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US High Production Volume Chemical Program

Category Summary

For

Low Benzene Naphthas Category

Prepared by:

Olefins Panel of the American Chemistry Council

Revised May 5, 2009

EXECUTIVE SUMMARY

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

- Present results of an assessment to demonstrate that the 12 CAS numbers which are present in 9 production streams are adequately characterized with the existing data from representative gasoline blending streams and hydrocarbon constituents of the production streams, as described in the Low Benzene Naphthas Category test plan.
- Summarize the SIDS (Screening Information Data Set) physicochemical, environmental fate and effects, and human health HPV program endpoints for the Low Benzene Naphthas Category.
- Provide a description of manufacturing processes, potential exposure sources, and uses for Low Benzene Naphtha streams.
- Demonstrate that the extensive body of data available on chemical composition, and on mammalian and environmental endpoints on representative constituents of products in this category, and in gasoline blending streams of similar complex hydrocarbon composition are sufficient to fully define the Low Benzene Naphthas Category.

The Low Benzene Naphthas Category is comprised of 9 ethylene manufacturing streams that exhibit commonalities of manufacturing process and composition. The 12 CAS numbers in this category each represent at least one production stream but may represent more than one stream. The production streams consist of complex hydrocarbon reaction products, predominantly C5 through C12, and may be correctly represented by more than one CAS number.

Aromatic hydrocarbons represent the major chemical class in all these streams. The benzene content is usually less than 5%.

Most of the low benzene naphthas produced are used as blending stocks for gasoline. The low benzene naphthas are compositionally most similar to the high aromatic naphtha gasoline blending streams. For these reasons, the mammalian and environmental test data developed for the API Gasoline Blending Streams test plan have been used as "read-across" results for the Low Benzene Naphthas Category endpoints, along with data developed for this test plan.

Exposure

The product streams in the Low Benzene Naphthas Category are isolated from pyrolysis gasoline (7 streams) or are produced from aromatic processing units (2 streams). Production is performed in closed systems and products are distributed to petroleum refineries by pipeline, barge, tank cars or tank trucks for blending into gasoline. Environmental exposure can occur through accidental spills, fugitive emissions, leakage or release of light-end vapors into the atmosphere during tankage or delivery, or as components of gasoline during delivery, storage or refueling.

Exposure of workers is minimal because low benzene naphtha streams are isolated in production or used in closed system process units. Exposure would occur by inhalation of low level concentrations of fugitive emissions from process units or storage tanks, from sampling, or by displaced emissions during loading of bulk transportation vessels, and dermally by accidental spillage. The general population is not usually exposed to low benzene naphthas but may be exposed to gasoline during refueling, from emissions into ambient air, or possibly through leakage into groundwater. Inhalation exposure would be primarily to the lighter more volatile fraction of the gasoline, which contains far less aromatic compounds and fewer large chain (C7 and longer) aliphatic hydrocarbons.

Human Health

Evaluation of available mammalian data and "read-across" from gasoline blending streams of similar carbon number range and composition indicate that Low Benzene Naphthas are not acutely toxic (Oral LD50 >5000mg/kg; Inhalation LC50 >5000mg/m^3), are irritating to skin but minimally or not irritating to eyes and are not skin sensitizers.

Extrapolation from repeat dose inhalation studies of representative high aromatic gasoline blending streams indicate that Low Benzene Naphthas may induce irritation of nasal passages and lungs, cause effects on the hematopoietic system and liver weights at concentrations above 1030mg/m^3 for wholly vaporized materials, or above 1970–9250 mg/m^3 for partially vaporized materials, depending on degree of vaporization. Most of these effects would be resolved with cessation of exposure. Hydrocarbon nephropathy, a male rat specific effect not relevant to humans (U.S. EPA, 1991) may also occur. No neurotoxicity was observed.

Based on data from rat and mouse studies, Low Benzene Naphthas are unlikely to induce genetic damage *in vivo*. NOAELs were 2.5-3.0g/kg intraperitoneally for rat bone marrow chromosome aberrations and mouse bone marrow micronucleus assays. For representative high aromatic gasoline blending stream samples, *in vitro* mutation in mammalian cells (Mouse lymphoma L5178Y cells) occurred primarily in the presence of metabolic activation and correlated with the level of aromatic constituents for samples containing 60-80% aromatics. The heavy aromatic distillate that is part of the Low Benzene Naphthas Category did not induce gene mutation or DNA perturbation in mammalian (CHO) cells.

No significant reproductive or developmental toxicity was observed from representative high aromatic streams. Parental systemic effects observed at the highest dose of a light catalytic reformed naphtha distillate (27,750mg/m^3), slightly reduced body weight, changes in liver and kidney weights for males, did not have any effect on reproductive performance or fertility. No histologic changes were seen in reproductive organs of either sex. For a full range catalytic reformed naphtha, exposure at a maximum concentration of 7800mg/m^3 from gestation days 6-19 did not cause adverse effects on any fetal parameter. Fetal effects or overt neurobehavioral changes in offspring similar to those reported for toluene were not observed with these materials, even though tested materials contained up to 29% toluene. The absence of significant reproductive toxicity for these endpoints from exposure to high aromatic naphthas is supported by comparable data on gasoline and on individual components found in other high aromatic streams: benzene, xylenes and aromatics of C9 and above. On this basis, Low Benzene Naphthas containing less than 30% toluene are unlikely to induce reproductive or developmental toxicity. Three streams in this category contain levels of toluene greater than 55 % (Pyrolysis C7s, Pyrolysis C7-C8 fraction and Toluene Extract). It is not known whether the developmental effects of the mixed hydrocarbon streams containing 55-80% toluene will induce developmental effects similar to those reported for toluene (decreased pup weight and delayed ossification). However, due to the uncertainty and in order to be conservative, the developmental NOAEL (2250 mg/m3) identified for toluene was used to "read across" to identify a developmental NOAEL for streams containing high toluene content.

Environmental

For environmental endpoints, measured data on components present in the products of the Low Benzene Naphthas Category, and on other complex products that contain a similar range of chemical classes and carbon numbers were used. These data demonstrate that the hydrocarbons that comprise this category have a very low potential to hydrolyze and do not photodegrade directly due to a minimal capacity to absorb appreciable light energy above 290nm. However, atmospheric oxidation constitutes a significant route of degradation. Calculation of atmospheric half-lives of representative constituent chemicals identified a range of 2.3-31.8 hours as a result of indirect hydrolysis by hydroxyl radical attack. Fugacity modeling demonstrated that members of this category partition primarily into the air, with slight partitioning into water and soil, and minimal partitioning into sediment. Read-across data indicate that these products are likely to biodegrade significantly and have the potential to produce a moderate level of toxicity in freshwater algae and a moderate level of acute toxicity in freshwater fish and invertebrates. Aquatic toxicity for products in this category can be predicted based on carbon number, measured or calculated toxicities of constituent hydrocarbons and constituent composition.

The extensive body of data available for mammalian and environmental endpoints on representative constituents of products in this category and on gasoline blending streams of similar complex hydrocarbon composition are sufficient to fully characterize the potential toxicity for materials in this category and demonstrate the integrity of the category, itself.

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

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1 CATEGORY DESCRIPTION AND JUSTIFICATION

1.1 Category Identification

The Low Benzene Naphthas Category was developed for the HPV program (Olefins Panel, 2003) by grouping ethylene manufacturing streams that exhibit commonalities from both manufacturing process and compositional perspectives. The category includes nine production streams and twelve Chemical Abstract Services (CAS) registry numbers (Table 1). Each CAS number represents at least one production stream. All of these process streams are complex products containing many chemical components and are assigned CAS numbers described by broad process and physical chemical property descriptions. Certain single streams may be correctly represented by more than one CAS number, and a CAS number may be applicable to more than one stream. A description of the ethylene and associated stream production processes is included in Appendix 1.

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

Production Streams	CAS RN	CAS RN Name
Pyrolysis C7s	68527-23-1	Naphtha, petroleum, light steam-cracked arom.
	68478-10-4	Naphtha, petroleum, light steam-cracked, debenzenized, C8-16-cycloalkadiene conc.
Pyrolysis C7-C12 fraction	68516-20-1	Naphtha, petroleum, steam-cracked middle arom.
	64742-83-2	Naphtha, petroleum, light steam-cracked
	68476-45-9	Hydrocarbons, C5-10 arom. conc., ethylene-manuf.-by-product
Pyrolysis C7-C8 fraction	68527-23-1	Naphtha, petroleum, light steam-cracked arom.
	68919-15-3	Hydrocarbons, C6-12, benzene-recovery
C9+ from xylene unit	68333-88-0	Aromatic hydrocarbons, C9-C17
	68553-14-0 [2]	Hydrocarbons, C8-11
Hydrotreated C7+ fraction	64742-48-9	Naphtha, petroleum, hydrotreated heavy
Hydrotreated C8-C10 fraction	68512-78-7[2]	Solvent naphtha, petroleum, light arom., hydrotreated
	64742-48-9	Naphtha, petroleum, hydrotreated heavy
Hydrotreated C7-C12 fraction	64742-48-9	Naphtha, petroleum, hydrotreated heavy
	68516-20-1	Naphtha, petroleum, steam-cracked middle arom.
Hydrotreated C5/C9 Blend	64742-49-0	Naphtha, petroleum, hydrotreated light
Toluene Extract	64741-98-6	Extract, petroleum, heavy naphtha solvent

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

[2] This CAS number, although not included in the original test plan for this category, may also be used to represent the corresponding stream. The CAS number has been added to this summary report to further utilize the results of the HPV initiative for this stream.

The streams in this category consist of complex hydrocarbon reaction products that are predominantly C5 through C12. The complex hydrocarbon streams represent a category because they each share many of the same components, although distribution of those components may vary somewhat. Most of the streams in this category include the pyrolysis C7 fraction and are isolated by distillation from pyrolysis gasoline.

Aromatics represent the major chemical class in all of the streams, varying from approximately 45 to 95 percent. The benzene content is usually less than five percent. The typical compositions of the streams are shown in Appendix 2, Table A2-1. The category is designated Low Benzene Naphthas.

Most of the Low Benzene Naphthas produced are used as blending stocks for gasoline. The range of composition of the Low Benzene Naphthas falls within the range of composition of gasoline blending streams presented in the API Gasoline Blending Streams HPV test plan (see Fig. 1 and 2), and are compositionally most similar to the high aromatic C7 – C12 streams. A small percentage of Low Benzene Naphthas are used as industrial solvents or blended into fuel oil.

The CAS numbers in the Low Benzene Naphthas category are associated with nine streams that are commercial products or isolated intermediates:

1 – 3. Pyrolysis C7s, C7-C12, and C7-C8 fractions: Pyrolysis gasoline is separated by distillation into various boiling-point-range fractions as an intermediate step in preparation for further processing. Many carbon number distribution fractions are technically feasible. the compositions of these fractions vary depending on the ethylene process feedstock, the cracking furnaces operating conditions and the ethylene process configuration.

1. Pyrolysis C7s: the reported composition is 75% toluene with the balance primarily C7 non-aromatics, largely unsaturates. The stream may contain low levels of benzene.

2. Pyrolysis C7-C12 fraction: The typical composition reported included about 2% benzene, 23% toluene, 28% C8 aromatics and 8% naphthalene. The balance is expected to be largely unsaturated hydrocarbons and other aromatics.

3. Pyrolysis C7-C8 fraction: The reported compositions indicate C7-C8 streams that contain 45 to 80% toluene and other streams with 11 to 78% C8 aromatics. The typical benzene concentration reported was 2% with a maximum of 5%.

4. C9+ from Xylene Unit: This stream is a coproduct from process units that produce o- or p-xylene. The carbon distribution for the stream is C8 to C12 hydrocarbon compounds with a boiling point of 65°F or higher. The stream is predominantly aromatics.

5 – 8. Hydrotreated Pyrolysis Fractions (Hydrotreated C8-C10, C7-C12, and C7+fractions, and C5/C9 blend): Pyrolysis gasoline, or distillate fractions of pyrolysis gasoline are typically treated with hydrogen over catalyst. The hydrogenation process may be either a 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 to alkyl aromatics,

for example, styrene to ethylbenzene. The two-stage process is typically a vapor-phase, more severe hydrogenation that hydrogenates essentially all of the contained mono- and diolefins to paraffins. A pygas fraction that will be processed by extraction or extractive distillation to produce aromatics (toluene or xylenes in this case) is subject to two-stage hydrogenation. Pygas fractions may be forwarded to hydrodealkylation units (less common) for benzene production after one-stage of hydrogenation. Pygas fractions intended for use as a gasoline blending stock are frequently subject to only one-stage hydrogenation. The streams may result from fractionation of hydrotreated pyrolysis gasoline or from hydrotreating pyrolysis gasoline fractions followed by distillation. Reformate fractions from petroleum refineries are sometimes mixed with these pyrolysis fractions.

5. Hyrdotreated C8-C10 fraction: The carbon number distribution for this stream is C6 -C12, but is predominately C8-C10. The reported typical concentration includes 0.3% benzene, 2.4% toluene, and 24% C8 aromatics with the balance primarily of C9 and C10 aromatics and lesser amounts of paraffins, isoparaffins and naphthenes in this carbon range.

6. Hydrotreated C7-C12 fraction: The carbon number distribution for this distillate fraction of hydrogenated pygas is predominately C7- C12, with lesser amounts of C6. The reported typical concentration includes 1% benzene, 23% toluene, and 25% C8 aromatics, with the balance primarily other aromatics and lesser amounts of monoolefins and paraffins.

7. Hydrotreated C7+ fraction: This stream is derived as distillation residue after removing the C5 and C6 fractions from a hydrogenated pygas stream. (Alternately the stream could be hydrotreated after distillation.) The carbon number distribution is predominantly greater than C6, although the reported analysis does not report compounds greater than C12. The reported typical analysis includes 23% toluene, 32% C8 aromatics, and 1% naphthalene, with the balance primarily other aromatics and lesser amounts of paraffins.

8. Hydrotreated C5/C9 blend: This stream is produced by blending C5 and C9 pyrolysis fractions, hydrogenated either before or after blending. Reported typical analysis includes about 2% benzene, 40% C5's in the blend, 9% C8 aromatics, 19% C9 aromatics, and 25% C10+.

9. Toluene Extract: This stream is produced as a co-product of a benzene extraction unit. The stream may contain significant concentrations of xylenes.

1.2 Purity/Impurities/Additives

CAS numbers in this category are extremely complex mixtures of hydrocarbons in the C5 – C12 carbon range. Typically there are no impurities in the streams in this category. Typical stream compositions for streams in the Low Benzene Naphthas Category are presented in Table A2-1.

1.3 Physico-Chemical Properties

Properties for the Low Benzene Naphthas category have been estimated from calculated and measured values for representative constituents of the category. Commercial substances in this category consist of complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C12. The seven chemicals selected to represent physico-chemical properties of the category are C5 –C11 hydrocarbons that can be found in substances identified by the 12 CAS numbers. Calculated data has been derived using subroutines of the EPIWIN© version 3.04 computer model [EPIWIN, 1999] described in the US EPA document "The Use of Structure-Activity Relations (SAR) in the High Production Volume Chemical Challenge Program (US EPA, 1999). The representative constituents are isopentane, toluene, m-xylene, styrene, naphthalene, tricyclodecane and methylnaphthalene. Robust summaries for Physico-Chemical property studies are in Attachment 3.

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

Substance Costituent	**Melting Point (°C)**	**Boiling Point (°C@760mm Hg)**	**Vapor Pressure (hPa@ 25°C)**	**Log K_{ow} (@ 25^0C)**	**Water Solubility (mg/L@25^0C)**
Isopentane	-119.04	30.18	9.17 E2	2.72	184.6
toluene	-59.17	125.72	31.60	2.54	832.7
m-xylene	-40.69	148.29	8.83	3.09	258.4
styrene	-48.31	146.65	6.73	2.89	386.7
naphthalene	5.01	231.64	0.11	3.17	183.8
tricyclodecane	-19.15	171.25	2.64	3.59	21.5
methyl-naphthalene	22.15	249.60	4.60 E-2	3.72	54.6

Calculated values determined by EPIWIN [EPIWIN (1999). Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.].

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

Substance Costituent	**Melting Point (°C)**	**Boiling Point (°C@760mm Hg)**	**Vapor Pressure (hPa@ 25°C)**	**Log K_{ow} (@ 25^0C)**	**Water Solubility (mg/L@25^0C)**
Isopentane	-159.9	27.8	9.19 E2	n.a	n.a.
toluene	-94.9	110.6	37.86	2.73	573.1
m-xylene	-47.8	139.1	11.05	3.20	207.2
styrene	-31.0	145.0	8.53	2.95	343.7
naphthalene	80.2	217.9	0.05	3.30	142.1
tricyclodecane	n.a.	n.a.	n.a.	n.a.	n.a.
methyl-naphthalene	34.4	241.1	7.33 E-2	3.86	41.4

Measured values from the experimental database in EPIWIN [EPIWIN (1999). Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.].

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

1.3.1 Melting Point (Range)

The calculated melting points [by subroutine MPBPWIN, version 1.40] for some representative constituents that are present in the category streams vary from -119.04 to 22.15 °C. The measured melting points of these same constituents vary from -159.9 to 80.2°C. Although this does not define the actual melting points of the category streams, it offers an indication of a range that might be expected to encompass the melting points of these complex streams with variable compositions. Melting points outside these ranges may be possible for some category streams.

1.3.2 Boiling Point (Range)

The calculated boiling points [by subroutine MPBPWIN, version 1.40] for some representative constituents that are present in the category streams vary from 30.18 to 249.60°C @ 760 mm Hg. The measured boiling points of these same constituents vary from 27.8 to 241.1°C @ 760 mm Hg. Although this does not define the actual boiling points of the category streams, it offers an indication of a range that might be expected to encompass the boiling points of these complex streams with variable compositions. Boiling points outside these ranges may be possible for some category streams.

1.3.3 Vapor Pressure (Range)

The calculated vapor pressures [by subroutine MPBPWIN, version 1.40] for some representative constituents that are present in the category streams vary from 4.60 E-2 to 9.17 E2 hPa @ 25°C. The measured vapor pressures of these same constituents vary from 7.33 E-2 to 9.19 E2 hPa @ 25°C. Although this does not define the actual vapor pressures of the category streams, it offers an indication of a range that might be expected to encompass the vapor pressures of these complex streams with variable compositions. Vapor pressure outside these ranges may be possible for some category streams.

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

The calculated log K_{ow} [by subroutine KOWWIN, version 1.65] for some representative constituents that are present in the category streams vary from 2.54 to 3.72 @ 25°C. The measured log K_{ow} of these same constituents vary from 2.73 to 3.86 @ 25°C. Although this does not define the actual log K_{ow} of the category streams, it offers an indication of a range that might be expected to encompass the log K_{ow} of these complex streams with variable compositions. Log K_{ow} values outside these ranges may be possible for some category streams.

1.3.5 Water Solubility (Range)

The calculated water solubility [by subroutine WSKOWWIN, version 1.36] for some representative constituents that are present in the category streams vary from 21.5 to 832.7 mg/L @ 25°C. The measured water solubility of these same constituents vary from 41.4 to 573.1 mg/L @ 25°C. Although this does not define the actual water solubility of the category streams, it offers an indication of a range that might be expected to encompass the water solubility of these complex streams with variable compositions. Water solubilities outside these ranges may be possible for some category streams.

1.3.6 Comparison with High Aromatic Gasoline Blending Streams

Some relevant physico-chemical properties of the high aromatic gasoline blending streams [C7-C12] are: boiling range 35-230^{0}C (measured); Reid vapor pressure 3 psia; Water solubility 3-2000mg/L (range of components), Water accommodated Fraction [WAF] value =14ppm; partition coefficient 2.13 - 4.76 at 25^{0}C (calculated). Properties for the other representative gasoline blending streams, high in paraffins, olefins, or naphthenes, are: boiling range –20 to 230^{0}C (measured); Reid vapor pressure 1.2 psia [naphthenic] – 10.3 psia[olefinic]; Water solubility 3- 2000mg/L (range of components), WAF range =0.9 – 7.9ppm; partition coefficient 2.13 – 4.85 at 25^{0}C (calculated)

1.4 Category Justification

Approximately 90% of the Low Benzene Naphthas produced are used as blending stocks for gasoline. The range of composition of the Low Benzene Naphthas falls within the range of composition of gasoline blending streams presented in the 2003 API gasoline blending streams HPV test plan (see Fig. 4 and 5), and are compositionally most similar to the high aromatic C7 – C12 streams. The large volume of toxicology data on gasoline and gasoline blending streams is particularly useful for characterizing the naphthas in this category. Gasoline blending streams were evaluated by collecting a complete set of screening level mammalian and environmental data on representative streams containing relatively high amounts of one of the major hydrocarbon classes – **P**araffins, **O**lefins, **N**aphthenes and **A**romatics [**PONA**]. Each stream also contained overlapping amounts of the other classes. More than 75 mammalian and environmental studies [physicochemical, environmental fate and aquatic] are available on gasoline blending streams and on gasoline, the product. These include 14 acutes [oral, dermal, inhalation], 2 repeat dermal and 7 repeat inhalation studies, 15 *in vitro* and *in vivo* genetic toxicity studies, and 8 reproduction/developmental toxicity studies, as well as 23 aquatic toxicity studies. Low benzene naphtha streams are compositionally most similar to the high aromatic gasoline blending streams [30-95% aromatic content], for which toxicity studies on three streams of varying aromatic content have been performed. Results demonstrated similar patterns of activity in the same organ systems for all streams tested. Overall, toxic effects in mammalian systems from gasoline blending streams and gasoline were observed in the same organ systems consistently at high exposure levels. Small changes in composition did not appear to significantly affect outcome. Environmentally, gasoline stream hydrocarbons also demonstrated similar modes of action. Specific information on this program and robust summaries of the studies are available on in the API Gasoline Blending Streams Test Plan on the US EPA HPV website.

The strategy for characterizing the physical-chemical properties, human health and environmental hazards of products in the Low Benzene Naphthas category has been to evaluate data from similar products and/or components of materials in this category found in the published literature, or developed as part of other EPA HPV, OECD SIDS, and ICCA HPV programs. Two approaches have been taken to evaluate environmental endpoints, or mammalian and aquatic toxicity. The similarity of the Low Benzene Naphthas to gasoline blending streams in composition and their use as gasoline feedstocks allows the use of toxicity data from these complex blending streams to “read-across” to the low benzene naphthas. In addition toxicity testing has also been performed on CAS # 64742-48-9, hydrotreated C8-C10, a member of the Low Benzene Naphthas category. These data are summarized in Attachment 1.

For environmental endpoints, a constituent approach is equally efficient; evaluating measured data on components present in the products of the low benzene naphthas category and on other complex products that contain a similar range of chemical classes and carbon numbers. Where measured data do not exist, calculated data for selected constituents of these naphthas have been developed using the Epiwin© computer models described by EPA.

2 EXPOSURE AND USE INFORMATION

The Category & HPV Stream Production: The HPV Low Benzene Naphthas Category includes the nine commercial product streams[1] from the Olefins Process that typically have a carbon range of C6 to C12 and that contain little or no benzene. One of the category streams (C5/C9 Blend) includes C5 hydocarbons. The category streams are complex mixtures of variable composition. They are gasoline-like streams and liquids at ambient conditions. Most of the streams (accounting for 91.5% of the category volume) are isolated intermediates that are transported under controlled conditions to a limited number of locations within the same company or to second parties that use the streams to produce gasoline.

Seven of the category streams are isolated from pyrolysis gasoline (pygas), a complex mixture of hydrocarbons produced by the ethylene manufacturing process. Two of the category streams, the C9+ (from the xylene unit) and, aromatic extract (from the benzene extraction unit), are produced from aromatics processing units. These two category streams make up 7% of the category volume, and are represented as “other” in Figure 1. The sponsors of the Low Benzene Naphthas category produce nearly all of the category-defined pygas streams that are isolated in the US. In contrast, the volume of the two category steams not derived from pygas and produced by the sponsors is expected to be a small percentage of the total US production.

The individual components or hydrocarbon compounds that make up the complex mixtures or streams in this category are also produced by other industrial processes, and they are naturally occurring substances. Potential exposures from these individual components from other manufacturing processes or from natural sources are considered to be out of scope for this assessment. This assessment is limited to potential exposures to the streams in the category, although some data are presented on a few of the components contained in the streams.

This assessment does not address potential exposures within the petroleum industry arising from the use of the category streams. These streams make up only a small portion of the similar streams managed by that industry. Exposures assessment of the potential exposures resulting from use of category streams as solvents is not included in this report[2].

