

**HIGH PRODUCTION VOLUME (HPV)
CHEMICAL CHALLENGE PROGRAM**

REVISED TEST PLAN

For The

High Benzene Naphthas Category

Prepared by:

**American Chemistry Council
Olefins Panel
HPV Implementation Task Group**

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PLAIN ENGLISH SUMMARY

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

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

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

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

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

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

EXECUTIVE SUMMARY

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

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

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

Human Health Effects

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

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

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

Physicochemical Properties, Environmental Fate, and Aquatic Toxicity

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

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

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

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

(a) Hydrotreated C6 Fraction

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

(b) Hydrotreated C6-C7 Fraction

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

(c) Hydrotreated C6-C8 Fraction

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

4. Quench Loop Pyrolysis Oil and Compressor Oil

Quench Loop Pyrolysis Oil (Pyoil) represents higher boiling hydrocarbons that condense in the water quench system of an ethylene plant, typically at an ethylene unit cracking ethane, propane or butane. The stream can also include liquids collected at the cracked gas compressor knock out drums, which may include compressor injection oil. The carbon number distribution for Pyoil is C4 (or even lower) through heavier hydrocarbons such as naphthalene or even heavier. The reported typical composition includes 10 to 22% benzene and 5 to 11% toluene.

5. Recovered Oil from Wastewater Treatment

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

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

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

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

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

Subchronic Toxicity

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

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

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

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

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

Developmental Toxicity

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

Reproductive Toxicity

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

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

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

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

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

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

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

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

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

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

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

