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ROBUST SUMMARIES PART 1

CRUDE BUTADIENE C4 ROBUST SUMMARIES

ARE ALSO USED FOR PYROLYSIS C3+ AND C4+

**ROBUST SUMMARIES OF STUDIES USED TO CHARACTERIZE THE
CRUDE BUTADIENE C4 CATEGORY ARE ALSO USED FOR
PYROLYSIS C3+ AND C4+**

PHYSICO-CHEMICAL ROBUST SUMMARIES

Melting Point

Test Substance*:	Other TS		
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: (FT - TC) <ul style="list-style-type: none"> Note: Concentration prep., vessel type, replication, test conditions. 	<p>Melting Point estimations performed by MPBPWIN are based on the average result of the calculation 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.</p>		
Results: (FT - RS) Units/Value: <ul style="list-style-type: none"> Note: Deviations from protocol or guideline, analytical method. 	<u>Chemical</u>	<u>Calculated MP (°C)</u>	<u>Measured* MP (°C)</u>
	Isobutane	-132.55	-138.3
	n-butane	-120.28	-138.2
	isobutylene	-130.88	-140.4
	cis-butene-2	-120.41	-105.5
	trans-butene-2	-120.41	-105.5
	butene-1	-121.74	-145.0
	1,3-butadiene	-123.21	-108.9
	* Experimental values are supplied by the MPBPWIN program database (EXP_MBVP.DB) which contains more		

	<p>than 11,000 organic compounds with reliably measured values which are taken from SRC's PHYSPROP Database.</p> <p>Commercial products in this category can have a carbon number distribution predominantly between C3 and C5. These products can contain significant levels of 1,3-butadiene and similar low molecular weight olefins, which is why they are considered a category for purposes of the High Production Volume Chemical Program, and designated <u>Crude Butadiene C4</u>.</p> <p>The seven chemicals selected to represent the melting range of this category are C4 hydrocarbons that are common across the 10 CAS numbers. Crude butadiene category products arise from production processes associated with ethylene manufacturing. More information on the Crude Butadiene C4 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 Crude Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
<p>Test Substance: (FT - TS)</p>	<p>25167-67-3 Butenes 68477-41-8 Distillate (Petroleum), Extractive C3-5 68955-28-2 Gases, (Petroleum) Light Steam Cracked, Butadiene Concentrate 68476-44-8 Hydrocarbons, >C3 68512-91-4 Hydrocarbons C3 – C4 Rich Petroleum Distillates 68187-60-0 Hydrocarbons, C4, Ethane-Propane Cracked 68476-52-8 Hydrocarbons, C4, Ethylene Manufactured By-Product 68956-54-7 Hydrocarbons C4, Unsaturated 69103-05-5 Hydrocarbons, C4-7, Butadiene Manufactured By-Product 64742-83-2 Naphtha, (Petroleum), Light Steam-Cracked</p>
<p>Conclusion: (FT - CL)</p>	<p>Based on the calculated values, products in this category can have a melting range of -132.55 to -120.28 °C. Based on the measured values, products in this category can have a melting range of -145.0 to -105.5°C.</p>
<p>Reliability: (FT - RL)</p>	<p>(2) Reliable with restrictions The results include calculated values based on the chemical</p>

	structure and experimental values available in the MPBPWIN program and represent a potential melting range for products with the 10 CAS numbers listed under <u>Test Substance</u> .
Reference: (FT - RE)	Meylan, M., SRC 1994-1999. WSKOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
Other (source): (FT - SO)	American Chemistry Council, Olefins Panel

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "melting point". Selecting this option refers the reader to information in the "freetext" field for "test substance".

FT - Freetext

IUCLID fields include:

- RL - Reliability
- TC - Test Conditions
- RE - Reference
- RS - Results
- TS - Test Substance
- SO - Source
- CL - Conclusion

Boiling Point

Test Substance*:	Other TS																										
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: (FT - TC) <ul style="list-style-type: none"> Note: Concentration prep., vessel type, replication, test conditions. 	Boiling Point estimations performed by MPBPWIN are 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: (FT - RS) Units/Value: <ul style="list-style-type: none"> Note: Deviations from protocol or guideline, analytical method. 	<table border="1"> <thead> <tr> <th><u>Chemical</u></th> <th><u>Calculated BP (°C)</u></th> <th><u>Measured* BP (°C)</u></th> </tr> </thead> <tbody> <tr> <td>Isobutane</td> <td>3.21</td> <td>-11.7</td> </tr> <tr> <td>n-butane</td> <td>19.58</td> <td>-0.5</td> </tr> <tr> <td>isobutylene</td> <td>10.18</td> <td>-6.9</td> </tr> <tr> <td>cis-butene-2</td> <td>27.82</td> <td>0.8</td> </tr> <tr> <td>trans-butene-2</td> <td>27.82</td> <td>0.8</td> </tr> <tr> <td>butene-1</td> <td>17.57</td> <td>-1.3</td> </tr> <tr> <td>1,3-butadiene</td> <td>15.55</td> <td>-4.4</td> </tr> </tbody> </table>	<u>Chemical</u>	<u>Calculated BP (°C)</u>	<u>Measured* BP (°C)</u>	Isobutane	3.21	-11.7	n-butane	19.58	-0.5	isobutylene	10.18	-6.9	cis-butene-2	27.82	0.8	trans-butene-2	27.82	0.8	butene-1	17.57	-1.3	1,3-butadiene	15.55	-4.4	<p>* Experimental values are supplied by the MPBPWIN program database (EXP_MBVP.DB) which contains more than 11,000 organic compounds with reliably measured values which are taken from SRC's PHYSPROP Database.</p> <p>Commercial products in this category can have a carbon number distribution predominantly between C3 and C5. These products can contain significant levels of 1,3-butadiene and similar low molecular weight olefins, which is why they are considered a category for purposes of the High Production Volume Chemical Program, and designated <u>Crude Butadiene C4</u>.</p> <p>The seven chemicals selected to represent the boiling range of this category are C4 hydrocarbons that are common</p>	
<u>Chemical</u>	<u>Calculated BP (°C)</u>	<u>Measured* BP (°C)</u>																									
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	<p>across the 10 CAS numbers. Crude butadiene category products arise from production processes associated with ethylene manufacturing. More information on the Crude Butadiene C4 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 Crude Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.</p>
Test Substance: (FT - TS)	<p>25167-67-3 Butenes 68477-41-8 Distillate (Petroleum), Extractive C3-5 68955-28-2 Gases, (Petroleum) Light Steam Cracked, Butadiene Concentrate 68476-44-8 Hydrocarbons, >C3 68512-91-4 Hydrocarbons C3 – C4 Rich Petroleum Distillates 68187-60-0 Hydrocarbons, C4, Ethane-Propane Cracked 68476-52-8 Hydrocarbons, C4, Ethylene Manufactured By-Product 68956-54-7 Hydrocarbons C4, Unsaturated 69103-05-5 Hydrocarbons, C4-7, Butadiene Manufactured By-Product 64742-83-2 Naphtha, (Petroleum), Light Steam-Cracked</p>
Conclusion: (FT - CL)	<p>Based on the calculated values, products in this category can have a boiling range of 3.21 to 27.82 °C. Based on the measured values, products in this category can have a boiling range of -11.7 to 0.8°C.</p>
Reliability: (FT - RL)	<p>(2) Reliable with restrictions</p> <p>The results include calculated values based on the chemical structure and experimental values available in the MPBPWIN program and represent a potential boiling point range for products with the 10 CAS numbers listed under <u>Test Substance</u>.</p>
Reference: (FT - RE)	<p>Meylan, M., SRC 1994-1999. WSKOWWIN 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): (FT - SO)	<p>American Chemistry Council, Olefins Panel</p>

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "boiling point". Selecting this option refers the reader to information in the "freetext" field for "test substance".

FT - Freetext

IUCLID fields include:

RL - Reliability

TC - Test Conditions

RE - Reference

RS - Results

TS - Test Substance

SO - Source

CL - Conclusion

Vapor Pressure

Test Substance*:	Other TS																										
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: (FT - TC) <ul style="list-style-type: none"> Note: Concentration prep., vessel type, replication, test conditions. 	<p>Vapor Pressure estimations performed by MPBPWIN are based on the average result of the calculation 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: (FT - RS) Units/Value: <ul style="list-style-type: none"> Note: Deviations from protocol or guideline, analytical method. 	<table border="1"> <thead> <tr> <th><u>Chemical</u></th> <th><u>Calculated VP (hPa)</u></th> <th><u>Measured* VP (hPa)</u></th> </tr> </thead> <tbody> <tr> <td>Isobutane</td> <td>3.45 E³</td> <td>3.08 E³</td> </tr> <tr> <td>n-butane</td> <td>2.41 E³</td> <td>2.43 E³</td> </tr> <tr> <td>isobutylene</td> <td>2.97 E³</td> <td>3.08 E³</td> </tr> <tr> <td>cis-butene-2</td> <td>2.31 E³</td> <td>2.33 E³</td> </tr> <tr> <td>trans-butene-2</td> <td>2.31 E³</td> <td>2.33 E³</td> </tr> <tr> <td>butene-1</td> <td>2.48 E³</td> <td>3.00 E³</td> </tr> <tr> <td>1,3-butadiene</td> <td>2.73 E³</td> <td>2.81 E³</td> </tr> </tbody> </table>	<u>Chemical</u>	<u>Calculated VP (hPa)</u>	<u>Measured* VP (hPa)</u>	Isobutane	3.45 E ³	3.08 E ³	n-butane	2.41 E ³	2.43 E ³	isobutylene	2.97 E ³	3.08 E ³	cis-butene-2	2.31 E ³	2.33 E ³	trans-butene-2	2.31 E ³	2.33 E ³	butene-1	2.48 E ³	3.00 E ³	1,3-butadiene	2.73 E ³	2.81 E ³	<p>* Experimental values are supplied by the MPBPWIN program database (EXP_MBVP.DB) which contains more than 11,000 organic compounds with reliably measured values which are taken from SRC's PHYSPROP Database.</p> <p>Commercial products in this category can have a carbon number distribution predominantly between C3 and C5. These products can contain significant levels of 1,3-</p>	
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	<p>butadiene and similar low molecular weight olefins, which is why they are considered a category for purposes of the High Production Volume Chemical Program, and designated <u>Crude Butadiene C4</u>.</p> <p>The seven chemicals selected to represent the vapor pressure range of this category are C4 hydrocarbons that are common across the 10 CAS numbers. Crude butadiene category products arise from production processes associated with ethylene manufacturing. More information on the Crude Butadiene C4 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 Crude Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.</p>
Test Substance: (FT - TS)	<p>25167-67-3 Butenes 68477-41-8 Distillate (Petroleum), Extractive C3-5 68955-28-2 Gases, (Petroleum) Light Steam Cracked, Butadiene Concentrate 68476-44-8 Hydrocarbons, >C3 68512-91-4 Hydrocarbons C3 – C4 Rich Petroleum Distillates 68187-60-0 Hydrocarbons, C4, Ethane-Propane Cracked 68476-52-8 Hydrocarbons, C4, Ethylene Manufactured By-Product 68956-54-7 Hydrocarbons C4, Unsaturated 69103-05-5 Hydrocarbons, C4-7, Butadiene Manufactured By-Product 64742-83-2 Naphtha, (Petroleum), Light Steam-Cracked</p>
Conclusion: (FT - CL)	<p>Based on the calculated values, products in this category can have a vapor pressure range of 2.31 E³ to 3.45 E³ hPa. Based on the measured values, products in this category can have a vapor pressure range of 2.33 E³ to 3.08 E³ hPa.</p>
Reliability: (FT - RL)	<p>(2) Reliable with restrictions</p> <p>The results include calculated values based on the chemical structure and experimental values available in the MPBPWIN program and represent a potential vapor pressure range for products with the 10 CAS numbers listed under <u>Test Substance</u>.</p>
Reference: (FT - RE)	<p>Meylan, M., SRC 1994-1999. MPBPWIN is contained in the</p>

	computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
Other (source): (FT - SO)	American Chemistry Council, Olefins Panel

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "vapor pressure". Selecting this option refers the reader to information in the "freetext" field for "test substance".

FT - Freetext

IUCLID fields include:

- RL - Reliability
- TC - Test Conditions
- RE - Reference
- RS - Results
- TS - Test Substance
- SO - Source
- CL - Conclusion

Partition Coefficient

Test Substance*:	Other TS		
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: (FT - TC) <ul style="list-style-type: none"> Note: Concentration prep., vessel type, replication, test conditions. 	Octanol / Water Partition Coefficient estimations performed by KOWWIN are 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: (FT - RS) Units/Value: <ul style="list-style-type: none"> Note: Deviations from protocol or guideline, analytical method. 	<u>Chemical</u>	<u>Calculated</u> <u>log K_{ow}</u>	<u>Measured*</u> <u>log K_{ow}</u>
	Isobutane	2.23	2.76
	n-butane	2.31	2.89
	isobutylene	2.23	2.34
	cis-butene-2	2.09	2.31
	trans-butene-2	2.09	2.33
	butene-1	2.17	2.40
	1,3-butadiene	2.03	1.99
	* Experimental K _{ow} values supplied by the KOWWIN program database (EXPKOW.DB) which contains more than 13,000 organic compounds with reliably measured values.		
	Commercial products in this category can have a carbon number distribution predominantly between C3 and C5. These products can contain significant levels of 1,3-butadiene and similar low molecular weight olefins, which is why they are considered a category for purposes of the High Production Volume Chemical Program, and designated <u>Crude Butadiene C4</u> .		
	The seven chemicals selected to represent the partition coefficient range of this category are C4 hydrocarbons that		

	<p>are common across the 10 CAS numbers. Crude butadiene category products arise from production processes associated with ethylene manufacturing. More information on the Crude Butadiene C4 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 Crude Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.</p>
Test Substance: (FT - TS)	<p>25167-67-3 Butenes 68477-41-8 Distillate (Petroleum), Extractive C3-5 68955-28-2 Gases, (Petroleum) Light Steam Cracked, Butadiene Concentrate 68476-44-8 Hydrocarbons, >C3 68512-91-4 Hydrocarbons C3 – C4 Rich Petroleum Distillates 68187-60-0 Hydrocarbons, C4, Ethane-Propane Cracked 68476-52-8 Hydrocarbons, C4, Ethylene Manufactured By-Product 68956-54-7 Hydrocarbons C4, Unsaturated 69103-05-5 Hydrocarbons, C4-7, Butadiene Manufactured By-Product 64742-83-2 Naphtha, (Petroleum), Light Steam-Cracked</p>
Conclusion: (FT - CL)	<p>Based on the calculated K_{ow} values, products in this category can have a partition coefficient range of 2.03 to 2.31. Based on the measured K_{ow} values, products in this category can have a partition coefficient range of 1.99 to 2.89.</p>
Reliability: (FT - RL)	<p>(2) Reliable with restrictions</p> <p>The results include calculated values based on the chemical structure and experimental values available in the KOWWIN program and represent a potential partition coefficient range for products with the 10 CAS numbers listed under <u>Test Substance</u>.</p>
Reference: (FT - RE)	<p>Meylan, M., SRC 1994-1999. KOWWIN 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): (FT - SO)	<p>American Chemistry Council, Olefins Panel</p>

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "partition coefficient". Selecting this option refers the reader to information in the "freetext" field for "test substance".

FT - Freetext

IUCLID fields include:

- RL - Reliability
- TC - Test Conditions
- RE - Reference
- RS - Results
- TS - Test Substance
- SO - Source
- CL - Conclusion

Water Solubility

Test Substance*:	Other TS		
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: (FT - TC) <ul style="list-style-type: none"> Note: Concentration prep., vessel type, replication, test conditions. 	Water Solubility estimations performed by WSKOWWIN are 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: (FT - RS) Units/Value: <ul style="list-style-type: none"> Note: Deviations from protocol or guideline, analytical method. 	<u>Chemical</u>	<u>Calculated WS (mg/L)</u>	<u>Measured* WS (mg/L)</u>
	Isobutane	496.4	175.1
	n-butane	424.1	135.6
	isobutylene	495.6	399.2
	cis-butene-2	652.7	423.5
	trans-butene-2	652.7	407.1
	butene-1	557.7	354.8
	1,3-butadiene	732.4	792.3
	* Experimental K _{ow} values supplied by the WSKOWWIN program database (EXPKOW.DB) which contains more than 13,000 organic compounds with reliably measured values.		
	Commercial products in this category can have a carbon number distribution predominantly between C3 and C5. These products can contain significant levels of 1,3-butadiene and similar low molecular weight olefins, which is why they are considered a category for purposes of the High Production Volume Chemical Program, and designated <u>Crude Butadiene C4</u> .		
	The seven chemicals selected to represent the water solubility range of this category are C4 hydrocarbons that		

	<p>are common across the 10 CAS numbers. Crude butadiene category products arise from production processes associated with ethylene manufacturing. More information on the Crude Butadiene C4 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 Crude Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.</p>
Test Substance: (FT - TS)	<p>25167-67-3 Butenes 68477-41-8 Distillate (Petroleum), Extractive C3-5 68955-28-2 Gases, (Petroleum) Light Steam Cracked, Butadiene Concentrate 68476-44-8 Hydrocarbons, >C3 68512-91-4 Hydrocarbons C3 – C4 Rich Petroleum Distillates 68187-60-0 Hydrocarbons, C4, Ethane-Propane Cracked 68476-52-8 Hydrocarbons, C4, Ethylene Manufactured By-Product 68956-54-7 Hydrocarbons C4, Unsaturated 69103-05-5 Hydrocarbons, C4-7, Butadiene Manufactured By-Product 64742-83-2 Naphtha, (Petroleum), Light Steam-Cracked</p>
Conclusion: (FT - CL)	<p>Based on the calculated K_{ow} values, products in this category can have a water solubility range of 424.1 to 732.4 mg/L. Based on the measured K_{ow} values, products in this category can have a water solubility range of 135.6 to 792.3 mg/L.</p>
Reliability: (FT - RL)	<p>(2) Reliable with restrictions</p> <p>The results include values estimated using calculated K_{ow} and experimental K_{ow} values available in the WSKOWWIN program and represent a potential water solubility range for products with the 10 CAS numbers listed under <u>Test Substance</u>.</p>
Reference: (FT - RE)	<p>Meylan, M., SRC 1994-1999. WSKOWWIN 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): (FT - SO)	<p>American Chemistry Council, Olefins Panel</p>

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "water solubility". Selecting this option refers the reader to information in the "freetext" field for "test substance".

FT - Freetext

IUCLID fields include:

- RL - Reliability
- TC - Test Conditions
- RE - Reference
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- TS - Test Substance
- SO - Source
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ENVIRONMENTAL FATE ROBUST SUMMARIES

Photodegradation (Direct)

Test Substance*:	Other TS
Method/Guideline:	Other: Technical discussion
Year (guideline):	Not applicable
GLP (Y/N):	Not applicable
Year (study performed):	Not applicable
Type (air, soil, water, other):	Not applicable
Light Source:	Not applicable
Light Spectrum: <ul style="list-style-type: none"> • Wave length value (upper/lower) 	Not applicable
Relative Intensity:	Not applicable
Test Substance Spectrum:	Not applicable
Test Conditions: (FT - TC) <ul style="list-style-type: none"> • Note: Concentration, temperature, test system type, replication, deviations from guideline or protocol 	Not applicable
Direct Photolysis**: Results: half-life, % degradation, quantum yield	<p>Summary</p> <p>In the environment, photolysis will not significantly contribute to the degradation of chemicals in the Crude Butadiene C4 Category (C4 refers to a chemical with 4 carbons). The Crude Butadiene C4 Category includes two process streams:</p> <ul style="list-style-type: none"> • C4 Crude Butadiene • Butadiene Unit Heavy Ends <p>Ten CAS numbers (see <u>Test Substance</u>) 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, products in this</p>

category do not contain component chemicals that will undergo direct photolysis.

The Crude Butadiene C4 Category

A process stream is a mixture of chemicals that arises from a chemical reaction or separation activity. Process streams containing 10 to 92% butadiene are referred to as “crude butadiene.” The CAS numbers or streams in this category consist of complex mixtures of hydrocarbons.

Most commercial products in this category have a carbon number distribution predominantly between C3 and C5. All of these streams contain significant levels of 1,3-butadiene and olefins, which is why this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated Crude Butadiene C4.

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).

Crude butadiene streams arise from production processes associated with ethylene manufacturing. More information on the Crude Butadiene C4 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 two process streams in this category are:

- **C4 Crude Butadiene** is produced by the distillation of a condensed portion of cracked gas in an ethylene process. C4 Crude Butadiene typically contains 40% to about 60% 1,3-butadiene, but could contain between 10% and 82% butadiene. Other chemicals in this mixed stream are predominately chemicals containing 4 carbons.
- **Butadiene Unit Heavy Ends** is produced by extractive distillation of cracked gas. The 1,3-butadiene content of this mixed stream ranges from 13% to 92%. Other chemicals in this mixed stream are predominately chemicals containing 4 carbons. Only three companies report isolating this stream which is more typically an unisolated intermediate.

Photolysis of Hydrocarbons

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

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

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

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

	Hydrocarbon	λ below 290 nm	
		λ_{\max}	ϵ
		Ethylene	193
	1,3-Butadiene	217	2,090
Direct Photolysis**: (cont.) Results: half-life, % degradation, quantum yield	<p>Olefins with one double bond, two conjugated double bonds, or multiple un-conjugated bonds, which constitute the majority of the chemicals in the Crude Butadiene C4 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 Crude Butadiene C4 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"> 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Crude Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. Virginia, USA. 2. Harris, J. C. 1982. "Rate of Aqueous Photolysis," Chapter 8 in: W. J. Lyman, W. F. Reehl, and D. H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, USA. 3. Zepp, R. G. and D. M. Cline. 1977. Rates of Direct Photolysis in the Aqueous Environment, Environ. Sci. Technol., 11:359-366. 		
Indirect Photolysis**: <ul style="list-style-type: none"> • Results: type of sensitizer, concentration of sensitizer, rate constant, % degradation, half-life 	Not applicable		
Degradation Products**: <ul style="list-style-type: none"> • Note: Identification, concentration 	Unknown		

Test Substance: (FT - TS)	25167-67-3 Butenes 68477-41-8 Distillate (Petroleum), Extractive C3-5 68955-28-2 Gases, (Petroleum) Light Steam Cracked, Butadiene Concentrate 68476-44-8 Hydrocarbons, >C3 68512-91-4 Hydrocarbons C3 – C4 Rich Petroleum Distillates 68187-60-0 Hydrocarbons, C4, Ethane-Propane Cracked 68476-52-8 Hydrocarbons, C4, Ethylene Manufactured By-Product 68956-54-7 Hydrocarbons C4, Unsaturated 69103-05-5 Hydrocarbons, C4-7, Butadiene Manufactured By-Product 64742-83-2 Naphtha, (Petroleum), Light Steam-Cracked
Conclusion: (FT - CL)	Not applicable
Reliability: (FT - RL)	Not applicable
Reference: (FT - RE)	American Chemistry Council, Olefins Panel. 2002. Hydrolysis: Crude Butadiene C4 Category. Rosslyn, VA, USA.
Other (source): (FT - SO)	American Chemistry Council, Olefins Panel

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "photodegradation". Selecting this option refers the reader to information in the "freetext" field for "test substance".

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

FT - Freetext

IUCLID fields include:

- RL - Reliability
- TC - Test Conditions
- RE - Reference
- RS - Results
- TS - Test Substance
- SO - Source
- CL - Conclusion

Photodegradation (Indirect)

Test Substance*:	Other TS
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: (FT - TC) • Note: Concentration, temperature, test system type, replication, deviations from guideline or protocol	Indirect photodegradation, or atmospheric oxidation potential, is based on the structure-activity relationship methods developed by R. Atkinson. Temperature: 25°C Sensitizer: OH radical Concentration of Sensitizer: 1.5 E ⁶ OH radicals/cm ³
Direct Photolysis**: Results: half-life, % degradation, quantum yield	Not applicable
Indirect Photolysis**: • Results: type of sensitizer, concentration of sensitizer, rate constant, % degradation, half-life	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 (1,2). The rate at which an organic compound reacts with OH- radicals is a direct measure of its atmospheric persistence (3). AOPWIN estimates the rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. The rate constants estimated by the program are then used to calculate atmospheric half-lives for organic compounds based upon

average atmospheric concentrations of hydroxyl radicals.

Since the reactions only take place in the presence of sunlight, the atmospheric half-lives are normalized for a 12-hour day.

<u>Chemical</u>	<u>Calculated* half-life (hrs)</u>	<u>OH- Rate Constant (cm³/molecule-sec)</u>
Isobutane	52.6	2.4 E ⁻¹²
n-butane	48.8	2.6 E ⁻¹²
isobutylene	2.5	51.7 E ⁻¹²
cis-butene-2	2.3	56.7 E ⁻¹²
trans-butene-2	2.0	64.3 E ⁻¹²
butene-1	4.7	27.4 E ⁻¹²
1,3-butadiene	1.9	66.6 E ⁻¹²

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

Commercial products in this category can have a carbon number distribution predominantly between C3 and C5. These products can contain significant levels of 1,3-butadiene and similar low molecular weight olefins, which is why they are considered a category for purposes of the High Production Volume Chemical Program, and designated Crude Butadiene C4.

The seven chemicals selected to represent the atmospheric half-life range of this category are C4 hydrocarbons that are common across the 10 CAS numbers listed under Test Substance. Crude butadiene category products arise from production processes associated with ethylene manufacturing. More information on the Crude Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (4).

References:

1. Atkinson, R. 1988. Estimation of gas-phase hydroxyl radical rate constants for organic chemicals. *Environ. Toxicol. Chem.* **7**:435-442.
2. Atkinson, R. 1989. Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds. *J. Phys. Chem. Ref. Data Monograph No. 1*, Amer. Inst. Physics & Amer. Chem. Soc., NY.
3. Meylan, W.M. and P.H. Howard. 1993. Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. *Chemosphere* **12**:2293-2299.
4. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Crude Butadiene C4

	Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Degradation Products**: • Note: Identification, concentration	Unknown
Test Substance: (FT - TS)	25167-67-3 Butenes 68477-41-8 Distillate (Petroleum), Extractive C3-5 68955-28-2 Gases, (Petroleum) Light Steam Cracked, Butadiene Concentrate 68476-44-8 Hydrocarbons, >C3 68512-91-4 Hydrocarbons C3 – C4 Rich Petroleum Distillates 68187-60-0 Hydrocarbons, C4, Ethane-Propane Cracked 68476-52-8 Hydrocarbons, C4, Ethylene Manufactured By-Product 68956-54-7 Hydrocarbons C4, Unsaturated 69103-05-5 Hydrocarbons, C4-7, Butadiene Manufactured By-Product 64742-83-2 Naphtha, (Petroleum), Light Steam-Cracked
Conclusion: (FT - CL)	Atmospheric oxidation vial hydroxyl radical 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 1.9 to 52.6 hours as a result of indirect photolysis by hydroxyl radical attack.
Reliability: (FT - RL)	(2) Reliable with restrictions The results include values calculated using the AOPWIN program and represent a potential atmospheric half-life range for products with the 10 CAS numbers listed under <u>Test Substance</u> .
Reference: (FT - RE)	Meylan, M., SRC 1994-1999. AOPWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
Other (source): (FT - SO)	American Chemistry Council, Olefins Panel

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "photodegradation". Selecting this option refers the reader to information in the "freetext" field for "test substance".

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

FT - Freetext

IUCLID fields include:

RL - Reliability

TC - Test Conditions

RE - Reference
RS - Results
TS - Test Substance
SO - Source
CL - Conclusion

Hydrolysis (Stability in Water)

Test Substance*:	Other TS
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: (FT - TC) <ul style="list-style-type: none"> Note: Concentration preparation, vessel type, volume, replication, deviations from guideline or protocol 	Not applicable
Results: (FT - RS) Units/Value: <ul style="list-style-type: none"> Note: Analytical method, observations, half-lives by pH, degradation products 	Not applicable
Test Substance: (FT - TS)	25167-67-3 Butenes 68477-41-8 Distillate (Petroleum), Extractive C3-5 68955-28-2 Gases, (Petroleum) Light Steam Cracked, Butadiene Concentrate 68476-44-8 Hydrocarbons, >C3 68512-91-4 Hydrocarbons C3 – C4 Rich Petroleum Distillates 68187-60-0 Hydrocarbons, C4, Ethane-Propane Cracked 68476-52-8 Hydrocarbons, C4, Ethylene Manufactured By-Product 68956-54-7 Hydrocarbons C4, Unsaturated 69103-05-5 Hydrocarbons, C4-7, Butadiene Manufactured By-Product 64742-83-2 Naphtha, (Petroleum), Light Steam-Cracked
Conclusion: (FT - CL)	Summary In the environment, hydrolysis will not contribute to the

degradation of chemicals in the Crude Butadiene C4 Category (C4 refers to a chemical with 4 carbons). This category includes two process streams:

- **C4 Crude Butadiene**
- **Butadiene Unit Heavy Ends**

Ten CAS numbers (see Test Substance) identify products derived from these process streams. As discussed below, the chemicals in these streams are composed of carbon and hydrogen and are not amenable to hydrolysis because of their molecular structure and the chemical reaction required for this type of transformation to occur.