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[1] The Olefins Panel also sponsored Naphtha and Condensate, which are sometimes imported and used as feedstocks to the Olefins units, the products o- and p-xylene, and the raffinate stream from aromatics extraction units. However, these streams are sponsored by others in the HPV program, and not included in this assessment.

[2] For information about screening level assessments of exposure potentials related to hydrocarbon solvent the reader is referenced to the HPV category reports provided by the Hydrocarbons Solvents Panel of the American Chemistry Council.

There are twelve CAS numbers that are used by the Olefins Industry to represent these nine category streams. Some of the CAS numbers used in this Category may also be used to describe products that are not in the Low Benzene Naphthas Category. This assessment addresses the use of the CAS numbers for the Low Benzene Naphtha Category streams. The Olefins Industry or others may use these same CAS numbers to represent substances that may be, in various degrees, dissimilar to the category streams or may be managed differently.

Distribution of the 5 billion pounds/year of category production[3] among the category streams is shown in Figure 1.

Figure 1. Low Benzene Naphthas Category Production

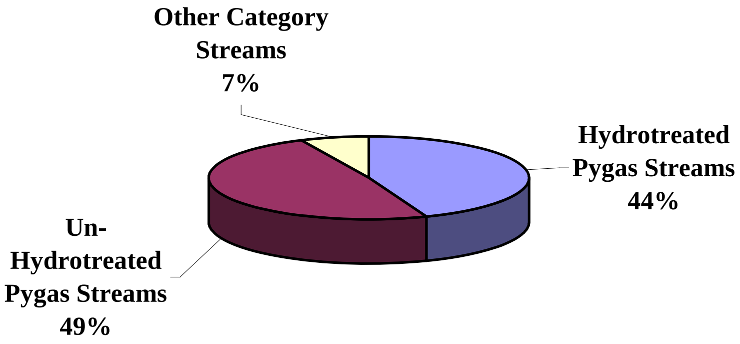

Table 4 – Low Benzene Naphthas Category Streams

Hydrotreated Pygas Streams	Un-Hydrotreated Pygas Streams	Other Category Streams
Hydrotreated C8-C10	Pyrolysis C7s	C9+ (from Xylene Unit)
Hydrotreated C7-C12	Pyrolysis C7-C12	Toluene Extract
Hydrotreated C7+	Pyrolysis C7-C8	
Hydrotreated C5/C9 Blend		

Storage and Transportation of Category Streams: Most of the Low Benzene Naphtha streams are either used on-site where they were produced, or shipped to other industrial sites for additional processing or use. When shipped between industrial sites, the Low Benzene Naphtha category streams are usually transported in bulk in closed systems by pipeline or barge, with lesser quantities moved by tank car or tank truck.

Use: Uses of the category streams are shown in Figure 2[4]. As indicated, the major use of the Low Benzene Naphtha Category streams (91.5% of the category volume) is for production of

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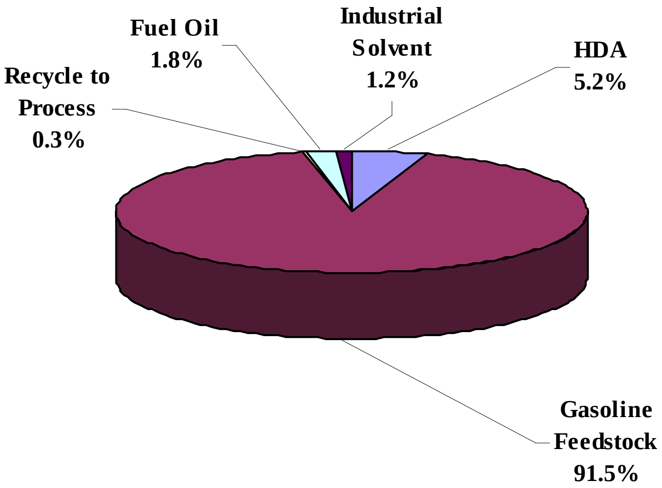
[3] 5 billion lbs/yr is approximately the total commercial production of category streams reported by sponsors of the HPV Low Benzene Naphthas Category, and based on their 1998 TSCA IUR report.

[4] The percentage use of the category steams is based on data received from 8 of the 9 category sponsors. Although similar information was not available from the other two sponsors at the time this report was written, the uses shown in Figure 2 are expected to be representative of the industry.

motor gasoline. About 5.2% of the category volume was used in the reporting year in HDA (Hydrodealkylation) process units for the production of benzene. About 1.2% of the category use is as industrial solvents. The solvent use reportedly includes use as a solvent for a broad range of oilfield chemicals, pesticides, and fuel additives, and as a well fracture/well stimulation fluid.

FIGURE 2
USE OF THE LOW BENZENE NAPHTHA CATEGORY STREAMS



Potential Exposure: The category streams are liquids at ambient conditions, with volatility similar to gasoline. Inhalation is a likely route of potential exposure due to the volatility of the streams. There may also be a potential for dermal exposure as a results of accidental contact. The streams or components in the streams are slightly soluble in water and therefore groundwater contamination is possible in the event of spills or leaks from transportation or storage equipment. Most of these streams contain significant concentrations of toluene[5]. "Occupational exposure to toluene may occur through inhalation and dermal contact with this compound at workplaces where toluene is produced or used. The general population may be exposed to toluene via inhalation of ambient air, ingestion of food and drinking water, handling of gasoline, and exposure to some consumer products where toluene is used as a solvent [6]."

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[5] "The majority of toluene produced is unrecovered (i.e., not isolated from other aromatic constituents) and is consumed as a constituent of various refinery streams. The largest concentrations of toluene are recovered from catalytic reformate (a refinery operation) and pyrolysis gasoline (a coproduct of ethylene manufacture) streams. In 2002, approximately 89% of toluene recovered in the United States was from catalytic reformate and 7% was from pyrolysis gasoline. Additional quantities are obtained as a by-product of styrene manufacture and xylene isomerization as well as extraction from coke-oven light oil. Recovered toluene consumption in the United States decreased to 1,460 million gallons (4,801 thousand metric tons) in 2002." (http://ceh.sric.sri.com/Public/Reports/454.0000/).

[6] Hazardous Substances Databank, a database of the National Library of Medicine's TOXNET system, (http://toxnet.nlm.nih.gov) downloaded on February 3, 2004.

Sources of Potential Exposure: Exposure to the category streams for workers in the Olefins Industry process units where the category streams are isolated or used is low because that equipment and those processes are closed systems. Emissions from storage and loading equipment is typically controlled by using floating roof storage tanks or by routing vents from fixed roof storage tanks and loading equipment to control or recovery systems, or back to process. For the industrial workers at these facilities, the most likely exposure potential occurs through inhalation of low-level concentrations in air of vapors that escape from the closed process, such as fugitive emissions from valve packing and from pump seals. Other potential exposures may result during operations such as sampling, loading of bulk transportation vessels (tank cars and barges); emissions from floating roof storage tanks, or during infrequent opening of equipment for maintenance; and from emissions from control devices, such as flares.

The above-described sources of emissions of the category streams may present a potential for exposure to the public and to the environment adjacent to the industrial facilities that use or produce or use the category streams.

Most of the category streams contain significant concentrations of toluene. “Toluene is released into the atmosphere principally from the volatilization of petroleum fuels and toluene-based solvents and thinners and from motor vehicle exhaust. Toluene's production and use as an intermediate in the production of benzoic acid, benzaldehyde, benzene, explosives, dyes and many other organic compounds may also result in its release to the environment through various waste streams. Toluene has been detected in emissions from volcanoes, forest fires and crude oil.[6]”

Controls that Limit Exposure: Neither OSHA nor ACGIH have established occupational exposure limits for the complex mixtures in this category. However OSHA has established occupational exposure limits[7] for some of the components typically present in the streams. In addition ACGIH has established guidelines for some components in the category streams. For example, the OSHA PEL for Toluene (a major component in most of the category streams is 200 ppm; and the ACGIH TLV is 50 ppm. Five of the eight sponsors of category streams reported that they have programs that assess exposure to the category streams, and in three cases they included specific measurements for toluene. Industrial hygiene programs for a specific production site are typically unique to the site and address the specific chemical exposure issues. Components typically present in some of the category streams that have OSHA PELs or ACGIH TLVs are shown in Table 5.

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[7] http://www.osha.gov/pls/oshaweb/owadisp.show_document?p_table=STANDARDS&p_id=9991

Table 5

Components Typically present in Some Streams in the Low Benzene Naphthas Category & That Have OSHA PELs or ACGIH TLVs

Component	OSHA PEL	ACGIH TLV	Component	OSHA PEL	ACGIH TLV	Component	OSHA PEL	ACGIH TLV
Biphenyl	0.2	0.2	Ethylbenzene	100	100	Pentane Isomers	1000	600
Cumene	50	50	Heptane	500	400	Styrene	100	20
CPD	75	75	Indene	-	10	Toluene	200	50
Cyclopentane	--	600	Naphthalene	10	10	Vinyltoluene	100	50
DCPD	-	5	Octane isomer	500	300	Xylenes Isomers	100	100

Among other reasons, the release of the category steams from process, storage and transportation equipment at industrial facilities is avoided because the streams are flammable liquids, similar in flammability and volatility characteristics to gasoline.

The category streams are mixtures of volatile organic compound (VOC) and are therefore subject to USEPA and state environmental regulations that limit VOC emissions. The USEPA new source performance standards of 40CFR Part 60 limit emissions of VOC at new or modified Olefins process units where the streams in the category are produced and used. Subpart VV of 40CFR Part 60 limits emission from equipment leaks, Subpart NNN limits emissions from distillation operations, subpart RRR limits emissions from reactor systems and subpart Kb limits emissions from VOC storage tanks. Facilities that produce and use the category streams are also typically subject to state operating permits and state regulations that further limit VOC emissions.

Ambient Air Concentration Data: Ambient air concentration data for the complex category streams is not available. Most of the category streams contain significant concentrations of toluene. "In a survey of 3,195 samples obtained from urban areas in the US, toluene was detected at concentrations of 0-85 ppb (11 ppb median). Average toluene concentrations in US cities range from 0.8-37 ppb with max values ranging from 6.5-1,110 ppb. Daily variations in concentrations and ratios of toluene to benzene indicate that auto traffic is the most common source of atmospheric toluene.[6]"

Estimates of Potentially Exposed Workers: Information not developed.

Category Emissions: Emissions of the individual streams in the category are not readily available because the streams are multi-component mixtures. The components that make up these mixtures are industrial compounds and for at least some, emissions are reported to the EPA and made available to the public in the Toxics Release Inventory (TRI) [8]. This inventory was established under the Emergency Planning and Community Right-to-Know Act of 1986 (EPCRA) and expanded by the Pollution Prevention Act of 1990.

Toluene is a component found at significant concentrations in most of the category streams. The

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[8] EPA website for TRI: http://www.epa.gov/tri/

TRI data indicate that emissions of toluene have significantly decreased since 1988. The TRI data from 2001 indicate that emissions of toluene reported in the TRI for the chemical sector (sic 28) have declined by 77% since 1988. However the relevance of individual component emissions values with regard to the category streams is uncertain, because the category streams likely account for a minor portion of the total emissions for specific components.

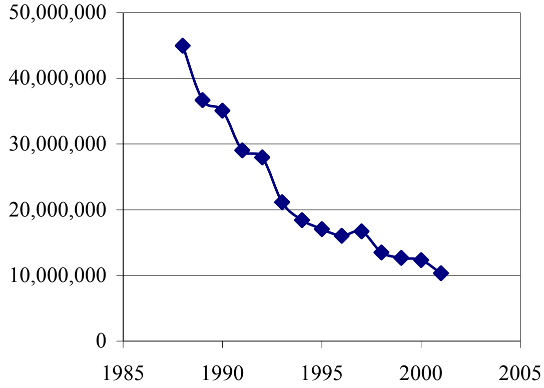

Figure 3
TRI Toluene Emissions (lbs/year) Chemical Sector SIC 28 Only 1988 - 2001

2.1.1 Summary of Exposure Assessment

The HPV Low Benzene Naphthas Category includes the nine commercial product streams from the Olefins Industry processes that typically have a carbon range of C6 to C12 and that contain little or no benzene. The category streams are complex mixtures of variable composition. They are gasoline-like streams, liquids at ambient conditions. The major use for the category streams is in production of motor gasoline. Seven of the nine streams are derived from pyrolysis gasoline, a complex mixture of hydrocarbons produced by the ethylene manufacturing process. The other two category streams are similar to the pyrolysis gasoline streams, but are derived from the industry's aromatics processing units. The Olefins Industry uses twelve CAS numbers to represent these nine category streams. The 5 billion pounds annual commercial production for the category is made up of the pyrolysis gasoline streams, hydrotreated or un-hydrotreated, which represent 44% and 49% of the category volume. Two aromatics-processing streams account for the remaining 7%.

The category streams are typically used at the same location where they are produced, or transported in bulk by pipeline or barge with lesser quantities moved by tank car or truck car. About 91.5% of the commercial volume is used in the production of motor gasoline, 5% is used in the reporting year in Hydrodealkylation units for the production of benzene, 1.8% is used as industrial or commercial fuel oil, 1.2% is used as an industrial solvent, and 0.3% is recycled back to the olefins industry processes.

Inhalation is a likely route of potential exposure to the category streams due to the volatility of the streams, which is similar to gasoline. There may also be a potential for dermal exposure as a results of accidental contact to these streams that are liquids at ambient conditions. The streams or components in the streams are slightly soluble in water and therefore groundwater contamination is possible in the event of spills or leaks from transportation or storage equipment.

Exposure to the category streams for workers in the Olefins Industry process units where the category streams are isolated or used is low because that equipment and those processes are closed systems.

Most of the category streams contain significant concentrations of toluene, a naturally occurring aromatic hydrocarbon that is also produced by other industrial and combustion processes. Occupational exposure to toluene may occur through inhalation and dermal contact with this compound at workplaces where toluene is produced or used. The general population may be exposed to toluene via inhalation of ambient air, ingestion of food and drinking water, handling of gasoline, and exposure to some consumer products where toluene is used as a solvent. Toluene is released into the atmosphere principally from the volatilization of petroleum fuels and toluene-based solvents and thinners and from motor vehicle exhaust.

Neither OSHA nor ACGIH have established occupational exposure limits for the complex mixtures in this category. However OSHA has established occupational exposure limits for some of the components typically present in the streams. In addition ACGIH has established guidelines for some components in the category streams. For example, the OSHA PEL for Toluene (a major component in most of the category streams) is 200 ppm; and the ACGIH TLV is 50 ppm. The category streams are mixtures of volatile organic compound (VOC) and are therefore subject to USEPA and state environmental regulations that limit VOC emissions.

In a survey of 3,195 samples obtained from urban areas in the US, toluene was detected at concentrations of 0-85 ppb (11 ppb median). Average toluene concentrations in US cities range from 0.8-37 ppb with max values ranging from 6.5-1,110 ppb. Daily variations in concentrations and ratios of toluene to benzene indicate that auto traffic is the most common source of atmospheric toluene.

Toluene is a component found at significant concentrations in most of the category streams. The TRI data indicate that emissions of toluene have significantly decreased since 1988. The TRI data from 2001 indicate that emissions of toluene reported in the TRI for the chemical sector (SIC 28) have declined by 77% since 1988.

This assessment did not address potential exposures as a result of use of the category streams at petroleum refineries where the steams are used to produce gasoline, or as a result of the use (of a limited amount) of the streams as a hydrocarbon solvent, primarily and industrial solvent.

3. Environmental Fate

Photodegradation

3.1.1 Direct photodegradation: The absorption of light in the ultraviolet (UV) visible range (110-750nm) can induce electronic excitation of an organic molecule. The stratospheric ozone layer allows only light in wavelengths in the 290-750nm range to reach earth's surface with the potential to result in photochemical transformation in the environment. To estimate photochemical degradation, it is assumed that degradation will occur in proportion to the amount of light wavelengths greater than 290nm absorbed by the molecule. Saturated hydrocarbons (paraffins and naphthenics), olefins with one double bond or two conjugated double bonds, and single ring aromatics do not absorb appreciable light energy above 290nm. For this class of materials, only aromatic with 2 or more rings absorb light above 290nm. Examples of absorbance maxima (λ max) and associated molar absorptivities (ϵ) for representative hydrocarbons are shown below.

Table 6. Characteristic Absorbance Maxima (λmax) and Associated Molar (ε) for Representative Hydrocarbons of the Low Benzene Naphthas Category

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

Only naphthalene demonstrated some photochemical degradation at wavelengths above 290nm.

Products in the Low Benzene Naphthas category do not contain component molecules that will undergo direct photolysis. This process will not contribute a measurable degradative removal of chemical components in this category from the environment.

3.1.2 Atmospheric Oxidation (Indirect photodegradation): Atmospheric oxidation as a result of hydroxyl radical attack is not direct photochemical degradation but an indirect degradation process. Hydrocarbons such as those in the Low Benzene Naphthas Category have the potential to volatilize to air where they can react with hydroxyl radicals (OH-). The rate at which an organic compound reacts with OH- radicals is a direct measure of its atmospheric persistence. The AOPWIN version 1.89 computer program [subroutine of EPIWIN 3.04] was used here to estimate the rate constants for OH- radical reactions of representative organic constituents of the products in the Low Benzene Naphthas category, which are then used to calculate atmospheric half-lives for these constituents as shown below:

Table 7. Hydroxy Radical Photodegradation Half-lives of Representative Hydrocarbons of the Low Benzene Naphthas Category

Chemical	Calculated* half-life (hrs)	OH- Rate Constant (cm^3/molecule-sec)
isopentane	31.8	4.0 E^{-12}
toluene	24.6	5.2 E^{-12}
m-xylene	9.5	13.6 E^{-12}
styrene	4.6	28.1 E^{-12}
naphthalene	5.9	21.6 E^{-12}
tricyclodecane	5.6	22.9 E^{-12}
methylnaphthalene	2.3	56.5 E^{-12}

* Atmospheric half-life values are based on a 12-hr day.

Based on these calculated values, for several representative stream constituents, products in the Low Benzene Naphthas category can have an atmospheric half-life range of 2.3 –31.8 hours, indicating that atmospheric oxidation can be a significant route of degradation for products in this category. These values fall within the calculated atmospheric half-lives for gasoline blending streams, which range from a minimum of 38.4 minutes to approximately 16 days based on the concentration of components in each stream.

Stability in Water

Hydrolysis is unlikely for product streams in the Low Benzene Naphthas category and for gasoline blending streams. Hydrolysis is a nucleophilic substitution reaction in which a water molecule or hydroxide ion reacts with an organic molecule to form a new carbon-oxygen bond. Carbon to carbon double bonds are too stable to be cleaved by nucleophilic substitution and the carbon atom lacks sufficient electronegativity to be a good "leaving group". Chemicals that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters and sulfonic acid esters. The chemical components of the Low Benzene Naphthas are hydrocarbons that are not included in these groups and have very low potential to hydrolyze. This degradative process will not contribute to removal of these hydrocarbons in the environment.

Distribution in the Environment

Substances in the Low Benzene Naphthas category are calculated to partition primarily into air with negligible percentages partitioning in water, soil and sediment. Relatively high vapor pressure and water solubility largely control the partitioning behavior of constituent chemicals in substances from this category.

The EQC level 1 fugacity model (MacKay et al., 1996) recommended by U.S. EPA (1999b) was used to determine partitioning of representative chemical constituents into different environmental compartments under steady state conditions, in order to estimate the partitioning behavior for the category substances. Mackay level 1 distribution values, calculated and measured, for 7 representative constituents of products in this category are presented below:

Table 8. Environmental Distribution as Calculated by EQC Level I Fugacity Model for Representative Hydrocarbons of the Low Benzene Naphthas Category

Chemical	**Percent Distribution: Calculated[a] [Measured][b]**			
	Air	Water	Soil	Sediment
Isopentane	99.98 [99.98]	0.01 [0.01]	0.01 [0.01]	----
Toluene	98.17 [98.80]	1.40 [0.81]	0.43 [0.39]	----
m-Xylene	97.19 [97.91]	1.33 [0.86]	1.45 [1.20]	0.03 [0.03]
Styrene	95.55 [96.65]	2.61 [1.85]	1.80 [1.46]	0.04 [0.04]
Naphthalene	24.47 [42.27]	32.28 [20.56]	42.28 [36.33]	0.94 [0.81]
Tricyclodecane	98.68 [NA]	0.29 [NA]	1.01 [NA]	0.02 [NA]
Methylnaphthalene	97.68 [98.53]	0.40 [0.19]	1.88 [1.25]	0.04 [0.03]

NA =Data not available

a- Values determined using calculated input data from EPIWIN program

b- Values determined using input data from the EPIWIN program experimental database.

With the exception of naphthalene, the representative components partition into air at >95%; water 0.01 – 2.61%; soil 0.01 – 1.9% and sediment <1.0%. These values are similar to those calculated for classes in the gasoline blending streams test plan. These complex hydrocarbon mixtures partition at >97% to air, where hydrocarbons are rapidly oxidized by OH radicals; partitioning into soil and water does not exceed 1.25 or 2.7% respectively, and partitioning in sediment is minimal.

Biodegradation

The biodegradability of products in the Low Benzene Naphthas category is readily determined from data developed for constituent chemicals of products in this category and from complex products (e.g. gasoline naphtha blending streams) containing similar compounds (aromatic, naphthenics, olefins, paraffins) present in products in this category. The data in Appendix 3, Table A3-1 demonstrate that chemicals in the C5-C12 carbon range found in low benzene naphtha products have biodegraded from 63 - 100% after 14 or 28 days, while results for complex products range from 21 – 96% after 28 days. Table A3-2 summarizes the chemical composition of the gasoline blending streams for which bioavailability data are available, and demonstrates the compositional similarities of these streams to members of the Low Benzene Naphthas category. Much of these data were developed using a manometric respiratory test procedure that employs continuous stirring in closed systems. These data suggest that products in the Low Benzene Naphthas category are expected to demonstrate relatively high biodegradability and hence are not expected to persist in the environment.

4. HUMAN HEALTH HAZARDS

Effects on Human Health

A substantial amount of toxicity data is available for many of the components of the streams in the Low Benzene Naphthas category. Some of the components are SIDS materials, and some components will be tested by other category test plans or by other groups within the EPA or ICCA HPV programs. In addition, a significant amount of testing has already been completed on hydrocarbon streams of similar composition and boiling point ranges.

The streams in the Low Benzene Naphthas category are primarily transferred to the petroleum refining industry for use in blending unleaded gasoline. The API Petroleum HPV Testing Group's Gasoline Blending Streams Test Plan addresses naphtha streams used to formulate unleaded gasoline that are similar in carbon number range and composition to streams in the Low Benzene Naphthas category. The gasoline blending streams are all volatile hydrocarbon liquids at standard temperature and pressure with a boiling range of –20^{0}C to 230^{0}C and a carbon range of C5-C12. Streams in the Low Benzene Naphthas Category are most similar in composition to the high aromatic class (30-95% aromatics) of gasoline blending streams, although they still maintain some similarities to other blending streams.

The API Petroleum HPV Testing Group has reported studies on naphtha streams high in aromatic constituents. These streams include Full Range Catalytic Reformed Naphtha (FRCRN) containing approximately 63% aromatics with approximately 2% benzene, a Light Catalytic Reformed Naphtha (LCRN, 31% aromatics), and a Heavy Catalytic Reformed Naphtha (HCRN, 93% aromatics). Selected properties are presented below. Because of these similarities in composition, toxicity data from the Gasoline Blending Streams Category has been used to characterize the human health hazards of the members of the Low Benzene Naphthas category. Additional details and robust summaries for these studies are available in Gasoline Blending Streams Test Plan located on the US EPA HPV website. Results of studies on a Heavy Aromatic Distillate (CAS #64742-48-9; HAD), HPV stream name Hydrotreated C8-C10, specified in the Low Benzene Naphthas Category are also summarized and robust summaries are provided for these studies [see Attachments 2a-2b]. In addition, developmental toxicity data and in vitro gene tox data from pure toluene will be used to supplement the assessment for the three streams containg high levels of toluene. Results for toluene studies can be found in the European Union Risk assessment report for toluene.

