calculate atmospheric half-lives for organic compounds based upon average atmospheric concentrations of hydroxyl radicals. Since the reactions only take place in the presence of sunlight, the atmospheric half-lives are normalized for a 12-hour day.

Indirect Photolysis: (cont'd)** **Results: type of sensitizer, concentration of sensitizer, rate constant, % degradation, half-life**	Chemical / Calculated* half-life (hrs) / OH- Rate Constant (cm^3/molecule-sec) Isoprene 1.2 105.1 E^{-12} n-pentane 31.7 4.0 E^{-12} 1,3-cyclopentadiene 0.9 142.6 E^{-12} Isohexane 22.4 5.7 E^{-12} n-hexane 23.5 5.5 E^{-12} methylcyclopentane 22.7 5.7 E^{-12} benzene 65.8 1.9 E^{-12} toluene 24.6 5.2 E^{-12} m-xylene 9.5 13.6 E^{-12} styrene 4.6 28.1 E^{-12} dicyclopentadiene 1.1 119.2 E^{-12} naphthalene 5.9 21.6 E^{-12} * Atmospheric half-life values are based on a 12-hr day. More information on the High Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (Olefins Panel, 2001). References: 1. Atkinson, R. 1988. Estimation of gas-phase hydroxyl radical rate constants for organic chemicals. *Environ. Toxicol. Chem*. **7**:435-442. 2. Atkinson, R. 1989. Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds. J. Phys. Chem. Ref. Data Monograph No. 1, Amer. Inst. Physics & Amer. Chem. Soc., NY. 3. Meylan, W.M. and P.H. Howard. 1993. Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. *Chemosphere* **12**:2293-2299. 4. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Degradation Products:** • **Note: Identification, concentration**	Unknown
Test Substance:	The High Benzene Naphthas Category includes the following CAS numbers: 64741-99-7 Extracts, petroleum, light naphtha solvent 64742-49-0 Naphtha, petroleum, hydrotreated light 64742-73-0 Naphtha, petroleum, hydrodesulfurized light

	64742-83-2 Naphtha, petroleum, light steam-cracked 64742-91-2 Distillates, petroleum, steam-cracked 67891-79-6 Distillates, petroleum, heavy aromatic 67891-80-9 Distillates, petroleum, light aromatic 68410-97-9 Distillates, petroleum, light distillate hydrotreating process, low-boiling 68475-70-7 Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived 68476-45-9 Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product 68526-77-2 Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum 68606-10-0 Gasoline, pyrolysis, debutanizer bottoms 68606-28-0 Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic 68921-67-5 Hydrocarbons, ethylene-manufacture-by-product distillation residues 68955-29-3 Distillates, petroleum, light thermal cracked, debutanized aromatic 68956-52-5 Hydrocarbons, C4-8 68956-70-7 Petroleum products, C5-12, reclaimed, wastewater treatment 69013-21-4 Fuel oil, pyrolysis 8030-30-6 Naphtha
Conclusion:	Atmospheric oxidation via hydroxyl radicals can be a significant route of degradation for products in this category. Based on calculated values, products in this category can have an atmospheric half-life range of 0.9 to 65.8 hours as a result of indirect photolysis by hydroxyl radical attack.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by AOPWIN. The data represent a potential atmospheric half-life range for substances represented by the 19 CAS numbers under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the High Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for atmospheric half-life range based on constituent data.
Reference:	Meylan, M., SRC 1994-1999. AOPWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
Other (source):	American Chemistry Council, Olefins Panel (Prepared 10/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Photodegradation (Indirect). Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.
** In IUCLID, provide additional discussion if needed in the results free text

HIGH BENZENE NAPHTHAS ROBUST SUMMARY

Partition Coefficient

Test Substance*:	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]
Method/Guideline:	Calculated values using KOWWIN version 1.65, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Octanol / Water Partition Coefficient is calculated by the KOWWIN subroutine, which is based on an atom/fragment contribution method of W. Meylan and P. Howard in "Atom/fragment contribution method for estimating octanol-water partition coefficients". 1995. *J. Pharm. Sci*. 84:83-92.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Calculated and measured log K_{ow} data for representative constituents of the High Benzene Naphthas Category are listed below. The data identify a potential log K_{ow} range for substances represented by the 19 CAS numbers under Test Substance. Substances in this category do not have a specific log K_{ow} value. Actual log K_{ow} ranges for substances in this category will vary dependent on their constituent composition. Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C11. The 12 chemicals selected to represent the log K_{ow} range of this category are C5-C10 hydrocarbons that can be found in substances identified by the 19 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.

Results: (continued) **Units/Value:** **Note: Deviations from protocol or guideline, analytical method.**	Substance Constituent — Calculated log K_{ow} @ 25°C — Measured* log K_{ow} @ 25°C Isoprene 2.58 2.42 n-pentane 2.80 3.39 1,3-cyclopentadiene 2.25 na Isohexane 3.21 3.60 n-hexane 3.29 3.90 methylcyclopentane 3.10 3.37 benzene 1.99 2.13 toluene 2.54 2.73 m-xylene 3.09 3.20 styrene 2.89 2.95 dicyclopentadiene 3.16 na naphthalene 3.17 3.30 * Experimental values from EPIWIN database. na = not available The data represent a potential log K_{ow} range for substances represented by the 19 CAS numbers under Test Substance.
Test Substance:	The High Benzene Naphthas Category includes the following CAS numbers: 64741-99-7 Extracts, petroleum, light naphtha solvent 64742-49-0 Naphtha, petroleum, hydrotreated light 64742-73-0 Naphtha, petroleum, hydrodesulfurized light 64742-83-2 Naphtha, petroleum, light steam-cracked 64742-91-2 Distillates, petroleum, steam-cracked 67891-79-6 Distillates, petroleum, heavy aromatic 67891-80-9 Distillates, petroleum, light aromatic 68410-97-9 Distillates, petroleum, light distillate hydrotreating process, low-boiling 68475-70-7 Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived 68476-45-9 Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product 68526-77-2 Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum 68606-10-0 Gasoline, pyrolysis, debutanizer bottoms 68606-28-0 Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic 68921-67-5 Hydrocarbons, ethylene-manufacture-by-product distillation residues 68955-29-3 Distillates, petroleum, light thermal cracked, debutanized aromatic 68956-52-5 Hydrocarbons, C4-8 68956-70-7 Petroleum products, C5-12, reclaimed, wastewater treatment 69013-21-4 Fuel oil, pyrolysis 8030-30-6 Naphtha High Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 19 CAS numbers are used to describe the ten process streams arising from the ethylene process and other associated

	manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%. More information on the High Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	The calculated log K_{ow} for some representative constituents that are present in the category streams vary from 1.99 to 3.29 @ 25°C. The measured log K_{ow} of these same constituents vary from 2.13 to 3.90 @ 25°C. Although this does not define the actual log K_{ow} of the category streams, it offers an indication of a range that might be expected to encompass the log K_{ow} of these complex streams with variable compositions. Log K_{ow} values outside of these ranges may be possible for some category streams.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential log K_{ow} range for substances represented by the 19 CAS numbers under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the High Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for log K_{ow} range based on constituent data.
Reference:	EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Log K_{ow} values were calculated by the KOWWIN subroutine and measured data came from the database in the computer program.)
Other (source):	American Chemistry Council, Olefins Panel (Prepared 7/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Partition Coefficient. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

HIGH BENZENE NAPHTHAS ROBUST SUMMARY

Transport / Distribution (Fugacity)

Test Substance*:	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]
Method/Guideline:	Calculated according to Mackay Level I, EQC Model version 1.01
Year (guideline):	1997
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment. Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.04 program (1). Measured input values were also used where available and obtained from the EPIWIN database (1). Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, sediment, suspended sediment, biota). 1. EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

Results:

Units/Value:

- **Note: Deviations from protocol or guideline, analytical method.**

Calculated partitioning data for representative constituents of the High Benzene Naphthas Category are listed below. The data identify a potential distribution for substances represented by the 19 CAS numbers under Test Substance. Actual distribution of substances in this category will vary dependent on their constituent composition.

Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C11. The 12 chemicals selected to represent the boiling point range of this category are C5-C10 hydrocarbons that can be found in substances identified by the 19 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.

The range of distribution data for constituent chemicals in each of the compartments can be used as an estimate of the partitioning behavior for category substances.

The following Mackay Level I model distribution values for representative constituents of substances in this category were determined using physicochemical input data calculated using the EPIWIN program:

	Calculated* Percent Distribution			
Chemical	Air	Water	Soil	Sediment
Isoprene	99.97	0.02	0.01	-
n-pentane	99.97	0.02	0.01	-
1,3-cyclopentadiene	99.93	0.06	0.01	-
Isohexane	99.96	0.02	0.02	-
n-hexane	99.95	0.02	0.02	-
methylcyclopentane	99.94	0.03	0.03	-
benzene	98.46	1.42	0.12	-
toluene	98.17	1.40	0.43	-
m-xylene	97.19	1.33	1.45	0.03
styrene	95.55	2.61	1.80	0.04
dicyclopentadiene	98.00	0.87	1.11	0.02
naphthalene	24.47	32.28	42.28	0.94

* Distribution values determined using calculated input data from EPIWIN program

Results: (cont'd) **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Measured** Percent Distribution Chemical / Air / Water / Soil / Sediment Isoprene 99.96 0.03 0.01 - n-pentane 99.99 0.01 - - 1,3-cyclopentadiene 99.93 0.06 0.01 - Isohexane 99.97 0.01 0.02 - n-hexane 99.96 - 0.04 - methylcyclopentane 99.95 0.02 0.03 - benzene 98.89 1.00 0.11 - toluene 98.80 0.81 0.39 - m-xylene 97.91 0.86 1.20 0.03 styrene 96.65 1.85 1.46 0.04 dicyclopentadiene 98.55 0.63 0.80 0.02 naphthalene 42.27 20.56 36.33 0.81 ** Distribution values determined using input data from the EPIWIN program experimental database
Test Substance:	The High Benzene Naphthas Category includes the following CAS numbers: 64741-99-7 Extracts, petroleum, light naphtha solvent 64742-49-0 Naphtha, petroleum, hydrotreated light 64742-73-0 Naphtha, petroleum, hydrodesulfurized light 64742-83-2 Naphtha, petroleum, light steam-cracked 64742-91-2 Distillates, petroleum, steam-cracked 67891-79-6 Distillates, petroleum, heavy aromatic 67891-80-9 Distillates, petroleum, light aromatic 68410-97-9 Distillates, petroleum, light distillate hydrotreating process, low-boiling 68475-70-7 Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived 68476-45-9 Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product 68526-77-2 Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum 68606-10-0 Gasoline, pyrolysis, debutanizer bottoms 68606-28-0 Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic 68921-67-5 Hydrocarbons, ethylene-manufacture-by-product distillation residues 68955-29-3 Distillates, petroleum, light thermal cracked, debutanized aromatic 68956-52-5 Hydrocarbons, C4-8 68956-70-7 Petroleum products, C5-12, reclaimed, wastewater treatment 69013-21-4 Fuel oil, pyrolysis 8030-30-6 Naphtha High Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 19 CAS numbers are used to describe the ten process streams arising from the ethylene process and other associated

	manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%. More information on the High Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	The partitioning data represent a potential distribution range for substances in the 19 CAS numbers listed under Test Substance. Substances in the High Benzene Naphthas Category are calculated to partition primarily to air with a small percentage partitioning to water, soil, and sediment. Relatively high vapor pressure and high water solubility largely control the partitioning behavior of constituent chemicals in substances from this category. The input data used to run the EQC Level I model included estimated values calculated by the EPIWIN program based on chemical structure and measured data from the EPIWIN database. A comparison of the distribution data developed using either all calculated input values or measured values where data were available indicate a similar partitioning behavior and support the use of the dataset for chemicals without any measured data.
Reliability:	(2) Reliable with restrictions The input data used to run the EQC Level I model include calculated and experimental values available through the EPIWIN program. The data represent a potential environmental distribution range for substances with the 19 CAS numbers listed under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the High Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for distribution range based on constituent data.
Reference:	Mackay, D.A. DiGuardo, S. Paterson, and C. Cowan. EQC Model Version 1.01. 1997. Available from the Environmental Modeling Centre, Trent University, Canada.
Other (source):	American Chemistry Council, Olefins Panel (Prepared 7/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Transport-Distribution. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

