

201-15522B1

Attachment 2a.

Robust Summaries

PhysicoChemical and Environmental Fate

01/15/2015 11:15

01/15/2015

LOW BENZENE NAPHTHAS ROBUST SUMMARY

Boiling Point

Test Substance*:	Other TS [CAS # 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3]
Method/Guideline:	Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Pressure:	760 mm Hg
Test Conditions: <ul style="list-style-type: none"> Note: Concentration prep., vessel type, replication, test conditions. 	Boiling Point is calculated by the MPBPWIN subroutine, which is based on the calculation method of S. Stein and R. Brown in "Estimation of Normal Boiling Points from Group Contributions". 1994. J. Chem. Inf. Comput. Sci. 34: 581-587.
Results: Units/Value: <ul style="list-style-type: none"> Note: Deviations from protocol or guideline, analytical method. 	<p>Calculated and measured boiling point data for representative constituents of the Low Benzene Naphthas Category are listed below. The data identify a potential boiling point range for substances represented by the 10 CAS numbers under <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 complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C12. The seven chemicals selected to represent the boiling point range of this category are C5-C11 hydrocarbons that can be found in substances identified by the 10 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.</p>

HPV CHEMICAL CATEGORY SUMMARY (DRAFT): LOW BENZENE NAPHTHAS

<p>Results: (continued)</p> <p>Units/Value:</p> <p>Note: Deviations from protocol or guideline, analytical method.</p>	<table border="1"> <thead> <tr> <th>Substance <u>Constituent</u></th> <th>Calculated <u>BP (°C)</u></th> <th>Measured* <u>BP (°C)</u></th> </tr> </thead> <tbody> <tr> <td>isopentane</td> <td>30.18</td> <td>27.8</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>naphthalene</td> <td>231.64</td> <td>217.9</td> </tr> <tr> <td>tricyclodecane</td> <td>171.25</td> <td>na</td> </tr> <tr> <td>methylnaphthalene</td> <td>249.60</td> <td>241.1</td> </tr> </tbody> </table> <p>* Experimental values from EPIWIN database. na = not available</p> <p>The data represent a potential boiling point range for substances represented by the 10 CAS numbers under <u>Test Substance</u>.</p>	Substance <u>Constituent</u>	Calculated <u>BP (°C)</u>	Measured* <u>BP (°C)</u>	isopentane	30.18	27.8	toluene	125.72	110.6	m-xylene	148.29	139.1	styrene	146.65	145.0	naphthalene	231.64	217.9	tricyclodecane	171.25	na	methylnaphthalene	249.60	241.1
Substance <u>Constituent</u>	Calculated <u>BP (°C)</u>	Measured* <u>BP (°C)</u>																							
isopentane	30.18	27.8																							
toluene	125.72	110.6																							
m-xylene	148.29	139.1																							
styrene	146.65	145.0																							
naphthalene	231.64	217.9																							
tricyclodecane	171.25	na																							
methylnaphthalene	249.60	241.1																							
<p>Test Substance:</p>	<p>The Low Benzene Naphthas Category includes the following CAS numbers:</p> <p>64741-98-6 Extract, petroleum, heavy naphtha solvent 64742-48-9 Naphtha, petroleum, hydrotreated heavy 64742-49-0 Naphtha, petroleum, hydrotreated light 64742-83-2 Naphtha, petroleum, light steam-cracked 68333-88-0 Aromatic hydrocarbons, C9-C17 68476-45-9 Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product 68478-10-4 Naphtha, petroleum, light steam-cracked, debezenized, C8-16-cycloalkadiene concentrate 68516-20-1 Naphtha, petroleum, steam-cracked middle aromatic 68527-23-1 Naphtha, petroleum, light steam-cracked aromatic 68919-15-3 Hydrocarbons, C6-12, benzene-recovery</p> <p>Low Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 10 CAS numbers are used to describe the nine process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry. Aromatics represent the major constituents in all of the streams, varying from approximately 45 to 95 percent. The benzene content is usually less than five percent.</p> <p>More information on the Low 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.</p>																								

HPV CHEMICAL CATEGORY SUMMARY (DRAFT): LOW BENZENE NAPHTHAS

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

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

LOW BENZENE NAPHTHAS ROBUST SUMMARY

Melting Point

Test Substance*:	Other TS [CAS # 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3]
Method/Guideline:	Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Test Conditions: <ul style="list-style-type: none"> Note: Concentration prep., vessel type, replication, test conditions. 	<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 $T_m = 0.5839T_b$, where T_m is the melting point in Kelvin and T_b 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>
Results: Units/Value: <ul style="list-style-type: none"> Note: Deviations from protocol or guideline, analytical method. 	<p>Calculated and measured melting point data for representative constituents of the Low Benzene Naphthas Category are listed below. The data identify a potential melting point range for substances represented by the 10 CAS numbers under <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 complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C12. The seven chemicals selected to represent the melting point range of this category are C5-C11 hydrocarbons that can be found in substances identified by the 10 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.</p>

HPV CHEMICAL CATEGORY SUMMARY (DRAFT): LOW BENZENE NAPHTHAS

<p>Results: (continued)</p> <p>Units/Value:</p> <p>Note: Deviations from protocol or guideline, analytical method.</p>	<table border="1"> <thead> <tr> <th>Substance <u>Constituent</u></th> <th>Calculated <u>MP (°C)</u></th> <th>Measured* <u>MP (°C)</u></th> </tr> </thead> <tbody> <tr> <td>isopentane</td> <td>-119.04</td> <td>-159.9</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>naphthalene</td> <td>5.01</td> <td>80.2</td> </tr> <tr> <td>tricyclodecane</td> <td>-19.15</td> <td>na</td> </tr> <tr> <td>methylnaphthalene</td> <td>22.15</td> <td>34.4</td> </tr> </tbody> </table> <p>* Experimental values from EPIWIN database. na = not available</p> <p>The data represent a potential melting point range for substances represented by the 10 CAS numbers under <u>Test Substance</u>.</p>	Substance <u>Constituent</u>	Calculated <u>MP (°C)</u>	Measured* <u>MP (°C)</u>	isopentane	-119.04	-159.9	toluene	-59.17	-94.9	m-xylene	-40.69	-47.8	styrene	-48.31	-31.0	naphthalene	5.01	80.2	tricyclodecane	-19.15	na	methylnaphthalene	22.15	34.4
Substance <u>Constituent</u>	Calculated <u>MP (°C)</u>	Measured* <u>MP (°C)</u>																							
isopentane	-119.04	-159.9																							
toluene	-59.17	-94.9																							
m-xylene	-40.69	-47.8																							
styrene	-48.31	-31.0																							
naphthalene	5.01	80.2																							
tricyclodecane	-19.15	na																							
methylnaphthalene	22.15	34.4																							
<p>Test Substance:</p>	<p>The Low Benzene Naphthas Category includes the following CAS numbers:</p> <p>64741-98-6 Extract, petroleum, heavy naphtha solvent 64742-48-9 Naphtha, petroleum, hydrotreated heavy 64742-49-0 Naphtha, petroleum, hydrotreated light 64742-83-2 Naphtha, petroleum, light steam-cracked 68333-88-0 Aromatic hydrocarbons, C9-C17 68476-45-9 Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product 68478-10-4 Naphtha, petroleum, light steam-cracked, debezenized, C8-16-cycloalkadiene concentrate 68516-20-1 Naphtha, petroleum, steam-cracked middle aromatic 68527-23-1 Naphtha, petroleum, light steam-cracked aromatic 68919-15-3 Hydrocarbons, C6-12, benzene-recovery</p> <p>Low Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 10 CAS numbers are used to describe the nine process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry. Aromatics represent the major constituents in all of the streams, varying from approximately 45 to 95 percent. The benzene content is usually less than five percent.</p> <p>More information on the Low 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.</p>																								

HPV CHEMICAL CATEGORY SUMMARY (DRAFT): LOW BENZENE NAPHTHAS

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

- 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.

