

201-15727B

RECEIVED  
OPPT CRIC  
04 DEC 14 PM 12:48

**ATTACHMENT 1A**

**HIGH BENZENE NAPHTHAS ROBUST SUMMARIES:  
PHYSICAL-CHEMICAL PROPERTIES AND ENVIRONMENTAL FATE**

## HIGH BENZENE NAPHTHAS ROBUST SUMMARY

### Boiling Point

<b>Test Substance*:</b>	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]											
<b>Method/Guideline:</b>	Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04											
<b>Year (guideline):</b>	1999											
<b>Type (test type):</b>	Not applicable											
<b>GLP:</b>	Not applicable											
<b>Year (study performed):</b>	Not applicable											
<b>Estimation Pressure:</b>	760 mm Hg											
<b>Test Conditions:</b>	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.											
<b>Note: Concentration prep., vessel type, replication, test conditions.</b>												
<b>Results:</b> <b>Units/Value:</b> <ul style="list-style-type: none"> <li><b>Note: Deviations from protocol or guideline, analytical method.</b></li> </ul>	<p>Calculated and measured boiling point data for representative constituents of the High Benzene Naphthas Category are listed below. The data identify a potential boiling point range for substances represented by the 19 CAS numbers under <u>Test Substance</u>. 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.</p> <p>Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C11. The 12 chemicals selected to represent the boiling point range of this category are C5-C10 hydrocarbons that can be found in substances identified by the 19 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.</p>											
<b>Results: (continued)</b> <b>Units/Value:</b> <b>Note: Deviations from protocol or guideline, analytical method.</b>	<table border="1"> <thead> <tr> <th><u>Substance Constituent</u></th> <th><u>Calculated BP (°C)</u></th> <th><u>Measured* BP (°C)</u></th> </tr> </thead> <tbody> <tr> <td>Isoprene</td> <td>34.95</td> <td>34.0</td> </tr> <tr> <td>n-pentane</td> <td>46.01</td> <td>36.0</td> </tr> </tbody> </table>	<u>Substance Constituent</u>	<u>Calculated BP (°C)</u>	<u>Measured* BP (°C)</u>	Isoprene	34.95	34.0	n-pentane	46.01	36.0		
<u>Substance Constituent</u>	<u>Calculated BP (°C)</u>	<u>Measured* BP (°C)</u>										
Isoprene	34.95	34.0										
n-pentane	46.01	36.0										

	<table> <tr><td>1,3-cyclopentadiene</td><td>69.17</td><td>41.0</td></tr> <tr><td>Isohexane</td><td>56.26</td><td>63.2</td></tr> <tr><td>n-hexane</td><td>71.53</td><td>68.7</td></tr> <tr><td>methylcyclopentane</td><td>80.34</td><td>71.8</td></tr> <tr><td>benzene</td><td>102.24</td><td>80.0</td></tr> <tr><td>toluene</td><td>125.72</td><td>110.6</td></tr> <tr><td>m-xylene</td><td>148.29</td><td>139.1</td></tr> <tr><td>styrene</td><td>146.65</td><td>145.0</td></tr> <tr><td>dicyclopentadiene</td><td>176.78</td><td>170.0</td></tr> <tr><td>naphthalene</td><td>231.64</td><td>217.9</td></tr> </table> <p>* Experimental values from EPIWIN database. The data represent a potential boiling point range for substances represented by the 19 CAS numbers under <u>Test Substance</u>.</p>	1,3-cyclopentadiene	69.17	41.0	Isohexane	56.26	63.2	n-hexane	71.53	68.7	methylcyclopentane	80.34	71.8	benzene	102.24	80.0	toluene	125.72	110.6	m-xylene	148.29	139.1	styrene	146.65	145.0	dicyclopentadiene	176.78	170.0	naphthalene	231.64	217.9								
1,3-cyclopentadiene	69.17	41.0																																					
Isohexane	56.26	63.2																																					
n-hexane	71.53	68.7																																					
methylcyclopentane	80.34	71.8																																					
benzene	102.24	80.0																																					
toluene	125.72	110.6																																					
m-xylene	148.29	139.1																																					
styrene	146.65	145.0																																					
dicyclopentadiene	176.78	170.0																																					
naphthalene	231.64	217.9																																					
<b>Test Substance:</b>	<p>The High Benzene Naphthas Category includes the following CAS numbers:</p> <table> <tr><td>64741-99-7</td><td>Extracts, petroleum, light naphtha solvent</td></tr> <tr><td>64742-49-0</td><td>Naphtha, petroleum, hydrotreated light</td></tr> <tr><td>64742-73-0</td><td>Naphtha, petroleum, hydrodesulfurized light</td></tr> <tr><td>64742-83-2</td><td>Naphtha, petroleum, light steam-cracked</td></tr> <tr><td>64742-91-2</td><td>Distillates, petroleum, steam-cracked</td></tr> <tr><td>67891-79-6</td><td>Distillates, petroleum, heavy aromatic</td></tr> <tr><td>67891-80-9</td><td>Distillates, petroleum, light aromatic</td></tr> <tr><td>68410-97-9</td><td>Distillates, petroleum, light distillate hydrotreating process, low-boiling</td></tr> <tr><td>68475-70-7</td><td>Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived</td></tr> <tr><td>68476-45-9</td><td>Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product</td></tr> <tr><td>68526-77-2</td><td>Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum</td></tr> <tr><td>68606-10-0</td><td>Gasoline, pyrolysis, debutanizer bottoms</td></tr> <tr><td>68606-28-0</td><td>Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic</td></tr> <tr><td>68921-67-5</td><td>Hydrocarbons, ethylene-manufacture-by-product distillation residues</td></tr> <tr><td>68955-29-3</td><td>Distillates, petroleum, light thermal cracked, debutanized aromatic</td></tr> <tr><td>68956-52-5</td><td>Hydrocarbons, C4-8</td></tr> <tr><td>68956-70-7</td><td>Petroleum products, C5-12, reclaimed, wastewater treatment</td></tr> <tr><td>69013-21-4</td><td>Fuel oil, pyrolysis</td></tr> <tr><td>8030-30-6</td><td>Naphtha</td></tr> </table> <p>High Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 19 CAS numbers are used to describe the ten process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%.</p> <p>More information on the High Benzene Naphthas Category can be</p>	64741-99-7	Extracts, petroleum, light naphtha solvent	64742-49-0	Naphtha, petroleum, hydrotreated light	64742-73-0	Naphtha, petroleum, hydrodesulfurized light	64742-83-2	Naphtha, petroleum, light steam-cracked	64742-91-2	Distillates, petroleum, steam-cracked	67891-79-6	Distillates, petroleum, heavy aromatic	67891-80-9	Distillates, petroleum, light aromatic	68410-97-9	Distillates, petroleum, light distillate hydrotreating process, low-boiling	68475-70-7	Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived	68476-45-9	Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product	68526-77-2	Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum	68606-10-0	Gasoline, pyrolysis, debutanizer bottoms	68606-28-0	Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic	68921-67-5	Hydrocarbons, ethylene-manufacture-by-product distillation residues	68955-29-3	Distillates, petroleum, light thermal cracked, debutanized aromatic	68956-52-5	Hydrocarbons, C4-8	68956-70-7	Petroleum products, C5-12, reclaimed, wastewater treatment	69013-21-4	Fuel oil, pyrolysis	8030-30-6	Naphtha
64741-99-7	Extracts, petroleum, light naphtha solvent																																						
64742-49-0	Naphtha, petroleum, hydrotreated light																																						
64742-73-0	Naphtha, petroleum, hydrodesulfurized light																																						
64742-83-2	Naphtha, petroleum, light steam-cracked																																						
64742-91-2	Distillates, petroleum, steam-cracked																																						
67891-79-6	Distillates, petroleum, heavy aromatic																																						
67891-80-9	Distillates, petroleum, light aromatic																																						
68410-97-9	Distillates, petroleum, light distillate hydrotreating process, low-boiling																																						
68475-70-7	Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived																																						
68476-45-9	Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product																																						
68526-77-2	Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum																																						
68606-10-0	Gasoline, pyrolysis, debutanizer bottoms																																						
68606-28-0	Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic																																						
68921-67-5	Hydrocarbons, ethylene-manufacture-by-product distillation residues																																						
68955-29-3	Distillates, petroleum, light thermal cracked, debutanized aromatic																																						
68956-52-5	Hydrocarbons, C4-8																																						
68956-70-7	Petroleum products, C5-12, reclaimed, wastewater treatment																																						
69013-21-4	Fuel oil, pyrolysis																																						
8030-30-6	Naphtha																																						

	<p>found in the American Chemistry Council, Olefins Panel test plan for this category (1).</p> <ol style="list-style-type: none"> <li>Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.</li> </ol>
<b>Conclusion:</b>	<p>The calculated boiling points for some representative constituents that are present in the category streams vary from 34.95 to 231.64°C @ 760 mm Hg. The measured boiling points of these same constituents vary from 34.0 to 217.9°C @ 760 mm Hg. Although this does not define the actual boiling points of the category streams, it offers an indication of a range that might be expected to encompass the boiling points of these complex streams with variable compositions. Boiling points outside of these ranges may be possible for some category streams.</p>
<b>Reliability:</b>	<p>(2) Reliable with restrictions</p> <p>The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential boiling point range for substances represented by the 19 CAS numbers listed under <u>Test Substance</u>. This robust summary has a reliability rating of 2 because the data are not for specific substances in High Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for boiling point range based on constituent data.</p>
<b>Reference:</b>	<p>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.)</p>
<b>Other (source):</b>	<p>American Chemistry Council, Olefins Panel (Prepared 7/03)</p>

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

## HIGH BENZENE NAPHTHAS ROBUST SUMMARY

### Melting Point

<b>Test Substance*:</b>	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]
<b>Method/Guideline:</b>	Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
<b>Year (guideline):</b>	1999
<b>Type (test type):</b>	Not applicable
<b>GLP:</b>	Not applicable
<b>Year (study performed):</b>	Not applicable
<b>Test Conditions:</b> <ul style="list-style-type: none"> <li><b>Note: Concentration prep., vessel type, replication, test conditions.</b></li> </ul>	<p>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.</p> <p>Joback's Method is described in Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In <u>The Properties of Gases and Liquids</u>. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds.</p> <p>The Gold and Ogle Method simply uses the formula <math>T_m = 0.5839T_b</math>, where <math>T_m</math> is the melting point in Kelvin and <math>T_b</math> is the boiling point in Kelvin. The Gold and Ogle Method is described by Lyman, W.J., 1985, In: <u>Environmental Exposure from Chemicals</u>. Volume 1. Neely, W.B. and Blau, G.E. (eds), Boca Raton, FL, CRC Press, Inc., Chapter 2.</p>
<b>Results:</b> <b>Units/Value:</b> <ul style="list-style-type: none"> <li><b>Note: Deviations from protocol or guideline, analytical method.</b></li> </ul>	<p>Calculated and measured melting point data for representative constituents of the High Benzene Naphthas Category are listed below. The data identify a potential melting point range for substances represented by the 19 CAS numbers under <u>Test Substance</u>. 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.</p> <p>Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C11. The 12 chemicals selected to represent the melting point range of this category are C5-C10 hydrocarbons that can be found in substances identified by the 19 CAS numbers. Constituents representing category members were selected on the basis of</p>
<b>Results: (continued)</b>	carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category

<p><b>Units/Value:</b></p> <p><b>Note: Deviations from protocol or guideline, analytical method.</b></p>	<p>substances, and olefinic process (distillation) knowledge.</p> <table border="1" data-bbox="623 237 1417 699"> <thead> <tr> <th>Substance Constituent</th> <th>Calculated MP (°C)</th> <th>Measured* MP (°C)</th> </tr> </thead> <tbody> <tr><td>Isoprene</td><td>-118.89</td><td>-145.9</td></tr> <tr><td>n-pentane</td><td>-106.92</td><td>-129.7</td></tr> <tr><td>1,3-cyclopentadiene</td><td>-91.83</td><td>-85.0</td></tr> <tr><td>Isohexane</td><td>-105.80</td><td>-162.9</td></tr> <tr><td>n-hexane</td><td>-93.84</td><td>-95.3</td></tr> <tr><td>methylcyclopentane</td><td>-85.82</td><td>-142.5</td></tr> <tr><td>benzene</td><td>-77.92</td><td>5.5</td></tr> <tr><td>toluene</td><td>-59.17</td><td>-94.9</td></tr> <tr><td>m-xylene</td><td>-40.69</td><td>-47.8</td></tr> <tr><td>styrene</td><td>-48.31</td><td>-31.0</td></tr> <tr><td>dicyclopentadiene</td><td>-16.78</td><td>32.0</td></tr> <tr><td>naphthalene</td><td>5.01</td><td>80.2</td></tr> </tbody> </table> <p>* Experimental values from EPIWIN database. The data represent a potential melting point range for substances represented by the 19 CAS numbers under <u>Test Substance</u>.</p>	Substance Constituent	Calculated MP (°C)	Measured* MP (°C)	Isoprene	-118.89	-145.9	n-pentane	-106.92	-129.7	1,3-cyclopentadiene	-91.83	-85.0	Isohexane	-105.80	-162.9	n-hexane	-93.84	-95.3	methylcyclopentane	-85.82	-142.5	benzene	-77.92	5.5	toluene	-59.17	-94.9	m-xylene	-40.69	-47.8	styrene	-48.31	-31.0	dicyclopentadiene	-16.78	32.0	naphthalene	5.01	80.2
Substance Constituent	Calculated MP (°C)	Measured* MP (°C)																																						
Isoprene	-118.89	-145.9																																						
n-pentane	-106.92	-129.7																																						
1,3-cyclopentadiene	-91.83	-85.0																																						
Isohexane	-105.80	-162.9																																						
n-hexane	-93.84	-95.3																																						
methylcyclopentane	-85.82	-142.5																																						
benzene	-77.92	5.5																																						
toluene	-59.17	-94.9																																						
m-xylene	-40.69	-47.8																																						
styrene	-48.31	-31.0																																						
dicyclopentadiene	-16.78	32.0																																						
naphthalene	5.01	80.2																																						
<p><b>Test Substance:</b></p>	<p>The High Benzene Naphthas Category includes the following CAS numbers:</p> <table border="0" data-bbox="623 911 1417 1728"> <tr><td>64741-99-7</td><td>Extracts, petroleum, light naphtha solvent</td></tr> <tr><td>64742-49-0</td><td>Naphtha, petroleum, hydrotreated light</td></tr> <tr><td>64742-73-0</td><td>Naphtha, petroleum, hydrodesulfurized light</td></tr> <tr><td>64742-83-2</td><td>Naphtha, petroleum, light steam-cracked</td></tr> <tr><td>64742-91-2</td><td>Distillates, petroleum, steam-cracked</td></tr> <tr><td>67891-79-6</td><td>Distillates, petroleum, heavy aromatic</td></tr> <tr><td>67891-80-9</td><td>Distillates, petroleum, light aromatic</td></tr> <tr><td>68410-97-9</td><td>Distillates, petroleum, light distillate hydrotreating process, low-boiling</td></tr> <tr><td>68475-70-7</td><td>Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived</td></tr> <tr><td>68476-45-9</td><td>Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product</td></tr> <tr><td>68526-77-2</td><td>Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum</td></tr> <tr><td>68606-10-0</td><td>Gasoline, pyrolysis, debutanizer bottoms</td></tr> <tr><td>68606-28-0</td><td>Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic</td></tr> <tr><td>68921-67-5</td><td>Hydrocarbons, ethylene-manufacture-by-product distillation residues</td></tr> <tr><td>68955-29-3</td><td>Distillates, petroleum, light thermal cracked, debutanized aromatic</td></tr> <tr><td>68956-52-5</td><td>Hydrocarbons, C4-8</td></tr> <tr><td>68956-70-7</td><td>Petroleum products, C5-12, reclaimed, wastewater treatment</td></tr> <tr><td>69013-21-4</td><td>Fuel oil, pyrolysis</td></tr> <tr><td>8030-30-6</td><td>Naphtha</td></tr> </table>	64741-99-7	Extracts, petroleum, light naphtha solvent	64742-49-0	Naphtha, petroleum, hydrotreated light	64742-73-0	Naphtha, petroleum, hydrodesulfurized light	64742-83-2	Naphtha, petroleum, light steam-cracked	64742-91-2	Distillates, petroleum, steam-cracked	67891-79-6	Distillates, petroleum, heavy aromatic	67891-80-9	Distillates, petroleum, light aromatic	68410-97-9	Distillates, petroleum, light distillate hydrotreating process, low-boiling	68475-70-7	Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived	68476-45-9	Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product	68526-77-2	Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum	68606-10-0	Gasoline, pyrolysis, debutanizer bottoms	68606-28-0	Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic	68921-67-5	Hydrocarbons, ethylene-manufacture-by-product distillation residues	68955-29-3	Distillates, petroleum, light thermal cracked, debutanized aromatic	68956-52-5	Hydrocarbons, C4-8	68956-70-7	Petroleum products, C5-12, reclaimed, wastewater treatment	69013-21-4	Fuel oil, pyrolysis	8030-30-6	Naphtha	
64741-99-7	Extracts, petroleum, light naphtha solvent																																							
64742-49-0	Naphtha, petroleum, hydrotreated light																																							
64742-73-0	Naphtha, petroleum, hydrodesulfurized light																																							
64742-83-2	Naphtha, petroleum, light steam-cracked																																							
64742-91-2	Distillates, petroleum, steam-cracked																																							
67891-79-6	Distillates, petroleum, heavy aromatic																																							
67891-80-9	Distillates, petroleum, light aromatic																																							
68410-97-9	Distillates, petroleum, light distillate hydrotreating process, low-boiling																																							
68475-70-7	Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived																																							
68476-45-9	Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product																																							
68526-77-2	Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum																																							
68606-10-0	Gasoline, pyrolysis, debutanizer bottoms																																							
68606-28-0	Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic																																							
68921-67-5	Hydrocarbons, ethylene-manufacture-by-product distillation residues																																							
68955-29-3	Distillates, petroleum, light thermal cracked, debutanized aromatic																																							
68956-52-5	Hydrocarbons, C4-8																																							
68956-70-7	Petroleum products, C5-12, reclaimed, wastewater treatment																																							
69013-21-4	Fuel oil, pyrolysis																																							
8030-30-6	Naphtha																																							
<p><b>Test Substance: (continued)</b></p>	<p>High Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 19 CAS numbers are used to describe the ten process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon</p>																																							