ATTACHMENT 1B

HIGH BENZENE NAPHTHAS ROBUST SUMMARIES:

BIODEGRADATION OF BENZENE

HIGH BENZENE NAPHTHAS ROBUST SUMMARY

Biodegradation

Test Substance:	CAS No. 71-43-2; Benzene
Method/Guideline:	OECD 301F
Year (guideline):	1993
Type (test type):	Ready Biodegradability, Manometric Respirometry Test
GLP:	Yes
Year (study performed):	2000
Inoculum:	Domestic activated sludge
Exposure Period:	28 days
Test Conditions: (FT - TC) • **Note: Concentration prep., vessel type, replication, test conditions.**	Activated sludge and test medium were combined prior to test material addition. Test medium consisted of glass distilled water and mineral salts (Phosphate buffer, Ferric chloride, Magnesium sulfate, Calcium chloride, EDTA). Test vessels were 500 mL dark glass bottles placed on a magnetic stirrer and electronically monitored for oxygen consumption. Test material and blanks were tested in triplicate, controls were tested in duplicate. Test material (benzene) concentration was 17mg/L. Sodium benzoate (positive control) concentration was 30mg/L. Toxicity control with benzene and Na Benzoate concentrations at 17 and 30 mg/L, respectively. Test temperature was 22 +/- 2 Deg C. All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.
Results: (FT - RS) **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Test material was readily biodegradable. Half-life was <2 weeks. By day 28, 63.0% degradation of the test material was observed. 10% biodegradation was achieved in less than 5 days, 50% biodegradation on approximately day 5. By day 5, >60% biodegradation of positive control was observed, which meets the guideline requirement. No excursions from the protocol were noted. Biodegradation was based on oxygen consumption and the theoretical oxygen demand of the test material as calculated using results of an elemental analysis of the test material.

Sample	% Degradation* (day 28)	Mean % Degradation (day 28)
Benzene	54, 72, 63	63
Na Benzoate	65, 75	70
Toxicity Control	59, 65	62

* replicate data

Conclusion: (FT - CL)	Test material was readily biodegradable. Half-life was <2 weeks
Reliability: (FT - RL)	(1) Reliable without restriction
Reference: (FT - RE)	Brixham Environmental Laboratory. 2001. OECD 301F, Ready biodegradability: Manometric respirometry. Study # AH0378/A.
Other (source): (FT - SO)	Olefins Panel, American Chemistry Council

* IUCLID field abbreviations include:
FT - Freetext
TC - Test Conditions
RS - Results
CL - Conclusion
RL - Reliability
RE - Reference
SO - Source

ATTACHMENT 1C

HIGH BENZENE NAPHTHAS ROBUST SUMMARIES:

MAMMALIAN TOXICITY

Robust Summary: High Benzene Naphthas

Acute Toxicity

Test Substance	**Dripolene**. Yellow, homogeneous liquid, stable for 5 years at ambient temperature. (CRU #93329). Olefins Panel HVP Stream: Pyrolysis Gasoline. Typical composition ranges for Pyrolysis Gasoline are shown in Table 2 of the Test Plan.
Method	
Method/guideline followed	Not specified
Type (test type)	Acute, limit test
GLP	Yes
Year	1994
Species/Strain	Rat, Sprague-Dawley
Sex	Males and females
No. of animals per sex /dose	5
Vehicle	None
Route of administration	Oral gavage
Test Conditions	Sprague Dawley rats (180-350g) were individually housed in stainless steel suspended cages and fasted overnight prior to administration of 2g/kg neat dripolene. The study room was maintained at 68-72^{0}F with a relative humidity of 35-63% and a 12 hr light-dark cycle. Water and chow diet were available ad lib after dosing. Test article was administered once on day 1 by oral gavage through a blunted needle. Rats were observed for clinical signs approx. 30 min, 1hr, and 4hr, after dosing, and daily thereafter until sacrifice on day 15. Rats were checked once a day for mortality and moribundity. Observations were not made on weekends. Body wts were recorded prior to fasting and on days 1, 8 and 15.
Results	
LD_{50} with confidence limits.	The LD_{50} was not reached at 2g/kg. There were no deaths and all rats gained some weight during the study. Clinical signs noted in one or more rats were salivation, decreased activity, rales, lacrimation, chromodacryorrhea, ataxia, head shaking, chromorhinorrhea, miosis, slight tremors, mydriasis, hyperactivity, hypothermia, urogenital discharge, nasal discharge, decreased food consumption, decreased fecal output, vocalization, and decreased stool size. No gross pathological findings were noted at necropsy.
Remarks	
Conclusions (study author)	The LD_{50} was not reached at 2g/kg.
Data Quality	
Reliability	**1.** Reliable without restriction.
References	Rodriguez, S.C. and Dalbey, W.E. 1994. Acute oral toxicity of dripolene in Sprague Dawley Rats. Study #65642. Stonybrook Laboratories, Princeton, NJ. for Mobil Chemical Co., Edison, NJ.
Other	
Last changed	10/23/2001 (Prepared by a contractor to the Olefins Panel)

Robust Summary: High Benzene Naphthas

Acute Toxicity

Test Substance	**Dripolene**. Yellow, homogeneous liquid, stable for 5 years at ambient temperature. (CRU #93329). Olefins Panel HVP Stream: Pyrolysis Gasoline. Typical composition ranges for Pyrolysis Gasoline are shown in Table 2 of the Test Plan.
Method	
Method/guideline followed	Not specified
Type (test type)	Acute, limit test
GLP	Yes
Year	1994
Species/Strain	Rabbit, New Zealand White
Sex	Males and females
No. of animals per sex/dose	3
Vehicle	None
Route of administration	dermal
Test Conditions	Rabbits, weighing at least 2kg, were individually housed in stainless steel suspended cages in a study room maintained at 69-72^{0}F with a relative humidity of 40-85% and a 12 hr light-dark cycle. Water and chow diet were available ad lib. The dorsal skin surface extending down from the front to rear legs and from left to right lower flanks was clipped free of hair the day prior to test article administration. Test article was spread evenly over the clipped area (approx. 10% of body surface area) at a dose of 2g/kg. A layer of 8-ply gauze was placed on the dorsal site, and a rubber dam sleeve was fitted snugly over the gauze pad and around the trunk. Edges of the dam were taped in place. An Elizabethan collar was affixed to the neck to prevent oral ingestion of test article and mechanical irritation of the test site. After 24 hrs, the collar and wrappings were removed and residual test article was wiped off. Body wts were recorded on days 1, 8 and 15. Rabbits were observed for toxicity at about 1 and 2 hr post-dose and daily thereafter on weekdays, through day 14. Observations for mortality/moribundity were made daily. Rabbits were sacrificed on day 15 and necropsies were performed.
Results	
LD_{50} with confidence limits.	The LD_{50} was not reached at 2g/kg. There were no deaths during the study and rabbits either gained some weight or remained at day 1 body wt. Signs that might have resulted from treatment in one or more rabbits were: decreased fecal output, decreased fecal pellet size, soft stool, and decreased food consumption. No gross pathological findings were noted at necropsy.
Remarks	
Conclusions	
(study author)	The LD_{50} was not reached at 2g/kg.
Data Quality	
Reliability	**1.** Reliable without restriction.
References	Rodriguez, S.C. and Dalbey, W.E. 1994. Dermal toxicity of dripolene in the New Zealand White rabbit. Study #65643. Stonybrook Laboratories, Princeton, NJ. for Mobil Chemical Co., Edison, NJ.
Other	
Last changed	10/23/2001 (Prepared by a contractor to the Olefins Panel)

Robust Summary: High Benzene Naphthas

Acute Toxicity

Test Substance	**Hydrogenated Pyrolysis Gasoline** CAS# 68410-97-9. Clear liquid, aromatic odor. Olefins Panel HVP Stream: Hydrotreated C6-C8.
Method	
Method/guideline followed	Standard method (not referenced) with doses based on a limit test and range-finding study
Type (test type)	Acute LD50
GLP	Yes
Year	1984
Species/Strain	Rat, Fischer 344
Sex	Males and females
No. of animals per sex per dose	5
Vehicle	None
Route of administration	Oral
Test Conditions	Rats (99.9-134.0 g; 57 days old) were individually housed in screen-bottomed cages in a room with 70.6^{0}F temperature, relative humidity of 59% and a 12 hr light/dark cycle. Chow diet and tap water from an automatic watering system were available ad lib. Rats were fasted for 24 hours prior to dosing at 4.2, 4.6, 5.0, and 5.4g/kg and observed at 1 and 4 hrs after dosing on day 1, and daily thereafter, over 14 days for clinical signs, morbidity and mortality. Gross necropsies were performed on all rats. LD50 was calculated by Probit analysis.
Results	
LD_{50} with confidence limits.	LD50 = 5.17g/kg (95% confidence limits: 5.02-5.45g/kg) On day 1, males and females showed dose responsive increases in ataxia, harsh respiratory sounds, and a non-dose responsive increase in red ocular discharge.
Remarks	Soft feces were observed in treated males and females on day 2. Frequency of clinical signs decreased by day 3 and signs were absent by day 5. There were no changes in body weight gain among the groups. Male and female mortalities were combined to calculate an LD50. Mortality from a previously performed limit test, conducted at 5.0g/kg was combined with results from the 5.0g/kg dose in this definitive study, raising that group number to 20. Mortalities were: 0/10 at 4.2, and 4.6g/kg, 7/20 at 5.0g/kg, 7/10 at 5.4g/kg. Gross necropsies revealed red lungs, gas-filled stomach and intestine, mottled liver, discoloration of kidney, and opaque eyes in rats that died during the study. These observations, with the exception of opacity in the left eye of one 5.4g/kg female, were absent in rats sacrificed at study termination (day 15).
Conclusions (study author)	The acute median lethal dose (LD50) for Hydrogenated Pyrolysis Gasoline in male and female rats was 5.17g/kg. A descriptive classification of Practically Non-toxic for acute oral exposure was assigned.
Data Quality	
Reliability	**1.** Reliable without restrictions.
References	Rausina, G.A. 1984. Acute oral toxicity study in rats of hydrogenated pyrolysis gasoline. Proj. #2091. Gulf Life Sciences Center, Pittsburgh, PA
Other	
Last change	5/7/2001 (Prepared by a contractor to the Olefins Panel)