LOW BENZENE NAPHTHAS ROBUST SUMMARY

Vapor Pressure

Test Substance*:	Other TS [CAS # 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3]
Method/Guideline:	Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: <ul style="list-style-type: none"> Note: Concentration prep., vessel type, replication, test conditions. 	<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>
Results: Units/Value: <ul style="list-style-type: none"> Note: Deviations from protocol or guideline, analytical method. 	<p>Calculated and measured vapor pressure data for representative constituents of the Low Benzene Naphthas Category are listed below. The data identify a potential vapor pressure range for substances represented by the 10 CAS numbers under <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 complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C12. The seven chemicals selected to represent the vapor pressure range of this category are C5-C11 hydrocarbons that can be found in substances identified by the 10 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.</p>

HPV CHEMICAL CATEGORY SUMMARY (DRAFT): LOW BENZENE NAPHTHAS

<p>Results (continued):</p> <p>Units/Value:</p> <p>Note: Deviations from protocol or guideline, analytical method.</p>	<table border="1"> <thead> <tr> <th data-bbox="623 170 781 237">Substance Constituent</th> <th data-bbox="862 170 1052 237">Calculated VP (hPa @ 25°C)</th> <th data-bbox="1101 170 1291 237">Measured* VP (hPa @ 25°C)</th> </tr> </thead> <tbody> <tr> <td data-bbox="623 268 773 300">isopentane</td> <td data-bbox="899 268 1015 300">9.17 E2</td> <td data-bbox="1149 268 1265 300">9.19 E2</td> </tr> <tr> <td data-bbox="623 304 724 336">toluene</td> <td data-bbox="899 304 976 336">31.60</td> <td data-bbox="1138 304 1218 336">37.86</td> </tr> <tr> <td data-bbox="623 340 748 371">m-xylene</td> <td data-bbox="911 340 976 371">8.83</td> <td data-bbox="1138 340 1218 371">11.05</td> </tr> <tr> <td data-bbox="623 375 724 407">styrene</td> <td data-bbox="911 375 976 407">6.73</td> <td data-bbox="1149 375 1214 407">8.53</td> </tr> <tr> <td data-bbox="623 411 789 443">naphthalene</td> <td data-bbox="911 411 976 443">0.11</td> <td data-bbox="1149 411 1214 443">0.05</td> </tr> <tr> <td data-bbox="623 447 813 478">tricyclodecane</td> <td data-bbox="911 447 976 478">2.64</td> <td data-bbox="1161 447 1203 478">na</td> </tr> <tr> <td data-bbox="623 483 873 514">methylnaphthalene</td> <td data-bbox="899 483 1031 514">4.60 E-2</td> <td data-bbox="1149 483 1281 514">7.33 E-2</td> </tr> </tbody> </table> <p data-bbox="623 541 1224 604">* Experimental values from EPIWIN database. na = not available</p> <p data-bbox="623 625 1406 720">The data represent a potential vapor pressure range for substances represented by the 10 CAS numbers under <u>Test Substance</u>.</p>	Substance Constituent	Calculated VP (hPa @ 25°C)	Measured* VP (hPa @ 25°C)	isopentane	9.17 E2	9.19 E2	toluene	31.60	37.86	m-xylene	8.83	11.05	styrene	6.73	8.53	naphthalene	0.11	0.05	tricyclodecane	2.64	na	methylnaphthalene	4.60 E-2	7.33 E-2
Substance Constituent	Calculated VP (hPa @ 25°C)	Measured* VP (hPa @ 25°C)																							
isopentane	9.17 E2	9.19 E2																							
toluene	31.60	37.86																							
m-xylene	8.83	11.05																							
styrene	6.73	8.53																							
naphthalene	0.11	0.05																							
tricyclodecane	2.64	na																							
methylnaphthalene	4.60 E-2	7.33 E-2																							
<p>Test Substance:</p>	<p data-bbox="623 747 1406 810">The Low Benzene Naphthas Category includes the following CAS numbers:</p> <p data-bbox="623 831 1341 863">64741-98-6 Extract, petroleum, heavy naphtha solvent</p> <p data-bbox="623 867 1317 898">64742-48-9 Naphtha, petroleum, hydrotreated heavy</p> <p data-bbox="623 903 1292 934">64742-49-0 Naphtha, petroleum, hydrotreated light</p> <p data-bbox="623 938 1317 970">64742-83-2 Naphtha, petroleum, light steam-cracked</p> <p data-bbox="623 974 1208 1005">68333-88-0 Aromatic hydrocarbons, C9-C17</p> <p data-bbox="623 1010 1382 1062">68476-45-9 Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product</p> <p data-bbox="623 1066 1325 1161">68478-10-4 Naphtha, petroleum, light steam-cracked, debezenized, C8-16-cycloalkadiene concentrate</p> <p data-bbox="623 1165 1349 1228">68516-20-1 Naphtha, petroleum, steam-cracked middle aromatic</p> <p data-bbox="623 1232 1317 1295">68527-23-1 Naphtha, petroleum, light steam-cracked aromatic</p> <p data-bbox="623 1299 1317 1331">68919-15-3 Hydrocarbons, C6-12, benzene-recovery</p> <p data-bbox="623 1352 1406 1682">Low Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 10 CAS numbers are used to describe the nine process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry. Aromatics represent the major constituents in all of the streams, varying from approximately 45 to 95 percent. The benzene content is usually less than five percent.</p> <p data-bbox="623 1719 1377 1814">More information on the Low Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1).</p> <p data-bbox="623 1852 1390 1948">1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low Benzene Naphthas</p>																								

HPV CHEMICAL CATEGORY SUMMARY (DRAFT): LOW BENZENE NAPHTHAS

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

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

LOW BENZENE NAPHTHAS ROBUST SUMMARY

Hydrolysis (Stability in Water)

Test Substance*:	Other TS [CAS # 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3]
Method/Guideline:	Other: Technical discussion
Year (guideline):	Not applicable
Type (test type):	Not applicable
GLP (Y/N):	Not applicable
Year (study performed):	Not applicable
Analytical Monitoring:	Not applicable
Test Conditions: <ul style="list-style-type: none"> Note: Concentration preparation, vessel type, volume, replication, deviations from guideline or protocol 	Not applicable
Results: Units/Value: <ul style="list-style-type: none"> Note: Analytical method, observations, half-lives by pH, degradation products 	Not applicable
Test Substance:	The Low Benzene Naphthas Category includes the following CAS numbers: 64741-98-6 Extract, petroleum, heavy naphtha solvent 64742-48-9 Naphtha, petroleum, hydrotreated heavy 64742-49-0 Naphtha, petroleum, hydrotreated light 64742-83-2 Naphtha, petroleum, light steam-cracked 68333-88-0 Aromatic hydrocarbons, C9-C17 68476-45-9 Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product 68478-10-4 Naphtha, petroleum, light steam-cracked, debezenized, C8-16-cycloalkadiene concentrate 68516-20-1 Naphtha, petroleum, steam-cracked middle aromatic 68527-23-1 Naphtha, petroleum, light steam-cracked aromatic 68919-15-3 Hydrocarbons, C6-12, benzene-recovery Low Benzene Naphthas Category substances arise from

HPV CHEMICAL CATEGORY SUMMARY (DRAFT): LOW BENZENE NAPHTHAS

	<p>production processes associated with ethylene manufacturing. The 10 CAS numbers are used to describe the nine process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry. Aromatics represent the major constituents in all of the streams, varying from approximately 45 to 95 percent. The benzene content is usually less than five percent.</p> <p>More information on the Low 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"> 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
<p>Conclusion:</p>	<p><u>Summary</u></p> <p>In the environment, hydrolysis will not contribute to the degradation of constituent chemicals in the Low Benzene Naphthas Category. The Low Benzene Naphthas Category includes nine process streams:</p> <ul style="list-style-type: none"> • Pyrolysis C7s Fraction • Pyrolysis C7-C12 Fraction • Pyrolysis C7-C8 Fraction • C9+ From Xylene Unit • Hydrotreated C8-C10 Fraction • Hydrotreated C7-C12 Fraction • Hydrotreated C7+ Fraction • Hydrotreated C5/C9 blend • Toluene Extract <p>Ten CAS numbers (see <u>Test Substance</u>) identify products derived from these process streams. As discussed below, the chemicals in these streams are composed of carbon and hydrogen and are not amenable to hydrolysis because of their molecular structure and the chemical reaction required for this type of transformation to occur.</p> <p><u>The Low Benzene Naphthas Category</u></p> <p>A process stream is a mixture of chemicals that arises from a chemical reaction or separation activity. The category includes hydrocarbon product streams associated with the ethylene industry. Aromatics represent the major constituents in all of the streams, varying from approximately 45 to 95 percent. The benzene content is usually less than five percent. This grouping of CAS numbers represents hydrocarbon streams with a carbon number distribution that is predominantly C5-C12. That is why this group is considered a category for purposes of the High</p>

	<p>Production Volume (HPV) Chemical Program, and designated <u>Low Benzene Naphthas</u>.</p> <p>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).</p> <p>More information on the Low Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). The plan is available on the U.S. Environmental Protection Agency website under the HPV Chemical Program. A brief description of the production and composition of the nine process streams in this category are:</p> <ul style="list-style-type: none"> • Pyrolysis Fractions (C7s, C7-C12, and C7-C8 Fractions) are separated by distillation into various boiling-point range fractions as intermediates in preparation for further processing. Many carbon number distribution fractions are technically feasible. The compositions of these fractions vary depending on the ethylene process feedstock, the cracking furnaces operating conditions and the ethylene process configuration. <ol style="list-style-type: none"> 1. Pyrolysis C7s Fraction has a carbon number distribution that is 75% toluene with the balance primarily C7 non-aromatics, largely unsaturates. The stream may contain low levels of benzene. 2. Pyrolysis C7-C12 Fraction has a typical composition including about 2% benzene, 23% toluene, 28% C8 aromatics and 8% naphthalene, with the balance expected to be largely unsaturated hydrocarbons and other aromatics. 3. Pyrolysis C7-C8 Fraction has a carbon number distribution that is predominantly C7 to C8. The reported compositions range from 45 to 80% with 11 to 78% C8 aromatics. The typical benzene concentration reported is 2% with a maximum of 5%. <ul style="list-style-type: none"> • C9+ from Xylene Unit is a co-product from process units that produce o- or p-xylene. The carbon distribution for the stream is C8+ with some hydrocarbon compounds having a boiling point of 650°F or higher. The stream is predominantly aromatics. • Hydrotreated Pyrolysis Fractions (C8-C10, C7-C12, C7+ Fractions, and C5/C9 Blend) are pyrolysis gasoline or distillate fractions of pyrolysis gasoline that are treated with hydrogen over catalyst. The hydrogenation process may
--	---