	<p>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%.</p> <p>More information on the High Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1).</p> <ol style="list-style-type: none"> <li>1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.</li> </ol>
<b>Conclusion:</b>	<p>The calculated melting points for some representative constituents that are present in the category streams vary from -118.89 to 5.01 °C. The measured melting points of these same constituents vary from -162.9 to 80.2°C. Although this does not define the actual melting points of the category streams, it offers an indication of a range that might be expected to encompass the melting points of these complex streams with variable compositions. Melting points outside of these ranges may be possible for some category streams.</p>
<b>Reliability:</b>	<p>(2) Reliable with restrictions</p> <p>The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential melting point range for substances represented by the 19 CAS numbers listed under <u>Test Substance</u>. This robust summary has a reliability rating of 2 because the data are not for specific substances in the High Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for melting point range based on constituent data.</p>
<b>Reference:</b>	<p>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.)</p>
<b>Other (source):</b>	<p>American Chemistry Council, Olefins Panel (Prepared 7/03)</p>

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

## HIGH BENZENE NAPHTHAS ROBUST SUMMARY

### Vapor Pressure

<b>Test Substance*:</b>	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]
<b>Method/Guideline:</b>	Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
<b>Year (guideline):</b>	1999
<b>Type (test type):</b>	Not applicable
<b>GLP:</b>	Not applicable
<b>Year (study performed):</b>	Not applicable
<b>Estimation Temperature:</b>	25°C
<b>Test Conditions:</b> <ul style="list-style-type: none"> <li><b>Note: Concentration prep., vessel type, replication, test conditions.</b></li> </ul>	<p>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.</p> <p>The Antoine Method is described in the <u>Handbook of Chemical Property Estimation</u>, Chapter 14. W.J. Lyman, W.F. Reehl and D.H. Rosenblatt, Eds. Washington, D.C.: American Chemical Society. 1990.</p> <p>A modified Grain Method is described on page 31 of Neely and Blau's <u>Environmental Exposure from Chemicals</u>, Volume 1, CRC Press. 1985.</p>
<b>Results:</b> <b>Units/Value:</b> <ul style="list-style-type: none"> <li><b>Note: Deviations from protocol or guideline, analytical method.</b></li> </ul>	<p>Calculated and measured vapor pressure data for representative constituents of the High Benzene Naphthas Category are listed below. The data identify a potential vapor pressure range for substances represented by the 19 CAS numbers under <u>Test Substance</u>. 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.</p> <p>Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C11. The 12 chemicals selected to represent the vapor pressure range of this category are C5-C10 hydrocarbons that can be found in substances identified by the 19 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.</p>

	<table border="1"> <thead> <tr> <th data-bbox="618 254 769 317"><u>Substance Constituent</u></th> <th data-bbox="873 254 1040 317"><u>Calculated VP (hPa @ 25°C)</u></th> <th data-bbox="1110 254 1278 317"><u>Measured* VP (hPa @ 25°C)</u></th> </tr> </thead> <tbody> <tr><td data-bbox="618 344 732 373">Isoprene</td><td data-bbox="915 344 998 373">7.35 E<sup>2</sup></td><td data-bbox="1154 344 1237 373">7.33 E<sup>2</sup></td></tr> <tr><td data-bbox="618 375 748 405">n-pentane</td><td data-bbox="915 375 998 405">6.84 E<sup>2</sup></td><td data-bbox="1154 375 1237 405">6.85 E<sup>2</sup></td></tr> <tr><td data-bbox="618 407 862 436">1,3-cyclopentadiene</td><td data-bbox="915 407 998 436">5.69 E<sup>2</sup></td><td data-bbox="1154 407 1237 436">5.80 E<sup>2</sup></td></tr> <tr><td data-bbox="618 438 748 468">Isohexane</td><td data-bbox="915 438 998 468">2.48 E<sup>2</sup></td><td data-bbox="1154 438 1237 468">2.53 E<sup>2</sup></td></tr> <tr><td data-bbox="618 470 732 499">n-hexane</td><td data-bbox="915 470 998 499">2.00 E<sup>2</sup></td><td data-bbox="1154 470 1237 499">2.01 E<sup>2</sup></td></tr> <tr><td data-bbox="618 501 862 531">methylcyclopentane</td><td data-bbox="915 501 998 531">1.77 E<sup>2</sup></td><td data-bbox="1154 501 1237 531">1.84 E<sup>2</sup></td></tr> <tr><td data-bbox="618 533 716 562">benzene</td><td data-bbox="915 533 998 562">1.16 E<sup>2</sup></td><td data-bbox="1154 533 1237 562">1.26 E<sup>2</sup></td></tr> <tr><td data-bbox="618 564 699 594">toluene</td><td data-bbox="899 564 982 594">31.60</td><td data-bbox="1138 564 1221 594">37.86</td></tr> <tr><td data-bbox="618 596 732 625">m-xylene</td><td data-bbox="915 596 964 625">8.83</td><td data-bbox="1138 596 1221 625">11.05</td></tr> <tr><td data-bbox="618 627 699 657">styrene</td><td data-bbox="915 627 964 657">6.73</td><td data-bbox="1138 627 1221 657">8.53</td></tr> <tr><td data-bbox="618 659 829 688">dicyclopentadiene</td><td data-bbox="915 659 964 688">2.20</td><td data-bbox="1138 659 1221 688">3.05</td></tr> <tr><td data-bbox="618 690 764 720">naphthalene</td><td data-bbox="915 690 964 720">0.05</td><td data-bbox="1138 690 1221 720">0.11</td></tr> </tbody> </table> <p data-bbox="618 743 1338 863">* Experimental values from EPIWIN database. The data represent a potential vapor pressure range for substances represented by the 19 CAS numbers under <u>Test Substance</u>.</p>	<u>Substance Constituent</u>	<u>Calculated VP (hPa @ 25°C)</u>	<u>Measured* VP (hPa @ 25°C)</u>	Isoprene	7.35 E <sup>2</sup>	7.33 E <sup>2</sup>	n-pentane	6.84 E <sup>2</sup>	6.85 E <sup>2</sup>	1,3-cyclopentadiene	5.69 E <sup>2</sup>	5.80 E <sup>2</sup>	Isohexane	2.48 E <sup>2</sup>	2.53 E <sup>2</sup>	n-hexane	2.00 E <sup>2</sup>	2.01 E <sup>2</sup>	methylcyclopentane	1.77 E <sup>2</sup>	1.84 E <sup>2</sup>	benzene	1.16 E <sup>2</sup>	1.26 E <sup>2</sup>	toluene	31.60	37.86	m-xylene	8.83	11.05	styrene	6.73	8.53	dicyclopentadiene	2.20	3.05	naphthalene	0.05	0.11
<u>Substance Constituent</u>	<u>Calculated VP (hPa @ 25°C)</u>	<u>Measured* VP (hPa @ 25°C)</u>																																						
Isoprene	7.35 E <sup>2</sup>	7.33 E <sup>2</sup>																																						
n-pentane	6.84 E <sup>2</sup>	6.85 E <sup>2</sup>																																						
1,3-cyclopentadiene	5.69 E <sup>2</sup>	5.80 E <sup>2</sup>																																						
Isohexane	2.48 E <sup>2</sup>	2.53 E <sup>2</sup>																																						
n-hexane	2.00 E <sup>2</sup>	2.01 E <sup>2</sup>																																						
methylcyclopentane	1.77 E <sup>2</sup>	1.84 E <sup>2</sup>																																						
benzene	1.16 E <sup>2</sup>	1.26 E <sup>2</sup>																																						
toluene	31.60	37.86																																						
m-xylene	8.83	11.05																																						
styrene	6.73	8.53																																						
dicyclopentadiene	2.20	3.05																																						
naphthalene	0.05	0.11																																						
<p data-bbox="168 911 375 940"><b>Test Substance:</b></p>	<p data-bbox="618 911 1406 974">The High Benzene Naphthas Category includes the following CAS numbers:</p> <table border="0" data-bbox="618 989 1382 1814"> <tr><td data-bbox="618 989 764 1018">64741-99-7</td><td data-bbox="786 989 1279 1018">Extracts, petroleum, light naphtha solvent</td></tr> <tr><td data-bbox="618 1020 764 1050">64742-49-0</td><td data-bbox="786 1020 1243 1050">Naphtha, petroleum, hydrotreated light</td></tr> <tr><td data-bbox="618 1052 764 1081">64742-73-0</td><td data-bbox="786 1052 1305 1081">Naphtha, petroleum, hydrodesulfurized light</td></tr> <tr><td data-bbox="618 1083 764 1113">64742-83-2</td><td data-bbox="786 1083 1268 1113">Naphtha, petroleum, light steam-cracked</td></tr> <tr><td data-bbox="618 1115 764 1144">64742-91-2</td><td data-bbox="786 1115 1224 1144">Distillates, petroleum, steam-cracked</td></tr> <tr><td data-bbox="618 1146 764 1176">67891-79-6</td><td data-bbox="786 1146 1230 1176">Distillates, petroleum, heavy aromatic</td></tr> <tr><td data-bbox="618 1178 764 1207">67891-80-9</td><td data-bbox="786 1178 1208 1207">Distillates, petroleum, light aromatic</td></tr> <tr><td data-bbox="618 1209 764 1239">68410-97-9</td><td data-bbox="786 1209 1365 1272">Distillates, petroleum, light distillate hydrotreating process, low-boiling</td></tr> <tr><td data-bbox="618 1274 764 1304">68475-70-7</td><td data-bbox="786 1274 1349 1337">Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived</td></tr> <tr><td data-bbox="618 1339 764 1369">68476-45-9</td><td data-bbox="786 1339 1325 1402">Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product</td></tr> <tr><td data-bbox="618 1404 764 1434">68526-77-2</td><td data-bbox="786 1404 1377 1467">Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum</td></tr> <tr><td data-bbox="618 1470 764 1499">68606-10-0</td><td data-bbox="786 1470 1268 1499">Gasoline, pyrolysis, debutanizer bottoms</td></tr> <tr><td data-bbox="618 1501 764 1551">68606-28-0</td><td data-bbox="786 1501 1344 1551">Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic</td></tr> <tr><td data-bbox="618 1554 764 1604">68921-67-5</td><td data-bbox="786 1554 1360 1617">Hydrocarbons, ethylene-manufacture-by-product distillation residues</td></tr> <tr><td data-bbox="618 1619 764 1669">68955-29-3</td><td data-bbox="786 1619 1305 1682">Distillates, petroleum, light thermal cracked, debutanized aromatic</td></tr> <tr><td data-bbox="618 1684 764 1713">68956-52-5</td><td data-bbox="786 1684 1029 1713">Hydrocarbons, C4-8</td></tr> <tr><td data-bbox="618 1715 764 1766">68956-70-7</td><td data-bbox="786 1715 1386 1778">Petroleum products, C5-12, reclaimed, wastewater treatment</td></tr> <tr><td data-bbox="618 1768 764 1797">69013-21-4</td><td data-bbox="786 1768 997 1797">Fuel oil, pyrolysis</td></tr> <tr><td data-bbox="618 1799 764 1829">8030-30-6</td><td data-bbox="786 1799 894 1829">Naphtha</td></tr> </table> <p data-bbox="618 1850 1354 1900">High Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing.</p>	64741-99-7	Extracts, petroleum, light naphtha solvent	64742-49-0	Naphtha, petroleum, hydrotreated light	64742-73-0	Naphtha, petroleum, hydrodesulfurized light	64742-83-2	Naphtha, petroleum, light steam-cracked	64742-91-2	Distillates, petroleum, steam-cracked	67891-79-6	Distillates, petroleum, heavy aromatic	67891-80-9	Distillates, petroleum, light aromatic	68410-97-9	Distillates, petroleum, light distillate hydrotreating process, low-boiling	68475-70-7	Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived	68476-45-9	Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product	68526-77-2	Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum	68606-10-0	Gasoline, pyrolysis, debutanizer bottoms	68606-28-0	Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic	68921-67-5	Hydrocarbons, ethylene-manufacture-by-product distillation residues	68955-29-3	Distillates, petroleum, light thermal cracked, debutanized aromatic	68956-52-5	Hydrocarbons, C4-8	68956-70-7	Petroleum products, C5-12, reclaimed, wastewater treatment	69013-21-4	Fuel oil, pyrolysis	8030-30-6	Naphtha	
64741-99-7	Extracts, petroleum, light naphtha solvent																																							
64742-49-0	Naphtha, petroleum, hydrotreated light																																							
64742-73-0	Naphtha, petroleum, hydrodesulfurized light																																							
64742-83-2	Naphtha, petroleum, light steam-cracked																																							
64742-91-2	Distillates, petroleum, steam-cracked																																							
67891-79-6	Distillates, petroleum, heavy aromatic																																							
67891-80-9	Distillates, petroleum, light aromatic																																							
68410-97-9	Distillates, petroleum, light distillate hydrotreating process, low-boiling																																							
68475-70-7	Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived																																							
68476-45-9	Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product																																							
68526-77-2	Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum																																							
68606-10-0	Gasoline, pyrolysis, debutanizer bottoms																																							
68606-28-0	Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic																																							
68921-67-5	Hydrocarbons, ethylene-manufacture-by-product distillation residues																																							
68955-29-3	Distillates, petroleum, light thermal cracked, debutanized aromatic																																							
68956-52-5	Hydrocarbons, C4-8																																							
68956-70-7	Petroleum products, C5-12, reclaimed, wastewater treatment																																							
69013-21-4	Fuel oil, pyrolysis																																							
8030-30-6	Naphtha																																							

	<p>The 19 CAS numbers are used to describe the ten process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%.</p> <p>More information on the High Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1).</p> <p>1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.</p>
<b>Conclusion:</b>	<p>The calculated vapor pressures for some representative constituents that are present in the category streams vary from 0.05 to 7.35 E<sup>2</sup> hPa @ 25°C. The measured vapor pressures of these same constituents vary from 0.11 to 7.33 E<sup>2</sup> hPa @ 25°C. Although this does not define the actual vapor pressures of the category streams, it offers an indication of a range that might be expected to encompass the vapor pressures of these complex streams with variable compositions. Vapor pressure outside of these ranges may be possible for some category streams.</p>
<b>Reliability:</b>	<p>(2) Reliable with restrictions</p> <p>The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential vapor pressure range for substances represented by the 19 CAS numbers under <u>Test Substance</u>. This robust summary has a reliability rating of 2 because the data are not for specific substances in the High Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for vapor pressure range based on constituent data.</p>
<b>Reference:</b>	<p>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.)</p>
<b>Other (source):</b>	<p>American Chemistry Council, Olefins Panel (Prepared 7/03)</p>