Table 9. Representative High Aromatic Gasoline Blending Streams

	LCRN	FRCRN	HCRN	Low Benzene Naphthas [Overall avgs.]
Carbon number range	C5 - C11	C4 – C12	C7 – C12	C5 – C12
Aromatic Content (%)	31	63	93	~50-100
Benzene	5	2	0	<0.1 – 5
Toluene	29	20	15	<0.1 - 80
Boiling Range ^{0}C	35 -190	30 - 220	90 - 230	27 - 241

Acute Toxicity

Studies in Animals

Table 8. Summary of Acute Toxicity Data

Route	FRCRN	HAD
Oral LD50	Males 6.62g/kg; Females 5.39g/kg	>6.0g/kg
Dermal LD50	> 2.0g/kg	-
Inhalation LC50 [4hr exposure]	> 5220mg/m^3 [fully vaporized]	>8500mg/m^3

Conclusion

High aromatic naphthas demonstrate minimal toxicity by the oral, dermal or inhalation routes of exposure. Acute toxicity results for gasoline streams high in paraffins, olefins and naphthenes were comparable: oral toxicity > 5g/kg, dermal toxicity > 2g/kg and inhalation toxicity > 5000mg/m3 (4 hr exposure). From the available data on materials of similar composition it can be concluded that Low Benzene Naphthas demonstrate minimal acute toxicity.

Irritation [Non-HPV SIDS Endpoints]

Skin Irritation

Studies in Animals

FRCRN: Rabbit: 0.5ml applied to intact or abraded skin, occluded for 24hrs, then dressing removed and residue wiped off. Primary irritation index = 3.1 (Draize scoring system, 24+72hr scores). Moderate skin irritant with erythema and edema of intact or abraded skin completely resolved by 14 days post-exposure.

Eye Irritation

Studies in Animals

FRCRN: Rabbit: 0.1ml applied to corneal surface. After 30 seconds eyes of some rabbits were flushed with lukewarm water; other rabbit eyes left unwashed. No corneal or irradial irritation in washed eyes, in unwashed eyes irradial irritation subsided after 24hrs. Non-irritating

HAD: Rabbit: similar procedure to above. Non-irritating

Conclusion

High aromatic naphtha streams are non-irritating to the eye and are moderate skin irritants. From the available data on materials of similar composition it can be concluded that Low Benzene Naphthas would induce moderate irritation to the skin and minimal to no eye irritation.

4.1.3 Sensitization [Non-HPV SIDS Endpoint]

Studies in Animals

Skin

Guinea pigs were induced with a 50% mixture FRCRN in paraffin oil for 6 hours under an occlusive dressing, once a week for 3 weeks. After a 2 week rest period animals were challenged at a previously untreated site with 25% FRCRN. The site was evaluated for erythema and edema at 24 and 48hrs after exposure. FRCRN did not induce skin sensitization in guinea pigs under conditions of occlusive epicutaneous application.

Conclusion

High aromatic naphtha streams are not expected to be skin sensitizers. From the available data on materials of similar composition it can be concluded that Low Benzene Naphthas are unlikely to be skin sensitizers.

4.1.4 Repeated Dose Toxicity

Studies in Animals

Inhalation

FRCRN (63% aromatics) was evaluated in a 13-week inhalation study using Sprague-Dawley rats. Animals were exposed to the volatile fraction (30-40% partially vaporized to simulate human exposure) at concentrations of 0, 96, 464 and 1894ppm (0, 410, 1970, and 8050 mg/m^3) 5 days/week. Higher kidney (13%) and liver (14%) weights were noted in the high dose males. However, no treatment related abnormalities were observed in any tissue upon histological examination. NOAEL = 1970mg/m^3

Sprague-Dawley rats were exposed by inhalation for 21 days (15 exposures) to wholly vaporized LCRN (31% aromatics) and HCRN (93% aromatics) at concentrations of 0, 544, 1591, and 5522ppm (0, 2000, 5850, and 20300 mg/m^3) and 0, 215, 587, and 2132ppm (0, 1030, 2810, and 10200 mg/m^3), respectively. LCRN induced small concentration-related increases in necrosis of renal tubules and an increased incidence and severity of hyaline droplets, typical of hydrocarbon nephropathy at all doses. No adverse kidney effects were noted after exposure to HCRN however, lung irritation was apparent. In a 13-week study, Sprague-Dawley rats were exposed to a light vapor fraction of LCRN at concentrations of 0, 750, 2500, and 7500ppm (0, 2775, 9250 and 27,750 mg/m^3). The light vapor was tested as the fraction to which humans are most likely exposed, and in this study contained 10% aromatics compared to 33% in the LCRN liquid. No test article related mortality or effects on physical signs, body weight, food consumption or clinical chemistry were observed. A significant decrease in total white blood cell and lymphocyte counts and a decrease in spleen weight were observed at terminal sacrifice in males exposed to 7500ppm, but were not present in animals after a 4-week recovery period. Statistically significant increases in kidney weight relative to body weight in high dose males correlated with microscopically observed hydrocarbon nephropathy. The only effect on neurobehavioral parameters was significantly higher motor activity in the high dose males after the four-week recovery period. However, there was no evidence of hyperactivity or abnormal behavior from the functional observation battery and no microscopic changes in neural tissue. NOAEL = 9250mg/m^3.

Wholly vaporized HAD was administered to Fischer 344 rats, 6hr/day for 5 days at concentrations of 0, 1200, 2700, and 5000mg/m^3. One death occurred during exposure to 5000mg/m^3. All other rats exhibited clinical signs including ocular discharge, eye closure and dry red material around nose/mouth, which increased in overall incidence in a dose related manner. No gross pathological lesions were attributed to test material administration. No histology was performed. LOEL = 1200mg/m^3.

Dermal

FRCRN was evaluated in a 28-day dermal toxicity study (New Zealand White rabbit) at doses of 0, 200, 1000, and 2000 mg/kg/day, 3 days/week. Moderate to severe skin irritation was noted at all doses. Three males (2 high dose, 1 mid dose) died. Deaths occurred on day 12 and 17 for high dose animals, and on day 19 at the mid dose. At 2000mg/kg/day, females showed no weight gain and males had an overall weight loss. Histopathologic examination revealed slight-moderate proliferative and inflammatory changes in skin at the highest dose concurrent with granulopoiesis of bone marrow, attributed to stress and other factors associated with skin irritation. No other significant findings were noted.

HAD was evaluated in a 4 week study with Fischer 344 rats at concentrations of 0, 500, 1000, and 1500mg/kg in paraffin oil vehicle, unoccluded, once a day, 5 days/wk. Severe skin irritation [including ulceration, acanthosis and hyperkeratosis] and decreased food consumption were observed. Significantly elevated WBC counts and mild anemia associated with decreased RBC, decreased hematocrit, hemoglobin in peripheral blood and elevated platelet counts also occurred.

Oral

No studies are available

Conclusion

Inhalation studies of high aromatic naphtha streams demonstrated some effects in the lung (irritation), blood and kidneys of treated rats at high doses. Effects on lung and blood were no longer observed after a 4-week recovery period. No significant neurobehavioral or neuropathologic effects were observed when measured. In studies where histopathology was performed, the only systemic effect was slight hydrocarbon nephropathy in male rats, a species and sex specific effect that is not relevant to human health (U.S. EPA, 1991). Inhalation studies of gasoline blending streams representing two of the other PONA classes –paraffins and olefins – resulted in similar results to the high aromatic naphtha stream data, including increases in liver weight and hyperplasia of the nasal epithelium (high olefins) which were not present after 4 weeks recovery. Increased male kidney weight and hydrocarbon nephropathy were consistently observed at the highest doses with more severe expression when alkane content was highest. NOAEL values for the other gasoline blending streams ranged from 5474 –8102mg/m^3, dependent on vapor composition. Results of repeated dose dermal studies of naphthas with relatively high aromatic content demonstrated that test materials induced skin irritation and systemic effects primarily related to skin damage and accompanying stress. Irritation and accompanying systemic effects were also seen in the other refinery streams relatively high in paraffin, olefins and napthenes. Mild anemia was also observed with exposure to HAD. The amount of toluene in gasoline blending streams did not appear to contribute to substantial neurobehavioral effects even at stream doses well above likely human exposure. Toluene itself has been reported to induce neurobehavioral effects in humans with long-term exposures above the 50ppm TLV and in animals at high concentrations. Toluene and gasoline have been demonstrated to induce neurotoxic effects at high exposure conditions of hydrocarbon abuse. Based on data from representative high aromatic naphtha blending streams, inhalation exposure to Low Benzene Naphthas at concentrations above 1030mg/m^3 for wholly vaporized samples or above 1970-9250mg/m^3 for partially vaporized samples may induce irritation in the nasal passages and lungs, and effects on the hematopoietic system and liver weights, most of which are resolved with cessation of exposure. Light hydrocarbon nephropathy, a male rat specific effect, not relevant to humans, may occur. Dermal exposure may cause skin irritation and at high doses, the related systemic effects due to severe irritation and stress.

4.1.5 Mutagenicity

In vivo Studies

FRCRN, LCRN, and HCRN were tested in rat chromosome aberration assays using a single intraperitoneal injection at concentrations of 0.0, 0.3, 1.0, and 2.5-3.0g/kg in corn oil. Rats were killed at 6, 24, and 48 hours post-dose to evaluate all stages of cell cycles in bone marrow lymphocytes. None of these materials induced chromosome aberrations or disruption of cell cycle kinetics in this assay.

HAD was tested in a mouse bone marrow micronucleus assay by oral administration of 0.0, 625, 1250 and 2500mg/kg in corn oil, 1dose/day for 2 days and 2500mg/kg for one dose only. One female given 2500mg/kg for 2 days died by day 4. Surviving animals did not demonstrate any significant changes in micronucleus formation or in the ratio of polychromatic/normochromatic erythrocytes as a measure of toxicity at any dose level.

In vitro Studies

LCRN (42% aromatic) did not induce mutagenic events in the mouse lymphoma (L5178Y TK+/-) forward mutation assay with or without metabolic activation. FRCRN (63% aromatic) was negative in the absence of metabolic activation and positive in the presence of metabolic activation. HCRN (90% aromatics) gave positive and equivocal results with and without activation, respectively. The occurrence of positive results in the presence of metabolic activation correlated with the concentrations of aromatic components greater than 60%. Polynuclear aromatic compounds can be converted to active mutagens by P450-rich liver homogenates used in both bacterial and mammalian cell systems.

Toluene did not induce gene mutations in the bacterial reverse mutation assay (Ames assay), Mouse Lymphoma assay or Sister Chromatid exchange assay.

HAD did not induce gene mutation in the Chinese hamster ovary (CHO) cell system with or without metabolic activation and did not cause DNA perturbation as measured by unscheduled DNA synthesis in rat primary hepatocyte cultures at any dose level.

Conclusion

In vitro mutagenic activity in mammalian cells demonstrated by naphtha streams high in aromatic content, when present, occured primarily with metabolic activation and correlated with higher ratios of aromatics in the test sample (60-90%). However, streams with high aromatic content largely due to the presence of toluene would not be expected to induce similar genetic toxicity. Only HCRN (90% aromatics) showed equivocal results on plates without metabolic activation. The heavy aromatic distillate that is part of the Low Benzene Naphthas category did not induce gene mutations or DNA perturbation in mammalian cells. *In vivo*, naphtha streams containing relatively high aromatic and low benzene content do not induce cytogenetic damage. Other gasoline blending streams (P-, O-, N-rich) did not induce *in vitro* genetic toxicity or cytogenetic damage in animals: NOAEL = 3000mg/kg [ip] or > 7400mg/m^3 by inhalation Overall, the Low Benzene Naphthas streams are expected to have a low potential for gene mutation or DNA perturbation.

4.1.6 Carcinogenicity [Non-HPV SIDS Endpoint]

In vivo Studies

No studies are available for low benzene naphthas or for any gasoline blending streams. For comparative purposes, a two-year inhalation carcinogenesis bioassay was performed with wholly vaporized unleaded gasoline at actual concentrations of 0, 67, 292 and 2056ppm (250, 1089, 7672mg/m^3) administered to rats and mice (McFarland et al, 1984). Mortality rates were unaffected. Rats and mice in the highest dose group had lower body weights throughout the study. In mice, liver tumors were present in high dose females. Kidney weights of male rats were elevated accompanied by light hydrocarbon nephropathy at interim sacrifices and dose related incidences of kidney tumor at terminal sacrifice. These kidney lesions have been determined to be species and sex specific and not relevant to humans (U.S. EPA, 1991). Nephrotoxic activity appeared attributable to the alkane constituents in gasoline (Halder et al., 1984).

In vitro Studies

HAD was tested in a mouse embryo (BALB/3T3) transformation assay, a predictive assay for possible carcinogenc potential. Heavy aromatic distillate did not induce cell transformation at any dose level tested.

Conclusions

In vitro data demonstrated that a representative low benzene naphtha did not induce cell transformation, a predictor of cancer potential, in mammalian cells. Although no carcinogenesis studies were available on low benzene naphthas, extrapolation from 2-year cancer bioassays on toluene and gasoline indicate the materials comprising this category that contain a higher proportion of aromatics and fewer alkanes, are unlikely to induce cancer relevant to human health, especially at the lower doses to which humans are most frequently exposed.

4.1.7 Toxicity for Reproduction

Effects on Fertility

A distillate of LCRN administered to male and female Sprague-Dawley rats by inhalation at target concentration of 0, 750, 2500, and 7500 ppm (0, 2775, 9250 and 27,750 mg/m^3) according to OECD protocol 421, did not affect reproductive performance, delivery data or live pups/litter. The light vapor was tested as the fraction to which humans are most likely exposed, and in this study contained 10% aromatics compared to 33% in the LCRN liquid. Offspring showed comparable body weights, weight gain, and viability at postnatal day four. Parental systemic effects observed at the highest dose were slightly reduced body weights, increased kidney to body weight and liver to body weight ratios in high dose males. No histological changes were seen in reproductive organs of treated rats. NOAEL reproduction = 27,750mg/m^3; NOAEL parental = 9250mg/m^3. Data from a toluene 2-generation reproductive toxicity study can be used to read across to those streams high in toluene content. Rats exposed to concentrations up to 7500 mg/m^3 did not exhibit adverse effects on any reproductive parameters (NOAEL repro 7500 mg/m^3).

Developmental Toxicity

FRCRN was tested in a developmental toxicity screen by exposing pregnant Sprague-Dawley rats to partially vaporized (30 – 40%) FRCRN, via inhalation at concentrations of 0, 508 and 1835 ppm (0, 2160, 7800 mg/m^3) on gestation days 6-19. Animals were sacrificed on day 20 of gestation. Maternal body weights, serum chemistry, and organ weights were unaffected. No adverse effects were observed on fetal parameters at sacrifice (viability, fetal body weight, external development) or subsequent skeletal and visceral examinations. In contrast, several studies on toluene have shown decreased fetal body weight and delayed development at concentrations greater than 2250 mg/m^3. NOAEL developmental = 7800mg/m^3.for streams with less than 30% toluene content and 2250 mg/m^3 for streams with higher toluene content.

Conclusion

No significant reproductive or developmental effects were observed for these high aromatic streams. Parental systemic effect observed at the highest dose of LCRN distillate, slightly reduced body weight for males, increased kidney to body weight and liver to body weight ratios, did not have any effect on reproductive performance or fertility. Reproductive and developmental toxicity studies with gasoline blending streams high in olefinic naphthenic, or paraffinic content (data not summarized here- see Gasoline Blending Streams Test Plan) had similar findings. The absence of naphtha-induced significant toxicity for these endpoints is supported by comparable data on gasoline and data on individual components found in other high aromatic streams: benzene, xylenes and C9 and above aromatics [Attachment 2]. No adverse reproductive effects were observed for toluene however, several developmental toxicity studies reported decreased fetal body weights and delayed development. Based on available data, Low Benzene Naphthas containing less than 30% toluene are unlikely to induce reproductive or developmental toxicity. For those streams higher in toluene content decreased fetal body weight and delayed development is possible.

4.2 Assessment Summary for Human Health

Existing data are sufficient to characterize human health hazards of substances included in the Low Benzene Naphthas Category and thus, satisfy HPV program requirements. From available data, and read-across from streams of similar composition in the API Gasoline Blending Streams test plan, it can be concluded that Low Benzene Naphthas are not acutely toxic, are irritating to the skin and minimal or not irritating to the eyes, and are not skin sensitizers. These materials do not induce genetic damage *in vivo*. *In vitro* mutagenesis in mammalian cells is correlated with the level of aromatic constituents in the stream tested. Repeated dose inhalation studies showed some effects at high doses which did not have histopathological correlates and appeared reversible after 4 weeks recovery, with the exception of light hydrocarbon nephropathy in male rats (a species and sex specific effect) and no neurobehavioral or neuropathologic effects. Neurotoxicity reportedly induced by toluene, a major constituent of some of the low benzene naphtha streams, has not been demonstrated in these blending stream studies, possibly because the concentration in the blended materials was not high enough or competitive inhibition with other hydrocarbons occurred. No significant reproductive or developmental toxicity was observed in streams containing less than 30% toluene. The results of these studies are similar to those from other naphtha streams, presented in the Gasoline Blending Streams Test Plan (API, 2003). These similarities demonstrate that hydrocarbon streams, comprised of the same molecules along a continuum of concentrations, affect the same organ/tissue systems. Small alterations in composition do not significantly alter the biological responses. The consistency of results in mammalian studies for materials representing this range of naphthas justifies the designation of Low Benzene Naphthas as a category for HPV.

5 HAZARDS TO THE ENVIRONMENT

5.1 Aquatic Effects

Acute Toxicity Test Results

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 Low Benzene Naphthas Category, there are sufficient read across data from constituent chemicals of those products and comparably complex products to fully characterize the toxicity of this category. Study specifics and robust summaries for high aromatic blending streams are available in the API Gasoline Blending Streams test plan on the US EPA HPV website. The use of data from selected read across materials to products in this category can be justified for the following reasons:
- Individual chemicals and complex products used for read across purposes contain a chemical class or combinations of chemical classes (i.e., olefins, aromatics, paraffins) that are found in 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 all act by a similar mode of toxic action.

The data in Appendix 4, Table A4-1 provides a comparison of the range of product compositions (i.e., carbon number, chemical class, weight percent) in the Low Benzene Naphthas Category to products that have been used to characterize the aquatic toxicity of this category. This comparison illustrates the similarity in carbon number ranges between products in this category and the selected products with read across data.

The data in Appendix 4, Tables A4-2 (Fish), A4-3 (Daphnia), and A4-4 (Algae) establish the range of toxicity for products in this category, based on the read across data. Generally, the fish, invertebrate, and alga studies followed the OECD Guidelines 203, 202, and 201, respectively. For complex products, the test procedures used to develop the test material exposure solutions also applied the OECD guidance described in "Guidance Document on Aquatic Toxicity Testing of Difficult Substances and Mixtures" (OECD, 1999). For these studies, the results are represented as lethal loading (LL) endpoints, a designation used to define results for multi-hydrocarbon mixtures, tested as water accommodated fractions [WAF], compared to the data developed for pure chemicals, which represent results as lethal concentration endpoints where test material is analytically verified. Low benzene naphthas are likely to produce moderate level of toxicity in freshwater algae and a moderate level of acute toxicity in freshwater fish and invertebrates.

For representative chemicals and products, experimental acute fish toxicity values range between 2.5 to 46.0 mg/L for two species (Table A4-2), while acute invertebrate (Daphnia) toxicity values range between 0.9 to 32 mg/L for one species (Table A4-3). In comparison, alga toxicity values for one species range between 1.0 to 64 mg/L (for biomass or growth rate endpoints), while alga loading rate NOELR values range between 1.0 to 51 mg/L (for biomass and growth rate endpoints) (Table A4-4).

The fairly narrow range of effect is expected because the chemical constituents of products in this category are neutral organic hydrocarbons whose toxic mode of action is non-polar narcosis. The mechanism of short-term toxicity for these chemicals is disruption of biological membrane function (Van Wezel and Opperhuizan, 1995), and the differences between measured toxicities (i.e., LC/LL50, EC/EL50) can be explained by the differences between the target tissue-partitioning behavior of the individual chemicals (Verbruggen, et al., 2000).

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

Chronic Toxicity Test Results [Non-HPV SIDS endpoint]

Light catalytic reformed naphtha, a high aromatic gasoline blending stream was tested as a water accommodated fraction (WAF) for 21 days with *Daphnia magna* and for 14 days with Fathead Minnow. Results were:

Daphnia Reproductive EL50 =14mg/L; NOEL <0.30mg/L.
Fathead Minnow LL50 [survival] = 5.2mg/L
NOEL [survival & growth] = 2.6mg/L

5.2 Assessment Summary for the Environment

The environmental impact of products in the Low Benzene Naphthas Category has been determined by evaluating data developed for chemical components found in the products in this category and for similar complex products. The hydrocarbons that comprise this category have a very low potential to hydrolyze and do not photodegrade directly due to a minimal capacity to absorb appreciable light energy above 290nm. However, atmospheric oxidation constitutes a significant route of degradation. Calculation of atmospheric half-lives of representative constituent chemicals identified a range of 2.3-31.8 hours as a result of indirect hydrolysis by hydroxyl radical attack. Fugacity modelling demonstrated that members of this category partition primarily into the air, with slight partitioning into water and soil, and minimal partitioning into sediment. Read-across data shows that these products are likely to biodegrade significantly and have the potential to produce a moderate level of toxicity in freshwater algae and a moderate level of acute toxicity in freshwater fish and invertebrates. Aquatic toxicity for products in this category can be predicted based on carbon number, measured or calculated toxicities of constituent hydrocarbons and constituent composition.

Extensive data on chemical components of the products in this category and on streams containing similar mixtures of complex hydrocarbons have demonstrated that, based on biological and physical degradation processes, products in the Low Benzene Naphthas Category, although moderately toxic to aquatic species at exposure, are not expected to persist in the environment. The consistency of results in environmental studies for these materials justifies the designation of Low Benzene Naphthas as a category for HPV.

6. PROGRAM SUMMARY AND RECOMMENDATIONS

The Low Benzene Naphthas Test Plan has addressed nine petrochemical streams (products) derived from ethylene and associated manufacturing processes. The category is comprised of 12 CAS numbers and 9 petrochemical streams. The category includes complex hydrocarbons mixtures containing primarily C5 through C12 olefins, paraffins, naphthenes and aromatic molecules. The benzene content of these streams is typically less than 2% but may be as high as 5%. All of these products are produced and transferred in closed system so that occupational and public exposure to individual or combined streams is very low.

The Low Benzene Naphthas category streams have many of the same components as gasoline blending streams outlined in the API Gasoline Blending Streams test plan (EPA HPV website, 2003) and about 90% of the low benzene naphthas category volume is blended into gasoline. The Low Benzene Naphthas are compositionally most similar to the high aromatic naphtha blending streams. For these reasons, the mammalian and environmental test data developed for the Gasoline Blending Streams test plan were appropriately used as ‘read-across’ results for Low Benzene Naphthas endpoints, and along with toluene data and data developed for this test plan, provide a well developed human health and environmental profile of Low Benzene Naphthas.

Human Health Effects: Evaluation of available mammalian data and “read-across” from streams of similar carbon number range and composition in the API Gasoline Blending Streams test plan, indicate that Low Benzene Naphthas are not acutely toxic, are irritating to the skin but minimally or not irritating to eyes, and are not skin sensitizers. These materials do not induce genetic damage *in vivo*. *In vitro* mutagenesis in mammalian cells is correlated with the level of aromatic constituents in the stream tested. Repeat dose inhalation studies of representative blending streams showed effects in some organ systems at high doses, which did not have histopathologic correlates and were not present after 4-weeks recovery. The exception was occurrence of hydrocarbon nephropathy in male rats, a species and sex specific effect not relevant to human health. No significant neurobehavioral or neuropathological effects were seen. No significant reproductive or developmental toxicity was observed for streams containing less than 30% toluene. However, decreased fetal body weights and delayed development is possible for those streams containing greater than 50% toluene.

Physicochemical, Environmental and Aquatic Endpoints: For environmental endpoints, measured data on components present in the products of the Low Benzene Naphthas category, and on other complex products that contain a similar range of chemical classes and carbon numbers were used. Where measured data do not exist, calculated data for selected constituents of these naphthas have been developed using the EPIWIN© computer models described by EPA. The hydrocarbons that comprise this category have a very low potential to hydrolyze and do not photodegrade directly due to a minimal capacity to absorb appreciable light energy above 290nm. However, atmospheric oxidation constitutes a significant route of degradation. Calculation of atmospheric half-lives of representative constituent chemicals identified a range of 2.3-31.8 hours as a result of indirect hydrolysis by hydroxyl radical attack. Fugacity modeling demonstrated that members of this category partition primarily into the air, with slight partitioning into water and soil, and minimal partitioning into sediment. Read-across data shows that these products are likely to biodegrade significantly and have the potential to produce a moderate level of toxicity in freshwater algae and a moderate level of acute toxicity in freshwater fish and invertebrates.