The Crude Butadiene C4 Category

A process stream is a mixture of chemicals that arises from a chemical reaction or separation activity. Process streams containing 10 to 92% butadiene are referred to as “crude butadiene.” The CAS numbers or streams in this category consist of complex mixtures of hydrocarbons.

Most commercial products in this category have a carbon number distribution predominantly between C3 and C5. All of these streams contain significant levels of 1,3-butadiene and olefins, which is why this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated Crude Butadiene C4.

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).

Crude butadiene streams arise from production processes associated with ethylene manufacturing. More information on the Crude Butadiene C4 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 two process streams in this category are:

- **C4 Crude Butadiene** is produced by the distillation of a condensed portion of cracked gas in an ethylene process. C4 Crude Butadiene typically contains 40% to about 60% 1,3-butadiene, but could contain between 10% and 82%

butadiene. Other chemicals in this mixed stream are predominately chemicals containing 4 carbons.

- **Butadiene Unit Heavy Ends** is produced by extractive distillation of cracked gas. The 1,3-butadiene content of this mixed stream ranges from 13% to 92%. Other chemicals in this mixed stream are predominately chemicals containing 4 carbons. Only three companies report isolating this stream which is more typically an un-isolated intermediate.

Hydrolysis of Hydrocarbons as a Function of Molecular Structure

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.

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

Under strongly acidic conditions the carbon-carbon double bond found in alkenes, such as those in the Crude Butadiene C4 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).

Chemicals that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (4). The chemicals in this 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 Crude Butadiene C4 Category have a very low potential to hydrolyze, and this degradative process will not contribute to their removal in the environment.

References

	<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 Crude Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA. 2. Gould, E.S. (1959), Mechanism and Structure in Organic Chemistry, Holt, Reinhart and Winston, New York, NY, USA. 3. Harris, J.C. (1982), "Rate of Hydrolysis," Chapter 7 in: W.J. Lyman, W.F. Reehl, and D.H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, NY, USA. 4. Neely, W. B. 1985. Hydrolysis. In: W. B. Neely and G. E. Blau, eds. Environmental Exposure from Chemicals. Vol I., pp. 157-173. CRC Press, Boca Raton, FL, USA.
Reliability: (FT - RL)	Not applicable
Reference: (FT - RE)	American Chemistry Council, Olefins Panel. 2002. Hydrolysis: Crude Butadiene C4 Category. Rosslyn, VA, USA.
Other (source): (FT - SO)	American Chemistry Council, Olefins Panel

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "hydrolysis". Selecting this option refers the reader to information in the "freetext" field for "test substance".

FT - Freetext

IUCLID fields include:

RL - Reliability

TC - Test Conditions

RE - Reference

RS - Results

TS - Test Substance

SO - Source

CL - Conclusion

Transport / Distribution (Fugacity)

Test Substance*:	Other TS																													
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																													
<p>Test Conditions: (FT - TC)</p> <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>Physical properties input into the model are those calculated by the EPIWIN Estimation v 3.04 program (1) or supplied by the databases of experimental values contained with EPIWIN. Output data from the equilibrium model provides basic information on the potential distribution 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>																													
<p>Results: (FT - RS)</p> <p>Units/Value:</p> <ul style="list-style-type: none"> Note: Deviations from protocol or guideline, analytical method. 	<p>The following chemicals are representative of products in the Crude Butadiene C4 Category, which are complex, multi-constituent substances. The range of partitioning data for component chemicals is an estimate of the partitioning behavior for category products.</p> <table border="1"> <thead> <tr> <th rowspan="2"><u>Chemical</u></th> <th colspan="2"><u>Calculated*</u></th> <th colspan="2"><u>Measured**</u></th> </tr> <tr> <th><u>Air</u></th> <th><u>Water</u></th> <th><u>Air</u></th> <th><u>Water</u></th> </tr> </thead> <tbody> <tr> <td>Isobutane</td> <td>99.99</td> <td>0.01</td> <td>99.99</td> <td>0.01</td> </tr> <tr> <td>n-butane</td> <td>99.98</td> <td>0.02</td> <td>99.99</td> <td>0.01</td> </tr> <tr> <td>isobutylene</td> <td>99.98</td> <td>0.02</td> <td>99.99</td> <td>0.01</td> </tr> <tr> <td>cis-butene-2</td> <td>99.97</td> <td>0.03</td> <td>99.98</td> <td>0.02</td> </tr> </tbody> </table>	<u>Chemical</u>	<u>Calculated*</u>		<u>Measured**</u>		<u>Air</u>	<u>Water</u>	<u>Air</u>	<u>Water</u>	Isobutane	99.99	0.01	99.99	0.01	n-butane	99.98	0.02	99.99	0.01	isobutylene	99.98	0.02	99.99	0.01	cis-butene-2	99.97	0.03	99.98	0.02
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cis-butene-2	99.97	0.03	99.98	0.02																										

	<table border="0"> <tr> <td>trans-butene-2</td> <td>99.97</td> <td>0.03</td> <td>99.98</td> <td>0.02</td> </tr> <tr> <td>butene-1</td> <td>99.98</td> <td>0.02</td> <td>99.99</td> <td>0.01</td> </tr> <tr> <td>1,3-butadiene</td> <td>99.97</td> <td>0.03</td> <td>99.97</td> <td>0.03</td> </tr> </table> <p>* Distribution values determined using input data calculated by the EPIWIN program</p> <p>**Distribution values determined using input data supplied by the EPIWIN program experimental databases (EXPKOW.DB, EXP_MBVP.DB, and EXP_MBVP.DB) which contain more than 11,000 organic compounds with reliably measured values.</p> <p>Distribution of each chemical to each remaining compartment (soil, sediment, suspended sediment, biota) was calculated as less than 0.01%. Mobility in the environment is expected to be high due to the relatively high water solubility and high vapor pressure of these chemicals.</p> <p>Commercial products in this category can have a carbon number distribution predominantly between C3 and C5. These products can contain significant levels of 1,3-butadiene and similar low molecular weight olefins, which is why they are considered a category for purposes of the High Production Volume Chemical Program, and designated <u>Crude Butadiene C4</u>.</p> <p>The seven chemicals selected to represent the transport / distribution range of this category are C4 hydrocarbons that are common across the 10 CAS numbers (see <u>Test Substance</u>) and can represent a significant proportion of a product. Crude butadiene category products arise from production processes associated with ethylene manufacturing. More information on the Crude Butadiene C4 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 Crude Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.</p>	trans-butene-2	99.97	0.03	99.98	0.02	butene-1	99.98	0.02	99.99	0.01	1,3-butadiene	99.97	0.03	99.97	0.03
trans-butene-2	99.97	0.03	99.98	0.02												
butene-1	99.98	0.02	99.99	0.01												
1,3-butadiene	99.97	0.03	99.97	0.03												
<p>Test Substance: (FT - TS)</p>	<p>25167-67-3 Butenes</p> <p>68477-41-8 Distillate (Petroleum), Extractive C3-5</p> <p>68955-28-2 Gases, (Petroleum) Light Steam Cracked, Butadiene Concentrate</p> <p>68476-44-8 Hydrocarbons, >C3</p> <p>68512-91-4 Hydrocarbons C3 – C4 Rich Petroleum Distillates</p> <p>68187-60-0 Hydrocarbons, C4, Ethane-Propane Cracked</p>															

	68476-52-8 Hydrocarbons, C4, Ethylene Manufactured By-Product 68956-54-7 Hydrocarbons C4, Unsaturated 69103-05-5 Hydrocarbons, C4-7, Butadiene Manufactured By-Product 64742-83-2 Naphtha, (Petroleum), Light Steam-Cracked
Conclusion: (FT - CL)	Products in the Crude Butadiene C4 Category are expected to distribute to air with a small percentage partitioning to water.
Reliability: (FT - RL)	(2) Reliable with restrictions The input data used to run the EQC Level I model include estimated values calculated by the EPIWIN program based on chemical structure, and experimental values supplied by the EPIWIN program databases. The partitioning data represent a potential distribution range for products with the 10 CAS numbers listed under <u>Test Substance</u> . Computer modeling is an accepted method of assessing environmental distribution of chemicals.
Reference: (FT - RE)	Mackay, D.A. DiGuardo, S. Paterson, and C. Cowan. EQC Model Version 1.01. 1997. Available from the Environmental Modeling Centre, Trent University, Canada.
Other (source): (FT - SO)	American Chemistry Council, Olefins Panel

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "transport / distribution". Selecting this option refers the reader to information in the "freetext" field for "test substance".

FT - Freetext

IUCLID fields include:

- RL - Reliability
- TC - Test Conditions
- RE - Reference
- RS - Results
- TS - Test Substance
- SO - Source
- CL - Conclusion

Biodegradation

Test Substance*:	Other TS
Method/Guideline:	Other: Technical discussion
Year (guideline):	Not applicable
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Inoculum:	Not applicable
Exposure Period:	Not applicable
Test Conditions: (FT - TC) <ul style="list-style-type: none"> Note: Concentration prep., vessel type, replication, test conditions. 	Not applicable
Results: (FT - RS) Units/Value: <ul style="list-style-type: none"> Note: Deviations from protocol or guideline, analytical method. 	Not applicable
Test Substance: (FT - TS)	25167-67-3 Butenes 68477-41-8 Distillate (Petroleum), Extractive C3-5 68955-28-2 Gases, (Petroleum) Light Steam Cracked, Butadiene Concentrate 68476-44-8 Hydrocarbons, >C3 68512-91-4 Hydrocarbons C3 – C4 Rich Petroleum Distillates 68187-60-0 Hydrocarbons, C4, Ethane-Propane Cracked 68476-52-8 Hydrocarbons, C4, Ethylene Manufactured By-Product 68956-54-7 Hydrocarbons C4, Unsaturated 69103-05-5 Hydrocarbons, C4-7, Butadiene Manufactured By-Product 64742-83-2 Naphtha, (Petroleum), Light Steam-Cracked
Conclusion: (FT - CL)	SUMMARY In the environment, biodegradation will not contribute significantly to the loss of chemicals in products from the

Crude Butadiene C4 Category (C4 refers to a chemical with 4 carbons). This category includes two process streams:

- **C4 Crude Butadiene**
- **Butadiene Unit Heavy Ends**

Ten CAS numbers (see Test Substance) identify products derived from these process streams. The products contain various chemicals composed of carbon and hydrogen. As discussed below, products in this category are gaseous. If they are released to the environment, their chemical components will partition primarily to the air where they can degrade rapidly by physicochemical reactions. It is far less likely that products from this category will partition to environmental compartments where they could be degraded by bacteria.

The Crude Butadiene C4 Category

A process stream is a mixture of chemicals that arises from a chemical reaction or separation activity. Process streams containing 10 to 92% butadiene are referred to as “crude butadiene.” The CAS numbers or streams in this category consist of complex mixtures of hydrocarbons.

Most commercial products in this category have a carbon number distribution predominantly between C3 and C5. All of these streams contain significant levels of 1,3-butadiene and olefins, which is why this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated Crude Butadiene C4.

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).

Crude butadiene streams arise from production processes associated with ethylene manufacturing. More information on the Crude Butadiene C4 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 three process streams in this category are:

- **C4 Crude Butadiene** is produced by the distillation of a condensed portion of cracked gas in an ethylene process.

C4 Crude Butadiene typically contains 40% to about 60% 1,3-butadiene, but could contain between 10% and 82% butadiene. Other chemicals in this mixed stream are predominately chemicals containing 4 carbons.

- **Butadiene Unit Heavy Ends** is produced by extractive distillation of cracked gas. The 1,3-butadiene content of this mixed stream ranges from 13% to 92%. Other chemicals in this mixed stream are predominately chemicals containing 4 carbons. Only three companies report isolating this stream which is more typically an unisolated intermediate.

Biodegradation of Hydrocarbons

Biodegradation is the use of a chemical by microorganisms as a source of energy and carbon. The parent chemical is broken down to simpler, smaller chemicals, which can be converted to inorganic forms such as carbon dioxide, nitrate, sulfate, and water.

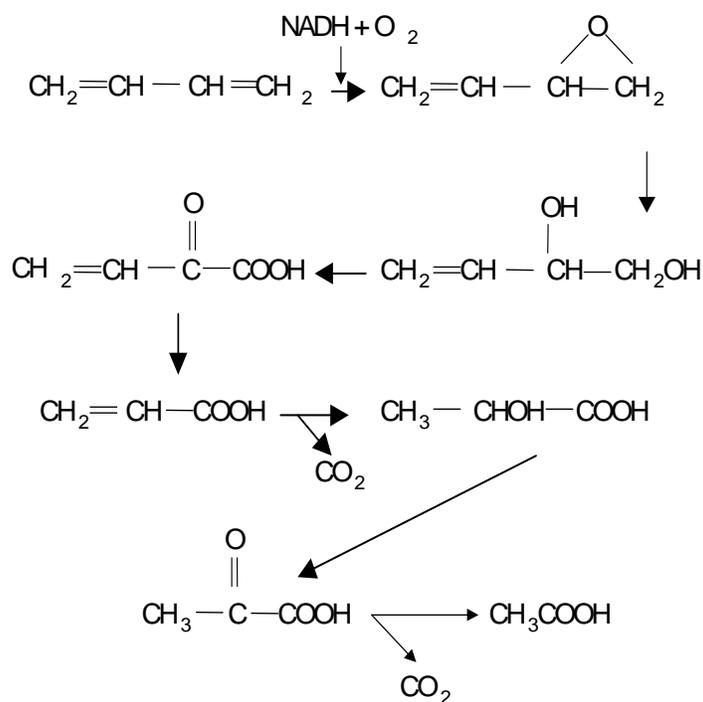
Products in the Crude Butadiene C4 Category are gaseous hydrocarbons, composed predominantly of chemicals with carbon numbers smaller than C5. However, the *Full-Range Butadiene Concentrates* process stream from this category, can contain hydrocarbons greater than C4. These chemicals when isolated individually are not gaseous, but relatively volatile liquids under most environmental conditions.

Several hydrocarbons as well as products that are mixtures of hydrocarbons with carbon numbers greater than C4 have been shown to biodegrade. If released to the environment, biodegradation of these chemicals will occur primarily in aquatic and terrestrial habitats. There is sufficient biodegradation data on hydrocarbons in this category that are greater than C4 to show that these chemicals have a potential to biodegrade to a great extent and not persist in the environment (see the *C5 Noncyclics, Low Benzene Naphtha, and High Benzene Naphtha* HPV Chemical Program test plans from the Olefins Panel of the American Chemistry Council, for specific data and a more detailed discussion of the biodegradability of selected hydrocarbons greater than C4.) The larger proportion of chemicals from this category are gaseous. Consequently, their availability to microbial degraders will be significantly limited.

Component chemicals from all three process streams in this category are simple hydrocarbons, the majority of which will partition primarily to the air where physical processes will contribute to their degradation [see the atmospheric oxidation potential (AOP) data (as mediated by hydroxyl radical

attack) for specific degradation rates of selected chemicals from this category; AOP data were developed for this category under the HPV Chemical Program]. All chemicals from this category that partition to the air are calculated to degrade rapidly due to physical processes and not persist. Because of the partitioning behavior of chemicals in this category, biodegradative processes will be less likely to contribute to their loss from the environment.

Products from the Crude Butadiene C4 Category do not lend themselves to being evaluated for biodegradability using standard experimental techniques because of their physical state. However, there is microbial metabolism information for one of the major chemicals, 1,3-butadiene, in this category that demonstrates that it can be biodegraded. Experimental studies to determine a catabolic pathway for 1,3-butadiene as mediated by a *Nocardia* sp. (3) resulted in the following proposed series of reactions:



The intermediary metabolic steps depicted above result in the production of acetic acid, CH₃COOH, which can be further metabolized. In addition, 1,3-butadiene has been estimated to have an aerobic aquatic biodegradation half-life ranging from 1 to 4 weeks (2).

The potential biodegradability of some of the higher molecular weight components including benzene, toluene, xylene, ethylbenzene, and naphthalene has been summarized

	<p>and metabolic pathways leading to their biodegradation have been described (4). These compounds have been shown to biodegrade to high extents such that if they were to partition to either a terrestrial or aqueous environment, they would be subject to biodegradative processes that would result in their removal from the environment.</p> <p>In summary, because the C4 and lighter chemical components of this category will partition to the air, physical degradative processes will dominate their fate. Data show that these chemicals are subject to rapid physical degradation. Chemical components of this category that are greater than C4 also have a potential to partition to the air to a great extent, where they will also degrade rapidly in a similar manner. However, they also have a potential to partition to aquatic and terrestrial environments where they are subject to biological processes that can result in their rapid biodegradation. Overall, products from this category and their component chemicals are expected to degrade rapidly in the environment and not persist.</p> <p>References</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 Crude Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. Virginia, USA. 2. Howard, P.H., R.S. Boethling, W.F. Jarvis, W.M. Meylan, and E.M. Michalenko. 1991. Handbook of Environmental Degradation Rates. H.T. Printup Ed. Lewis Publishers, Chelsea, MI, USA. 3. Watkinson, R.J. and H.J. Somerville. 1976. The Microbial Utilization of Butadiene. Shell Research Limited, Sittingbourne Research Centre, Kent, UK. 4. van Agteren, M.H., S. Keuning, and D.B. Janssen. 1998. Handbook on Biodegradation and Biological Treatment of Hazardous Organic Compounds. Kluwer Academic Publishers. Boston, CT, USA.
Reliability: (FT - RL)	Not applicable
Reference: (FT - RE)	American Chemistry Council, Olefins Panel. 2002. Hydrolysis: Crude Butadiene C4 Category. Rosslyn, VA, USA.
Other (source): (FT - SO)	American Chemistry Council, Olefins Panel

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "biodegradation". Selecting this option refers the reader to information in the "freetext" field for "test substance".

FT - Freetext

IUCLID fields include:

RL - Reliability

TC - Test Conditions

RE - Reference

RS - Results

TS - Test Substance

SO - Source

CL - Conclusion

HUMAN HEALTH ROBUST SUMMARIES

Acute Toxicity

<u>Test Substance</u>	
Remarks	Butadiene Concentrate, CAS# 68955-28-2 Gases (petroleum) light steam-cracked, butadiene conc. Approximately 45% 1,3-butadiene, 20% butanes, and 30% butenes.
<u>Method</u>	
Method/guideline followed	OECD 402.
Type (test type)	Acute inhalation.
GLP	Yes.
Year	1982.
Species/Strain	Rat/Fischer 344.
Sex	Males and females.
No. of animals per sex per dose	5/sex.
Vehicle	Not applicable.
Route of administration	Inhalation (gas).
Test Conditions	A group of ten rats (age: 12 weeks, weight: 143-234 grams) were exposed to 5,300 mg/m ³ (2,331 ppm) of the test substance in air for four hours. Analytical chamber concentrations were determined by gas chromatography every 15 minutes during the exposure; a single particle size sample was taken to show the absence of aerosol. Body weights were recorded prior to exposure and 7 and 14 days post-exposure. Individual clinical observations were recorded pre-exposure and daily for 14 days post-exposure. The rats were sacrificed on the fourteenth day and a gross necropsy performed.
<u>Results</u>	
LC50	Rat LC50 (4 hour) = >5,300 mg/m ³ (2,331 ppm)
Remarks	Observations noted following exposure were two male rats with respiratory sounds/wheezing or hyperexcitability and one female with minimal porphyrin around the eyes. All rats were normal from Days 2-14. No significant necropsy findings were reported, except one female with an ovary filled with red fluid. Body weight gains appeared normal.
<u>Conclusions</u>	
(study author)	No mortality or significant adverse effects were observed in rats exposed to 5,300 mg/m ³ (2,331 ppm) of the test substance.
<u>Data Quality</u>	
Reliability	Reliable without restrictions. Guideline study.
<u>References</u>	Gulf Oil Chemicals Company (1982). Acute LC50 Inhalation Toxicity Test in Rats with Butadiene Feedstock. Unpublished

	report (Project #82-060).
<i><u>Other</u></i>	Robust Summary prepared by ExxonMobil Biomedical Sciences, Inc.
<i>Last changed</i>	19-Oct-99

Acute Toxicity

<u>Test Substance</u>	1,3-butadiene CAS# 106-99-0
<u>Method</u>	
Method/guideline followed	Other.
Type (test type)	Acute inhalation.
GLP	Pre-GLP.
Year	1969.
Species/Strain	Rat and mouse (strains not specified).
Sex	Not specified.
No. of animals per sex per dose	Not specified.
Vehicle	Not applicable.
Route of administration	Inhalation (gas).
Test Conditions	Age, number, and sex of test animals not specified. Number of groups and exposure concentrations not specified. Dynamic flow exposure system; no description of exposure chambers or conditions. Rats exposed four hours; mice exposed two hours. No post-exposure observation period - mortality study only. Exposure concentrations "controlled" by gas chromatography.
<u>Results</u>	
LC50 with confidence limits	Rat LC50 (4 hour) = 285 mg/L (219-370 mg/L $p \leq 0.05$) Mouse LC50 (2 hour) = 270 mg/L (251-290 mg/L $p \leq 0.05$)
Remarks	No clinical observations or necropsy findings reported. Objective of study was to determine hydrocarbon concentrations in various tissues at lethal exposure concentrations.
<u>Conclusions</u>	
(study author)	LC50 value reported to be 285 mg/L (129,000 ppm) in rats, 270 mg/L (122,000 ppm) in mice.
<u>Data Quality</u>	
Reliability	Not assignable. Lethality study only; insufficient experimental detail to assess quality.
<u>References</u>	Shugaev, B.B. (1969) Concentrations of Hydrocarbons in Tissues as a Measure of Toxicity. Arch. Environ. Health 18:878-882.
<u>Other</u>	Robust Summary Prepared by ExxonMobil Biomedical Sciences, Inc.
<u>Last changed</u>	13-Oct-99

Acute Toxicity

<u>Test Substance</u>	Butadiene Concentrate, CAS# 68955-28-2 Gases (petroleum) light steam-cracked, butadiene conc. Approximately 67% 1,3-butadiene, 30% butenes, 2% 1,2-butadiene
<u>Method</u>	
Method/guideline followed	Other.
Type (test type)	Irritation screen in rabbits.
GLP	Yes.
Year	1985.
Species/Strain	Rabbit (New Zealand White).
Sex	1 male, 1 female.
Vehicle	Not applicable.
Route of administration	Eye and skin.
Remarks For Test Conditions	Two young adult rabbits were evaluated for eye and skin irritation. The test substance was dispensed immediately prior to dosing into a flask packed in dry ice. On the first treatment day, 0.1mL of the test substance was instilled into one eye of each rabbit. Irritation was scored at 24, 48, and 72 hours. The untreated eye served as the control. Twenty-four hours after treatment of the eye, 0.1mL of the test substance was applied to the skin of the rabbits and occluded with a rubber dam. The test sites were evaluated 1, 3, and 7 days after dosing.
<u>Results</u>	
Remarks	The eye irritation scores were 0 at all observation intervals. The treated skin sites were virtually free of irritation at all observation intervals.
<u>Conclusions</u>	
(study author)	The test substance is estimated not to be irritating to the eye or skin.
<u>Data Quality</u>	
Reliability	Reliable with restrictions. Screening study.
<u>References</u>	Mobil Environmental and Health Sciences Laboratory (1985). Irritation Screen of Butadiene Concentrate in Albino Rabbits, Unpublished report (Study No. 41652).
<u>Other</u>	Robust Summary prepared by ExxonMobil Biomedical Sciences, Inc.
<i>Last changed</i>	24-Oct-99

Genetic Toxicity - *in vitro*

<u>Test Substance</u>	
<i>Test substance</i>	1,3-butadiene CAS# 106-99-0
<u>Method</u>	
Method/guideline followed	No data.
Type	Reverse mutation assay (<i>Ames Salmonella</i> test).
System of testing	Bacterial.
GLP	No data.
Year	1990.
Species/Strain	<i>Salmonella typhimurium</i> /TA97, TA98, TA100, TA1535.
Metabolic activation	With and without.
Species and cell type	Rat, mouse, and human liver S9 fraction.
Quantity	0.8 and 4.0 mg protein/plate.
Induced or not induced	Arochlor 1254-induced and uninduced rat, mouse, and human S9.
Concentrations tested	0, 30, 40, 50, and 60% butadiene in air.
Statistical Methods	Not specified.
Remarks for Test Conditions	Concentrations of butadiene gas were metered into specially constructed treatment chambers holding the agar plates overlaid with the bacteria and activation system. Actual gas concentrations were determined by gas chromatography before and after the 48 hour exposure period. Different treatment chambers were used for each activation system and for the non-activated treatment. S9 preparations were made according to the procedure of Ames <i>et al.</i> (1975).
<u>Results</u>	1,3-Butadiene (BD) induced revertants only in strain TA1535. Mouse S9 showed slightly higher activity than the uninduced rat or human S9 at 30% 1,3-butadiene in air. At concentrations greater than 30%, the number of revertants decreased in the presence of rat or human S9. Results from the human S9-activated treatments did not differ substantially from those of the non-activated treatments. Arochlor 1254-induced rat S9 gave similar results as mouse S9 (uninduced). Since the response was weak, the S9 concentration was increased from 0.8 mg/plate to 4.0 mg/plate. Increasing the concentration of Arochlor 1254-induced rat S9 had no effect on the number of revertants; slightly more revertants were observed using 4.0 than 0.8 mg/plate of uninduced rat S9.
<u>Conclusions</u>	
(study author)	<i>Salmonella typhimurium</i> reverse gene mutation (<i>Ames</i>) tests of 1,3-butadiene using strains TA1535, TA97, TA98, and TA100 and employing rat, mouse, and human liver S9 metabolic systems were barely 2-fold above background only in strain TA1535 at 30% butadiene in air with induced and uninduced rat S9 and mouse S9 (uninduced). In general, 1,3-butadiene was a weak <i>in vitro</i> genotoxin.
<u>Data Quality</u>	
<i>Reliabilities</i>	Reliable without restrictions. Comparable to guideline study.
<u>Reference</u>	Arce G.T., Vincent D.R., Cunningham M.J, Choy W.N., and Sarrif

	A.M. (1990). <i>In vitro</i> and <i>in vivo</i> genotoxicity of 1,3-butadiene and metabolites. Environ. Health Perspect. 86:75-8.
<u>Other</u>	Robust Summary Prepared by ExxonMobil Biomedical Sciences, Inc.
<i>Last changed</i>	18-Oct-99

Genetic Toxicity - *in vitro*

<u>Test Substance</u>	
Test substance	Butadiene Concentrate, CAS# 68955-28-2. Gases (petroleum) light steam-cracked, butadiene conc. Approximately 45% 1,3-butadiene, 20% butanes, and 30% butenes.
<u>Method</u>	
Method/guideline followed	OECD 482.
Type	Unscheduled DNA Synthesis (UDS).
System of testing	Primary hepatocytes derived from Fischer 344 rats.
GLP	Yes.
Year	1984.
Metabolic activation	No.
Concentrations tested	0, 1000, 5000, 10000, and 20000 ppm.
Control groups and treatment	Negative = air only; positive = 2-acetylaminofluorene (0.2ug/mL).
Statistical Methods	Group means and standard deviations for number of viable cells and nuclear grain counts. The test substance was considered positive if the mean nuclear grain count exceeded the negative control by at least 6 grains per nucleus and the negative control did not exceed 5.
Remarks for Test Conditions	Primary hepatocytes were derived from freshly perfused rat liver (1 male, 10 weeks age, 226 grams body weight). Cultures were seeded with approximately 10 ⁵ cells/mL on Day 1. Three cultures per group were exposed to ³ H-thymidine and the test substance for 18-20 hours. The culture flasks were placed in sealed dessicator jars for the exposure period, and the test substance added by injection via a 50cc syringe. Cells growing on coverslips were fixed on Day 2. On Day 3 the slides were dipped in autoradiograph emulsion and stored in the dark at 2-8°C. The autoradiographs were developed and stained on Day 21.
<u>Results</u>	<p>A separate range-finding study was conducted to establish levels of cytotoxicity based on relative cell viability. The test substance was toxic to primary hepatocytes at 10000 ppm where 64% relative viability was observed following 18 hour exposure. At 20000 ppm, the relative viability was 57%.</p> <p>In the UDS study, both positive and negative control groups gave expected responses. A weak positive response was observed at 20000 ppm (7.74 nuclear grain counts vs. 1.24 in the air control vs. 107.13 in the positive control). The 1000, 5000, and 10000 ppm groups were also slightly increased (4.29-5.14) from the air control but less than the criteria for a significant response.</p>
<u>Conclusions</u>	
(study author)	Cytotoxicity was observed at 10000 ppm. Increased unscheduled DNA synthesis was observed at 20000 ppm.
<u>Data Quality</u>	
<i>Reliabilities</i>	Reliable without restrictions. Guideline study.
<u>Reference</u>	Gulf Oil Chemicals Company (1984). Hepatocyte Primary Culture/DNA Repair Test of Butadiene Feedstock, Unpublished report (Project# 2073).