Robust Summary: High Benzene Naphthas

Acute Toxicity

Test Substance	**Hydrogenated Pyrolysis Gasoline** CAS# 68410-97-9. Clear liquid, aromatic odor. Olefins Panel HVP Stream: Hydrotreated C6-C8.
Method	
Method/guideline followed	Standard method (not referenced)
Type (test type)	Acute LC50
GLP	Yes
Year	1984
Species/Strain	Rat, Fischer 344
Sex	Males and females
No. of animals per sex /dose	5
Vehicle	Filtered air
Route of administration	Inhalation
Test Conditions	Rats (8 wks. old, 100-172g at initiation) were individually housed in stainless steel, screen-bottomed cages in a room maintained at 73.0^{0}F (75.5^{0}F during exposure) temperature, relative humidity of 51% (40% during exposure) and a 12 hr light/dark cycle. Rats received chow diet and tap water ad lib, except during exposure. One group of 10 rats was exposed to aerosolized test article generated by a ball jet nebulizer for 4 hrs. A condensing flask was used to prevent large particles from entering the chamber. Actual average chamber concentration was 12,408ppm (range 8,642-17,371ppm) determined by gas chromatography. Particulate phase was negligible. Rats were observed for clinical signs at 1 and 4 hrs after dosing on day 1 and daily thereafter over 14 days, and for morbidity and mortality twice daily on weekdays, once daily on weekends. Body wt. was determined at initiation and on days 8 and 15. Gross necropsies were performed on all rats at termination on day 15.
Results	
LC_{50} with confidence limits.	LC50>12,408ppm
Remarks	There were no deaths during the study, no effects on body wt gain, and no gross alterations were seen at necropsy. Immediately after exposure, all rats exhibited lethargy, increased and labored respiration, and ocular discharge; most animals showed twitching and dry red material around nose/mouth. There were a few instances of harsh respiratory sounds, trembling, and perianal soiling. These clinical signs decreased in frequency by 4 hr post-exposure and disappeared by day 2.
Conclusions (study author)	No deaths occurred at the dose of 12,408ppm of test article, indicating a descriptive classification of Practically Non-toxic for acute inhalation exposure. Clinical signs noted immediately after exposure (increased/labored respiration, twitching, trembling, lethargy, ocular discharge) were not observed by day 2 and thereafter.
Data Quality	
Reliability	**1.** Reliable without restrictions.
References	Rausina, G.A. 1984. Acute inhalation toxicity study in rats of hydrogenated pyrolysis gasoline. Proj. #2092. Gulf Life Sciences Center, Pittsburgh, PA
Other	
Last change	Revised 7/27/2001 (Prepared by a contractor to the Olefins Panel)

Robust Summary: High Benzene Naphthas

Genetic Toxicity - in Vitro

Test Substance	**Hydrogenated Pyrolysis Gasoline**, CAS #68410-97-9. clear liquid with aromatic odor, negligible solubility in water, contains <55.0% benzene, <25% toluene, <10% dimethyl benzene/xylene, <7% pentane, <7% ethylbenzene, <3% cyclohexane, <2% hexane. Olefins Panel HVP Stream: Hydrotreated C6-C8.
Test substance	
Method	
Method/guideline followed	Standard method per Ames et al
Type	Reverse mutation bacterial assay
System of testing	Salmonella typhimurium, Escherichia coli with and without metabolic activation
GLP	Yes
Year	1991
Species/Strain	S. typh. TA1535, TA1537, TA98, TA100; E. coli WP2(uvrA)
Metabolic activation	Yes
Species and cell type	Male Sprague Dawley rat liver (S9 fraction), Molecular Toxicology, Inc., Annapolis, MD
Quantity	20% S9 fraction in 0.5ml S9 mix/plate
Induced or not induced	Aroclor 1254 induced, rats given a single 500mg/kg ip dose
Concentrations tested	0, 33, 100, 333, 1000, 3333, 10,000µg/plate ± S9. All diluted in acetone (200mg/ml)
Statistical Methods	None specified. Test article considered mutagenic when it induces a reproductive, dose-related increase in number of revertants in one or more strains at 3 consecutive dose levels. A non-mutagen does not induce a dose-related increase in at least 2 independent tests.
Remarks for Test Conditions	Hydrogenated pyrolysis gasoline (HPG) was prepared in acetone immediately prior to use. At end of the study, an aliquot of the stock dilution was sent to PTRL West, Richmond, CA to confirm concentration. Salmonella (approx. 10^8cells/ml) were exposed to either test material or acetone in 3 plates/dose ± S9 by the plate incorporation method. Six dose levels from 33-10,000µg/plate were employed in both the range-finding trial using TA100 and the mutagenicity test with all strains of Salmonella and E. coli. Optimum level of S9 for the mutagenicity assay was determined by testing the highest non-toxic dose, 10,000µg per plate with metabolic activation systems containing 4, 20 or 80% S9 fraction. No noteworthy increases in revertants or cytotoxicity was observed at any S9 concentration; 20% S9 was used in the mutagenicity test. All plates were incubated at 37^0C for 48 hrs then revertant colonies were counted. Positive control compounds were: cultures-S9, sodium azide (5µg/plate) for TA1535, TA100; 9-aminoacridine (50µg/plate) for TA1537; 2-nitrofluorene (5µg/plate) for TA98; N-ethyl-N'-Nitro-N-Nitrosoguanidene (5ug/plate) for E. coli WP2, and cultures+S9, 2-anthramine (4µg/plate) for TA1535, TA1537, (2µg/plate) for TA98, TA100, and (20µg/plate) for E. coli WP2. Two independent assays were performed.
Results	
Genotoxic effects	HPG did not induce increases in number of revertant colonies and no toxicity was observed in any Salmonella strain or E. coli WP2 with or without 20% S9 metabolic activation in both studies. Positive control compounds performed appropriately.
Conclusions (contractor)	Hydrogenated pyrolysis gasoline is not mutagenic to bacteria under conditions of this assay.
Data Quality	
Reliabilities	**1**. Reliable without restriction

Reference	Riccio, E.S. and Stewart, K.R. 1991. Salmonella-Escherichia coli/microsome plate incorporation assay of Hydrogenated Pyrolysis Gasoline. SRI Study #2545-A03-91, Sponsor study #91-66. SRI International, Menlo Park, CA for Chevron Environmental Health Center, Richmond, CA
Other	
Last changed	5/7/2001 (Prepared by a contractor to the Olefins Panel)

Robust Summary: High Benzene Naphthas

Genetic Toxicity - in Vitro

Test Substance	**Hydrogenated Pyrolysis Gasoline,** CAS #68410-97-9. clear liquid with aromatic odor. Composition, purity and stability referred to sponsor. Olefins Panel HVP Stream: Hydrotreated C6-C8.
Test substance	
Method	
Method/guideline followed	Standard method based on Cortesi et al (1983), Dunkel et al (1981), Reznikoff et al (1973)
Type	In vitro cell transformation
System of testing	Mouse embryo cells
GLP	Yes
Year	1984
Species/Strain	BALB/3T3-A31-1-1 from T. Kakunaga, National Cancer Inst., 1983
Metabolic activation	No
Species and cell type	NA
Quantity	NA
Induced or not induced	NA
Concentrations tested	Cytotoxicity: 8, 16, 32, 64, 128, 256, 512, 1024, 2048, and 5000µg/ml; Transformation: 100, 250, 500, 1500µg/ml, all diluted in 10% Pluronic® polyol F68 (prepared in deionized water, mol. wt. 8350, 80% hydrophilic).
Exposure period	2 days
Statistical Methods	None employed. Criteria for positive response were a two-fold increase in type III foci at the highest dose over vehicle control (at least 2 type III foci if vehicle control had none) with or without a dose related response, or a two-fold increase at two or more consecutive doses. Test is equivocal if two-fold increase occurred at any one level other than the highest acceptable dose.
Remarks for Test Conditions	Sufficient Hydrogenated Pyrolysis Gasoline (HPG) was weighed separately for each dose level, 0.40ml of 10% F68 added per ml of final volume and medium (Eagles MEM with 10% heat-inactivated fetal calf serum) added as required to achieve final volume for testing. Test preparations were mixed just prior to addition to cultures at 50µl to each 5 ml culture. All cultures were incubated at 37^0C in 5% CO2 enriched humidified atmosphere. For cytotoxicity, 2 cultures/dose group, 2 cultures for vehicle F68 or medium negative control were seeded with $1x10^4$ cells/plate in day 1, exposed on days 2-3, trypsinized and counted with a Coulter Model ZB on day 4 for at least 20% survival. For transformation, 15 cultures ($1x10^4$ cells/flask/dose group)) and two colony-forming cultures (100 cells/plate/dose group) were seeded on day 1, exposed on days 2-3 and culture medium changed on day 4. For transformation cultures, medium continued to be changed weekly to day 29. Positive control was 3-methylcholanthrene (1µg/ml). Colony forming cultures were fixed, stained, and counted visually on day 10 to determine cloning efficiency (avg. number colonies/plate ÷ 100 cells seeded). Transformation cultures were fixed and stained on day 29 for focus counting and evaluation. Transformation frequency = total type III foci ÷ total flasks/dose group.
Results	
Genotoxic effects	HPG induced toxicity in BALB/3T3 cells after two days exposure beginning at 128 µg/ml (45.4% relative survival) with relative survivals of 26.7, 25.6, 3.2 and 0% at 512, 1024, 2048 and 5000µg/ml, respectively. In the transformation assay, toxicity was seen at all dose levels (relative cloning efficiencies of 53.7, 67.8, 78.5 and 0% at 100, 250, 500 and 1500µg/ml). At 1500µg/ml, the highest dose level, HPG induced 5 Type III foci; no other dose levels produced a positive response. Transformation frequencies were 0.13, 0, 0, 0.07 and 0.36 for medium control, vehicle control, 100, 250, 500 and 1500µg/ml, respectively. Positive and negative controls gave appropriate responses.

Conclusions (contractor)	Hydrogenated Pyrolysis Gasoline induced transformation in BALB/3T3 cells under conditions of this assay. Cytotoxicity and impairment of cloning efficiency were also observed. The positive response was observed only at the highest dose level, a level that appeared to be too toxic for cells to recover and form colonies (0% relative colony forming efficiency)
Data Quality *Reliabilities*	**1.** Reliable without restriction
Reference	Brecher, S. 1984. Transformation test of Hydrogenated Pyrolysis Gasoline. Proj. #2098. Gulf Life Sciences Center, Pittsburgh, PA for Gulf Oil Chemicals Co, Houston, TX Cortesi, E. et al. 1983. Teratogenesis, Carcinogenesis, Mutagenesis 3: 101-110. Dunkel, V.A. et al. 1981. J. Nat'l Cancer Inst. 67: 1303-1315. Reznikoff, C.A. et al. 1973. Cancer Res. 3239-3249.
Other *Last changed*	Revised 8/27/2001 (Prepared by a contractor to the Olefins Panel).