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

## HIGH BENZENE NAPHTHAS ROBUST SUMMARY

### Water Solubility

<b>Test Substance*:</b>	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]		
<b>Method/Guideline:</b>	Calculated values using WSKOWWIN version 1.36, a subroutine of the computer program EPIWIN version 3.04		
<b>Year (guideline):</b>	1999		
<b>Type (test type):</b>	Not applicable		
<b>GLP:</b>	Not applicable		
<b>Year (study performed):</b>	Not applicable		
<b>Estimation Temperature:</b>	25°C		
<b>Test Conditions:</b>	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". <i>Environ. Toxicol. Chem.</i> 15:100-106. 1995.		
<b>Results:</b> <b>Units/Value:</b>	Calculated and measured water solubility data for representative constituents of the High Benzene Naphthas Category are listed below. The data identify a potential water solubility range for substances represented by the 19 CAS numbers under <u>Test Substance</u> . 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).		
<ul style="list-style-type: none"><li><b>Note: Deviations from protocol or guideline, analytical method.</b></li></ul>	Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C11. The 12 chemicals selected to represent the water solubility range of this category are C5-C10 hydrocarbons that can be found in substances identified by the 19 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.		
<b>Results: (continued)</b> <b>Units/Value:</b>	<u>Substance</u>	<u>Calculated WS</u>	<u>Measured WS*</u>
<b>Note: Deviations from protocol or</b>	<u>Constituent</u>	<u>(mg/L @ 25°C)</u>	<u>(mg/L @ 25°C)</u>
	Isoprene	247.2	338.6

<b>guideline, analytical method.</b>	<table border="0"> <tr><td>n-pentane</td><td>159.70</td><td>49.8</td></tr> <tr><td>1,3-cyclopentadiene</td><td>470.6</td><td>na</td></tr> <tr><td>Isohexane</td><td>66.94</td><td>31.1</td></tr> <tr><td>n-hexane</td><td>57.42</td><td>17.2</td></tr> <tr><td>methylcyclopentane</td><td>83.95</td><td>49.4</td></tr> <tr><td>benzene</td><td>2634.0</td><td>2000.0</td></tr> <tr><td>toluene</td><td>832.7</td><td>573.1</td></tr> <tr><td>m-xylene</td><td>258.4</td><td>207.2</td></tr> <tr><td>styrene</td><td>386.7</td><td>343.7</td></tr> <tr><td>dicyclopentadiene</td><td>51.9</td><td>na</td></tr> <tr><td>naphthalene</td><td>183.8</td><td>142.1</td></tr> </table> <p>* Experimental values from EPIWIN database. na = not available</p> <p>The data represent a potential water solubility range for substances represented by the 19 CAS numbers under <u>Test Substance</u>.</p>	n-pentane	159.70	49.8	1,3-cyclopentadiene	470.6	na	Isohexane	66.94	31.1	n-hexane	57.42	17.2	methylcyclopentane	83.95	49.4	benzene	2634.0	2000.0	toluene	832.7	573.1	m-xylene	258.4	207.2	styrene	386.7	343.7	dicyclopentadiene	51.9	na	naphthalene	183.8	142.1					
n-pentane	159.70	49.8																																					
1,3-cyclopentadiene	470.6	na																																					
Isohexane	66.94	31.1																																					
n-hexane	57.42	17.2																																					
methylcyclopentane	83.95	49.4																																					
benzene	2634.0	2000.0																																					
toluene	832.7	573.1																																					
m-xylene	258.4	207.2																																					
styrene	386.7	343.7																																					
dicyclopentadiene	51.9	na																																					
naphthalene	183.8	142.1																																					
<b>Test Substance:</b>	<p>The High Benzene Naphthas Category includes the following CAS numbers:</p> <table border="0"> <tr><td>64741-99-7</td><td>Extracts, petroleum, light naphtha solvent</td></tr> <tr><td>64742-49-0</td><td>Naphtha, petroleum, hydrotreated light</td></tr> <tr><td>64742-73-0</td><td>Naphtha, petroleum, hydrodesulfurized light</td></tr> <tr><td>64742-83-2</td><td>Naphtha, petroleum, light steam-cracked</td></tr> <tr><td>64742-91-2</td><td>Distillates, petroleum, steam-cracked</td></tr> <tr><td>67891-79-6</td><td>Distillates, petroleum, heavy aromatic</td></tr> <tr><td>67891-80-9</td><td>Distillates, petroleum, light aromatic</td></tr> <tr><td>68410-97-9</td><td>Distillates, petroleum, light distillate hydrotreating process, low-boiling</td></tr> <tr><td>68475-70-7</td><td>Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived</td></tr> <tr><td>68476-45-9</td><td>Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product</td></tr> <tr><td>68526-77-2</td><td>Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum</td></tr> <tr><td>68606-10-0</td><td>Gasoline, pyrolysis, debutanizer bottoms</td></tr> <tr><td>68606-28-0</td><td>Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic</td></tr> <tr><td>68921-67-5</td><td>Hydrocarbons, ethylene-manufacture-by-product distillation residues</td></tr> <tr><td>68955-29-3</td><td>Distillates, petroleum, light thermal cracked, debutanized aromatic</td></tr> <tr><td>68956-52-5</td><td>Hydrocarbons, C4-8</td></tr> <tr><td>68956-70-7</td><td>Petroleum products, C5-12, reclaimed, wastewater treatment</td></tr> <tr><td>69013-21-4</td><td>Fuel oil, pyrolysis</td></tr> <tr><td>8030-30-6</td><td>Naphtha</td></tr> </table>	64741-99-7	Extracts, petroleum, light naphtha solvent	64742-49-0	Naphtha, petroleum, hydrotreated light	64742-73-0	Naphtha, petroleum, hydrodesulfurized light	64742-83-2	Naphtha, petroleum, light steam-cracked	64742-91-2	Distillates, petroleum, steam-cracked	67891-79-6	Distillates, petroleum, heavy aromatic	67891-80-9	Distillates, petroleum, light aromatic	68410-97-9	Distillates, petroleum, light distillate hydrotreating process, low-boiling	68475-70-7	Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived	68476-45-9	Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product	68526-77-2	Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum	68606-10-0	Gasoline, pyrolysis, debutanizer bottoms	68606-28-0	Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic	68921-67-5	Hydrocarbons, ethylene-manufacture-by-product distillation residues	68955-29-3	Distillates, petroleum, light thermal cracked, debutanized aromatic	68956-52-5	Hydrocarbons, C4-8	68956-70-7	Petroleum products, C5-12, reclaimed, wastewater treatment	69013-21-4	Fuel oil, pyrolysis	8030-30-6	Naphtha
64741-99-7	Extracts, petroleum, light naphtha solvent																																						
64742-49-0	Naphtha, petroleum, hydrotreated light																																						
64742-73-0	Naphtha, petroleum, hydrodesulfurized light																																						
64742-83-2	Naphtha, petroleum, light steam-cracked																																						
64742-91-2	Distillates, petroleum, steam-cracked																																						
67891-79-6	Distillates, petroleum, heavy aromatic																																						
67891-80-9	Distillates, petroleum, light aromatic																																						
68410-97-9	Distillates, petroleum, light distillate hydrotreating process, low-boiling																																						
68475-70-7	Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived																																						
68476-45-9	Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product																																						
68526-77-2	Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum																																						
68606-10-0	Gasoline, pyrolysis, debutanizer bottoms																																						
68606-28-0	Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic																																						
68921-67-5	Hydrocarbons, ethylene-manufacture-by-product distillation residues																																						
68955-29-3	Distillates, petroleum, light thermal cracked, debutanized aromatic																																						
68956-52-5	Hydrocarbons, C4-8																																						
68956-70-7	Petroleum products, C5-12, reclaimed, wastewater treatment																																						
69013-21-4	Fuel oil, pyrolysis																																						
8030-30-6	Naphtha																																						
<b>Test Substance: (cont'd)</b>	<p>High Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 19 CAS numbers are used to describe the ten process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%.</p>																																						

	<p>More information on the High Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1).</p> <p>1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.</p>
<b>Conclusion:</b>	<p>The calculated water solubility for some representative constituents that are present in the category streams vary from 51.9 to 2634.0 mg/L @ 25°C. The measured water solubility of these same constituents vary from 17.2 to 2000.0 mg/L @ 25°C. Although this does not define the actual water solubility of the category streams, it offers an indication of a range that might be expected to encompass the water solubility of these complex streams with variable compositions. Water solubilities outside of these ranges may be possible for some category streams.</p>
<b>Reliability:</b>	<p>(2) Reliable with restrictions</p> <p>The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential water solubility range for substances represented by the 19 CAS numbers under <u>Test Substance</u>. This robust summary has a reliability rating of 2 because the data are not for specific substances in the High Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for water solubility range based on constituent data.</p>
<b>Reference:</b>	<p>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.)</p>
<b>Other (source):</b>	<p>American Chemistry Council, Olefins Panel (Prepared 7/03)</p>

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

## HIGH BENZENE NAPHTHAS ROBUST SUMMARY

### Hydrolysis (Stability in Water)

<b>Test Substance*:</b>	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]
<b>Method/Guideline:</b>	Other: Technical discussion
<b>Year (guideline):</b>	Not applicable
<b>Type (test type):</b>	Not applicable
<b>GLP (Y/N):</b>	Not applicable
<b>Year (study performed):</b>	Not applicable
<b>Analytical Monitoring:</b>	Not applicable
<b>Test Conditions:</b> <ul style="list-style-type: none"> <li><b>Note: Concentration preparation, vessel type, volume, replication, deviations from guideline or protocol</b></li> </ul>	Not applicable
<b>Results:</b> <b>Units/Value:</b> <ul style="list-style-type: none"> <li><b>Note: Analytical method, observations, half-lives by pH, degradation products</b></li> </ul>	Not applicable
<b>Test Substance:</b>	The High Benzene Naphthas Category includes the following CAS numbers: 64741-99-7 Extracts, petroleum, light naphtha solvent 64742-49-0 Naphtha, petroleum, hydrotreated light 64742-73-0 Naphtha, petroleum, hydrodesulfurized light 64742-83-2 Naphtha, petroleum, light steam-cracked 64742-91-2 Distillates, petroleum, steam-cracked 67891-79-6 Distillates, petroleum, heavy aromatic 67891-80-9 Distillates, petroleum, light aromatic 68410-97-9 Distillates, petroleum, light distillate hydrotreating process, low-boiling 68475-70-7 Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived 68476-45-9 Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product

	<p>68526-77-2 Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum  68606-10-0 Gasoline, pyrolysis, debutanizer bottoms  68606-28-0 Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic  68921-67-5 Hydrocarbons, ethylene-manufacture-by-product distillation residues  68955-29-3 Distillates, petroleum, light thermal cracked, debutanized aromatic  68956-52-5 Hydrocarbons, C4-8  68956-70-7 Petroleum products, C5-12, reclaimed, wastewater treatment  69013-21-4 Fuel oil, pyrolysis  8030-30-6 Naphtha</p> <p>High Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 19 CAS numbers are used to describe the ten process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%.</p> <p>More information on the High Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1).</p> <ol style="list-style-type: none"> <li>1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.</li> </ol>
<p><b>Conclusion:</b></p>	<p><b><u>Summary</u></b></p> <p>In the environment, hydrolysis will not contribute to the degradation of chemicals in the High Benzene Naphthas Category. The High Benzene Naphthas Category includes ten process streams:</p> <ul style="list-style-type: none"> <li>• <b>Pyrolysis Gasoline</b></li> <li>• <b>Pyrolysis C6 Fraction</b></li> <li>• <b>Pyrolysis C6-C8 Fraction</b></li> <li>• <b>Pyrolysis C5-C6 Fraction</b></li> <li>• <b>Hydrotreated C6 Fraction</b></li> <li>• <b>Hydrotreated C6-C7 Fraction</b></li> <li>• <b>Hydrotreated C6-C8 Fraction</b></li> <li>• <b>Quench Loop Pyrolysis Oil and Compressor Oil</b></li> <li>• <b>Recovered Oil from Waste Water Treatment</b></li> <li>• <b>Extract from Benzene Extraction</b></li> </ul> <p>Nineteen CAS numbers (see <u>Test Substance</u>) identify substances derived from these process streams. As discussed below, the chemicals in these streams are composed of carbon and hydrogen and are not amenable to hydrolysis because of their molecular structure and the chemical reaction required for this type of transformation to occur.</p>

### **The High Benzene Naphthas Category**

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

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

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

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

	<ul style="list-style-type: none"> <li>• <b>Pyrolysis Gasoline Fractions (C5-C6, C6, and C6-C8 Fractions)</b> are separated by distillation into various boiling-point range fractions as intermediates in preparation for further processing. In some cases, petroleum refinery streams such as a C6 reformat fraction are combined with the pyrolysis gasoline prior to this separation. Similar to the situation for Pygas, the composition of these fractions vary depending on the ethylene process feedstock and the other operating variables.       <ol style="list-style-type: none"> <li>1. <b>Pyrolysis C5-C6 Fraction</b> has a carbon number distribution that is predominantly C5 to C6. One typical composition for this stream is reported as 70% benzene and 10% pentenes.</li> <li>2. <b>Pyrolysis C6 Fraction</b> has a carbon number distribution that is predominantly C6. Reported compositions vary from 35 to 77% benzene, 0.5 to 5% toluene with the balance primarily C6 non-aromatics, which are expected to be largely unsaturates.</li> <li>3. <b>Pyrolysis C6-C8 Fraction</b> has a carbon number distribution that is predominantly C6 to C8. The reported compositions range from 30 to 80% benzene, 15 to 25% toluene and 3 to 23% C8 aromatics.</li> </ol> </li> <li>• <b>Hydrotreated Pyrolysis Fractions (C6, C6-C7, and C6-C8 Fractions)</b> are Pyrolysis gasoline or distillate fractions of pyrolysis gasoline that are treated with hydrogen over catalyst to saturate or partially saturate diolefins and/or olefins. In some cases, petroleum refinery streams such as a C6 reformat fraction are combined with the pyrolysis gasoline prior to this step. The hydrogenation process may be either one-stage or two-stage. The one-stage process is typically a liquid-phase process where the primary objective is to selectively convert diolefins to mono-olefins and to convert vinyl aromatics, for example, styrene to ethylbenzene. The second stage in a two-stage hydrogenation process is typically a vapor-phase, more severe hydrogenation that converts essentially all of the contained olefins to saturated hydrocarbons. A pygas fraction that will be processed by extraction or extractive distillation to produce high purity aromatics (benzene, toluene, or xylenes) is subjected to two-stage hydrogenation. Pygas fractions may be forwarded to hydrodealkylation units (less common) for benzene production after one-stage of hydrogenation. Hydrotreated Pyrolysis fractions may be the result of either one- or two-stage hydrogenation.       <ol style="list-style-type: none"> <li>1. <b>Hydrotreated C6 Fraction</b> is very similar to the Pyrolysis C6 fraction except that the non-aromatics present in the hydrotreated stream are essentially all saturates. The reported composition for the Hydrotreated C6 stream indicates typical benzene content of 75%.</li> <li>2. <b>Hydrotreated C6-C7 Fraction</b> has a carbon number distribution that is predominantly C6-C7 and the reported values indicate 40 to 70% benzene, and 3 to 15% toluene.</li> <li>3. <b>Hydrotreated C6-C8 Fraction</b> has a reported typical composition of 40 to 60% benzene, 10 to 25% toluene, and 3 to 10% C8</li> </ol> </li> </ul>
--	---

aromatics.