<i><u>Other</u></i>	Robust Summary Prepared by ExxonMobil Biomedical Sciences, Inc.
<i>Last changed</i>	18-Oct-99

Genetic Toxicity - *in vitro*

<u>Test Substance</u>	
<i>Test substance</i>	Butadiene Concentrate, CAS# 68955-28-2 Gases (petroleum) light steam-cracked, butadiene conc. Approximately 45% 1,3-butadiene, 20% butanes, and 30% butenes.
<u>Method</u>	
<i>Method/guideline followed</i>	Other.
<i>Type</i>	Mammalian cell transformation test.
<i>System of testing</i>	BALB/3T3-A31-1-1 cells.
<i>GLP</i>	Yes.
<i>Year</i>	1983.
<i>Metabolic activation</i>	No.
<i>Concentrations tested</i>	0, 1000, 5000, 10000, and 20000 ppm.
<i>Control groups and treatment</i>	Negative = air only; positive = 3-methylcholanthrene (1.0 ug/mL).
<i>Statistical Methods</i>	Group means and standard deviations for number of viable cells, cloning efficiency, and transformed foci per culture. The test substance was considered positive if there was a two-fold increase in foci compared to the negative control group.
<i>Remarks for Test Conditions</i>	Each treatment group consisted of 12 flask cultures for cell transformation seeded with 10000 cells and 2 plate cultures for cloning efficiency with 250 cells. The cultures were placed in sealed dessicator jars and exposed to the test substance for two days. The test substance was added to the jars by injection via a 50cc syringe and samples of the exposure atmosphere were analyzed by gas chromatography. The mediums were changed on Day 4 and then weekly. Plate cultures were fixed and stained on Day 8 and flask cultures on Day 29. Foci in transformation cultures were counted and examined microscopically to determine type.
<u>Results</u>	Cloning efficiency was used as a measure of toxicity under culture conditions. Toxicity was observed at 5000 ppm where a relative cloning efficiency of 53.8% was observed. The negative and positive control gave expected responses for transformation. The response for the test substance was not increased from the negative control group at any level tested.
<u>Conclusions</u>	
<i>(study author)</i>	The test substance was negative for cell transformation.
<u>Data Quality</u>	
<i>Reliabilities</i>	Reliable without restrictions. Comparable to draft OECD guideline.
<u>Reference</u>	Gulf Oil Chemicals Company (1983). BALB/3T3 Transformation Test Using Butadiene Feedstock, Unpublished report (Project# 2074).
<u>Other</u>	Robust Summary Prepared by ExxonMobil Biomedical Sciences, Inc.
<i>Last changed</i>	18-Oct-99

Genetic Toxicity - *in vitro*

<u>Test Substance</u>	
Remarks	Butadiene Concentrate, CAS# 68955-28-2 Gases (petroleum) light steam-cracked, butadiene conc. Approximately 67% 1,3-butadiene, 30% butenes, 2% 1,2-butadiene.
<u>Method</u>	
Method/guideline followed	No data.
Type	Reverse mutation assay (Ames <i>Salmonella</i> test).
System of testing	Bacterial.
GLP	Yes.
Year	1985.
Species/Strain	<i>Salmonella typhimurium</i> / TA98, TA100, TA1535, TA1537, TA1538.
Metabolic activation	With and without.
Species and cell type	Rat liver S9 fraction.
Quantity	0.6 mL.
Induced or not induced	Arochlor 1254-induced.
Concentrations tested	25, 50, 75, or 100 μ L.
Statistical Methods	The test substance was considered mutagenic if it produced a dose-related two-fold increase in mean revertant value compared to the negative control.
Remarks for Test Conditions	The test substance was stored in a dry ice/ethanol slurry to prevent loss of volatile components and dosed by microdispenser into sterile septa-capped culture tubes. Sodium phosphate buffer or S-9/bacteria mix was injected through the septa into the tubes containing the test substance and pre-incubated for 20 minutes at 37°C. After the pre-incubation period, the contents of the tubes were overlayed on agar and incubated for 48 hours at 37°C. Revertant colonies were counted by automatic colony counter. Positive control chemicals were: 2.0 μ g 2-aminoanthracene, 15.0 μ g 9-aminoacridine, 20.0 μ g 2-nitrofluorene, and 5.0 μ g N-methyl-N-nitro-N-nitrosoguanidine, in 50 μ l DMSO per plate.
<u>Results</u>	A preliminary toxicity/initial mutagenicity assay was conducted over a range of 10 to 500 μ l per plate in two strains (TA100 and TA1537) with and without S-9. Toxicity was exhibited at $\geq 75 \mu$ L in TA100, and $\geq 100 \mu$ L in TA1537. Some inconsistencies in toxicity with increasing dose level were noted that were attributed to the volatility of the test substance. Based on the toxicity data, the test substance was tested in the pre-incubation mutagenicity assay at volumes of 25, 50, 75, and 100 μ l per plate. None of the five strains with or without induced rat liver S-9 exhibited reversion frequencies substantially different from spontaneous controls in this assay.
<u>Conclusions</u>	
(study author)	The test substance was not considered a mutagen with or without metabolic activation in this test system.

<u>Data Quality</u>	
<i>Reliabilities</i>	Reliable without restrictions. Comparable to guideline study.
<u>Reference</u>	Mobil Environmental and Health Sciences Laboratory (1985). An Ames Salmonella/Mammalian Microsome Mutagenesis Assay For Determination of Potential Mutagenicity of Butadiene Concentrate, Unpublished report (Study No. 41653).
<u>Other</u>	Robust Summary Prepared by ExxonMobil Biomedical Sciences, Inc.
<i>Last changed</i>	24-Oct-99

Genetic Toxicity - *in vitro*

<u>Test Substance</u>	
Remarks	Butadiene Concentrate, CAS# 68955-28-2 Gases (petroleum) light steam-cracked, butadiene conc. Approximately 67% 1,3-butadiene, 30% butenes, 2% 1,2-butadiene.
<u>Method</u>	
Method/guideline followed	Other.
Type	Mouse lymphoma mutagenesis assay.
System of testing	Mammalian cell.
GLP	Yes.
Year	1985.
Species/Strain	Mouse lymphoma cells/ L5178Y (TK+/-; subclone 3.7.2C).
Metabolic activation	With and without.
Species and cell type	Rat liver S9 fraction.
Quantity	4.0 mL.
Induced or not induced	Arochlor 1242/1254-induced.
Concentrations tested	Nonactivated assays: 10.0, 12.5, 15.0, 17.5, 20.0, 22.5, 25.0, 27.5, 30.0, 35.0 40.0, or 45.0 uL/mL media. S-9 activated assays: 2.5, 5.0, 7.5, 10.0, 12.5, 15.0, 17.5, 20.0, 22.5, or 25.0 uL/mL.
Statistical Methods	The test substance was considered mutagenic if it produced a dose-related or toxicity-related two-fold increase in average mutant frequency compared to the negative controls, at concentrations exhibiting acceptable total growths (10% or greater).
Remarks for Test Conditions	The positive control chemical for the S-9 activated assays was 7, 12-dimethylbenz[a]anthracene (DMBA) at 2.5 and 5.0 ug/mL, and ethylmethane sulfonate (EMS) for the nonactivated assays at 0.5 and 1.0 uL/mL. An initial toxicity assay was performed with and without activation at concentrations ranging from 10 to 100 uL/mL. The dosing regimen for the mutagenesis assay was designed to produce 10-90% lethality. Six mLs of cell suspension (10 ⁶ cells/mL) were exposed for 3 hours to the test or positive control substances. An expression period of 2 days followed with determinations of cell population densities and growth. Cultures selected for mutant analysis and cloning efficiencies were incubated for 10-12 days.
<u>Results</u>	Without activation, mutant frequencies and total number of mutants were significantly increased at the two highest concentrations (20.0 and 22.5 uL/mL). Although total growth was very low (5.1% and 5.5%), these levels were considered mutagenic since there was no reduction in cloning efficiency. There were no significant differences in mutant frequency for the S-9 activated cultures.
<u>Conclusions</u>	
(study author)	The test substance induced a significant increase in mutant frequency of mouse lymphoma cells without metabolic activation, but was evaluated as non-mutagenic in the presence of S-9 activation.

<u>Data Quality</u>	
<i>Reliabilities</i>	Reliable without restrictions. Comparable to guideline study.
<u>Reference</u>	Mobil Environmental and Health Sciences Laboratory (1985). Evaluation of the Mutagenic Potential of Butadiene Concentrate in the Mouse Lymphoma (L5178Y/TK+/-) Mutagenesis Assay, Unpublished report (Study No. 41654).
<u>Other</u>	Robust Summary Prepared by ExxonMobil Biomedical Sciences, Inc.
<i>Last changed</i>	24-Oct-99

Genetic Toxicity - *in vivo*

<u>Test Substance</u>	
Remarks	1,3-butadiene CAS# 106-99-0
<u>Method</u>	
Method/guideline followed	Other.
Type	Mammalian erythrocyte micronucleus assay.
GLP	No data.
Year	1994.
Species	Rat and mouse.
Strain	Rat: Wistar. Mouse: CB6F1
Sex	Rat: Male. Mouse: Female.
Route of administration	Inhalation (gas).
Doses/concentration levels	0, 50, 200, or 500 ppm.
Exposure period	6 hours/day for 5 days.
Statistical methods	Student's two-tailed t-test for differences between groups.
Remarks for Test Conditions.	Twenty female CB6F1 mice (approximately 25g, 8-10 weeks old) and ten male Wistar rats (300-350g, 10 weeks old) per group were exposed for 5 days, 6 h/day 0, 50, 200, or 500 ppm of 1,3-butadiene (BD) by inhalation. An additional high concentration group of mice was exposed to 1300 ppm. Exposure concentrations were monitored by infrared spectroscopy (rats) and gas chromatography (mice). The animals were sacrificed 1 day after the last exposure and smears of blood and bone marrow erythrocytes were prepared and stained.
<u>Results</u>	In the rats, no effects on micronuclei frequencies were observed either in the peripheral blood or bone marrow at all exposure levels. A slight toxic effect in rat bone marrow cells (decreased polychromatic/normochromatic ratio) was observed at the 500 ppm level. In the mice, a clear dose-dependent increase in micronuclei frequency was observed in both blood and bone marrow cells at all exposure levels tested.
<u>Conclusions</u>	
(study author)	1,3-butadiene was active in inducing micronuclei in peripheral blood and bone marrow erythrocytes in mice at levels ≥ 50 ppm, but not in rats. The genotoxic effects observed in this study parallel the species differences observed in cancer studies.
<u>Data Quality</u>	
<u>Reliabilities</u>	Reliable without restrictions. Comparable to guideline study.
<u>References</u>	Autio, K., Renzi, L., Catalan, J., Albrecht, O.E., and Sorsa, M. (1994). Induction of Micronuclei in Peripheral Blood and Bone Marrow Erythrocytes of Rats and Mice Exposed to 1,3-Butadiene by Inhalation. <i>Mut. Res.</i> 309:315-320.
	Robust Summary Prepared by ExxonMobil Biomedical Sciences, Inc.
<u>Last changed</u>	25-Oct-99

Genetic Toxicity - *in vivo*

<u>Test Substance</u>	
Remarks	Butadiene Concentrate, CAS# 68955-28-2 Gases (petroleum) light steam-cracked, butadiene conc. Approximately 45% 1,3-butadiene, 20% butanes, and 30% butenes.
<u>Method</u>	
Method/guideline followed	OECD 474
Type	Mammalian erythrocyte micronucleus test
GLP	Yes
Year	1984
Species	Mouse
Strain	CrI:CD-1 BR Swiss
Sex	Male and female
Route of administration	Inhalation (gas)
Doses/concentration levels	10,780; 20,671; 35,430 ppm
Exposure period	2 hours/day for 2 consecutive days
No. of animals per dose	10/sex/group
Control groups and treatment	10/sex negative (air) control; 5/sex positive control (cyclophosphamide, 75 mg/kg intraperitoneal injection)
Statistical methods	Group mean body weights, total polychromatic erythrocytes (PCEs), normochromatic erythrocytes (NORMs), PCEs with micronuclei, and NORMs with micronuclei were compared by t-test ($p < 0.05$ = positive).
Remarks for Test Conditions.	Mice were 11 weeks old and 25-42 grams weight at study initiation. Test and control substances were administered on Days 1 and 2. Exposure concentrations determined by gas chromatography. Animals were observed daily and body weights were recorded on Days 1, 3, and 4. Five mice/sex/group were sacrificed on Days 3 and 4 and bone marrow smears prepared; positive controls (5/sex) were sacrificed on Day 3 only.
<u>Results</u>	No mice died during the study; the only clinical observations were an apparent unconsciousness during exposure. There were no significant body weight differences. The negative and positive control groups produced negative and positive results, respectively. Mice in the exposed groups showed increased micronuclei formation at all levels in both sexes. Females were statistically increased from control at all levels on Day 3 and at 20,671 ppm and 35,430 ppm on Day 4; males were significantly increased only at 35,430 ppm on both days. There was no significant change in the PCE/NORM ratio in any group.
<u>Conclusions</u>	
(study author)	The test material produced an increased frequency of micronucleated erythrocytes in the bone marrow of mice at all levels tested.
<u>Data Quality</u>	
<u>Reliabilities</u>	Reliable without restrictions. Guideline study.
<u>References</u>	Gulf Oil Chemicals Company (1984). Micronucleus Test in Mouse Bone Marrow: Butadiene Feedstock Administered by

	Inhalation For 2 Hours/Day For 2 Days, Unpublished report (Project #2014).
<i>Other</i>	Robust Summary Prepared by ExxonMobil Biomedical Sciences, Inc.
<i>Last changed</i>	13-Oct-99

Repeated Dose Toxicity

<u>Test Substance</u>	
Remarks	1,3-butadiene, CAS# 106-99-0 Rubber grade, containing 0.02% t-butyl catechol; purity ≥98.94%.
<u>Method</u>	
Method/guideline followed	Other
Test type	14-week inhalation study
GLP	Yes
Year	1977
Species	Mouse
Strain	B6C3F1
Route of administration	Inhalation (gas)
Duration of test	14 weeks
Doses/concentration levels	0, 625, 1250, 2500, 5000, or 8000 ppm
Sex	10 male, 10 female per group
Exposure period	6 hours/day
Frequency of treatment	5 days/week, total of 63 or 64 exposures
Control group and treatment	10 male, 10 female, air-only exposed
Post exposure observation period	Not applicable
Statistical methods	Group means and standard deviations calculated for body weights.
Test Conditions	Groups of 10 mice/sex /group (4-5 weeks age at study initiation) were exposed to various levels of 1,3-butadiene for 6 hrs/day, 5 days/week for 14 weeks (64 exposures). Because four male mice in the high exposure group died by day 4, another 2 groups of 10 male mice each were restarted (control and 8000 ppm). Mice were observed once daily for morbidity and mortality; moribund animals were sacrificed. Body weights were recorded weekly. At the end of the 95 or 93-day (restart) studies, surviving mice were sacrificed. Necropsies were performed and tissues preserved. Histopathologic examinations were performed on all controls, high exposure (8000 ppm), and early deaths.
<u>Results</u>	
NOAEL (NOEL)	1250 ppm.
LOAEL (LOEL)	2500 ppm, based on reduced body weight gains.
Remarks	Six of ten males and 1/10 females exposed at 8000 ppm, 6/10 males and 1/10 females at 5000 ppm, and 1/10 males at 2500 or 1250 ppm died prior to study termination or were sacrificed in a moribund condition. Body weight gains were decreased in males at 2500, 5000, and 8000 ppm, and at 5000 and 8000 ppm in the females. No exposure-related histopathologic effects were observed in the high (8000 ppm) group.
<u>Conclusions</u>	Based on the results of this study, exposure levels of 625 and 1250 ppm were selected for a 2-year carcinogenicity study in

	mice based on reduced body weight gains and mortality in higher exposure groups.
<u>Data Quality</u>	
Reliabilities	Reliable with restrictions. Acceptable, well-documented study report but deficient by current guidelines. No organ weights, hematology or clinical chemistry evaluations were performed.
<u>References</u>	National Toxicology Program, Toxicology and Carcinogenesis Studies of 1,3-Butadiene (CAS No. 106-99-0) in B6C3F1 Mice (Inhalation Studies), NTP Technical Report Series No. 288, NIH Publication 84-2544 (1984).
<u>Other</u>	Robust Summary Prepared by ExxonMobil Biomedical Sciences, Inc.
Last changed	8-Dec-99

Repeated Dose Toxicity

<u>Test Substance</u>	
Remarks	1,3-butadiene, CAS# 106-99-0 Purity >99.2%, containing 120 ppm t-butyl catechol.
<u>Method</u>	
Method/guideline followed	Other.
Test type	13-week inhalation study.
GLP	No data.
Year	1977.
Species	Rat.
Strain	CD (Sprague-Dawley).
Route of administration	Inhalation (gas).
Duration of test	14 weeks.
Doses/concentration levels	0, 1000, 2000, 4000, or 8000 ppm.
Sex	40 male, 40 female per group.
Exposure period	6 hours/day.
Frequency of treatment	5 days/week for 13 weeks.
Control group and treatment	40 male, 40 female, exposed to filtered air only.
Post exposure observation period	Not applicable.
Statistical methods	Analysis of variance for body weights, food consumption, urinalysis, hematology, clinical chemistry, organ weights.
Test Conditions	Groups of 40 rats/sex /group (approx. 5 weeks age at study initiation) were exposed to various levels of 1,3-butadiene for 6 hrs/day, 5 days/week for 13 weeks. All animals were observed daily; individual body weights and food consumption were recorded weekly. Interim sacrifices of 10 rats/sex/group were performed after 2 and 6 weeks of exposure. Three urine samples were obtained from each animal during the 1-2 weeks prior to sacrifice. Blood samples were collected from all rats prior to the 2, 6, and 13 week sacrifices. Brain cholinesterase activity was measured using half the brain of 5 rats/sex/group at the 2 and 6-week sacrifices and all rats at the terminal sacrifice. Organ weights were recorded for the adrenals, brain, gonads, heart, kidneys, liver, lung, pituitary, spleen, and thyroid. Necropsies were performed and tissues preserved. Histopathologic examinations were performed on all control and high exposure (8000 ppm) tissues.
<u>Results</u>	
NOAEL (NOEL)	8000 ppm.
LOAEL (LOEL)	>8000 ppm.
Remarks	Increased salivation was observed in the females after 8 weeks exposure and decreased grooming (stained fur) in the males after 10 weeks. No other exposure-related conditions were observed. Male rats showed slight (non-statistically significant) reductions in body weight gains compared to the controls; female body weights at 1000 and 4000 ppm were statistically higher than the controls.

	<p>Neuromuscular function tests using a modified rotating cone gave some random group differences, but were not considered exposure-related. There were no toxicologically significant differences in hematology, blood chemistry, brain cholinesterase measurements, or urine analysis. Organ weight and organ to brain weight ratios showed some scattered statistically significant differences among the groups but did not indicate any treatment-related effects.</p> <p>Microscopic examination of the tissues of the exposed rats showed a similar incidence and severity of histopathologic findings to the control group.</p>
<u>Conclusions</u>	
(study author)	Rats exposed to butadiene gas at concentrations up to 8000 ppm showed no significant effects related to exposure.
<u>Data Quality</u>	
Reliabilities	Reliable without restrictions. Comparable to guideline study.
<u>References</u>	Crouch, C.N., Pullinger, D.H., and Gaunt, I.F. (1979) Inhalation Toxicity Studies With 1,3-butadiene - 2. 3 Month Toxicity Study in Rats. Am. Ind. Hyg. Assoc. J. 40:796-802.
<u>Other</u>	Robust Summary Prepared by ExxonMobil Biomedical Sciences, Inc.
Last changed	18-Oct-99

Repeated Dose Toxicity

<u>Test Substance</u>	
Remarks	Butadiene feedstock, CAS# 68955-28-2 Gases (petroleum) light steam-cracked, butadiene conc. Approximately 45% 1,3-butadiene, 20% butanes, and 30% butenes.
<u>Method</u>	
Method/guideline followed	Other.
Test type	9-day inhalation study.
GLP	Yes
Year	1982
Species	Rat
Strain	Fischer 344
Route of administration	Inhalation (gas)
Duration of test	12 days (9 exposures)
Doses/concentration levels	0, 2500, and 25100 mg/m ³ (0, 1110, and 11140 ppm)
Sex	5 male, 5 female per group.
Exposure period	6 hours/day.
Frequency of treatment	9 exposure days
Control group and treatment	5 male, 5 female, exposed to air only.
Post exposure observation period	Not applicable.
Statistical methods	Bartlett's test and analysis of variance for body and organ weights. If the Bartlett's test indicated homogeneity, Dunnett's test was also performed; if non-homogeneous, a modified t-test was done.
Remarks for Test Conditions	Three groups of 5 rats/sex /group (8 weeks age and 120-198 grams at study initiation) were exposed to 0, 2500, or 25100 mg/m ³ of the test substance for 6 hrs/day for a total of 9 exposures. The exposure regimen was 5 days of exposure , 2 days off, 4 days of exposure, then one day for the terminal sacrifice (12 days). Analytical chamber concentrations were determined by gas chromatography, 5 to 16 times per day in the low and high exposure chambers or approximately every 1.5 hours for the control chamber. A particle size sample was performed once daily for each exposure chamber to confirm the absence of aerosol. Individual animal observations were performed twice daily on exposure days and once daily on non-exposure days. Body weights were recorded prior to the first exposure and on Days 1, 7, and 12. Blood samples were obtained from all rats prior to sacrifice on Day 12. A gross necropsy was performed and organ weights recorded for the brain, heart, kidneys, liver, lung, and spleen. These organs plus the testes and ovaries were preserved and examined microscopically.
<u>Results</u>	
NOAEL (NOEL)	11140 ppm
LOAEL (LOEL)	>11140 ppm
Remarks	Most rats in both exposure groups appeared normal throughout

	the study. Nasal discharge was observed in some rats of both groups, and at a greater incidence in the high exposure group. There were no statistically significant differences between the control and exposed groups for mean body weight, organ weight, hematology, or blood chemistry values. There were no exposure-related histopathologic changes in any of the organs and tissues examined.
<u>Conclusions</u>	
(study author)	The 9-day repeated inhalation exposure of up to 11140 ppm (25100 mg/m ³) resulted in no significant adverse effects in rats.
<u>Data Quality</u>	
Reliabilities	Reliable without restrictions. Comparable to guideline study (OECD 412).
<u>References</u>	Gulf Oil Chemicals Company (1983). Nine-day Repeated Dose Inhalation Study in Rats Using Butadiene Feedstock, Unpublished report (Project #82-090). (1983). Gulf Life Sciences Center, Pittsburgh PA
<u>Other</u>	Robust summary prepared by ExxonMobil Biomedical Sciences, Inc.
Last changed	19-Oct-99

Developmental Toxicity/Teratogenicity

<u>Test Substance</u>	
Remarks	1,3-butadiene, CAS# 106-99-0 Purity 99.88%
<u>Method</u>	
Method/guideline followed	OECD 414.
Test type	Developmental toxicity (teratogenicity) study.
GLP	Yes.
Year	1987.
Species	Mouse.
Strain	CD-1 (Swiss).
Route of administration	Inhalation (gas).
Concentration levels	0, 40, 200, or 1000 ppm.
Sex	18-22 pregnant females per group.
Exposure period	Days 6-15 of gestation.
Frequency of treatment	6 hours/day.
Control group and treatment	Air-exposed only.
Duration of test	Females sacrificed on gestation day 18.
Statistical methods	Analysis of variance for body weights, number of resorptions, implants, live, dead or affected fetuses per litter. Significant differences among the groups were also analyzed by Duncan's multiple range test or arcsin transformation of the response proportion. Binary-response variables between groups were compared using chi-square or Fisher's exact test.
Remarks for Test Conditions.	Female mice were mated to unexposed males and exposed from days 6-15 of gestation to 0, 40, 200, or 1000 ppm of the test substance. Analytical chamber concentrations were measured by on-line gas chromatography. Body weights were recorded on gestation days 0, 6, 11, 16, and 18. Maternal animals were observed daily for mortality, morbidity, and signs of toxicity and examined for gross tissue abnormalities at necropsy (day 18). The uterus and placenta was removed and weighed; the number of implantation sites, resorptions, live and dead fetuses were recorded. Live fetuses were weighed and subjected to external, visceral, and skeletal examinations. Approximately 50% of the fetal heads were sectioned and examined.
<u>Results</u>	
NOAEL maternal toxicity	40 ppm.
NOAEL developmental toxicity	40 ppm.
	There were decreases in maternal body weight gains in the 200 and 1000 ppm groups. Fetal weights were significantly reduced in both males and females at 200 and 1000 ppm; placenta weights were significantly reduced for corresponding male fetuses at 200 ppm and for both males and females at 1000 ppm. There were no significant differences in percent resorptions or malformations per litter, although there was an increase in fetal variations (supernumary ribs and reduced ossification of sternbrae) at 200 and 1000 ppm.
<u>Conclusions</u>	

(study author)	Developmental toxicity was observed in mice in the presence of maternal toxicity at 200 and 1000 ppm. A slight statistically significant decrease in male fetal weight (95% of control) was also observed, but the biological significance of this finding has been questioned.
<u>Data Quality</u>	
<u>Reliabilities</u>	Reliable without restrictions. Guideline study.
<u>References</u>	Morrissey, R.E., Schwetz, B.A., Hackett, P.L., Sikov, M.R., Hardin, B.D., McClanahan, B.J., Decker, J.R., and Mast, T.J. (1990). Overview of Reproductive and Developmental Toxicity Studies of 1,3-Butadiene in Rodents. Environ. Health Perspect. 86:79-84.
<u>Other</u>	Robust Summary Prepared by ExxonMobil Biomedical Sciences, Inc.
<u>Last changed</u>	20-Oct-99

Developmental Toxicity/Teratogenicity

<u>Test Substance</u>	
Remarks	1,3-butadiene, CAS# 106-99-0 Purity 99.88%
<u>Method</u>	
Method/guideline followed	OECD 414.
Test type	Developmental toxicity (teratogenicity) study.
GLP	Yes.
Year	1987.
Species	Rat.
Strain	CD (Sprague-Dawley).
Route of administration	Inhalation (gas).
Concentration levels	0, 40, 200, or 1000 ppm.
Sex	24-28 pregnant females per group.
Exposure period	Days 6-15 of gestation.
Frequency of treatment	6 hours/day.
Control group and treatment	Air-exposed only.
Duration of test	Females sacrificed on gestation day 20.
Statistical methods	Analysis of variance for body weights, number of resorptions, implants, live, dead or affected fetuses per litter. Significant differences among the groups were also analyzed by Duncan's multiple range test or arcsin transformation of the response proportion. Binary-response variables between groups were compared using chi-square or Fisher's exact test.
Remarks for Test Conditions.	Female rats were mated to unexposed males and exposed from days 6-15 of gestation to 0, 40, 200, or 1000 ppm of the test substance. Analytical chamber concentrations were measured by on-line gas chromatography. Body weights were recorded on gestation days 0, 6, 11, 16, and 20. Maternal animals were observed daily for mortality, morbidity, and signs of toxicity and examined for gross tissue abnormalities at necropsy (day 20). The uterus and placenta was removed and weighed; the number of implantation sites, resorptions, live and dead fetuses were recorded. Live fetuses were weighed and subjected to external, visceral, and skeletal examinations. Approximately 50% of the fetal heads were sectioned and examined.
<u>Results</u>	
NOAEL maternal toxicity	200 ppm
NOAEL developmental toxicity	1000 ppm
toxicity	The only toxicity observed was decreased body weight gains in the dams at 1000 ppm. The percentage of pregnant animals and number of litters with live fetuses were unaffected by treatment. There were no significant differences among the groups for number of live fetuses per litter, percent resorptions or malformations per litter, placental or fetal body weights, or sex ratio.
<u>Conclusions</u>	