Robust Summary - Group 5: High Benzene Naphthas

Genetic Toxicity - in Vitro

Test Substance	**Hydrogenated Pyrolysis Gasoline**, CAS #68410-97-9. clear liquid with aromatic odor. Composition, purity and stability referred to sponsor. Olefins Panel HVP Stream: Hydrotreated C6-C8.
Test substance	
Method	
Method/guideline followed	Standard method based on Williams et al (1977, 1982)
Type	In vitro mammalian DNA repair assay
System of testing	Unscheduled DNA synthesis (UDS) in primary hepatocyte cultures
GLP	Yes
Year	1984
Species/Strain	Fischer 344 male rat (10 wks old)
Metabolic activation	No
Species and cell type	NA
Quantity	NA
Induced or not induced	NA
Concentrations tested	8, 16, 32, 64, 128, 256, 512, 1024µg/ml diluted in 10% Pluronic F68 (prepared in deionized water, mol. wt 8350, 80% hydrophilic)
Exposure period	18 hrs.
Statistical Methods	None specified. Criteria for positive response are incorporation of radioactive precursor (^{3}H-thymidine) in cells that are not normally synthesizing DNA, indicating repair of damage. A positive response is defined as a mean net nuclear grain count at any treatment level that exceeds concurrent negative control by at least 6 grains/nucleus; negative control value must not exceed 5 grains. If this criterion is not met, a positive response can be identified if there is a significant difference ($p<0.01$) in % cells in repair at any dose level and negative control value. This indicator defines whether a small fraction of cells is undergoing repair (Casciano & Gaylor, 1983). A positive response need not be dose related.
Remarks for Test Conditions	Sufficient Hydrogenated Pyrolysis Gasoline (HPG) was weighed separately for each dose level, 0.40ml of 10% F68 added per ml of final volume and sufficient medium (Williams Medium E with 10% fetal bovine serum and insulin) added to achieve final volume. Test preparations were mixed just prior to addition at 20µl to each 2ml culture. The conc. of ^{3}H-thymidine (½ life 12.4 yrs.) used in these assays was 1mCi/ml. All cultures were incubated at 37^{0}C in 5% CO2 enriched humidified atmosphere. No range finding assay was performed. In the UDS assay, 2x10^5 cells/ml were seeded into coverslip cultures, exposed to ^{3}H-thymidine and test substance for 18 hours (3 cultures/dose level, 8 dose levels), untreated controls, vehicle F68 control and positive control, 2-acetyl aminofluorene (0.01µg/ml). Cells growing on coverslips were rinsed, fixed and glued to microscope slides on day 2. On day 3, slides were dipped in autoradiographic emulsion and stored in the dark at 2-8^{0}C. Autoradiographs were developed, stained and coverslipped on day 10. Numbers of grains overlying 50 randomly selected nuclei/slide were counted. The highest of 3 cytoplasmic grain counts/cell were subtracted and this number was divided by a conversion factor (unspecified) to obtain net nuclear grain count. Avg. net nuclear grain count/slide (sum of net nuclear grain count ÷ 50) and mean net nuclear grain count (avg. net nuclear grain count/slide ÷3) were calculated. In addition, % cells in repair were determined for each dose level.
Results	
Genotoxic effects	HPG induced toxicity in primary hepatocytes following 18 hr exposure that left too few cells for UDS analysis at doses of 512 and 1024µg/ml. HPG did not induce unscheduled DNA synthesis at any dose level with sufficient cells to be analyzed. Positive and negative controls gave appropriate responses.

Conclusions (contractor)	Hydrogenated Pyrolysis Gasoline did not induce unscheduled DNA synthesis in primary cultures of rat hepatocytes under conditions of this assay.
Data Quality *Reliabilities*	**2**. Reliable with restrictions. No table of cell counts/viability. No individual data to verify calculations and identify conversion factor. Statistical criteria are mentioned but method is not cited.
Reference	Brecher, S. 1984. Hepatocyte primary culture/DNA repair test of Hydrogenated Pyrolysis Gasoline. Proj. # 2097. Gulf Life Sciences Center, Pittsburgh, PA for Gulf Oil Chemicals Co., Houston, TX Williams, G.M. 1977. Cancer Res. 37: 1845-1851 Williams et al. 1977. In Vitro 13: 809-817 Williams et al. 1982. Mut. Res. 97:359-370 Casciano, D.A. and Gaylor, D.W. 1983. Mut. Res. 122:81-86
Other *Last changed*	5/7/2001 (Prepared by a contractor to the Olefins Panel)

Robust Summary - Group 5: High Benzene Naphthas

Genetic Toxicity - in Vivo

Test Substance	**Hydrogenated Pyrolysis Gasoline**, CAS #68410-97-9. Clear liquid with
Remarks	aromatic odor. Compositional analysis, purity and stability referred to sponsor. Olefins Panel HVP Stream: Hydrotreated C6-C8.
Method	
Method/guideline followed	None specified. Comparable to standard assay.
Type	Mammalian bone marrow erythrocyte micronucleus assay
GLP	Yes
Year	1984
Species	Mice
Strain	Crl:CD-1(ICR)BR Swiss
Sex	Male and female. Range-finding 2M, 2F (10 wks old)/group; 3 groups; Micronucleus test 10M, 10F (11 wks old)/group in 4 groups, 15M, 15F in one group.
Route of administration	Oral gavage
Doses/concentration levels	0, 0.5, 1.0, 2.0g/kg (2doses), 2.0g/kg (1 dose) undiluted
Exposure period	1 dose/day for 2 days: one group- 1 dose, 1 day only
Statistical methods	Values from treated groups for daily mean body weights, group means and std. dev. for polychromatic erythrocytes (PCEs) with micronuclei (MN) , and group mean ratios of PCE to normochromatic erythrocytes (NORMs) were calculated and compared with vehicle control values by Student's t-test. Positive response was indicated by statistically significant ($p<0.05$) increases in micronucleated PCE at any dose level with a dose related response evident. Results were considered equivocal if only one of these criteria was met.
Remarks for Test Conditions.	Animals in the range-finding study (2M, 2F/group), 3 treated groups (no control group) were given 1.25, 2.5, and 5.0g/kg neat hydrogenated pyrolysis gasoline (HPG) by gavage once each day for two days. Eighty percent of the dose level that produced ≤50% mortality was selected for the maximum dose in the micronucleus study. In the micronucleus study, three groups of mice were given undiluted HPG by oral gavage daily for two days at doses of 0.5, 1.0, 2.0g/kg, negative control mice were given corn oil (5g/kg). One-half of each treated group and negative control (5M, 5F) was killed on day 3 and the remainder on day 4. One group (15M, 15F), given 2.0 g/kg by gavage in a single dose for 1 day only, was killed on days 2, 3, 4 (5/sex/day). Positive control mice (4M, 4F) given cyclophosphamide (75 mg/kg) ip daily for 2 days were killed on day 3. Survival, body wt, and clinical signs were observed and recorded daily. Slides of femoral bone marrow smears were prepared, stained with May-Grunewald/Giemsa stain and examined microscopically. For each mouse, 1000 PCE and all associated mature erythrocytes (NORMs) were counted. Data collected included group mean body weights for each day, total PCEs, total NORMs, PCEs with MN, and NORMs with MN.
Results	
Genotoxic effects	
NOAEL (NOEL)	NOAELmortality = 1.0g/kg; NOELgenetics > 2.0g/kg (Assigned by reviewer)
LOAEL (LOEL)	In the range-finding study, half of the animals given HPG at conc of 5.0g/kg died on or before day 2. Gross necropsy of dead mice was unremarkable. In the micronucleus test, 1/10 males given 2.0g/kg (2 doses) died on day 2. No other mortality or significant wt changes were observed. Lethargy was observed among high dose mice. Surviving mice treated with HPG did not show any significant increase in micronucleus formation in PCE and no significant changes in ratio of PCE/NORM compared to negative controls. Negative and positive

	controls gave appropriate results.
Conclusions (study authors)	Oral treatment of mice with Hydrogenated Pyrolysis Gasoline for 1-2 days at doses up to 2.0g/kg/day had no effect on frequency of micronucleated polychromatic erythrocytes in bone marrow under these test conditions. HPG did not induce cytogenetic damage.
Data Quality *Reliabilities*	**1.** Reliable without restriction
References	Khan, S.H. 1984. Micronucleus test of Hydrogenated Pyrolysis Gasoline. Proj. #2096. Gulf Life Sciences Center, Pittsburgh, PA for Gulf Oil Chemicals Co., Houston, TX
Other *Last changed*	5/7/2001 (Prepared by a contractor to the Olefins Panel)

Robust Summary - Group 5: High Benzene Naphthas

Repeated Dose Toxicity

Test Substance	**Hydrogenated Pyrolysis Gasoline** CAS #68410-97-9, Clear liquid with aromatic odor. Olefins Panel HVP Stream: Hydrotreated C6-C8.
Remarks	
Method	
Method/guideline followed	Standard method, method not referenced
Test type	Subacute
GLP	Yes
Year	1984
Species	Rat
Strain	Fischer 344
Route of administration	Inhalation
Duration of test	8 days
Doses/concentration levels	0, 4869±470, 9137±917ppm±SD, actual exposure conc.
Sex	Males and females (5/sex/group)
Exposure period	6 hrs.
Frequency of treatment	once daily for 5 days (d1-5)
Control group and treatment	5M, 5F; filtered air
Post exposure observation period	2 days
Statistical methods	Body wt variance compared by Bartlett's test and one way analysis of variance. Group mean body wt compared either with Dunnett's test or a modified t-test to assess significance.
Test Conditions	Rats (9 wks old, 113-195g at initiation) were housed individually in stainless steel, screen-bottomed cages. Rooms were maintained at 72.2^{0}F (exposure chamber 75^{0}F) with relative humidity of 54% (exposure chamber 50%), and 12 hr light/dark cycle. Rats received chow diet and tap water ad lib throughout the study, except during exposure. Three groups of 10 rats (5M, 5F/group) each, were exposed to test article or air. Test article was aerosolized with a ball jet nebulizer; an in-line condensing flask was used to prevent large particles from entering the exposure chamber. Chamber concentration of test article was measured by gas chromatography. Rats were observed twice daily on weekdays and once daily on weekends for morbidity/mortality, and once daily for clinical signs immediately after exposure on days 1-5. Surviving rats were sacrificed on day 8. Gross necropsies were performed on all rats.
Results	
NOAEL (NOEL)	NOAEL< 4869ppm (estimated by reviewer)
LOAEL (LOEL)	LOAEL= 4869ppm (estimated by reviewer) based on clinical observations, reduced wt gain.
Remarks	Two rats (1M, 1F) from group 3 (9137ppm) died on day 2; one female from group 3 died during exposure on day 1. Rats in groups 2 and 3 showed ocular discharge throughout d1-5. Rats in group 2 showed increased respiratory rate and dry red material around nose and mouth. All rats in group 2 were lethargic and showed labored respiration. Many rats in group 3 were lethargic and exhibited twitching and harsh respiratory sounds during days 1-5. All rats in group 2 and all but one survivor in group 3 appeared normal on day 8. Group mean body wt was significantly decreased in a dose related manner. No test article related effects were seen at gross necropsy on day 8; the male rat that died during the study showed gas in the G.I. tract and red-tinged fluid in the stomach.
Conclusions	
(study authors)	Exposure to test article caused a significant decrease in group mean body wt of

	male and female rats of low and high dose groups that was correlated with exposure level. Three deaths occurred in the high dose group during exposure. Major clinical signs were lethargy, twitching, harsh respiratory sounds and ocular discharge. No gross alterations were found in rats surviving to sacrifice.
Quality	
Reliabilities	**1.** Reliable without restrictions
References	Rausina, G.A. 1984. Five-day repeated dose inhalation toxicity study in rats of Hydrogenated Pyrolysis Gasoline. Proj. #2099. Gulf Life Sciences Center, Pittsburgh, PA
Other	
Last changed	Revised 7/27/2001 (Prepared by a contractor to the Olefins Panel)

Robust Summary: High Benzene Naphthas

Acute Toxicity

Test Substance	**Pyrolysis gasoline (Rerun Tower Overheads**). Yellow, homogeneous liquid; 40% benzene, 26% C5, 13% toluene, 20% other. Test substance is described as a sample of a Pyrolysis Gasoline distillate fraction and is similar to Pyrolysis gasoline, a stream included in the test plan.
Method	
Method/guideline followed	Not specified
Type (test type)	Acute, limit test
GLP	Yes
Year	1994
Species/Strain	Rat, Sprague-Dawley
Sex	Males and females
No. of animals per sex /dose	5
Vehicle	None
Route of administration	Oral gavage
Test Conditions	Sprague Dawley rats (180-350g) were individually housed in stainless steel suspended cages and fasted overnight prior to administration of 2g/kg neat pyrolysis gasoline. The study room was maintained at 68-72^{0}F with a relative humidity of 35-63% and a 12 hr light-dark cycle. Water and chow diet were available ad lib after dosing. Test article was administered once on day 1 by oral gavage through a blunted needle. Rats were observed for clinical signs approx. 30 min, 1hr and 4hr, after dosing, and daily thereafter until sacrifice on day 15. Rats were checked once a day for mortality and moribundity. Observations were not made on weekends. Body wts were recorded prior to fasting and on days 1, 8 and 15.
Results	
LD_{50} with confidence limits.	The LD_{50} was not reached at 2g/kg. There were no deaths and all rats gained some weight during the study. Clinical signs noted in one or more rats were salivation, decreased activity, rales, lacrimation, chromodacryorrhea, ataxia, chromorhinorrhea, miosis, slight tremors, mydriasis, hyperactivity, hypothermia, urogenital discharge, nasal discharge, decreased food consumption, decreased fecal output, vocalization, and penile discharge. No gross pathological findings were noted at necropsy.
Remarks	
Conclusions	
(study author)	The LD_{50} was not reached at 2g/kg.
Data Quality	
Reliability	**1.** Reliable without restriction.
References	Rodriguez, S.C. and Dalbey, W.E. 1994. Acute oral toxicity of pyrolysis gasoline in Sprague Dawley Rats. Study #65636. Stonybrook Laboratories, Princeton, NJ. for Mobil Chemical Co., Edison, NJ.
Other	
Last changed	10/16/2001 (Prepared by a contractor to the Olefins Panel)