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

#### **Hydrolysis of Hydrocarbons as a Function of Molecular Structure**

Hydrolysis of an organic molecule occurs when a molecule (R-X) reacts with water (H<sub>2</sub>O) 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

	<p>in alkenes, such as those in the High Benzene Naphthas Category, will react with water by an addition reaction mechanism (2). The reaction product is an alcohol. This reaction is not considered to be hydrolysis because the carbon-carbon linkage is not cleaved and because the reaction is freely reversible (3). Substances that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (4).</p> <p>The substances in the High Benzene Naphthas Category are primarily olefins that contain at least one double bond (alkenes). The remaining chemicals are saturated hydrocarbons (alkanes). These two groups of chemicals contain only carbon and hydrogen. As such, their molecular structure is not subject to the hydrolytic mechanism discussed above. Therefore, chemicals in the High Benzene Naphthas Category have a very low potential to hydrolyze, and this degradative process will not contribute to their removal in the environment.</p> <p><b>References</b></p> <ol style="list-style-type: none"> <li>1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.</li> <li>2. Gould, E.S. (1959), Mechanism and Structure in Organic Chemistry, Holt, Reinhart and Winston, New York, NY, USA.</li> <li>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.</li> <li>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.</li> </ol>
<b>Reliability:</b>	These data represent a key study for characterizing the potential of substances in the High Benzene Naphthas Category to undergo hydrolysis.
<b>Reference:</b>	American Chemistry Council, Olefins Panel. 2003. Hydrolysis High Benzene Naphthas Category. Rosslyn, VA, USA.
<b>Other (source):</b>	American Chemistry Council, Olefins Panel (Prepared 7/03)

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

## HIGH BENZENE NAPHTHAS ROBUST SUMMARY

### Photodegradation (Direct)

<b>Test Substance*:</b>	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]
<b>Method/Guideline:</b>	Other: Technical discussion
<b>Year (guideline):</b>	Not applicable
<b>GLP (Y/N):</b>	Not applicable
<b>Year (study performed):</b>	Not applicable
<b>Type (air, soil, water, other):</b>	Water
<b>Light Source:</b>	Not applicable
<b>Light Spectrum:</b> • Wave length value (upper/lower)	Not applicable
<b>Relative Intensity:</b>	Not applicable
<b>Test Substance Spectrum:</b>	Not applicable
<b>Test Conditions:</b> • Note: Concentration, temperature, test system type, replication, deviations from guideline or protocol	Not applicable
<b>Direct Photolysis**:</b> • Results: half-life, % degradation, quantum yield	<p><b><u>Summary</u></b></p> <p>In the environment, direct photolysis will not significantly contribute to the degradation of constituent chemicals in the High Benzene Naphthas Category. The High Benzene Naphthas Category includes ten process streams:</p> <ul style="list-style-type: none"> <li>• <b>Pyrolysis Gasoline</b></li> <li>• <b>Pyrolysis C6 Fraction</b></li> <li>• <b>Pyrolysis C6-C8 Fraction</b></li> <li>• <b>Pyrolysis C5-C6 Fraction</b></li> <li>• <b>Hydrotreated C6 Fraction</b></li> <li>• <b>Hydrotreated C6-C7 Fraction</b></li> <li>• <b>Hydrotreated C6-C8 Fraction</b></li> <li>• <b>Quench Loop Pyrolysis Oil and Compressor Oil</b></li> <li>• <b>Recovered Oil from Waste Water Treatment</b></li> </ul>

- **Extract from Benzene Extraction**

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

### **The High Benzene Naphthas Category**

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

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

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

- **Pyrolysis Gasoline (Pygas)** consists predominantly of C5+ hydrocarbons produced by the ethylene cracking furnaces. Typically the stream is derived from (1) the bottoms product from the debutanizer, (2) oils separated from furnace effluent quench systems, and (3) “drips” or condensate resulting from compression of the cracked gas. The oils from the quench systems and the “drips” may be stabilized to remove lights before blending with Pygas from the other sources. Depending on the plant configuration, Pygas may contain all of these intermediate streams, or the quench oils and stabilized drips may be transferred as separate streams. Low concentrations (e.g. 3% total) of C4 and lighter hydrocarbons may be present in the stream. A detailed analysis of Pygas may identify 60 or more hydrocarbon components or component groups, primarily unsaturated hydrocarbons and aromatics. Benzene, toluene, and dicyclopentadiene together may account for more than 50% of a Pygas stream and typically no other single component is present at a level greater than about 5%. The benzene concentration of

	<p>Pygas is typically about 40% and the reported values range from 15 to 62%. The concentrations of individual hydrocarbon components in Pygas vary depending on the type of feedstock used by the ethylene plant, the mode of operation of the cracking furnaces (i.e. severity) and the ethylene process configuration. One non-typical Pygas stream is reported to contain vinylacetate at a concentration of up to about 10%. Vinylacetate is not typically found in ethylene process streams.</p> <ul style="list-style-type: none"> <li>• <b>Pyrolysis Gasoline Fractions (C5-C6, C6, and C6-C8 Fractions)</b> are separated by distillation into various boiling-point range fractions as intermediates in preparation for further processing. In some cases, petroleum refinery streams such as a C6 reformat fraction are combined with the pyrolysis gasoline prior to this separation. Similar to the situation for Pygas, the composition of these fractions vary depending on the ethylene process feedstock and the other operating variables.</li> </ul> <ol style="list-style-type: none"> <li>4. <b>Pyrolysis C5-C6 Fraction</b> has a carbon number distribution that is predominantly C5 to C6. One typical composition for this stream is reported as 70% benzene and 10% pentenes.</li> <li>5. <b>Pyrolysis C6 Fraction</b> has a carbon number distribution that is predominantly C6. Reported compositions vary from 35 to 77% benzene, 0.5 to 5% toluene with the balance primarily C6 non-aromatics, which are expected to be largely unsaturates.</li> <li>6. <b>Pyrolysis C6-C8 Fraction</b> has a carbon number distribution that is predominantly C6 to C8. The reported compositions range from 30 to 80% benzene, 15 to 25% toluene and 3 to 23% C8 aromatics.</li> </ol> <ul style="list-style-type: none"> <li>• <b>Hydrotreated Pyrolysis Fractions (C6, C6-C7, and C6-C8 Fractions)</b> are Pyrolysis gasoline or distillate fractions of pyrolysis gasoline that are treated with hydrogen over catalyst to saturate or partially saturate diolefins and/or olefins. In some cases, petroleum refinery streams such as a C6 reformat fraction are combined with the pyrolysis gasoline prior to this step. The hydrogenation process may be either one-stage or two-stage. The one-stage process is typically a liquid-phase process where the primary objective is to selectively convert diolefins to mono-olefins and to convert vinyl aromatics, for example, styrene to ethylbenzene. The second stage in a two-stage hydrogenation process is typically a vapor-phase, more severe hydrogenation that converts essentially all of the contained olefins to saturated hydrocarbons. A pygas fraction that will be processed by extraction or extractive distillation to produce high purity aromatics (benzene, toluene, or xylenes) is subjected to two-stage hydrogenation. Pygas fractions may be forwarded to hydrodealkylation units (less common) for benzene production after one-stage of hydrogenation. Hydrotreated Pyrolysis fractions may be the result of either one- or two-stage hydrogenation.</li> </ul> <ol style="list-style-type: none"> <li>4. <b>Hydrotreated C6 Fraction</b> is very similar to the Pyrolysis C6 fraction except that the non-aromatics present in the hydrotreated stream are essentially all saturates. The reported composition for the Hydrotreated C6 stream indicates typical benzene content of</li> </ol>
--	---

75%.

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

#### **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 ( $\lambda_{max}$ ) and associated molar absorptivities ( $\epsilon$ ) for selected unsaturated hydrocarbons are shown below (2):

<u>Hydrocarbon</u>	$\lambda$ below 290 nm		$\lambda$ above 290 nm	
	$\lambda_{max}$	$\epsilon$	$\lambda_{max}$	$\epsilon$
Ethylene	193	10,000	-	-
Benzene	255	215	-	-
Styrene	244	12,000	-	-
Naphthalene	282	450		
	221	100,000	311	250
	270	5,000		

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

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

#### References

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

<p><b>Indirect Photolysis**:</b></p> <ul style="list-style-type: none"> <li>• <b>Results: type of sensitizer, concentration of sensitizer, rate constant, % degradation, half-life</b></li> </ul>	Not applicable
<p><b>Degradation Products**:</b></p> <ul style="list-style-type: none"> <li>• <b>Note: Identification, concentration</b></li> </ul>	Unknown
<p><b>Test Substance:</b></p>	<p>The High Benzene Naphthas Category includes the following CAS numbers:</p> <p>64741-99-7 Extracts, petroleum, light naphtha solvent  64742-49-0 Naphtha, petroleum, hydrotreated light  64742-73-0 Naphtha, petroleum, hydrodesulfurized light  64742-83-2 Naphtha, petroleum, light steam-cracked  64742-91-2 Distillates, petroleum, steam-cracked  67891-79-6 Distillates, petroleum, heavy aromatic  67891-80-9 Distillates, petroleum, light aromatic  68410-97-9 Distillates, petroleum, light distillate hydrotreating process, low-boiling  68475-70-7 Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived  68476-45-9 Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product  68526-77-2 Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum  68606-10-0 Gasoline, pyrolysis, debutanizer bottoms  68606-28-0 Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic  68921-67-5 Hydrocarbons, ethylene-manufacture-by-product distillation residues  68955-29-3 Distillates, petroleum, light thermal cracked, debutanized aromatic  68956-52-5 Hydrocarbons, C4-8  68956-70-7 Petroleum products, C5-12, reclaimed, wastewater treatment  69013-21-4 Fuel oil, pyrolysis  8030-30-6 Naphtha</p>
<p><b>Conclusion:</b></p>	Not applicable
<p><b>Reliability:</b></p>	<p>These data represent a key study for characterizing the potential of substances in the High Benzene Naphthas Category to undergo direct photodegradation.</p>
<p><b>Reference:</b></p>	<p>American Chemistry Council, Olefins Panel. 2003. Photodegradation (Direct): High Benzene Naphthas Category. Rosslyn, VA, USA.</p>
<p><b>Other (source):</b></p>	<p>American Chemistry Council, Olefins Panel (Prepared 7/03)</p>

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

## HIGH BENZENE NAPHTHAS ROBUST SUMMARY

### Photodegradation (Indirect)

<b>Test Substance*:</b>	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]
<b>Method/Guideline:</b>	Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.04
<b>Year (guideline):</b>	1999
<b>GLP (Y/N):</b>	Not applicable
<b>Year (study performed):</b>	Not applicable
<b>Type (air, soil, water, other):</b>	Not applicable
<b>Light Source:</b>	Sunlight
<b>Light Spectrum:</b> • Wave length value (upper/lower)	Natural sunlight
<b>Relative Intensity:</b>	1
<b>Test Substance Spectrum:</b>	Not applicable
<b>Test Conditions:</b> • 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: $1.5 \text{ E}^6 \text{ OH radicals/cm}^3$
<b>Direct Photolysis**:</b> <b>Results: half-life, % degradation, quantum yield</b>	Not applicable

<p><b>Indirect Photolysis**:</b></p> <ul style="list-style-type: none"> <li><b>Results: type of sensitizer, concentration of sensitizer, rate constant, % degradation, half-life</b></li> </ul>	<p><b><u>The High Benzene Naphthas Category</u></b></p> <p>High Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 19 CAS numbers are used to describe the ten process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%.</p> <p>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>High Benzene Naphthas</u>.</p> <p>The 12 chemicals selected to represent the atmospheric oxidation potential of this category are C5-C10 hydrocarbons that can be found in substances identified by the 19 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.</p> <p><b><u>Atmospheric Oxidation of Hydrocarbons</u></b></p> <p>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).</p> <p>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.</p> <p>Since the reactions only take place in the presence of sunlight, the atmospheric half-lives are normalized for a 12-hour day.</p>
---	--

<b>Indirect Photolysis**:</b> (cont'd) <b>Results:</b> type of sensitizer, concentration of sensitizer, rate constant, % degradation, half-life	<table border="1"> <thead> <tr> <th><u>Chemical</u></th> <th><u>Calculated* half-life (hrs)</u></th> <th><u>OH- Rate Constant (cm<sup>3</sup>/molecule-sec)</u></th> </tr> </thead> <tbody> <tr><td>Isoprene</td><td>1.2</td><td>105.1 E<sup>-12</sup></td></tr> <tr><td>n-pentane</td><td>31.7</td><td>4.0 E<sup>-12</sup></td></tr> <tr><td>1,3-cyclopentadiene</td><td>0.9</td><td>142.6 E<sup>-12</sup></td></tr> <tr><td>Isohexane</td><td>22.4</td><td>5.7 E<sup>-12</sup></td></tr> <tr><td>n-hexane</td><td>23.5</td><td>5.5 E<sup>-12</sup></td></tr> <tr><td>methylcyclopentane</td><td>22.7</td><td>5.7 E<sup>-12</sup></td></tr> <tr><td>benzene</td><td>65.8</td><td>1.9 E<sup>-12</sup></td></tr> <tr><td>toluene</td><td>24.6</td><td>5.2 E<sup>-12</sup></td></tr> <tr><td>m-xylene</td><td>9.5</td><td>13.6 E<sup>-12</sup></td></tr> <tr><td>styrene</td><td>4.6</td><td>28.1 E<sup>-12</sup></td></tr> <tr><td>dicyclopentadiene</td><td>1.1</td><td>119.2 E<sup>-12</sup></td></tr> <tr><td>naphthalene</td><td>5.9</td><td>21.6 E<sup>-12</sup></td></tr> </tbody> </table> <p>* Atmospheric half-life values are based on a 12-hr day.</p> <p>More information on the High Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (Olefins Panel, 2001).</p> <p><u>References:</u></p> <ol style="list-style-type: none"> <li>1. Atkinson, R. 1988. Estimation of gas-phase hydroxyl radical rate constants for organic chemicals. <i>Environ. Toxicol. Chem.</i> <b>7</b>:435-442.</li> <li>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 &amp; Amer. Chem. Soc., NY.</li> <li>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. <i>Chemosphere</i> <b>12</b>:2293-2299.</li> <li>4. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.</li> </ol>	<u>Chemical</u>	<u>Calculated* half-life (hrs)</u>	<u>OH- Rate Constant (cm<sup>3</sup>/molecule-sec)</u>	Isoprene	1.2	105.1 E <sup>-12</sup>	n-pentane	31.7	4.0 E <sup>-12</sup>	1,3-cyclopentadiene	0.9	142.6 E <sup>-12</sup>	Isohexane	22.4	5.7 E <sup>-12</sup>	n-hexane	23.5	5.5 E <sup>-12</sup>	methylcyclopentane	22.7	5.7 E <sup>-12</sup>	benzene	65.8	1.9 E <sup>-12</sup>	toluene	24.6	5.2 E <sup>-12</sup>	m-xylene	9.5	13.6 E <sup>-12</sup>	styrene	4.6	28.1 E <sup>-12</sup>	dicyclopentadiene	1.1	119.2 E <sup>-12</sup>	naphthalene	5.9	21.6 E <sup>-12</sup>
<u>Chemical</u>	<u>Calculated* half-life (hrs)</u>	<u>OH- Rate Constant (cm<sup>3</sup>/molecule-sec)</u>																																						
Isoprene	1.2	105.1 E <sup>-12</sup>																																						
n-pentane	31.7	4.0 E <sup>-12</sup>																																						
1,3-cyclopentadiene	0.9	142.6 E <sup>-12</sup>																																						
Isohexane	22.4	5.7 E <sup>-12</sup>																																						
n-hexane	23.5	5.5 E <sup>-12</sup>																																						
methylcyclopentane	22.7	5.7 E <sup>-12</sup>																																						
benzene	65.8	1.9 E <sup>-12</sup>																																						
toluene	24.6	5.2 E <sup>-12</sup>																																						
m-xylene	9.5	13.6 E <sup>-12</sup>																																						
styrene	4.6	28.1 E <sup>-12</sup>																																						
dicyclopentadiene	1.1	119.2 E <sup>-12</sup>																																						
naphthalene	5.9	21.6 E <sup>-12</sup>																																						
<b>Degradation Products**:</b> <ul style="list-style-type: none"> <li>• <b>Note: Identification, concentration</b></li> </ul>	Unknown																																							
<b>Test Substance:</b>	The High Benzene Naphthas Category includes the following CAS numbers: 64741-99-7 Extracts, petroleum, light naphtha solvent 64742-49-0 Naphtha, petroleum, hydrotreated light 64742-73-0 Naphtha, petroleum, hydrodesulfurized light																																							

	<p>64742-83-2 Naphtha, petroleum, light steam-cracked  64742-91-2 Distillates, petroleum, steam-cracked  67891-79-6 Distillates, petroleum, heavy aromatic  67891-80-9 Distillates, petroleum, light aromatic  68410-97-9 Distillates, petroleum, light distillate hydrotreating process, low-boiling  68475-70-7 Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived  68476-45-9 Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product  68526-77-2 Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum  68606-10-0 Gasoline, pyrolysis, debutanizer bottoms  68606-28-0 Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic  68921-67-5 Hydrocarbons, ethylene-manufacture-by-product distillation residues  68955-29-3 Distillates, petroleum, light thermal cracked, debutanized aromatic  68956-52-5 Hydrocarbons, C4-8  68956-70-7 Petroleum products, C5-12, reclaimed, wastewater treatment  69013-21-4 Fuel oil, pyrolysis  8030-30-6 Naphtha</p>
<b>Conclusion:</b>	<p>Atmospheric oxidation via hydroxyl radicals can be a significant route of degradation for products in this category. Based on calculated values, products in this category can have an atmospheric half-life range of 0.9 to 65.8 hours as a result of indirect photolysis by hydroxyl radical attack.</p>
<b>Reliability:</b>	<p>(2) Reliable with restrictions</p> <p>The results include calculated data based on chemical structure as modeled by AOPWIN. The data represent a potential atmospheric half-life range for substances represented by the 19 CAS numbers under <u>Test Substance</u>. This robust summary has a reliability rating of 2 because the data are not for specific substances in the High Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for atmospheric half-life range based on constituent data.</p>
<b>Reference:</b>	<p>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.</p>
<b>Other (source):</b>	<p>American Chemistry Council, Olefins Panel (Prepared 10/03)</p>