(study author)	There was no evidence of teratogenicity or adverse reproductive effects in any of the exposed groups.
<u>Data Quality</u>	
<u>Reliabilities</u>	Reliable without restrictions. Guideline study.
<u>References</u>	Morrissey, R.E., Schwetz, B.A., Hackett, P.L., Sikov, M.R., Hardin, B.D., McClanahan, B.J., Decker, J.R., and Mast, T.J. (1990). Overview of Reproductive and Developmental Toxicity Studies of 1,3-Butadiene in Rodents. Environ. Health Perspect. 86:79-84.
<u>Other</u>	Robust Summary Prepared by ExxonMobil Biomedical Sciences, Inc.
<u>Last changed</u>	20-Oct-99

Toxicity to Reproduction

<u>Test Substance</u>	
Remarks	1,3-butadiene, CAS# 106-99-0 Purity 99.88%
<u>Method</u>	
Method/guideline followed	Other.
Test type	Sperm-head morphology assay.
GLP	Yes.
Year	1987.
Species	Mouse.
Strain	B6C3F1.
Route of administration	Inhalation (gas).
Concentration levels	0, 200, 1000, and 5000 ppm.
Sex	20 males per group.
Exposure period	6 hours/day.
Frequency of treatment	5 days.
Control group and treatment	Air-exposed only.
Duration of test	Males sacrificed 5 weeks post-exposure.
Statistical methods	Normal and abnormal sperm heads were expressed as percentage of the total number of cells examined. These data were subjected to arcsin transformation and evaluated by analysis of variance. If significant, Duncan's multiple range test was used for intergroup differences. Dose response trends were determined by orthogonal contrast.
Remarks for Test Conditions.	The mice were observed twice daily and body weights recorded weekly. During the fifth week post-exposure the mice were sacrificed and examined for lesions of the reproductive tract and other gross abnormalities. Sperm was obtained from the cauda of the right epididymis. Slides were prepared, stained, and examined microscopically. The morphology of at least 500 sperm heads per mouse was categorized.
<u>Results</u>	
NOAEL	200 ppm The percentage of abnormal sperm heads increased with exposure concentration: 1.61% (0 ppm), 1.95% (200 ppm), 2.79% (1000 ppm), and 3.79% (5000 ppm). Only the values for the 1000 and 5000 ppm groups were significantly different from the control ($p < 0.05$). Only a single timepoint was examined, so the effect on all stages of spermatogenesis could not be determined.
<u>Conclusions</u>	
(Study author)	These results suggest that the test substance affected spermatogenesis in mice at 1000 and 5000 ppm, but the effect of this observation on other reproductive endpoints is not known.
<u>Data Quality</u>	
Reliabilities	Reliable with restrictions. Acceptable, well-documented publication which meets basic scientific principles.
<u>References</u>	
Morrissey, R.E., Schwetz, B.A., Hackett, P.L., Sikov, M.R.,	

	Hardin, B.D., McClanahan, B.J., Decker, J.R., and Mast, T.J. (1990). Overview of Reproductive and Developmental Toxicity Studies of 1,3-Butadiene in Rodents. Environ. Health Perspect. 86:79-84.
<i>Other</i>	Robust Summaries Prepared by ExxonMobil Biomedical Sciences, Inc.
<i>Last changed</i>	20-Oct-99

Toxicity to Reproduction

<u>Test Substance</u>	
Remarks	1,3-butadiene, CAS# 106-99-0 Purity 99.88%
<u>Method</u>	
Method/guideline followed	Other.
Test type	Rodent dominant lethal test.
GLP	Yes.
Year	1987.
Species	Mouse
Strain	CD-1 (Swiss).
Route of administration	Inhalation (gas).
Concentration levels	0, 200, 1000, and 5000 ppm.
Sex	20 males per group.
Exposure period	6 hours/day.
Frequency of treatment	5 days.
Control group and treatment	Air-exposed only.
Duration of test	8 weeks post-exposure.
Statistical methods	The number of implantation sites and intrauterine deaths per litter for each week were analyzed by analysis of variance. When appropriate, proportions of resorptions and dead or live fetuses per implant were subjected to arcsin transformation and evaluated by analysis of variance. If significant, Duncan's multiple range test was used for intergroup differences.
Remarks for Test Conditions.	After five days of exposure, the male mice were mated with unexposed females (two females per week for each male for 8 consecutive weeks). Females were removed from cohabitation after 7 days sacrificed 12 days later and the uterine contents examined. Observations included: the total number, position, and status of implantations; the numbers of early and late resorptions; and numbers of live and dead fetuses.
<u>Results</u>	Slight statistically significant effects were noted in the mated females for three endpoints during the first 2 weeks post-exposure: ratio of dead to total implants, percentage of females with ≥ 2 dead implants, and number of dead implants per pregnancy. However, these observations only occurred in the two lower exposure groups (except for increased number dead implants/pregnancy in the 5000 ppm group during week 1). There were no differences for number of pregnant females, implantations per litter, number of live fetuses, dead implantations per total implantations, or number of resorptions during weeks 1 and 2. There were no differences for any endpoint during weeks 3-8.
<u>Conclusions</u>	
(Study author)	The authors concluded that the results observed during the first two weeks are consistent with an adverse effect on more mature germ cells (spermatozoa and spermatids) however considering the lack of effects in the high exposure group the findings are not clear for a

	dose-dependent response.
<u>Data Quality</u>	
<i>Reliabilities</i>	Reliable with restrictions. Acceptable, well-documented publication which meets basic scientific principles.
<u>References</u>	Morrissey, R.E., Schwetz, B.A., Hackett, P.L., Sikov, M.R., Hardin, B.D., McClanahan, B.J., Decker, J.R., and Mast, T.J. (1990). Overview of Reproductive and Developmental Toxicity Studies of 1,3-Butadiene in Rodents. Environ. Health Perspect. 86:79-84.
<u>Other</u>	Robust Summary Prepared by Exxon Biomedical Sciences, Inc.
<i>Last changed</i>	20-Oct-99

Genetic Toxicity - *in vivo*

<u>Test Substance</u>	
Remarks	C4 Crude Butadiene (Low 1,3-Butadiene Content) approx. composition: 10% 1,3-butadiene, 4% isobutane, 4% n-butane, 29% trans-2-butene, 29% 1-butene, 11% isobutylene, 12% cis-2-butene Primary CAS #: 68476-52-8 Other CAS #s in the stream: 25167-67-3, 64742-83-2, 68187-60-0, 68476-44-8, 68955-28-2, and 68956-54-7.
<u>Method</u>	
Method/guideline followed	U.S. EPA OPPTS 870.5395 (1998) and OECD # 474 (1997) guidelines.
Type	Mammalian erythrocyte micronucleus assay.
GLP	Yes.
Year	2001.
Species	Mouse.
Strain	B6C3F1
Sex	Male and Female
Route of administration	Inhalation (gas).
Doses/concentration levels	0, 0.5, 10.0, or 20.0 mg/L.
Exposure period	4 hours/day for 2 days.
Statistical methods	The raw data on the counts of MN-PCE for each animal were first transformed by adding one (1) to each count and then taking the natural log of the adjusted number. The transformed MN-PCE data and the data on percent PCE were analyzed separately by a two-way analysis of variance (Winer, 1971). The sex-by-dose interaction in the two-way analysis was reviewed and if significant, a one-way analysis was performed for each sex. Pairwise comparisons of treated vs. control groups were done, if the dose effect was significant, by Dunnett's t-test, one-sided (upper) for MNPCE and two-sided for the percent PCE (Winer 1971). Linear dose-related trend tests were performed only if any of the pairwise comparisons yielded significant differences. The alpha level at which all tests were conducted was 0.05.
Remarks for Test Conditions.	Groups of six male B6C3F1 mice (approximately 26g, 9 weeks old) and six female B6C3F1 mice (approximately 21g, 9 weeks old) were exposed whole-body inhalation to target concentrations of 0, 0.5, 10.0, and 20.0 mg/L of the C4 Crude Butadiene, Low 1,3-Butadiene Content. All inhalation exposures occurred under dynamic airflow conditions and chamber concentrations were monitored by analytical methods. Inhalation exposures occurred on two consecutive days, 4 hours per day. A positive control group was dosed by oral gavage with 120 mg/kg of cyclophosphamide approximately 24 hours before sacrifice. Groups of animals (6/sex/dose) were sacrificed at 24 hours after the second treatment for the collection of femoral bone marrow to evaluate the incidence of micronuclei (MN) in polychromatic erythrocytes (2000 PCE/animal) The proportion of PCE among erythrocytes in the bone marrow was estimated by examining 200

	erythrocytes/animal.
<u>Results</u>	Statistically significant increases in the frequencies of MN-PCE in both sexes of all groups treated with the test material were observed as compared to the negative controls. Although statistical analyses indicated a significant dose response, the difference in MN-PCE incidence at the high- (20 mg/L) and low- (0.5 mg/L) dose was minimal. The positive control treatment induced a significant increase in the frequency of MN-PCE. The mean proportion of PCE among the erythrocytes (200/animal) in the bone marrow was not affected following exposure to the test material while the positive control treatment significantly reduced this value.
<u>Conclusions</u>	
(study author)	C4 Crude Butadiene (low 1,3-butadiene content) was positive for the induction of micronuclei in this test system under the experimental conditions used.
<u>Data Quality</u>	
<u>Reliabilities</u>	Reliable without restrictions.
<u>References</u>	<p>Organisation for Economic Co-Operation and Development (OECD) (1997). Guidelines for Testing of Chemicals. #474. Genetic Toxicology: Micronucleus Test, OECD Publication Service, 2 Rue Andre-Pascal, 75775 Paris Cedex 16, France.</p> <p>U.S. EPA (1998). Office of Prevention, Pesticides and Toxic Substances, OPPTS 870.5395. <i>In Vivo Mammalian Bone Marrow Cytogenetic Tests - Micronucleus assay</i></p> <p>Winer, B. J. (1971). <i>Statistical Principles in Experimental Design</i> (2nd Edition). McGraw-Hill, New York, New York.</p> <p>Spencer, T.J., Hammond, T.A., Houtman, C.E. and Marty, G.T. (2001). The valuation of C4 crude butadiene (low 1,3-butadiene content) in the mouse bone marrow micronucleus test by an inhalation exposure - multiple exposures followed by a single sampling point. Report of The Dow Chemical Company conducted for the American Chemistry Council, Olefins Panel.</p>
<u>Other</u>	Last updated: Robust summary prepared by contractor to Olefins Panel

Repeated Dose Toxicity

<u>Test Substance</u>	
Remarks	C4 Crude Butadiene (low 1,3-Butadiene Content), approx. composition: 10% 1,3-butadiene, 4% isobutane, 4% n-butane, 29% trans-2-butene, 29% 1-butene, 11% isobutylene, 12% cis-2-butene Primary CAS#: 68476-52-8; Other CAS #s used to represent this stream : 25167-67-3, 64742-83-2, 68187-60-0, 68476-44-8, 68955-28-2, and 68956-54-7
<u>Method</u>	
Method/guideline followed	OECD 422
Test type	Combined repeated exposure inhalation toxicity study with the reproduction / developmental screening test
GLP	Yes
Year	2001
Species	Rat
Strain	CrI:CD [®] (Sprague-Dawley) IGS BR
Route of administration	Inhalation (vapor).
Duration of test	36-37 days
Doses/concentration levels	0, 2, 10, or 20 mg/L (0; 2,000; 10,000; or 20,000 mg/m ³)
Sex	12 male, 12 female per group.
Exposure period	6 hours/day.
Frequency of treatment	7 days/week
Control group and treatment	12 male, 12 female, air-only exposed.
Post exposure observation period	Not applicable.
Statistical methods	Adult body weights, body weight gains, feed consumption, organ weights, clinical chemistry data and appropriate hematologic data were evaluated by ANOVA. Detailed clinical observation incidence scores for ranked observations and sensory evaluation scores were statistically analyzed by a z-test of proportions. Rectal temperature and grip performance were analyzed by an analysis of covariance with dose as the factor and time as the covariate. Motor activity was analyzed by a repeated-measure design with treatment as a between-subjects factor and the repeated factor of time.
Test Conditions	Groups of 12 male and 12 female CD rats were exposed to vapors of the test material daily by inhalation for approximately six hours/day at exposure levels of 0, 2, 10, or 20 mg/L (0; 2,000; 10,000; or 20,000 mg/m ³). The main study (repeated-exposure general toxicity and neurotoxicity endpoints) males and females were exposed for 36 and 37 days, respectively. Effects on general toxicity, neurobehavioral activity, clinical chemistry, and hematology were evaluated. In addition, a gross necropsy with extensive histopathologic examination of tissues was conducted. The study also contained reproductive and developmental toxicity satellite groups (summarized separately).

<u>Results</u>	
NOAEL (NOEL)	20 mg/L (20,000 mg/m ³).
LOAEL (LOEL)	Not applicable.
Remarks	<p>Actual time-weighted averages for total olefins for the 2, 10 and 20 mg/L (2,000; 10,000; or 20,000 mg/m³) exposure groups were 2.17 ± 0.461, 9.81 ± 1.66, 19.1 ± 2.63 mg/L, respectively, over the 37 exposure days in the study. Owing in part to the nature of the test material, there were technical difficulties in generating vapors from the test material, such that targeted exposure concentrations were not met on one entire day and for brief periods on a few other days. However, the affected instances were limited relative to the total duration of the study and were considered to have no significant impact on study integrity.</p> <p>There were no deaths or treatment-related clinical observations noted. No significant differences in body weights or feed consumption were observed for the males or females at any dose level tested throughout the duration of the study. Sensory evaluation, rectal temperature, and fore/hindlimb grip performance data revealed no treatment-related findings. Treatment did not affect motor activity total counts (treatment-by-time interaction, p = 0.0930). However, the treatment-by-time-by-epoch interaction was significant (p = 0.0098). Examination of the data suggested that this effect could be reasonably attributed to the significant time-by-epoch interaction (p = 0.0001) rather than to a true treatment effect. This was confirmed following calculation of linear contrasts to determine which group(s), if any, were different from the control group. These analyses revealed that none of the three treatment groups were significantly different from control (alpha > 0.02) when the time-by-epoch-by-treatment interaction was considered.</p> <p>There were no treatment-related changes for males and females at any dose level for prothrombin time, hematology values or clinical chemistry measures. Females exposed to 2 mg/L had a statistically identified increase in hematocrit value, and a statistically identified decrease in serum total protein. Given the lack of dose response, effects on related parameters, and similar effects in males, these were considered incidental findings that were toxicologically insignificant. There were no effects of exposure on organ weights, gross pathology or histopathology in any of the treated groups when compared to their respective controls.</p>
<u>Conclusions</u>	Repeated inhalation exposure of C4 Crude Butadiene, Low 1,3-Butadiene to male and female Sprague Dawley rats at levels of 0, 2, 10, or 20 mg/L (0; 2,000; 10,000; or 20,000 mg/m ³) produced no evidence of any adverse effects on clinical observations, organ weights, gross or histopathology, neurobehavioral activity, clinical chemistry or hematology endpoints. Based on these data, the no-observable-effect level

	(NOEL) for repeated dose toxicity was 20 mg/L, the highest concentration tested.
<u>Data Quality</u>	
Reliabilities	Klimisch value = 1 (Reliable without restrictions).
<u>References</u>	Carney, E.W., Liberacki, A.B., Thomas, J., Houtman, C.E. and Marable, B.R. (2001). C4 Crude butadiene, low 1,3-butadiene content: a combined repeated exposure inhalation toxicity study with the reproduction/developmental screening test in Sprague Dawley rats. Report of The Dow Chemical Company conducted for the American Chemistry Council, Olefins Panel.
<u>Other</u>	
Last changed	6-Aug-01 Robust summary prepared by contract to Olefins Panel

Toxicity to Reproduction

<u>Test Substance</u>	
Remarks	C4 Crude Butadiene (low 1,3-Butadiene Content) approx. composition: 10% 1,3-butadiene, 4% isobutane, 4% n-butane, 29% trans-2-butene, 29% 1-butene, 11% isobutylene, 12% cis-2-butene Primary CAS#: 68476-52-8; Other CAS #s used to represent this stream: 25167-67-3, 64742-83-2, 68187-60-0, 68476-44-8, 68955-28-2, and 68956-54-7
<u>Method</u>	
Method/guideline followed	OECD 422
Test type	Combined repeated exposure inhalation toxicity study with the reproduction / developmental screening test
GLP	Yes.
Year	2001
Species	Rat
Strain	CrI:CD [®] (Sprague-Dawley) IGS BR
Route of administration	Inhalation (vapor).
Duration of test	Two weeks prior to breeding, during breeding (up to two weeks), and continuing through day 19 of gestation. The dams were then allowed to deliver their litters, which were retained until postnatal day 4. The males were exposed for 36-37 days.
Doses/concentration levels	0, 2, 10, or 20 mg/L (0; 2,000; 10,000; or 20,000 mg/m ³)
Sex	12 male, 12 female per group.
Exposure period	6 hours/day.
Frequency of treatment	7 days/week
Control group and treatment	12 male, 12 female, air-only exposed.
Post exposure observation period	Not applicable.
Statistical methods	Adult body weights and feed consumption, maternal body weight gains, and pup body weights were analyzed by ANOVA. Gestation length, average time to mating (precoital interval) and litter size were analyzed using a nonparametric ANOVA. Pregnancy rates and mating, conception, fertility and gestation indices were analyzed by the Fisher exact probability test. Evaluation of the neonatal sex ratio was performed by the binomial distribution test. Post-implantation loss, pup survival indices, and other incidence data among neonates were analyzed using the litter as the experimental unit by a censored Wilcoxon test.
Test Conditions	Groups of 12 male and 12 female Sprague Dawley rats were exposed to vapors of the test material daily by inhalation for approximately six hours/day at exposure levels of 0, 2, 10, or 20 mg/L (0; 2,000; 10,000; or 20,000 mg/m ³). The study design included a main study for repeated dose toxicity end points (summarized separately) and reproductive / developmental toxicity satellite groups of 12 females per exposure level. The reproductive and developmental toxicity satellite groups were

	<p>exposed for two weeks prior to breeding, during breeding (up to two weeks), and continuing through day 19 of gestation. Males from the main study were used to breed these females. The dams were allowed to deliver their litters, which were retained until postnatal day 4. Effects on general toxicity, gonadal function, mating behavior, implantation, and general fertility were evaluated in the satellite group adults, followed by a gross necropsy of the satellite group females on lactation day 5. Litter size, pup survival, sex, body weight, and the presence of gross external malformations was assessed in the offspring. The males were exposed for a total of 36 to 37 days, and were then necropsied. In addition to the repeated dose toxicity end points assessed (discussed separately), reproductive assessment of the males included mating, conception and fertility indices, reproductive organ weights and gross/histopathology of the reproductive tract. Testis histopathology included a qualitative assessment of stages of the spermatogenic cycle.</p>
Results	
NOAEL (NOEL)	20 mg/L (20,000 mg/m ³).
LOAEL (LOEL)	Not applicable.
Remarks	<p>Actual time-weighted averages for total olefins for the 2, 10 and 20 mg/L (2,000; 10,000; or 20,000 mg/m³) exposure groups were 2.17 ± 0.461, 9.81 ± 1.66, 19.1 ± 2.63 mg/L, respectively, over the 37 exposure days in the study. Owing in part to the nature of the test material, there were technical difficulties in generating vapors from the test material, such that targeted exposure concentrations were not met on one entire day and for brief periods on a few other days. However, the affected instances were limited relative to the total duration of the study and were considered to have no significant impact on study integrity.</p> <p>There were no deaths or treatment-related clinical observations noted. No significant differences in parental body weights, body weight gains or feed consumption were observed at any dose level tested throughout the duration of the study. The only exception to this was a statistically identified increase in feed consumption noted for the 10 mg/L satellite females during the premating period (days 7-14). However, this increase was considered spurious, as feed consumption increases were not noted during subsequent gestation and lactation periods and similar changes in feed consumption were not observed at the highest exposure level of 20 mg/L.</p> <p>There were no treatment-related effects at any dose level on any of the reproductive parameters evaluated in this study. These included measures of reproductive performance (mating, conception and fertility, time to mating, gestation length, litter size), offspring survival (gestation and postnatal survival indices, percent pre- and post-implantation loss), pup body weight and pup sex ratio. The only statistically identified</p>

	change in any of these parameters was an increase in post-implantation loss occurring only at the low-dose. This was considered a spurious finding, given the lack of a dose response. Of the 12 females mated in each group, the number of viable litters produced was 11, 11, 11, and 12 for the 0, 2, 10 and 20 mg/L (0; 2,000; 10,000; or 20,000 mg/m ³) exposure level groups, respectively. External morphological alterations observed in the pups were limited to a hernia observed in a single pup from the high dose group. Given the low incidence of this finding, it was considered spurious and unrelated to exposure.
<u>Conclusions</u>	Repeated inhalation exposure of C4 Crude Butadiene, Low 1,3-Butadiene to male and female Sprague Dawley rats at levels of 0, 2, 10, or 20 mg/L (0; 2,000; 10,000; or 20,000 mg/m ³) produced no evidence of adverse effects on any measures of reproductive function. Based on these data, the no-observable-effect level (NOEL) for reproductive toxicity was 20 mg/L, the highest concentration tested.
<u>Data Quality</u>	
Reliabilities	Klimisch value = 1 (Reliable without restrictions).
<u>References</u>	Carney, E.W., Liberacki, A.B., Thomas, J., Houtman, C.E. and Marable, B.R. (2001). C4 Crude butadiene, low 1,3-butadiene content: a combined repeated exposure inhalation toxicity study with the reproduction/developmental screening test in Sprague Dawley rats. Report of The Dow Chemical Company conducted for the American Chemistry Council, Olefins Panel.
<u>Other</u>	
Last changed	6-Aug-01 Robust summary prepared by contractor to Olefins Panel

Developmental Toxicity/Teratogenicity

<u>Test Substance</u>	
Remarks	C4 Crude Butadiene (low 1,3-Butadiene Content), approx. composition: 10% 1,3-butadiene, 4% isobutane, 4% n-butane, 29% trans-2-butene, 29% 1-butene, 11% isobutylene, 12% cis-2-butene Primary CAS#: 68476-52-8; Other CAS #s used to represent this stream : 25167-67-3, 64742-83-2, 68187-60-0, 68476-44-8, 68955-28-2, and 68956-54-7
<u>Method</u>	
Method/guideline followed	OECD 422
Test type	Combined repeated exposure inhalation toxicity study with the reproduction / developmental screening test
GLP	Yes.
Year	2001
Species	Rat
Strain	CrI:CD [®] (Sprague-Dawley) IGS BR
Route of administration	Inhalation (vapor).
Duration of test	Two weeks prior to breeding, during breeding (up to two weeks), and continuing through day 19 of gestation. The dams were then allowed to deliver their litters, which were retained until postnatal day 4.
Doses/concentration levels	0, 2, 10, or 20 mg/L
Sex	12 male, 12 female per group.
Exposure period	6 hours/day.
Frequency of treatment	7 days/week
Control group and treatment	12 male, 12 female, air-only exposed.
Post exposure observation period	Not applicable.
Statistical methods	Adult body weights and feed consumption, maternal body weight gains, and pup body weights were analyzed by ANOVA. Gestation length, average time to mating (precoital interval) and litter size were analyzed using a nonparametric ANOVA. Pregnancy rates and mating, conception, fertility and gestation indices were analyzed by the Fisher exact probability test. Evaluation of the neonatal sex ratio was performed by the binomial distribution test. Post-implantation loss, pup survival indices, and other incidence data among neonates were analyzed using the litter as the experimental unit by a censored Wilcoxon test.
Test Conditions	Groups of 12 male and 12 female Sprague Dawley rats were exposed to vapors of the test material daily by inhalation for approximately six hours/day at exposure levels of 0, 2, 10, or 20 mg/L. The study design included a main study for repeated dose toxicity end points (summarized separately) and reproductive / developmental toxicity satellite groups of 12 females per exposure level. The reproductive and developmental toxicity satellite groups were exposed for two weeks prior to breeding,

	during breeding (up to two weeks), and continuing until day 19 of gestation. Males from the main study were used to breed these females. The dams were allowed to deliver their litters, which were retained until postnatal day 4. Effects on general toxicity, gonadal function, mating behavior, implantation, and general fertility were evaluated in the satellite group adults, followed by a gross necropsy of the satellite group females on lactation day 5. Litter size, pup survival, sex, body weight, and the presence of gross external malformations was assessed in the offspring.
<u>Results</u>	
NOAEL (NOEL)	20 mg/L.
LOAEL (LOEL)	Not applicable.
Remarks	<p>Actual time-weighted averages for total olefins for the 2, 10 and 20 mg/L exposure groups were 2.17 ± 0.461, 9.81 ± 1.66, 19.1 ± 2.63 mg/L, respectively, over the 37 exposure days in the study. Owing in part to the nature of the test material, there were technical difficulties in generating vapors from the test material, such that targeted exposure concentrations were not met on one entire day and for brief periods on a few other days. However, the affected instances were limited relative to the total duration of the study and were considered to have no significant impact on study integrity.</p> <p>There were no deaths or treatment-related clinical observations noted. No significant differences in parental body weights, body weight gains or feed consumption were observed at any dose level tested throughout the duration of the study. There were no treatment-related effects at any dose level on any of the reproductive parameters evaluated in this study. These included measures of reproductive performance (mating, conception and fertility, time to mating, gestation length, litter size), offspring survival (gestation and postnatal survival indices, percent pre- and post-implantation loss), pup body weight and pup sex ratio. The only statistically identified change in any of these parameters was an increase in post-implantation loss occurring only at the low-dose. This was considered a spurious finding, given the lack of a dose response. Of the 12 females mated in each group, the number of viable litters produced was 11, 11, 11, and 12 for the 0, 2, 10 and 20 mg/L exposure level groups, respectively. External morphological alterations observed in the pups were limited to a hernia observed in a single pup from the high dose group. Given the low incidence of this finding, it was considered to be a spontaneous finding unrelated to exposure.</p>
<u>Conclusions</u>	Repeated inhalation exposure of C4 Crude Butadiene, Low 1,3-Butadiene to male and female Sprague Dawley rats at levels of 0, 2, 10, or 20 mg/L produced no evidence of developmental toxicity or teratogenicity, as assessed in the OECD 422 study design. Based on these data, the no-observable-effect level (NOEL) for developmental toxicity was 20 mg/L, the highest

	concentration tested.
<u>Data Quality</u>	
Reliabilities	Klimisch value = 1 (Reliable without restrictions).
<u>References</u>	Carney, E.W., Liberacki, A.B., Thomas, J., Houtman, C.E. and Marable, B.R. (2001). C4 Crude butadiene, low 1,3-butadiene content: a combined repeated exposure inhalation toxicity study with the reproduction/developmental screening test in Sprague Dawley rats. Report of The Dow Chemical Company conducted for the American Chemistry Council Olefins Panel.
<u>Other</u>	
Last changed	6-Aug-01 Robust summary prepared by contractor to Olefins Panel