Robust Summary - Group 5: High Benzene Naphthas

Acute Toxicity

Test Substance	Pyrolysis gasoline (Rerun Tower Overheads). Yellow, homogeneous liquid; 40% benzene, 26% C5, 13% toluene, 20% other. Test substance is described as a sample of a Pyrolysis Gasoline distillate fraction and is similar to Pyrolysis gasoline, a stream included in the test plan.
Method	
Method/guideline followed	Not specified
Type (test type)	Acute, limit test
GLP	Yes
Year	1994
Species/Strain	Rabbit, New Zealand White
Sex	Males and females
No. of animals per sex /dose	3
Vehicle	None
Route of administration	dermal
Test Conditions	Rabbits, weighing at least 2kg, were individually housed in stainless steel suspended cages in a study room maintained at 69-72^{0}F with a relative humidity of 38-85% and a 12 hr light-dark cycle. Water and chow diet were available ad lib. The dorsal skin surface extending down from the front to rear legs and from left to right lower flanks was clipped free of hair the day prior to test article administration. Test article was spread evenly over the clipped area (approx. 10% of body surface area) at a dose of 2g/kg. A layer of 8-ply gauze was placed on the dorsal site, and a rubber dam sleeve was fitted snugly over the gauze pad and around the trunk. Edges of the dam were taped in place. An Elizabethan collar was affixed to the neck to prevent oral ingestion of test article and mechanical irritation of the test site. After 24 hrs, the collar and wrappings were removed and residual test article was wiped off. Body wts were recorded on days 1, 8 and 15. Rabbits were observed for toxicity at about 1 and 2 hr post-dose and daily thereafter on weekdays through day 14. Observations for mortality/moribundity were made daily. Rabbits were sacrificed on day 15 and necropsies were performed.
Results	
LD_{50} with confidence limits.	The LD_{50} was not reached at 2g/kg. There were no deaths during the study and rabbits either gained some weight or remained at day 1 body wt. Signs that might have resulted from treatment in one or more rabbits were: soft stool, decreased fecal pellet size, nasal discharge, and test site erythema. No gross pathological findings were noted at necropsy.
Remarks	
Conclusions	
(study author)	The LD_{50} was not reached at 2g/kg.
Data Quality	
Reliability	**1.** Reliable without restriction.
References	Rodriguez, S.C. and Dalbey, W.E. 1994. Dermal toxicity of pyrolysis gasoline in the New Zealand White rabbit. Study #65637. Stonybrook Laboratories, Princeton, NJ. for Mobil Chemical Co., Edison, NJ.
Other	
Last changed	10/16/2001 (Prepared by a contractor to the Olefins Panel)

Robust Summary - Group 5: High Benzene Naphthas

Genetic Toxicity - in Vitro

Test Substance	**Rerun Tower Overheads** from Olefins/Aromatics Plant (light thermal cracked naphtha) CAS # 64741-74-8. Straw colored liquid; 40% benzene, 26% C5, 13% toluene, 20% other. Test substance is described as a sample of a Pyrolysis Gasoline distillate fraction and is similar to Pyrolysis gasoline, a stream included in the test plan.
Test substance	
Method	
Method/guideline followed	Standard method based on Ames et al, 1975
Type	Reverse mutation bacterial assay
System of testing	Salmonella typhimurium with and without metabolic activation
GLP	Yes
Year	1981
Species/Strain	S. typhimurium TA 98, TA100, TA1535, TA1537, and TA1538.
Metabolic activation	Yes
Species and cell type	Sprague Dawley male rat liver (S9 fraction) from Litton Bionetics, Kensington, MD
Quantity	50ul S9 fraction in 0.5ml S9 mix/plate
Induced or not induced	Aroclor 1254-induced, rats were given a single ip 500mg/kg dose, 5 days prior to sacrifice.
Concentrations tested	0, 0.029, 0.094, 0.30, 0.97µl/plate –S9, and 0.094, 0.30, 0.97, and 3.1µl/plate + S9; samples diluted in dimethyl sulfoxide (DMSO). Negative control 50µl DMSO
Statistical Method	None. Criteria for a positive response were an increase in revertant colonies at least two-fold that of negative control at the lowest active dose, and a dose response curve. Positive results must be reproducible in an independent repeat assay.
Remarks for Test Conditions	Rerun tower overheads test solutions were prepared in DMSO immediately prior to use. Salmonella (Approx. 1.4-2x10^8 cells/ml) were exposed to either test solution or DMSO ±S9 by the preincubation method. Doses of 0.029-0.97µl/plate-S9 and 0.094-3.1µl/plate +S9 were determined by a pretest toxicity test in TA 100 and TA1537±S9 using incremental doses from 0.01-10µl/plate. Culture tubes containing 50µl test solution or DMSO, 0.1ml Salmonella and 0.5 ml phosphate buffer or S9 mix were combined and incubated with shaking (150 rpm) for 20 minutes at 37^{0}C. At the end of the preincubation period, top agar was added, mixed and cultures were overlaid on minimal agar plates, 3 plates/dose/strain. Plates were incubated at 37^{0}C for 48 hrs, then counted automatically (Biotran II) and background lawn evaluated by stereomicroscope. Positive control compounds were: -S9, 2-nitrofluorene (2-NF, 20µg/plate) for TA98 and TA1538; N-methyl-N'-nitro-N-nitrosoguanidine (MNNG, 2.0µg/plate) for TA100 and TA1535; 9-aminoacridine (9-AA, 25µg/plate) for TA1537; +S9 2-aminoanthracene (2µg/plate) for all strains except TA1537.
Results	
Genotoxic effects	The preliminary toxicity test exhibited severe toxicity at 10µl/plate with activation and at 3.1 and 10µl/plate without activation (individual data not shown). In the mutagenicity test, none of the 5 strains of Salmonella exhibited revertant frequencies substantially different from the solvent or spontaneous controls at any dose level with or without metabolic activation (e.g. TA98-S9: 16, 15, 12, 12, and 0 average revertants/plate and TA100-S9: 111, 115, 107, 94, and 0 at 0[DMSO], 0.029, 0.094, 0.30, and 0.97µl/plate, respectively: TA98+S9: 33, 26, 26, 22, and 0 revertants/plate, and TA100+S9: 128, 161, 128, 118, and 0 revertants/plate at 0[DMSO], 0.094, 0.30, 0.97 and 3.1µl/plate, respectively). Clearing of background lawn and microcolonies were observed at the maximum doses (0.97µl/plate-S9; 3.1µl/plate+S9). Positive control compounds (2 plates/strain) performed

	appropriately (-S9: MNNG 1906, 1883 revertants/plate in TA 100 and TA1535, respectively; 9-AA 586 revertants/plate in TA1537; 2-NF 2114, 1214 revertants/plate in TA98 and TA1538, respectively; and +S9 2- aminoanthracene 406-2307 revertants/plate for all strains except TA1537). The results of this assay indicate that rerun tower overheads had no mutagenic activity in this test system. (Reviewer's note: Due to toxicity, tests were performed over a low dose range; 3 of 4 doses were non-toxic and showed sufficient growth to evaluate mutagenicity. Testing at any lower doses was impractical).
Conclusions (contractor)	Rerun Tower Overheads did not induce an increase in revertant colonies in any Salmonella strain, tested at any dose level with or without metabolic activation in this single Ames test.
Data Quality *Reliabilities*	**1.** Reliable without restriction
Reference	Blackburn, G.R. 1981. An Ames Salmonella/mammalian microsome mutagenesis assay for the determination of potential mutagenicity of Rerun Tower Overheads from an olefins/aromatics plant. Study No. 1781-80. Mobil Environmental and Health Sciences Laboratory, Princeton, NJ. Ames B. N. et al. 1975. Mutat. Res. 31: 347-364.
Other *Last changed*	10/02/2001 (Prepared by a contractor for the Olefins Panel)

Robust Summary - Group 5: High Benzene Naphthas

Genetic Toxicity - in Vitro

Test Substance	**Rerun Tower Overheads** from Olefins/Aromatics Plant (light thermal cracked naphtha) CAS # 64741-74-8. Straw colored liquid; 40% benzene, 26% C5, 13% toluene, 20% other. Test substance is described as a sample of a Pyrolysis Gasoline distillate fraction and is similar to Pyrolysis gasoline, a stream included in the test plan.
Test substance	
Method	
Method/guideline followed	None specified. Standard method based on Slater et al., 1971, Green and Muriel, 1976, and Ames et al., 1973.
Type	Bacterial DNA repair
System of testing	Escherichia coil, Salmonella typhimurium
GLP	Not specified
Year	1978
Species/Strain	*E. coli* WP2 uvrA^{+} recA^{+}, WP100 uvrA^{-} recA^{-}; *S. typh*. TA1978 uvrB^{+}, TA1538 uvrB^{-}
Metabolic activation	Yes
Species and cell type	Sprague Dawley male rat liver (S9 fraction)
Quantity	50µl S9 fraction in 1.0ml S9 mix/plate
Induced or not induced	Aroclor 1254 induced (single ip injection of 500mg/kg, 5 days prior to sacrifice)
Concentrations tested	Spot test: 10µl/plate undiluted
Statistical Methods	None. Compounds that cause damage to DNA will more severely affect repair deficient strains than repair proficient stains. Toxic compounds that do not affect DNA will not induce differential toxicity.
Remarks for Test Conditions	Tester strains were stored in liquid nitrogen and fresh cultures were inoculated directly from frozen stock, grown overnight at 37^{0}C, re-diluted and grown to final cell concentration of 2x10^{8} cells/ml. Each test article-strain combination was plated in triplicate with and without metabolic activation. Log phase cultures (0.1ml) added to 2.5ml top agar were poured on Vogel-Bonner minimal medium plates. For plates without activation, a 6.5mm paper disc (antibiotic type) was placed in the center of each plate; 10µl test article is placed on disc. For plates with S9 activation, after top agar sets, a 9.5mm diameter hole was cut in agar in the center of the plate, the well was sealed with 0.1ml top agar, and 150µl of S9 mix/control or test article mix (14:1) added to the well. All inverted plates were incubated at 37^{0}C for 24hr. The diameter of any resulting zone of inhibition was measured in mm. Zone diameter of a repair deficient strain was divided by the zone diameter of the repair proficient parent strain. Positive control compounds were 4-nitro-quinoline-1-oxide (4-NQO; 30µg/plate) –S9, 2-aminofluorene (2-AF; 250µg/plate) +S9, and negative control was 25µg/plate penicillin. Tests were performed twice ± S9.
Results	
Genotoxic effects	In duplicate tests, average inhibition ratios induced by Rerun tower overheads –S9 were 1.4, 1.8 for *E. coli* WP100/WP2, and 1.3, 1.5 for *S. typh*. TA1538/TA1978 compared to negative control values of 1.0, 1.1, and 1.1, 1.2 in *E coli* strains and *S. typh*. strains, respectively, suggesting a weak differential killing of repair deficient strains without metabolic activation. Positive control ratios for 4-NQ –S9 were 2.3, 2.5 for *E coli* WP100/WP2, and 1.7, 1.6 for *S. typh*. TA1538/TA1978. In tests with metabolic activation (+S9), average inhibition ratios were 1.0, 1.0 for *E.coli* strains and 1.0, 1.0 for *S. typh*. strains in duplicate tests compared to negative control values of 1.1, 1.1, and 1.1, 1.1 in *E. coli* and *S. typh*. strains, respectively, indicating no test article induced toxicity. Positive control, 2-AF, inhibition ratios were 2.1, 2.1 for *E. coli* WP100/WP2, and 1.9, 1.4 for *S. typh*. TA1538/TA1978.