	<p>be either one-stage or two-stage. The one-stage process is typically a liquid-phase process where the primary objective is to selectively convert diolefins to mono-olefins and to convert vinyl aromatics, for example, styrene to ethylbenzene. The second stage in a two-stage hydrogenation process is typically a vapor-phase, more severe hydrogenation that converts essentially all of the contained mono- and diolefins to paraffins. A pygas fraction that will be processed by extraction or extractive distillation to produce high purity aromatics (toluene or xylenes in this case) is subjected to two-stage hydrogenation. Pygas fractions may be forwarded to hydrodealkylation units (less common) for benzene production after one-stage of hydrogenation. Pygas fractions intended for use as a gasoline blending stock are frequently subject to only one-stage hydrogenation. The streams may result from fractionation of hydrotreated pyrolysis gasoline or from hydrotreating pyrolysis gasoline fractions followed by distillation. Reformate fractions from petroleum refineries are sometimes mixed with these pyrolysis fractions.</p> <ol style="list-style-type: none"> 1. Hydrotreated C8-C10 Fraction has a carbon number distribution of C6 to C12, but is predominantly C8 to C10. Typical concentration includes 0.3% benzene, 2.4% toluene, 24% C8 aromatics with the balance primarily C9 and C10 aromatics and lesser amounts of paraffins, isoparaffins and naphthenes in this carbon range. 2. Hydrotreated C7-C12 Fraction is a distillate fraction of hydrogenated pygas with a carbon number distribution that is predominantly C7-C12, with lesser amounts of C6. Typical reported values indicate 1% benzene, 23% toluene, 25% C8 aromatics, with the balance primarily other aromatics and lesser amounts of monoolefins and paraffins. 3. Hydrotreated C7+ Fraction is derived as distillation residue after removing the C5 and C6 fractions from a hydrogenated pygas stream (alternately the stream could be hydrotreated after distillation). The carbon number distribution is predominantly greater than C6, although the reported analysis does not report compounds greater than C12. Typical reported values include 23% toluene, 32% C8 aromatics, 1% naphthalene, with the balance primarily other aromatics and lesser amounts of paraffins. 4. Hydrotreated C5/C9 Blend is produced by blending C5 and C9 pyrolysis fractions, hydrogenated either before or after blending. Typical reported values includes approximately 2% benzene, 40% C5's in the blend, 9% C8 aromatics, 19% C9 aromatics, and 25% C10+. <ul style="list-style-type: none"> • Toluene Extract is produced as a co-product of a benzene
--	--

	<p>extraction unit. The stream may contain significant concentrations of xylenes.</p>
	<p><u>Hydrolysis of Hydrocarbons as a Function of Molecular Structure</u></p> <p>Hydrolysis of an organic molecule occurs when a molecule (R-X) reacts with water (H₂O) 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.</p> <p>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.</p> <p>Under strongly acidic conditions the carbon-carbon double bond found in alkenes, such as those in the Low Benzene Naphthas Category, will react with water by an addition reaction mechanism (2). The reaction product is an alcohol. This reaction is not considered to be hydrolysis because the carbon-carbon linkage is not cleaved and because the reaction is freely reversible (3). Substances that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (4).</p> <p>The substances in the Low Benzene Naphthas Category are primarily olefins that contain at least one double bond (alkenes). The remaining chemicals are saturated hydrocarbons (alkanes). These two groups of chemicals contain only carbon and hydrogen. As such, their molecular structure is not subject to the hydrolytic mechanism discussed above. Therefore, chemicals in the Low Benzene Naphthas Category have a very low potential to hydrolyze, and this degradative process will not contribute to their removal in the environment.</p> <p><u>References</u></p> <ol style="list-style-type: none"> 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA. 2. Gould, E.S. (1959), Mechanism and Structure in Organic Chemistry, Holt, Reinhart and Winston, New York, NY, USA. 3. Harris, J.C. (1982), "Rate of Hydrolysis," Chapter 7 in: W.J.

HPV CHEMICAL CATEGORY SUMMARY (DRAFT): LOW BENZENE NAPHTHAS

	<p>Lyman, W.F. Reehl, and D.H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, NY, USA.</p> <p>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.</p>
Reliability:	These data represent a key study for characterizing the potential of substances in the Low Benzene Naphthas Category to undergo hydrolysis.
Reference:	American Chemistry Council, Olefins Panel. 2003. Hydrolysis Low Benzene Naphthas Category. Rosslyn, VA, USA.
Other (source):	American Chemistry Council, Olefins Panel (Prepared 7/03)

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

LOW BENZENE NAPHTHAS ROBUST SUMMARY

Partition Coefficient

Test Substance*:	Other TS [CAS # 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3]
Method/Guideline:	Calculated values using KOWWIN version 1.65, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: <ul style="list-style-type: none"> Note: Concentration prep., vessel type, replication, test conditions. 	Octanol / Water Partition Coefficient is calculated by the KOWWIN subroutine, which is based on an atom/fragment contribution method of W. Meylan and P. Howard in "Atom/fragment contribution method for estimating octanol-water partition coefficients". 1995. <i>J. Pharm. Sci.</i> 84:83-92.
Results: Units/Value: <ul style="list-style-type: none"> Note: Deviations from protocol or guideline, analytical method. 	<p>Calculated and measured log K_{ow} data for representative constituents of the Low Benzene Naphthas Category are listed below. The data identify a potential log K_{ow} range for substances represented by the 10 CAS numbers under <u>Test Substance</u>. Substances in this category do not have a specific log K_{ow} value. Actual log K_{ow} ranges for substances in this category will vary dependent on their constituent composition.</p> <p>Commercial substances in this category consist of complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C12. The seven chemicals selected to represent the log K_{ow} range of this category are C5-C11 hydrocarbons that can be found in substances identified by the 10 CAS numbers listed under <u>Test Substance</u>. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.</p>

HPV CHEMICAL CATEGORY SUMMARY (DRAFT): LOW BENZENE NAPHTHAS

<p>Results: (continued)</p> <p>Units/Value:</p> <p>Note: Deviations from protocol or guideline, analytical method.</p>	<table border="1"> <thead> <tr> <th>Substance Constituent</th> <th>Calculated log K_{ow} @ 25°C</th> <th>Measured* log K_{ow} @ 25°C</th> </tr> </thead> <tbody> <tr> <td>isopentane</td> <td>2.72</td> <td>na</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>naphthalene</td> <td>3.17</td> <td>3.30</td> </tr> <tr> <td>tricyclodecane</td> <td>3.59</td> <td>na</td> </tr> <tr> <td>methylnaphthalene</td> <td>3.72</td> <td>3.86</td> </tr> </tbody> </table> <p>* Experimental values from EPIWIN database. na = not available The data represent a potential log K_{ow} range for substances represented by the 10 CAS numbers under Test Substance.</p>	Substance Constituent	Calculated log K _{ow} @ 25°C	Measured* log K _{ow} @ 25°C	isopentane	2.72	na	toluene	2.54	2.73	m-xylene	3.09	3.20	styrene	2.89	2.95	naphthalene	3.17	3.30	tricyclodecane	3.59	na	methylnaphthalene	3.72	3.86
Substance Constituent	Calculated log K _{ow} @ 25°C	Measured* log K _{ow} @ 25°C																							
isopentane	2.72	na																							
toluene	2.54	2.73																							
m-xylene	3.09	3.20																							
styrene	2.89	2.95																							
naphthalene	3.17	3.30																							
tricyclodecane	3.59	na																							
methylnaphthalene	3.72	3.86																							
<p>Test Substance:</p>	<p>The Low Benzene Naphthas Category includes the following CAS numbers:</p> <p>64741-98-6 Extract, petroleum, heavy naphtha solvent 64742-48-9 Naphtha, petroleum, hydrotreated heavy 64742-49-0 Naphtha, petroleum, hydrotreated light 64742-83-2 Naphtha, petroleum, light steam-cracked 68333-88-0 Aromatic hydrocarbons, C9-C17 68476-45-9 Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product 68478-10-4 Naphtha, petroleum, light steam-cracked, debezenized, C8-16-cycloalkadiene concentrate 68516-20-1 Naphtha, petroleum, steam-cracked middle aromatic 68527-23-1 Naphtha, petroleum, light steam-cracked aromatic 68919-15-3 Hydrocarbons, C6-12, benzene-recovery</p> <p>Low Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 10 CAS numbers are used to describe the nine process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry. Aromatics represent the major constituents in all of the streams, varying from approximately 45 to 95 percent. The benzene content is usually less than five percent.</p> <p>More information on the Low 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 Low Benzene Naphthas</p>																								