AQUATIC TOXICITY ROBUST SUMMARIES

Fish Acute Toxicity

Test Substance*:	Other TS																								
Method/Guideline*:	Other: ECOSAR Computer Model																								
Year (guideline):	1999																								
Type (test type):	Acute Fish Toxicity Calculation; LC50																								
GLP:	Not applicable																								
Year (study performed):	Not applicable																								
Species:	Freshwater Fish (calculated toxicity values are not species specific)																								
Analytical Monitoring:	Not applicable																								
Exposure Period:	96 hours																								
Statistical Method: (FT - ME)*	Not applicable																								
Test Conditions: (FT - TC) <ul style="list-style-type: none"> Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading. 	<p>Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2). KOWWIN also has a database of experimental Kow values (EXPKOW.DB).</p> <p>The following chemicals are representative of products in the Crude Butadiene C4 Category, which are complex, multi-constituent substances. The range of toxicity data for component chemicals is an estimate of the potential toxicity of category products.</p> <table border="1"> <thead> <tr> <th><u>Chemical</u></th> <th>Calculated <u>log K_{ow}</u></th> <th>Measured* <u>log K_{ow}</u></th> </tr> </thead> <tbody> <tr> <td>Isobutane</td> <td>2.23</td> <td>2.76</td> </tr> <tr> <td>n-butane</td> <td>2.31</td> <td>2.89</td> </tr> <tr> <td>isobutylene</td> <td>2.23</td> <td>2.34</td> </tr> <tr> <td>cis-butene-2</td> <td>2.09</td> <td>2.31</td> </tr> <tr> <td>trans-butene-2</td> <td>2.09</td> <td>2.33</td> </tr> <tr> <td>butene-1</td> <td>2.17</td> <td>2.40</td> </tr> <tr> <td>1,3-butadiene</td> <td>2.03</td> <td>1.99</td> </tr> </tbody> </table>	<u>Chemical</u>	Calculated <u>log K_{ow}</u>	Measured* <u>log K_{ow}</u>	Isobutane	2.23	2.76	n-butane	2.31	2.89	isobutylene	2.23	2.34	cis-butene-2	2.09	2.31	trans-butene-2	2.09	2.33	butene-1	2.17	2.40	1,3-butadiene	2.03	1.99
<u>Chemical</u>	Calculated <u>log K_{ow}</u>	Measured* <u>log K_{ow}</u>																							
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	<p>* Experimental K_{ow} values supplied by the KOWWIN program database (EXPKOW.DB) which contains more than 13,000 organic compounds with reliably measured values.</p> <p>Commercial products in this category can have a carbon number distribution predominantly between C3 and C5. These products can contain significant levels of 1,3-butadiene and similar low molecular weight olefins, which is why they are considered a category for purposes of the High Production Volume Chemical Program, and designated <u>Crude Butadiene C4</u>.</p> <p>The seven chemicals selected to represent the fish acute toxicity range of this category are C4 hydrocarbons that are common across the 10 CAS numbers (see <u>Test Substance</u>). Crude butadiene category products arise from production processes associated with ethylene manufacturing. More information on the Crude Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (3).</p> <ol style="list-style-type: none"> 1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92. 2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. 3. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Crude Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA. 																								
<p>Results: (FT - RS)</p> <p>Units/Value:</p> <ul style="list-style-type: none"> • Note: Deviations from protocol or guideline, analytical method, biological observations, control survival. 	<p>Calculated fish acute toxicity values for 7 chemicals representative of products in the Crude Butadiene C4 Category are as follows:</p> <table border="1" data-bbox="634 1514 1385 1871"> <thead> <tr> <th><u>Chemical</u></th> <th><u>Calculated log K_{ow}</u></th> <th><u>Fish Acute 96-hr LC50 (mg/L)</u></th> </tr> </thead> <tbody> <tr> <td>Isobutane</td> <td>2.23</td> <td>26.19</td> </tr> <tr> <td>n-butane</td> <td>2.31</td> <td>22.03</td> </tr> <tr> <td>isobutylene</td> <td>2.23</td> <td>25.28</td> </tr> <tr> <td>cis-butene-2</td> <td>2.09</td> <td>34.23</td> </tr> <tr> <td>trans-butene-2</td> <td>2.09</td> <td>34.23</td> </tr> <tr> <td>butene-1</td> <td>2.17</td> <td>28.79</td> </tr> <tr> <td>1,3-butadiene</td> <td>2.03</td> <td>37.59</td> </tr> </tbody> </table>	<u>Chemical</u>	<u>Calculated log K_{ow}</u>	<u>Fish Acute 96-hr LC50 (mg/L)</u>	Isobutane	2.23	26.19	n-butane	2.31	22.03	isobutylene	2.23	25.28	cis-butene-2	2.09	34.23	trans-butene-2	2.09	34.23	butene-1	2.17	28.79	1,3-butadiene	2.03	37.59
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	<u>Chemical</u>	Measured* <u>log K_{ow}</u>	Fish Acute <u>96-hr LC50 (mg/L)</u>
	Isobutane	2.76	8.32
	n-butane	2.89	6.28
	isobutylene	2.34	19.93
	cis-butene-2	2.31	21.26
	trans-butene-2	2.33	20.36
	butene-1	2.40	17.50
	1,3-butadiene	1.99	40.98
	* Experimental K _{ow} values supplied by the KOWWIN program database (EXPKOW.DB) which contains more than 13,000 organic compounds with reliably measured values.		
Test Substance: (FT - TS)	25167-67-3 Butenes 68477-41-8 Distillate (Petroleum), Extractive C3-5 68955-28-2 Gases, (Petroleum) Light Steam Cracked, Butadiene Concentrate 68476-44-8 Hydrocarbons, >C3 68512-91-4 Hydrocarbons C3 – C4 Rich Petroleum Distillates 68187-60-0 Hydrocarbons, C4, Ethane-Propane Cracked 68476-52-8 Hydrocarbons, C4, Ethylene Manufactured By-Product 68956-54-7 Hydrocarbons C4, Unsaturated 69103-05-5 Hydrocarbons, C4-7, Butadiene Manufactured By-Product 64742-83-2 Naphtha, (Petroleum), Light Steam-Cracked		
Conclusion: (FT - CL)	Based on the calculated Kow values, products in this category are expected to have a fish 96-hour LC50 range of 22.03 to 37.59 mg/L. Based on the measured Kow values, products in this category are expected to have a fish 96-hour LC50 range of 6.28 to 40.98 mg/L.		
Reliability: (FT - RL)	(2) Reliable with restrictions The toxicity values are calculated.		
Reference: (FT - RE)	Cash, G. and V. Nabholz. 1999. ECOSAR Classes for Microsoft Windows, ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment Division. Washington, DC, USA.		
Other (source): (FT - SO)	American Chemistry Council, Olefins Panel		

* **Other TS** is an option in the "test substance" pick list within the IUCLID data entry field for "acute toxicity to fish ". Selecting this option refers the reader to information in the "freetext" field for "test substance".

FT - Freetext

IUCLID fields include:

RL - Reliability

TC - Test Conditions

RE - Reference

RS - Results

TS - Test Substance

SO - Source

CL - Conclusion

Daphnid Acute Toxicity

Test Substance*:	Other TS																								
Method/Guideline*:	Other: ECOSAR Computer Model																								
Year (guideline):	1999																								
Type (test type):	Acute Daphnid Toxicity Calculation; LC50																								
GLP:	Not applicable																								
Year (study performed):	Not applicable																								
Species:	Daphnid (calculated toxicity values are not species specific)																								
Analytical Monitoring:	Not applicable																								
Exposure Period:	48 hours																								
Statistical Method: (FT - ME)*	Not applicable																								
Test Conditions: (FT - TC) <ul style="list-style-type: none"> Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading. 	<p>Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2). KOWWIN also has a database of experimental Kow values (EXPKOW.DB).</p> <p>The following chemicals are representative of products in the Crude Butadiene C4 Category, which are complex, multi-constituent substances. The range of toxicity data for component chemicals is an estimate of the potential toxicity of category products.</p> <table border="1"> <thead> <tr> <th><u>Chemical</u></th> <th><u>Calculated log K_{ow}</u></th> <th><u>Measured* log K_{ow}</u></th> </tr> </thead> <tbody> <tr> <td>Isobutane</td> <td>2.23</td> <td>2.76</td> </tr> <tr> <td>n-butane</td> <td>2.31</td> <td>2.89</td> </tr> <tr> <td>isobutylene</td> <td>2.23</td> <td>2.34</td> </tr> <tr> <td>cis-butene-2</td> <td>2.09</td> <td>2.31</td> </tr> <tr> <td>trans-butene-2</td> <td>2.09</td> <td>2.33</td> </tr> <tr> <td>butene-1</td> <td>2.17</td> <td>2.40</td> </tr> <tr> <td>1,3-butadiene</td> <td>2.03</td> <td>1.99</td> </tr> </tbody> </table> <p>* Experimental K_{ow} values supplied by the KOWWIN program database (EXPKOW.DB) which contains more than 13,000 organic compounds with reliably measured</p>	<u>Chemical</u>	<u>Calculated log K_{ow}</u>	<u>Measured* log K_{ow}</u>	Isobutane	2.23	2.76	n-butane	2.31	2.89	isobutylene	2.23	2.34	cis-butene-2	2.09	2.31	trans-butene-2	2.09	2.33	butene-1	2.17	2.40	1,3-butadiene	2.03	1.99
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	<p>values.</p> <p>Commercial products in this category can have a carbon number distribution predominantly between C3 and C5. These products can contain significant levels of 1,3-butadiene and similar low molecular weight olefins, which is why they are considered a category for purposes of the High Production Volume Chemical Program, and designated <u>Crude Butadiene C4</u>.</p> <p>The seven chemicals selected to represent the daphnid acute toxicity range of this category are C4 hydrocarbons that are common across the 10 CAS numbers (see <u>Test Substance</u>). Crude butadiene category products arise from production processes associated with ethylene manufacturing. More information on the Crude Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (3).</p> <ol style="list-style-type: none"> 1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92. 2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. 3. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Crude Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA. 																											
<p>Results: (FT - RS)</p> <p>Units/Value:</p> <ul style="list-style-type: none"> • Note: Deviations from protocol or guideline, analytical method, biological observations, control survival. 	<p>Calculated daphnid acute toxicity values for 7 chemicals representative of products in the Crude Butadiene C4 Category are as follows:</p> <table border="1" data-bbox="634 1444 1385 1919"> <thead> <tr> <th><u>Chemical</u></th> <th>Calculated <u>log K_{ow}</u></th> <th>Daphnid Acute 48-hr LC50 (mg/L)</th> </tr> </thead> <tbody> <tr> <td>Isobutane</td> <td>2.23</td> <td>28.51</td> </tr> <tr> <td>n-butane</td> <td>2.31</td> <td>24.11</td> </tr> <tr> <td>isobutylene</td> <td>2.23</td> <td>27.53</td> </tr> <tr> <td>cis-butene-2</td> <td>2.09</td> <td>36.91</td> </tr> <tr> <td>trans-butene-2</td> <td>2.09</td> <td>36.91</td> </tr> <tr> <td>butene-1</td> <td>2.17</td> <td>31.21</td> </tr> <tr> <td>1,3-butadiene</td> <td>2.03</td> <td>40.27</td> </tr> <tr> <td><u>Chemical</u></td> <td>Measured* <u>log K_{ow}</u></td> <td>Daphnid Acute 48-hr LC50 (mg/L)</td> </tr> </tbody> </table>	<u>Chemical</u>	Calculated <u>log K_{ow}</u>	Daphnid Acute 48-hr LC50 (mg/L)	Isobutane	2.23	28.51	n-butane	2.31	24.11	isobutylene	2.23	27.53	cis-butene-2	2.09	36.91	trans-butene-2	2.09	36.91	butene-1	2.17	31.21	1,3-butadiene	2.03	40.27	<u>Chemical</u>	Measured* <u>log K_{ow}</u>	Daphnid Acute 48-hr LC50 (mg/L)
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	<p>Isobutane 2.76 9.39 n-butane 2.89 7.15 isobutylene 2.34 21.86 cis-butene-2 2.31 23.28 trans-butene-2 2.33 22.32 butene-1 2.40 19.28 1,3-butadiene 1.99 43.88</p> <p>* Experimental K_{ow} values supplied by the KOWWIN program database (EXPKOW.DB) which contains more than 13,000 organic compounds with reliably measured values.</p>
Test Substance: (FT - TS)	<p>25167-67-3 Butenes 68477-41-8 Distillate (Petroleum), Extractive C3-5 68955-28-2 Gases, (Petroleum) Light Steam Cracked, Butadiene Concentrate 68476-44-8 Hydrocarbons, >C3 68512-91-4 Hydrocarbons C3 – C4 Rich Petroleum Distillates 68187-60-0 Hydrocarbons, C4, Ethane-Propane Cracked 68476-52-8 Hydrocarbons, C4, Ethylene Manufactured By-Product 68956-54-7 Hydrocarbons C4, Unsaturated 69103-05-5 Hydrocarbons, C4-7, Butadiene Manufactured By-Product 64742-83-2 Naphtha, (Petroleum), Light Steam-Cracked</p>
Conclusion: (FT - CL)	<p>Based on the calculated Kow values, products in this category are expected to have a daphnid 48-hour LC50 range of 24.11 to 40.27 mg/L. Based on the measured Kow values, products in this category are expected to have a daphnid 48-hour LC50 range of 7.15 to 43.88 mg/L.</p>
Reliability: (FT - RL)	<p>(2) Reliable with restrictions The toxicity values are calculated.</p>
Reference: (FT - RE)	<p>Cash, G. and V. Nabholz. 1999. ECOSAR Classes for Microsoft Windows, ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment Division. Washington, DC, USA.</p>
Other (source): (FT - SO)	<p>American Chemistry Council, Olefins Panel</p>

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "acute toxicity to aquatic invertebrates". Selecting this option refers the reader to information in the "freetext" field for "test substance".

FT - Freetext

IUCLID fields include:

RL - Reliability
TC - Test Conditions
RE - Reference
RS - Results
TS - Test Substance
SO - Source
CL - Conclusion

Alga Toxicity

Test Substance*:	Other TS																								
Method/Guideline*:	Other: ECOSAR Computer Model																								
Year (guideline):	1999																								
Type (test type):	Green Alga Toxicity Calculation; EC50																								
GLP:	Not applicable																								
Year (study performed):	Not applicable																								
Species:	Freshwater Green Alga (calculated toxicity values are not species specific)																								
Analytical Monitoring:	Not applicable																								
Exposure Period:	96 hours																								
Statistical Method: (FT - ME)*	Not applicable																								
Test Conditions: (FT - TC) <ul style="list-style-type: none"> Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading. 	<p>Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2). KOWWIN also has a database of experimental Kow values (EXPKOW.DB).</p> <p>The following chemicals are representative of products in the Crude Butadiene C4 Category, which are complex, multi-constituent substances. The range of toxicity data for component chemicals is an estimate of the potential toxicity of category products.</p> <table border="1"> <thead> <tr> <th><u>Chemical</u></th> <th>Calculated <u>log K_{ow}</u></th> <th>Measured* <u>log K_{ow}</u></th> </tr> </thead> <tbody> <tr> <td>Isobutane</td> <td>2.23</td> <td>2.76</td> </tr> <tr> <td>n-butane</td> <td>2.31</td> <td>2.89</td> </tr> <tr> <td>isobutylene</td> <td>2.23</td> <td>2.34</td> </tr> <tr> <td>cis-butene-2</td> <td>2.09</td> <td>2.31</td> </tr> <tr> <td>trans-butene-2</td> <td>2.09</td> <td>2.33</td> </tr> <tr> <td>butene-1</td> <td>2.17</td> <td>2.40</td> </tr> <tr> <td>1,3-butadiene</td> <td>2.03</td> <td>1.99</td> </tr> </tbody> </table> <p>* Experimental K_{ow} values supplied by the KOWWIN program database (EXPKOW.DB) which contains more</p>	<u>Chemical</u>	Calculated <u>log K_{ow}</u>	Measured* <u>log K_{ow}</u>	Isobutane	2.23	2.76	n-butane	2.31	2.89	isobutylene	2.23	2.34	cis-butene-2	2.09	2.31	trans-butene-2	2.09	2.33	butene-1	2.17	2.40	1,3-butadiene	2.03	1.99
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	<u>Chemical</u>	<u>log K_{ow}</u>	<u>96-hr EC50 (mg/L)</u>
	Isobutane	2.76	6.13
	n-butane	2.89	4.71
	isobutylene	2.34	13.94
	cis-butene-2	2.31	14.81
	trans-butene-2	2.33	14.22
	butene-1	2.40	12.33
	1,3-butadiene	1.99	27.42
	* Experimental K _{ow} values supplied by the KOWWIN program database (EXPKOW.DB) which contains more than 13,000 organic compounds with reliably measured values.		
Test Substance: (FT - TS)	25167-67-3 Butenes 68477-41-8 Distillate (Petroleum), Extractive C3-5 68955-28-2 Gases, (Petroleum) Light Steam Cracked, Butadiene Concentrate 68476-44-8 Hydrocarbons, >C3 68512-91-4 Hydrocarbons C3 – C4 Rich Petroleum Distillates 68187-60-0 Hydrocarbons, C4, Ethane-Propane Cracked 68476-52-8 Hydrocarbons, C4, Ethylene Manufactured By-Product 68956-54-7 Hydrocarbons C4, Unsaturated 69103-05-5 Hydrocarbons, C4-7, Butadiene Manufactured By-Product 64742-83-2 Naphtha, (Petroleum), Light Steam-Cracked		
Conclusion: (FT - CL)	Based on the calculated Kow values, products in this category are expected to have an alga 96-hour EC50 range of 15.35 to 25.27 mg/L. Based on the measured Kow values, products in this category are expected to have an alga 96-hour EC50 range of 4.71 to 27.42 mg/L.		
Reliability: (FT - RL)	(2) Reliable with restrictions The toxicity values are calculated.		
Reference: (FT - RE)	Cash, G. and V. Nabholz. 1999. ECOSAR Classes for Microsoft Windows, ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment Division. Washington, DC, USA.		
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FT - Freetext

IUCLID fields include:

RL - Reliability

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ROBUST SUMMARIES PART 2

**HIGH BENZENE NAPHTHAS ROBUST SUMMARIES:
PHYSICAL-CHEMICAL PROPERTIES AND ENVIRONMENTAL FATE
ARE ALSO USED FOR PYROLYSIS C3+ AND C4+**

HIGH BENZENE NAPHTHAS ROBUST SUMMARY

Boiling Point

Test Substance*:	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]											
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:	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.											
Note: Concentration prep., vessel type, replication, test conditions.												
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 High Benzene Naphthas Category are listed below. The data identify a potential boiling point range for substances represented by the 19 CAS numbers under <u>Test Substance</u>. Substances in this category do not have a specific boiling point value. Actual boiling point ranges for substances in this category will vary dependent on their constituent composition.</p> <p>Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C11. The 12 chemicals selected to represent the boiling point range of this category are C5-C10 hydrocarbons that can be found in substances identified by the 19 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.</p>											
Results: (continued) Units/Value: Note: Deviations from protocol or guideline, analytical method.	<table border="1"> <thead> <tr> <th><u>Substance Constituent</u></th> <th><u>Calculated BP (°C)</u></th> <th><u>Measured* BP (°C)</u></th> </tr> </thead> <tbody> <tr> <td>Isoprene</td> <td>34.95</td> <td>34.0</td> </tr> <tr> <td>n-pentane</td> <td>46.01</td> <td>36.0</td> </tr> </tbody> </table>	<u>Substance Constituent</u>	<u>Calculated BP (°C)</u>	<u>Measured* BP (°C)</u>	Isoprene	34.95	34.0	n-pentane	46.01	36.0		
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	<p>found in the American Chemistry Council, Olefins Panel test plan for this category (1).</p> <p>1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.</p>
Conclusion:	<p>The calculated boiling points for some representative constituents that are present in the category streams vary from 34.95 to 231.64°C @ 760 mm Hg. The measured boiling points of these same constituents vary from 34.0 to 217.9°C @ 760 mm Hg. Although this does not define the actual boiling points of the category streams, it offers an indication of a range that might be expected to encompass the boiling points of these complex streams with variable compositions. Boiling points outside of these ranges may be possible for some category streams.</p>
Reliability:	<p>(2) Reliable with restrictions</p> <p>The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential boiling point range for substances represented by the 19 CAS numbers listed under <u>Test Substance</u>. This robust summary has a reliability rating of 2 because the data are not for specific substances in High Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for boiling point range based on constituent data.</p>
Reference:	<p>EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Boiling point values were calculated by the MPBPWIN subroutine and measured data came from the database in the computer program.)</p>
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 Boiling Point. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

HIGH BENZENE NAPHTHAS ROBUST SUMMARY

Melting Point

Test Substance*:	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]
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 High Benzene Naphthas Category are listed below. The data identify a potential melting point range for substances represented by the 19 CAS numbers under <u>Test Substance</u>. Substances in this category do not have a specific melting point value. Actual melting point ranges for substances in this category will vary dependent on their constituent composition.</p> <p>Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C11. The 12 chemicals selected to represent the melting point range of this category are C5-C10 hydrocarbons that can be found in substances identified by the 19 CAS numbers. Constituents representing category members were selected on the basis of</p>
Results: (continued)	carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category

<p>Units/Value:</p> <p>Note: Deviations from protocol or guideline, analytical method.</p>	<p>substances, and olefinic process (distillation) knowledge.</p> <table border="1" data-bbox="620 233 1414 695"> <thead> <tr> <th>Substance Constituent</th> <th>Calculated MP (°C)</th> <th>Measured* MP (°C)</th> </tr> </thead> <tbody> <tr><td>Isoprene</td><td>-118.89</td><td>-145.9</td></tr> <tr><td>n-pentane</td><td>-106.92</td><td>-129.7</td></tr> <tr><td>1,3-cyclopentadiene</td><td>-91.83</td><td>-85.0</td></tr> <tr><td>Isohexane</td><td>-105.80</td><td>-162.9</td></tr> <tr><td>n-hexane</td><td>-93.84</td><td>-95.3</td></tr> <tr><td>methylcyclopentane</td><td>-85.82</td><td>-142.5</td></tr> <tr><td>benzene</td><td>-77.92</td><td>5.5</td></tr> <tr><td>toluene</td><td>-59.17</td><td>-94.9</td></tr> <tr><td>m-xylene</td><td>-40.69</td><td>-47.8</td></tr> <tr><td>styrene</td><td>-48.31</td><td>-31.0</td></tr> <tr><td>dicyclopentadiene</td><td>-16.78</td><td>32.0</td></tr> <tr><td>naphthalene</td><td>5.01</td><td>80.2</td></tr> </tbody> </table> <p>* Experimental values from EPIWIN database. The data represent a potential melting point range for substances represented by the 19 CAS numbers under <u>Test Substance</u>.</p>	Substance Constituent	Calculated MP (°C)	Measured* MP (°C)	Isoprene	-118.89	-145.9	n-pentane	-106.92	-129.7	1,3-cyclopentadiene	-91.83	-85.0	Isohexane	-105.80	-162.9	n-hexane	-93.84	-95.3	methylcyclopentane	-85.82	-142.5	benzene	-77.92	5.5	toluene	-59.17	-94.9	m-xylene	-40.69	-47.8	styrene	-48.31	-31.0	dicyclopentadiene	-16.78	32.0	naphthalene	5.01	80.2
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<p>Test Substance: (continued)</p>	<p>High Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 19 CAS numbers are used to describe the ten process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon</p>																																							

	<p>product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%.</p> <p>More information on the High Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1).</p> <ol style="list-style-type: none"> 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	<p>The calculated melting points for some representative constituents that are present in the category streams vary from -118.89 to 5.01 °C. The measured melting points of these same constituents vary from -162.9 to 80.2°C. Although this does not define the actual melting points of the category streams, it offers an indication of a range that might be expected to encompass the melting points of these complex streams with variable compositions. Melting points outside of these ranges may be possible for some category streams.</p>
Reliability:	<p>(2) Reliable with restrictions</p> <p>The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential melting point range for substances represented by the 19 CAS numbers listed under <u>Test Substance</u>. This robust summary has a reliability rating of 2 because the data are not for specific substances in the High Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for melting point range based on constituent data.</p>
Reference:	<p>EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Melting point values were calculated by the MPBPWIN subroutine and measured data came from the database in the computer program.)</p>
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* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Melting Point. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

HIGH BENZENE NAPHTHAS ROBUST SUMMARY

Vapor Pressure

Test Substance*:	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]
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 High Benzene Naphthas Category are listed below. The data identify a potential vapor pressure range for substances represented by the 19 CAS numbers under <u>Test Substance</u>. Substances in this category do not have a specific vapor pressure value. Actual vapor pressure ranges for substances in this category will vary dependent on their constituent composition.</p> <p>Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C11. The 12 chemicals selected to represent the vapor pressure range of this category are C5-C10 hydrocarbons that can be found in substances identified by the 19 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.</p>

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	<p>The 19 CAS numbers are used to describe the ten process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%.</p> <p>More information on the High Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1).</p> <p>1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.</p>
Conclusion:	<p>The calculated vapor pressures for some representative constituents that are present in the category streams vary from 0.05 to 7.35 E² hPa @ 25°C. The measured vapor pressures of these same constituents vary from 0.11 to 7.33 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 of these ranges may be possible for some category streams.</p>
Reliability:	<p>(2) Reliable with restrictions</p> <p>The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential vapor pressure range for substances represented by the 19 CAS numbers under <u>Test Substance</u>. This robust summary has a reliability rating of 2 because the data are not for specific substances in the High Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for vapor pressure range based on constituent data.</p>
Reference:	<p>EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Vapor pressure values were calculated by the MPBPWIN subroutine and measured data came from the database in the computer program.)</p>
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 Vapor Pressure. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

HIGH BENZENE NAPHTHAS ROBUST SUMMARY

Water Solubility

Test Substance*:	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]		
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:	Calculated and measured water solubility data for representative constituents of the High Benzene Naphthas Category are listed below. The data identify a potential water solubility range for substances represented by the 19 CAS numbers under <u>Test Substance</u> . Substances in this category do not have a specific water solubility value. Actual water solubility ranges for substances in this category will vary dependent on their loading rate (i.e., weight of test material added to a volume of water).		
<ul style="list-style-type: none">• Note: Deviations from protocol or guideline, analytical method.	Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C11. The 12 chemicals selected to represent the water solubility range of this category are C5-C10 hydrocarbons that can be found in substances identified by the 19 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.		
Results: (continued) Units/Value:	<u>Substance</u>	<u>Calculated WS</u>	<u>Measured WS*</u>
Note: Deviations from protocol or	<u>Constituent</u>	<u>(mg/L @ 25°C)</u>	<u>(mg/L @ 25°C)</u>
	Isoprene	247.2	338.6

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

	<p>More information on the High Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1).</p> <p>1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.</p>
Conclusion:	<p>The calculated water solubility for some representative constituents that are present in the category streams vary from 51.9 to 2634.0 mg/L @ 25°C. The measured water solubility of these same constituents vary from 17.2 to 2000.0 mg/L @ 25°C. Although this does not define the actual water solubility of the category streams, it offers an indication of a range that might be expected to encompass the water solubility of these complex streams with variable compositions. Water solubilities outside of these ranges may be possible for some category streams.</p>
Reliability:	<p>(2) Reliable with restrictions</p> <p>The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential water solubility range for substances represented by the 19 CAS numbers under <u>Test Substance</u>. This robust summary has a reliability rating of 2 because the data are not for specific substances in the High Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for water solubility range based on constituent data.</p>
Reference:	<p>EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Water solubility values were calculated by the WSKOWWIN subroutine and measured data came from the database in the computer program.)</p>
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 Water Solubility. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

HIGH BENZENE NAPHTHAS ROBUST SUMMARY

Hydrolysis (Stability in Water)

Test Substance*:	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]
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 High Benzene Naphthas Category includes the following CAS numbers: 64741-99-7 Extracts, petroleum, light naphtha solvent 64742-49-0 Naphtha, petroleum, hydrotreated light 64742-73-0 Naphtha, petroleum, hydrodesulfurized light 64742-83-2 Naphtha, petroleum, light steam-cracked 64742-91-2 Distillates, petroleum, steam-cracked 67891-79-6 Distillates, petroleum, heavy aromatic 67891-80-9 Distillates, petroleum, light aromatic 68410-97-9 Distillates, petroleum, light distillate hydrotreating process, low-boiling 68475-70-7 Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived 68476-45-9 Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product

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

The High Benzene Naphthas Category

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

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

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

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

- **Pyrolysis Gasoline Fractions (C5-C6, C6, and C6-C8 Fractions)** are separated by distillation into various boiling-point range fractions as intermediates in preparation for further processing. In some cases, petroleum refinery streams such as a C6 reformat fraction are combined with the pyrolysis gasoline prior to this separation. Similar to the situation for Pygas, the composition of these fractions vary depending on the ethylene process feedstock and the other operating variables.
 1. **Pyrolysis C5-C6 Fraction** has a carbon number distribution that is predominantly C5 to C6. One typical composition for this stream is reported as 70% benzene and 10% pentenes.
 2. **Pyrolysis C6 Fraction** has a carbon number distribution that is predominantly C6. Reported compositions vary from 35 to 77% benzene, 0.5 to 5% toluene with the balance primarily C6 non-aromatics, which are expected to be largely unsaturates.
 3. **Pyrolysis C6-C8 Fraction** has a carbon number distribution that is predominantly C6 to C8. The reported compositions range from 30 to 80% benzene, 15 to 25% toluene and 3 to 23% C8 aromatics.
- **Hydrotreated Pyrolysis Fractions (C6, C6-C7, and C6-C8 Fractions)** are Pyrolysis gasoline or distillate fractions of pyrolysis gasoline that are treated with hydrogen over catalyst to saturate or partially saturate diolefins and/or olefins. In some cases, petroleum refinery streams such as a C6 reformat fraction are combined with the pyrolysis gasoline prior to this step. The hydrogenation process may be either one-stage or two-stage. The one-stage process is typically a liquid-phase process where the primary objective is to selectively convert diolefins to mono-olefins and to convert vinyl aromatics, for example, styrene to ethylbenzene. The second stage in a two-stage hydrogenation process is typically a vapor-phase, more severe hydrogenation that converts essentially all of the contained olefins to saturated hydrocarbons. A pygas fraction that will be processed by extraction or extractive distillation to produce high purity aromatics (benzene, toluene, or xylenes) is subjected to two-stage hydrogenation. Pygas fractions may be forwarded to hydrodealkylation units (less common) for benzene production after one-stage of hydrogenation. Hydrotreated Pyrolysis fractions may be the result of either one- or two-stage hydrogenation.
 1. **Hydrotreated C6 Fraction** is very similar to the Pyrolysis C6 fraction except that the non-aromatics present in the hydrotreated stream are essentially all saturates. The reported composition for the Hydrotreated C6 stream indicates typical benzene content of 75%.
 2. **Hydrotreated C6-C7 Fraction** has a carbon number distribution that is predominantly C6-C7 and the reported values indicate 40 to 70% benzene, and 3 to 15% toluene.
 3. **Hydrotreated C6-C8 Fraction** has a reported typical composition of 40 to 60% benzene, 10 to 25% toluene, and 3 to 10% C8

aromatics.