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

\*\* In IUCLID, provide additional discussion if needed in the results free text

## HIGH BENZENE NAPHTHAS ROBUST SUMMARY

### Partition Coefficient

<b>Test Substance*:</b>	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]
<b>Method/Guideline:</b>	Calculated values using KOWWIN version 1.65, a subroutine of the computer program EPIWIN version 3.04
<b>Year (guideline):</b>	1999
<b>Type (test type):</b>	Not applicable
<b>GLP:</b>	Not applicable
<b>Year (study performed):</b>	Not applicable
<b>Estimation Temperature:</b>	25°C
<b>Test Conditions:</b>	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. <i>J. Pharm. Sci.</i> 84:83-92.
<b>Results:</b> <b>Units/Value:</b> <ul style="list-style-type: none"> <li>• <b>Note: Deviations from protocol or guideline, analytical method.</b></li> </ul>	<p>Calculated and measured log K<sub>ow</sub> data for representative constituents of the High Benzene Naphthas Category are listed below. The data identify a potential log K<sub>ow</sub> range for substances represented by the 19 CAS numbers under <u>Test Substance</u>. Substances in this category do not have a specific log K<sub>ow</sub> value. Actual log K<sub>ow</sub> ranges for substances in this category will vary dependent on their constituent composition.</p> <p>Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C11. The 12 chemicals selected to represent the log K<sub>ow</sub> range of this category are C5-C10 hydrocarbons that can be found in substances identified by the 19 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.</p>

<p><b>Results: (continued)</b></p> <p><b>Units/Value:</b></p> <p><b>Note: Deviations from protocol or guideline, analytical method.</b></p>	<table border="1"> <thead> <tr> <th data-bbox="626 239 764 296">Substance Constituent</th> <th data-bbox="841 239 1027 296">Calculated log K<sub>ow</sub> @ 25°C</th> <th data-bbox="1078 239 1265 296">Measured* log K<sub>ow</sub> @ 25°C</th> </tr> </thead> <tbody> <tr><td>Isoprene</td><td>2.58</td><td>2.42</td></tr> <tr><td>n-pentane</td><td>2.80</td><td>3.39</td></tr> <tr><td>1,3-cyclopentadiene</td><td>2.25</td><td>na</td></tr> <tr><td>Isohexane</td><td>3.21</td><td>3.60</td></tr> <tr><td>n-hexane</td><td>3.29</td><td>3.90</td></tr> <tr><td>methylcyclopentane</td><td>3.10</td><td>3.37</td></tr> <tr><td>benzene</td><td>1.99</td><td>2.13</td></tr> <tr><td>toluene</td><td>2.54</td><td>2.73</td></tr> <tr><td>m-xylene</td><td>3.09</td><td>3.20</td></tr> <tr><td>styrene</td><td>2.89</td><td>2.95</td></tr> <tr><td>dicyclopentadiene</td><td>3.16</td><td>na</td></tr> <tr><td>naphthalene</td><td>3.17</td><td>3.30</td></tr> </tbody> </table> <p>* Experimental values from EPIWIN database. na = not available The data represent a potential log K<sub>ow</sub> range for substances represented by the 19 CAS numbers under <u>Test Substance</u>.</p>	Substance Constituent	Calculated log K <sub>ow</sub> @ 25°C	Measured* log K <sub>ow</sub> @ 25°C	Isoprene	2.58	2.42	n-pentane	2.80	3.39	1,3-cyclopentadiene	2.25	na	Isohexane	3.21	3.60	n-hexane	3.29	3.90	methylcyclopentane	3.10	3.37	benzene	1.99	2.13	toluene	2.54	2.73	m-xylene	3.09	3.20	styrene	2.89	2.95	dicyclopentadiene	3.16	na	naphthalene	3.17	3.30
Substance Constituent	Calculated log K <sub>ow</sub> @ 25°C	Measured* log K <sub>ow</sub> @ 25°C																																						
Isoprene	2.58	2.42																																						
n-pentane	2.80	3.39																																						
1,3-cyclopentadiene	2.25	na																																						
Isohexane	3.21	3.60																																						
n-hexane	3.29	3.90																																						
methylcyclopentane	3.10	3.37																																						
benzene	1.99	2.13																																						
toluene	2.54	2.73																																						
m-xylene	3.09	3.20																																						
styrene	2.89	2.95																																						
dicyclopentadiene	3.16	na																																						
naphthalene	3.17	3.30																																						
<p><b>Test Substance:</b></p>	<p>The High Benzene Naphthas Category includes the following CAS numbers:</p> <p>64741-99-7 Extracts, petroleum, light naphtha solvent</p> <p>64742-49-0 Naphtha, petroleum, hydrotreated light</p> <p>64742-73-0 Naphtha, petroleum, hydrodesulfurized light</p> <p>64742-83-2 Naphtha, petroleum, light steam-cracked</p> <p>64742-91-2 Distillates, petroleum, steam-cracked</p> <p>67891-79-6 Distillates, petroleum, heavy aromatic</p> <p>67891-80-9 Distillates, petroleum, light aromatic</p> <p>68410-97-9 Distillates, petroleum, light distillate hydrotreating process, low-boiling</p> <p>68475-70-7 Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived</p> <p>68476-45-9 Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product</p> <p>68526-77-2 Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum</p> <p>68606-10-0 Gasoline, pyrolysis, debutanizer bottoms</p> <p>68606-28-0 Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic</p> <p>68921-67-5 Hydrocarbons, ethylene-manufacture-by-product distillation residues</p> <p>68955-29-3 Distillates, petroleum, light thermal cracked, debutanized aromatic</p> <p>68956-52-5 Hydrocarbons, C4-8</p> <p>68956-70-7 Petroleum products, C5-12, reclaimed, wastewater treatment</p> <p>69013-21-4 Fuel oil, pyrolysis</p> <p>8030-30-6 Naphtha</p> <p>High Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 19 CAS numbers are used to describe the ten process streams arising from the ethylene process and other associated</p>																																							

	<p>manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%.</p> <p>More information on the High Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1).</p> <ol style="list-style-type: none"> <li>1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.</li> </ol>
<b>Conclusion:</b>	<p>The calculated log <math>K_{ow}</math> for some representative constituents that are present in the category streams vary from 1.99 to 3.29 @ 25°C. The measured log <math>K_{ow}</math> of these same constituents vary from 2.13 to 3.90 @ 25°C. Although this does not define the actual log <math>K_{ow}</math> of the category streams, it offers an indication of a range that might be expected to encompass the log <math>K_{ow}</math> of these complex streams with variable compositions. Log <math>K_{ow}</math> values outside of these ranges may be possible for some category streams.</p>
<b>Reliability:</b>	<p>(2) Reliable with restrictions</p> <p>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 <math>K_{ow}</math> range for substances represented by the 19 CAS numbers under <u>Test Substance</u>. This robust summary has a reliability rating of 2 because the data are not for specific substances in the High Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for log <math>K_{ow}</math> range based on constituent data.</p>
<b>Reference:</b>	<p>EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Log <math>K_{ow}</math> values were calculated by the KOWWIN subroutine and measured data came from the database in the computer program.)</p>
<b>Other (source):</b>	<p>American Chemistry Council, Olefins Panel (Prepared 7/03)</p>

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

## HIGH BENZENE NAPHTHAS ROBUST SUMMARY

### Transport / Distribution (Fugacity)

<b>Test Substance*:</b>	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]
<b>Method/Guideline:</b>	Calculated according to Mackay Level I, EQC Model version 1.01
<b>Year (guideline):</b>	1997
<b>Type (test type):</b>	Not applicable
<b>GLP:</b>	Not applicable
<b>Year (study performed):</b>	Not applicable
<b>Estimation Temperature:</b>	25°C
<b>Test Conditions:</b> <ul style="list-style-type: none"> <li>• <b>Note: Concentration prep., vessel type, replication, test conditions.</b></li> </ul>	<p>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.</p> <p>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).</p> <p>1. EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.</p>

**Results:**

**Units/Value:**

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

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

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

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

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

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

\* Distribution values determined using calculated input data from EPIWIN program

<p><b>Results: (cont'd)</b></p> <p><b>Units/Value:</b></p> <ul style="list-style-type: none"> <li><b>Note: Deviations from protocol or guideline, analytical method.</b></li> </ul>	<table border="1"> <thead> <tr> <th rowspan="2"><u>Chemical</u></th> <th colspan="4"><u>Measured**</u></th> </tr> <tr> <th><u>Air</u></th> <th><u>Water</u></th> <th><u>Soil</u></th> <th><u>Sediment</u></th> </tr> </thead> <tbody> <tr> <td>Isoprene</td> <td>99.96</td> <td>0.03</td> <td>0.01</td> <td>-</td> </tr> <tr> <td>n-pentane</td> <td>99.99</td> <td>0.01</td> <td>-</td> <td>-</td> </tr> <tr> <td>1,3-cyclopentadiene</td> <td>99.93</td> <td>0.06</td> <td>0.01</td> <td>-</td> </tr> <tr> <td>Isohexane</td> <td>99.97</td> <td>0.01</td> <td>0.02</td> <td>-</td> </tr> <tr> <td>n-hexane</td> <td>99.96</td> <td>-</td> <td>0.04</td> <td>-</td> </tr> <tr> <td>methylcyclopentane</td> <td>99.95</td> <td>0.02</td> <td>0.03</td> <td>-</td> </tr> <tr> <td>benzene</td> <td>98.89</td> <td>1.00</td> <td>0.11</td> <td>-</td> </tr> <tr> <td>toluene</td> <td>98.80</td> <td>0.81</td> <td>0.39</td> <td>-</td> </tr> <tr> <td>m-xylene</td> <td>97.91</td> <td>0.86</td> <td>1.20</td> <td>0.03</td> </tr> <tr> <td>styrene</td> <td>96.65</td> <td>1.85</td> <td>1.46</td> <td>0.04</td> </tr> <tr> <td>dicyclopentadiene</td> <td>98.55</td> <td>0.63</td> <td>0.80</td> <td>0.02</td> </tr> <tr> <td>naphthalene</td> <td>42.27</td> <td>20.56</td> <td>36.33</td> <td>0.81</td> </tr> </tbody> </table> <p>** Distribution values determined using input data from the EPIWIN program experimental database</p>	<u>Chemical</u>	<u>Measured**</u>				<u>Air</u>	<u>Water</u>	<u>Soil</u>	<u>Sediment</u>	Isoprene	99.96	0.03	0.01	-	n-pentane	99.99	0.01	-	-	1,3-cyclopentadiene	99.93	0.06	0.01	-	Isohexane	99.97	0.01	0.02	-	n-hexane	99.96	-	0.04	-	methylcyclopentane	99.95	0.02	0.03	-	benzene	98.89	1.00	0.11	-	toluene	98.80	0.81	0.39	-	m-xylene	97.91	0.86	1.20	0.03	styrene	96.65	1.85	1.46	0.04	dicyclopentadiene	98.55	0.63	0.80	0.02	naphthalene	42.27	20.56	36.33	0.81
<u>Chemical</u>	<u>Measured**</u>																																																																					
	<u>Air</u>	<u>Water</u>	<u>Soil</u>	<u>Sediment</u>																																																																		
Isoprene	99.96	0.03	0.01	-																																																																		
n-pentane	99.99	0.01	-	-																																																																		
1,3-cyclopentadiene	99.93	0.06	0.01	-																																																																		
Isohexane	99.97	0.01	0.02	-																																																																		
n-hexane	99.96	-	0.04	-																																																																		
methylcyclopentane	99.95	0.02	0.03	-																																																																		
benzene	98.89	1.00	0.11	-																																																																		
toluene	98.80	0.81	0.39	-																																																																		
m-xylene	97.91	0.86	1.20	0.03																																																																		
styrene	96.65	1.85	1.46	0.04																																																																		
dicyclopentadiene	98.55	0.63	0.80	0.02																																																																		
naphthalene	42.27	20.56	36.33	0.81																																																																		
<p><b>Test Substance:</b></p>	<p>The High Benzene Naphthas Category includes the following CAS numbers:</p> <p>64741-99-7 Extracts, petroleum, light naphtha solvent</p> <p>64742-49-0 Naphtha, petroleum, hydrotreated light</p> <p>64742-73-0 Naphtha, petroleum, hydrodesulfurized light</p> <p>64742-83-2 Naphtha, petroleum, light steam-cracked</p> <p>64742-91-2 Distillates, petroleum, steam-cracked</p> <p>67891-79-6 Distillates, petroleum, heavy aromatic</p> <p>67891-80-9 Distillates, petroleum, light aromatic</p> <p>68410-97-9 Distillates, petroleum, light distillate hydrotreating process, low-boiling</p> <p>68475-70-7 Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived</p> <p>68476-45-9 Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product</p> <p>68526-77-2 Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum</p> <p>68606-10-0 Gasoline, pyrolysis, debutanizer bottoms</p> <p>68606-28-0 Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic</p> <p>68921-67-5 Hydrocarbons, ethylene-manufacture-by-product distillation residues</p> <p>68955-29-3 Distillates, petroleum, light thermal cracked, debutanized aromatic</p> <p>68956-52-5 Hydrocarbons, C4-8</p> <p>68956-70-7 Petroleum products, C5-12, reclaimed, wastewater treatment</p> <p>69013-21-4 Fuel oil, pyrolysis</p> <p>8030-30-6 Naphtha</p> <p>High Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 19 CAS numbers are used to describe the ten process streams arising from the ethylene process and other associated</p>																																																																					

	<p>manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%.</p> <p>More information on the High Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1).</p> <ol style="list-style-type: none"> <li>1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.</li> </ol>
<b>Conclusion:</b>	<p>The partitioning data represent a potential distribution range for substances in the 19 CAS numbers listed under <u>Test Substance</u>. Substances in the High Benzene Naphthas Category are calculated to partition primarily to air with a small percentage partitioning to water, soil, and sediment. Relatively high vapor pressure and high water solubility largely control the partitioning behavior of constituent chemicals in substances from this category.</p> <p>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.</p>
<b>Reliability:</b>	<p>(2) Reliable with restrictions</p> <p>The input data used to run the EQC Level I model include calculated and experimental values available through the EPIWIN program. The data represent a potential environmental distribution range for substances with the 19 CAS numbers listed under <u>Test Substance</u>. This robust summary has a reliability rating of 2 because the data are not for specific substances in the High Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for distribution range based on constituent data.</p>
<b>Reference:</b>	<p>Mackay, D.A. DiGuardo, S. Paterson, and C. Cowan. EQC Model Version 1.01. 1997. Available from the Environmental Modeling Centre, Trent University, Canada.</p>
<b>Other (source):</b>	<p>American Chemistry Council, Olefins Panel (Prepared 7/03)</p>

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

**ATTACHMENT 1B**

**HIGH BENZENE NAPHTHAS ROBUST SUMMARIES:**

**BIODEGRADATION OF BENZENE**

## HIGH BENZENE NAPHTHAS ROBUST SUMMARY

### Biodegradation

<b>Test Substance:</b>	CAS No. 71-43-2; Benzene
<b>Method/Guideline:</b>	OECD 301F
<b>Year (guideline):</b>	1993
<b>Type (test type):</b>	Ready Biodegradability, Manometric Respirometry Test
<b>GLP:</b>	Yes
<b>Year (study performed):</b>	2000
<b>Inoculum:</b>	Domestic activated sludge
<b>Exposure Period:</b>	28 days
<b>Test Conditions: (FT - TC)</b>	Activated sludge and test medium were combined prior to test material addition. Test medium consisted of glass distilled water and mineral salts (Phosphate buffer, Ferric chloride, Magnesium sulfate, Calcium chloride, EDTA). Test vessels were 500 mL dark glass bottles placed on a magnetic stirrer and electronically monitored for oxygen consumption. Test material and blanks were tested in triplicate, controls were tested in duplicate. Test material (benzene) concentration was 17mg/L. Sodium benzoate (positive control) concentration was 30mg/L. Toxicity control with benzene and Na Benzoate concentrations at 17 and 30 mg/L, respectively. Test temperature was 22 +/- 2 Deg C. All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.
<ul style="list-style-type: none"><li><b>Note: Concentration prep., vessel type, replication, test conditions.</b></li></ul>	

### **Results: (FT - RS)**

#### **Units/Value:**

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

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

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

\* replicate data

**Conclusion: (FT - CL)** Test material was readily biodegradable. Half-life was <2 weeks

**Reliability: (FT - RL)** (1) Reliable without restriction

**Reference: (FT - RE)** Brixham Environmental Laboratory. 2001. OECD 301F, Ready biodegradability: Manometric respirometry. Study # AH0378/A.