HPV CHEMICAL CATEGORY SUMMARY (DRAFT): LOW BENZENE NAPHTHAS

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

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

LOW BENZENE NAPHTHAS ROBUST SUMMARY

Photodegradation (Direct)

Test Substance*:	Other TS [CAS # 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3]
Method/Guideline:	Other: Technical discussion
Year (guideline):	Not applicable
GLP (Y/N):	Not applicable
Year (study performed):	Not applicable
Type (air, soil, water, other):	Water
Light Source:	Not applicable
Light Spectrum: • Wave length value (upper/lower)	Not applicable
Relative Intensity:	Not applicable
Test Substance Spectrum:	Not applicable
Test Conditions: • Note: Concentration, temperature, test system type, replication, deviations from guideline or protocol	Not applicable
Direct Photolysis**: • Results: half-life, % degradation, quantum yield	<p><u>Summary</u></p> <p>In the environment, direct photolysis will not significantly contribute to the degradation of constituent chemicals in the Low Benzene Naphthas Category. The Low Benzene Naphthas Category includes nine process streams:</p> <ul style="list-style-type: none"> • Pyrolysis C7s Fraction • Pyrolysis C7-C12 Fraction • Pyrolysis C7-C8 Fraction • C9+ From Xylene Unit • Hydrotreated C8-C10 Fraction • Hydrotreated C7-C12 Fraction • Hydrotreated C7+ Fraction • Hydrotreated C5/C9 blend • Toluene Extract

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

The Low Benzene Naphthas Category

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

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

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

- **Pyrolysis Fractions (C7s, C7-C12, and C7-C8 Fractions)** are separated by distillation into various boiling-point range fractions as intermediates in preparation for further processing. Many carbon number distribution fractions are technically feasible. The compositions of these fractions vary depending on the ethylene process feedstock, the cracking furnaces operating conditions and the ethylene process configuration.
4. **Pyrolysis C7s Fraction** has a carbon number distribution that is 75% toluene with the balance primarily C7 non-aromatics, largely unsaturates. The stream may contain low levels of benzene.
 5. **Pyrolysis C7-C12 Fraction** has a typical composition

	<p>including about 2% benzene, 23% toluene, 28% C8 aromatics and 8% naphthalene, with the balance expected to be largely unsaturated hydrocarbons and other aromatics.</p> <p>6. Pyrolysis C7-C8 Fraction has a carbon number distribution that is predominantly C7 to C8. The reported compositions range from 45 to 80% with 11 to 78% C8 aromatics. The typical benzene concentration reported is 2% with a maximum of 5%.</p> <ul style="list-style-type: none"> • C9+ from Xylene Unit is a co-product from process units that produce o- or p-xylene. The carbon distribution for the stream is C8+ with some hydrocarbon compounds having a boiling point of 650°F or higher. The stream is predominantly aromatics. • Hydrotreated Pyrolysis Fractions (C8-C10, C7-C12, C7+ Fractions, and C5/C9 Blend) are pyrolysis gasoline or distillate fractions of pyrolysis gasoline that are treated with hydrogen over catalyst. The hydrogenation process may be either one-stage or two-stage. The one-stage process is typically a liquid-phase process where the primary objective is to selectively convert diolefins to mono-olefins and to convert vinyl aromatics, for example, styrene to ethylbenzene. The second stage in a two-stage hydrogenation process is typically a vapor-phase, more severe hydrogenation that converts essentially all of the contained mono- and diolefins to paraffins. A pygas fraction that will be processed by extraction or extractive distillation to produce high purity aromatics (toluene or xylenes in this case) is subjected to two-stage hydrogenation. Pygas fractions may be forwarded to hydrodealkylation units (less common) for benzene production after one-stage of hydrogenation. Pygas fractions intended for use as a gasoline blending stock are frequently subject to only one-stage hydrogenation. The streams may result from fractionation of hydrotreated pyrolysis gasoline or from hydrotreating pyrolysis gasoline fractions followed by distillation. Reformate fractions from petroleum refineries are sometimes mixed with these pyrolysis fractions. <p>5. Hydrotreated C8-C10 Fraction has a carbon number distribution of C6 to C12, but is predominantly C8 to C10. Typical concentration includes 0.3% benzene, 2.4% toluene, 24% C8 aromatics with the balance primarily C9 and C10 aromatics and lesser amounts of paraffins, isoparaffins and naphthenes in this carbon range.</p> <p>6. Hydrotreated C7-C12 Fraction is a distillate fraction of hydrogenated pygas with a carbon number distribution that is predominantly C7-C12, with lesser amounts of C6. Typical reported values indicate 1% benzene, 23% toluene, 25% C8 aromatics, with the balance primarily other aromatics and</p>
--	---

lesser amounts of monoolefins and paraffins.

7. **Hydrotreated C7+ Fraction** is derived as distillation residue after removing the C5 and C6 fractions from a hydrogenated pygas stream (alternately the stream could be hydrotreated after distillation). The carbon number distribution is predominantly greater than C6, although the reported analysis does not report compounds greater than C12. Typical reported values include 23% toluene, 32% C8 aromatics, 1% naphthalene, with the balance primarily other aromatics and lesser amounts of paraffins.
 8. **Hydrotreated C5/C9 Blend** is produced by blending C5 and C9 pyrolysis fractions, hydrogenated either before or after blending. Typical reported values includes approximately 2% benzene, 40% C5's in the blend, 9% C8 aromatics, 19% C9 aromatics, and 25% C10+.
- **Toluene Extract** is produced as a co-product of a benzene extraction unit. The stream may contain significant concentrations of xylenes.

Photolysis of Hydrocarbons

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

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

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

A conservative approach to estimating a photochemical degradation rate is to assume that degradation will occur in proportion to the amount of light wavelengths >290 nm absorbed

HPV CHEMICAL CATEGORY SUMMARY (DRAFT): LOW BENZENE NAPHTHAS

	<p>by the molecule (3). Saturated hydrocarbons do not absorb light above 200 nm. Some characteristic absorbance maxima (λ_{\max}) and associated molar absorptivities (ϵ) for selected unsaturated hydrocarbons are shown below (2):</p>																																					
	<table border="1" data-bbox="586 373 1438 667"> <thead> <tr> <th rowspan="2">Hydrocarbon</th> <th colspan="2">λ below 290 nm</th> <th colspan="2">λ above 290 nm</th> </tr> <tr> <th>λ_{\max}</th> <th>ϵ</th> <th>λ_{\max}</th> <th>ϵ</th> </tr> </thead> <tbody> <tr> <td>Ethylene</td> <td>193</td> <td>10,000</td> <td>-</td> <td>-</td> </tr> <tr> <td>Benzene</td> <td>255</td> <td>215</td> <td>-</td> <td>-</td> </tr> <tr> <td rowspan="2">Styrene</td> <td>244</td> <td>12,000</td> <td>-</td> <td>-</td> </tr> <tr> <td>282</td> <td>450</td> <td></td> <td></td> </tr> <tr> <td rowspan="2">Naphthalene</td> <td>221</td> <td>100,000</td> <td>311</td> <td>250</td> </tr> <tr> <td>270</td> <td>5,000</td> <td></td> <td></td> </tr> </tbody> </table> <p>Olefins with one double bond, or two conjugated double bonds, which constitute the majority of the chemicals in the Low Benzene Naphthas category, do not absorb appreciable light energy above 290 nm. The absorption of UV light to cause cis-trans isomerism about the double bond of an olefin occurs only if it is in conjugation with an aromatic ring (2).</p> <p>Products in the Low Benzene Naphthas Category do not contain component molecules that will undergo direct photolysis. Therefore, this fate process will not contribute to a measurable degradative removal of chemical components in this category from the environment.</p> <p>References</p> <ol style="list-style-type: none"> Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA. 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. Zepp, R. G. and D. M. Cline. 1977. Rates of Direct Photolysis in the Aqueous Environment, Environ. Sci. Technol., 11:359-366. 	Hydrocarbon	λ below 290 nm		λ above 290 nm		λ_{\max}	ϵ	λ_{\max}	ϵ	Ethylene	193	10,000	-	-	Benzene	255	215	-	-	Styrene	244	12,000	-	-	282	450			Naphthalene	221	100,000	311	250	270	5,000		
Hydrocarbon	λ below 290 nm		λ above 290 nm																																			
	λ_{\max}	ϵ	λ_{\max}	ϵ																																		
Ethylene	193	10,000	-	-																																		
Benzene	255	215	-	-																																		
Styrene	244	12,000	-	-																																		
	282	450																																				
Naphthalene	221	100,000	311	250																																		
	270	5,000																																				
<p>Indirect Photolysis**:</p> <ul style="list-style-type: none"> Results: type of sensitizer, concentration of sensitizer, rate constant, % degradation, half-life 	<p>Not applicable</p>																																					