The extensive body of data available for mammalian and environmental endpoints on representative constituents of products in this category and on gasoline blending streams of similar complex hydrocarbon composition are sufficient to fully characterize the potential toxicity for materials in this category and demonstrate the integrity of the category, itself. No additional testing is needed to fulfill the requirements of the HPV program.

Table 11. Physico-Chemical and Environmental Data Used to Characterize Streams and CAS RNs in the Low Benzene Naphthas Category

ENDPOINT	Low Benzene Naphthas Category Streams and CAS RNs								
	Pyrolysis C7s 68527-23-1 + 68478-10-4	Pyrolysis C7-C12 fraction 68516-20-1 + 64742-83-2 + 68476-45-9	Pyrolysis C7-C8 fraction 68527-23-1 + 68919-15-3	Hydrotreated C7+ fraction 64742-48-9	Hydrotreated C7-C12 fraction 64742-48-9 + 68516-20-1	Hydrotreated C8-C10 fraction 68512-78-7 + 64742-48-9	Hydrotreated C5/C9 Blend 64742-49-0	C9+ from xylene unit 68333-88-0 + 68553-14-0	Toluene Extract 64741-98-6
Boiling Point Range (°C @760 mm Hg)	27.8 to 241.1 (b, m)								
Vapor Pressure Range (hPa @ 25 °C)	0.05 to 9.19E2 (b, m)								
Log P_{ow} Range (25 °C)	2.54 to 3.72 (a, c)					2.72 to 3.72 (a-1, c)			2.54 to 3.72 (a, c)
Melting Point/ Range (°C)	-159.9 to 80.2 (b, m)								
Water Solubility/ Range (mg/L @ 25 °C)	21.5 to 832.7 (a, c)					21.5 to 386.7 (a-1, c)			21.5 to 832.7 (a, c)
Direct Photodegradation	Direct Photolysis will not contribute to degradation								
Indirect (OH-) Photodegradation (half-life, hrs)	2.3 to 31.8 (c,d)								
Hydrolysis	Hydrolysis will not contribute to degradation								
Distribution (c)	95 to 99% air; 0.01 to 2.6% water, 0.01 to 1.9% soil; <1.0% sediment (e-1)	24 to 99% air; 0.01 to 3.2% water; 0.01 to 42% soil; <1.0% sediment (e-2)	95 to 99% partitions to air; 0.01 to 2.6% to water, 0.01 to 1.9% to soil; <1.0% to sediment (e-1)			24 to 99% to air; 0.01 to 3.2% to water; 0.01 to 42% to soil; <1.0% sediment (e-2)			95 to 99% to air; 0.01 to 2.6% water, 0.01 to 1.9% soil; <1.0% to sediment (e-1)

(a) Constituent chemicals used to define selected endpoints are isopentane, toluene, m-xylene, styrene, naphthalene, tricyclodecane, methyl-naphthalene
(a-1) All of a except toluene: (b) Constituent chemicals used to define selected endpoints are toluene, m-xylene, styrene, naphthalene, methyl-naphthalene
(m) Measured values (c) Calculated values (d) Atmospheric half-life values are based on a 12-hr. day.
(e-1) Constituent chemicals are isopentane, toluene, m-xylene, styrene, tricyclodecane, methyl naphthalene; (e-2) All of e-1 + naphthalene**Table**

Table 11 . Physico-Chemical and Environmental Data Used to Characterize Streams and CAS RNs in the Low Benzene Naphthas Category

ENDPOINT	Low Benzene Naphthas Category Streams and CAS RNs								
	Pyrolysis C7s 68527-23-1 + 68478-10-4	Pyrolysis C7-C12 fraction 68516-20-1 + 64742-83-2 + 68476-45-9	Pyrolysis C7-C8 fraction 68527-23-1 + 68919-15-3	Hydrotreated C7+ fraction 64742-48-9	Hydrotreated C7-C12 fraction 64742-48-9 + 68516-20-1	Hydrotreated C8-C10 fraction 68512-78-7 + 64742-48-9	Hydrotreated C5/C9 Blend 64742-49-0	C9+ from xylene unit 68333-88-0 + 68553-14-0	Toluene Extract 64741-98-6
Biodegradation	63 to 100% degradation after 14 or 28days (RA from individual C5-C12 chemicals, a); 21 to 96% degradation after 28 days (RA from C5-C12 hydrocarbon mixtures, b)								
96-hr Fish LC50/ LL50 (mg/L)	LC50 =14.6 LL50 = 46 (RA-c)	LC50 range = 2.5 to 16.4 (RA from individual C5-C12 chemicals, d); LL50 range = 3.0 to 48 (RA from C5-C12 hydrocarbon mixtures, b)						3.0 to 34 (RA-i)	LC50 = 2.6 to 16.4 (RA-l)
14 day Fish	LL50 [survival] = 5.2mg/l; NOEL [survival and growth] = 2.6mg/L (RA from LCRN) Non-HPV SIDS endpoint								
48-hr Invertebrate EC50/EL50 (mg/L)	EC50 = 14.9 EL50 = 18.0 (RA-c)	EC50 range = 0.9 to 18.0 (RA from individual C5-C12 chemicals, e); EL50 range = 3.0 to 32 (RA from C5-C12 hydrocarbon mixtures, f)						3.0 to 21.3 (RA-j)	EC50 = 1.0 to 14.9 (RA from toluene, o-, m-xylene)
21 day Invertebrate	Reproductive EL50 = 14mg/L; NOEL < 0.30mg/L (RA from LCRN) Non-HPV SIDS endpoint								
72-hr Alga EC50/EL50 (mg/L)	$EL50_B$ = 64 (RA from LCCN)	$EL50_B$ range = 1.0 to 64 (RA-g) $EL50_R$ = 1.0 (RA from C8-C10 and C8-C14 aromatics); $EC50_R$ = 7.5 (RA from n-pentane for C5/C9 blend only)						$EL50_B$ = 1 to 8.5 $EL50_R$ = 1-3 (RA-k)	$EL50_B$ = 8.5 (RA from LCRN [29% toluene])
72-hr Alga NOEC/NOELR (mg/L)	$NOELR_B$ = 51 (RA from LCCN	$NOELR_B$ range = 5.0 to 51 (RA from C5-C12 hydrocarbon mixtures, h) $NOELR_R$ range = 1.0 to 2.0 (RA from n-pentane, C8-C10 and C8-C14 aromatics)						$NOELR_B$ = 1.0 $NOELR_R$ = 1.0 (RA from C8-C10 & C8-C14 aromatics)	$NOELR_B$ = 5.0 (RA from LCRN [29% toluene])

RA = Read across B = Algal biomass R = Algal growth rate

a = Based on results from n-pentane, isopentane, cyclohexane, 1-hexene (linear), benzene, toluene, p-xylene, styrene.

b = Based on results from Alkenes, C6 rich or C7-C9, C8 rich, Light Alkylate Naphtha [LAN], Light Catalytically Cracked Naphtha [LCCN], Light Catalytically Reformed Naphtha [LCRN], C8-C10 Aromatics (C9 alkylbenzene) and C8-C14 Aromatics (alkyl naphthalenes and naphthalene).

c = Based on results from toluene [concentration values] and LCCN [loading values].

d = Based on results from n-pentane, n-hexane, benzene, toluene, xylenes (o, p), ethyl benzene, 1,2, trimethyl benzene.

e = Based on results from n-pentane, n-hexane, cyclopentane, benzene, toluene, xylenes (o, m), naphthalene.

f = Based on results from LCRN, LAN, LCCN, C8-C10 Aromatics (C9 alkylbenzene) and C8-C14 Aromatics (alkyl naphthalenes and naphthalene).

g = Based on results from benzene, LCRN, LAN, LCCN, C8-C10 Aromatics (C9 alkylbenzene) and C8-C14 Aromatics (alkyl naphthalenes & naphthalene).

h = Based on results from LCRN, LAN, LCCN, C8-C10 Aromatics (C9 alkylbenzene) and C8-C14 Aromatics (alkyl naphthalenes & naphthalene).

i = Based on results from ethyl benzene, 1,2,4 trimethylbenzene, LCRN, C8-C10 Aromatics (C9 alkylbenzene) and C8-C14 Aromatics (alkyl naphthalenes & naphthalene).

j = Based on results from naphthalene, LCRN, C8-C10 Aromatics (C9 alkylbenzene) and C8-C14 Aromatics (alkyl naphthalenes & naphthalene).

k = Based on results from LCRN, C8-C10 Aromatics (C9 alkylbenzene) and C8-C14 Aromatics (alkyl naphthalenes & naphthalene).

l = Based on results from toluene, ethyl benzene and xylenes (o, p).

12 . Human Health Data to Characterize Streams and CAS RNs in the Low Benzene Naphthas Category

<table>
<tr><th rowspan="2">ENDPOINT</th><th colspan="9">Low Benzene Naphthas Category Streams and CAS RNs</th></tr>
<tr><th>Pyrolysis C7s
68527-23-1 + 68478-10-4
(70% toluene)</th><th>Pyrolysis C7-C12 fraction
68516-20-1 + 64742-83-2 + 68476-45-9</th><th>Pyrolysis C7-C8 fraction
68527-23-1 + 68919-15-3</th><th>Hydrotreated C7+ fraction
64742-48-9</th><th>Hydrotreated C7-C12 fraction
64742-48-9 + 68516-20-1</th><th>Hydrotreated C8-C10 fraction
68512-78-7 + 64742-48-9
(HAD)</th><th>Hydrotreated C5/C9 Blend
64742-49-0</th><th>C9+ from xylene unit
68333-88-0 + 68553-14-0</th><th>Toluene Extract
64741-98-6
(75 - 80% toluene)</th></tr>
<tr><td>Acute Toxicity (oral, rat)</td><td colspan="5">> 5.0g/kg (RA FRCRN, HAD, toluene)</td><td>>6.0g/kg</td><td colspan="3">> 5.0g/kg (RA FRCRN, HAD, toluene)</td></tr>
<tr><td>Acute Toxicity (dermal, rabbit)</td><td colspan="9">>2.0g/kg (RA FRCRN)</td></tr>
<tr><td>Acute Toxicity (inhalation, rat)</td><td colspan="5">>5000mg/m^3 (RA FRCRN)</td><td>>8500mg/m^3</td><td colspan="3">>5000mg/m^3 (RA FRCRN)</td></tr>
<tr><td>Eye Irritation (rabbit)</td><td colspan="5">Non-irritating (RA FRCRN, HAD)</td><td>Non-irritating</td><td colspan="3">Non-irritating (RA FRCRN, HAD)</td></tr>
<tr><td>Skin Irritation (rabbit)</td><td colspan="9">Moderate skin irritant (RA FRCRN)</td></tr>
<tr><td>Skin Sensitization</td><td colspan="9">Not a skin sensitizer in guinea pigs (RA FRCRN, toluene)</td></tr>
<tr><td>Repeat Dose Toxicity (inhalation, rat)</td><td colspan="5">LOAEL = 1030-2000mg/m^3; 21 d (RA LCRN, HCRN, HAD whole vapor)
NOAEL = 1970–9250mg/m^3 13 wks (RA FRCRN, LCRN partial vapor)</td><td>LOAEL=1200 mg/m^3 whole vapor (5 days)</td><td colspan="3">LOAEL = 1030-2000mg/m^3; 21 d (RA LCRN, HCRN, HAD whole vapor)
NOAEL = 1970–9250mg/m^3 13 wks (RA FRCRN, LCRN partial vapor)</td></tr>
<tr><td>Repeat Dose Toxicity (dermal)</td><td colspan="5">NOAEL = 1000mg/kg (3d/wk; 28 days, rabbit) (RA FRCRN)</td><td>LOAEL male =500mg/kg; NOAEL female= 1000mg/kg (5d/4wk rat)</td><td colspan="3">NOAEL = 1000mg/kg (3d/wk; 28 days, rabbit) (RA FRCRN)</td></tr>
</table>

Table 12 . Human Health Data to Characterize Streams and CAS RNs in the Low Benzene Naphthas Category [cont]

<table>
<tr><th rowspan="2">ENDPOINT</th><th colspan="9">Low Benzene Naphthas Category Streams and CAS RNs</th></tr>
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64742-48-9 + 68516-20-1</th><th>Hydrotreated C8-C10 fraction
68512-78-7 + 64742-48-9
(HAD)</th><th>Hydrotreated C5/C9 Blend
64742-49-0</th><th>C9+ from xylene unit
68333-88-0 + 68553-14-0</th><th>Toluene Extract
64741-98-6
(75 - 80% toluene)</th></tr>
<tr><td>Genetic Toxicity <i>in vitro</i></td><td>Negative) (RA toluene [Ames, ML, SCE])</td><td>Positive (RA FRCN, HCRN [ML])</td><td>Negative (RA HAD [CHO, UDS] and toluene [Ames, ML, SCE])</td><td colspan="2">Positive (RA FRCN, HCRN [ML])</td><td>Negative (CHO, UDS)</td><td>Negative (RA HAD [CHO, UDS], LCRN [ML])</td><td>Positive (RA FRCN, HCRN [ML])</td><td>Negative (RA toluene [Ames, ML, SCE])</td></tr>
<tr><td>Genetic Toxicity <i>in vivo</i></td><td>Negative – SCE, CA (RA toluene)</td><td colspan="4">Negative CA (RA FRCRN, LCRN, HCRN)
Negative MN (RA HAD, toluene)</td><td>Negative -MN</td><td colspan="2">Negative CA (RA FRCRN, LCRN, HCRN)
Negative MN (RA HAD, toluene</td><td>Negative – SCE, CA (RA toluene)</td></tr>
<tr><td>Reproductive Toxicity (inhalation, rat)</td><td>NOAELrepro = 7500mg/m^3 2-generation (RA toluene)</td><td>NOAEL repro = 27,750mg/m^3 (RA LCRN light ends OECD 421)</td><td>NOAELrepro= 7500mg/m^3 2-generation (RA toluene)</td><td colspan="5">NOAEL repro = 27,750mg/m^3 (RA LCRN light ends OECD 421)</td><td>NOAELrepro= 7500mg/m^3 2-generation (RA toluene)</td></tr>
<tr><td>Developmental Toxicity (inhalation, rat)</td><td>NOAEL = 2250mg/m^3 (600ppm) (RA toluene)</td><td>NOAEL = 7800mg/m^3 (RA FRCRN [30-40% vaporized])</td><td>NOAEL = 2250mg/m^3 (600ppm) (RA toluene)</td><td colspan="5">NOAEL = 7800mg/m^3 (RA FRCRN [30-40% vaporized])</td><td>NOAEL = 2250mg/m^3 (600ppm) (RA toluene)</td></tr>
</table>

RA = Read-across data

FRCRN = Full range catalytic reformed naphtha; **LCRN** = Light catalytic reformed naphtha; **HCRN** = Heavy catalytic reformed naphtha.

CHO = Chinese Hamster Ovary cells; **UDS** = Unscheduled DNA synthesis; **ML** = Mouse lymphoma cells; **SCE** = Sister Chromatid Exchange;

Ames =Ames Salmonella assay; **MN** = Mammalian Bone Marrow Erythrocyte Micronucleus assay; **CA** = Bone Marrow Chromosome Aberrations

7. References

American Petroleum Institute (API) 1993. Gasoline Vapor Exposure Assessment at Service Stations. Clayton Environmental Consultants API Publication #4553. Washington, DC: API.

API Monthly Statistical Report vol. 23, no.12. December, 1999. Washington, DC:

API Petroleum HPV Testing Group. 2003. Gasoline Blending Streams Test Plan and Robust SummariesAPI, Washington, D.C. EPA website for HPV Chemical Challenge test plans: http://www.epa.gov/chemrtk/viewsrch.htm.

CONCAWE, the Oil Companies' European Organization for Environmental and Health Protection. Gasolines. 1992: Product dossier No. 92/103. Brussels, Belgium: CONCAWE.

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

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

European Union [Danish Environmental Protection Agency] 2003. Risk Assessment Report: Toluene in accordance with Council regulation (ECC 793/93). SIAR 10888.

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

Halder, C.A., Warne, T.M., and Hatoum, N.S. 1984. Renal toxicity of gasoline and related petroleum naphthas in male rats. Chapter VI in Renal Effects of Petroleum Hydrocarbons, Mehlman et al., Eds. Princeton Scientific Publishers, Princeton, NJ pp. 73-88

MacFarland, H.N., Ulrich, C.E., Holdsworth, C.E., Kitchen, D.N., Halliwell, W.H., Blum, S.C. A chronic inhalation study with unleaded gasoline vapor. *J. Am. Coll. Toxicol*. 1984; 3: 231-248.

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

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

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

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

Olefins Panel HPV Implementation Task Group. 2003. High Production Volume (HPV) Chemical Challenge Program Test Plan (Revised) for the Low Benzene Naphthas Category. American Chemical Council, VA. USA. EPA website for HPV Chemical Challenge test plans: http://www.epa.gov/chemrtk/viewsrch.htm.

Roberts, L., White, R., Bui, Q., Daughtrey, W., Koschier, F., Rodney, S., Schreiner, C., Steup, D., Breglia, R., Rhoden., Schroeder., and Newton, P. 2001. Developmental toxicity evaluation of unleaded gasoline vapor in the rat. Reproductive Toxicol. 15:

U.S. Environmental Protection Agency (U.S. EPA). 1991. Alpha 2 microglobulin: association with chemically induced renal toxicity and neoplasia in the male rat. In Risk Assessment Forum. US Government Printing Office, Washington, DC: EPA:85

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

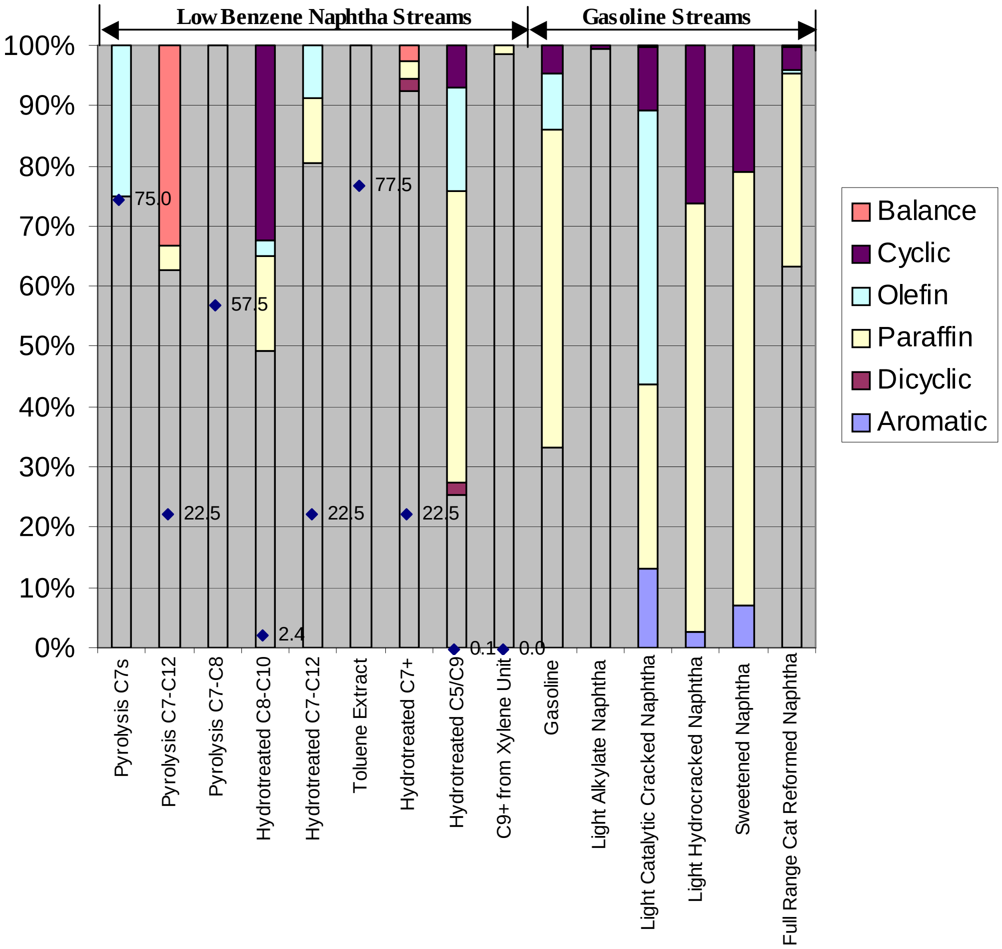
U.S. EPA. 1999b. Determining the Adequacy of Existing Data. OPPT, EPA., Washington, DC, USA.

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

Verbruggen et al. 2000. Polyacrylate-Coated SPME Fibers as a Tool To Simulate Body Residues and Target Concentrations of Complex Organic Mixtures for Estimation of Baseline Toxicity. Environ. Sci. Technol. 34: 324-331

Figure 4.

Composition Data - Low Benzene Naphthas Category Streams and Gasoline Streams.

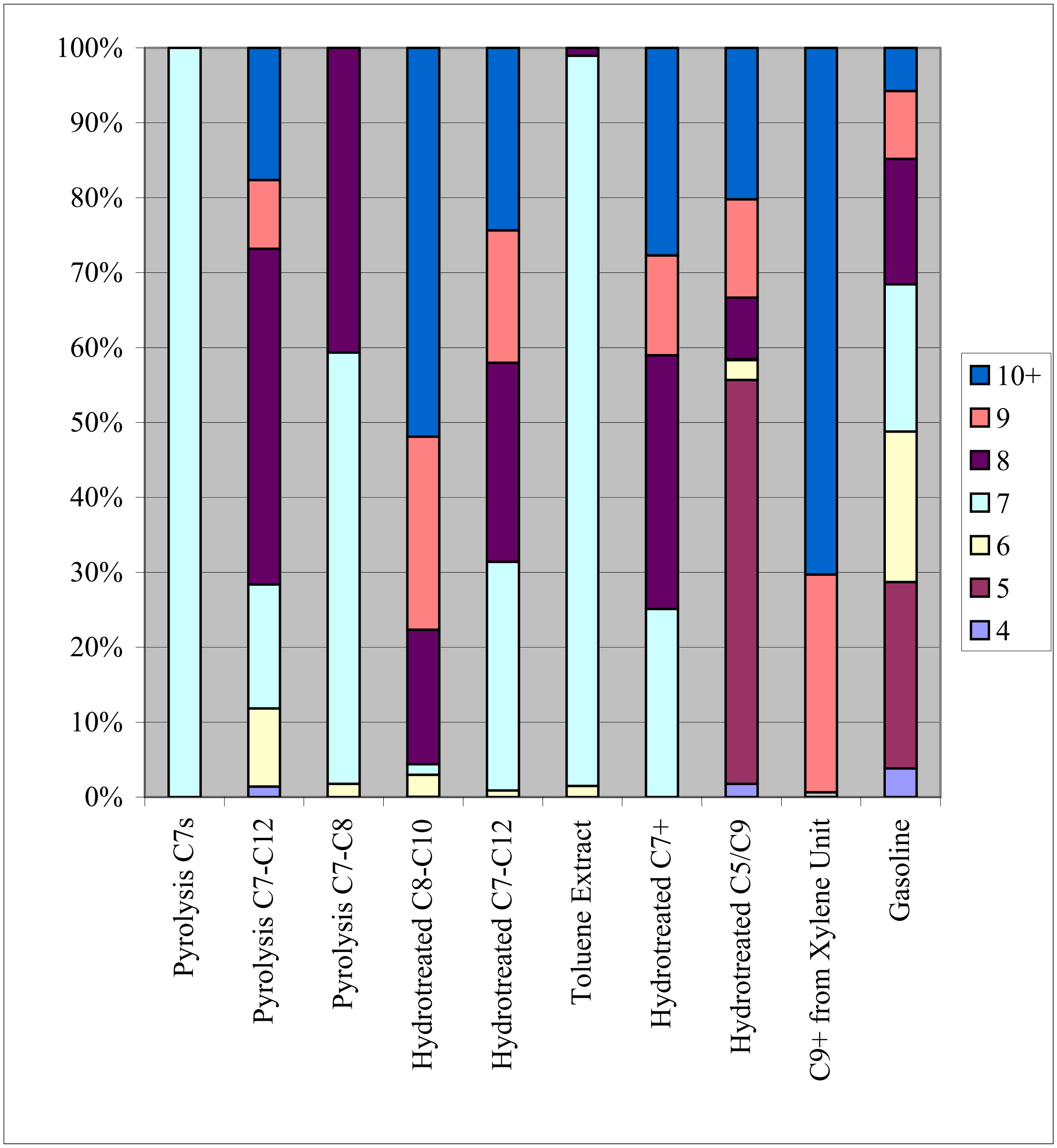


Compositions for the low benzene naphthas in Figure 1 above are averages of the ranges reported for these complex, variable composition streams. In some cases, because of overlaps and variations in the way components were sometimes grouped in individual reports, the sum of the averages for streams exceeded 100%. In those cases, compositions were normalized for plotting. When the total of the averages were less than 100%, a balance was added and included in the figure. Average wt% toluene content (actual average of reported values) of the streams is shown as points in the above figure.