**Other (source): (FT - SO)** Olefins Panel, American Chemistry Council

\* IUCLID field abbreviations include:

FT - Freetext  
TC - Test Conditions  
RS - Results  
CL - Conclusion  
RL - Reliability  
RE - Reference  
SO - Source

**ATTACHMENT 1C**  
**HIGH BENZENE NAPHTHAS ROBUST SUMMARIES:**  
**MAMMALIAN TOXICITY**

## Robust Summary: High Benzene Naphthas

### Acute Toxicity

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

## Robust Summary: High Benzene Naphthas

### Acute Toxicity

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

## Robust Summary: High Benzene Naphthas

### Acute Toxicity

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

## Robust Summary: High Benzene Naphthas

### Acute Toxicity

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

## Robust Summary: High Benzene Naphthas

### Genetic Toxicity - in Vitro

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



## Robust Summary: High Benzene Naphthas

### Genetic Toxicity - in Vitro

<p><b><u>Test Substance</u></b> <i>Test substance</i></p> <p><b><u>Method</u></b> Method/guideline followed</p> <p>Type System of testing GLP Year Species/Strain Metabolic activation Species and cell type Quantity Induced or not induced Concentrations tested</p> <p>Exposure period Statistical Methods</p> <p>Remarks for Test Conditions</p> <p><b><u>Results</u></b> Genotoxic effects</p>	<p><b>Hydrogenated Pyrolysis Gasoline</b>, CAS #68410-97-9. clear liquid with aromatic odor. Composition, purity and stability referred to sponsor. Olefins Panel HVP Stream: Hydrotreated C6-C8.</p> <p>Standard method based on Cortesi et al (1983), Dunkel et al (1981), Reznikoff et al (1973)</p> <p>In vitro cell transformation Mouse embryo cells Yes 1984 BALB/3T3-A31-1-1 from T. Kakunaga, National Cancer Inst., 1983 No NA NA NA Cytotoxicity: 8, 16, 32, 64, 128, 256, 512, 1024, 2048, and 5000µg/ml; Transformation: 100, 250, 500, 1500µg/ml, all diluted in 10% Pluronic® polyol F68 (prepared in deionized water, mol. wt. 8350, 80% hydrophilic). 2 days 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.</p> <p>Sufficient Hydrogenated Pyrolysis Gasoline (HPG) was weighed separately for each dose level, 0.40ml of 10% F68 added per ml of final volume and medium (Eagles MEM with 10% heat-inactivated fetal calf serum) added as required to achieve final volume for testing. Test preparations were mixed just prior to addition to cultures at 50µl to each 5 ml culture. All cultures were incubated at 37°C in 5% CO2 enriched humidified atmosphere. For cytotoxicity, 2 cultures/dose group, 2 cultures for vehicle F68 or medium negative control were seeded with 1x10<sup>4</sup> cells/plate in day 1, exposed on days 2-3, trypsinized and counted with a Coulter Model ZB on day 4 for at least 20% survival. For transformation, 15 cultures (1x10<sup>4</sup> cells/flask/dose group) and two colony-forming cultures (100 cells/plate/dose group) were seeded on day 1, exposed on days 2-3 and culture medium changed on day 4. For transformation cultures, medium continued to be changed weekly to day 29. Positive control was 3-methylcholanthrene (1µg/ml). Colony forming cultures were fixed, stained, and counted visually on day 10 to determine cloning efficiency (avg. number colonies/plate ÷ 100 cells seeded). Transformation cultures were fixed and stained on day 29 for focus counting and evaluation. Transformation frequency = total type III foci ÷ total flasks/dose group.</p> <p>HPG induced toxicity in BALB/3T3 cells after two days exposure beginning at 128 µg/ml (45.4% relative survival) with relative survivals of 26.7, 25.6, 3.2 and 0% at 512, 1024, 2048 and 5000µg/ml, respectively. In the transformation assay, toxicity was seen at all dose levels (relative cloning efficiencies of 53.7, 67.8, 78.5 and 0% at 100, 250, 500 and 1500µg/ml). At 1500µg/ml, the highest dose level, HPG induced 5 Type III foci; no other dose levels produced a positive response. Transformation frequencies were 0.13, 0, 0, 0.07 and 0.36 for medium control, vehicle control, 100, 250, 500 and 1500µg/ml, respectively. Positive and negative controls gave appropriate responses.</p>
---	---

<p><b><u>Conclusions</u></b> (contractor)</p> <p><b><u>Data Quality</u></b> <i>Reliabilities</i></p> <p><b><u>Reference</u></b></p> <p><b><u>Other</u></b> <i>Last changed</i></p>	<p>Hydrogenated Pyrolysis Gasoline induced transformation in BALB/3T3 cells under conditions of this assay. Cytotoxicity and impairment of cloning efficiency were also observed. The positive response was observed only at the highest dose level, a level that appeared to be too toxic for cells to recover and form colonies (0% relative colony forming efficiency)</p> <p>1. Reliable without restriction</p> <p>Brecher, S. 1984. Transformation test of Hydrogenated Pyrolysis Gasoline. Proj. #2098. Gulf Life Sciences Center, Pittsburgh, PA for Gulf Oil Chemicals Co, Houston, TX</p> <p>Cortesi, E. et al. 1983. Teratogenesis, Carcinogenesis, Mutagenesis 3: 101-110.</p> <p>Dunkel, V.A. et al. 1981. J. Nat'l Cancer Inst. 67: 1303-1315.</p> <p>Reznikoff, C.A. et al. 1973. Cancer Res. 3239-3249.</p> <p>Revised 8/27/2001 (Prepared by a contractor to the Olefins Panel).</p>
--	---

## Robust Summary - Group 5: High Benzene Naphthas

### Genetic Toxicity - in Vitro

<p><b><u>Test Substance</u></b> <i>Test substance</i></p> <p><b><u>Method</u></b> Method/guideline followed Type System of testing GLP Year Species/Strain Metabolic activation Species and cell type Quantity Induced or not induced Concentrations tested  Exposure period Statistical Methods</p> <p>Remarks for Test Conditions</p> <p><b><u>Results</u></b> Genotoxic effects</p>	<p><b>Hydrogenated Pyrolysis Gasoline</b>, CAS #68410-97-9. clear liquid with aromatic odor. Composition, purity and stability referred to sponsor. Olefins Panel HVP Stream: Hydrotreated C6-C8.</p> <p>Standard method based on Williams et al (1977, 1982) In vitro mammalian DNA repair assay Unscheduled DNA synthesis (UDS) in primary hepatocyte cultures Yes 1984 Fischer 344 male rat (10 wks old) No NA NA NA 8, 16, 32, 64, 128, 256, 512, 1024µg/ml diluted in 10% Pluronic F68 (prepared in deionized water, mol. wt 8350, 80% hydrophilic) 18 hrs. None specified. Criteria for positive response are incorporation of radioactive precursor (<sup>3</sup>H-thymidine) in cells that are not normally synthesizing DNA, indicating repair of damage. A positive response is defined as a mean net nuclear grain count at any treatment level that exceeds concurrent negative control by at least 6 grains/nucleus; negative control value must not exceed 5 grains. If this criterion is not met, a positive response can be identified if there is a significant difference (p&lt;0.01) in % cells in repair at any dose level and negative control value. This indicator defines whether a small fraction of cells is undergoing repair (Casciano &amp; Gaylor, 1983). A positive response need not be dose related.</p> <p>Sufficient Hydrogenated Pyrolysis Gasoline (HPG) was weighed separately for each dose level, 0.40ml of 10% F68 added per ml of final volume and sufficient medium (Williams Medium E with 10% fetal bovine serum and insulin) added to achieve final volume. Test preparations were mixed just prior to addition at 20µl to each 2ml culture. The conc. of <sup>3</sup>H-thymidine (½ life 12.4 yrs.) used in these assays was 1mCi/ml. All cultures were incubated at 37°C in 5% CO2 enriched humidified atmosphere. No range finding assay was performed. In the UDS assay, 2x10<sup>5</sup> cells/ml were seeded into coverslip cultures, exposed to <sup>3</sup>H-thymidine and test substance for 18 hours (3 cultures/dose level, 8 dose levels), untreated controls, vehicle F68 control and positive control, 2-acetyl aminofluorene (0.01µg/ml). Cells growing on coverslips were rinsed, fixed and glued to microscope slides on day 2. On day 3, slides were dipped in autoradiographic emulsion and stored in the dark at 2-8°C. Autoradiographs were developed, stained and coverslipped on day 10. Numbers of grains overlying 50 randomly selected nuclei/slide were counted. The highest of 3 cytoplasmic grain counts/cell were subtracted and this number was divided by a conversion factor (unspecified) to obtain net nuclear grain count. Avg. net nuclear grain count/slide (sum of net nuclear grain count ÷ 50) and mean net nuclear grain count (avg. net nuclear grain count/slide ÷3) were calculated. In addition, % cells in repair were determined for each dose level.</p> <p>HPG induced toxicity in primary hepatocytes following 18 hr exposure that left too few cells for UDS analysis at doses of 512 and 1024µg/ml. HPG did not induce unscheduled DNA synthesis at any dose level with sufficient cells to be analyzed. Positive and negative controls gave appropriate responses.</p>
--	---

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

## Robust Summary - Group 5: High Benzene Naphthas

### Genetic Toxicity - in Vivo

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

<p><b><u>Conclusions</u></b> (study authors)</p> <p><b><u>Data Quality</u></b> <i>Reliabilities</i></p> <p><b><u>References</u></b></p> <p><b><u>Other</u></b> <i>Last changed</i></p>	<p>controls gave appropriate results.</p> <p>Oral treatment of mice with Hydrogenated Pyrolysis Gasoline for 1-2 days at doses up to 2.0g/kg/day had no effect on frequency of micronucleated polychromatic erythrocytes in bone marrow under these test conditions. HPG did not induce cytogenetic damage.</p> <p>1. Reliable without restriction</p> <p>Khan, S.H. 1984. Micronucleus test of Hydrogenated Pyrolysis Gasoline. Proj. #2096. Gulf Life Sciences Center, Pittsburgh, PA for Gulf Oil Chemicals Co., Houston, TX</p> <p>5/7/2001 (Prepared by a contractor to the Olefins Panel)</p>
--	---

## Robust Summary - Group 5: High Benzene Naphthas

### Repeated Dose Toxicity

<p><b><u>Test Substance</u></b> Remarks</p> <p><b><u>Method</u></b> Method/guideline followed Test type GLP Year Species Strain Route of administration Duration of test Doses/concentration levels Sex Exposure period Frequency of treatment Control group and treatment Post exposure observation period</p> <p>Statistical methods</p> <p>Test Conditions</p> <p><b><u>Results</u></b> NOAEL (NOEL) LOAEL (LOEL) Remarks</p> <p><b><u>Conclusions</u></b> (study authors)</p>	<p><b>Hydrogenated Pyrolysis Gasoline</b> CAS #68410-97-9, Clear liquid with aromatic odor. Olefins Panel HVP Stream: Hydrotreated C6-C8.</p> <p>Standard method, method not referenced Subacute Yes 1984 Rat Fischer 344 Inhalation 8 days 0, 4869±470, 9137±917ppm±SD, actual exposure conc. Males and females (5/sex/group) 6 hrs. once daily for 5 days (d1-5) 5M, 5F; filtered air 2 days</p> <p>Body wt variance compared by Bartlett's test and one way analysis of variance. Group mean body wt compared either with Dunnett's test or a modified t-test to assess significance.</p> <p>Rats (9 wks old, 113-195g at initiation) were housed individually in stainless steel, screen-bottomed cages. Rooms were maintained at 72.2<sup>0</sup>F (exposure chamber 75<sup>0</sup>F) with relative humidity of 54% (exposure chamber 50%), and 12 hr light/dark cycle. Rats received chow diet and tap water ad lib throughout the study, except during exposure. Three groups of 10 rats (5M, 5F/group) each, were exposed to test article or air. Test article was aerosolized with a ball jet nebulizer; an in-line condensing flask was used to prevent large particles from entering the exposure chamber. Chamber concentration of test article was measured by gas chromatography. Rats were observed twice daily on weekdays and once daily on weekends for morbidity/mortality, and once daily for clinical signs immediately after exposure on days 1-5. Surviving rats were sacrificed on day 8. Gross necropsies were performed on all rats.</p> <p>NOAEL&lt; 4869ppm (estimated by reviewer) LOAEL= 4869ppm (estimated by reviewer) based on clinical observations, reduced wt gain. Two rats (1M, 1F) from group 3 (9137ppm) died on day 2; one female from group 3 died during exposure on day 1. Rats in groups 2 and 3 showed ocular discharge throughout d1-5. Rats in group 2 showed increased respiratory rate and dry red material around nose and mouth. All rats in group 2 were lethargic and showed labored respiration. Many rats in group 3 were lethargic and exhibited twitching and harsh respiratory sounds during days 1-5. All rats in group 2 and all but one survivor in group 3 appeared normal on day 8. Group mean body wt was significantly decreased in a dose related manner. No test article related effects were seen at gross necropsy on day 8; the male rat that died during the study showed gas in the G.I. tract and red-tinged fluid in the stomach.</p> <p>Exposure to test article caused a significant decrease in group mean body wt of</p>
---	---

<p><b><u>Quality</u></b> Reliabilities</p> <p><b><u>References</u></b></p> <p><b><u>Other</u></b> Last changed</p>	<p>male and female rats of low and high dose groups that was correlated with exposure level. Three deaths occurred in the high dose group during exposure. Major clinical signs were lethargy, twitching, harsh respiratory sounds and ocular discharge. No gross alterations were found in rats surviving to sacrifice.</p> <p>1. Reliable without restrictions</p> <p>Rausina, G.A. 1984. Five-day repeated dose inhalation toxicity study in rats of Hydrogenated Pyrolysis Gasoline. Proj. #2099. Gulf Life Sciences Center, Pittsburgh, PA</p> <p>Revised 7/27/2001 (Prepared by a contractor to the Olefins Panel)</p>
--	--

## Robust Summary: High Benzene Naphthas

### Acute Toxicity

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

## Robust Summary - Group 5: High Benzene Naphthas

### Acute Toxicity

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

## Robust Summary - Group 5: High Benzene Naphthas

### Genetic Toxicity - in Vitro

<p><b><u>Test Substance</u></b> <i>Test substance</i></p>	<p><b>Rerun Tower Overheads</b> from Olefins/Aromatics Plant (light thermal cracked naphtha) CAS # 64741-74-8. Straw colored liquid; 40% benzene, 26% C5, 13% toluene, 20% other. Test substance is described as a sample of a Pyrolysis Gasoline distillate fraction and is similar to Pyrolysis gasoline, a stream included in the test plan.</p>
<p><b><u>Method</u></b> Method/guideline followed Type System of testing GLP Year Species/Strain Metabolic activation Species and cell type Quantity Induced or not induced Concentrations tested Statistical Method</p>	<p>Standard method based on Ames et al, 1975 Reverse mutation bacterial assay Salmonella typhimurium with and without metabolic activation Yes 1981 S. typhimurium TA 98, TA100, TA1535, TA1537, and TA1538. Yes Sprague Dawley male rat liver (S9 fraction) from Litton Bionetics, Kensington, MD 50ul S9 fraction in 0.5ml S9 mix/plate Aroclor 1254-induced, rats were given a single ip 500mg/kg dose, 5 days prior to sacrifice. 0, 0.029, 0.094, 0.30, 0.97µl/plate –S9, and 0.094, 0.30, 0.97, and 3.1µl/plate + S9; samples diluted in dimethyl sulfoxide (DMSO). Negative control 50µl DMSO None. Criteria for a positive response were an increase in revertant colonies at least two-fold that of negative control at the lowest active dose, and a dose response curve. Positive results must be reproducible in an independent repeat assay.</p>
<p>Remarks for Test Conditions</p>	<p>Rerun tower overheads test solutions were prepared in DMSO immediately prior to use. Salmonella (Approx. <math>1.4-2 \times 10^8</math> cells/ml) were exposed to either test solution or DMSO ±S9 by the preincubation method. Doses of 0.029-0.97µl/plate-S9 and 0.094-3.1µl/plate +S9 were determined by a pretest toxicity test in TA 100 and TA1537±S9 using incremental doses from 0.01-10µl/plate. Culture tubes containing 50µl test solution or DMSO, 0.1ml Salmonella and 0.5 ml phosphate buffer or S9 mix were combined and incubated with shaking (150 rpm) for 20 minutes at 37°C. At the end of the preincubation period, top agar was added, mixed and cultures were overlaid on minimal agar plates, 3 plates/dose/strain. Plates were incubated at 37°C for 48 hrs, then counted automatically (Biotran II) and background lawn evaluated by stereomicroscope. Positive control compounds were: -S9, 2-nitrofluorene (2-NF, 20µg/plate) for TA98 and TA1538; N-methyl-N'-nitro-N-nitrosoguanidine (MNNG, 2.0µg/plate) for TA100 and TA1535; 9-aminoacridine (9-AA, 25µg/plate) for TA1537; +S9 2-aminoanthracene (2µg/plate) for all strains except TA1537.</p>
<p><b><u>Results</u></b> Genotoxic effects</p>	<p>The preliminary toxicity test exhibited severe toxicity at 10µl/plate with activation and at 3.1 and 10µl/plate without activation (individual data not shown). In the mutagenicity test, none of the 5 strains of Salmonella exhibited revertant frequencies substantially different from the solvent or spontaneous controls at any dose level with or without metabolic activation (e.g. TA98-S9: 16, 15, 12, 12, and 0 average revertants/plate and TA100-S9: 111, 115, 107, 94, and 0 at 0[DMSO], 0.029, 0.094, 0.30, and 0.97µl/plate, respectively; TA98+S9: 33, 26, 26, 22, and 0 revertants/plate, and TA100+S9: 128, 161, 128, 118, and 0 revertants/plate at 0[DMSO], 0.094, 0.30, 0.97 and 3.1µl/plate, respectively). Clearing of background lawn and microcolonies were observed at the maximum doses (0.97µl/plate-S9; 3.1µl/plate+S9). Positive control compounds (2 plates/strain) performed</p>