HPV CHEMICAL CATEGORY SUMMARY (DRAFT): LOW BENZENE NAPHTHAS

<p>Degradation Products**:</p> <ul style="list-style-type: none"> Note: Identification, concentration 	<p>Unknown</p>
<p>Test Substance:</p>	<p>The Low Benzene Naphthas Category includes the following CAS numbers:</p> <p>64741-98-6 Extract, petroleum, heavy naphtha solvent 64742-48-9 Naphtha, petroleum, hydrotreated heavy 64742-49-0 Naphtha, petroleum, hydrotreated light 64742-83-2 Naphtha, petroleum, light steam-cracked 68333-88-0 Aromatic hydrocarbons, C9-C17 68476-45-9 Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product 68478-10-4 Naphtha, petroleum, light steam-cracked, debezenized, C8-16-cycloalkadiene concentrate 68516-20-1 Naphtha, petroleum, steam-cracked middle aromatic 68527-23-1 Naphtha, petroleum, light steam-cracked aromatic 68919-15-3 Hydrocarbons, C6-12, benzene-recovery</p>
<p>Conclusion:</p>	<p>Not applicable</p>
<p>Reliability:</p>	<p>These data represent a key study for characterizing the potential of substances in the Low Benzene Naphthas Category to undergo direct photodegradation.</p>
<p>Reference:</p>	<p>American Chemistry Council, Olefins Panel. 2003. Photodegradation (Direct): Low Benzene Naphthas Category. Rosslyn, VA, USA.</p>
<p>Other (source):</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.

LOW BENZENE NAPHTHAS ROBUST SUMMARY

Photodegradation (Indirect)

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

<p>Indirect Photolysis**:</p> <ul style="list-style-type: none"> • Results: type of sensitizer, concentration of sensitizer, rate constant, % degradation, half-life 	<p><u>The Low Benzene Naphthas Category</u></p> <p>Low Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 10 CAS numbers are used to describe nine process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry. Aromatics represent the major constituents in all of the streams, varying from approximately 45 to 95 percent. The benzene content is usually less than five percent.</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>Low Benzene Naphthas</u>.</p> <p>The seven chemicals selected to represent the atmospheric oxidation potential of this category are C5-C11 hydrocarbons that can be found in substances identified by the 10 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.</p> <p><u>Atmospheric Oxidation of Hydrocarbons</u></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>
---	--

HPV CHEMICAL CATEGORY SUMMARY (DRAFT): LOW BENZENE NAPHTHAS

<p>Indirect Photolysis**: (cont'd)</p> <p>Results: type of sensitizer, concentration of sensitizer, rate constant, % degradation, half-life</p>	<table border="1"> <thead> <tr> <th><u>Chemical</u></th> <th><u>Calculated* half-life (hrs)</u></th> <th><u>OH- Rate Constant (cm³/molecule-sec)</u></th> </tr> </thead> <tbody> <tr> <td>isopentane</td> <td>31.8</td> <td>4.0 E⁻¹²</td> </tr> <tr> <td>toluene</td> <td>24.6</td> <td>5.2 E⁻¹²</td> </tr> <tr> <td>m-xylene</td> <td>9.5</td> <td>13.6 E⁻¹²</td> </tr> <tr> <td>styrene</td> <td>4.6</td> <td>28.1 E⁻¹²</td> </tr> <tr> <td>naphthalene</td> <td>5.9</td> <td>21.6 E⁻¹²</td> </tr> <tr> <td>tricyclodecane</td> <td>5.6</td> <td>22.9 E⁻¹²</td> </tr> <tr> <td>methylnaphthalene</td> <td>2.3</td> <td>56.5 E⁻¹²</td> </tr> </tbody> </table> <p>* Atmospheric half-life values are based on a 12-hr day.</p> <p>More information on the Low Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (Olefins Panel, 2001).</p> <p><u>References:</u></p> <ol style="list-style-type: none"> 1. Atkinson, R. 1988. Estimation of gas-phase hydroxyl radical rate constants for organic chemicals. <i>Environ. Toxicol. Chem.</i> 7:435-442. 2. Atkinson, R. 1989. Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds. J. Phys. Chem. Ref. Data Monograph No. 1, Amer. Inst. Physics & Amer. Chem. Soc., NY. 3. Meylan, W.M. and P.H. Howard. 1993. Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. <i>Chemosphere</i> 12:2293-2299. 4. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA. 	<u>Chemical</u>	<u>Calculated* half-life (hrs)</u>	<u>OH- Rate Constant (cm³/molecule-sec)</u>	isopentane	31.8	4.0 E ⁻¹²	toluene	24.6	5.2 E ⁻¹²	m-xylene	9.5	13.6 E ⁻¹²	styrene	4.6	28.1 E ⁻¹²	naphthalene	5.9	21.6 E ⁻¹²	tricyclodecane	5.6	22.9 E ⁻¹²	methylnaphthalene	2.3	56.5 E ⁻¹²
<u>Chemical</u>	<u>Calculated* half-life (hrs)</u>	<u>OH- Rate Constant (cm³/molecule-sec)</u>																							
isopentane	31.8	4.0 E ⁻¹²																							
toluene	24.6	5.2 E ⁻¹²																							
m-xylene	9.5	13.6 E ⁻¹²																							
styrene	4.6	28.1 E ⁻¹²																							
naphthalene	5.9	21.6 E ⁻¹²																							
tricyclodecane	5.6	22.9 E ⁻¹²																							
methylnaphthalene	2.3	56.5 E ⁻¹²																							
<p>Degradation Products**:</p> <ul style="list-style-type: none"> • Note: Identification, concentration 	<p>Unknown</p>																								
<p>Test Substance:</p>	<p>The Low Benzene Naphthas Category includes the following CAS numbers:</p> <p>64741-98-6 Extract, petroleum, heavy naphtha solvent 64742-48-9 Naphtha, petroleum, hydrotreated heavy 64742-49-0 Naphtha, petroleum, hydrotreated light 64742-83-2 Naphtha, petroleum, light steam-cracked 68333-88-0 Aromatic hydrocarbons, C9-C17 68476-45-9 Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product 68478-10-4 Naphtha, petroleum, light steam-cracked,</p>																								

HPV CHEMICAL CATEGORY SUMMARY (DRAFT): LOW BENZENE NAPHTHAS

	<p>debezenized, C8-16-cycloalkadiene concentrate</p> <p>68516-20-1 Naphtha, petroleum, steam-cracked middle aromatic</p> <p>68527-23-1 Naphtha, petroleum, light steam-cracked aromatic</p> <p>68919-15-3 Hydrocarbons, C6-12, benzene-recovery</p>
Conclusion:	<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 2.3 to 31.8 hours as a result of indirect photolysis by hydroxyl radical attack.</p>
Reliability:	<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 10 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 Low Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for atmospheric half-life range based on constituent data.</p>
Reference:	<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>
Other (source):	<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 freetext

LOW BENZENE NAPHTHAS ROBUST SUMMARY

Transport / Distribution (Fugacity)

Test Substance*:	Other TS [CAS # 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3]
Method/Guideline:	Calculated according to Mackay Level I, EQC Model version 1.01
Year (guideline):	1997
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: <ul style="list-style-type: none"> Note: Concentration prep., vessel type, replication, test conditions. 	<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>

HPV CHEMICAL CATEGORY SUMMARY (DRAFT): LOW BENZENE NAPHTHAS

<p>Results:</p> <p>Units/Value:</p> <ul style="list-style-type: none"> Note: Deviations from protocol or guideline, analytical method. 	<p>Calculated partitioning data for representative constituents of the Low Benzene Naphthas Category are listed below. The data identify a potential distribution for substances represented by the 10 CAS numbers under <u>Test Substance</u>. Actual distribution of substances in this category will vary dependent on their constituent composition.</p> <p>Commercial substances in this category consist of complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C12. The seven chemicals selected to represent the environmental distribution range of this category are C5-C11 hydrocarbons that can be found in substances identified by the 10 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.</p> <p>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.</p> <p>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:</p> <table border="1" data-bbox="625 1108 1323 1480"> <thead> <tr> <th rowspan="2"><u>Chemical</u></th> <th colspan="4"><u>Calculated*</u> <u>Percent Distribution</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>isopentane</td> <td>99.98</td> <td>0.01</td> <td>0.01</td> <td>-</td> </tr> <tr> <td>toluene</td> <td>98.17</td> <td>1.40</td> <td>0.43</td> <td>-</td> </tr> <tr> <td>m-xylene</td> <td>97.19</td> <td>1.33</td> <td>1.45</td> <td>0.03</td> </tr> <tr> <td>styrene</td> <td>95.55</td> <td>2.61</td> <td>1.80</td> <td>0.04</td> </tr> <tr> <td>naphthalene</td> <td>24.47</td> <td>32.28</td> <td>42.28</td> <td>0.94</td> </tr> <tr> <td>tricyclodecane</td> <td>98.68</td> <td>0.29</td> <td>1.01</td> <td>0.02</td> </tr> <tr> <td>methylnaphthalene</td> <td>97.68</td> <td>0.40</td> <td>1.88</td> <td>0.04</td> </tr> </tbody> </table> <p>* Distribution values determined using calculated input data from EPIWIN program</p>	<u>Chemical</u>	<u>Calculated*</u> <u>Percent Distribution</u>				<u>Air</u>	<u>Water</u>	<u>Soil</u>	<u>Sediment</u>	isopentane	99.98	0.01	0.01	-	toluene	98.17	1.40	0.43	-	m-xylene	97.19	1.33	1.45	0.03	styrene	95.55	2.61	1.80	0.04	naphthalene	24.47	32.28	42.28	0.94	tricyclodecane	98.68	0.29	1.01	0.02	methylnaphthalene	97.68	0.40	1.88	0.04
<u>Chemical</u>	<u>Calculated*</u> <u>Percent Distribution</u>																																												
	<u>Air</u>	<u>Water</u>	<u>Soil</u>	<u>Sediment</u>																																									
isopentane	99.98	0.01	0.01	-																																									
toluene	98.17	1.40	0.43	-																																									
m-xylene	97.19	1.33	1.45	0.03																																									
styrene	95.55	2.61	1.80	0.04																																									
naphthalene	24.47	32.28	42.28	0.94																																									
tricyclodecane	98.68	0.29	1.01	0.02																																									
methylnaphthalene	97.68	0.40	1.88	0.04																																									