Gasoline and the gasoline streams represented in Figure 1 are not streams in this category. However, the primary use of streams in this category is for blending to formulate unleaded gasoline. Composition data for gasoline and the gasoline streams were taken from Table 1 in the Gasoline Blending Streams Test Plan (API HPV Testing Group).

As can be seen in the above Figure 1, the paraffin, naphthene (or cyclic), olefin, and aromatic makeup of the low benzene naphtha streams is similar to the petroleum industry gasoline blending streams, and represented in the composition of gasoline. [Naphthenes are identified as cyclics and dicyclics.]

Figure 5.
Stream Carbon Range Content - Low Benzene Naphthas Category
(see note on Gasoline below)



Carbon range contents were normalized. Gasoline is not a stream in this category. However, the primary use of the streams in this category is for blending to formulate unleaded gasoline. Carbon range percentages for gasoline were estimated from Figure 2 in the Gasoline Blending Streams Test Plan (API HPV Testing Group).

As can be in seen in the above Figure 2, the carbon range for each of the low benzene naphthas streams is bounded by the carbon range distribution of gasoline (last bar on the right in Figure 2).

Appendix 1: Ethylene Process Description

A. The Ethylene Process

1. Steam Cracking

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

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

2. Refinery Gas Separation

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

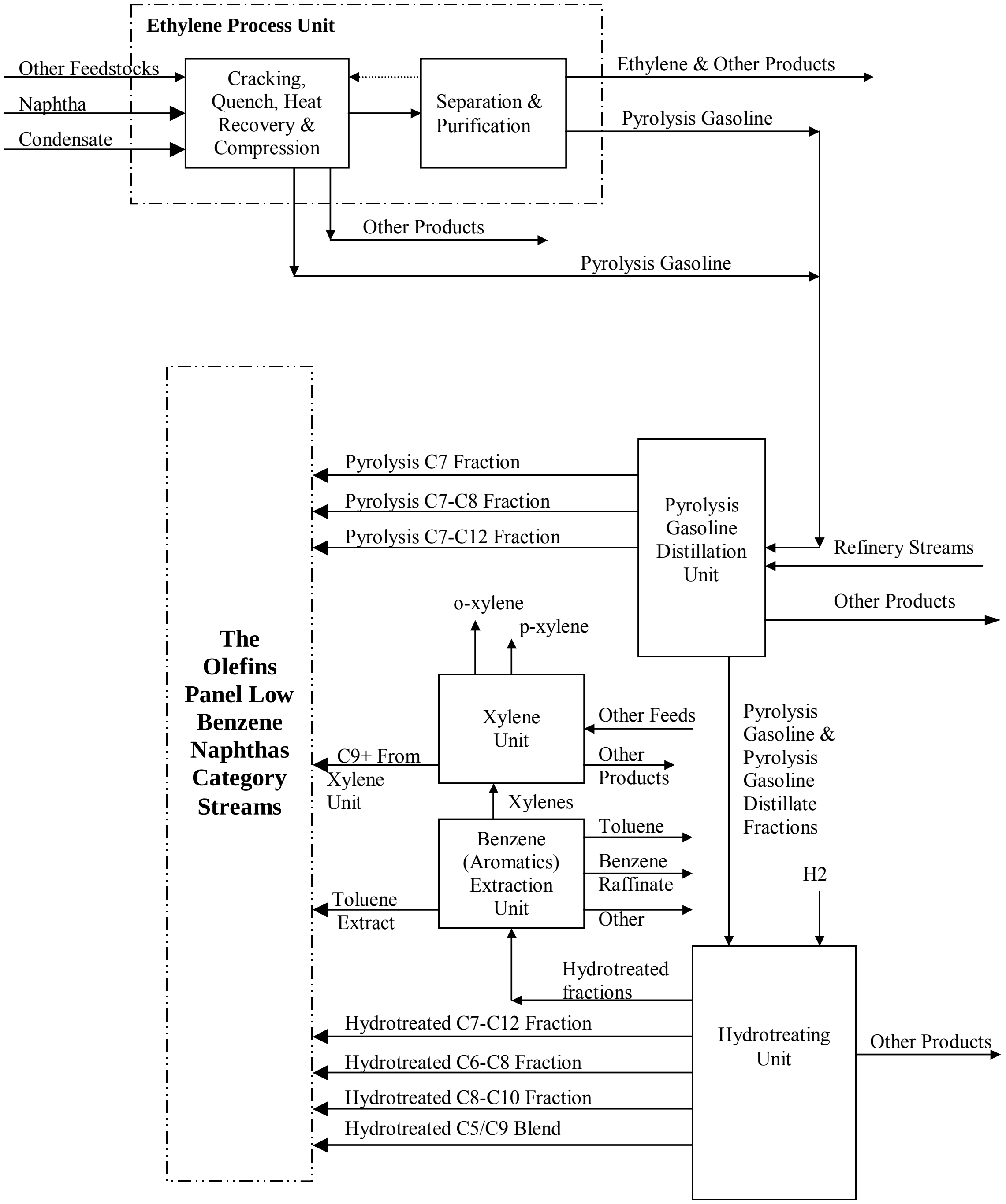
B. Products of the Ethylene Process

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

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

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

Figure A1-1. Chemical Process Operations Associated with Process Streams in the Low Benzene Naphthas Category.



Appendix 2: Composition

Table A2-1 Typical Stream Compositions (wt. %) for the Low Benzene Naphthas Category.

Component Name	Pyrolysis C7s	Pyrolysis C7-C12	Pyrolysis C7-C8 Fraction	C9+ from O-xylene Unit	Hydro-treated C8-C10	Hydro-treated C7-C12	Hydro-treated C7+	Hydro-treated C5/C9 Blend	Toluene Extract
C4's								0.2 - 3.6	
C4 and C5		2							
Isopentane (2-methylbutane)								3 - 7	
1-Pentene (Amylene)								0.5 - 1	
2-Methyl-1-Butene								1 - 2	
Pentene-2 (isomer mix)								7 - 15	
Pentane								2 - 5	
2-Methyl-2-Butene								4 - 8	
Cyclopentene								4 - 8	
Cyclopentane								1 - 3	
2-methylpentane								0.5 - 4	
3-methylpentane (Isohexane)								0.1 - 1	
C6 Hydrocarbons		9							
Hexane		4			3.7				
Remaining C6 to C7 non-Aromatic Hydrocarbons			0.2 - 12						
Benzene		1.5 - 2	5		0 - 0.4	1		3	<0.1
Cyclohexane					1				
heptenes						5			
2-methylhexane						5			
Heptane						2	1 - 3		
C8								3	
C7 Olefins	25								
i-octane						5			
C7-Non-aromatics		1							
Toluene	75	22 - 23	45 - 80		2.4	20 - 25	15 - 30		75-80

Table A2-1 Typical Stream Compositions (wt. %) for the Low Benzene Naphthas Category (cont).

Component Name	Pyrolysis C7s	Pyrolysis C7-C12	Pyrolysis C7-C8 Fraction	C9+ from O-xylene Unit	Hydro-treated C8-C10	Hydro-treated C7-C12	Hydro-treated C7+	Hydro-treated C5/C9 Blend	Toluene Extract
nonaromatics			10 - 20						
C8 Paraffins & Naphthenes		35			0.1				
C8 olefin					0.8				
Octane							1		
Ethylbenzene		3 - 5	7 - 25		2.4 - 10.7	10 - 15	10 - 20	9	5-20
C8 Aromatics				0.9					
C9 Olefins					3.3				
i-nonene						5			
Xylenes, mixed		9 - 17	3.5 - 45		3.3 - 17.9	10 - 15	10 - 20	0.3 - 3	5-20
C8's		1							
Styrene		10 - 11	0.5				1 - 3	0.5 - 5	
isopropylbenzene (cumene)					0.9		1 - 3		
C10 Isoparaffins					1.1				
Propylbenzene				1.8	3 - 3.5		1 - 3		
C9 Aromatics					4.6	10 - 20		19	
Ethyltoluenes				52.82	6		1 - 5		
C9 Paraffins and Naphthenes					2.3				
1,4-methylethylbenzene					9.4				
C10+		17						25	
C-10 Naphthenes					4.9				
1,2,4-Trimethylbenzen (pseudocumene)		3							
Trimethylbenzenes				4.4	5		2 -4		
Dicyclopentadiene							1 - 3	1 - 4	
Vinyl Toluene							1		
Propenylbenzene							2		
C9's		10							

Table A2-1 Typical Stream Compositions (wt. %) for the Low Benzene Naphthas Category. (cont.)

Component Name	Pyrolysis C7s	Pyrolysis C7-C12	Pyrolysis C7-C8 Fraction	C9+ from O-xylene Unit	Hydro-treated C8-C10	Hydro-treated C7-C12	Hydro-treated C7+	Hydro-treated C5/C9 Blend	Toluene Extract
Indane (indan)					8.5				
sec-butylcyclohexane					8.8				
3-ethylnonane					1.5				
C9+ Paraffins				2.88					
C9+ Naphthenes				0.94					
C9+ Aromatics				96.18					
C10 Aromatics					1.8	10 - 20			
C-11 Isoparaffins					18				
diethylbenzenes					1.3				
Indene							2		
dimethyl-ethylbenzenes					0.8				
C10-C11 Alkylbenzenes							13 - 35		
C11+ Aromatics						10 - 15			
Naphthalene		7 - 9		11.5	0.2 - 7.8		2	0.2 - 4	
tricyclodecane					44				
2-Methylnaphthalene				8.7					
1,1'-Biphenyl				0.5					
C10 Paraffins & Naphthenes					0.8				
Heavy Hydrocarbons and Polycyclic Aromatics				22.4					

Note 1:The balance of these streams is expected to be other hydrocarbons that have boiling points in the range of the listed components.
Note 2: The listed ranges should not be considered absolute values. They are instead the approximate highs and lows of the reported values, and are expected to be typical limit values.
Note 3: 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 stream (composition).

Appendix 3: Biodegradation

Table A3-1

Read Across Data used to Characterize the Biodegradability of the Low Benzene Naphthas Category

from Chemicals Contained by Products in this Category and Chemically Complex Products not in this Category, but that Contain Like-Chemicals.

CHEMICAL / PRODUCT	CARBON NUMBER	PERCENT BIODEGRADATION[a] (28 days)	REFERENCE
n-Pentane	5	87	IHSC[e]
Isopentane	5	71	IHSC[e]
Cyclohexane	6	77	IHSC[e]
Alkenes, C6 Rich	6[b]	21	HOP[f]
1-Hexene (linear)	6	67-98[c]	[g]
Benzene	6	63	[h]
Toluene	7	80-86% (20 days) [c]	Price et al., 1974[k]
Alkenes, C7-C9, C8 Rich	7-9	29	HOP[f]
p-Xylene	8	89	XIC[i]
Styrene	8	100 (14 days) [c]	[g]
Naphtha (Petroleum), light alkylate (gasoline stream)	5-8	42[d]	API[j]
Naphtha (Petroleum), Light Catalytically Cracked (gasoline stream)	5-8	74 [d]	API[j]
Naphtha (Petroleum), Light Catalytically Reformed (gasoline stream)	5-9	96 [d]	API[j]
C8-C10 Aromatics, Predominantly C9 Alkylbenzenes	9 [b]	78	IHSC[e]
C8-C14 Aromatics, Predominantly Alkyl Naphthalenes and Naphthalene	10-12 [b]	61	IHSC[e]

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

i	Part of the Xylene ICCA Consortium and were reviewed by OECD at SIAM 16
j	Robust summary from the American Petroleum Institute: Gasoline Blending Streams Test Plan (2003)
k	Price, K.S., Waggy, G.T. and Comway, R.A. 1974. Brine shrimp bioassay and seawater BOD of petrochemicals. J Water Pollut Control Fed. 46: 63-77. In EU Toluene SIAR 10888

Table A3-2
Composition (Weight Percent) of Three Gasoline Streams with Biodegradation Data Used to Read Across to Products in the Low Benzene Naphthas Category.

Naphtha, (Pet.) Light Alkylate		**Naphtha, (Pet.) Light Catalytically Cracked**		**Naphtha, (Pet.) Light Catalytically Reformed**	
CAS# 64741-66-8	Weight %	CAS# 64741-55-5	Weight %	CAS# 64741-63-5	Weight %
Isopentane	12.61	n-hexane	1.69	n-heptane	3.59
2,3 dimethyl butane	4.74	n-pentane	1.71	n-hexane	4.69
2,4 dimethyl pentane	4.09	isopentane	4.7	n-pentane	8.05
2,3 dimethyl pentane	2.25	2,3 dimethyl pentane	1.12	Isopentane	11.39
2,2,4 trimethyl pentane	23.92	2 methyl hexane	1.58	2,2 dimethyl butane	1.26
2,2,3 trimethyl pentane	1.76	3 methyl hexane	1.45	2,3 dimethyl butane	1.11
2,3,3 trimethyl pentane	8.99	2 methyl pentane	3.64	2,3 dimethyl pentane	1.70
2,3,4 trimethyl pentane	11.56	3 methyl pentane	2.20	2 methyl hexane	4.30
2,3,5 trimethyl hexane	1.25	methyl cyclopentane	1.87	3 methyl hexane	5.18
2,5 dimethyl hexane	4.34	methyl cyclohexane	1.19	2 methyl pentane	5.17
2,4 dimethyl hexane	3.60	1-pentene	1.25	3 methyl pentane	4.00
2,3 dimethyl hexane	2.60	2-methyl-1-butene	2.31	benzene	8.37
1methyl-1ethyl cyclopentane	9.44	2-methyl-2-butene	5.35	toluene	29.77
		trans-2-pentene	3.33		
		cis-2-pentene	1.94		
		2-methyl-1-pentene	2.31		
		cis-3-hexene	1.67		
		trans-2-hexene	1.97		
		2-methyl-2-pentene	1.83		
		1-methyl cyclopentene	1.85		
		ethylbenzene	1.47		
		m-xylene	3.05		
		p-xylene	1.34		
		o-xylene	1.83		
		benzene	1.48		
		toluene	6.73		

Appendix 4: Aquatic Toxicity

Table A4-1

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

Substance Name	Olefins		Aromatics		Paraffins		Naphthenes	
	% (wt.)	**C #[b]**	**% (wt.)**	**C #[b]**	**% (wt.)**	**C #[b]**	**% (wt)**	**C #[b]**
Products in Low Benzene Naphtha Category	**0-25**	**5-10+**	**25-100**	**7-10+**	**0-48**	**5-10+**	**0-33**	**5-10+**
Alkenes, C6 Rich	**100**	**5-7**	**0**	**-**	**0**	**-**	**0**	**-**
Alkenes, C7-9, C8 Rich	**100**	**7-9**	**0**	**-**	**0**	**-**	**0**	**-**
C8-C10 Aromatics, Predominantly C9 Aromatics	**0**	**-**	**>97**	**8-10**	**-**	**-**	**<3**	**-**
C8-C14 Aromatics, Predominantly Alkyl Naphthalenes and Naphthalene	**0**	**-**	**>94**	**10-14**	**-**	**-**	**<6**	**-**
Naphtha (petroleum), Light Alkylate (gasoline stream)	**0**	**-**	**0**	**-**	**82**	**5-8**	**9**	**8**
Naphtha (petroleum), Light Catalytically Cracked (gasoline stream)	**22**	**5-6**	**16**	**6-8**	**18**	**5-7**	**5**	**6-7**
Naphtha (petroleum), Light Catalytically Reformed (gasoline stream)	**0**	**-**	**38**	**6-7**	**50**	**5-7**	**0**	**-**

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

b Predominant carbon number range

Table A4-2

Acute Fish Toxicity Data for Selected Chemicals and Complex Products used to Characterize the Toxicity of Products in the Low Benzene Naphthas Category

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

a Endpoint is mortality; LC = Lethal Concentration; LL = Lethal Loading; values cited as "concentration" are based on measured values
b Predominant carbon number or range
c 93-hour value
d Covered by the International Hydrocarbon Solvents Consortium: Contained in selected SIAR (expected to be submitted at SIAM 19)
e Benzene is in the OECD program and was reviewed as part of SIAM 15 (Galassi, et. al., 1988)
f Robust summary from the Higher Olefins Panel HPV Test Plan (2003)
g Xylenes are part of the Xylene ICCA Consortium and were reviewed by OECD at SIAM 16
h Ethylbenzene is in the OECD program and was reviewed as part of SIAM 15
i Robust summary from the American Petroleum Institute: Gasoline Blending Streams Test Plan (2003)

Table A4-3

Acute Invertebrate Toxicity Data for Selected Chemicals and Complex Products used to Characterize the Toxicity of Products in the Low Benzene Naphthas Category.

CHEMICAL / PRODUCT	CARBON NUMBER	ORGANISM	AQUATIC TOXICITY [a] (48-hr, mg/L)	REFERENCE
n-Pentane	5	Daphnia magna	EC50 = 2.7	IHSC[e]
n-Hexane	6	Daphnia magna	EC50 = 2.1	IHSC[e]
Cyclohexane	6	Daphnia magna	EC50 = 0.9	IHSC[e]
Benzene	6	Daphnia magna	EC50 = 18[b]	[f]
Toluene	7	Daphnia magna	EC50 = 14.9	Hermens et al[J]
o-Xylene	8	Daphnia magna	EC50 = 1.0	XIC[g]
m-Xylene	8	Daphnia magna	EC50 = 4.7	XIC[g]
Naphtha (Petroleum), Light Catalytically Reformed (gasoline stream)	5-7[c]	Daphnia magna	EL50 = 10	API[h]
Naphtha (Petroleum), Light Alkylate (gasoline stream)	5-8 [c]	Daphnia magna	EL50 = 32	API[h]
Naphtha (Petroleum), Light Catalytically Cracked (gasoline stream)	5-8 [c]	Daphnia magna	EL50 = 18	API[h]
C8-C10 Aromatics, Predominantly C9 Aromatics	8-10 [c]	Daphnia magna	EL50 = 21.3	IHSC[e]
Naphthalene	10	Daphnia magna	EL50 = 16.7 [d]	[i]
C8-C14 Aromatics, Predominantly Alkyl Naphthalenes and Naphthalene	10-12 [c]	Daphnia magna	EL50 = 3.0	IHSC[e]

a Endpoint is immobility; EC = Effect Concentration; EL = Effect Loading; values cited as “concentration” are based on measured values

b 24-hour study

c Predominant carbon number or range

d Based on nominal values

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

f Benzene is in the OECD program and was reviewed as part of SIAM 15 (Galassi, et. al., 1988)

g Xylenes are part of the Xylene ICCA Consortium and were reviewed by OECD at SIAM 16

h Robust summary from the American Petroleum Institute: Gasoline Blending Streams Test Plan (2003)

i Naphthalene is part of the OECD program and was reviewed in SIAM 13

j Hermens, J., Canton, H., Janssen, P., and deJong, R. (1984). Quantitative structure-activity relationships and toxicity studies of mixtures of chemicals with anesthetic potency: acute lethal and sublethal toxicity to *Daphnia magna*. Aquat Toxicol 5: 143 –154. In EU Toluene SIAR 10888

Table A4-4

Alga Toxicity Data for Selected Chemicals and Complex Products Used to Characterize the Toxicity of Products in the Low Benzene Naphthas Category

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

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

[b] Formally known as *Selenastrum capricornutum*

[c] Predominant carbon number or range

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

[e] Benzene is in the OECD program and was reviewed as part of SIAM 15 (Galassi, et. al., 1988)

[f] Robust summary from the American Petroleum Institute: Gasoline Blending Streams Test Plan (2003)

Appendix 5

American Chemistry Council

Olefins Panel Sponsored HPV Test Categories.

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

Attachments [Separate documents]

Attachment 1. Summary of High Aromatic Studies for Reproductive Toxicity

Attachment 2a. Robust Summaries: PhysicoChemical and Environmental Fate

Attachment 2b. Robust Summaries: Mammalian Toxicology – Heavy Aromatic Distillate

Attachment 2a.

Robust Summaries

PhysicoChemical and Environmental Fate

LOW BENZENE NAPHTHAS ROBUST SUMMARY

Boiling Point

Test Substance*:	Other TS [CAS # 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3]
Method/Guideline:	Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Pressure:	760 mm Hg
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Boiling Point is calculated by the MPBPWIN subroutine, which is based on the calculation method of S. Stein and R. Brown in "Estimation of Normal Boiling Points from Group Contributions". 1994. J. Chem. Inf. Comput. Sci. 34: 581-587.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Calculated and measured boiling point data for representative constituents of the Low Benzene Naphthas Category are listed below. The data identify a potential boiling point range for substances represented by the 10 CAS numbers under Test Substance. Substances in this category do not have a specific boiling point value. Actual boiling point ranges for substances in this category will vary dependent on their constituent composition. Commercial substances in this category consist of complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C12. The seven chemicals selected to represent the boiling point range of this category are C5-C11 hydrocarbons that can be found in substances identified by the 10 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.

Results: (continued)

Units/Value:

Note: Deviations from protocol or guideline, analytical method.

Substance Constituent	Calculated BP (°C)	Measured* BP (°C)
isopentane	30.18	27.8
toluene	125.72	110.6
m-xylene	148.29	139.1
styrene	146.65	145.0
naphthalene	231.64	217.9
tricyclodecane	171.25	na
methylnaphthalene	249.60	241.1

* Experimental values from EPIWIN database.
na = not available

The data represent a potential boiling point range for substances represented by the 10 CAS numbers under Test Substance.

Test Substance:

The Low Benzene Naphthas Category includes the following CAS numbers:

64741-98-6	Extract, petroleum, heavy naphtha solvent
64742-48-9	Naphtha, petroleum, hydrotreated heavy
64742-49-0	Naphtha, petroleum, hydrotreated light
64742-83-2	Naphtha, petroleum, light steam-cracked
68333-88-0	Aromatic hydrocarbons, C9-C17
68476-45-9	Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product
68478-10-4	Naphtha, petroleum, light steam-cracked, debezenized, C8-16-cycloalkadiene concentrate
68516-20-1	Naphtha, petroleum, steam-cracked middle aromatic
68527-23-1	Naphtha, petroleum, light steam-cracked aromatic
68919-15-3	Hydrocarbons, C6-12, benzene-recovery

Low Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 10 CAS numbers are used to describe the nine process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry. Aromatics represent the major constituents in all of the streams, varying from approximately 45 to 95 percent. The benzene content is usually less than five percent.

More information on the Low Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1).

1. Olefins Panel, HPV Implementation Task Group. 2001.

	High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	The calculated boiling points for some representative constituents that are present in the category streams vary from 30.18 to 249.60°C @ 760 mm Hg. The measured boiling points of these same constituents vary from 27.8 to 241.1°C @ 760 mm Hg. Although this does not define the actual boiling points of the category streams, it offers an indication of a range that might be expected to encompass the boiling points of these complex streams with variable compositions. Boiling points outside these ranges may be possible for some category streams.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential boiling point range for substances represented by the 10 CAS numbers listed under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in Low Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for boiling point range based on constituent data.
Reference:	EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Boiling point values were calculated by the MPBPWIN subroutine and measured data came from the database in the computer program.)
Other (source):	American Chemistry Council, Olefins Panel (Prepared 7/03)

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

LOW BENZENE NAPHTHAS ROBUST SUMMARY

Melting Point

Test Substance*:	Other TS [CAS # 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3]
Method/Guideline:	Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Melting Point is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of K. Joback and Gold and Ogle. Joback's Method is described in Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds. The Gold and Ogle Method simply uses the formula $Tm = 0.5839Tb$, where Tm is the melting point in Kelvin and Tb is the boiling point in Kelvin. The Gold and Ogle Method is described by Lyman, W.J., 1985, In: Environmental Exposure from Chemicals. Volume 1. Neely, W.B. and Blau, G.E. (eds), Boca Raton, FL, CRC Press, Inc., Chapter 2.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Calculated and measured melting point data for representative constituents of the Low Benzene Naphthas Category are listed below. The data identify a potential melting point range for substances represented by the 10 CAS numbers under Test Substance. Substances in this category do not have a specific melting point value. Actual melting point ranges for substances in this category will vary dependent on their constituent composition. Commercial substances in this category consist of complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C12. The seven chemicals selected to represent the melting point range of this category are C5-C11 hydrocarbons that can be found in substances identified by the 10 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.