<p><b><u>Conclusions</u></b> (contractor)</p> <p><b><u>Data Quality</u></b> <i>Reliabilities</i></p> <p><b><u>Reference</u></b></p> <p><b><u>Other</u></b> <i>Last changed</i></p>	<p>appropriately (-S9: MNNG 1906, 1883 revertants/plate in TA 100 and TA1535, respectively; 9-AA 586 revertants/plate in TA1537; 2-NF 2114, 1214 revertants/plate in TA98 and TA1538, respectively; and +S9 2- aminoanthracene 406-2307 revertants/plate for all strains except TA1537). The results of this assay indicate that rerun tower overheads had no mutagenic activity in this test system. (Reviewer's note: Due to toxicity, tests were performed over a low dose range; 3 of 4 doses were non-toxic and showed sufficient growth to evaluate mutagenicity. Testing at any lower doses was impractical).</p> <p>Rerun Tower Overheads did not induce an increase in revertant colonies in any Salmonella strain, tested at any dose level with or without metabolic activation in this single Ames test.</p> <p>1. Reliable without restriction</p> <p>Blackburn, G.R. 1981. An Ames Salmonella/mammalian microsome mutagenesis assay for the determination of potential mutagenicity of Rerun Tower Overheads from an olefins/aromatics plant. Study No. 1781-80. Mobil Environmental and Health Sciences Laboratory, Princeton, NJ. Ames B. N. et al. 1975. Mutat. Res. 31: 347-364.</p> <p>10/02/2001 (Prepared by a contractor for the Olefins Panel)</p>
--	---

## Robust Summary - Group 5: High Benzene Naphthas

### Genetic Toxicity - in Vitro

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

<p><b><u>Conclusions</u></b> (contractor)</p> <p><b><u>Data Quality</u></b> <i>Reliabilities</i></p> <p><b><u>Reference</u></b></p> <p><b><u>Other</u></b> <i>Last changed</i></p>	<p>Rerun tower overheads did cause weak differential killing in DNA repair deficient strains, <i>E. coli</i> WP100 and <i>S. typhimurium</i>. TA1538 in the absence of metabolic activation, suggesting that the test article can cause direct acting damage to bacterial DNA. No differential killing was observed in the presence of metabolic activation.</p> <p>1. Reliable without restriction</p> <p>Haworth, S.R. 1978. Bacterial DNA repair assay of Mobil Chemical Company Compound MCTR-125-78 (MRI #110). E. G. and G. Mason Research Institute, Rockville, MD. for Mobil Chemical Co, Edison, NJ  Slater, E.E. et al. 1971. Cancer Res. 31: 970-973.  Green, M.H.L. and Muriel, W.J. 1976. Mutat. Res. 38:3-32  Ames, B.N. et al. 1973. Proc. Natl. Acad. Sci., USA 70: 782-786.</p> <p>2/28/2002 (Prepared by a contractor to the Olefins Panel)</p>
--	---

## Robust Summary: High Benzene Naphthas

### Genetic Toxicity - in Vitro

<p><b><u>Test Substance</u></b> <i>Test substance</i></p>	<p><b>Rerun Tower Overheads</b> from Olefins/Aromatics Plant (light thermal cracked naphtha) CAS # 64741-74-8. Straw colored liquid; 40% benzene, 26% C5, 13% toluene, 20% other. Test substance is described as a sample of a Pyrolysis Gasoline distillate fraction and is similar to Pyrolysis gasoline, a stream included in the test plan.</p>
<p><b><u>Method</u></b> Method/guideline followed Type System of testing GLP Year Species/Strain Metabolic activation Species and cell type Quantity Induced or not induced Concentrations tested</p>	<p>Standard method, no guideline specified Cell transformation Mouse embryo cells Yes 1981 BALB-c/3T3 mouse cell line No NA NA NA Initial cytotoxicity: 0, 0.01, 0.1, 1.0, 10.0, 100.0µg/ml medium; Transformation: 0.0.8, 4.0, 20.0 and 100µg/ml, diluted in dimethyl sulfoxide. Negative control was DMSO at 2.5% vol. concentration.</p>
<p>Statistical Method</p>	<p>T-test specified. Standard criteria for positive response is a two fold increase in type III foci at highest dose over vehicle control with or without a dose related response or a 2 fold increase at 2 or more consecutive doses.</p>
<p>Remarks for Test Conditions</p>	<p>Routine procedures were referred to Appendix 1 Standard Operating Procedures, which was not included with this report. Only specifics unique to this assay are presented. Due to the volatile nature of test material, the cytotoxicity assay and transformation assays were conducted in tightly capped T-25 flasks in sealed plastic bags. The pH of medium during the 72hr exposure period was maintained at 7.4 by 0.02M Hepes buffer in flasks. RTO was prepared as a 1% stock solution in DMSO, which, when added to culture medium at a 2.5% vol. conc. was a suspension. Despite limited solubility, RTO produced a dose-dependent cytotoxic effect after a 3-day exposure period. In the initial toxicity assay, RTO was added to flasks, seeded with BALB-c/3T3 cells, at concentrations of 0, 0.01, 0.1, 1.0, 10.0 and 100.0µg/ml, incubated for 3 days at 37<sup>0</sup>C in a CO<sub>2</sub> in air incubator, after which cells were counted for survival. In the transformation assay, RTO was tested at 0, 0.8, 4.0, 20.0 and 100µg/ml. In a standard BALB-c/3T3 transformation assay, colony formation cultures (approx. 100 cells/culture) and transformation cultures (approx. 10<sup>4</sup> cells/culture, 20 cultures/dose) were seeded on day 1, exposed to test material for 2-3 days, and culture medium was changed on day 4. For transformation cultures, medium continued to be changed weekly to day 29. Colony formation cultures were fixed, stained and counted visually on day 8 to determine cloning efficiency; transformation cultures were fixed and stained on day 29 for focus counting and evaluation. Transformation frequency = total type III foci ÷ total cultures/dose. Positive control compound was 3-methyl cholanthrene (2µg/ml).</p>
<p><b><u>Results</u></b> Genotoxic effects</p>	<p>RTO induced toxicity in BALB-c/3T3 cells after 3 days exposure at concentrations of 10µg/ml (59% viability) and at 100µg/ml (18% viability). In the transformation assay, inhibition of cloning efficiency (CE, clones/100 cells) occurred at 4.0µg/ml (89% CE), 20.0µg/ml (81% CE) and 100µg/ml (65% C.E.); cell toxicity was</p>

<p><b><u>Conclusions</u></b> (contractor)</p> <p><b><u>Data Quality</u></b> <i>Reliabilities</i></p> <p><b><u>Reference</u></b></p> <p><b><u>Other</u></b> <i>Last changed</i></p>	<p>somewhat less than in the initial cytotoxicity assay [40% viability at 100µg/ml]. RTO did not induce statistically significant increased incidence of transformed foci compared to negative controls at any dose level. Values were 0.10 foci/flask, 2/20 flasks with foci at 100µg/ml, 0.0 foci/flask, 0/20 flasks with foci at 20.0µg/ml, 0.15 foci/flask, 3/20 flasks with foci at 4.0µg/ml, 0.10 foci /flask, 2/20 flasks with foci at 0.8µg/ml compared to 0.05 foci/flask, 1/20 flasks with foci in negative control group. [Reviewer's note: Negative control value of 1 focus/20 flasks was lower than control values in other concurrent studies on 2 other compounds in this series where negative controls had 4 foci in 20 flasks (0.20 foci/flask)]. Positive control compound, 3 methyl cholanthrene, induced 56 foci/19 flasks (2.95 foci/flask), 18/19 flasks with foci.</p> <p>Rerun tower overheads did not induce neoplastic transformation in BALB-c/3T3 cells and was not active in this test system.</p> <p>2. Reliable with restrictions. Complete details of assay methods are not included in the report. Specifics of statistics are not supplied.</p> <p>Tu, A.S. and Sivak, A. 1981. BALB-c/3T3 Neoplastic transformation assay on 0818802, 08188003 and 08188005 (Rerun tower overheads). ALD Ref. #86374. Arthur D. Little, Inc. Cambridge, MA for Mobil Oil Corp, Study #1771-80, Princeton, NJ</p> <p>Roy, T.A., 1981. Analysis of rerun tower bottom oil by combined capillary gas chromatography/mass spectrometry. Study #1272-81-. Toxicology division, Mobil Oil Co., Princeton, NJ</p> <p>12/07/01 (Prepared by a contractor to the Olefins Panel)</p>
--	---

## Robust Summary: High Benzene Naphthas

### Genetic Toxicity - in Vitro

<p><b><u>Test Substance</u></b> <i>Test substance</i></p> <p><b><u>Method</u></b> Method/guideline followed Type System of testing GLP Year Species/Strain Metabolic activation Species and cell type Quantity Induced or not induced Concentrations tested</p> <p>Statistical Methods</p> <p>Remarks for Test Conditions</p>	<p><b>Rerun Tower Overheads</b> from Olefins/Aromatics Plant (light thermal cracked naphtha) CAS # 64741-74-8. Straw colored liquid; 40% benzene, 26% C5, 13% toluene, 20% other. Test substance is described as a sample of a Pyrolysis Gasoline distillate fraction and is similar to Pyrolysis gasoline, a stream included in the test plan.</p> <p>None specified. Standard method based on Clive and Spector, 1975 Mammalian cell mutation assay Mouse lymphoma cells Not specified 1979 Mouse lymphoma L5178Y TK+/- cells Yes Sprague Dawley males rat liver (S9 fraction) 50µl S9 fraction/ml S9mix) Aroclor 1254 induced (single ip injection of 500mg/kg, 5 days prior to sacrifice) -S9 cloned doses: 0.0, 0.013, 0.018, 0.024, 0.032, 0.042, 0.056, 0.075, and 0.10µl/ml +S9 cloned doses: 0.0, 0.048, 0.063, 0.085, 0.11, 0.15, 0.20, 0.27, and 0.36µl/ml. All doses diluted in acetone</p> <p>None. Compound was designated as mutagenic if it induced a mutation frequency (mutant cells/10<sup>4</sup> surviving cells) greater than 3 times the standard error (S.E. [f]) calculated by formula from the viable counts and total mutant cells (trifluorothymidine resistant cells) at each dose level.</p> <p>Freshly prepared actively growing cultures of L5178Y cells (1x10<sup>6</sup> cells/ml) were dispensed in 6ml aliquots into 44 polypropylene centrifuge tubes. Rerun tower overheads, solubilized in acetone, beginning at a concentration equal to LD90 from a preliminary toxicity test, was diluted over 15 serial 1/8 log dilutions, producing 16 dose levels decreasing approximately 100 fold from highest to lowest, and added to cells in the centrifuge tubes. Four ml of S9 activation mixture or 4ml culture medium was added, yielding a final cell suspension of 0.6x10<sup>6</sup> cells/ml. Positive control compounds were ethyl methyl sulfonate (EMS, 1.0µl/ml) -S9 and 7,12-dimethylbenzanthracene (7,12-DMBA, 2.5µl/ml) +S9 cultures. All tubes were gassed with 5% CO<sub>2</sub>/air and placed on a roller drum for 4hrs at 37°C in the dark. At the end of exposure, calls were washed with fresh medium, re-suspended, gassed, replaced on roller drum at 37°C and incubated for 3 days with a cell population adjustment every 24 hrs to maintain a cell population density of 0.3x10<sup>6</sup> cells/ml. After 3 days expression, 8 cultures ± S9, which exhibited toxicity from 10-90% growth inhibition during the expression period, were selected for cloning. At cloning, cells were placed in restrictive suspension medium containing trifluorothymidine (TFT, 1µg/ml) that allows only TK-/- cells to grow. Two Florence flasks/concentration ± S9, one for restrictive medium, one for viable cell counts, were filled with 100ml cloning medium and maintained at 37°C. Six 100mm petri plates/concentration ± S9 were prepared, 3 for restrictive medium, 3 for viable cell counts. Cell counts were made from each centrifuge tube to determine the volume of cell population = 3x10<sup>6</sup> cells. This volume was retained, centrifuged and the supernatant discarded except for 2ml in which cells were re-suspended and placed in restrictive medium flask. A 5x10<sup>-4</sup> dilution was prepared and added to the appropriate viable count flask containing 100ml cloning medium. After this dilution, 1 ml of TFT stock solution was added to the restrictive medium flask and incubated</p>
---	--

	<p>with shaking (125rpm) at 37<sup>0</sup>C for 15min. Flasks were removed, 33ml of cell suspension was pipetted into each of 3 appropriately labeled plates and placed in the cold (4<sup>0</sup>C) for 20 min to accelerate gelling. Plates were removed and incubated at 37<sup>0</sup>C in humidified 5% CO2/air for 10 days. At the end of incubation, plates were scored for total number of colonies/plate, 3 counts/plate, on an automated colony counter. Mutation frequency (MF) = avg. number of colonies in 3 restrictive medium plates ÷ avg. number of colonies x10<sup>4</sup> in 3 corresponding viable count plates. Induced mutation frequency (IMF) = MF test article – MF solvent control.</p>
<p><b><u>Results</u></b> Genotoxic effects</p>	<p>In cultures without metabolic activation, the two highest concentrations cloned, 0.10µl/ml (MF=1.4, IMF=0.8) and 0.075µl/ml (MF=1.0, IMF=0.4) exhibited slight dose related increases in IMF compared with acetone control (MF=0.6); only the 0.10µl/ml concentration caused a doubling of MF over controls. EMS positive control values were MF=27.1, IMF=26. The first activated assay was discarded due to loss of positive control cultures by contamination. In the repeat test with metabolic activation, 2 dose concentrations had MF 2 times greater than acetone controls: the highest dose cloned, 0.36µl/ml (MF=0.8, IMF=0.4) and 0.15µl/ml, the 4<sup>th</sup> highest dose cloned (MF=0.9, IMF=0.5) versus control (MF=0.4). However, intervening cloned doses of 0.20, and 0.27µl/ml did not show increased MF; the values for the positive doses were not dose related and were within the range of experimental error for the assay. Positive control values +S9 for 7,12- DMBA were MF=2.6, IMF=2.0.</p>
<p><b><u>Conclusions</u></b> (contractor)</p>	<p>Without metabolic activation, Rerun tower overheads appears to induce a weak mutagenic response at the two highest doses only; a dose response trend was not observed in the 6 lower doses cloned. Test article did not induce significant mutagenic activity in cultures containing S9, suggesting that any mutagenic activity is suppressed or inactivated by the presence of the liver microsome metabolizing system.</p>
<p><b><u>Data Quality</u></b> Reliabilities</p>	<p>1. Reliable without restriction.</p>
<p><b><u>Reference</u></b></p>	<p>Kirby, P.E. et al., 1979. An evaluation of mutagenic potential of MCTR-125-78 (MRI #110) employing the L5178Y TK+/- mouse lymphoma assay. E.G. and G. Mason Research Institute, Rockville, MD for Mobil Chemical Co., Edison, NJ Clive, D., and Spector, J.F.S. 1975. Mutat. Res. 31: 17-29</p>
<p><b><u>Other</u></b> Last changed</p>	<p>2/28/2002 (Prepared by a contractor to the Olefins Panel)</p>