HPV CHEMICAL CATEGORY SUMMARY (DRAFT): LOW BENZENE NAPHTHAS

<p>Results: (cont'd)</p> <p>Units/Value:</p> <ul style="list-style-type: none"> Note: Deviations from protocol or guideline, analytical method. 	<p style="text-align: center;">Measured**</p> <p style="text-align: center;"><u>Percent Distribution</u></p> <table border="1"> <thead> <tr> <th><u>Chemical</u></th> <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>Isopentane</td> <td>99.98</td> <td>0.01</td> <td>0.01</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>naphthalene</td> <td>42.27</td> <td>20.56</td> <td>36.33</td> <td>0.81</td> </tr> <tr> <td>tricyclodecane</td> <td>na</td> <td>na</td> <td>na</td> <td>na</td> </tr> <tr> <td>methylnaphthalene</td> <td>98.53</td> <td>0.19</td> <td>1.25</td> <td>0.03</td> </tr> </tbody> </table> <p>** Distribution values determined using measured input data from the EPIWIN program experimental database. na = not available</p>	<u>Chemical</u>	<u>Air</u>	<u>Water</u>	<u>Soil</u>	<u>Sediment</u>	Isopentane	99.98	0.01	0.01	-	toluene	98.80	0.81	0.39	-	m-xylene	97.91	0.86	1.20	0.03	styrene	96.65	1.85	1.46	0.04	naphthalene	42.27	20.56	36.33	0.81	tricyclodecane	na	na	na	na	methylnaphthalene	98.53	0.19	1.25	0.03
<u>Chemical</u>	<u>Air</u>	<u>Water</u>	<u>Soil</u>	<u>Sediment</u>																																					
Isopentane	99.98	0.01	0.01	-																																					
toluene	98.80	0.81	0.39	-																																					
m-xylene	97.91	0.86	1.20	0.03																																					
styrene	96.65	1.85	1.46	0.04																																					
naphthalene	42.27	20.56	36.33	0.81																																					
tricyclodecane	na	na	na	na																																					
methylnaphthalene	98.53	0.19	1.25	0.03																																					
<p>Test Substance:</p>	<p>The Low Benzene Naphthas Category includes the following CAS numbers:</p> <p>64741-98-6 Extract, petroleum, heavy naphtha solvent 64742-48-9 Naphtha, petroleum, hydrotreated heavy 64742-49-0 Naphtha, petroleum, hydrotreated light 64742-83-2 Naphtha, petroleum, light steam-cracked 68333-88-0 Aromatic hydrocarbons, C9-C17 68476-45-9 Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product 68478-10-4 Naphtha, petroleum, light steam-cracked, debezenized, C8-16-cycloalkadiene concentrate 68516-20-1 Naphtha, petroleum, steam-cracked middle aromatic 68527-23-1 Naphtha, petroleum, light steam-cracked aromatic 68919-15-3 Hydrocarbons, C6-12, benzene-recovery</p> <p>Low Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 10 CAS numbers are used to describe the nine process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry. Aromatics represent the major constituents in all of the streams, varying from approximately 45 to 95 percent. The benzene content is usually less than five percent.</p> <p>More information on the Low 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 Low Benzene Naphthas Category. American Chemistry Council, Olefins Panel,</p>																																								

HPV CHEMICAL CATEGORY SUMMARY (DRAFT): LOW BENZENE NAPHTHAS

HPV Implementation Task Group. VA, USA.	
Conclusion:	<p>The partitioning data represent a potential distribution range for substances in the 10 CAS numbers listed under <u>Test Substance</u>. Substances in the Low Benzene Naphthas Category are calculated to partition primarily to air with a negligible percentage partitioning to water, soil, and sediment. Relatively high vapor pressure and high water solubility largely control the partitioning behavior of constituent chemicals in substances from this category.</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>
Reliability:	<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 10 CAS numbers listed under <u>Test Substance</u>. This robust summary has a reliability rating of 2 because the data are not for specific substances in the Low Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for distribution range based on constituent data.</p>
Reference:	<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>
Other (source):	<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.

LOW BENZENE NAPHTHAS ROBUST SUMMARY

Water Solubility

Test Substance*:	Other TS [CAS # 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3]
Method/Guideline:	Calculated values using WSKOWWIN version 1.36, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions:	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.
Results: Units/Value: <ul style="list-style-type: none"> Note: Concentration prep., vessel type, replication, test conditions. Note: Deviations from protocol or guideline, analytical method. 	<p>Calculated and measured water solubility data for representative constituents of the Low Benzene Naphthas Category are listed below. The data identify a potential water solubility range for substances represented by the 10 CAS numbers under <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).</p> <p>Commercial substances in this category consist of complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C12. The seven chemicals selected to represent the water solubility range of this category are C5-C11 hydrocarbons that can be found in substances identified by the 10 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.</p>

HPV CHEMICAL CATEGORY SUMMARY (DRAFT): LOW BENZENE NAPHTHAS

<p>Results: (continued)</p> <p>Units/Value:</p> <p>Note: Deviations from protocol or guideline, analytical method.</p>	<table border="1"> <thead> <tr> <th>Substance Constituent</th> <th>Calculated WS (mg/L @ 25°C)</th> <th>Measured WS* (mg/L @ 25°C)</th> </tr> </thead> <tbody> <tr> <td>isopentane</td> <td>184.6</td> <td>na</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>naphthalene</td> <td>183.8</td> <td>142.1</td> </tr> <tr> <td>tricyclodecane</td> <td>21.5</td> <td>na</td> </tr> <tr> <td>methylnaphthalene</td> <td>54.6</td> <td>41.4</td> </tr> </tbody> </table> <p>* Experimental values from EPIWIN database. na = not available The data represent a potential water solubility range for substances represented by the 10 CAS numbers under <u>Test Substance</u>.</p>	Substance Constituent	Calculated WS (mg/L @ 25°C)	Measured WS* (mg/L @ 25°C)	isopentane	184.6	na	toluene	832.7	573.1	m-xylene	258.4	207.2	styrene	386.7	343.7	naphthalene	183.8	142.1	tricyclodecane	21.5	na	methylnaphthalene	54.6	41.4
Substance Constituent	Calculated WS (mg/L @ 25°C)	Measured WS* (mg/L @ 25°C)																							
isopentane	184.6	na																							
toluene	832.7	573.1																							
m-xylene	258.4	207.2																							
styrene	386.7	343.7																							
naphthalene	183.8	142.1																							
tricyclodecane	21.5	na																							
methylnaphthalene	54.6	41.4																							
<p>Test Substance:</p>	<p>The Low Benzene Naphthas Category includes the following CAS numbers:</p> <p>64741-98-6 Extract, petroleum, heavy naphtha solvent 64742-48-9 Naphtha, petroleum, hydrotreated heavy 64742-49-0 Naphtha, petroleum, hydrotreated light 64742-83-2 Naphtha, petroleum, light steam-cracked 68333-88-0 Aromatic hydrocarbons, C9-C17 68476-45-9 Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product 68478-10-4 Naphtha, petroleum, light steam-cracked, debezenized, C8-16-cycloalkadiene concentrate 68516-20-1 Naphtha, petroleum, steam-cracked middle aromatic 68527-23-1 Naphtha, petroleum, light steam-cracked aromatic 68919-15-3 Hydrocarbons, C6-12, benzene-recovery</p> <p>Low Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 10 CAS numbers are used to describe the nine process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry. Aromatics represent the major constituents in all of the streams, varying from approximately 45 to 95 percent. The benzene content is usually less than five percent.</p> <p>More information on the Low 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</p>																								

