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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

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## **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.

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## **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 reformat 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 reformat 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 Hydrotreated 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 to 11% 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 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 Cyclohexene 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 <sup>59</sup>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).

## 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<sub>50</sub> = 347 to 820 mg/kg, inhalation LC<sub>50</sub> = 359 to >500 but < 1000 ppm). The oral LD<sub>50</sub> for cyclopentadiene was 1.66 g/kg and the LD<sub>50</sub>s for the other components were greater than 2 g/kg. The inhalation LC<sub>50</sub>s for the components other than dicyclopentadiene ranged from 3680 to 120,000 ppm. The two streams that were tested had oral LD<sub>50</sub>s greater than 2 g/kg and the one stream tested for acute inhalation toxicity had an LC<sub>50</sub> 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 Cycloidiene 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<sup>®</sup> 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<sup>-</sup>).

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<sup>-</sup> reaction rate constant, a 12-hr day, and a given OH<sup>-</sup> 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.

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

<b>CAS Number</b>	<b>CAS Number Description</b>
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).





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 embryoletality 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 <sup>1</sup> – 1990; HSDB <sup>2</sup> ; ATSDR – 1992 <sup>4</sup>

<sup>1</sup> IRIS: EPA Integrated Risk Information System

<sup>2</sup> 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 <sup>3</sup> ; ATSDR <sup>4</sup> - 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 <sup>5</sup> - 1999

<sup>3</sup> ECETOC: European Centre for Ecotoxicology and Toxicology of Chemicals

<sup>4</sup> ATSDR: U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry

<sup>5</sup> IARC: International Agency for Research on Cancer

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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 addressed 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 <u>With 50/50 blend of n-butane and n-pentane</u> , 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

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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 <sup>6</sup> , RTECS <sup>7</sup> , 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

<sup>6</sup> ACGIH: American Conference of Governmental Industrial Hygienists

<sup>7</sup> RTECS: Registry of Toxic Effects of Chemical Substances

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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 <sup>8</sup> – 1999; rat chrom. ab. report in HSDB <sup>9</sup>
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

<sup>8</sup> ATSDR: U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry

<sup>9</sup> 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 tetragenic	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] <sup>10</sup> ; EU Risk Assessment – 2000 [Draft]  Bamberger, 1996; Kreckman, 1997; Malley, 1996 a,b

<sup>10</sup> 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 <sup>11</sup> – 2000; IARC <sup>12</sup> – 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 <sup>13</sup> - 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 <sup>14</sup> ; ECETOC - 1986

<sup>11</sup> ATSDR: U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry

<sup>12</sup> IARC: International Agency for Research on Cancer

<sup>13</sup> ATSDR: U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry

<sup>14</sup> 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 <sup>15</sup> – 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 <sup>16</sup> – 1991  JETOC <sup>17</sup> Issue 3 No. 32, 1998 [CHL chrom. ab and OECD 422 studies]; NTP <sup>18</sup> [CHO chrom. ab.]

<sup>15</sup> IARC: International Agency for Research on Cancer

<sup>16</sup> ECETOC: European Centre for Ecotoxicology and Toxicology of Chemicals

<sup>17</sup> JETOC: Japanese Chemical Industry Ecology – Toxicology and Information Center

<sup>18</sup> 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 <sup>19</sup> – 1995; EU Risk Assessment Document – Draft 2001

<sup>19</sup> ATSDR: U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry

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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
<b>Streams</b>								
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.**

<b>CHEMICAL / PRODUCT</b>	<b>CARBON NUMBER</b>	<b>PERCENT BIODEGRADATION(a) (28 days)</b>	<b>REFERENCE</b>
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.**

<b>Naphtha, (Pet.) Light Alkylate</b>		<b>Naphtha, (Pet.) Light Catalytically Cracked</b>		<b>Naphtha, (Pet.) Light Catalytically Reformed</b>	
CAS#	Weight %	CAS#	Weight %	CAS#	Weight %
64741-66-8		64741-55-5		64741-55-5	
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	
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**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	<b>1-34</b>	<b>5-9</b>	<b>&gt;40-100</b>	<b>6-11</b>	<b>&gt;4-75</b>	<b>5-10</b>
Alkenes, C6 Rich	<b>100</b>	<b>5-7</b>	<b>0</b>	<b>-</b>	<b>0</b>	<b>-</b>
Alkenes, C7-9, C8 Rich	<b>100</b>	<b>7-9</b>	<b>0</b>	<b>-</b>	<b>0</b>	<b>-</b>
C8-C10 Aromatics, Predominantly C9 Aromatics	<b>0</b>	<b>-</b>	<b>&gt;97</b>	<b>8-10</b>	<b>&lt;3</b>	<b>-</b>
C8-C14 Aromatics, Predominantly Alkyl Naphthalenes and Naphthalene	<b>0</b>	<b>-</b>	<b>&gt;94</b>	<b>10-14</b>	<b>&lt;6</b>	<b>-</b>
Naphtha (petroleum), Light Alkylate (gasoline stream)	<b>0</b>	<b>-</b>	<b>0</b>	<b>-</b>	<b>92</b>	<b>5-8</b>
Naphtha (petroleum), Light Catalytically Cracked (gasoline stream)	<b>24</b>	<b>5-6</b>	<b>16</b>	<b>6-8</b>	<b>21</b>	<b>5-7</b>
Naphtha (petroleum), Light Catalytically Reformed (gasoline stream)	<b>0</b>	<b>-</b>	<b>38</b>	<b>6-7</b>	<b>50</b>	<b>5-7</b>