Conclusions (contractor)	Rerun tower overheads did cause weak differential killing in DNA repair deficient strains, *E. coli* WP100 and *S. typhimurium*. TA1538 in the absence of metabolic activation, suggesting that the test article can cause direct acting damage to bacterial DNA. No differential killing was observed in the presence of metabolic activation.	
Data Quality *Reliabilities*	**1.** Reliable without restriction	
Reference	Haworth, S.R. 1978. Bacterial DNA repair assay of Mobil Chemical Company Compound MCTR-125-78 (MRI #110). E. G. and G. Mason Research Institute, Rockville, MD. for Mobil Chemical Co, Edison, NJ Slater, E.E. et al. 1971. Cancer Res. 31: 970-973. Green, M.H.L. and Muriel, W.J. 1976. Mutat. Res. 38:3-32 Ames, B.N. et al. 1973. Proc. Natl. Acad. Sci., USA 70: 782-786.	
Other *Last changed*	2/28/2002 (Prepared by a contractor to the Olefins Panel)	

Robust Summary: High Benzene Naphthas

Genetic Toxicity - in Vitro

Test Substance	**Rerun Tower Overheads** from Olefins/Aromatics Plant (light thermal cracked naphtha) CAS # 64741-74-8. Straw colored liquid; 40% benzene, 26% C5, 13% toluene, 20% other. Test substance is described as a sample of a Pyrolysis Gasoline distillate fraction and is similar to Pyrolysis gasoline, a stream included in the test plan.
Test substance	
Method	
Method/guideline followed	Standard method, no guideline specified
Type	Cell transformation
System of testing	Mouse embryo cells
GLP	Yes
Year	1981
Species/Strain	BALB-c/3T3 mouse cell line
Metabolic activation	No
Species and cell type	NA
Quantity	NA
Induced or not induced	NA
Concentrations tested	Initial cytotoxicity: 0, 0.01, 0.1, 1.0, 10.0, 100.0µg/ml medium; Transformation: 0. 0.8, 4.0, 20.0 and 100µg/ml, diluted in dimethyl sulfoxide. Negative control was DMSO at 2.5% vol. concentration.
Statistical Method	T-test specified. Standard criteria for positive response is a two fold increase in type III foci at highest dose over vehicle control with or without a dose related response or a 2 fold increase at 2 or more consecutive doses.
Remarks for Test Conditions	Routine procedures were referred to Appendix 1 Standard Operating Procedures, which was not included with this report. Only specifics unique to this assay are presented. Due to the volatile nature of test material, the cytotoxicity assay and transformation assays were conducted in tightly capped T-25 flasks in sealed plastic bags. The pH of medium during the 72hr exposure period was maintained at 7.4 by 0.02M Hepes buffer in flasks. RTO was prepared as a 1% stock solution in DMSO, which, when added to culture medium at a 2.5% vol. conc. was a suspension. Despite limited solubility, RTO produced a dose-dependent cytotoxic effect after a 3-day exposure period. In the initial toxicity assay, RTO was added to flasks, seeded with BALB-c/3T3 cells, at concentrations of 0, 0.01, 0.1, 1.0, 10.0 and 100.0µg/ml, incubated for 3 days at 37^0C in a CO_2 in air incubator, after which cells were counted for survival. In the transformation assay, RTO was tested at 0, 0.8, 4.0, 20.0 and 100µg/ml. In a standard BALB-c/3T3 transformation assay, colony formation cultures (approx. 100 cells/culture) and transformation cultures (approx. 10^4 cells/culture, 20 cultures/dose) were seeded on day 1, exposed to test material for 2-3 days, and culture medium was changed on day 4. For transformation cultures, medium continued to be changed weekly to day 29. Colony formation cultures were fixed, stained and counted visually on day 8 to determine cloning efficiency; transformation cultures were fixed and stained on day 29 for focus counting and evaluation. Transformation frequency = total type III foci ÷ total cultures/dose. Positive control compound was 3-methyl cholanthrene (2µg/ml).
Results	
Genotoxic effects	RTO induced toxicity in BALB-c/3T3 cells after 3 days exposure at concentrations of 10µg/ml (59% viability) and at 100µg/ml (18% viability). In the transformation assay, inhibition of cloning efficiency (CE, clones/100 cells) occurred at 4.0µg/ml (89% CE), 20.0µg/ml (81% CE) and 100µg/ml (65% C.E.); cell toxicity was

	somewhat less than in the initial cytotoxicity assay [40% viability at 100µg/ml]. RTO did not induce statistically significant increased incidence of transformed foci compared to negative controls at any dose level. Values were 0.10 foci/flask, 2/20 flasks with foci at 100µg/ml, 0.0 foci/flask, 0/20 flasks with foci at 20.0µg/ml, 0.15 foci/flask, 3/20 flasks with foci at 4.0µg/ml, 0.10 foci /flask, 2/20 flasks with foci at 0.8µg/ml compared to 0.05 foci/flask, 1/20 flasks with foci in negative control group. [Reviewer's note: Negative control value of 1 focus/20 flasks was lower than control values in other concurrent studies on 2 other compounds in this series where negative controls had 4 foci in 20 flasks (0.20 foci/flask)]. Positive control compound, 3 methyl cholanthrene, induced 56 foci/19 flasks (2.95 foci/flask), 18/19 flasks with foci.
Conclusions (contractor)	Rerun tower overheads did not induce neoplastic transformation in BALB-c/3T3 cells and was not active in this test system.
Data Quality *Reliabilities*	**2**. Reliable with restrictions. Complete details of assay methods are not included in the report. Specifics of statistics are not supplied.
Reference	Tu, A.S. and Sivak, A. 1981. BALB-c/3T3 Neoplastic transformation assay on 0818802, 08188003 and 08188005 (Rerun tower overheads). ALD Ref. #86374. Arthur D. Little, Inc. Cambridge, MA for Mobil Oil Corp, Study #1771-80, Princeton, NJ Roy, T.A., 1981. Analysis of rerun tower bottom oil by combined capillary gas chromatography/mass spectrometry. Study #1272-81-. Toxicology division, Mobil Oil Co., Princeton, NJ
Other *Last changed*	12/07/01 (Prepared by a contractor to the Olefins Panel)

Robust Summary: High Benzene Naphthas

Genetic Toxicity - in Vitro

Test Substance	**Rerun Tower Overheads** from Olefins/Aromatics Plant (light thermal cracked naphtha) CAS # 64741-74-8. Straw colored liquid; 40% benzene, 26% C5, 13% toluene, 20% other. Test substance is described as a sample of a Pyrolysis Gasoline distillate fraction and is similar to Pyrolysis gasoline, a stream included in the test plan.
Test substance	
Method	
Method/guideline followed	None specified. Standard method based on Clive and Spector, 1975
Type	Mammalian cell mutation assay
System of testing	Mouse lymphoma cells
GLP	Not specified
Year	1979
Species/Strain	Mouse lymphoma L5178Y TK+/- cells
Metabolic activation	Yes
Species and cell type	Sprague Dawley males rat liver (S9 fraction)
Quantity	50µl S9 fraction/ml S9mix)
Induced or not induced	Aroclor 1254 induced (single ip injection of 500mg/kg, 5 days prior to sacrifice)
Concentrations tested	-S9 cloned doses: 0.0, 0.013, 0.018, 0.024, 0.032, 0.042, 0.056, 0.075, and 0.10µl/ml +S9 cloned doses: 0.0, 0.048, 0.063, 0.085, 0. 11, 0.15, 0.20, 0.27, and 0.36µl/ml. All doses diluted in acetone
Statistical Methods	None. Compound was designated as mutagenic if it induced a mutation frequency (mutant cells/10^4 surviving cells) greater than 3 times the standard error (S.E. [f]) calculated by formula from the viable counts and total mutant cells (trifluorothymidine resistant cells) at each dose level.
Remarks for Test Conditions	Freshly prepared actively growing cultures of L5178Y cells ($1x10^6$ cells/ml) were dispensed in 6ml aliquots into 44 polypropylene centrifuge tubes. Rerun tower overheads, solubilized in acetone, beginning at a concentration equal to LD90 from a preliminary toxicity test, was diluted over 15 serial 1/8 log dilutions, producing 16 dose levels decreasing approximately 100 fold from highest to lowest, and added to cells in the centrifuge tubes. Four ml of S9 activation mixture or 4ml culture medium was added, yielding a final cell suspension of $0.6x10^6$ cells/ml. Positive control compounds were ethyl methyl sulfonate (EMS, 1.0µl/ml) –S9 and 7,12-dimethylbenzanthracene (7,12-DMBA, 2.5µl/ml) +S9 cultures. All tubes were gassed with 5% CO2/air and placed on a roller drum for 4hrs at 37^0C in the dark. At the end of exposure, calls were washed with fresh medium, re-suspended, gassed, replaced on roller drum at 37^0C and incubated for 3 days with a cell population adjustment every 24 hrs to maintain a cell population density of $0.3x10^6$ cells/ml. After 3 days expression, 8 cultures ± S9, which exhibited toxicity from 10-90% growth inhibition during the expression period, were selected for cloning. At cloning, cells were placed in restrictive suspension medium containing trifluorothymidine (TFT, 1µg/ml) that allows only TK-/- cells to grow. Two Florence flasks/concentration ± S9, one for restrictive medium, on for viable cell counts, were filled with 100ml cloning medium and maintained at 37^0C. Six 100mm petri plates/concentration ± S9 were prepared, 3 for restrictive medium, 3 for viable cell counts. Cell counts were made from each centrifuge tube to determine the volume of cell population = $3x10^6$cells. This volume was retained, centrifuged and the supernatant discarded except for 2ml in which cells were re-suspended and placed in restrictive medium flask. A $5x10^{-4}$ dilution was prepared and added to the appropriate viable count flask containing 100ml cloning medium. After this dilution, 1 ml of TFT stock solution was added to the restrictive medium flask and incubated

	with shaking (125rpm) at 37^{0}C for 15min. Flasks were removed, 33ml of cell suspension was pipetted into each of 3 appropriately labeled plates and placed in the cold (4^{0}C) for 20 min to accelerate gelling. Plates were removed and incubated at 37^{0}C in humidified 5% CO2/air for 10 days. At the end of incubation, plates were scored for total number of colonies/plate, 3 counts/plate, on an automated colony counter. Mutation frequency (MF) = avg. number of colonies in 3 restrictive medium plates ÷ avg. number of colonies x10^4 in 3 corresponding viable count plates. Induced mutation frequency (IMF) = MF test article – MF solvent control.
Results Genotoxic effects	In cultures without metabolic activation, the two highest concentrations cloned, 0.10µl/ml (MF=1.4, IMF=0.8) and 0.075µl/ml (MF=1.0, IMF=0.4) exhibited slight dose related increases in IMF compared with acetone control (MF=0.6); only the 0.10µl/ml concentration caused a doubling of MF over controls. EMS positive control values were MF=27.1, IMF=26. The first activated assay was discarded due to loss of positive control cultures by contamination. In the repeat test with metabolic activation, 2 dose concentrations had MF 2 times greater than acetone controls: the highest dose cloned, 0.36µl/ml (MF=0.8, IMF=0.4) and 0.15µl/ml, the 4th highest dose cloned (MF=0.9, IMF=0.5) versus control (MF=0.4). However, intervening cloned doses of 0.20, and 0.27µl/ml did not show increased MF; the values for the positive doses were not dose related and were within the range of experimental error for the assay. Positive control values +S9 for 7,12- DMBA were MF=2.6, IMF=2.0.
Conclusions (contractor)	Without metabolic activation, Rerun tower overheads appears to induce a weak mutagenic response at the two highest doses only; a dose response trend was not observed in the 6 lower doses cloned. Test article did not induce significant mutagenic activity in cultures containing S9, suggesting that any mutagenic activity is suppressed or inactivated by the presence of the liver microsome metabolizing system.
Data Quality *Reliabilities*	**1.** Reliable without restriction.
Reference	Kirby, P.E. et al., 1979. An evaluation of mutagenic potential of MCTR-125-78 (MRI #110) employing the L5178Y TK+/- mouse lymphoma assay. E.G. and G. Mason Research Institute, Rockville, MD for Mobil Chemical Co., Edison, NJ Clive, D., and Spector, J.F.S. 1975. Mutat. Res. 31: 17-29
Other *Last changed*	2/28/2002 (Prepared by a contractor to the Olefins Panel)