HPV CHEMICAL CATEGORY SUMMARY (DRAFT): LOW BENZENE NAPHTHAS

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

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

201-15522B₂

Attachment 2b

Robust Summaries

Heavy Aromatic Distillate, CAS# 64742-48-9

Mammalian Toxicity

04 AUG 2010 11:16

00000000

Robust Summary - Group 6: Low Benzene Naphthas

Acute Toxicity

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

Robust Summary – Group 6: Low Benzene Naphthas**Acute Toxicity**

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

Robust Summary - Group 6: Low Benzene Naphthas

Genetic Toxicity - in Vitro

<p><u>Test Substance</u> <i>Test substance</i></p>	<p>Heavy Aromatic Distillate, Gulf. CAS #64742-48-9. Water-white liquid with characteristic aromatic odor. Composition analysis, purity and stability referred to sponsor.</p>
<p><u>Method</u> 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 based on Hsie et al. (1981), O'Neill & Hsie (1979) In vitro mammalian cell forward mutation Chinese hamster ovary (CHO) cell culture Yes 1984 CHO-K-1 heterozygous for hypoxanthine-guanine phosphoribosyl transferase (HGPRT+/-) from Oak Ridge National Laboratory, TN. Yes Rat liver (S9) fraction purchased from Litton Bionetics, Kensington, MD 1.0mg S9 fraction/ml treatment medium (0.3ml S9 fraction in 3 ml medium/flask) Aroclor 1254 induced (treatment not specified) Cytotoxicity, final conc. (trial 2): 128, 256, 512, 1024µg/ml ± S9; Mutagenicity, final conc. (trial 2): 64, 128, 256, 512, 750, 1024µg/ml –S9; 128, 256, 512, 1024, 1500, 2048µg/ml +S9, all diluted in 10% Pluronic® polyol F68 (prepared in dionized water, mol. wt. 8350)</p>
<p>Statistical Methods</p>	<p>Frequency of mutant colonies per million clonable cells was calculated and comparisons of treated cultures with vehicle controls made on transformed data using a two-tailed t-test (Irr & Snee, 1979). Criteria for positive results were significant (p<0.05) increase in mutant colonies (HGPRT+/- → HGPRT-/-) at any dose level and a dose related response. If only one criterion is met, results are considered equivocal.</p>
<p>Remarks for Test Conditions</p>	<p>Sufficient Heavy Aromatic Distillate (HAD) was weighed separately for each dose level into 10 ml volumetric flasks, 1.8ml of 10% F68 added per ml of final volume and medium (Ham's F-12 without hypoxanthine) added as required to achieve final 10ml volume for testing. All dosing preparations were vortexed just after addition of medium and just prior to use when 20µl of each preparation was added to 3ml treatment medium/culture vessel. All cultures were incubated at 37°C in 5% CO2 enriched, humidified atmosphere. Positive control mutagens were ethyl methanesulfonate (100µg/ml) for –S9 cultures, and benzo(a)pyrene (4µg/ml) for +S9 cultures. For cytotoxicity, each dose group was composed of 2 flasks, one –S9, one+S9, negative controls ± S9, seeded with 5x10⁵ cells on day 1. Cultures were exposed to test compound for 5 hours on day 2. On day 3, cells were trypsinized and counted with a Coulter Model ZB, then 200 cells were transferred into each of 3 60mm culture dishes. These viability plates were incubated until day 10, fixed in methanol and stained with Giemsa. Colonies were counted visually or with an Artek Model 981 colony counter. Absolute survival = total colony count ÷ number of cells seeded/flask. Relative survival = absolute survival in treated cultures ÷ vehicle control survival. Acceptable survival level is at least 10%. For mutagenicity, cells were seeded on day 1 into 6 flasks/dose group, 3-S9, 3+S9; on day 2 approximately 10⁶ cells were exposed to HAD for 5 hours. Vehicle control had 12 flasks, 6-S9, 6+S9. On day 3, cultures with excessive cytotoxicity were discarded. From remaining cultures, 200 cells were seeded to each of 4 viability plates/dose level; incubated to day 10, fixed with methanol, stained with Giemsa, and colonies counted for survival. Expression cultures (10⁵-10⁶ cells/one dish/dose) were seeded on day 3; subcultured three times until day 10 when 200 cells were seeded on each of 4 viability plates/dose and 2x10⁵ cells seeded on each of 5 mutagenicity plates/dose with selective medium containing 10⁻⁵M 6-thioguanine to allow expression of HGPRT mutation. Cultures were incubated undisturbed until day 17 when they were fixed and stained. For mutagenicity, a ratio of total colony counts in mutagenicity plates over absolute survival in viability plates was calculated for each treatment group. Frequency of</p>

Robust Summary - Group 6: Low Benzene Naphthas**Genetic Toxicity - in Vitro**

<p><u>Test Substance</u> <i>Test substance</i></p>	<p>Heavy Aromatic Distillate, Gulf. CAS #64742-48-9. Water-white liquid with characteristic aromatic odor. Composition analysis, purity and stability referred to sponsor.</p>
<p><u>Method</u> 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>Exposure period Statistical Methods</p>	<p>Standard method based on Cortesi et al (1983), Dunkel et al (1981), Reznikoff et al (1973) In vitro cell transformation Mouse embryo cells Yes 1984 BALB/3T3-A31-1-1 from T. Kakunaga, National Cancer Inst., 1982 No NA NA NA Cytotoxicity: 8, 16, 32, 64, 128, 256, 512, 1024, 2048, 5000µg/ml; Transformation: 16, 32, 64, 200µg/ml, all diluted in 10% Pluronic[®] polyol F68 (prepared in deionized water, mol. wt. 8350, 80% hydrophilic). 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>Remarks for Test Conditions</p>	<p>Sufficient Heavy Aromatic Distillate (HAD) was weighed separately for each dose level, 0.45ml of 10% F68 added per ml of final volume and medium (Eagles MEM with 10% heat-inactivated fetal calf serum) added as required to achieve final volume for testing. Test preparations were mixed just prior to addition to cultures at 50µl to each 5 ml culture. All cultures were incubated at 37°C in 5% CO₂ enriched humidified atmosphere. For cytotoxicity, 2 plate cultures/dose group, 2 plate cultures for vehicle F68 or medium negative control were seeded with 1x10⁴ cells/plate in day 1, exposed on days 2-3, trypsinized and counted with a Coulter Model ZB on day 4 for at least 20% survival. For transformation, 15 flasks (1x10⁴ cells/flask/dose group) and two cloning flasks (100 cells per flask/dose group) were seeded on day 1, exposed on days 2-3 and culture medium changed on day 4. For transformation flask cultures, medium continued to be changed weekly to day 29. Positive control was 3-methylcholanthrene (1µg/ml). Cloning flask cultures were fixed, stained, and counted visually on day 8 to determine cloning efficiency (avg. number colonies/plate ÷ 100 cells seeded). Flask cultures were fixed and stained on day 29 for focus counting and evaluation. Transformation frequency = total type III foci ÷ total flasks/dose group.</p>
<p><u>Results</u> Genotoxic effects</p>	<p>In the first trial, HAD induced toxicity in BALB/3T3 cells after two days exposure beginning at 32µg/ml (59.9% relative survival), increasing with dose level to 2.9% relative survival at 5000µg/ml. The first trial was discarded due to loss of many cultures (27/105) due to contamination. Results of the second transformation trial indicated no treatment related cell transformation induced by HAD. Toxicity was evident 32µg/ml (67.2% relative cloning efficiency), increasing sharply at 200µg/ml (28.8% cloning efficiency). Positive and negative controls gave expected results.</p>
<p><u>Conclusions</u> (contractor)</p>	<p>Heavy Aromatic Distillate did not induce transformation in BALB/3T3 cells at any dose level under conditions of this assay.</p>
<p><u>Data Quality</u> <i>Reliabilities</i></p>	<p>1. Reliable without restriction. Study conforms to standard design. GLPs have been followed.</p>