Results: (continued)

Units/Value:

Note: Deviations from protocol or guideline, analytical method.

Substance Constituent	Calculated MP (°C)	Measured* MP (°C)
isopentane	-119.04	-159.9
toluene	-59.17	-94.9
m-xylene	-40.69	-47.8
styrene	-48.31	-31.0
naphthalene	5.01	80.2
tricyclodecane	-19.15	na
methylnaphthalene	22.15	34.4

* Experimental values from EPIWIN database.
na = not available

The data represent a potential melting point range for substances represented by the 10 CAS numbers under Test Substance.

Test Substance:

The Low Benzene Naphthas Category includes the following CAS numbers:

64741-98-6	Extract, petroleum, heavy naphtha solvent
64742-48-9	Naphtha, petroleum, hydrotreated heavy
64742-49-0	Naphtha, petroleum, hydrotreated light
64742-83-2	Naphtha, petroleum, light steam-cracked
68333-88-0	Aromatic hydrocarbons, C9-C17
68476-45-9	Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product
68478-10-4	Naphtha, petroleum, light steam-cracked, debezenized, C8-16-cycloalkadiene concentrate
68516-20-1	Naphtha, petroleum, steam-cracked middle aromatic
68527-23-1	Naphtha, petroleum, light steam-cracked aromatic
68919-15-3	Hydrocarbons, C6-12, benzene-recovery

Low Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 10 CAS numbers are used to describe the nine process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry. Aromatics represent the major constituents in all of the streams, varying from approximately 45 to 95 percent. The benzene content is usually less than five percent.

More information on the Low Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1).

1. Olefins Panel, HPV Implementation Task Group. 2001.

	High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	The calculated melting points for some representative constituents that are present in the category streams vary from -119.04 to 22.15 °C. The measured melting points of these same constituents vary from -159.9 to 80.2°C. Although this does not define the actual melting points of the category streams, it offers an indication of a range that might be expected to encompass the melting points of these complex streams with variable compositions. Melting points outside these ranges may be possible for some category streams.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential melting point range for substances represented by the 10 CAS numbers listed under <u>Test Substance</u>. This robust summary has a reliability rating of 2 because the data are not for specific substances in the Low Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for melting point range based on constituent data.
Reference:	EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Melting point values were calculated by the MPBPWIN subroutine and measured data came from the database in the computer program.)
Other (source):	American Chemistry Council, Olefins Panel (Prepared 7/03)

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

LOW BENZENE NAPHTHAS ROBUST SUMMARY

Vapor Pressure

Test Substance*:	Other TS [CAS # 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3]
Method/Guideline:	Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Vapor Pressure is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of Antoine and Grain. Both methods use boiling point for the calculation. The Antoine Method is described in the Handbook of Chemical Property Estimation. Chapter 14. W.J. Lyman, W.F. Reehl and D.H. Rosenblatt, Eds. Washington, D.C.: American Chemical Society. 1990. A modified Grain Method is described on page 31 of Neely and Blau's Environmental Exposure from Chemicals, Volume 1, CRC Press. 1985.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Calculated and measured vapor pressure data for representative constituents of the Low Benzene Naphthas Category are listed below. The data identify a potential vapor pressure range for substances represented by the 10 CAS numbers under Test Substance. Substances in this category do not have a specific vapor pressure value. Actual vapor pressure ranges for substances in this category will vary dependent on their constituent composition. Commercial substances in this category consist of complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C12. The seven chemicals selected to represent the vapor pressure range of this category are C5-C11 hydrocarbons that can be found in substances identified by the 10 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.

Results (continued):

Units/Value:

Note: Deviations from protocol or guideline, analytical method.

Substance Constituent	Calculated VP (hPa @ 25°C)	Measured* VP (hPa @ 25°C)
isopentane	9.17 E2	9.19 E2
toluene	31.60	37.86
m-xylene	8.83	11.05
styrene	6.73	8.53
naphthalene	0.11	0.05
tricyclodecane	2.64	na
methylnaphthalene	4.60 E-2	7.33 E-2

* Experimental values from EPIWIN database.
na = not available

The data represent a potential vapor pressure range for substances represented by the 10 CAS numbers under Test Substance.

Test Substance:

The Low Benzene Naphthas Category includes the following CAS numbers:

64741-98-6	Extract, petroleum, heavy naphtha solvent
64742-48-9	Naphtha, petroleum, hydrotreated heavy
64742-49-0	Naphtha, petroleum, hydrotreated light
64742-83-2	Naphtha, petroleum, light steam-cracked
68333-88-0	Aromatic hydrocarbons, C9-C17
68476-45-9	Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product
68478-10-4	Naphtha, petroleum, light steam-cracked, debezenized, C8-16-cycloalkadiene concentrate
68516-20-1	Naphtha, petroleum, steam-cracked middle aromatic
68527-23-1	Naphtha, petroleum, light steam-cracked aromatic
68919-15-3	Hydrocarbons, C6-12, benzene-recovery

Low Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 10 CAS numbers are used to describe the nine process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry. Aromatics represent the major constituents in all of the streams, varying from approximately 45 to 95 percent. The benzene content is usually less than five percent.

More information on the Low Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1).

1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low Benzene Naphthas

	Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	The calculated vapor pressures for some representative constituents that are present in the category streams vary from 4.60 E-2 to 9.17 E2 hPa @ 25°C. The measured vapor pressures of these same constituents vary from 7.33 E-2 to 9.19 E2 hPa @ 25°C. Although this does not define the actual vapor pressures of the category streams, it offers an indication of a range that might be expected to encompass the vapor pressures of these complex streams with variable compositions. Vapor pressure outside these ranges may be possible for some category streams.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential vapor pressure range for substances represented by the 10 CAS numbers under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the Low Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for vapor pressure range based on constituent data.
Reference:	EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Vapor pressure values were calculated by the MPBPWIN subroutine and measured data came from the database in the computer program.)
Other (source):	American Chemistry Council, Olefins Panel (Prepared 7/03)

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

LOW BENZENE NAPHTHAS ROBUST SUMMARY

Hydrolysis (Stability in Water)

Test Substance*:	Other TS [CAS # 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3]
Method/Guideline:	Other: Technical discussion
Year (guideline):	Not applicable
Type (test type):	Not applicable
GLP (Y/N):	Not applicable
Year (study performed):	Not applicable
Analytical Monitoring:	Not applicable
Test Conditions: • **Note: Concentration preparation, vessel type, volume, replication, deviations from guideline or protocol**	Not applicable
Results: **Units/Value:** • **Note: Analytical method, observations, half-lives by pH, degradation products**	Not applicable
Test Substance:	The Low Benzene Naphthas Category includes the following CAS numbers: 64741-98-6 Extract, petroleum, heavy naphtha solvent 64742-48-9 Naphtha, petroleum, hydrotreated heavy 64742-49-0 Naphtha, petroleum, hydrotreated light 64742-83-2 Naphtha, petroleum, light steam-cracked 68333-88-0 Aromatic hydrocarbons, C9-C17 68476-45-9 Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product 68478-10-4 Naphtha, petroleum, light steam-cracked, debezenized, C8-16-cycloalkadiene concentrate 68516-20-1 Naphtha, petroleum, steam-cracked middle aromatic 68527-23-1 Naphtha, petroleum, light steam-cracked aromatic 68919-15-3 Hydrocarbons, C6-12, benzene-recovery Low Benzene Naphthas Category substances arise from

	production processes associated with ethylene manufacturing. The 10 CAS numbers are used to describe the nine process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry. Aromatics represent the major constituents in all of the streams, varying from approximately 45 to 95 percent. The benzene content is usually less than five percent. More information on the Low Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	**Summary** In the environment, hydrolysis will not contribute to the degradation of constituent chemicals in the Low Benzene Naphthas Category. The Low Benzene Naphthas Category includes nine process streams: • **Pyrolysis C7s Fraction** • **Pyrolysis C7-C12 Fraction** • **Pyrolysis C7-C8 Fraction** • **C9+ From Xylene Unit** • **Hydrotreated C8-C10 Fraction** • **Hydrotreated C7-C12 Fraction** • **Hydrotreated C7+ Fraction** • **Hydrotreated C5/C9 blend** • **Toluene Extract** Ten CAS numbers (see Test Substance) identify products derived from these process streams. As discussed below, the chemicals in these streams are composed of carbon and hydrogen and are not amenable to hydrolysis because of their molecular structure and the chemical reaction required for this type of transformation to occur. **The Low Benzene Naphthas Category** A process stream is a mixture of chemicals that arises from a chemical reaction or separation activity. The category includes hydrocarbon product streams associated with the ethylene industry. Aromatics represent the major constituents in all of the streams, varying from approximately 45 to 95 percent. The benzene content is usually less than five percent. This grouping of CAS numbers represents hydrocarbon streams with a carbon number distribution that is predominantly C5-C12. That is why this group is considered a category for purposes of the High

Production Volume (HPV) Chemical Program, and designated Low Benzene Naphthas.

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

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

- **Pyrolysis Fractions (C7s, C7-C12, and C7-C8 Fractions)** are separated by distillation into various boiling-point range fractions as intermediates in preparation for further processing. Many carbon number distribution fractions are technically feasible. The compositions of these fractions vary depending on the ethylene process feedstock, the cracking furnaces operating conditions and the ethylene process configuration.

1. **Pyrolysis C7s Fraction** has a carbon number distribution that is 75% toluene with the balance primarily C7 non-aromatics, largely unsaturates. The stream may contain low levels of benzene.

2. **Pyrolysis C7-C12 Fraction** has a typical composition including about 2% benzene, 23% toluene, 28% C8 aromatics and 8% naphthalene, with the balance expected to be largely unsaturated hydrocarbons and other aromatics.

3. **Pyrolysis C7-C8 Fraction** has a carbon number distribution that is predominantly C7 to C8. The reported compositions range from 45 to 80% with 11 to 78% C8 aromatics. The typical benzene concentration reported is 2% with a maximum of 5%.

- **C9+ from Xylene Unit** is a co-product from process units that produce o- or p-xylene. The carbon distribution for the stream is C8+ with some hydrocarbon compounds having a boiling point of 650°F or higher. The stream is predominantly aromatics.

- **Hydrotreated Pyrolysis Fractions (C8-C10, C7-C12, C7+ Fractions, and C5/C9 Blend)** are pyrolysis gasoline or distillate fractions of pyrolysis gasoline that are treated with hydrogen over catalyst. 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 mono- and diolefins to paraffins. A pygas fraction that will be processed by extraction or extractive distillation to produce high purity aromatics (toluene or xylenes in this case) is subjected to two-stage hydrogenation. Pygas fractions may be forwarded to hydrodealkylation units (less common) for benzene production after one-stage of hydrogenation. Pygas fractions intended for use as a gasoline blending stock are frequently subject to only one-stage hydrogenation. The streams may result from fractionation of hydrotreated pyrolysis gasoline or from hydrotreating pyrolysis gasoline fractions followed by distillation. Reformate fractions from petroleum refineries are sometimes mixed with these pyrolysis fractions.

1. **Hydrotreated C8-C10 Fraction** has a carbon number distribution of C6 to C12, but is predominantly C8 to C10. Typical concentration includes 0.3% benzene, 2.4% toluene, 24% C8 aromatics with the balance primarily C9 and C10 aromatics and lesser amounts of paraffins, isoparaffins and naphthenes in this carbon range.

2. **Hydrotreated C7-C12 Fraction** is a distillate fraction of hydrogenated pygas with a carbon number distribution that is predominantly C7-C12, with lesser amounts of C6. Typical reported values indicate 1% benzene, 23% toluene, 25% C8 aromatics, with the balance primarily other aromatics and lesser amounts of monoolefins and paraffins.

3. **Hydrotreated C7+ Fraction** is derived as distillation residue after removing the C5 and C6 fractions from a hydrogenated pygas stream (alternately the stream could be hydrotreated after distillation). The carbon number distribution is predominantly greater than C6, although the reported analysis does not report compounds greater than C12. Typical reported values include 23% toluene, 32% C8 aromatics, 1% naphthalene, with the balance primarily other aromatics and lesser amounts of paraffins.

4. **Hydrotreated C5/C9 Blend** is produced by blending C5 and C9 pyrolysis fractions, hydrogenated either before or after blending. Typical reported values includes approximately 2% benzene, 40% C5's in the blend, 9% C8 aromatics, 19% C9 aromatics, and 25% C10+.

- **Toluene Extract** is produced as a co-product of a benzene extraction unit. The stream may contain significant concentrations of xylenes.

<u>Hydrolysis of Hydrocarbons as a Function of Molecular Structure</u>

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

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

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

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

<u>References</u>

1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
2. Gould, E.S. (1959), Mechanism and Structure in Organic Chemistry, Holt, Reinhart and Winston, New York, NY, USA.
3. Harris, J.C. (1982), "Rate of Hydrolysis," Chapter 7 in: W.J.

	Lyman, W.F. Reehl, and D.H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, NY, USA. 4. Neely, W. B. 1985. Hydrolysis. In: W. B. Neely and G. E. Blau, eds. Environmental Exposure from Chemicals. Vol I., pp. 157-173. CRC Press, Boca Raton, FL, USA.
Reliability:	These data represent a key study for characterizing the potential of substances in the Low Benzene Naphthas Category to undergo hydrolysis.
Reference:	American Chemistry Council, Olefins Panel. 2003. Hydrolysis Low Benzene Naphthas Category. Rosslyn, VA, USA.
Other (source):	American Chemistry Council, Olefins Panel (Prepared 7/03)

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

LOW BENZENE NAPHTHAS ROBUST SUMMARY

Partition Coefficient

Test Substance*:	Other TS [CAS # 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3]
Method/Guideline:	Calculated values using KOWWIN version 1.65, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Octanol / Water Partition Coefficient is calculated by the KOWWIN subroutine, which is based on an atom/fragment contribution method of W. Meylan and P. Howard in "Atom/fragment contribution method for estimating octanol-water partition coefficients". 1995. *J. Pharm. Sci*. 84:83-92.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Calculated and measured log K_{ow} data for representative constituents of the Low Benzene Naphthas Category are listed below. The data identify a potential log K_{ow} range for substances represented by the 10 CAS numbers under <u>Test Substance</u>. Substances in this category do not have a specific log K_{ow} value. Actual log K_{ow} ranges for substances in this category will vary dependent on their constituent composition. Commercial substances in this category consist of complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C12. The seven chemicals selected to represent the log K_{ow} range of this category are C5-C11 hydrocarbons that can be found in substances identified by the 10 CAS numbers listed under <u>Test Substance</u>. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.

Results: (continued)

Units/Value:

Note: Deviations from protocol or guideline, analytical method.

Substance Constituent	Calculated log K_{ow} @ 25°C	Measured* log K_{ow} @ 25°C
isopentane	2.72	na
toluene	2.54	2.73
m-xylene	3.09	3.20
styrene	2.89	2.95
naphthalene	3.17	3.30
tricyclodecane	3.59	na
methylnaphthalene	3.72	3.86

* Experimental values from EPIWIN database.
na = not available
The data represent a potential log K_{ow} range for substances represented by the 10 CAS numbers under Test Substance.

Test Substance:

The Low Benzene Naphthas Category includes the following CAS numbers:

64741-98-6	Extract, petroleum, heavy naphtha solvent
64742-48-9	Naphtha, petroleum, hydrotreated heavy
64742-49-0	Naphtha, petroleum, hydrotreated light
64742-83-2	Naphtha, petroleum, light steam-cracked
68333-88-0	Aromatic hydrocarbons, C9-C17
68476-45-9	Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product
68478-10-4	Naphtha, petroleum, light steam-cracked, debezenized, C8-16-cycloalkadiene concentrate
68516-20-1	Naphtha, petroleum, steam-cracked middle aromatic
68527-23-1	Naphtha, petroleum, light steam-cracked aromatic
68919-15-3	Hydrocarbons, C6-12, benzene-recovery

Low Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 10 CAS numbers are used to describe the nine process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry. Aromatics represent the major constituents in all of the streams, varying from approximately 45 to 95 percent. The benzene content is usually less than five percent.

More information on the Low Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1).

1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low Benzene Naphthas

	Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	The calculated log K_{ow} for some representative constituents that are present in the category streams vary from 2.54 to 3.72 @ 25°C. The measured log K_{ow} of these same constituents vary from 2.73 to 3.86 @ 25°C. Although this does not define the actual log K_{ow} of the category streams, it offers an indication of a range that might be expected to encompass the log K_{ow} of these complex streams with variable compositions. Log K_{ow} values outside these ranges may be possible for some category streams.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential log K_{ow} range for substances represented by the 10 CAS numbers under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the Low Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for log K_{ow} range based on constituent data.
Reference:	EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Log K_{ow} values were calculated by the KOWWIN subroutine and measured data came from the database in the computer program.)
Other (source):	American Chemistry Council, Olefins Panel (Prepared 7/03)

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

LOW BENZENE NAPHTHAS ROBUST SUMMARY

Photodegradation (Direct)

Test Substance*:	Other TS [CAS # 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3]
Method/Guideline:	Other: Technical discussion
Year (guideline):	Not applicable
GLP (Y/N):	Not applicable
Year (study performed):	Not applicable
Type (air, soil, water, other):	Water
Light Source:	Not applicable
Light Spectrum: • **Wave length value (upper/lower)**	Not applicable
Relative Intensity:	Not applicable
Test Substance Spectrum:	Not applicable
Test Conditions: • **Note: Concentration, temperature, test system type, replication, deviations from guideline or protocol**	Not applicable
Direct Photolysis:** • **Results: half-life, % degradation, quantum yield**	**Summary** In the environment, direct photolysis will not significantly contribute to the degradation of constituent chemicals in the Low Benzene Naphthas Category. The Low Benzene Naphthas Category includes nine process streams: • **Pyrolysis C7s Fraction** • **Pyrolysis C7-C12 Fraction** • **Pyrolysis C7-C8 Fraction** • **C9+ From Xylene Unit** • **Hydrotreated C8-C10 Fraction** • **Hydrotreated C7-C12 Fraction** • **Hydrotreated C7+ Fraction** • **Hydrotreated C5/C9 blend** • **Toluene Extract**

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

The Low Benzene Naphthas Category

A process stream is a mixture of chemicals that arises from a chemical reaction or separation activity. The category includes hydrocarbon product streams associated with the ethylene industry. Aromatics represent the major constituents in all of the streams, varying from approximately 45 to 95 percent. The benzene content is usually less than five percent. This grouping of CAS numbers represents hydrocarbon streams with a carbon number distribution that is predominantly C5-C12. That is why this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated Low Benzene Naphthas.

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

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

- **Pyrolysis Fractions (C7s, C7-C12, and C7-C8 Fractions)** are separated by distillation into various boiling-point range fractions as intermediates in preparation for further processing. Many carbon number distribution fractions are technically feasible. The compositions of these fractions vary depending on the ethylene process feedstock, the cracking furnaces operating conditions and the ethylene process configuration.

4. **Pyrolysis C7s Fraction** has a carbon number distribution that is 75% toluene with the balance primarily C7 non-aromatics, largely unsaturates. The stream may contain low levels of benzene.

5. **Pyrolysis C7-C12 Fraction** has a typical composition

including about 2% benzene, 23% toluene, 28% C8 aromatics and 8% naphthalene, with the balance expected to be largely unsaturated hydrocarbons and other aromatics.

6. Pyrolysis C7-C8 Fraction has a carbon number distribution that is predominantly C7 to C8. The reported compositions range from 45 to 80% with 11 to 78% C8 aromatics. The typical benzene concentration reported is 2% with a maximum of 5%.

- **C9+ from Xylene Unit** is a co-product from process units that produce o- or p-xylene. The carbon distribution for the stream is C8+ with some hydrocarbon compounds having a boiling point of 650°F or higher. The stream is predominantly aromatics.

- **Hydrotreated Pyrolysis Fractions (C8-C10, C7-C12, C7+ Fractions, and C5/C9 Blend)** are pyrolysis gasoline or distillate fractions of pyrolysis gasoline that are treated with hydrogen over catalyst. 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 mono- and diolefins to paraffins. A pygas fraction that will be processed by extraction or extractive distillation to produce high purity aromatics (toluene or xylenes in this case) is subjected to two-stage hydrogenation. Pygas fractions may be forwarded to hydrodealkylation units (less common) for benzene production after one-stage of hydrogenation. Pygas fractions intended for use as a gasoline blending stock are frequently subject to only one-stage hydrogenation. The streams may result from fractionation of hydrotreated pyrolysis gasoline or from hydrotreating pyrolysis gasoline fractions followed by distillation. Reformate fractions from petroleum refineries are sometimes mixed with these pyrolysis fractions.

5. **Hydrotreated C8-C10 Fraction** has a carbon number distribution of C6 to C12, but is predominantly C8 to C10. Typical concentration includes 0.3% benzene, 2.4% toluene, 24% C8 aromatics with the balance primarily C9 and C10 aromatics and lesser amounts of paraffins, isoparaffins and naphthenes in this carbon range.

6. **Hydrotreated C7-C12 Fraction** is a distillate fraction of hydrogenated pygas with a carbon number distribution that is predominantly C7-C12, with lesser amounts of C6. Typical reported values indicate 1% benzene, 23% toluene, 25% C8 aromatics, with the balance primarily other aromatics and

lesser amounts of monoolefins and paraffins.

7. **Hydrotreated C7+ Fraction** is derived as distillation residue after removing the C5 and C6 fractions from a hydrogenated pygas stream (alternately the stream could be hydrotreated after distillation). The carbon number distribution is predominantly greater than C6, although the reported analysis does not report compounds greater than C12. Typical reported values include 23% toluene, 32% C8 aromatics, 1% naphthalene, with the balance primarily other aromatics and lesser amounts of paraffins.

8. **Hydrotreated C5/C9 Blend** is produced by blending C5 and C9 pyrolysis fractions, hydrogenated either before or after blending. Typical reported values includes approximately 2% benzene, 40% C5's in the blend, 9% C8 aromatics, 19% C9 aromatics, and 25% C10+.

- **Toluene Extract** is produced as a co-product of a benzene extraction unit. The stream may contain significant concentrations of xylenes.

Photolysis of Hydrocarbons

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

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

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

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

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

Olefins with one double bond, or two conjugated double bonds, which constitute the majority of the chemicals in the Low Benzene Naphthas category, do not absorb appreciable light energy above 290 nm. The absorption of UV light to cause cis-trans isomerism about the double bond of an olefin occurs only if it is in conjugation with an aromatic ring (2).

Products in the Low Benzene Naphthas Category do not contain component molecules that will undergo direct photolysis. Therefore, this fate process will not contribute to a measurable degradative removal of chemical components in this category from the environment.

References

1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
2. Harris, J. C. 1982. "Rate of Aqueous Photolysis," Chapter 8 in: W. J. Lyman, W. F. Reehl, and D. H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, USA.
3. Zepp, R. G. and D. M. Cline. 1977. Rates of Direct Photolysis in the Aqueous Environment, Environ. Sci. Technol., 11:359-366.