Robust Summary: High Benzene Naphthas

Genetic Toxicity - in Vitro

Test Substance	**Rerun Tower Overheads** from Olefins/Aromatics Plant (light thermal cracked naphtha) CAS # 64741-74-8. Straw colored liquid; 40% benzene, 26% C5, 13% toluene, 20% other. Test substance is described as a sample of a Pyrolysis Gasoline distillate fraction and is similar to Pyrolysis gasoline, a stream included in the test plan.
Test substance	
Method	
Method/guideline followed	None specified. Standard method based on Bertram, 1977
Type	Mammalian cell transformation assay
System of testing	Mouse C3H embryo cells
GLP	Not specified
Year	1978
Species/Strain	Mouse embryo cells/ C3H 10T½
Metabolic activation	No
Species and cell type	NA
Quantity	NA
Induced or not induced	NA
Concentrations tested	0, 0.625, 1.25, 2.5 and 5.0µl/ml, all diluted in acetone
Statistical Methods	None. A positive response is determined by the appearance of any type II foci (50% can be malignantly transformed) and type III foci (85% can be malignantly transformed) compared to negative controls. The C3H 10T½ cell line has no spontaneous transformation.
Remarks for Test Conditions	For the preliminary toxicity assay, cells (200/plate) were exposed to Rerun tower overheads diluted in acetone, over a range of concentrations from 0.0003-5.0µl/ml, at 2-fold dilutions for 18hrs; cells were then washed, re-fed with fresh Eagle's basal medium and incubated for 10 days in 5% CO2/air at 37^0C. After incubation, cells were washed, fixed with absolute methanol (20 min) and stained with Giemsa (30 min); number of cells/plate were counted and cloning efficiency (CE) determined=Avg. number colonies/plate ÷ number cells plated x100. In the transformation assay, cells in late log phase were plated at a concentration of $1x10^3$ cells/60mm petri dish. Cultures for concurrent toxicity determination were prepared at 200 cells/plate. After 24 hrs, cultures were treated with appropriate test article concentrations in 25µl volumes at 4 dose levels, 12 plates/dose, in decreasing 2-fold dilutions from concentrations which exhibit 25-75% relative CE. Positive control compound was 7, 12-dimethylbenzanthracene (7, 12-DMBA, 0.5µg/ml). After 18hr treatment, test article was removed, cultures were re-fed, and re-incubated. Toxicity plates were incubated for 10 days, stained and CE determined. Transformation cultures were re-fed weekly until 35 days after removal of test article had elapsed. All plate cultures were washed, fixed, stained and scored for the presence of type II and type III foci by macroscopic and microscopic examination. Type II foci show massive piling up in virtually opaque monolayers, cells are moderately polar. Type III foci are composed of highly polar, fibroblastic, multilayered, criss-crossed arrays of densely stained cells.
Results	
Genotoxic effects	Rerun tower overheads induced 71% relative cloning efficiency at 5.0µl/ml; transformation assay was performed at 2-fold dilutions from 5.0µl/ml. In the toxicity study conducted in parallel with the transformation assay, test article induced 100% cell death at 5.0µl/ml. In the transformation assay, sufficient cells survived to form a confluent layer in 8/12 plates at 5.0µl/ml dose level after 35 days. No indication of type II or type III foci were induced by rerun tower overheads at any dose level. Positive control, 7,12-DMBA induced 9 type II and

	12 type III foci on 12 plates.
Conclusions (contractor)	Rerun tower overheads does not induce cell transformation in mouse embryo C3H 10T½ cells.
Data Quality *Reliabilities*	**1.** Reliable without restriction
Reference	Jensen, E.M., and Thilager, A.K. 1978. C3H 10T½ cell transformation assay, Mobil Chemical Co. Compound MCTR-125-78 (MRI #110). E.G. and G. Mason Research Institute, Rockville, MD Bertram, J.S. 1977. Cancer Res. 37: 514-523
Other *Last changed*	2/28/2002 (Prepared by a contractor to the Olefins Panel)

Robust Summary - Group 5: High Benzene Naphthas

Genetic Toxicity - in Vivo

Test Substance	
Remarks	**Rerun Tower Overheads** from Olefins/Aromatics Plant (light thermal cracked naphtha) CAS # 64741-74-8. Straw colored liquid; 40% benzene, 26% C5, 13% toluene, 20% other. Test substance is described as a sample of a Pyrolysis Gasoline distillate fraction and is similar to Pyrolysis gasoline, a stream included in the test plan.
Method	
Method/guideline followed	None specified. Standard method based on Bowman, 1969; Lewis, 1954; Mendelson, 1976
Type	*Drosophila* assays for point mutation, chromosome aberrations & chromosome loss
GLP	Not specified
Year	1979
Species	Drosophila melanogaster
Strain	Dominant lethal: Canton S; Y chromosome loss: males red/white eye; females white/white eye; Somatic reversion: males white ivory ($\underline{w^i}$), yellow body ($\underline{y}$), echinus ($\underline{ec}$); females $\underline{w^i}/\underline{w^i}$; Bithrox test: males Ultrabithorax ($\underline{Ubx}$); females bithorax ($\underline{bx^{34e}}$); Sex-linked recessive lethal: males Canton S; females $\underline{Basc}/\underline{Basc}$
Sex	Males and females
Route of administration	Aerosol
Doses/concentration levels	0.3ml in 50ml air
Exposure period	10 min.
Statistical methods	Events in these tests have very low probabilities. Analysis based on Poisson distribution with fiducial limits computed according to Stevens, 1942.
Remarks for Test Conditions.	*Drosophila* stocks were maintained in agar/corn meal/sugar/yeast medium at 23^0C. One set of stocks was transferred each week to isolate virgin females for breeding. Four days are required for maturation of *Drosophila* sperm cells after meiosis. In all assays, treated males were mated for 3 days only to assure use of a uniform sample of treated sperm. In all assays, test article was administered as an aerosol, 0.3ml in 50ml volume of air.when administered for 1hr anesthesized flies and killed approximately 30%. Longer treatments reduced fertility. Exposure in all assays was 10 minutes in duration. Somatic reversion of white-ivory: Larvae from mating of males carrying 5 copies of white-ivory gene on the X chromosome ($\underline{w^i}$, $\underline{y}$, $\underline{ec}$) with $\underline{w^i}/\underline{w^i}$ females were treated with aerosolized test article for 10 min. Positive control compound was 0.04M mitomycin C. Larvae were washed and transferred to culture bottles to complete development. After eclosion, female offspring, genotype Qn(1)$\underline{w^i}$, $\underline{y}$, $\underline{ec}/\underline{w^i}$ were scored for red spots in the eye, which signals reversion of $\underline{w^i}$ to a pigment cell. Y chromosome loss: Males carrying a duplication of the gene for normal (red) eyes on Y chromosome and a mutant allele, white ($\underline{w}$) on the X chromosome were treated with aerosolized test article for 10 min and mated to white-eyed females ($\underline{w}/\underline{w}$). Positive control were males exposed to 3kr X-rays. Frequency of occurrence of white-eyed male progeny measured frequency of Y chromosome loss. Dominant lethal mutations: Defined as any genetic change that blocks development prior to hatching. Treated Canton S males were mated with untreated females in nylon net cages on Welch's grape juice solidified with 2% agar. After 12 hr, agar plates were removed and stored at room temp. (23^0C) for 30 hrs. Positive control was 0.04M ethyl methane sulfonate. Eggs were scored for hatching after 30hrs.

	Bithorax test of Lewis: Occurrence of rearrangements with one breakpoint between centromere and the locus of bithorax (bx) was determined by scoring offspring of treated Ultrabithorax males and bithorax females. Males treated with 3kr X-rays were the positive controls. Distinctive phenotype was the presence of a mesonotum Sex-linked recessive lethals: Canton-S males, treated with test article, were mated with Basc (balancer X chromosome) females. Individual (F1) female progeny were mated with Basc males. Any single female culture containing at least 20 flies (F2), at least 8 of which are males, but no males are wild type, is scored as a lethal. Ethyl methane sulfonate (0.04M) treated males were the positive controls. A repeat study was performed due to loss of cultures to dessication.
Results Genotoxic effects NOAEL (NOEL) LOAEL (LOEL)	Rerun tower overheads did not induce genetic damage in *Drosophila melanogaster* under experimental conditions in any test employed. The repeated sex-linked recessive lethal test, performed due to technical problems in the initial assay, did not demonstrate any genetic damage in *Drosophila* from exposure to the test article
Conclusions (study authors)	Rerun tower overheads did not induce genetic damage in *Drosophila melanogaster*.
Data Quality *Reliabilities*	**1.** Reliable without restrictions.
References	Bowman, J.T. 1979. *Drosophila* mutagenicity assays of Mobil Chemical Compound MCTR-125-78. MRI #110. E.G. and G. Mason Research Institute, Rockville, MD, for Mobil Chemical Co., Edison, NJ. Bowman, J.T. 1969. Mutat. Res. 7: 409-415 Lewis, E.B. 1954. Am. Nat. 88: 225-239 Mendelson, D. 1976. Mutat. Res. 41: 269-276 Stevens, W.L. 1942. J. Genetics 43: 301-307
Other *Last changed*	2/28/2002 (Prepared by a contractor to the Olefins Panel)