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

Hydrolysis of Hydrocarbons as a Function of Molecular Structure

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.

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

Under strongly acidic conditions the carbon-carbon double bond found

	<p>in alkenes, such as those in the High Benzene Naphthas Category, will react with water by an addition reaction mechanism (2). The reaction product is an alcohol. This reaction is not considered to be hydrolysis because the carbon-carbon linkage is not cleaved and because the reaction is freely reversible (3). Substances that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (4).</p> <p>The substances in the High Benzene Naphthas Category are primarily olefins that contain at least one double bond (alkenes). The remaining chemicals are saturated hydrocarbons (alkanes). These two groups of chemicals contain only carbon and hydrogen. As such, their molecular structure is not subject to the hydrolytic mechanism discussed above. Therefore, chemicals in the High Benzene Naphthas Category have a very low potential to hydrolyze, and this degradative process will not contribute to their removal in the environment.</p> <p>References</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 High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA. 2. Gould, E.S. (1959), Mechanism and Structure in Organic Chemistry, Holt, Reinhart and Winston, New York, NY, USA. 3. Harris, J.C. (1982), "Rate of Hydrolysis," Chapter 7 in: W.J. Lyman, W.F. Reehl, and D.H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, NY, USA. 4. Neely, W. B. 1985. Hydrolysis. In: W. B. Neely and G. E. Blau, eds. Environmental Exposure from Chemicals. Vol I., pp. 157-173. CRC Press, Boca Raton, FL, USA.
Reliability:	These data represent a key study for characterizing the potential of substances in the High Benzene Naphthas Category to undergo hydrolysis.
Reference:	American Chemistry Council, Olefins Panel. 2003. Hydrolysis High 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.

HIGH BENZENE NAPHTHAS ROBUST SUMMARY

Photodegradation (Direct)

Test Substance*:	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]
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 High Benzene Naphthas Category. The High Benzene Naphthas Category includes ten process streams:</p> <ul style="list-style-type: none"> • Pyrolysis Gasoline • Pyrolysis C6 Fraction • Pyrolysis C6-C8 Fraction • Pyrolysis C5-C6 Fraction • Hydrotreated C6 Fraction • Hydrotreated C6-C7 Fraction • Hydrotreated C6-C8 Fraction • Quench Loop Pyrolysis Oil and Compressor Oil • Recovered Oil from Waste Water Treatment

- **Extract from Benzene Extraction**

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

The High Benzene Naphthas Category

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

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

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

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

	<p>Pygas is typically about 40% and the reported values range from 15 to 62%. The concentrations of individual hydrocarbon components in Pygas vary depending on the type of feedstock used by the ethylene plant, the mode of operation of the cracking furnaces (i.e. severity) and the ethylene process configuration. One non-typical Pygas stream is reported to contain vinylacetate at a concentration of up to about 10%. Vinylacetate is not typically found in ethylene process streams.</p> <ul style="list-style-type: none"> • Pyrolysis Gasoline Fractions (C5-C6, C6, and C6-C8 Fractions) are separated by distillation into various boiling-point range fractions as intermediates in preparation for further processing. In some cases, petroleum refinery streams such as a C6 reformat fraction are combined with the pyrolysis gasoline prior to this separation. Similar to the situation for Pygas, the composition of these fractions vary depending on the ethylene process feedstock and the other operating variables. <ol style="list-style-type: none"> 4. Pyrolysis C5-C6 Fraction has a carbon number distribution that is predominantly C5 to C6. One typical composition for this stream is reported as 70% benzene and 10% pentenes. 5. Pyrolysis C6 Fraction has a carbon number distribution that is predominantly C6. Reported compositions vary from 35 to 77% benzene, 0.5 to 5% toluene with the balance primarily C6 non-aromatics, which are expected to be largely unsaturates. 6. Pyrolysis C6-C8 Fraction has a carbon number distribution that is predominantly C6 to C8. The reported compositions range from 30 to 80% benzene, 15 to 25% toluene and 3 to 23% C8 aromatics. <ul style="list-style-type: none"> • Hydrotreated Pyrolysis Fractions (C6, C6-C7, and C6-C8 Fractions) are Pyrolysis gasoline or distillate fractions of pyrolysis gasoline that are treated with hydrogen over catalyst to saturate or partially saturate diolefins and/or olefins. In some cases, petroleum refinery streams such as a C6 reformat fraction are combined with the pyrolysis gasoline prior to this step. The hydrogenation process may be either one-stage or two-stage. The one-stage process is typically a liquid-phase process where the primary objective is to selectively convert diolefins to mono-olefins and to convert vinyl aromatics, for example, styrene to ethylbenzene. The second stage in a two-stage hydrogenation process is typically a vapor-phase, more severe hydrogenation that converts essentially all of the contained olefins to saturated hydrocarbons. A pygas fraction that will be processed by extraction or extractive distillation to produce high purity aromatics (benzene, toluene, or xylenes) is subjected to two-stage hydrogenation. Pygas fractions may be forwarded to hydrodealkylation units (less common) for benzene production after one-stage of hydrogenation. Hydrotreated Pyrolysis fractions may be the result of either one- or two-stage hydrogenation. <ol style="list-style-type: none"> 4. Hydrotreated C6 Fraction is very similar to the Pyrolysis C6 fraction except that the non-aromatics present in the hydrotreated stream are essentially all saturates. The reported composition for the Hydrotreated C6 stream indicates typical benzene content of
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75%.

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

Photolysis of Hydrocarbons

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

The absorption of light in the ultra violet (UV)-visible range, 110-750 nm, can result in the electronic excitation of an organic molecule. Light in this range contains energy of the same order of magnitude as

covalent bond dissociation energies (2). Higher wavelengths (e.g. infrared) result only in vibrational and rotational transitions, which do not tend to produce structural changes to a molecule.

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

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

<u>Hydrocarbon</u>	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	-	-
Naphthalene	282	450	311	250
	221	100,000		
	270	5,000		

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

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

References

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

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

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

HIGH BENZENE NAPHTHAS ROBUST SUMMARY

Photodegradation (Indirect)

Test Substance*:	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]
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 High Benzene Naphthas Category</u></p> <p>High Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 19 CAS numbers are used to describe the ten process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%.</p> <p>Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C11. That is why this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated <u>High Benzene Naphthas</u>.</p> <p>The 12 chemicals selected to represent the atmospheric oxidation potential of this category are C5-C10 hydrocarbons that can be found in substances identified by the 19 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.</p> <p><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>
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<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>Isoprene</td> <td>1.2</td> <td>105.1 E⁻¹²</td> </tr> <tr> <td>n-pentane</td> <td>31.7</td> <td>4.0 E⁻¹²</td> </tr> <tr> <td>1,3-cyclopentadiene</td> <td>0.9</td> <td>142.6 E⁻¹²</td> </tr> <tr> <td>Isohexane</td> <td>22.4</td> <td>5.7 E⁻¹²</td> </tr> <tr> <td>n-hexane</td> <td>23.5</td> <td>5.5 E⁻¹²</td> </tr> <tr> <td>methylcyclopentane</td> <td>22.7</td> <td>5.7 E⁻¹²</td> </tr> <tr> <td>benzene</td> <td>65.8</td> <td>1.9 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>dicyclopentadiene</td> <td>1.1</td> <td>119.2 E⁻¹²</td> </tr> <tr> <td>naphthalene</td> <td>5.9</td> <td>21.6 E⁻¹²</td> </tr> </tbody> </table> <p>* Atmospheric half-life values are based on a 12-hr day.</p> <p>More information on the High Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (Olefins Panel, 2001).</p> <p><u>References:</u></p> <ol style="list-style-type: none"> 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 High 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>	Isoprene	1.2	105.1 E ⁻¹²	n-pentane	31.7	4.0 E ⁻¹²	1,3-cyclopentadiene	0.9	142.6 E ⁻¹²	Isohexane	22.4	5.7 E ⁻¹²	n-hexane	23.5	5.5 E ⁻¹²	methylcyclopentane	22.7	5.7 E ⁻¹²	benzene	65.8	1.9 E ⁻¹²	toluene	24.6	5.2 E ⁻¹²	m-xylene	9.5	13.6 E ⁻¹²	styrene	4.6	28.1 E ⁻¹²	dicyclopentadiene	1.1	119.2 E ⁻¹²	naphthalene	5.9	21.6 E ⁻¹²
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Conclusion:	Atmospheric oxidation via hydroxyl radicals can be a significant route of degradation for products in this category. Based on calculated values, products in this category can have an atmospheric half-life range of 0.9 to 65.8 hours as a result of indirect photolysis by hydroxyl radical attack.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by AOPWIN. The data represent a potential atmospheric half-life range for substances represented by the 19 CAS numbers under <u>Test Substance</u> . This robust summary has a reliability rating of 2 because the data are not for specific substances in the High Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for atmospheric half-life range based on constituent data.
Reference:	Meylan, M., SRC 1994-1999. AOPWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
Other (source):	American Chemistry Council, Olefins Panel (Prepared 10/03)

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

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

HIGH BENZENE NAPHTHAS ROBUST SUMMARY

Partition Coefficient

Test Substance*:	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]
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 High Benzene Naphthas Category are listed below. The data identify a potential log K_{ow} range for substances represented by the 19 CAS numbers under <u>Test Substance</u>. Substances in this category do not have a specific log K_{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 both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C11. The 12 chemicals selected to represent the log K_{ow} range of this category are C5-C10 hydrocarbons that can be found in substances identified by the 19 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.</p>

<p>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="630 237 768 300">Substance Constituent</th> <th data-bbox="841 237 1027 300">Calculated log K_{ow} @ 25°C</th> <th data-bbox="1076 237 1263 300">Measured* log K_{ow} @ 25°C</th> </tr> </thead> <tbody> <tr><td>Isoprene</td><td>2.58</td><td>2.42</td></tr> <tr><td>n-pentane</td><td>2.80</td><td>3.39</td></tr> <tr><td>1,3-cyclopentadiene</td><td>2.25</td><td>na</td></tr> <tr><td>Isohexane</td><td>3.21</td><td>3.60</td></tr> <tr><td>n-hexane</td><td>3.29</td><td>3.90</td></tr> <tr><td>methylcyclopentane</td><td>3.10</td><td>3.37</td></tr> <tr><td>benzene</td><td>1.99</td><td>2.13</td></tr> <tr><td>toluene</td><td>2.54</td><td>2.73</td></tr> <tr><td>m-xylene</td><td>3.09</td><td>3.20</td></tr> <tr><td>styrene</td><td>2.89</td><td>2.95</td></tr> <tr><td>dicyclopentadiene</td><td>3.16</td><td>na</td></tr> <tr><td>naphthalene</td><td>3.17</td><td>3.30</td></tr> </tbody> </table> <p>* Experimental values from EPIWIN database. na = not available The data represent a potential log K_{ow} range for substances represented by the 19 CAS numbers under <u>Test Substance</u>.</p>	Substance Constituent	Calculated log K _{ow} @ 25°C	Measured* log K _{ow} @ 25°C	Isoprene	2.58	2.42	n-pentane	2.80	3.39	1,3-cyclopentadiene	2.25	na	Isohexane	3.21	3.60	n-hexane	3.29	3.90	methylcyclopentane	3.10	3.37	benzene	1.99	2.13	toluene	2.54	2.73	m-xylene	3.09	3.20	styrene	2.89	2.95	dicyclopentadiene	3.16	na	naphthalene	3.17	3.30
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	<p>manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%.</p> <p>More information on the High Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1).</p> <p>1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.</p>
Conclusion:	<p>The calculated log K_{ow} for some representative constituents that are present in the category streams vary from 1.99 to 3.29 @ 25°C. The measured log K_{ow} of these same constituents vary from 2.13 to 3.90 @ 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 of these ranges may be possible for some category streams.</p>
Reliability:	<p>(2) Reliable with restrictions</p> <p>The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential log K_{ow} range for substances represented by the 19 CAS numbers under <u>Test Substance</u>. This robust summary has a reliability rating of 2 because the data are not for specific substances in the High Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for log K_{ow} range based on constituent data.</p>
Reference:	<p>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.)</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 Partition Coefficient. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

HIGH BENZENE NAPHTHAS ROBUST SUMMARY

Transport / Distribution (Fugacity)

Test Substance*:	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]
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>

Results:

Units/Value:

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

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

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

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

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

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

* Distribution values determined using calculated input data from EPIWIN program

<p>Results: (cont'd)</p> <p>Units/Value:</p> <ul style="list-style-type: none"> Note: Deviations from protocol or guideline, analytical method. 	<table border="1"> <thead> <tr> <th rowspan="2"><u>Chemical</u></th> <th colspan="4"><u>Measured**</u></th> </tr> <tr> <th><u>Air</u></th> <th><u>Water</u></th> <th><u>Soil</u></th> <th><u>Sediment</u></th> </tr> </thead> <tbody> <tr><td>Isoprene</td><td>99.96</td><td>0.03</td><td>0.01</td><td>-</td></tr> <tr><td>n-pentane</td><td>99.99</td><td>0.01</td><td>-</td><td>-</td></tr> <tr><td>1,3-cyclopentadiene</td><td>99.93</td><td>0.06</td><td>0.01</td><td>-</td></tr> <tr><td>Isohexane</td><td>99.97</td><td>0.01</td><td>0.02</td><td>-</td></tr> <tr><td>n-hexane</td><td>99.96</td><td>-</td><td>0.04</td><td>-</td></tr> <tr><td>methylcyclopentane</td><td>99.95</td><td>0.02</td><td>0.03</td><td>-</td></tr> <tr><td>benzene</td><td>98.89</td><td>1.00</td><td>0.11</td><td>-</td></tr> <tr><td>toluene</td><td>98.80</td><td>0.81</td><td>0.39</td><td>-</td></tr> <tr><td>m-xylene</td><td>97.91</td><td>0.86</td><td>1.20</td><td>0.03</td></tr> <tr><td>styrene</td><td>96.65</td><td>1.85</td><td>1.46</td><td>0.04</td></tr> <tr><td>dicyclopentadiene</td><td>98.55</td><td>0.63</td><td>0.80</td><td>0.02</td></tr> <tr><td>naphthalene</td><td>42.27</td><td>20.56</td><td>36.33</td><td>0.81</td></tr> </tbody> </table> <p>** Distribution values determined using input data from the EPIWIN program experimental database</p>	<u>Chemical</u>	<u>Measured**</u>				<u>Air</u>	<u>Water</u>	<u>Soil</u>	<u>Sediment</u>	Isoprene	99.96	0.03	0.01	-	n-pentane	99.99	0.01	-	-	1,3-cyclopentadiene	99.93	0.06	0.01	-	Isohexane	99.97	0.01	0.02	-	n-hexane	99.96	-	0.04	-	methylcyclopentane	99.95	0.02	0.03	-	benzene	98.89	1.00	0.11	-	toluene	98.80	0.81	0.39	-	m-xylene	97.91	0.86	1.20	0.03	styrene	96.65	1.85	1.46	0.04	dicyclopentadiene	98.55	0.63	0.80	0.02	naphthalene	42.27	20.56	36.33	0.81
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	<p>manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%.</p> <p>More information on the High Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1).</p> <ol style="list-style-type: none"> 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	<p>The partitioning data represent a potential distribution range for substances in the 19 CAS numbers listed under <u>Test Substance</u>. Substances in the High Benzene Naphthas Category are calculated to partition primarily to air with a small percentage partitioning to water, soil, and sediment. Relatively high vapor pressure and high water solubility largely control the partitioning behavior of constituent chemicals in substances from this category.</p> <p>The input data used to run the EQC Level I model included estimated values calculated by the EPIWIN program based on chemical structure and measured data from the EPIWIN database. A comparison of the distribution data developed using either all calculated input values or measured values where data were available indicate a similar partitioning behavior and support the use of the dataset for chemicals without any measured data.</p>
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 19 CAS numbers listed under <u>Test Substance</u>. This robust summary has a reliability rating of 2 because the data are not for specific substances in the High Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for distribution range based on constituent data.</p>
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.

ATTACHMENT 1B

HIGH BENZENE NAPHTHAS ROBUST SUMMARIES:

BIODEGRADATION OF BENZENE

HIGH BENZENE NAPHTHAS ROBUST SUMMARY

Biodegradation

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

Results: (FT - RS)

Units/Value:

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

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

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

* replicate data

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

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

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

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

* IUCLID field abbreviations include:

FT - Freetext

TC - Test Conditions

RS - Results

CL - Conclusion

RL - Reliability

RE - Reference

SO - Source

ROBUST SUMMARIES PART 3
HIGH BENZENE NAPHTHAS ROBUST SUMMARIES:
MAMMALIAN TOXICITY
ARE ALSO USED FOR PYROLYSIS C3+ AND C4+

Robust Summary: High Benzene Naphthas

Acute Toxicity

<p><u>Test Substance</u></p> <p><u>Method</u> Method/guideline followed Type (test type) GLP Year Species/Strain Sex No. of animals per sex /dose Vehicle Route of administration</p> <p>Test Conditions</p> <p><u>Results</u> LD₅₀ with confidence limits.</p> <p>Remarks</p> <p><u>Conclusions</u> (study author)</p> <p><u>Data Quality</u> Reliability</p> <p><u>References</u></p> <p><u>Other</u> Last changed</p>	<p>Dripolene. Yellow, homogeneous liquid, stable for 5 years at ambient temperature. (CRU #93329). Olefins Panel HVP Stream: Pyrolysis Gasoline. Typical composition ranges for Pyrolysis Gasoline are shown in Table 2 of the Test Plan.</p> <p>Not specified Acute, limit test Yes 1994 Rat, Sprague-Dawley Males and females 5 None Oral gavage</p> <p>Sprague Dawley rats (180-350g) were individually housed in stainless steel suspended cages and fasted overnight prior to administration of 2g/kg neat dripolene. The study room was maintained at 68-72°F with a relative humidity of 35-63% and a 12 hr light-dark cycle. Water and chow diet were available ad lib after dosing. Test article was administered once on day 1 by oral gavage through a blunted needle. Rats were observed for clinical signs approx. 30 min, 1hr, and 4hr, after dosing, and daily thereafter until sacrifice on day 15. Rats were checked once a day for mortality and moribundity. Observations were not made on weekends. Body wts were recorded prior to fasting and on days 1, 8 and 15.</p> <p>The LD₅₀ was not reached at 2g/kg. There were no deaths and all rats gained some weight during the study. Clinical signs noted in one or more rats were salivation, decreased activity, rales, lacrimation, chromodacryorrhea, ataxia, head shaking, chromorhinorrhea, miosis, slight tremors, mydriasis, hyperactivity, hypothermia, urogenital discharge, nasal discharge, decreased food consumption, decreased fecal output, vocalization, and decreased stool size. No gross pathological findings were noted at necropsy.</p> <p>The LD₅₀ was not reached at 2g/kg.</p> <p>1. Reliable without restriction.</p> <p>Rodriguez, S.C. and Dalbey, W.E. 1994. Acute oral toxicity of dripolene in Sprague Dawley Rats. Study #65642. Stonybrook Laboratories, Princeton, NJ. for Mobil Chemical Co., Edison, NJ.</p> <p>10/23/2001 (Prepared by a contractor to the Olefins Panel)</p>
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Robust Summary: High Benzene Naphthas

Acute Toxicity

<p><u>Test Substance</u></p>	<p>Dripolene. Yellow, homogeneous liquid, stable for 5 years at ambient temperature. (CRU #93329). Olefins Panel HVP Stream: Pyrolysis Gasoline. Typical composition ranges for Pyrolysis Gasoline are shown in Table 2 of the Test Plan.</p>
<p><u>Method</u> Method/guideline followed Type (test type) GLP Year Species/Strain Sex No. of animals per sex/dose Vehicle Route of administration</p>	<p>Not specified Acute, limit test Yes 1994 Rabbit, New Zealand White Males and females 3 None dermal</p>
<p>Test Conditions</p>	<p>Rabbits, weighing at least 2kg, were individually housed in stainless steel suspended cages in a study room maintained at 69-72⁰F with a relative humidity of 40-85% and a 12 hr light-dark cycle. Water and chow diet were available ad lib. The dorsal skin surface extending down from the front to rear legs and from left to right lower flanks was clipped free of hair the day prior to test article administration. Test article was spread evenly over the clipped area (approx. 10% of body surface area) at a dose of 2g/kg. A layer of 8-ply gauze was placed on the dorsal site, and a rubber dam sleeve was fitted snugly over the gauze pad and around the trunk. Edges of the dam were taped in place. An Elizabethan collar was affixed to the neck to prevent oral ingestion of test article and mechanical irritation of the test site. After 24 hrs, the collar and wrappings were removed and residual test article was wiped off. Body wts were recorded on days 1, 8 and 15. Rabbits were observed for toxicity at about 1 and 2 hr post-dose and daily thereafter on weekdays, through day 14. Observations for mortality/morbidity were made daily. Rabbits were sacrificed on day 15 and necropsies were performed.</p>
<p><u>Results</u> LD₅₀ with confidence limits.</p>	<p>The LD₅₀ was not reached at 2g/kg. There were no deaths during the study and rabbits either gained some weight or remained at day 1 body wt. Signs that might have resulted from treatment in one or more rabbits were: decreased fecal output, decreased fecal pellet size, soft stool, and decreased food consumption. No gross pathological findings were noted at necropsy.</p>
<p>Remarks</p>	
<p><u>Conclusions</u> (study author)</p>	<p>The LD₅₀ was not reached at 2g/kg.</p>
<p><u>Data Quality</u> Reliability</p>	<p>1. Reliable without restriction.</p>
<p><u>References</u></p>	<p>Rodriguez, S.C. and Dalbey, W.E. 1994. Dermal toxicity of dripolene in the New Zealand White rabbit. Study #65643. Stonybrook Laboratories, Princeton, NJ. for Mobil Chemical Co., Edison, NJ.</p>
<p><u>Other</u> Last changed</p>	<p>10/23/2001 (Prepared by a contractor to the Olefins Panel)</p>

Robust Summary: High Benzene Naphthas

Acute Toxicity

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

Acute Toxicity

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

Genetic Toxicity - in Vitro

<p><u>Test Substance</u> <i>Test substance</i></p> <p><u>Method</u> Method/guideline followed Type System of testing GLP Year Species/Strain Metabolic activation Species and cell type</p> <p>Quantity Induced or not induced Concentrations tested</p> <p>Statistical Methods</p> <p>Remarks for Test Conditions</p> <p><u>Results</u> Genotoxic effects</p> <p><u>Conclusions</u> (contractor)</p> <p><u>Data Quality</u> <i>Reliabilities</i></p>	<p>Hydrogenated Pyrolysis Gasoline, CAS #68410-97-9. clear liquid with aromatic odor, negligible solubility in water, contains <55.0% benzene, <25% toluene, <10% dimethyl benzene/xylene, <7% pentane, <7% ethylbenzene, <3% cyclohexane, <2% hexane. Olefins Panel HVP Stream: Hydrotreated C6-C8.</p> <p>Standard method per Ames et al Reverse mutation bacterial assay Salmonella typhimurium, Escherichia coli with and without metabolic activation Yes 1991 S. typh. TA1535, TA1537, TA98, TA100; E. coli WP2(uvrA) Yes Male Sprague Dawley rat liver (S9 fraction), Molecular Toxicology, Inc., Annapolis, MD 20% S9 fraction in 0.5ml S9 mix/plate Aroclor 1254 induced, rats given a single 500mg/kg ip dose 0, 33, 100, 333, 1000, 3333, 10,000µg/plate ± S9. All diluted in acetone (200mg/ml)</p> <p>None specified. Test article considered mutagenic when it induces a reproductive, dose-related increase in number of revertants in one or more strains at 3 consecutive dose levels. A non-mutagen does not induce a dose-related increase in at least 2 independent tests.</p> <p>Hydrogenated pyrolysis gasoline (HPG) was prepared in acetone immediately prior to use. At end of the study, an aliquot of the stock dilution was sent to PTRL West, Richmond, CA to confirm concentration. Salmonella (approx. 10⁸ cells/ml) were exposed to either test material or acetone in 3 plates/dose ± S9 by the plate incorporation method. Six dose levels from 33-10,000µg/plate were employed in both the range-finding trial using TA100 and the mutagenicity test with all strains of Salmonella and E. coli. Optimum level of S9 for the mutagenicity assay was determined by testing the highest non-toxic dose, 10,000µg per plate with metabolic activation systems containing 4, 20 or 80% S9 fraction. No noteworthy increases in revertants or cytotoxicity was observed at any S9 concentration; 20% S9 was used in the mutagenicity test. All plates were incubated at 37°C for 48 hrs then revertant colonies were counted. Positive control compounds were: cultures-S9, sodium azide (5µg/plate) for TA1535, TA100; 9-aminoacridine (50µg/plate) for TA1537; 2-nitrofluorene (5µg/plate) for TA98; N-ethyl-N'-Nitro-N-Nitrosoguanidene (5ug/plate) for E. coli WP2, and cultures+S9, 2-anthramine (4µg/plate) for TA1535, TA1537, (2µg/plate) for TA98, TA100, and (20µg/plate) for E. coli WP2. Two independent assays were performed.</p> <p>HPG did not induce increases in number of revertant colonies and no toxicity was observed in any Salmonella strain or E. coli WP2 with or without 20% S9 metabolic activation in both studies. Positive control compounds performed appropriately.</p> <p>Hydrogenated pyrolysis gasoline is not mutagenic to bacteria under conditions of this assay.</p> <p>1. Reliable without restriction</p>
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Robust Summary: High Benzene Naphthas