- 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	<i>Oncorhynchus mykiss</i>	LC50 = 4.3	IHSC*
n-Hexane	6	<i>Pimephales promelas</i>	LC50 = 2.5	IHSC*
Benzene	6	<i>Oncorhynchus mykiss</i>	LC50 = 5.9	****
Alkenes, C6 Rich	5-7(b)	<i>Oncorhynchus mykiss</i>	LL50 = 12.8	HOP**
Mixed Cycloparaffins, C7-8, C7 Rich	7	<i>Oncorhynchus mykiss</i>	LC50 = 5.4(c)	IHSC*
Toluene	7	<i>Pimephales promelas</i>	LC50 = 14.6	IHSC*
Alkenes, C7-9, C8 Rich	7-9(b)	<i>Oncorhynchus mykiss</i>	LL50 = 8.9	HOP**
o-Xylene	8	<i>Pimephales promelas</i>	LC50 = 16.4	IHSC*
p-Xylene	8	<i>Oncorhynchus mykiss</i>	LC50 = 2.6	IHSC*
p-Xylene	8	<i>Pimephales promelas</i>	LC50 = 8.9	IHSC*
Ethylbenzene	8	<i>Pimephales promelas</i>	LC50 = 12.1	IHSC*
Naphtha (Petroleum), Light Alkylate (gasoline stream)	5-8(b)	<i>Pimephales promelas</i>	LL50 = 8.2	API***
Naphtha (petroleum), Light Catalytically Cracked (gasoline stream)	5-8(b)	<i>Pimephales promelas</i>	LL50 = 46	API***
Naphtha (petroleum), Light Catalytically Reformed (gasoline stream)	5-7(b)	<i>Pimephales promelas</i>	LL50 = 34	API***
1,2,4-Trimethyl-benzene	9	<i>Pimephales promelas</i>	LC50 = 7.7	IHSC*
C8-C10 Aromatics, Predominantly C9 Aromatics	8-10(b)	<i>Oncorhynchus mykiss</i>	LL50 = 18.0	IHSC*
C8-C14 Aromatics, Predominantly alkyl Naphthalenes and Naphthalene	10-12(b)	<i>Oncorhynchus mykiss</i>	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	<i>Daphnia magna</i>	EC50 = 2.7	IHSC*
n-Hexane	6	<i>Daphnia magna</i>	EC50 = 2.1	IHSC*
Cyclohexane	6	<i>Daphnia magna</i>	EC50 = 0.9	IHSC*
Benzene	6	<i>Daphnia magna</i>	EC50 = 18(b)	***
o-Xylene	8	<i>Daphnia magna</i>	EC50 = 1.0	IHSC*
m-Xylene	8	<i>Daphnia magna</i>	EC50 = 4.7	IHSC*
Naphtha (Petroleum), Light Catalytically Reformed (gasoline stream)	5-7(c)	<i>Daphnia magna</i>	EL50 = 10	API**
Naphtha (Petroleum), Light Alkylate (gasoline stream)	5-8(c)	<i>Daphnia magna</i>	EL50 = 32	API**
Naphtha (Petroleum), Light Catalytically Cracked (gasoline stream)	5-8(c)	<i>Daphnia magna</i>	EL50 = 18	API**
C8-C10 Aromatics, Predominantly C9 Aromatics	8-10(c)	<i>Daphnia magna</i>	EL50 = 21.3	IHSC*
Naphthalene	10	<i>Daphnia magna</i>	EL50 = 16.7(d)	IHSC*
C8-C14 Aromatics, Predominantly Alkyl Naphthalenes and Naphthalene	10-12(c)	<i>Daphnia magna</i>	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.**

<b>CHEMICAL / PRODUCT</b>	<b>CARBON NUMBER</b>	<b>ORGANISM</b>	<b>AQUATIC TOXICITY (a) (72-hr, mg/L)</b>	<b>REFERENCE</b>
n-Pentane	5	<i>Pseudokirchneriella subcapitata</i> (b)	EbC50 = 10.7 ErC50 = 7.5 NOECb = 1.3 NOECr = 2.0	IHSC*
Benzene	6	<i>Pseudokirchneriella subcapitata</i>	EbL50 = 29	***
Naphtha (Petroleum), Light Catalytically reformed (gasoline stream)	5-7(c)	<i>Pseudokirchneriella subcapitata</i>	EbL50 = 8.5 NOELRb = 5.0	API**
Naphtha (Petroleum), Light alkylate (gasoline stream)	5-8(c)	<i>Pseudokirchneriella subcapitata</i>	EbL50 = 45 NOELRb = 18	API**
Naphtha (Petroleum), Light Catalytically Cracked (gasoline stream)	5-8(c)	<i>Pseudokirchneriella subcapitata</i>	EbL50 = 64 NOELRb = 51	API**
C8-C10 Aromatics, Predominantly C9 Aromatics	8-10(c)	<i>Pseudokirchneriella subcapitata</i>	EbL50 = 2.6 ErL50 = 2.9 NOELRb = 1.0 NOELRr = 1.0	IHSC*
C8-C14 Aromatics, Predominantly Alkyl Naphthalenes and Naphthalene	10-12(c)	<i>Pseudokirchneriella subcapitata</i>	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. <sup>1</sup>	Environmental Fate			
	Acute Toxicity	Genetic Point Mut.	Genetic Chrom.	Sub-chronic	Developmental	Reproduction	Acute Fish	Acute Invert.	Algal Toxicity		Photo-deg.	Hydrolysis	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 TD Technical Discussion proposed RA Read Across (see Sec. III.C. and D.)  
 ACD Adequate existing component data for read across (see Sec. III.A.) CM Computer Modeling proposed

**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 (C<sub>2</sub>+). 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**