Robust Summary: High Benzene Naphthas

Repeated Dose Toxicity

Test Substance	**Rerun Tower Overheads** from Olefins/Aromatics Plant (light thermal cracked naphtha) CAS # 64741-74-8. Straw colored liquid; 40% benzene, 26% C5, 13% toluene, 20% other. Test substance is described as a sample of a Pyrolysis Gasoline distillate fraction and is similar to Pyrolysis gasoline, a stream included in the test plan.
Remarks	
Method	
Method/guideline followed	None specified, comparable to standard methods
Test type	Subacute
GLP	Not specified
Year	1980
Species	Rabbit (4/sex/group)
Strain	New Zealand White
Route of administration	Dermal
Duration of test	21 days
Doses/concentration levels	0, 0.1, 0.5, and 1.0ml/kg/day
Sex	Male and females
Exposure period	Continuous (no wipe-off)
Frequency of treatment	Once/day
Control group and treatment	Males and females (4M, 4F), saline (0.9%), 1ml/kg/day
Post exposure observation period	3 days
Statistical methods	Bartletts test, analysis of variance, Scheffe's multiple pair wise comparison, Gaines and Howell's multiple pair wise comparison
Test Conditions	Rabbits were housed individually in stainless steel cages and received water and rabbit chow diet, ad lib. Initial body wt ranged from 2455-3005g for males and 2455-3035g for females. Four rabbits of each sex were assigned to treatment groups of 0, 0.1, 0.5, and 1.0ml of neat test article/kg/day. Control rabbits received 1.0ml/kg/day of 0.9%NaCl. Prior to initiation, the dorsal dosing area was clipped free of hair and clipping was done periodically during the study. The exposure area was abraded with minor incisions deep enough to penetrate the stratum corneum but not deep enough to produce bleeding. Abrasions were made prior to the first application, and thereafter, on the first day of each week. Test article was applied to the skin once a day, starting on day 1, for 21 consecutive days; rabbits were sacrificed between day 22 and day 24. Each rabbit wore a plexiglass collar for the entire study to retard ingestion of test article. Rabbits were observed daily for mortality and moribundity, food/water intake, general appearance/behavior, toxic/pharmacological effects, and dermal reactions for 24 consecutive days. Dermal irritation was graded each morning prior to dosing. Food consumption was determined 3 times /wk and body weight on days1, 8, 15, and at termination. Prior to study initiation and during wk 3, hematocrit (Hct), hemoglobin (Hgb), erythrocyte count (RBC), total leukocyte count (WBC) and differential leukocyte count, mean cell volume (MCV), mean corpuscular hemoglobin (MCH), mean corpuscular hemoglobin conc. (MCHC), serum glutamate pyruvate transaminase (SGPT), serum glutamate oxaloacetate transaminase (SGOT), alkaline phosphatase (Alk Phos), fasting glucose, and blood urea nitrogen (BUN); urine (pH, specific gravity, glucose, ketones, total protein, bilirubin[BIH]), and microscopic examination of sediment were evaluated. Rabbits were sacrificed on day 24; necropsies were performed and gross observations recorded for all rabbits. Liver, kidney, thyroid, and adrenals were weighed and preserved for microscopic analysis along with brain, pituitary, lung, heart, spleen, pancreas, urinary bladder, testis/ovary, skin, and any unusual lesions.

Results	
NOAEL (NOEL) LOAEL (LOEL) Remarks	NOAEL <0.10ml/kg/day both sexes (skin irr). LOAEL = 0.1ml/kg/day both sexes (skin irr) NOAEL = 1.0ml/kg/day both sexes (systemic effects). LOAEL >1.0ml/kg/day both sexes (systemic effects). Two rabbits died during the study from cardiac puncture blood sampling. No test article induced effects were noted during clinical observations. Two 0.1ml/kg/day group males and one female showed erythema from day 10 to termination; 3 0.5ml/kg/day group males showed erythema from day 8 to termination; all 0.5ml/kg/day males and females, and 1.0ml/kg/day males and females had well defined erythema from day 9 to termination. Edema was not present in any rabbits. Skin thickening was noted in all test article groups from wk 1 to termination. Fissuring was seen in 3 0.1ml/kg/day males, 3 0.5ml/kg/day males and all 1.0ml/kg/day males; all test article treated females showed fissuring. Necrosis was present in 2males and 3 females given 0.1ml/kg/day, 3males and all females given 0.5ml/kg/day, and all males and females given 1.0ml/kg/day. There were no significant changes in body wt or food consumption between controls and treatment groups. Terminal basophilic values were elevated in all male test article treated groups; all other hematology values were comparable to controls. Urinalysis findings were unremarkable. There were no significant differences in organ wt between control and any treatment group. Histological evaluation for the skin showed effects consistent with gross observations with no dose-related gradation of severity between doses, including hyperkeratosis, acanthosis, accumulation of heterophils, and cellular debris in stratum corneum, and hyperplasia of sebaceous glands. There were no abnormal microscopic findings attributable to test article administration in organs from the three treatment levels compared to controls.
Conclusions (study authors)	Daily epidermal application of test article resulted in skin irritation at the application site.
Quality Reliabilities	**2.** Reliable with restriction. There was no mention of GLP.
References	Fieser, S., Alsaker, R.D., Brown, H.R., and Wolfe, G.W. 1980. 21-Day dermal irritation study in rabbits. Proj. #230-213. Hazleton Laboratories America, Inc., Vienna, VA. For Mobil Chemical Co., Edison NJ (This study was actually for subacute toxicity, not only skin irritation)
Other Last changed	2/28/2002 (Prepared by a contractor to the Olefins Panel)

Robust Summary: High Benzene Naphthas

Developmental Toxicity/Teratogenicity

Test Substance	**Rerun Tower Overheads** from Olefins/Aromatics Plant (light thermal cracked naphtha) CAS # 64741-74-8. Straw colored liquid; 40% benzene, 26% C5, 13% toluene, 20% other. Test substance is described as a sample of a Pyrolysis Gasoline distillate fraction and is similar to Pyrolysis gasoline, a stream included in the test plan.
Remarks	
Method	
Method/guideline followed	None specified, conforms to standard method
Test type	Teratology
GLP	Yes
Year	1981
Species	Rabbit
Strain	New Zealand White
Route of administration	Oral gavage
Concentration levels	0, 10, 25, and 50mg/kg/day, diluted in corn oil
Sex	Pregnant females (16/group)
Exposure period	Day 6-28 of gestation
Frequency of treatment	Once/day
Control group and treatment	16 pregnant females received 0.5ml/kg/day corn oil
Duration of test	29 days
Statistical methods	Chi square with Yates' correction for 2x2 contingency table and /or Fisher's exact probability test; Mann-Whitney U test; analysis of variance (one-way), Bartlett's test and t-test using Dunnett's multiple comparison tables. Level of significance $p<0.05$.
Remarks for Test Conditions.	In an initial study, RTO was administered by oral gavage, undiluted to 16 pregnant rabbits/group at levels of 0 (distilled water), 10, 25 and 50 mg/kg/day. Forty-two rabbits died: 14, 11, 13, and 13 in the 0, 10, 25 and 50mg/kg/day groups respectively. Due to excess mortality in all treated groups and the controls, the study was terminated and repeated at the same concentrations diluted in corn oil. Sixty-four sexually mature virgin female rabbits (7 months old, 3.46-4.19kg at study initiation) were acclimated for 59 days, assigned a unique animal number and ear-tagged when placed on study. All rabbits were individually housed in suspended wire cages and maintained in a temperature, humidity, and light (12 hr light/dark cycle) controlled environment. Certified rabbit chow and tap water were available ad lib. Only coccidiosis-free rabbits were used in the study. Prior to insemination, females were randomly assigned to groups (16/group) according to body wt, by a computer-generated program. Sperm was collected from each of 6 proven breeder males of the same source and strain, using an artificial vagina. Semen was immediately evaluated for motility, and was used for insemination only if motility was≥50%. Useable ejaculate was diluted in 0.9%NaCl at 35^0C; 0.25-0.50ml of dilute semen was introduced into the anterior vagina. Ovulation was induced by injection of 100 units chorionic gonadotropin (Ayerst, NY) in the marginal ear vein of the female immediately after insemination. Semen from one male was used to inseminate an equal number of females in each group. Inseminations were performed on two consecutive days; an equal number of females was inseminated in each group/day, designated as day 0 of gestation. RTO was mixed with corn oil daily at appropriate doses and shaken by hand. No analysis of dosing solution was reported. Negative control dams were given 0.5ml corn oil/kg/day, the volume equal to the highest treatment group. Individual doses were determined from individual body wt on day 6 of gestation. Females

	were observed daily for mortality, overt changes in appearance and behavior, and, from day 6-29 of gestation, for clinical signs of toxicity. One dam aborted on gest. day 19 and remained on study until scheduled sacrifice; aborted material was discarded. Body wt was recorded on gestation days 0, 6, 12, 18, 24, and 29. On gest. day 29, all females were sacrificed by overdose of sodium pentabarbitol, uteri were excised and weighed prior to removal of fetuses. Number and location of viable and non-viable fetuses, early and late resorptions, number of total implantations, and corpora lutea were recorded. Abdominal and thoracic cavity and organs of dams were examined grossly and discarded. Uteri from apparently non-gravid animals were opened and placed in 10% ammonium sulfide solution to confirm pregnancy status. All fetuses were individually weighed and examined for external malformations and variations. Each fetus was internally sexed and examined for internal malformations and variations, including the brain by mid-coronal slice. The heart was dissected using Staples' technique. Eviscerated, skinned fetuses were individually numbered and tagged, fixed in alcohol, macerated and stained with Alizarin Red S for skeletal examination. Fetal findings were classified as malformations or genetic or developmental variations.
Results	
NOAEL maternal toxicity	NOAEL maternal = 25mg/kg/day (based on 1 abortion at 50mg/kg/day)
NOAEL developmental toxicity	NOAEL developmental = 50mg/kg/day; both values assigned by reviewer
Maternal effects	Maternal survival was 100% in all groups. Slight increase in matted haircoat (primarily in nasal region) and slight reduction in fecal material beneath cages was noted in 50mg/kg/day rabbits. Occasional instances of nasal discharge, soft stool, hair loss and scabbing were noted in all groups during gestation. One 50mg/kg/day rabbit aborted on day 19 of gestation. Maternal body wt in treated rabbits at all doses were comparable to controls throughout treatment (gest. day 6-28) and gestation (day 0-29) periods. Mean maternal adjusted body wt (minus gravid uterus) at termination in all groups was comparable to controls. Pregnancy ratio was 87.5, 81.3, 81.3, 93.8 in 0, 10, 25 and 50mg/kg/day groups, respectively. Two control dams and one 50mg/kg/day dam had all resorptions. There were no biologically or statistically significant differences in mean number of corpora lutea, total implantations, early or late resorptions, postimplantation loss, viable fetuses, fetal sex index, or mean fetal body wt in any RTO treated group compared to controls.
Embryo/fetal effects	Average litter size was 6.1, 6.5, 6.4, and 5.9 and average fetal body wt (both sexes) was 38.9, 43.0, 42.5, and 42.4g in 0, 10, 25, and 50mg/kg/day groups, respectively. There were no biologically or statistically significant differences in number of litters with malformations (external, soft tissue, skeletal) in any treated group compared to controls: 5/12 litters (85 pups), 1/13 litters (84 pups), 3/13 litters (83 pups) and 5/13 litters (82 pups examined) in 0, 10, 25, and 50mg/kg/day, respectively. In the 50mg/kg/day group, one occurrence of atlas-occipital anomaly and one occurrence of enlarged heart with great vessel anomaly, were observed in 2 separate litters. Scoliosis was present in all groups including control, with slightly higher incidence in the 50mg/kg/day group., but incidences were within the range of historical control data for this laboratory. Fetuses and litters with genetic or developmental variations were comparable in all groups.
Conclusions (study authors)	Rerun tower overhead did not produce a teratogenic response in pregnant New Zealand White rabbits when administered orally in corn oil vehicle at dose levels of 10, 25 and 50mg/kg/day. With the exception of one 50mg/kg/day female that aborted, minimal maternal toxicity was observed at any dose level.

Data Quality *Reliabilities*	**2.** Reliable with restrictions. Analysis of test article concentration in corn oil vehicle was not performed.
References	Schardein, J.L. 1981. Teratology study in rabbits: Rerun tower overheads (MRTC-171-79) IRDC #450-011. International Research and Development Corp., Mattawan, MI. for Mobil Petrochemicals Division, Edison, NJ
Other L*ast changed*	2/28/2002 (Prepared by a contractor to the Olefins Panel)