Genetic Toxicity - in Vitro

<p><u>Test Substance</u> <i>Test substance</i></p> <p><u>Method</u> Method/guideline followed</p> <p>Type System of testing GLP Year Species/Strain Metabolic activation Species and cell type Quantity Induced or not induced Concentrations tested</p> <p>Exposure period Statistical Methods</p> <p>Remarks for Test Conditions</p> <p><u>Results</u> Genotoxic effects</p>	<p>Hydrogenated Pyrolysis Gasoline, CAS #68410-97-9. clear liquid with aromatic odor. Composition, purity and stability referred to sponsor. Olefins Panel HVP Stream: Hydrotreated C6-C8.</p> <p>Standard method based on Cortesi et al (1983), Dunkel et al (1981), Reznikoff et al (1973)</p> <p>In vitro cell transformation Mouse embryo cells Yes 1984 BALB/3T3-A31-1-1 from T. Kakunaga, National Cancer Inst., 1983 No NA NA NA Cytotoxicity: 8, 16, 32, 64, 128, 256, 512, 1024, 2048, and 5000µg/ml; Transformation: 100, 250, 500, 1500µg/ml, all diluted in 10% Pluronic® polyol F68 (prepared in deionized water, mol. wt. 8350, 80% hydrophilic). 2 days None employed. Criteria for positive response were a two-fold increase in type III foci at the highest dose over vehicle control (at least 2 type III foci if vehicle control had none) with or without a dose related response, or a two-fold increase at two or more consecutive doses. Test is equivocal if two-fold increase occurred at any one level other than the highest acceptable dose.</p> <p>Sufficient Hydrogenated Pyrolysis Gasoline (HPG) was weighed separately for each dose level, 0.40ml of 10% F68 added per ml of final volume and medium (Eagles MEM with 10% heat-inactivated fetal calf serum) added as required to achieve final volume for testing. Test preparations were mixed just prior to addition to cultures at 50µl to each 5 ml culture. All cultures were incubated at 37°C in 5% CO2 enriched humidified atmosphere. For cytotoxicity, 2 cultures/dose group, 2 cultures for vehicle F68 or medium negative control were seeded with 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 cultures (1x10⁴ cells/flask/dose group) and two colony-forming cultures (100 cells/plate/dose group) were seeded on day 1, exposed on days 2-3 and culture medium changed on day 4. For transformation cultures, medium continued to be changed weekly to day 29. Positive control was 3-methylcholanthrene (1µg/ml). Colony forming cultures were fixed, stained, and counted visually on day 10 to determine cloning efficiency (avg. number colonies/plate ÷ 100 cells seeded). Transformation cultures were fixed and stained on day 29 for focus counting and evaluation. Transformation frequency = total type III foci ÷ total flasks/dose group.</p> <p>HPG induced toxicity in BALB/3T3 cells after two days exposure beginning at 128 µg/ml (45.4% relative survival) with relative survivals of 26.7, 25.6, 3.2 and 0% at 512, 1024, 2048 and 5000µg/ml, respectively. In the transformation assay, toxicity was seen at all dose levels (relative cloning efficiencies of 53.7, 67.8, 78.5 and 0% at 100, 250, 500 and 1500µg/ml). At 1500µg/ml, the highest dose level, HPG induced 5 Type III foci; no other dose levels produced a positive response. Transformation frequencies were 0.13, 0, 0, 0.07 and 0.36 for medium control, vehicle control, 100, 250, 500 and 1500µg/ml, respectively. Positive and negative controls gave appropriate responses.</p>
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<p><u>Conclusions</u> (contractor)</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>Hydrogenated Pyrolysis Gasoline induced transformation in BALB/3T3 cells under conditions of this assay. Cytotoxicity and impairment of cloning efficiency were also observed. The positive response was observed only at the highest dose level, a level that appeared to be too toxic for cells to recover and form colonies (0% relative colony forming efficiency)</p> <p>1. Reliable without restriction</p> <p>Brecher, S. 1984. Transformation test of Hydrogenated Pyrolysis Gasoline. Proj. #2098. Gulf Life Sciences Center, Pittsburgh, PA for Gulf Oil Chemicals Co, Houston, TX</p> <p>Cortesi, E. et al. 1983. Teratogenesis, Carcinogenesis, Mutagenesis 3: 101-110.</p> <p>Dunkel, V.A. et al. 1981. J. Nat'l Cancer Inst. 67: 1303-1315.</p> <p>Reznikoff, C.A. et al. 1973. Cancer Res. 3239-3249.</p> <p>Revised 8/27/2001 (Prepared by a contractor to the Olefins Panel).</p>
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Robust Summary - Group 5: High Benzene Naphthas

Genetic Toxicity - in Vitro

<p><u>Test Substance</u> <i>Test substance</i></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 Exposure period Statistical Methods</p> <p>Remarks for Test Conditions</p> <p><u>Results</u> Genotoxic effects</p>	<p>Hydrogenated Pyrolysis Gasoline, CAS #68410-97-9. clear liquid with aromatic odor. Composition, purity and stability referred to sponsor. Olefins Panel HVP Stream: Hydrotreated C6-C8.</p> <p>Standard method based on Williams et al (1977, 1982) In vitro mammalian DNA repair assay Unscheduled DNA synthesis (UDS) in primary hepatocyte cultures Yes 1984 Fischer 344 male rat (10 wks old) No NA NA NA 8, 16, 32, 64, 128, 256, 512, 1024µg/ml diluted in 10% Pluronic F68 (prepared in deionized water, mol. wt 8350, 80% hydrophilic) 18 hrs. None specified. Criteria for positive response are incorporation of radioactive precursor (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. If this criterion is not met, a positive response can be identified if there is a significant difference (p<0.01) in % cells in repair at any dose level and negative control value. This indicator defines whether a small fraction of cells is undergoing repair (Casciano & Gaylor, 1983). A positive response need not be dose related.</p> <p>Sufficient Hydrogenated Pyrolysis Gasoline (HPG) was weighed separately for each dose level, 0.40ml of 10% F68 added per ml of final volume and sufficient medium (Williams Medium E with 10% fetal bovine serum and insulin) added to achieve final volume. Test preparations were mixed just prior to addition at 20µl to each 2ml culture. The conc. of ³H-thymidine (½ life 12.4 yrs.) used in these assays was 1mCi/ml. All cultures were incubated at 37°C in 5% CO2 enriched humidified atmosphere. No range finding assay was performed. In the UDS assay, 2x10⁵ cells/ml were seeded into coverslip cultures, exposed to ³H-thymidine and test substance for 18 hours (3 cultures/dose level, 8 dose levels), untreated controls, vehicle F68 control and positive control, 2-acetyl aminofluorene (0.01µg/ml). Cells growing on coverslips were rinsed, fixed and glued to microscope slides on day 2. On day 3, slides were dipped in autoradiographic emulsion and stored in the dark at 2-8°C. Autoradiographs were developed, stained and coverslipped on day 10. Numbers of grains overlying 50 randomly selected nuclei/slide were counted. The highest of 3 cytoplasmic grain counts/cell were subtracted and this number was divided by a conversion factor (unspecified) to obtain net nuclear grain count. Avg. net nuclear grain count/slide (sum of net nuclear grain count ÷ 50) and mean net nuclear grain count (avg. net nuclear grain count/slide ÷3) were calculated. In addition, % cells in repair were determined for each dose level.</p> <p>HPG induced toxicity in primary hepatocytes following 18 hr exposure that left too few cells for UDS analysis at doses of 512 and 1024µg/ml. HPG did not induce unscheduled DNA synthesis at any dose level with sufficient cells to be analyzed. Positive and negative controls gave appropriate responses.</p>
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<p><u>Conclusions</u> (contractor)</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>Hydrogenated Pyrolysis Gasoline did not induce unscheduled DNA synthesis in primary cultures of rat hepatocytes under conditions of this assay.</p> <p>2. Reliable with restrictions. No table of cell counts/viability. No individual data to verify calculations and identify conversion factor. Statistical criteria are mentioned but method is not cited.</p> <p>Brecher, S. 1984. Hepatocyte primary culture/DNA repair test of Hydrogenated Pyrolysis Gasoline. Proj. # 2097. Gulf Life Sciences Center, Pittsburgh, PA for Gulf Oil Chemicals Co., Houston, TX Williams, G.M. 1977. Cancer Res. 37: 1845-1851 Williams et al. 1977. In Vitro 13: 809-817 Williams et al. 1982. Mut. Res. 97:359-370 Casciano, D.A. and Gaylor, D.W. 1983. Mut. Res. 122:81-86</p> <p>5/7/2001 (Prepared by a contractor to the Olefins Panel)</p>
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Robust Summary - Group 5: High Benzene Naphthas

Genetic Toxicity - in Vivo

<p><u>Test Substance</u> Remarks</p> <p><u>Method</u> Method/guideline followed Type GLP Year Species Strain Sex</p> <p>Route of administration Doses/concentration levels Exposure period</p> <p>Statistical methods</p> <p>Remarks for Test Conditions.</p> <p><u>Results</u> Genotoxic effects NOAEL (NOEL) LOAEL (LOEL)</p>	<p>Hydrogenated Pyrolysis Gasoline, CAS #68410-97-9. Clear liquid with aromatic odor. Compositional analysis, purity and stability referred to sponsor. Olefins Panel HVP Stream: Hydrotreated C6-C8.</p> <p>None specified. Comparable to standard assay. Mammalian bone marrow erythrocyte micronucleus assay Yes 1984 Mice Crl:CD-1(ICR)BR Swiss Male and female. Range-finding 2M, 2F (10 wks old)/group; 3 groups; Micronucleus test 10M, 10F (11 wks old)/group in 4 groups, 15M, 15F in one group. Oral gavage 0, 0.5, 1.0, 2.0g/kg (2doses), 2.0g/kg (1 dose) undiluted 1 dose/day for 2 days: one group- 1 dose, 1 day only</p> <p>Values from treated groups for daily mean body weights, group means and std. dev. for polychromatic erythrocytes (PCEs) with micronuclei (MN), and group mean ratios of PCE to normochromatic erythrocytes (NORMs) were calculated and compared with vehicle control values by Student's t-test. Positive response was indicated by statistically significant ($p < 0.05$) increases in micronucleated PCE at any dose level with a dose related response evident. Results were considered equivocal if only one of these criteria was met.</p> <p>Animals in the range-finding study (2M, 2F/group), 3 treated groups (no control group) were given 1.25, 2.5, and 5.0g/kg neat hydrogenated pyrolysis gasoline (HPG) by gavage once each day for two days. Eighty percent of the dose level that produced $\leq 50\%$ mortality was selected for the maximum dose in the micronucleus study. In the micronucleus study, three groups of mice were given undiluted HPG by oral gavage daily for two days at doses of 0.5, 1.0, 2.0g/kg, negative control mice were given corn oil (5g/kg). One-half of each treated group and negative control (5M, 5F) was killed on day 3 and the remainder on day 4. One group (15M, 15F), given 2.0 g/kg by gavage in a single dose for 1 day only, was killed on days 2, 3, 4 (5/sex/day). Positive control mice (4M, 4F) given cyclophosphamide (75 mg/kg) ip daily for 2 days were killed on day 3. Survival, body wt, and clinical signs were observed and recorded daily. Slides of femoral bone marrow smears were prepared, stained with May-Grunewald/Giemsa stain and examined microscopically. For each mouse, 1000 PCE and all associated mature erythrocytes (NORMs) were counted. Data collected included group mean body weights for each day, total PCEs, total NORMs, PCEs with MN, and NORMs with MN.</p> <p>NOAELmortality = 1.0g/kg; NOELgenetics > 2.0g/kg (Assigned by reviewer) In the range-finding study, half of the animals given HPG at conc of 5.0g/kg died on or before day 2. Gross necropsy of dead mice was unremarkable. In the micronucleus test, 1/10 males given 2.0g/kg (2 doses) died on day 2. No other mortality or significant wt changes were observed. Lethargy was observed among high dose mice. Surviving mice treated with HPG did not show any significant increase in micronucleus formation in PCE and no significant changes in ratio of PCE/NORM compared to negative controls. Negative and positive</p>
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<p><u>Conclusions</u> (study authors)</p> <p><u>Data Quality</u> <i>Reliabilities</i></p> <p><u>References</u></p> <p><u>Other</u> <i>Last changed</i></p>	<p>controls gave appropriate results.</p> <p>Oral treatment of mice with Hydrogenated Pyrolysis Gasoline for 1-2 days at doses up to 2.0g/kg/day had no effect on frequency of micronucleated polychromatic erythrocytes in bone marrow under these test conditions. HPG did not induce cytogenetic damage.</p> <p>1. Reliable without restriction</p> <p>Khan, S.H. 1984. Micronucleus test of Hydrogenated Pyrolysis Gasoline. Proj. #2096. Gulf Life Sciences Center, Pittsburgh, PA for Gulf Oil Chemicals Co., Houston, TX</p> <p>5/7/2001 (Prepared by a contractor to the Olefins Panel)</p>
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Robust Summary - Group 5: High Benzene Naphthas

Repeated Dose Toxicity

<p><u>Test Substance</u> Remarks</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</p> <p>Statistical methods</p> <p>Test Conditions</p> <p><u>Results</u> NOAEL (NOEL) LOAEL (LOEL) Remarks</p> <p><u>Conclusions</u> (study authors)</p>	<p>Hydrogenated Pyrolysis Gasoline CAS #68410-97-9, Clear liquid with aromatic odor. Olefins Panel HVP Stream: Hydrotreated C6-C8.</p> <p>Standard method, method not referenced Subacute Yes 1984 Rat Fischer 344 Inhalation 8 days 0, 4869±470, 9137±917ppm±SD, actual exposure conc. Males and females (5/sex/group) 6 hrs. once daily for 5 days (d1-5) 5M, 5F; filtered air 2 days</p> <p>Body wt variance compared by Bartlett's test and one way analysis of variance. Group mean body wt compared either with Dunnett's test or a modified t-test to assess significance.</p> <p>Rats (9 wks old, 113-195g at initiation) were housed individually in stainless steel, screen-bottomed cages. Rooms were maintained at 72.2^oF (exposure chamber 75^oF) with relative humidity of 54% (exposure chamber 50%), and 12 hr light/dark cycle. Rats received chow diet and tap water ad lib throughout the study, except during exposure. Three groups of 10 rats (5M, 5F/group) each, were exposed to test article or air. Test article was aerosolized with a ball jet nebulizer; an in-line condensing flask was used to prevent large particles from entering the exposure chamber. Chamber concentration of test article was measured by gas chromatography. Rats were observed twice daily on weekdays and once daily on weekends for morbidity/mortality, and once daily for clinical signs immediately after exposure on days 1-5. Surviving rats were sacrificed on day 8. Gross necropsies were performed on all rats.</p> <p>NOAEL< 4869ppm (estimated by reviewer) LOAEL= 4869ppm (estimated by reviewer) based on clinical observations, reduced wt gain. Two rats (1M, 1F) from group 3 (9137ppm) died on day 2; one female from group 3 died during exposure on day 1. Rats in groups 2 and 3 showed ocular discharge throughout d1-5. Rats in group 2 showed increased respiratory rate and dry red material around nose and mouth. All rats in group 2 were lethargic and showed labored respiration. Many rats in group 3 were lethargic and exhibited twitching and harsh respiratory sounds during days 1-5. All rats in group 2 and all but one survivor in group 3 appeared normal on day 8. Group mean body wt was significantly decreased in a dose related manner. No test article related effects were seen at gross necropsy on day 8; the male rat that died during the study showed gas in the G.I. tract and red-tinged fluid in the stomach.</p> <p>Exposure to test article caused a significant decrease in group mean body wt of</p>
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<p><u>Quality</u> Reliabilities</p> <p><u>References</u></p> <p><u>Other</u> Last changed</p>	<p>male and female rats of low and high dose groups that was correlated with exposure level. Three deaths occurred in the high dose group during exposure. Major clinical signs were lethargy, twitching, harsh respiratory sounds and ocular discharge. No gross alterations were found in rats surviving to sacrifice.</p> <p>1. Reliable without restrictions</p> <p>Rausina, G.A. 1984. Five-day repeated dose inhalation toxicity study in rats of Hydrogenated Pyrolysis Gasoline. Proj. #2099. Gulf Life Sciences Center, Pittsburgh, PA</p> <p>Revised 7/27/2001 (Prepared by a contractor to the Olefins Panel)</p>
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Robust Summary: High Benzene Naphthas

Acute Toxicity

<p><u>Test Substance</u></p>	<p>Pyrolysis gasoline (Rerun Tower Overheads). Yellow, homogeneous liquid; 40% benzene, 26% C5, 13% toluene, 20% other. Test substance is described as a sample of a Pyrolysis Gasoline distillate fraction and is similar to Pyrolysis gasoline, a stream included in the test plan.</p>
<p><u>Method</u> Method/guideline followed Type (test type) GLP Year Species/Strain Sex No. of animals per sex /dose Vehicle Route of administration</p>	<p>Not specified Acute, limit test Yes 1994 Rat, Sprague-Dawley Males and females 5 None Oral gavage</p>
<p>Test Conditions</p>	<p>Sprague Dawley rats (180-350g) were individually housed in stainless steel suspended cages and fasted overnight prior to administration of 2g/kg neat pyrolysis gasoline. The study room was maintained at 68-72^oF with a relative humidity of 35-63% and a 12 hr light-dark cycle. Water and chow diet were available ad lib after dosing. Test article was administered once on day 1 by oral gavage through a blunted needle. Rats were observed for clinical signs approx. 30 min, 1hr and 4hr, after dosing, and daily thereafter until sacrifice on day 15. Rats were checked once a day for mortality and moribundity. Observations were not made on weekends. Body wts were recorded prior to fasting and on days 1, 8 and 15.</p>
<p><u>Results</u> LD₅₀ with confidence limits.</p>	<p>The LD₅₀ was not reached at 2g/kg. There were no deaths and all rats gained some weight during the study. Clinical signs noted in one or more rats were salivation, decreased activity, rales, lacrimation, chromodacryorrhea, ataxia, chromorhinorrhea, miosis, slight tremors, mydriasis, hyperactivity, hypothermia, urogenital discharge, nasal discharge, decreased food consumption, decreased fecal output, vocalization, and penile discharge. No gross pathological findings were noted at necropsy.</p>
<p>Remarks</p>	
<p><u>Conclusions</u> (study author)</p>	<p>The LD₅₀ was not reached at 2g/kg.</p>
<p><u>Data Quality</u> Reliability</p>	<p>1. Reliable without restriction.</p>
<p><u>References</u></p>	<p>Rodriguez, S.C. and Dalbey, W.E. 1994. Acute oral toxicity of pyrolysis gasoline in Sprague Dawley Rats. Study #65636. Stonybrook Laboratories, Princeton, NJ. for Mobil Chemical Co., Edison, NJ.</p>
<p><u>Other</u> Last changed</p>	<p>10/16/2001 (Prepared by a contractor to the Olefins Panel)</p>

Robust Summary - Group 5: High Benzene Naphthas

Acute Toxicity

<p><u>Test Substance</u></p>	<p>Pyrolysis gasoline (Rerun Tower Overheads). Yellow, homogeneous liquid; 40% benzene, 26% C5, 13% toluene, 20% other. Test substance is described as a sample of a Pyrolysis Gasoline distillate fraction and is similar to Pyrolysis gasoline, a stream included in the test plan.</p>
<p><u>Method</u> Method/guideline followed Type (test type) GLP Year Species/Strain Sex No. of animals per sex /dose Vehicle Route of administration</p>	<p>Not specified Acute, limit test Yes 1994 Rabbit, New Zealand White Males and females 3 None dermal</p>
<p>Test Conditions</p>	<p>Rabbits, weighing at least 2kg, were individually housed in stainless steel suspended cages in a study room maintained at 69-72^oF with a relative humidity of 38-85% and a 12 hr light-dark cycle. Water and chow diet were available ad lib. The dorsal skin surface extending down from the front to rear legs and from left to right lower flanks was clipped free of hair the day prior to test article administration. Test article was spread evenly over the clipped area (approx. 10% of body surface area) at a dose of 2g/kg. A layer of 8-ply gauze was placed on the dorsal site, and a rubber dam sleeve was fitted snugly over the gauze pad and around the trunk. Edges of the dam were taped in place. An Elizabethan collar was affixed to the neck to prevent oral ingestion of test article and mechanical irritation of the test site. After 24 hrs, the collar and wrappings were removed and residual test article was wiped off. Body wts were recorded on days 1, 8 and 15. Rabbits were observed for toxicity at about 1 and 2 hr post-dose and daily thereafter on weekdays through day 14. Observations for mortality/moribundity were made daily. Rabbits were sacrificed on day 15 and necropsies were performed.</p>
<p><u>Results</u> LD₅₀ with confidence limits.</p>	<p>The LD₅₀ was not reached at 2g/kg. There were no deaths during the study and rabbits either gained some weight or remained at day 1 body wt. Signs that might have resulted from treatment in one or more rabbits were: soft stool, decreased fecal pellet size, nasal discharge, and test site erythema. No gross pathological findings were noted at necropsy.</p>
<p>Remarks</p>	
<p><u>Conclusions</u> (study author)</p>	<p>The LD₅₀ was not reached at 2g/kg.</p>
<p><u>Data Quality</u> Reliability</p>	<p>1. Reliable without restriction.</p>
<p><u>References</u></p>	<p>Rodriguez, S.C. and Dalbey, W.E. 1994. Dermal toxicity of pyrolysis gasoline in the New Zealand White rabbit. Study #65637. Stonybrook Laboratories, Princeton, NJ. for Mobil Chemical Co., Edison, NJ.</p>
<p><u>Other</u> Last changed</p>	<p>10/16/2001 (Prepared by a contractor to the Olefins Panel)</p>

Robust Summary - Group 5: High Benzene Naphthas

Genetic Toxicity - in Vitro

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

<p><u>Conclusions</u> (contractor)</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>appropriately (-S9: MNNG 1906, 1883 revertants/plate in TA 100 and TA1535, respectively; 9-AA 586 revertants/plate in TA1537; 2-NF 2114, 1214 revertants/plate in TA98 and TA1538, respectively; and +S9 2- aminoanthracene 406-2307 revertants/plate for all strains except TA1537). The results of this assay indicate that rerun tower overheads had no mutagenic activity in this test system. (Reviewer's note: Due to toxicity, tests were performed over a low dose range; 3 of 4 doses were non-toxic and showed sufficient growth to evaluate mutagenicity. Testing at any lower doses was impractical).</p> <p>Rerun Tower Overheads did not induce an increase in revertant colonies in any Salmonella strain, tested at any dose level with or without metabolic activation in this single Ames test.</p> <p>1. Reliable without restriction</p> <p>Blackburn, G.R. 1981. An Ames Salmonella/mammalian microsome mutagenesis assay for the determination of potential mutagenicity of Rerun Tower Overheads from an olefins/aromatics plant. Study No. 1781-80. Mobil Environmental and Health Sciences Laboratory, Princeton, NJ. Ames B. N. et al. 1975. Mutat. Res. 31: 347-364.</p> <p>10/02/2001 (Prepared by a contractor for the Olefins Panel)</p>
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Robust Summary - Group 5: High Benzene Naphthas

Genetic Toxicity - in Vitro

<p><u>Test Substance</u> Test substance</p> <p><u>Method</u> Method/guideline followed</p> <p>Type System of testing GLP Year Species/Strain Metabolic activation Species and cell type Quantity Induced or not induced Concentrations tested</p> <p>Statistical Methods</p> <p>Remarks for Test Conditions</p> <p><u>Results</u> Genotoxic effects</p>	<p>Rerun Tower Overheads from Olefins/Aromatics Plant (light thermal cracked naphtha) CAS # 64741-74-8. Straw colored liquid; 40% benzene, 26% C5, 13% toluene, 20% other. Test substance is described as a sample of a Pyrolysis Gasoline distillate fraction and is similar to Pyrolysis gasoline, a stream included in the test plan.</p> <p>None specified. Standard method based on Slater et al., 1971, Green and Muriel, 1976, and Ames et al., 1973.</p> <p>Bacterial DNA repair Escherichia coil, Salmonella typhimurium Not specified 1978 <i>E. coli</i> WP2 <i>uvrA</i>⁺ <i>recA</i>⁺, WP100 <i>uvrA</i>⁻ <i>recA</i>⁻; <i>S. typh.</i> TA1978 <i>uvrB</i>⁺, TA1538 <i>uvrB</i>⁻ Yes Sprague Dawley male rat liver (S9 fraction) 50µl S9 fraction in 1.0ml S9 mix/plate Aroclor 1254 induced (single ip injection of 500mg/kg, 5 days prior to sacrifice) Spot test: 10µl/plate undiluted</p> <p>None. Compounds that cause damage to DNA will more severely affect repair deficient strains than repair proficient stains. Toxic compounds that do not affect DNA will not induce differential toxicity.</p> <p>Tester strains were stored in liquid nitrogen and fresh cultures were inoculated directly from frozen stock, grown overnight at 37^oC, re-diluted and grown to final cell concentration of 2x10⁸ cells/ml. Each test article-strain combination was plated in triplicate with and without metabolic activation. Log phase cultures (0.1ml) added to 2.5ml top agar were poured on Vogel-Bonner minimal medium plates. For plates without activation, a 6.5mm paper disc (antibiotic type) was placed in the center of each plate; 10µl test article is placed on disc. For plates with S9 activation, after top agar sets, a 9.5mm diameter hole was cut in agar in the center of the plate, the well was sealed with 0.1ml top agar, and 150µl of S9 mix/control or test article mix (14:1) added to the well. All inverted plates were incubated at 37^oC for 24hr. The diameter of any resulting zone of inhibition was measured in mm. Zone diameter of a repair deficient strain was divided by the zone diameter of the repair proficient parent strain. Positive control compounds were 4-nitro-quinoline-1-oxide (4-NQO; 30µg/plate) –S9, 2-aminofluorene (2-AF; 250µg/plate) +S9, and negative control was 25µg/plate penicillin. Tests were performed twice ± S9.</p> <p>In duplicate tests, average inhibition ratios induced by Rerun tower overheads –S9 were 1.4, 1.8 for <i>E. coli</i> WP100/WP2, and 1.3, 1.5 for <i>S. typh.</i> TA1538/TA1978 compared to negative control values of 1.0, 1.1, and 1.1, 1.2 in <i>E. coli</i> strains and <i>S. typh.</i> strains, respectively, suggesting a weak differential killing of repair deficient strains without metabolic activation. Positive control ratios for 4-NQ –S9 were 2.3, 2.5 for <i>E. coli</i> WP100/WP2, and 1.7, 1.6 for <i>S. typh.</i> TA1538/TA1978. In tests with metabolic activation (+S9), average inhibition ratios were 1.0, 1.0 for <i>E. coli</i> strains and 1.0, 1.0 for <i>S. typh.</i> strains in duplicate tests compared to negative control values of 1.1, 1.1, and 1.1, 1.1 in <i>E. coli</i> and <i>S. typh.</i> strains, respectively, indicating no test article induced toxicity. Positive control, 2-AF, inhibition ratios were 2.1, 2.1 for <i>E. coli</i> WP100/WP2, and 1.9, 1.4 for <i>S. typh.</i> TA1538/TA1978.</p>
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<p><u>Conclusions</u> (contractor)</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>Rerun tower overheads did cause weak differential killing in DNA repair deficient strains, <i>E. coli</i> WP100 and <i>S. typhimurium</i>. TA1538 in the absence of metabolic activation, suggesting that the test article can cause direct acting damage to bacterial DNA. No differential killing was observed in the presence of metabolic activation.</p> <p>1. Reliable without restriction</p> <p>Haworth, S.R. 1978. Bacterial DNA repair assay of Mobil Chemical Company Compound MCTR-125-78 (MRI #110). E. G. and G. Mason Research Institute, Rockville, MD. for Mobil Chemical Co, Edison, NJ Slater, E.E. et al. 1971. Cancer Res. 31: 970-973. Green, M.H.L. and Muriel, W.J. 1976. Mutat. Res. 38:3-32 Ames, B.N. et al. 1973. Proc. Natl. Acad. Sci., USA 70: 782-786.</p> <p>2/28/2002 (Prepared by a contractor to the Olefins Panel)</p>
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Robust Summary: High Benzene Naphthas

Genetic Toxicity - in Vitro

<p><u>Test Substance</u> <i>Test substance</i></p>	<p>Rerun Tower Overheads from Olefins/Aromatics Plant (light thermal cracked naphtha) CAS # 64741-74-8. Straw colored liquid; 40% benzene, 26% C5, 13% toluene, 20% other. Test substance is described as a sample of a Pyrolysis Gasoline distillate fraction and is similar to Pyrolysis gasoline, a stream included in the test plan.</p>
<p><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, no guideline specified Cell transformation Mouse embryo cells Yes 1981 BALB-c/3T3 mouse cell line No NA NA NA Initial cytotoxicity: 0, 0.01, 0.1, 1.0, 10.0, 100.0µg/ml medium; Transformation: 0.0.8, 4.0, 20.0 and 100µg/ml, diluted in dimethyl sulfoxide. Negative control was DMSO at 2.5% vol. concentration.</p>
<p>Statistical Method</p>	<p>T-test specified. Standard criteria for positive response is a two fold increase in type III foci at highest dose over vehicle control with or without a dose related response or a 2 fold increase at 2 or more consecutive doses.</p>
<p>Remarks for Test Conditions</p>	<p>Routine procedures were referred to Appendix 1 Standard Operating Procedures, which was not included with this report. Only specifics unique to this assay are presented. Due to the volatile nature of test material, the cytotoxicity assay and transformation assays were conducted in tightly capped T-25 flasks in sealed plastic bags. The pH of medium during the 72hr exposure period was maintained at 7.4 by 0.02M Hepes buffer in flasks. RTO was prepared as a 1% stock solution in DMSO, which, when added to culture medium at a 2.5% vol. conc. was a suspension. Despite limited solubility, RTO produced a dose-dependent cytotoxic effect after a 3-day exposure period. In the initial toxicity assay, RTO was added to flasks, seeded with BALB-c/3T3 cells, at concentrations of 0, 0.01, 0.1, 1.0, 10.0 and 100.0µg/ml, incubated for 3 days at 37°C in a CO₂ in air incubator, after which cells were counted for survival. In the transformation assay, RTO was tested at 0, 0.8, 4.0, 20.0 and 100µg/ml. In a standard BALB-c/3T3 transformation assay, colony formation cultures (approx. 100 cells/culture) and transformation cultures (approx. 10⁴ cells/culture, 20 cultures/dose) were seeded on day 1, exposed to test material for 2-3 days, and culture medium was changed on day 4. For transformation cultures, medium continued to be changed weekly to day 29. Colony formation cultures were fixed, stained and counted visually on day 8 to determine cloning efficiency; transformation cultures were fixed and stained on day 29 for focus counting and evaluation. Transformation frequency = total type III foci ÷ total cultures/dose. Positive control compound was 3-methyl cholanthrene (2µg/ml).</p>
<p><u>Results</u> Genotoxic effects</p>	<p>RTO induced toxicity in BALB-c/3T3 cells after 3 days exposure at concentrations of 10µg/ml (59% viability) and at 100µg/ml (18% viability). In the transformation assay, inhibition of cloning efficiency (CE, clones/100 cells) occurred at 4.0µg/ml (89% CE), 20.0µg/ml (81% CE) and 100µg/ml (65% C.E.); cell toxicity was</p>