Indirect Photolysis:**

- **Results: type of sensitizer, concentration of sensitizer, rate constant, % degradation, half-life**

Not applicable

Degradation Products:** - **Note: Identification, concentration**	Unknown
Test Substance:	The Low Benzene Naphthas Category includes the following CAS numbers: 64741-98-6 Extract, petroleum, heavy naphtha solvent 64742-48-9 Naphtha, petroleum, hydrotreated heavy 64742-49-0 Naphtha, petroleum, hydrotreated light 64742-83-2 Naphtha, petroleum, light steam-cracked 68333-88-0 Aromatic hydrocarbons, C9-C17 68476-45-9 Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product 68478-10-4 Naphtha, petroleum, light steam-cracked, debezenized, C8-16-cycloalkadiene concentrate 68516-20-1 Naphtha, petroleum, steam-cracked middle aromatic 68527-23-1 Naphtha, petroleum, light steam-cracked aromatic 68919-15-3 Hydrocarbons, C6-12, benzene-recovery
Conclusion:	Not applicable
Reliability:	These data represent a key study for characterizing the potential of substances in the Low Benzene Naphthas Category to undergo direct photodegradation.
Reference:	American Chemistry Council, Olefins Panel. 2003. Photodegradation (Direct): Low Benzene Naphthas Category. Rosslyn, VA, USA.
Other (source):	American Chemistry Council, Olefins Panel (Prepared 7/03)

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

LOW BENZENE NAPHTHAS ROBUST SUMMARY

Photodegradation (Indirect)

Test Substance*:	Other TS [CAS # 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3]
Method/Guideline:	Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
GLP (Y/N):	Not applicable
Year (study performed):	Not applicable
Type (air, soil, water, other):	Not applicable
Light Source:	Sunlight
Light Spectrum: • **Wave length value (upper/lower)**	Natural sunlight
Relative Intensity:	1
Test Substance Spectrum:	Not applicable
Test Conditions: • **Note: Concentration, temperature, test system type, replication, deviations from guideline or protocol**	Indirect photodegradation, or atmospheric oxidation potential, is based on the structure-activity relationship methods developed by R. Atkinson. Temperature: 25°C Sensitizer: OH radical Concentration of Sensitizer: 1.5 E^6 OH radicals/cm^3
Direct Photolysis:** **Results: half-life, % degradation, quantum yield**	Not applicable

Indirect Photolysis:** - **Results: type of sensitizer, concentration of sensitizer, rate constant, % degradation, half-life**	**<u>The Low Benzene Naphthas Category</u>** Low Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 10 CAS numbers are used to describe nine process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry. Aromatics represent the major constituents in all of the streams, varying from approximately 45 to 95 percent. The benzene content is usually less than five percent. Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C11. That is why this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated <u>Low Benzene Naphthas.</u> The seven chemicals selected to represent the atmospheric oxidation potential of this category are C5-C11 hydrocarbons that can be found in substances identified by the 10 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge. **<u>Atmospheric Oxidation of Hydrocarbons</u>** In the environment, organic chemicals emitted into the troposphere are degraded by several important transformation processes. The dominant transformation process for most compounds is the daylight reaction with hydroxyl (OH-) radicals (Atkinson, 1988, 1989). The rate at which an organic compound reacts with OH- radicals is a direct measure of its atmospheric persistence (Meylan and Howard, 1993). AOPWIN estimates the rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. The rate constants estimated by the program are then used to calculate atmospheric half-lives for organic compounds based upon average atmospheric concentrations of hydroxyl radicals. Since the reactions only take place in the presence of sunlight, the atmospheric half-lives are normalized for a 12-hour day.

Indirect Photolysis: (cont'd)**

Results: type of sensitizer, concentration of sensitizer, rate constant, % degradation, half-life

Chemical	Calculated* half-life (hrs)	OH- Rate Constant (cm^3/molecule-sec)
isopentane	31.8	4.0 E^{-12}
toluene	24.6	5.2 E^{-12}
m-xylene	9.5	13.6 E^{-12}
styrene	4.6	28.1 E^{-12}
naphthalene	5.9	21.6 E^{-12}
tricyclodecane	5.6	22.9 E^{-12}
methylnaphthalene	2.3	56.5 E^{-12}

* Atmospheric half-life values are based on a 12-hr day.

More information on the Low Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (Olefins Panel, 2001).

References:

1. Atkinson, R. 1988. Estimation of gas-phase hydroxyl radical rate constants for organic chemicals. *Environ. Toxicol. Chem*. **7**:435-442.
2. Atkinson, R. 1989. Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds. J. Phys. Chem. Ref. Data Monograph No. 1, Amer. Inst. Physics & Amer. Chem. Soc., NY.
3. Meylan, W.M. and P.H. Howard. 1993. Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. *Chemosphere* **12**:2293-2299.
4. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.

Degradation Products:**

- **Note: Identification, concentration**

Unknown

Test Substance:

The Low Benzene Naphthas Category includes the following CAS numbers:

64741-98-6	Extract, petroleum, heavy naphtha solvent
64742-48-9	Naphtha, petroleum, hydrotreated heavy
64742-49-0	Naphtha, petroleum, hydrotreated light
64742-83-2	Naphtha, petroleum, light steam-cracked
68333-88-0	Aromatic hydrocarbons, C9-C17
68476-45-9	Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product
68478-10-4	Naphtha, petroleum, light steam-cracked,

	debezenized, C8-16-cycloalkadiene concentrate 68516-20-1 Naphtha, petroleum, steam-cracked middle aromatic 68527-23-1 Naphtha, petroleum, light steam-cracked aromatic 68919-15-3 Hydrocarbons, C6-12, benzene-recovery
Conclusion:	Atmospheric oxidation via hydroxyl radicals can be a significant route of degradation for products in this category. Based on calculated values, products in this category can have an atmospheric half-life range of 2.3 to 31.8 hours as a result of indirect photolysis by hydroxyl radical attack.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by AOPWIN. The data represent a potential atmospheric half-life range for substances represented by the 10 CAS numbers under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the Low Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for atmospheric half-life range based on constituent data.
Reference:	Meylan, M., SRC 1994-1999. AOPWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
Other (source):	American Chemistry Council, Olefins Panel (Prepared 10/03)

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

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

LOW BENZENE NAPHTHAS ROBUST SUMMARY

Transport / Distribution (Fugacity)

Test Substance*:	Other TS [CAS # 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3]
Method/Guideline:	Calculated according to Mackay Level I, EQC Model version 1.01
Year (guideline):	1997
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment. Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.04 program (1). Measured input values were also used where available and obtained from the EPIWIN database (1). Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, sediment, suspended sediment, biota). 1. EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

Results:

Units/Value:

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

Calculated partitioning data for representative constituents of the Low Benzene Naphthas Category are listed below. The data identify a potential distribution for substances represented by the 10 CAS numbers under Test Substance. Actual distribution of substances in this category will vary dependent on their constituent composition.

Commercial substances in this category consist of complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C12. The seven chemicals selected to represent the environmental distribution range of this category are C5-C11 hydrocarbons that can be found in substances identified by the 10 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.

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

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

	Calculated* Percent Distribution			
Chemical	Air	Water	Soil	Sediment
isopentane	99.98	0.01	0.01	-
toluene	98.17	1.40	0.43	-
m-xylene	97.19	1.33	1.45	0.03
styrene	95.55	2.61	1.80	0.04
naphthalene	24.47	32.28	42.28	0.94
tricyclodecane	98.68	0.29	1.01	0.02
methylnaphthalene	97.68	0.40	1.88	0.04

* Distribution values determined using calculated input data from
EPIWIN program

Results: (cont'd)

Units/Value:

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

	Measured** Percent Distribution			
Chemical	Air	Water	Soil	Sediment
Isopentane	99.98	0.01	0.01	-
toluene	98.80	0.81	0.39	-
m-xylene	97.91	0.86	1.20	0.03
styrene	96.65	1.85	1.46	0.04
naphthalene	42.27	20.56	36.33	0.81
tricyclodecane	na	na	na	na
methylnaphthalene	98.53	0.19	1.25	0.03

** Distribution values determined using measured input data from the EPIWIN program experimental database.
na = not available

Test Substance:

The Low Benzene Naphthas Category includes the following CAS numbers:

64741-98-6	Extract, petroleum, heavy naphtha solvent
64742-48-9	Naphtha, petroleum, hydrotreated heavy
64742-49-0	Naphtha, petroleum, hydrotreated light
64742-83-2	Naphtha, petroleum, light steam-cracked
68333-88-0	Aromatic hydrocarbons, C9-C17
68476-45-9	Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product
68478-10-4	Naphtha, petroleum, light steam-cracked, debezenized, C8-16-cycloalkadiene concentrate
68516-20-1	Naphtha, petroleum, steam-cracked middle aromatic
68527-23-1	Naphtha, petroleum, light steam-cracked aromatic
68919-15-3	Hydrocarbons, C6-12, benzene-recovery

Low Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 10 CAS numbers are used to describe the nine process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry. Aromatics represent the major constituents in all of the streams, varying from approximately 45 to 95 percent. The benzene content is usually less than five percent.

More information on the Low Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1).

1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low Benzene Naphthas Category. American Chemistry Council, Olefins Panel,

	HPV Implementation Task Group. VA, USA.
Conclusion:	The partitioning data represent a potential distribution range for substances in the 10 CAS numbers listed under Test Substance. Substances in the Low Benzene Naphthas Category are calculated to partition primarily to air with a negligible percentage partitioning to water, soil, and sediment. Relatively high vapor pressure and high water solubility largely control the partitioning behavior of constituent chemicals in substances from this category. The input data used to run the EQC Level I model included estimated values calculated by the EPIWIN program based on chemical structure and measured data from the EPIWIN database. A comparison of the distribution data developed using either all calculated input values or measured values where data were available indicate a similar partitioning behavior and support the use of the dataset for chemicals without any measured data.
Reliability:	(2) Reliable with restrictions The input data used to run the EQC Level I model include calculated and experimental values available through the EPIWIN program. The data represent a potential environmental distribution range for substances with the 10 CAS numbers listed under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the Low Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for distribution range based on constituent data.
Reference:	Mackay, D.A. DiGuardo, S. Paterson, and C. Cowan. EQC Model Version 1.01. 1997. Available from the Environmental Modeling Centre, Trent University, Canada.
Other (source):	American Chemistry Council, Olefins Panel (Prepared 7/03)

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

LOW BENZENE NAPHTHAS ROBUST SUMMARY

Water Solubility

Test Substance*:	Other TS [CAS # 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3]
Method/Guideline:	Calculated values using WSKOWWIN version 1.36, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Water Solubility is calculated by the WSKOWWIN subroutine, which is based on a Kow correlation method described by W. Meylan, P. Howard and R. Boethling in "Improved method for estimating water solubility from octanol/water partition coefficient". *Environ. Toxicol. Chem*. 15:100-106. 1995.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Calculated and measured water solubility data for representative constituents of the Low Benzene Naphthas Category are listed below. The data identify a potential water solubility range for substances represented by the 10 CAS numbers under Test Substance. Substances in this category do not have a specific water solubility value. Actual water solubility ranges for substances in this category will vary dependent on their loading rate (i.e., weight of test material added to a volume of water). Commercial substances in this category consist of complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C12. The seven chemicals selected to represent the water solubility range of this category are C5-C11 hydrocarbons that can be found in substances identified by the 10 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.

Results: (continued)

Units/Value:

Note: Deviations from protocol or guideline, analytical method.

Substance Constituent	Calculated WS (mg/L @ 25°C)	Measured WS* (mg/L @ 25°C)
isopentane	184.6	na
toluene	832.7	573.1
m-xylene	258.4	207.2
styrene	386.7	343.7
naphthalene	183.8	142.1
tricyclodecane	21.5	na
methylnaphthalene	54.6	41.4

* Experimental values from EPIWIN database.
na = not available
The data represent a potential water solubility range for substances represented by the 10 CAS numbers under Test Substance.

Test Substance:

The Low Benzene Naphthas Category includes the following CAS numbers:

64741-98-6	Extract, petroleum, heavy naphtha solvent
64742-48-9	Naphtha, petroleum, hydrotreated heavy
64742-49-0	Naphtha, petroleum, hydrotreated light
64742-83-2	Naphtha, petroleum, light steam-cracked
68333-88-0	Aromatic hydrocarbons, C9-C17
68476-45-9	Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product
68478-10-4	Naphtha, petroleum, light steam-cracked, debezenized, C8-16-cycloalkadiene concentrate
68516-20-1	Naphtha, petroleum, steam-cracked middle aromatic
68527-23-1	Naphtha, petroleum, light steam-cracked aromatic
68919-15-3	Hydrocarbons, C6-12, benzene-recovery

Low Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 10 CAS numbers are used to describe the nine process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry. Aromatics represent the major constituents in all of the streams, varying from approximately 45 to 95 percent. The benzene content is usually less than five percent.

More information on the Low Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1).

1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge

	Program Test Plan For The Low Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	The calculated water solubility for some representative constituents that are present in the category streams vary from 21.5 to 832.7 mg/L @ 25°C. The measured water solubility of these same constituents vary from 41.4 to 573.1 mg/L @ 25°C. Although this does not define the actual water solubility of the category streams, it offers an indication of a range that might be expected to encompass the water solubility of these complex streams with variable compositions. Water solubilities outside these ranges may be possible for some category streams.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential water solubility range for substances represented by the 10 CAS numbers under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the Low Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for water solubility range based on constituent data.
Reference:	EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Water solubility values were calculated by the WSKOWWIN subroutine and measured data came from the database in the computer program.)
Other (source):	American Chemistry Council, Olefins Panel (Prepared 7/03)

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

Attachment 2b

Robust Summaries

Heavy Aromatic Distillate, CAS# 64742-48-9

Mammalian Toxicity

Robust Summary - Group 6: Low Benzene Naphthas

Acute Toxicity

Test Substance	Heavy Aromatic Distillate, CAS# 64742-48-9
Method	
Method/guideline followed	No guideline specified, comparable to standard study
Type (test type)	Acute LD50
GLP	Yes
Year	1984
Species/Strain	Rat, Fischer 344
Sex	Male and female
No. of animals per sex per dose	5/dose/group (4 groups)
Vehicle	None
Route of administration	Oral gavage
Test Conditions	Rats were dosed once with undiluted heavy aromatic distillate at 4.5, 5.0, 5.5 and 6.0 g/kg, and were observed for 14 days post dosing for mortality, moribundity and clinical signs. Body weight was obtained at initiation, and after 7 and 14 days post dosing. Gross necropsies were performed on all rats at study termination.
Results	There were no deaths attributed to test article administration, and therefore, the LD50 was not reached in either sex at the highest dose. Body weight was not significantly changed over the 14-day observation period. Over the first week of study, there were instances of perianal soiling, dry material around the mouth, and soft feces. In sacrificed rats, there were no findings that could be attributable to test material administration.
LD_{50} with confidence limits.	
Remarks	
Conclusions	
(study author)	The LD50 was not reached at the highest dose of 6.0 g/kg.
Data Quality	
Reliability	**1**. Reliable without restrictions
References	Rausina, G. 1984. Acute oral toxicity study in albino rats using heavy aromatic distillate. Proj. # 2049. Gulf Life Sciences Center, Pittsburgh, PA for Gulf Oil Chemicals Co., Houston, TX.
Other	
Last changed	Rev 6/25/2001 (Prepared by a contractor to the Olefins Panel)

Robust Summary – Group 6: Low Benzene Naphthas

Acute Toxicity

Test Substance	Heavy aromatic distillate, CAS# 64742-48-9. No composition or purity analysis reported, refer to sponsor.
Method	
Method/guideline followed	No guideline specified but comparable to standard study
Type (test type)	Acute LC50
GLP	Yes
Year	1983
Species/Strain	Rat, Fischer 344
Sex	Male and female
No. of animals per sex/dose	5
Vehicle	filtered air
Route of administration	whole body inhalation
Test Conditions	Six groups of 10 rats (5M, 5F/group, 12-16 wks old, 145-307g) were individually housed and exposed in stainless steel/glass inhalation chambers to aerosolized test article or filtered air for 4 hours, followed by 14 days of observation post exposure for clinical signs, morbidity and death. Non-fasted rats were sacrificed on day 14 and necropsied for gross lesions. Nominal chamber concentrations (g/m^3) were 0.0, 12.2, 24.8, 25.8, 19.6, and 99 (uncorrected for large particle condensation), but actual chamber concentrations were 0, 6.0, 7.6, 8.6, 9.1, and 11.2 as determined by gas chromatography. Probit analysis was used to estimate an LC50.
Results	
LC_{50} with confidence limits.	LC50 was estimated to be 8.5 g/m^3 (actual chamber concentration).
Remarks	There was a large difference between nominal and actual concentrations in the inhalation chambers that was not addressed in the report. In the analyses, exposure concentration was estimated by comparing peak height (rather than peak area) with that of the neat sample. The method of calculating chamber concentration of test article in ppm was not reported (Comment by contractor). All animals in the high dose group died during exposure with congestion of lungs and nasal turbinates with red discharge. Six animals died in groups 4 and 5 during exposure, and were found with gas in the G.I. tract. Mean body wt of males and females decreased by day 7 but then increased over the remaining 7 days. Most rats exhibited nasal and ocular discharges, and in the higher dose groups showed signs of CNS effects, (hyperexcitablility, twitching, circling) that . were absent by day 2. Other clinical effects were absent by day 7. No test article related gross pathological lesions were observed.
Conclusions	LC50 was 8.5 g/m^3.
Data Quality	
Reliability	**1**. Reliable without restrictions. This study is acceptable for range-finding since the concentrations employed yielded a dose response curve covering the full range of biological response (0-100% fatalities).
References	Goode, J.W. 1983. LC50 Inhalation toxicity study in rats using heavy aromatic distillate. Proj. # 2050. Gulf Life Sciences Center, Pittsburgh, PA for Gulf Oil Chemicals Co., Houston, TX
Other	
Last changed	Rev. 7/2/2001 (Prepared by a contractor to the Olefins Panel)

Robust Summary - Group 6: Low Benzene Naphthas

Genetic Toxicity - in Vitro

Test Substance	
Test substance	Heavy Aromatic Distillate, Gulf. CAS #64742-48-9. Water-white liquid with characteristic aromatic odor. Composition analysis, purity and stability referred to sponsor.
Method	
Method/guideline followed	Standard method based on Hsie et al. (1981), O'Neill & Hsie (1979)
Type	In vitro mammalian cell forward mutation
System of testing	Chinese hamster ovary (CHO) cell culture
GLP	Yes
Year	1984
Species/Strain	CHO-K-1 heterozygous for hypoxanthine-guanine phosphoribosyl transferase (HGPRT+/-) from Oak Ridge National Laboratory, TN.
Metabolic activation	Yes
Species and cell type	Rat liver (S9) fraction purchased from Litton Bionetics, Kensington, MD
Quantity	1.0mg S9 fraction/ml treatment medium (0.3ml S9 fraction in 3 ml medium/flask)
Induced or not induced	Aroclor 1254 induced (treatment not specified)
Concentrations tested	Cytotoxicity, final conc. (trial 2): 128, 256, 512, 1024µg/ml ± S9; Mutagenicity, final conc. (trial 2): 64, 128, 256, 512, 750, 1024µg/ml –S9; 128, 256, 512, 1024, 1500, 2048µg/ml +S9, all diluted in 10% Pluronic® polyol F68 (prepared in dionized water, mol. wt. 8350)
Statistical Methods	Frequency of mutant colonies per million clonable cells was calculated and comparisons of treated cultures with vehicle controls made on transformed data using a two-tailed t-test (Irr & Snee, 1979). Criteria for positive results were significant ($p<0.05$) increase in mutant colonies (HGPRT+/- → HGPRT-/-) at any dose level and a dose related response. If only one criterion is met, results are considered equivocal.
Remarks for Test Conditions	Sufficient Heavy Aromatic Distillate (HAD) was weighed separately for each dose level into 10 ml volumetric flasks, 1.8ml of 10% F68 added per ml of final volume and medium (Ham's F-12 without hypoxanthine) added as required to achieve final 10ml volume for testing. All dosing preparations were vortexed just after addition of medium and just prior to use when 20µl of each preparation was added to 3ml treatment medium/culture vessel. All cultures were incubated at 37^0C in 5% CO$_2$ enriched, humidified atmosphere. Positive control mutagens were ethyl methanesulfonate (100µg/ml) for –S9 cultures, and benzo(a)pyrene (4µg/ml) for +S9 cultures. For cytotoxicity, each dose group was composed of 2 flasks, one –S9, one+S9, negative controls ± S9, seeded with 5x10^5 cells on day 1. Cultures were exposed to test compound for 5 hours on day 2. On day 3, cells were trypsinized and counted with a Coulter Model ZB, then 200 cells were transferred into each of 3 60mm culture dishes. These viability plates were incubated until day 10, fixed in methanol and stained with Giemsa. Colonies were counted visually or with an Artek Model 981 colony counter. Absolute survival = total colony count ÷ number of cells seeded/flask. Relative survival = absolute survival in treated cultures ÷ vehicle control survival. Acceptable survival level is at least 10%. For mutagenicity, cells were seeded on day 1 into 6 flasks/dose group, 3-S9, 3+S9; on day 2 approximately 10^6 cells were exposed to HAD for 5 hours. Vehicle control had 12 flasks, 6-S9, 6+S9. On day 3, cultures with excessive cytotoxicity were discarded. From remaining cultures, 200 cells were seeded to each of 4 viability plates/dose level; incubated to day 10, fixed with methanol, stained with Giemsa, and colonies counted for survival. Expression cultures (10^5-10^6 cells/one dish/dose) were seeded on day 3; subcultured three times until day 10 when 200 cells were seeded on each of 4 viability plates/dose and 2x10^5 cells seeded on each of 5 mutagenicity plates/dose with selective medium containing 10^{-5}M 6-thioguanine to allow expression of HGPRT mutation. Cultures were incubated undisturbed until day 17 when they were fixed and stained. For mutagenicity, a ratio of total colony counts in mutagenicity plates over absolute survival in viability plates was calculated for each treatment group. Frequency of

	mutant colonies/million clonable cells was calculated and statistical comparisons with negative control data were made.
Results Genotoxic effects	First trial was aborted after post treatment cell counts in the mutagenicity assay, because of disparity in cytotoxic response between cytotoxicity aspect and mutagenicity aspect of the trial. No cytotoxicity was seen in the mutagenicity aspect. Results of the second cytotoxicity trial demonstrated cytotoxicity at 512 µg/ml and higher in the –S9 portion and only a slight decrease in cell count at 1024 µg/ml in the activated portion but no cytotoxicity in colony count after treatment. The second mutagenicity trial indicated post treatment cell death in –S9 cultures beginning at 64 µg/ml with significant effects at 256 µg/ml and 100% toxicity at 750 µg/ml. In +S9 cultures, slight cell toxicity was seen at 1500 µg/ml and above. For both activated and non-activated cultures, no significant dose-related responses or significant increase in mutant frequency were observed at any dose level of HAD. Positive control compounds responded appropriately (EMS 5.2 fold increase and B(a)P 2.8 fold increase over vehicle control).
Conclusions (contractor)	Mutagenicity was not observed at any HAD dose level tested with or without metabolic activation. Heavy Aromatic Distillate does not induce gene point mutations in the CHO/HGPRT test under conditions of this assay.
Data Quality *Reliabilities*	**1**. Reliable without restrictions. Study conforms to standard design. GLPs have been followed
Reference	Papciak, M.S., Goode, J.W. 1984. CHO/HGPRT test: Heavy Aromatic Distillate. Proj. #2054. Gulf Life Sciences Center, Pittsburgh, PA for Gulf Oil Chemicals Co., Houston, TX Hsie, A.W. et al. 1981. Mut. Res. 86: 193-214 O'Neill, J.P. and Hsie, A.W. 1979. Banbury Report 2: 55-63 Irr, J.D. and Snee, R.D. 1979. Banbury Report 2: 263-275.
Other *Last changed*	Rev. 6/25/2001 (Prepared by a contractor to the Olefins Panel)

Robust Summary - Group 6: Low Benzene Naphthas

Genetic Toxicity - in Vitro

Test Substance _Test substance_	Heavy Aromatic Distillate, Gulf. CAS #64742-48-9. Water-white liquid with characteristic aromatic odor. Composition analysis, purity and stability referred to sponsor.
Method	
Method/guideline followed	Standard method based on Cortesi et al (1983), Dunkel et al (1981), Reznikoff et al (1973)
Type	In vitro cell transformation
System of testing	Mouse embryo cells
GLP	Yes
Year	1984
Species/Strain	BALB/3T3-A31-1-1 from T. Kakunaga, National Cancer Inst., 1982
Metabolic activation	No
Species and cell type	NA
Quantity	NA
Induced or not induced	NA
Concentrations tested	Cytotoxicity: 8, 16, 32, 64, 128, 256, 512, 1024, 2048, 5000µg/ml; Transformation: 16, 32, 64, 200µg/ml, all diluted in 10% Pluronic$^{®}$ polyol F68 (prepared in deionized water, mol. wt. 8350, 80% hydrophilic).
Exposure period	2 days
Statistical Methods	None employed. Criteria for positive response were a two-fold increase in type III foci at the highest dose over vehicle control (at least 2 type III foci if vehicle control had none) with or without a dose related response, or a two-fold increase at two or more consecutive doses. Test is equivocal if two-fold increase occurred at any one level other than the highest acceptable dose.
Remarks for Test Conditions	Sufficient Heavy Aromatic Distillate (HAD) was weighed separately for each dose level, 0.45ml of 10% F68 added per ml of final volume and medium (Eagles MEM with 10% heat-inactivated fetal calf serum) added as required to achieve final volume for testing. Test preparations were mixed just prior to addition to cultures at 50µl to each 5 ml culture. All cultures were incubated at 37^0C in 5% CO_2 enriched humidified atmosphere. For cytotoxicity, 2 plate cultures/dose group, 2 plate cultures for vehicle F68 or medium negative control were seeded with $1x10^4$ cells/plate in day 1, exposed on days 2-3, trypsinized and counted with a Coulter Model ZB on day 4 for at least 20% survival. For transformation, 15 flasks ($1x10^4$ cells/flask/dose group)) and two cloning flasks (100 cells per flask/dose group) were seeded on day 1, exposed on days 2-3 and culture medium changed on day 4. For transformation flask cultures, medium continued to be changed weekly to day 29. Positive control was 3-methylcholanthrene (1µg/ml). Cloning flask cultures were fixed, stained, and counted visually on day 8 to determine cloning efficiency (avg. number colonies/plate ÷ 100 cells seeded). Flask cultures were fixed and stained on day 29 for focus counting and evaluation. Transformation frequency = total type III foci ÷ total flasks/dose group.
Results Genotoxic effects	In the first trial, HAD induced toxicity in BALB/3T3 cells after two days exposure beginning at 32µg/ml (59.9% relative survival), increasing with dose level to 2.9% relative survival at 5000µg/ml. The first trial was discarded due to loss of many cultures (27/105) due to contamination. Results of the second transformation trial indicated no treatment related cell transformation induced by HAD. Toxicity was evident 32µg/ml (67.2% relative cloning efficiency), increasing sharply at 200µg/ml (28.8% cloning efficiency). Positive and negative controls gave expected results.
Conclusions (contractor)	Heavy Aromatic Distillate did not induce transformation in BALB/3T3 cells at any dose level under conditions of this assay.
Data Quality _Reliabilities_	**1.** Reliable without restriction. Study conforms to standard design. GLPs have been followed.