Robust Summary - Group 6: Low Benzene Naphthas**Genetic Toxicity - in Vitro**

<p><u>Test Substance</u> <i>Test substance</i></p>	<p>Heavy Aromatic Distillate, Gulf. CAS #64742-48-9. Water white liquid with characteristic aromatic odor. Composition analysis, purity and stability referred to sponsor.</p>
<p><u>Method</u> 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 based on Williams et al. (1977,1982) In vitro mammalian cell DNA repair assay Unscheduled DNA Synthesis (UDS) in primary hepatocyte cultures. Yes 1984 Fischer 344 male rat (13-14 wks old) – 1 rat per test No NA NA NA Range-finding: 8, 16, 32, 64, 128, 256, 512, 1024, 2048, 5000 µg/ml: UDS assay 10, 40, 100, 200 µg/ml; all diluted in 10% Pluronic® polyol F68 (prepared in deionized water, mol. wt 8350, 80% hydrophilic)</p>
<p>Exposure period Statistical Methods</p>	<p>18 hours None employed. Criteria for positive response are incorporation of radioactive precursor (³H-thymidine) in cells that are not normally synthesizing DNA, indicating repair of damage. A positive response is defined as a mean net nuclear grain count at any treatment level that exceeds concurrent negative control by at least 6 grains/nucleus; negative control value must not exceed 5 grains. A positive response need not be dose related.</p>
<p>Remarks for Test Conditions</p>	<p>Sufficient Heavy Aromatic Distillate (HAD) was weighed separately for each dose level, 0.45ml of 10% F68 added per ml of final volume and sufficient medium (Williams Medium E with 10% fetal bovine serum and insulin) added to achieve final volume. Test preparations were mixed just prior to addition at 30µl to each 3 ml culture. The conc. of ³H-thymidine (½ life 12.5 yrs.) used in these assays was 1mCi/ml. All cultures were incubated at 37°C in 5% CO₂ enriched humidified atmosphere. For range-finding, primary hepatocytes derived from freshly perfused rat liver were seeded (approx. 1x10⁵ cells/ml) into treatment vessels, exposed to test material for 18 hours (2 cultures/dose level; 2 untreated cultures, and two vehicle (F68) control cultures), then fixed in formalin and stained with trypan blue for viability determination. At least 50% viability needed for the assay. In the UDS assay, 1x10⁵ cells/ml were seeded into coverslip cultures, exposed to ³H-thymidine and test substance for 18 hours (3 cultures/dose level). Positive control was 2-acetyl aminofluorene (0.2µg/ml). Cells growing on coverslips were rinsed, fixed and glued to microscope slides on day 2. On day 3, slides were dipped in autoradiographic emulsion and stored in the dark at 2-8°C. Autoradiographs were developed, stained and coverslipped on day 14. Numbers of grains overlying 50 randomly selected nuclei/slide were counted. The highest of 3 cytoplasmic grain counts/cell were subtracted and this number was divided by a conversion factor of 2, to obtain net nuclear grain count. Avg. net nuclear grain count/slide (sum of net nuclear grain count ÷ 50) and mean net nuclear grain count (avg. net nuclear grain count/slide ÷ 3) were calculated.</p>
<p><u>Results</u> Genotoxic effects</p>	<p>HAD induced toxicity in primary hepatocytes beginning at 32-64µg/ml (72-80% relative viability) after 18 hours exposure, which increased with dose levels to 2% viability at 5000µg/ml. HAD did not cause unscheduled DNA synthesis at any dose level. Positive and negative controls gave expected results.</p>
<p><u>Conclusions</u> (contractor)</p>	<p>Unscheduled DNA synthesis was not observed in primary culture of rat hepatocytes at any dose level of Heavy Aromatic Distillate, indicating that this material does not damage DNA under conditions of this assay.</p>

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

Robust Summary - Group 6: Low Benzene Naphthas**Genetic Toxicity - in Vivo**

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

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

Robust Summary - Group 6: Low Benzene Naphthas

Repeated Dose Toxicity

<p><u>Test Substance</u> Remarks</p>	<p>Heavy Aromatic Distillate, CAS # 64742-48-9. No analysis of purity or composition reported; referred to sponsor.</p>
<p><u>Method</u> 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>No guidelines specified, comparable to standard study Subacute Yes 1983 Rat Fischer 344 Whole body inhalation 5 days 0, 1.2, 2.7, 5.0 g/m³ Males and females 5/sex/group 5 days 6 hours/day filtered air at 6 hrs/day for 5 days None Analysis of Variance, Dunnett's test</p>
<p>Test Conditions</p>	<p>Animals (13 weeks old at study initiation, 156-279g) were housed individually in screen-bottom cages with automatic watering in rooms maintained at approx. 74⁰F with relative humidity of 50%, and 12 hour light/ dark cycle. Chow diet and water were provided ad lib except during exposure. Chamber concentrations were monitored by GC; peak areas were compared with those of neat test article standards. Rats were monitored twice daily for morbidity and mortality, and observed once daily for clinical signs. Body weights were measured at initiation and termination. Necropsies were performed for gross lesions.</p>
<p><u>Results</u> NOAEL (NOEL) LOAEL (LOEL) Remarks</p>	<p>NOEL not determined LOEL = 1.2 g/m³ based on clinical observations: perianal staining, red material around nose/mouth, ocular porphyrin. (assessed by Reviewer). One female rat in the high dose group died during the initial exposure; all other rats survived until termination. Males and females exposed to 5.0g/m³, showed a dose related weight loss of approx. 8% after 5 days of dosing. Incidence of dry red material around nose/mouth, ocular porphyrin, clear discharge from the eyes, partially closed eyes and perianal staining occurred in all groups receiving test article. The two high dose groups showed purulent discharge from the eyes and bloody tears. Reviewer comment: The total incidence of clinical observations increased in a manner related to exposure concentration.</p>
<p><u>Conclusions</u></p>	<p>One death occurred during exposure of the high dose group. All other animals exhibited clinical signs that included ocular discharge, eye closure, and dry red material around the nose/mouth. Gross pathological lesions were not observed which could be directly attributable to test article administration.</p>
<p><u>Quality</u> Reliabilities</p>	<p>1. Reliable without restrictions.</p>
<p><u>References</u></p>	<p>Gordon, T. 1983. One week repeat dose inhalation toxicity study in the rat using heavy aromatic distillate. Proj. # 2062. Gulf Life Sciences Center, Pittsburgh, PA for Gulf Oil Chemicals Co., Houston, TX.</p>
<p><u>Other</u> Last changed</p>	<p>Rev. 7/3//2001 (Prepared by a contractor to the Olefins Panel)</p>

Robust Summary - Group 6: Low Benzene Naphthas**Repeated Dose Toxicity**

<u>Test Substance</u>	Heavy Aromatic Distillate, CAS #64742-48-9. No composition or purity analysis reported; refer to sponsor.
Remarks	
<u>Method</u>	
Method/guideline followed	No guideline specified; comparable to standard study.
Test type	Subacute
GLP	Yes
Year	1985
Species	Rat
Strain	Fischer 344
Route of administration	Dermal
Duration of test	4 weeks
Doses/concentration levels	0.0, 0.5, 1.0, 1.5 g/kg in paraffin oil vehicle
Sex	Males and female (10/sex/group), 72 days old at study initiation
Exposure period	6 hours/day
Frequency of treatment	once/day, 5 days/week
Control group and treatment	Paraffin oil, 2.18 ml/kg/day for 5 days/week
Post exposure observation period	None
Statistical methods	Bartlett's test for homogeneity, Dunnett's test for homogeneous data; modified t-test for non-homogeneous data.
Test Conditions	<p>Animals were housed individually in suspended stainless steel cages with wire mesh bottoms and fronts equipped with an automatic watering system, in a room maintained at 76.1⁰F with relative humidity of 56.6% and 12 hour light/dark cycle. Chow diet was provided ad lib. Test article dilutions in paraffin oil (75% v/v) were prepared weekly. Doses of test article were administered over 10% of body surface to the backs of rats clipped free of hair and fitted with Elizabethan collars to reduce ingestion. After 6 hours, collars were removed and residual oil wiped off. Observations for mortality and moribundity were made twice/day, and for clinical signs at least once daily (on dosing days). Dermal responses were scored at initiation and then weekly. Body weight was measured at initiation and then weekly. Food consumption was determined weekly. At sacrifice, gross necropsy was performed, organs/tissues (19/rat) weighed and preserved. Slides prepared for histopathologic examination for the following tissues/organs of control and high dose groups: brain, spinal cord, heart, lungs, thymus, left kidney, right kidney, liver, spleen, sternum, lymph nodes, testes, skin, adrenal glands, urinary bladder, and peripheral nerve.</p>
<u>Results</u>	
NOAEL (NOEL)	NOEL not determined.
LOAEL (LOEL)	LOEL males = 0.5g/kg (increased total WBC count, assigned by reviewer)
Remarks	LOEL females = 1.5 g/kg (hematologic alterations, skin irritation, assigned by reviewer)
	<p>No deaths or moribund rats were observed and no statistically or biologically significant differences in group mean body wt were noted at study termination. No clinical effects were observed that could be attributed to test article administration. Food consumption was significantly decreased in male rats given 1.5g/kg during wks 2 and 3, and in female rats given 1.0g/kg during wk 2. Severe erythema was observed in 1.5g/kg males and females by wk 3 which persisted for the duration of the study. At termination, moderate eschar formation was seen in 10/10 males and 7/10 females. Statistically significant changes in hematology and clinical chemistry parameters after 4 wks of dosing were: dose responsive increase in WBC (57-70%) of males and females in 1.5g/kg group; slight reduction of RBC in males and reduction of HGB and HCT of males and females given 1.5g/kg; elevated platelet counts (10-20%) in 1.5g/kg males and females, reduced total serum protein (10-13%) in 1.5g/kg males and females; reduced serum albumin (9-25%) in high dose males and females; dose responsive reduction in BUN (9-25%) in high dose animals. There were marked increases in segmented neutrophils (200-400%) and lymphocytes (20-30%) in males and females given 1.5g/kg, and an erratic but marked increase in atypical lymphocytes of males in low-high dose groups and increased eosinophils (485%) in 1.5g/kg males. There were several statistically significant but inconsistent changes in organ wt when expressed as</p>

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