## Robust Summary: High Benzene Naphthas

### Genetic Toxicity - in Vitro

<p><b><u>Test Substance</u></b> <i>Test substance</i></p>	<p><b>Rerun Tower Overheads</b> from Olefins/Aromatics Plant (light thermal cracked naphtha) CAS # 64741-74-8. Straw colored liquid; 40% benzene, 26% C5, 13% toluene, 20% other. Test substance is described as a sample of a Pyrolysis Gasoline distillate fraction and is similar to Pyrolysis gasoline, a stream included in the test plan.</p>
<p><b><u>Method</u></b> Method/guideline followed Type System of testing GLP Year Species/Strain Metabolic activation Species and cell type Quantity Induced or not induced Concentrations tested</p>	<p>None specified. Standard method based on Bertram, 1977 Mammalian cell transformation assay Mouse C3H embryo cells Not specified 1978 Mouse embryo cells/ C3H 10T½ No NA NA NA 0, 0.625, 1.25, 2.5 and 5.0µl/ml, all diluted in acetone</p>
<p>Statistical Methods</p>	<p>None. A positive response is determined by the appearance of any type II foci (50% can be malignantly transformed) and type III foci (85% can be malignantly transformed) compared to negative controls. The C3H 10T½ cell line has no spontaneous transformation.</p>
<p>Remarks for Test Conditions</p>	<p>For the preliminary toxicity assay, cells (200/plate) were exposed to Rerun tower overheads diluted in acetone, over a range of concentrations from 0.0003-5.0µl/ml, at 2-fold dilutions for 18hrs; cells were then washed, re-fed with fresh Eagle's basal medium and incubated for 10 days in 5% CO2/air at 37°C. After incubation, cells were washed, fixed with absolute methanol (20 min) and stained with Giemsa (30 min); number of cells/plate were counted and cloning efficiency (CE) determined=Avg. number colonies/plate ÷ number cells plated x100. In the transformation assay, cells in late log phase were plated at a concentration of 1x10<sup>3</sup> cells/60mm petri dish. Cultures for concurrent toxicity determination were prepared at 200 cells/plate. After 24 hrs, cultures were treated with appropriate test article concentrations in 25µl volumes at 4 dose levels, 12 plates/dose, in decreasing 2-fold dilutions from concentrations which exhibit 25-75% relative CE. Positive control compound was 7, 12-dimethylbenzanthracene (7, 12-DMBA, 0.5µg/ml). After 18hr treatment, test article was removed, cultures were re-fed, and re-incubated. Toxicity plates were incubated for 10 days, stained and CE determined. Transformation cultures were re-fed weekly until 35 days after removal of test article had elapsed. All plate cultures were washed, fixed, stained and scored for the presence of type II and type III foci by macroscopic and microscopic examination. Type II foci show massive piling up in virtually opaque monolayers, cells are moderately polar. Type III foci are composed of highly polar, fibroblastic, multilayered, criss-crossed arrays of densely stained cells.</p>
<p><b><u>Results</u></b> Genotoxic effects</p>	<p>Rerun tower overheads induced 71% relative cloning efficiency at 5.0µl/ml; transformation assay was performed at 2-fold dilutions from 5.0µl/ml. In the toxicity study conducted in parallel with the transformation assay, test article induced 100% cell death at 5.0µl/ml. In the transformation assay, sufficient cells survived to form a confluent layer in 8/12 plates at 5.0µl/ml dose level after 35 days. No indication of type II or type III foci were induced by rerun tower overheads at any dose level. Positive control, 7,12-DMBA induced 9 type II and</p>

<p><b><u>Conclusions</u></b> (contractor)</p> <p><b><u>Data Quality</u></b> <i>Reliabilities</i></p> <p><b><u>Reference</u></b></p> <p><b><u>Other</u></b> <i>Last changed</i></p>	<p>12 type III foci on 12 plates.</p> <p>Rerun tower overheads does not induce cell transformation in mouse embryo C3H 10T½ cells.</p> <p>1. Reliable without restriction</p> <p>Jensen, E.M., and Thilager, A.K. 1978. C3H 10T½ cell transformation assay, Mobil Chemical Co. Compound MCTR-125-78 (MRI #110). E.G. and G. Mason Research Institute, Rockville, MD</p> <p>Bertram, J.S. 1977. Cancer Res. 37: 514-523</p> <p>2/28/2002 (Prepared by a contractor to the Olefins Panel)</p>
--	---

## Robust Summary - Group 5: High Benzene Naphthas

### Genetic Toxicity - in Vivo

<p><b><u>Test Substance</u></b> Remarks</p> <p><b><u>Method</u></b> Method/guideline followed</p> <p>Type</p> <p>GLP</p> <p>Year</p> <p>Species</p> <p>Strain</p> <p>Sex</p> <p>Route of administration</p> <p>Doses/concentration levels</p> <p>Exposure period</p> <p>Statistical methods</p> <p>Remarks for Test Conditions.</p>	<p><b>Rerun Tower Overheads</b> from Olefins/Aromatics Plant (light thermal cracked naphtha) CAS # 64741-74-8. Straw colored liquid; 40% benzene, 26% C5, 13% toluene, 20% other. Test substance is described as a sample of a Pyrolysis Gasoline distillate fraction and is similar to Pyrolysis gasoline, a stream included in the test plan.</p> <p>None specified. Standard method based on Bowman, 1969; Lewis, 1954; Mendelson, 1976</p> <p><i>Drosophila</i> assays for point mutation, chromosome aberrations &amp; chromosome loss</p> <p>Not specified</p> <p>1979</p> <p><i>Drosophila melanogaster</i></p> <p>Dominant lethal: Canton S; Y chromosome loss: males red/white eye; females white/white eye; Somatic reversion: males white ivory (<u>w<sup>i</sup></u>), yellow body (<u>y</u>), echinus (<u>ec</u>); females <u>w<sup>i</sup>/w<sup>i</sup></u>; Bithorax test: males Ultrabithorax (<u>Ubx</u>); females bithorax (<u>bx<sup>34e</sup></u>); Sex-linked recessive lethal: males Canton S; females <u>Basc/Basc</u></p> <p>Males and females</p> <p>Aerosol</p> <p>0.3ml in 50ml air</p> <p>10 min.</p> <p>Events in these tests have very low probabilities. Analysis based on Poisson distribution with fiducial limits computed according to Stevens, 1942.</p> <p><i>Drosophila</i> stocks were maintained in agar/corn meal/sugar/yeast medium at 23<sup>0</sup>C. One set of stocks was transferred each week to isolate virgin females for breeding. Four days are required for maturation of <i>Drosophila</i> sperm cells after meiosis. In all assays, treated males were mated for 3 days only to assure use of a uniform sample of treated sperm. In all assays, test article was administered as an aerosol, 0.3ml in 50ml volume of air. when administered for 1hr anesthetized flies and killed approximately 30%. Longer treatments reduced fertility. Exposure in all assays was 10 minutes in duration.</p> <p><u>Somatic reversion of white-ivory</u>: Larvae from mating of males carrying 5 copies of white-ivory gene on the X chromosome (<u>w<sup>i</sup></u>, <u>y</u>, <u>ec</u>) with <u>w<sup>i</sup>/w<sup>i</sup></u> females were treated with aerosolized test article for 10 min. Positive control compound was 0.04M mitomycin C. Larvae were washed and transferred to culture bottles to complete development. After eclosion, female offspring, genotype Qn(1)<u>w<sup>i</sup></u>, <u>y</u>, <u>ec/w<sup>i</sup></u> were scored for red spots in the eye, which signals reversion of <u>w<sup>i</sup></u> to a pigment cell.</p> <p><u>Y chromosome loss</u>: Males carrying a duplication of the gene for normal (red) eyes on Y chromosome and a mutant allele, white (<u>w</u>) on the X chromosome were treated with aerosolized test article for 10 min and mated to white-eyed females (<u>w/w</u>). Positive control were males exposed to 3kr X-rays. Frequency of occurrence of white-eyed male progeny measured frequency of Y chromosome loss.</p> <p><u>Dominant lethal mutations</u>: Defined as any genetic change that blocks development prior to hatching. Treated Canton S males were mated with untreated females in nylon net cages on Welch's grape juice solidified with 2% agar. After 12 hr, agar plates were removed and stored at room temp. (23<sup>0</sup>C) for 30 hrs. Positive control was 0.04M ethyl methane sulfonate. Eggs were scored for hatching after 30hrs.</p>
---	---

<p><b><u>Results</u></b> Genotoxic effects NOAEL (NOEL) LOAEL (LOEL)</p> <p><b><u>Conclusions</u></b> (study authors)</p> <p><b><u>Data Quality</u></b> <i>Reliabilities</i></p> <p><b><u>References</u></b></p> <p><b><u>Other</u></b> <i>Last changed</i></p>	<p><b><u>Bithorax test of Lewis</u></b>: Occurrence of rearrangements with one breakpoint between centromere and the locus of bithorax (<u>bx</u>) was determined by scoring offspring of treated Ultrabithorax males and bithorax females. Males treated with 3kr X-rays were the positive controls. Distinctive phenotype was the presence of a mesonotum</p> <p><b><u>Sex-linked recessive lethals</u></b>: Canton-S males, treated with test article, were mated with Basc (balancer X chromosome) females. Individual (F1) female progeny were mated with Basc males. Any single female culture containing at least 20 flies (F2), at least 8 of which are males, but no males are wild type, is scored as a lethal. Ethyl methane sulfonate (0.04M) treated males were the positive controls. A repeat study was performed due to loss of cultures to dessication.</p> <p>Rerun tower overheads did not induce genetic damage in <i>Drosophila melanogaster</i> under experimental conditions in any test employed. The repeated sex-linked recessive lethal test, performed due to technical problems in the initial assay, did not demonstrate any genetic damage in <i>Drosophila</i> from exposure to the test article</p> <p>Rerun tower overheads did not induce genetic damage in <i>Drosophila melanogaster</i>.</p> <p>1. Reliable without restrictions.</p> <p>Bowman, J.T. 1979. <i>Drosophila</i> mutagenicity assays of Mobil Chemical Compound MCTR-125-78. MRI #110. E.G. and G. Mason Research Institute, Rockville, MD, for Mobil Chemical Co., Edison, NJ. Bowman, J.T. 1969. Mutat. Res. 7: 409-415 Lewis, E.B. 1954. Am. Nat. 88: 225-239 Mendelson, D. 1976. Mutat. Res. 41: 269-276 Stevens, W.L. 1942. J. Genetics 43: 301-307</p> <p>2/28/2002 (Prepared by a contractor to the Olefins Panel)</p>
---	--

## Robust Summary: High Benzene Naphthas

### Repeated Dose Toxicity

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

<p><b><u>Results</u></b>  NOAEL (NOEL)  LOAEL (LOEL)  Remarks</p> <p><b><u>Conclusions</u></b>  (study authors)</p> <p><b><u>Quality</u></b>  Reliabilities</p> <p><b><u>References</u></b></p> <p><b><u>Other</u></b>  Last changed</p>	<p>NOAEL &lt;0.10ml/kg/day both sexes (skin irr). LOAEL = 0.1ml/kg/day both sexes (skin irr)  NOAEL = 1.0ml/kg/day both sexes (systemic effects). LOAEL &gt;1.0ml/kg/day both sexes (systemic effects).  Two rabbits died during the study from cardiac puncture blood sampling. No test article induced effects were noted during clinical observations. Two 0.1ml/kg/day group males and one female showed erythema from day 10 to termination; 3 0.5ml/kg/day group males showed erythema from day 8 to termination; all 0.5ml/kg/day males and females, and 1.0ml/kg/day males and females had well defined erythema from day 9 to termination. Edema was not present in any rabbits. Skin thickening was noted in all test article groups from wk 1 to termination. Fissuring was seen in 3 0.1ml/kg/day males, 3 0.5ml/kg/day males and all 1.0ml/kg/day males; all test article treated females showed fissuring. Necrosis was present in 2males and 3 females given 0.1ml/kg/day, 3males and all females given 0.5ml/kg/day, and all males and females given 1.0ml/kg/day. There were no significant changes in body wt or food consumption between controls and treatment groups. Terminal basophilic values were elevated in all male test article treated groups; all other hematology values were comparable to controls. Urinalysis findings were unremarkable. There were no significant differences in organ wt between control and any treatment group. Histological evaluation for the skin showed effects consistent with gross observations with no dose-related gradation of severity between doses, including hyperkeratosis, acanthosis, accumulation of heterophils, and cellular debris in stratum corneum, and hyperplasia of sebaceous glands. There were no abnormal microscopic findings attributable to test article administration in organs from the three treatment levels compared to controls.</p> <p>Daily epidermal application of test article resulted in skin irritation at the application site.</p> <p>2. Reliable with restriction. There was no mention of GLP.</p> <p>Fieser, S., Alsaker, R.D., Brown, H.R., and Wolfe, G.W. 1980. 21-Day dermal irritation study in rabbits. Proj. #230-213. Hazleton Laboratories America, Inc., Vienna, VA. For Mobil Chemical Co., Edison NJ (This study was actually for subacute toxicity, not only skin irritation)</p> <p>2/28/2002 (Prepared by a contractor to the Olefins Panel)</p>
--	--

## Robust Summary: High Benzene Naphthas

### Developmental Toxicity/Teratogenicity

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

	<p>were observed daily for mortality, overt changes in appearance and behavior, and, from day 6-29 of gestation, for clinical signs of toxicity. One dam aborted on gest. day 19 and remained on study until scheduled sacrifice; aborted material was discarded. Body wt was recorded on gestation days 0, 6, 12, 18, 24, and 29. On gest. day 29, all females were sacrificed by overdose of sodium pentobarbitol, uteri were excised and weighed prior to removal of fetuses. Number and location of viable and non-viable fetuses, early and late resorptions, number of total implantations, and corpora lutea were recorded. Abdominal and thoracic cavity and organs of dams were examined grossly and discarded. Uteri from apparently non-gravid animals were opened and placed in 10% ammonium sulfide solution to confirm pregnancy status.</p> <p>All fetuses were individually weighed and examined for external malformations and variations. Each fetus was internally sexed and examined for internal malformations and variations, including the brain by mid-coronal slice. The heart was dissected using Staples' technique. Eviscerated, skinned fetuses were individually numbered and tagged, fixed in alcohol, macerated and stained with Alizarin Red S for skeletal examination. Fetal findings were classified as malformations or genetic or developmental variations.</p>
<p><b><u>Results</u></b>  NOAEL maternal toxicity  NOAEL developmental toxicity  Maternal effects</p>	<p>NOAEL maternal = 25mg/kg/day (based on 1 abortion at 50mg/kg/day)  NOAEL developmental = 50mg/kg/day; both values assigned by reviewer</p> <p>Maternal survival was 100% in all groups. Slight increase in matted haircoat (primarily in nasal region) and slight reduction in fecal material beneath cages was noted in 50mg/kg/day rabbits. Occasional instances of nasal discharge, soft stool, hair loss and scabbing were noted in all groups during gestation. One 50mg/kg/day rabbit aborted on day 19 of gestation. Maternal body wt in treated rabbits at all doses were comparable to controls throughout treatment (gest. day 6-28) and gestation (day 0-29) periods. Mean maternal adjusted body wt (minus gravid uterus) at termination in all groups was comparable to controls. Pregnancy ratio was 87.5, 81.3, 81.3, 93.8 in 0, 10, 25 and 50mg/kg/day groups, respectively. Two control dams and one 50mg/kg/day dam had all resorptions. There were no biologically or statistically significant differences in mean number of corpora lutea, total implantations, early or late resorptions, postimplantation loss, viable fetuses, fetal sex index, or mean fetal body wt in any RTO treated group compared to controls.</p>
<p>Embryo/fetal effects</p>	<p>Average litter size was 6.1, 6.5, 6.4, and 5.9 and average fetal body wt (both sexes) was 38.9, 43.0, 42.5, and 42.4g in 0, 10, 25, and 50mg/kg/day groups, respectively. There were no biologically or statistically significant differences in number of litters with malformations (external, soft tissue, skeletal) in any treated group compared to controls: 5/12 litters (85 pups), 1/13 litters (84 pups), 3/13 litters (83 pups) and 5/13 litters (82 pups examined) in 0, 10, 25, and 50mg/kg/day, respectively. In the 50mg/kg/day group, one occurrence of atlas-occipital anomaly and one occurrence of enlarged heart with great vessel anomaly, were observed in 2 separate litters. Scoliosis was present in all groups including control, with slightly higher incidence in the 50mg/kg/day group., but incidences were within the range of historical control data for this laboratory. Fetuses and litters with genetic or developmental variations were comparable in all groups.</p>
<p><b><u>Conclusions</u></b>  (study authors)</p>	<p>Rerun tower overhead did not produce a teratogenic response in pregnant New Zealand White rabbits when administered orally in corn oil vehicle at dose levels of 10, 25 and 50mg/kg/day. With the exception of one 50mg/kg/day female that aborted, minimal maternal toxicity was observed at any dose level.</p>

<p><b><u>Data Quality</u></b> <i>Reliabilities</i></p> <p><b><u>References</u></b></p> <p><b><u>Other</u></b> <i>Last changed</i></p>	<p>2. Reliable with restrictions. Analysis of test article concentration in corn oil vehicle was not performed.</p> <p>Schardein, J.L. 1981. Teratology study in rabbits: Rerun tower overheads (MRTC-171-79) IRDC #450-011. International Research and Development Corp., Mattawan, MI. for Mobil Petrochemicals Division, Edison, NJ</p> <p>2/28/2002 (Prepared by a contractor to the Olefins Panel)</p>
---	---