Reference	Brecher, S., Good, J.W. 1984. BALB/3T3 transformation test: Heavy Aromatic Distillate. Proj. #2057. Gulf Life Sciences Center, Pittsburgh, PA for Gulf Oil Chemicals Co, Houston, TX Cortesi, E. et al. 1983. Teratogenesis, Carcinogenesis, Mutagenesis 3: 101-110. Dunkel, V.A. et al. 1981. J. Nat'l Cancer Inst. 67: 1303-1315. Reznikoff, C.A. et al. 1973. Cancer Res. 3239-3249.
Other	
Last changed	4/11/2001 (prepared by a contractor to the Olefins Panel).

Robust Summary - Group 6: Low Benzene Naphthas

Genetic Toxicity - in Vitro

<u>Test Substance</u>	
Test substance	Heavy Aromatic Distillate, Gulf. CAS #64742-48-9. Water white liquid with characteristic aromatic odor. Composition analysis, purity and stability referred to sponsor.
<u>Method</u>	
Method/guideline followed	Standard method based on Williams et al. (1977,1982)
Type	In vitro mammalian cell DNA repair assay
System of testing	Unscheduled DNA Synthesis (UDS) in primary hepatocyte cultures.
GLP	Yes
Year	1984
Species/Strain	Fischer 344 male rat (13-14 wks old) – 1 rat per test
Metabolic activation	No
Species and cell type	NA
Quantity	NA
Induced or not induced	NA
Concentrations tested	Range-finding: 8, 16, 32, 64, 128, 256, 512, 1024, 2048, 5000 µg/ml: UDS assay 10, 40, 100, 200 µg/ml; all diluted in 10% Pluronic® polyol F68 (prepared in deionized water, mol. wt 8350, 80% hydrophilic)
Exposure period	18 hours
Statistical Methods	None employed. Criteria for positive response are incorporation of radioactive precursor (^{3}H-thymidine) in cells that are not normally synthesizing DNA, indicating repair of damage. A positive response is defined as a mean net nuclear grain count at any treatment level that exceeds concurrent negative control by at least 6 grains/nucleus; negative control value must not exceed 5 grains. A positive response need not be dose related.
Remarks for Test Conditions	Sufficient Heavy Aromatic Distillate (HAD) was weighed separately for each dose level, 0.45ml of 10% F68 added per ml of final volume and sufficient medium (Williams Medium E with 10% fetal bovine serum and insulin) added to achieve final volume. Test preparations were mixed just prior to addition at 30µl to each 3 ml culture. The conc. of ^{3}H-thymidine (½ life 12.5 yrs.) used in these assays was 1mCi/ml. All cultures were incubated at 37^{0}C in 5% CO_2 enriched humidified atmosphere. For range-finding, primary hepatocytes derived from freshly perfused rat liver were seeded (approx. 1x10^5 cells/ml) into treatment vessels, exposed to test material for 18 hours (2 cultures/dose level; 2 untreated cultures, and two vehicle (F68) control cultures), then fixed in formalin and stained with trypan blue for viability determination. At least 50% viability needed for the assay. In the UDS assay, 1x10^5 cells/ml were seeded into coverslip cultures, exposed to ^{3}H-thymidine and test substance for 18 hours (3 cultures/dose level). Positive control was 2-acetyl aminofluorene (0.2µg/ml). Cells growing on coverslips were rinsed, fixed and glued to microscope slides on day 2. On day 3, slides were dipped in autoradiographic emulsion and stored in the dark at 2-8^{0}C. Autoradiographs were developed, stained and coverslipped on day 14. Numbers of grains overlying 50 randomly selected nuclei/slide were counted. The highest of 3 cytoplasmic grain counts/cell were subtracted and this number was divided by a conversion factor of 2, to obtain net nuclear grain count. Avg. net nuclear grain count/slide (sum of net nuclear grain count ÷ 50) and mean net nuclear grain count (avg. net nuclear grain count/slide ÷3) were calculated.
<u>Results</u>	
Genotoxic effects	HAD induced toxicity in primary hepatocytes beginning at 32-64µg/ml (72-80% relative viability) after 18 hours exposure, which increased with dose levels to 2% viability at 5000µg/ml. HAD did not cause unscheduled DNA synthesis at any dose level. Positive and negative controls gave expected results.
<u>Conclusions</u>	
(contractor)	Unscheduled DNA synthesis was not observed in primary culture of rat hepatocytes at any dose level of Heavy Aromatic Distillate, indicating that this material does not damage DNA under conditions of this assay.

Data Quality *Reliabilities*	**1**. Reliable without restrictions. Study conforms to standard design. GLPs have been followed.
Reference	Brecher, S., Goode, J.W. 1984. Hepatocyte primary culture/DNA repair test of heavy aromatic distillate. Proj. #2056. Gulf Life Sciences Center, Pittsburgh, PA for Gulf Oil Chemicals Co., Houston, TX Williams, G.M. 1977. Cancer Res. 37: 1845-1851 Williams et al. 1977. In Vitro 13: 809-817 Williams et al. 1982. Mut. Res. 97:359-370
Other *Last changed*	4/11/2001 (Prepared by a contractor to the Olefins Panel)

Robust Summary - Group 6: Low Benzene Naphthas

Genetic Toxicity - in Vivo

Test Substance Remarks	Heavy Aromatic Distillate, Gulf CAS #64742-48-9. Water white liquid with aromatic odor. Compositional analysis, purity and stability referred to sponsor.
Method	
Method/guideline followed	Comparable to standard assay
Type	Mammalian bone marrow erythrocyte micronucleus
GLP	Yes
Year	1984
Species	Mouse
Strain/Sex	Crl:CD$^{®}$–1 (ICR) BR Swiss: Male and female: Range finding (RF): 2M, 2F/group; Micronucleus:.10M, 10F/group; 15M, 15 F in 1 group
Route of administration	Oral gavage
Doses/concentration levels	RF: 0, 1.25, 2.5, 5.0 g/kg in corn oil: Micronucleus: 0, 0.625, 1.25, 2.5 g/kg in corn oil
Exposure period	1 dose/day for 2 days; 1 group at 2.5 g/kg 1 dose, 1 day only
Statistical methods	Values from treated groups for daily mean body weights, group means and std. dev. for polychromatic erythrocytes (PCEs) with micronuclei (MN) , and group mean ratios of PCE to normochromatic erythrocytes (NORMs) were calculated and compared with vehicle control values by Student's t-test. Positive response was indicated by statistically significant ($p<0.05$) increases in micronucleated PCE at any dose level with a dose related response evident. Results were considered equivocal if only one of these criteria was met.
Remarks for Test Conditions.	Heavy Aromatic Distillate (HAD) dosing solutions were prepared fresh for each day of dosing –12.5 g HAD (RF) or 6.25 g HAD (micronucleus) mixed with corn oil to make 50 ml, blended by shaking. Based on results of the range finding study, three groups of mice were given HAD by oral gavage daily for two days. All mice were weighed on day 1 and on day of sacrifice. One half of each treated group and vehicle control (5M, 5F) was killed on day 3 and the remainder on day 4. One group (15M, 15F), given 2.5 g/kg by gavage in a single dose for 1 day only, was killed on days 2, 3, 4 (5/sex/day). Positive control mice given cyclophosphamide (75 mg/kg) ip daily for 2 days were killed on day 3. Slides of femoral bone marrow smears were prepared, stained with May-Grunewald/ Giemsa stain and examined microscopically. For each mouse, 1000 PCE and all associated mature erythrocytes (NORMs) were counted. Data collected included group mean body weights for each day, total PCEs, total NORMs, PCEs with MN, and NORMs with MN.
Results Genotoxic effects NOAEL (NOEL) LOAEL (LOEL)	In range finding test, 1/2males and ½ females died at 5.0 g/kg dose level by day 3. In the micronucleus test, 1/10 females in the 2.5 g/kg dose group (2 days of dosing) died by day 4. All other mice survived to study sacrifice. Body wts were comparable to negative controls for both sexes in all treatment groups and positive controls. Treatment with HAD did not show any significant changes in micronucleus formation or in the ratio of PCE/NORM at any dose level. Average PCE/NORM ratio was 0.9% for all HAD treatment groups and negative control; ratio for positive control was 0.5%. NOEL (systemic) = 1.25 g/kg: NOEL (genetic) = 2.5 g/kg
Conclusions (study authors)	Oral treatment of mice with Heavy AaromaticDistillate for 1 or 2 days at doses up to 2.5 g/kg did not cause increased frequency of micronucleated polychromatic erythrocytes in bone marrow of treated mice. Under these test conditions, Heavy Aromatic Distillate does not induce cytogenetic damage.
Data Quality *Reliabilities*	**1.** Reliable without restrictions. Study conforms to standard design. GLP followed.
References	Khan, S.H. and Goode, J.W. 1984. Micronucleus test in mouse bone marrow: Heavy Aromatic Distillate administered orally for 2 days. Proj. #2005. Gulf Life Sciences

	Center, Pittsburgh, PA for Gulf Oil Chemicals Co., Houston, TX
Other *Last changed*	Rev. 6/25/2001 (Prepared by a consultant to the Olefins Panel)

Robust Summary - Group 6: Low Benzene Naphthas

Repeated Dose Toxicity

Test Substance Remarks	Heavy Aromatic Distillate, CAS # 64742-48-9. No analysis of purity or composition reported; referred to sponsor.
Method	
Method/guideline followed	No guidelines specified, comparable to standard study
Test type	Subacute
GLP	Yes
Year	1983
Species	Rat
Strain	Fischer 344
Route of administration	Whole body inhalation
Duration of test	5 days
Doses/concentration levels	0, 1.2, 2.7, 5.0 g/m^3
Sex	Males and females 5/sex/group
Exposure period	5 days
Frequency of treatment	6 hours/day
Control group and treatment	filtered air at 6 hrs/day for 5 days
Post exposure observation period	None
Statistical methods	Analysis of Variance, Dunnett's test
Test Conditions	Animals (13 weeks old at study initiation, 156-279g) were housed individually in screen-bottom cages with automatic watering in rooms maintained at approx. 74^{0}F with relative humidity of 50%, and 12 hour light/ dark cycle. Chow diet and water were provided ad lib except during exposure. Chamber concentrations were monitored by GC; peak areas were compared with those of neat test article standards. Rats were monitored twice daily for morbidity and mortality, and observed once daily for clinical signs. Body weights were measured at initiation and termination. Necropsies were performed for gross lesions.
Results	
NOAEL (NOEL)	NOEL not determined
LOAEL (LOEL) Remarks	LOEL = 1.2 g/m^3 based on clinical observations: perianal staining, red material around nose/mouth, ocular porphyrin. (assessed by Reviewer). One female rat in the high dose group died during the initial exposure; all other rats survived until termination. Males and females exposed to 5.0g/m3, showed a dose related weight loss of approx. 8% after 5 days of dosing. Incidence of dry red material around nose/mouth, ocular porphyrin, clear discharge from the eyes, partially closed eyes and perianal staining occurred in all groups receiving test article. The two high dose groups showed purulent discharge from the eyes and bloody tears. Reviewer comment: The total incidence of clinical observations increased in a manner related to exposure concentration.
Conclusions	One death occurred during exposure of the high dose group. All other animals exhibited clinical signs that included ocular discharge, eye closure, and dry red material around the nose/mouth. Gross pathological lesions were not observed which could be directly attributable to test article administration.
Quality	
Reliabilities	1. Reliable without restrictions.
References	Gordon, T. 1983. One week repeat dose inhalation toxicity study in the rat using heavy aromatic distillate. Proj. # 2062. Gulf Life Sciences Center, Pittsburgh, PA for Gulf Oil Chemicals Co., Houston, TX.
Other	
Last changed	Rev. 7/3//2001 (Prepared by a contractor to the Olefins Panel)

Robust Summary - Group 6: Low Benzene Naphthas

Repeated Dose Toxicity

Test Substance	
Remarks	Heavy Aromatic Distillate, CAS #64742-48-9. No composition or purity analysis reported; refer to sponsor.
Method	
Method/guideline followed	No guideline specified; comparable to standard study.
Test type	Subacute
GLP	Yes
Year	1985
Species	Rat
Strain	Fischer 344
Route of administration	Dermal
Duration of test	4 weeks
Doses/concentration levels	0.0, 0.5, 1.0, 1.5 g/kg in paraffin oil vehicle
Sex	Males and female (10/sex/group), 72 days old at study initiation
Exposure period	6 hours/day
Frequency of treatment	once/day, 5 days/week
Control group and treatment	Paraffin oil, 2.18 ml/kg/day for 5 days/week
Post exposure observation period	None
Statistical methods	Bartlett's test for homogeneity, Dunnett's test for homogeneous data; modified t-test for non-homogeneous data.
Test Conditions	Animals were housed individually in suspended stainless steel cages with wire mesh bottoms and fronts equipped with an automatic watering system, in a room maintained at 76.1^0F with relative humidity of 56.6% and 12 hour light/dark cycle. Chow diet was provided ad lib. Test article dilutions in paraffin oil (75% v/v) were prepared weekly. Doses of test article were administered over 10% of body surface to the backs of rats clipped free of hair and fitted with Elizabethan collars to reduce ingestion. After 6 hours, collars were removed and residual oil wiped off. Observations for mortality and moribundity were made twice/day, and for clinical signs at least once daily (on dosing days). Dermal responses were scored at initiation and then weekly. Body weight was measured at initiation and then weekly. Food consumption was determined weekly. At sacrifice, gross necropsy was performed, organs/tissues (19/rat) weighed and preserved. Slides prepared for histopathologic examination for the following tissues/organs of control and high dose groups: brain, spinal cord, heart, lungs, thymus, left kidney, right kidney, liver, spleen, sternum, lymph nodes, testes, skin, adrenal glands, urinary bladder, and peripheral nerve.
Results	
NOAEL (NOEL)	NOEL not determined.
LOAEL (LOEL)	LOEL males = 0.5g/kg (increased total WBC count, assigned by reviewer) LOEL females =1.5 g/kg (hematologic alterations, skin irritation, assigned by reviewer)
Remarks	No deaths or moribund rats were observed and no statistically or biologically significant differences in group mean body wt were noted at study termination. No clinical effects were observed that could be attributed to test article administration. Food consumption was significantly decreased in male rats given 1.5g/kg during wks 2 and 3, and in female rats given 1.0g/kg during wk 2. Severe erythema was observed in 1.5g/kg males and females by wk 3 which persisted for the duration of the study. At termination, moderate eschar formation was seen in 10/10 males and 7/10 females. Statistically significant changes in hematology and clinical chemistry parameters after 4 wks of dosing were: dose responsive increase in WBC (57-70%) of males and females in 1.5g/kg group; slight reduction of RBC in males and reduction of HGB and HCT of males and females given 1.5g/kg; elevated platelet counts (10-20%) in 1.5g/kg males and females, reduced total serum protein (10-13%) in 1.5g/kg males and females; reduced serum albumin (9-25%) in high dose males and females; dose responsive reduction in BUN (9-25%) in high dose animals. There were marked increases in segmented neutrophils (200-400%) and lymphocytes (20-30%) in males and females given 1.5g/kg, and an erratic but marked increase in atypical lymphocytes of males in low-high dose groups and increased eosinophils (485%) in 1.5g/kg males. There were several statistically significant but inconsistent changes in organ wt when expressed as

	absolute wt, or per 100 g body wt. but these were not perceived as being biologically significant. There were no histopathological effects noted except those in the skin.
Conclusions	Repeated application of heavy aromatic distillate to male and female rats caused severe skin irritation and significantly decreased food consumption and body wt. Gross and microscopic lesions produced at the site of application, included ulceration, acanthosis and hyperkeratosis. In both male and female rats, treatment with heavy aromatic distillate was associated with significantly elevated WBC counts and mild anemia associated with decreased RBC counts, hematocrit, level of hemoglobin in peripheral blood, and elevated platelet count. The elevated WBC count was related to elevated levels of neutrophils and lymphocytes.
Quality Reliabilities	**2**. Reliable with restrictions. No analysis of test material preparations in paraffin oil.
References	Zellers, J.E. 1985. Four week repeated dose dermal toxicity study in rats using heavy aromatic distillate. Proj. #2063. Gulf Life Sciences Center, Pittsburgh, PA for Gulf Oil Chemicals Co., Houston, TX
Other Last changed	Rev. 7/2/2001 (Prepared by a contractor to the Olefins Panel)

201-16788D

Attachment 1: Summary of High Aromatic Studies for Reproductive Toxicity: Effect Levels & Exposure Duration

Test material	Species/Route of Exposure	NOAEL	LOAEL	Duration of Exposure	Reference
Gasoline 2-generation	Rats – males & females/Inhalation	7400ppm	No reproductive or fertility effects; no effects on offspring survival or growth	OECD protocol #416; OPPTS 870.3800 (1994) [0, 1850, 3700, 7400ppm]	McKee et al., 2000
Benzene 2-generation	Rat –female/inhalation	No maternal effects	116ppm- dec. pup wt no malformations	4 mon prior to impregnation & gestation; 2 generations	Vozovaya, 1975, 1976
1-generation	Rat- female/inhalation	No maternal effects 30ppm	300ppm – dec pup wt, no malformations	6h/d, 5d/wk for 60 d; 7d/wk for 35 days GD 1-20; LD 5-20	Kuna et al., 1992
Mixed Xylenes 1-generation	Rats- males & females/ inhalation	500ppm – max. dose parents & F1 offspring	None	151d, 5d/wk 35d, 7d/wk, 6hr/d gest. (1-20); lact.(5-20)	API, 1983
Male fertility	Rats- Males/ Inhalation	1000ppm – only dose, no effect on testes/acc organs	None	61 days, 18hr/d	Nylén et al., 1989
High Flash Aromatic Naphtha (C9) 3-generation	Rats – males & females/Inhalation offspring	500ppm [no reproductive effects at 1500ppm] 500ppm	1500ppm: dec parental body wt all gen., no repro effects 1500ppm: dec pup body wt all gen. after restart exposure. to dams at lact.day 5 F1 dams with undetected pregnant exposed to delivery had dec. litter size, birth wt and pup survival	10wk, 6hr/d, 5d/wk M&F; F0 6hr/d, 7d/wk GD0-20, LD5-21; F1 GD0-20 begun 5-7wk-old, LD5-21 F2 GD0-20, begun at weaning [3wk old]	McKee et al, 1990

Attachment 2. Summary of High Aromatic Studies for Reproductive Toxicity: Effect Levels & Exposure Duration (cont)

Test material	Species/Route of Exposure	NOAEL	LOAEL	Duration of Exposure	Reference
Aromatol (C9) **1-generation**	Rats – females/ Inhalation	120ppm	200ppm: maternal & pup body wt dec, also at 400ppm; no malformations	24h/d, 7d/wk GD7-15, natural delivery	Ungváry et al., 1983
	Rats – females/ Inhalation	400ppm	None: did not reproduce Ungváry et al, 1983 effects	24h/d, 7d/wk GD7-15, natural delivery	Lehotzky et al., 1985.
C10-C12 Naphtha	Rats- males & females/Inhalation	In Progress			ICCA Hydrocarbon Solvents HPV Test Program

References for Attachment 1

Gasoline:

McKee, R.H., Trinmer, G.W., Whitman, F.T., Nessel, C.S., Mackerer, C.R., Hagemann, R., Priston, R.A., Riley, A.J., Cruzan, G., Simpson, B.J., Urbanus, J.H. 2000. Assessment in rats of the reproductive toxicity of gasoline from a gasoline vapor recovery unit. *Reproductive Toxicol.* 14: 337-353.

Benzene:

Vozovaya, M.A. 1975. Action of low concentrations of benzene, dischloroethane and their combination on the generative function of animals and the development of progeny. *Gig. Tr. Prox. Label* 7: 20-23 [English abstract].

Vozovaya, M.A. 1975. The effect of small concentrations of benzene and dischloroethane separately and combined on the reproductive function of animals. *G. Sanit* 6: 100-102 [English abstract].

Kuna, R.A., Nicolich, M.J., Schroeder, R. E., and Rusch, G.M. 1992. A female rat fertility study with inhaled benzene. *J Am Coll Toxicol* 11: 275-282.

Xylene:

American Petroleum Institute. 1983. Parental and fetal reproduction inhalation toxicity study in rats with mixed xylenes. [performed at Bio/dynamics] API Medical Res. Report #31-31481**.** EPA/OTS FYI-AX-0983-0209. Washington, DC

Nylén, P, Ebendal, T., Eriksdotter-Nilsson, M., et al. 1989. Testicular atrophy and loss of nerve growth factor-immunoreactive germ cell line in rats exposed to n-hexane and a protective effect of simultaneous exposure to toluene or xylene. *Arch Toxicol*. 63: 296-307.

High Flash Aromatic Naphtha (C9)

McKee, R.H., Wong, Z.A., Schmitt, S., Beatty, P., Swanson, M., Schreiner, C.A., and Schardein, J.L. 1990. The reproductive and developmental toxicity of high flash aromatic naphtha. *Toxicol Indust Health* 6: 441-460.

Ungváry, G., Tatrái, E., Lorincz, M., Fittler, Z., and Barcza, G. 1983. Investigation of the embryonic effects of Aromatol, a new C9 aromatic mixture. *Egeszsegtudomany* 29: 138-148. [English abstract]

Lehotzky, K., SzeberenyI, J., Ungváry, G., and Kiss, A. 1985. The effect of prenatal Aromatol exposure on the nervous systems of offspring among rats. *Egeszsegtudomany* 29: 389-397. [English abstract]

Regulatory Documents

Benzene

Agency for Toxic Substances and Disease Registry (ASTDR). 1993. Toxicological Profile of Benzene. U.S. Dept. of Health and Human Services, U.S. Public Health Service, Atlanta, GA

European Union. 2000. Comprehensive risk assessment report of Benzene _EINECS-No. 200-753-7 DRAFT. Rapporteur, German Federal Institute for Occupational Safety and Health Notification Unit

Integrated Risk Information System (IRIS). 1998. Toxicological Review of Benzene (Noncancer effects). NCEA-S-0455. US EPA, Washington, DC.

Xylene

Agency for Toxic Substances and Disease Registry (ASTDR). 1995. Toxicological Profile of Xylenes: Update U.S. Dept. of Health and Human Services, U.S. Public Health Service, Atlanta, GA

Integrated Risk Information System (IRIS). 2002. Toxicological Review of Xylenes (CAS #1330-20-7)- Draft. NCEA-S-1203. US EPA, Washington, DC.

International Programme on Chemical Safety (IPCS). 1997. Environmental Health Criteria 190 Xylenes. World Health Organization, Geneva, Switzerland

IUCLID Hedset: para-xylene pp1-49