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

Genetic Toxicity - in Vitro

<p><u>Test Substance</u> <i>Test substance</i></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>Statistical Methods</p> <p>Remarks for Test Conditions</p>	<p>Rerun Tower Overheads from Olefins/Aromatics Plant (light thermal cracked naphtha) CAS # 64741-74-8. Straw colored liquid; 40% benzene, 26% C5, 13% toluene, 20% other. Test substance is described as a sample of a Pyrolysis Gasoline distillate fraction and is similar to Pyrolysis gasoline, a stream included in the test plan.</p> <p>None specified. Standard method based on Clive and Spector, 1975 Mammalian cell mutation assay Mouse lymphoma cells Not specified 1979 Mouse lymphoma L5178Y TK+/- cells Yes Sprague Dawley males rat liver (S9 fraction) 50µl S9 fraction/ml S9mix) Aroclor 1254 induced (single ip injection of 500mg/kg, 5 days prior to sacrifice) -S9 cloned doses: 0.0, 0.013, 0.018, 0.024, 0.032, 0.042, 0.056, 0.075, and 0.10µl/ml +S9 cloned doses: 0.0, 0.048, 0.063, 0.085, 0.11, 0.15, 0.20, 0.27, and 0.36µl/ml. All doses diluted in acetone</p> <p>None. Compound was designated as mutagenic if it induced a mutation frequency (mutant cells/10⁴ surviving cells) greater than 3 times the standard error (S.E. [f]) calculated by formula from the viable counts and total mutant cells (trifluorothymidine resistant cells) at each dose level.</p> <p>Freshly prepared actively growing cultures of L5178Y cells (1x10⁶ cells/ml) were dispensed in 6ml aliquots into 44 polypropylene centrifuge tubes. Rerun tower overheads, solubilized in acetone, beginning at a concentration equal to LD90 from a preliminary toxicity test, was diluted over 15 serial 1/8 log dilutions, producing 16 dose levels decreasing approximately 100 fold from highest to lowest, and added to cells in the centrifuge tubes. Four ml of S9 activation mixture or 4ml culture medium was added, yielding a final cell suspension of 0.6x10⁶ cells/ml. Positive control compounds were ethyl methyl sulfonate (EMS, 1.0µl/ml) -S9 and 7,12-dimethylbenzanthracene (7,12-DMBA, 2.5µl/ml) +S9 cultures. All tubes were gassed with 5% CO₂/air and placed on a roller drum for 4hrs at 37°C in the dark. At the end of exposure, calls were washed with fresh medium, re-suspended, gassed, replaced on roller drum at 37°C and incubated for 3 days with a cell population adjustment every 24 hrs to maintain a cell population density of 0.3x10⁶ cells/ml. After 3 days expression, 8 cultures ± S9, which exhibited toxicity from 10-90% growth inhibition during the expression period, were selected for cloning. At cloning, cells were placed in restrictive suspension medium containing trifluorothymidine (TFT, 1µg/ml) that allows only TK-/- cells to grow. Two Florence flasks/concentration ± S9, one for restrictive medium, one for viable cell counts, were filled with 100ml cloning medium and maintained at 37°C. Six 100mm petri plates/concentration ± S9 were prepared, 3 for restrictive medium, 3 for viable cell counts. Cell counts were made from each centrifuge tube to determine the volume of cell population = 3x10⁶ cells. This volume was retained, centrifuged and the supernatant discarded except for 2ml in which cells were re-suspended and placed in restrictive medium flask. A 5x10⁻⁴ dilution was prepared and added to the appropriate viable count flask containing 100ml cloning medium. After this dilution, 1 ml of TFT stock solution was added to the restrictive medium flask and incubated</p>
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<p><u>Results</u> Genotoxic effects</p> <p><u>Conclusions</u> (contractor)</p> <p><u>Data Quality</u> Reliabilities</p> <p><u>Reference</u></p> <p><u>Other</u> Last changed</p>	<p>with shaking (125rpm) at 37⁰C for 15min. Flasks were removed, 33ml of cell suspension was pipetted into each of 3 appropriately labeled plates and placed in the cold (4⁰C) for 20 min to accelerate gelling. Plates were removed and incubated at 37⁰C in humidified 5% CO2/air for 10 days. At the end of incubation, plates were scored for total number of colonies/plate, 3 counts/plate, on an automated colony counter. Mutation frequency (MF) = avg. number of colonies in 3 restrictive medium plates ÷ avg. number of colonies x10⁴ in 3 corresponding viable count plates. Induced mutation frequency (IMF) = MF test article – MF solvent control.</p> <p>In cultures without metabolic activation, the two highest concentrations cloned, 0.10µl/ml (MF=1.4, IMF=0.8) and 0.075µl/ml (MF=1.0, IMF=0.4) exhibited slight dose related increases in IMF compared with acetone control (MF=0.6); only the 0.10µl/ml concentration caused a doubling of MF over controls. EMS positive control values were MF=27.1, IMF=26. The first activated assay was discarded due to loss of positive control cultures by contamination. In the repeat test with metabolic activation, 2 dose concentrations had MF 2 times greater than acetone controls: the highest dose cloned, 0.36µl/ml (MF=0.8, IMF=0.4) and 0.15µl/ml, the 4th highest dose cloned (MF=0.9, IMF=0.5) versus control (MF=0.4). However, intervening cloned doses of 0.20, and 0.27µl/ml did not show increased MF; the values for the positive doses were not dose related and were within the range of experimental error for the assay. Positive control values +S9 for 7,12- DMBA were MF=2.6, IMF=2.0.</p> <p>Without metabolic activation, Rerun tower overheads appears to induce a weak mutagenic response at the two highest doses only; a dose response trend was not observed in the 6 lower doses cloned. Test article did not induce significant mutagenic activity in cultures containing S9, suggesting that any mutagenic activity is suppressed or inactivated by the presence of the liver microsome metabolizing system.</p> <p>1. Reliable without restriction.</p> <p>Kirby, P.E. et al., 1979. An evaluation of mutagenic potential of MCTR-125-78 (MRI #110) employing the L5178Y TK+/- mouse lymphoma assay. E.G. and G. Mason Research Institute, Rockville, MD for Mobil Chemical Co., Edison, NJ Clive, D., and Spector, J.F.S. 1975. Mutat. Res. 31: 17-29</p> <p>2/28/2002 (Prepared by a contractor to the Olefins Panel)</p>
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Robust Summary: High Benzene Naphthas

Genetic Toxicity - in Vitro

<p><u>Test Substance</u> <i>Test substance</i></p>	<p>Rerun Tower Overheads from Olefins/Aromatics Plant (light thermal cracked naphtha) CAS # 64741-74-8. Straw colored liquid; 40% benzene, 26% C5, 13% toluene, 20% other. Test substance is described as a sample of a Pyrolysis Gasoline distillate fraction and is similar to Pyrolysis gasoline, a stream included in the test plan.</p>
<p><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>None specified. Standard method based on Bertram, 1977 Mammalian cell transformation assay Mouse C3H embryo cells Not specified 1978 Mouse embryo cells/ C3H 10T½ No NA NA NA 0, 0.625, 1.25, 2.5 and 5.0µl/ml, all diluted in acetone</p>
<p>Statistical Methods</p>	<p>None. A positive response is determined by the appearance of any type II foci (50% can be malignantly transformed) and type III foci (85% can be malignantly transformed) compared to negative controls. The C3H 10T½ cell line has no spontaneous transformation.</p>
<p>Remarks for Test Conditions</p>	<p>For the preliminary toxicity assay, cells (200/plate) were exposed to Rerun tower overheads diluted in acetone, over a range of concentrations from 0.0003-5.0µl/ml, at 2-fold dilutions for 18hrs; cells were then washed, re-fed with fresh Eagle's basal medium and incubated for 10 days in 5% CO2/air at 37°C. After incubation, cells were washed, fixed with absolute methanol (20 min) and stained with Giemsa (30 min); number of cells/plate were counted and cloning efficiency (CE) determined=Avg. number colonies/plate ÷ number cells plated x100. In the transformation assay, cells in late log phase were plated at a concentration of 1x10³ cells/60mm petri dish. Cultures for concurrent toxicity determination were prepared at 200 cells/plate. After 24 hrs, cultures were treated with appropriate test article concentrations in 25µl volumes at 4 dose levels, 12 plates/dose, in decreasing 2-fold dilutions from concentrations which exhibit 25-75% relative CE. Positive control compound was 7, 12-dimethylbenzanthracene (7, 12-DMBA, 0.5µg/ml). After 18hr treatment, test article was removed, cultures were re-fed, and re-incubated. Toxicity plates were incubated for 10 days, stained and CE determined. Transformation cultures were re-fed weekly until 35 days after removal of test article had elapsed. All plate cultures were washed, fixed, stained and scored for the presence of type II and type III foci by macroscopic and microscopic examination. Type II foci show massive piling up in virtually opaque monolayers, cells are moderately polar. Type III foci are composed of highly polar, fibroblastic, multilayered, criss-crossed arrays of densely stained cells.</p>
<p><u>Results</u> Genotoxic effects</p>	<p>Rerun tower overheads induced 71% relative cloning efficiency at 5.0µl/ml; transformation assay was performed at 2-fold dilutions from 5.0µl/ml. In the toxicity study conducted in parallel with the transformation assay, test article induced 100% cell death at 5.0µl/ml. In the transformation assay, sufficient cells survived to form a confluent layer in 8/12 plates at 5.0µl/ml dose level after 35 days. No indication of type II or type III foci were induced by rerun tower overheads at any dose level. Positive control, 7,12-DMBA induced 9 type II and</p>

<p><u>Conclusions</u> (contractor)</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>12 type III foci on 12 plates.</p> <p>Rerun tower overheads does not induce cell transformation in mouse embryo C3H 10T½ cells.</p> <p>1. Reliable without restriction</p> <p>Jensen, E.M., and Thilager, A.K. 1978. C3H 10T½ cell transformation assay, Mobil Chemical Co. Compound MCTR-125-78 (MRI #110). E.G. and G. Mason Research Institute, Rockville, MD</p> <p>Bertram, J.S. 1977. Cancer Res. 37: 514-523</p> <p>2/28/2002 (Prepared by a contractor to the Olefins Panel)</p>
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Robust Summary - Group 5: High Benzene Naphthas

Genetic Toxicity - in Vivo

<p><u>Test Substance</u> Remarks</p> <p><u>Method</u> Method/guideline followed</p> <p>Type</p> <p>GLP</p> <p>Year</p> <p>Species</p> <p>Strain</p> <p>Sex</p> <p>Route of administration</p> <p>Doses/concentration levels</p> <p>Exposure period</p> <p>Statistical methods</p> <p>Remarks for Test Conditions.</p>	<p>Rerun Tower Overheads from Olefins/Aromatics Plant (light thermal cracked naphtha) CAS # 64741-74-8. Straw colored liquid; 40% benzene, 26% C5, 13% toluene, 20% other. Test substance is described as a sample of a Pyrolysis Gasoline distillate fraction and is similar to Pyrolysis gasoline, a stream included in the test plan.</p> <p>None specified. Standard method based on Bowman, 1969; Lewis, 1954; Mendelson, 1976</p> <p><i>Drosophila</i> assays for point mutation, chromosome aberrations & chromosome loss</p> <p>Not specified</p> <p>1979</p> <p><i>Drosophila melanogaster</i></p> <p>Dominant lethal: Canton S; Y chromosome loss: males red/white eye; females white/white eye; Somatic reversion: males white ivory (<u>w</u>ⁱ), yellow body (<u>y</u>), echinus (<u>ec</u>); females <u>w</u>ⁱ/<u>w</u>ⁱ; Bithrox test: males Ultrabithorax (<u>Ubx</u>); females bithorax (<u>bx</u>^{34e}); Sex-linked recessive lethal: males Canton S; females <u>Basc</u>/<u>Basc</u></p> <p>Males and females</p> <p>Aerosol</p> <p>0.3ml in 50ml air</p> <p>10 min.</p> <p>Events in these tests have very low probabilities. Analysis based on Poisson distribution with fiducial limits computed according to Stevens, 1942.</p> <p><i>Drosophila</i> stocks were maintained in agar/corn meal/sugar/yeast medium at 23^oC. One set of stocks was transferred each week to isolate virgin females for breeding. Four days are required for maturation of <i>Drosophila</i> sperm cells after meiosis. In all assays, treated males were mated for 3 days only to assure use of a uniform sample of treated sperm. In all assays, test article was administered as an aerosol, 0.3ml in 50ml volume of air. when administered for 1hr anesthetized flies and killed approximately 30%. Longer treatments reduced fertility. Exposure in all assays was 10 minutes in duration.</p> <p><u>Somatic reversion of white-ivory</u>: Larvae from mating of males carrying 5 copies of white-ivory gene on the X chromosome (<u>w</u>ⁱ, <u>y</u>, <u>ec</u>) with <u>w</u>ⁱ/<u>w</u>ⁱ females were treated with aerosolized test article for 10 min. Positive control compound was 0.04M mitomycin C. Larvae were washed and transferred to culture bottles to complete development. After eclosion, female offspring, genotype Qn(1)<u>w</u>ⁱ, <u>y</u>, <u>ec</u>/<u>w</u>ⁱ were scored for red spots in the eye, which signals reversion of <u>w</u>ⁱ to a pigment cell.</p> <p><u>Y chromosome loss</u>: Males carrying a duplication of the gene for normal (red) eyes on Y chromosome and a mutant allele, white (<u>w</u>) on the X chromosome were treated with aerosolized test article for 10 min and mated to white-eyed females (<u>w</u>/<u>w</u>). Positive control were males exposed to 3kr X-rays. Frequency of occurrence of white-eyed male progeny measured frequency of Y chromosome loss.</p> <p><u>Dominant lethal mutations</u>: Defined as any genetic change that blocks development prior to hatching. Treated Canton S males were mated with untreated females in nylon net cages on Welch's grape juice solidified with 2% agar. After 12 hr, agar plates were removed and stored at room temp. (23^oC) for 30 hrs. Positive control was 0.04M ethyl methane sulfonate. Eggs were scored for hatching after 30hrs.</p>
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<p><u>Results</u> Genotoxic effects NOAEL (NOEL) LOAEL (LOEL)</p> <p><u>Conclusions</u> (study authors)</p> <p><u>Data Quality</u> <i>Reliabilities</i></p> <p><u>References</u></p> <p><u>Other</u> <i>Last changed</i></p>	<p><u>Bithorax test of Lewis:</u> Occurrence of rearrangements with one breakpoint between centromere and the locus of bithorax (<u>bx</u>) was determined by scoring offspring of treated Ultrabithorax males and bithorax females. Males treated with 3kr X-rays were the positive controls. Distinctive phenotype was the presence of a mesonotum</p> <p><u>Sex-linked recessive lethals:</u> Canton-S males, treated with test article, were mated with Basc (balancer X chromosome) females. Individual (F1) female progeny were mated with Basc males. Any single female culture containing at least 20 flies (F2), at least 8 of which are males, but no males are wild type, is scored as a lethal. Ethyl methane sulfonate (0.04M) treated males were the positive controls. A repeat study was performed due to loss of cultures to dessication.</p> <p>Rerun tower overheads did not induce genetic damage in <i>Drosophila melanogaster</i> under experimental conditions in any test employed. The repeated sex-linked recessive lethal test, performed due to technical problems in the initial assay, did not demonstrate any genetic damage in <i>Drosophila</i> from exposure to the test article</p> <p>Rerun tower overheads did not induce genetic damage in <i>Drosophila melanogaster</i>.</p> <p>1. Reliable without restrictions.</p> <p>Bowman, J.T. 1979. <i>Drosophila</i> mutagenicity assays of Mobil Chemical Compound MCTR-125-78. MRI #110. E.G. and G. Mason Research Institute, Rockville, MD, for Mobil Chemical Co., Edison, NJ. Bowman, J.T. 1969. Mutat. Res. 7: 409-415 Lewis, E.B. 1954. Am. Nat. 88: 225-239 Mendelson, D. 1976. Mutat. Res. 41: 269-276 Stevens, W.L. 1942. J. Genetics 43: 301-307</p> <p>2/28/2002 (Prepared by a contractor to the Olefins Panel)</p>
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Robust Summary: High Benzene Naphthas

Repeated Dose Toxicity

<p><u>Test Substance</u> Remarks</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>Test Conditions</p>	<p>Rerun Tower Overheads from Olefins/Aromatics Plant (light thermal cracked naphtha) CAS # 64741-74-8. Straw colored liquid; 40% benzene, 26% C5, 13% toluene, 20% other. Test substance is described as a sample of a Pyrolysis Gasoline distillate fraction and is similar to Pyrolysis gasoline, a stream included in the test plan.</p> <p>None specified, comparable to standard methods Subacute Not specified 1980 Rabbit (4/sex/group) New Zealand White Dermal 21 days 0, 0.1, 0.5, and 1.0ml/kg/day Male and females Continuous (no wipe-off) Once/day Males and females (4M, 4F), saline (0.9%), 1ml/kg/day 3 days</p> <p>Bartlett's test, analysis of variance, Scheffe's multiple pair wise comparison, Gaines and Howell's multiple pair wise comparison</p> <p>Rabbits were housed individually in stainless steel cages and received water and rabbit chow diet, ad lib. Initial body wt ranged from 2455-3005g for males and 2455-3035g for females. Four rabbits of each sex were assigned to treatment groups of 0, 0.1, 0.5, and 1.0ml of neat test article/kg/day. Control rabbits received 1.0ml/kg/day of 0.9%NaCl. Prior to initiation, the dorsal dosing area was clipped free of hair and clipping was done periodically during the study. The exposure area was abraded with minor incisions deep enough to penetrate the stratum corneum but not deep enough to produce bleeding. Abrasions were made prior to the first application, and thereafter, on the first day of each week. Test article was applied to the skin once a day, starting on day 1, for 21 consecutive days; rabbits were sacrificed between day 22 and day 24. Each rabbit wore a plexiglass collar for the entire study to retard ingestion of test article. Rabbits were observed daily for mortality and morbidity, food/water intake, general appearance/behavior, toxic/pharmacological effects, and dermal reactions for 24 consecutive days. Dermal irritation was graded each morning prior to dosing. Food consumption was determined 3 times /wk and body weight on days 1, 8, 15, and at termination. Prior to study initiation and during wk 3, hematocrit (Hct), hemoglobin (Hgb), erythrocyte count (RBC), total leukocyte count (WBC) and differential leukocyte count, mean cell volume (MCV), mean corpuscular hemoglobin (MCH), mean corpuscular hemoglobin conc. (MCHC), serum glutamate pyruvate transaminase (SGPT), serum glutamate oxaloacetate transaminase (SGOT), alkaline phosphatase (Alk Phos), fasting glucose, and blood urea nitrogen (BUN); urine (pH, specific gravity, glucose, ketones, total protein, bilirubin[BIL]), and microscopic examination of sediment were evaluated. Rabbits were sacrificed on day 24; necropsies were performed and gross observations recorded for all rabbits. Liver, kidney, thyroid, and adrenals were weighed and preserved for microscopic analysis along with brain, pituitary, lung, heart, spleen, pancreas, urinary bladder, testis/ovary, skin, and any unusual lesions.</p>
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<p><u>Results</u> NOAEL (NOEL) LOAEL (LOEL) Remarks</p> <p><u>Conclusions</u> (study authors)</p> <p><u>Quality</u> Reliabilities</p> <p><u>References</u></p> <p><u>Other</u> Last changed</p>	<p>NOAEL <0.10ml/kg/day both sexes (skin irr). LOAEL = 0.1ml/kg/day both sexes (skin irr) NOAEL = 1.0ml/kg/day both sexes (systemic effects). LOAEL >1.0ml/kg/day both sexes (systemic effects). Two rabbits died during the study from cardiac puncture blood sampling. No test article induced effects were noted during clinical observations. Two 0.1ml/kg/day group males and one female showed erythema from day 10 to termination; 3 0.5ml/kg/day group males showed erythema from day 8 to termination; all 0.5ml/kg/day males and females, and 1.0ml/kg/day males and females had well defined erythema from day 9 to termination. Edema was not present in any rabbits. Skin thickening was noted in all test article groups from wk 1 to termination. Fissuring was seen in 3 0.1ml/kg/day males, 3 0.5ml/kg/day males and all 1.0ml/kg/day males; all test article treated females showed fissuring. Necrosis was present in 2males and 3 females given 0.1ml/kg/day, 3males and all females given 0.5ml/kg/day, and all males and females given 1.0ml/kg/day. There were no significant changes in body wt or food consumption between controls and treatment groups. Terminal basophilic values were elevated in all male test article treated groups; all other hematology values were comparable to controls. Urinalysis findings were unremarkable. There were no significant differences in organ wt between control and any treatment group. Histological evaluation for the skin showed effects consistent with gross observations with no dose-related gradation of severity between doses, including hyperkeratosis, acanthosis, accumulation of heterophils, and cellular debris in stratum corneum, and hyperplasia of sebaceous glands. There were no abnormal microscopic findings attributable to test article administration in organs from the three treatment levels compared to controls.</p> <p>Daily epidermal application of test article resulted in skin irritation at the application site.</p> <p>2. Reliable with restriction. There was no mention of GLP.</p> <p>Fieser, S., Alsaker, R.D., Brown, H.R., and Wolfe, G.W. 1980. 21-Day dermal irritation study in rabbits. Proj. #230-213. Hazleton Laboratories America, Inc., Vienna, VA. For Mobil Chemical Co., Edison NJ (This study was actually for subacute toxicity, not only skin irritation)</p> <p>2/28/2002 (Prepared by a contractor to the Olefins Panel)</p>
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Robust Summary: High Benzene Naphthas

Developmental Toxicity/Teratogenicity

<p><u>Test Substance</u> Remarks</p> <p><u>Method</u> Method/guideline followed Test type GLP Year Species Strain Route of administration Concentration levels Sex Exposure period Frequency of treatment Control group and treatment Duration of test</p> <p>Statistical methods</p> <p>Remarks for Test Conditions.</p>	<p>Rerun Tower Overheads from Olefins/Aromatics Plant (light thermal cracked naphtha) CAS # 64741-74-8. Straw colored liquid; 40% benzene, 26% C5, 13% toluene, 20% other. Test substance is described as a sample of a Pyrolysis Gasoline distillate fraction and is similar to Pyrolysis gasoline, a stream included in the test plan.</p> <p>None specified, conforms to standard method</p> <p>Teratology Yes 1981 Rabbit New Zealand White Oral gavage 0, 10, 25, and 50mg/kg/day, diluted in corn oil Pregnant females (16/group) Day 6-28 of gestation Once/day 16 pregnant females received 0.5ml/kg/day corn oil 29 days</p> <p>Chi square with Yates' correction for 2x2 contingency table and /or Fisher's exact probability test; Mann-Whitney U test; analysis of variance (one-way), Bartlett's test and t-test using Dunnett's multiple comparison tables. Level of significance $p < 0.05$.</p> <p>In an initial study, RTO was administered by oral gavage, undiluted to 16 pregnant rabbits/group at levels of 0 (distilled water), 10, 25 and 50 mg/kg/day. Forty-two rabbits died: 14, 11, 13, and 13 in the 0, 10, 25 and 50mg/kg/day groups respectively. Due to excess mortality in all treated groups and the controls, the study was terminated and repeated at the same concentrations diluted in corn oil.</p> <p>Sixty-four sexually mature virgin female rabbits (7 months old, 3.46-4.19kg at study initiation) were acclimated for 59 days, assigned a unique animal number and ear-tagged when placed on study. All rabbits were individually housed in suspended wire cages and maintained in a temperature, humidity, and light (12 hr light/dark cycle) controlled environment. Certified rabbit chow and tap water were available ad lib. Only coccidiosis-free rabbits were used in the study. Prior to insemination, females were randomly assigned to groups (16/group) according to body wt, by a computer-generated program. Sperm was collected from each of 6 proven breeder males of the same source and strain, using an artificial vagina. Semen was immediately evaluated for motility, and was used for insemination only if motility was $\geq 50\%$. Useable ejaculate was diluted in 0.9%NaCl at 35°C; 0.25-0.50ml of dilute semen was introduced into the anterior vagina. Ovulation was induced by injection of 100 units chorionic gonadotropin (Ayerst, NY) in the marginal ear vein of the female immediately after insemination. Semen from one male was used to inseminate an equal number of females in each group. Inseminations were performed on two consecutive days; an equal number of females was inseminated in each group/day, designated as day 0 of gestation. RTO was mixed with corn oil daily at appropriate doses and shaken by hand. No analysis of dosing solution was reported. Negative control dams were given 0.5ml corn oil/kg/day, the volume equal to the highest treatment group. Individual doses were determined from individual body wt on day 6 of gestation. Females</p>
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<p>Results NOAEL maternal toxicity NOAEL developmental toxicity Maternal effects</p> <p>Embryo/fetal effects</p> <p>Conclusions (study authors)</p>	<p>were observed daily for mortality, overt changes in appearance and behavior, and, from day 6-29 of gestation, for clinical signs of toxicity. One dam aborted on gest. day 19 and remained on study until scheduled sacrifice; aborted material was discarded. Body wt was recorded on gestation days 0, 6, 12, 18, 24, and 29. On gest. day 29, all females were sacrificed by overdose of sodium pentobarbitol, uteri were excised and weighed prior to removal of fetuses. Number and location of viable and non-viable fetuses, early and late resorptions, number of total implantations, and corpora lutea were recorded. Abdominal and thoracic cavity and organs of dams were examined grossly and discarded. Uteri from apparently non-gravid animals were opened and placed in 10% ammonium sulfide solution to confirm pregnancy status.</p> <p>All fetuses were individually weighed and examined for external malformations and variations. Each fetus was internally sexed and examined for internal malformations and variations, including the brain by mid-coronal slice. The heart was dissected using Staples' technique. Eviscerated, skinned fetuses were individually numbered and tagged, fixed in alcohol, macerated and stained with Alizarin Red S for skeletal examination. Fetal findings were classified as malformations or genetic or developmental variations.</p> <p>NOAEL maternal = 25mg/kg/day (based on 1 abortion at 50mg/kg/day) NOAEL developmental = 50mg/kg/day; both values assigned by reviewer</p> <p>Maternal survival was 100% in all groups. Slight increase in matted haircoat (primarily in nasal region) and slight reduction in fecal material beneath cages was noted in 50mg/kg/day rabbits. Occasional instances of nasal discharge, soft stool, hair loss and scabbing were noted in all groups during gestation. One 50mg/kg/day rabbit aborted on day 19 of gestation. Maternal body wt in treated rabbits at all doses were comparable to controls throughout treatment (gest. day 6-28) and gestation (day 0-29) periods. Mean maternal adjusted body wt (minus gravid uterus) at termination in all groups was comparable to controls. Pregnancy ratio was 87.5, 81.3, 81.3, 93.8 in 0, 10, 25 and 50mg/kg/day groups, respectively. Two control dams and one 50mg/kg/day dam had all resorptions. There were no biologically or statistically significant differences in mean number of corpora lutea, total implantations, early or late resorptions, postimplantation loss, viable fetuses, fetal sex index, or mean fetal body wt in any RTO treated group compared to controls.</p> <p>Average litter size was 6.1, 6.5, 6.4, and 5.9 and average fetal body wt (both sexes) was 38.9, 43.0, 42.5, and 42.4g in 0, 10, 25, and 50mg/kg/day groups, respectively. There were no biologically or statistically significant differences in number of litters with malformations (external, soft tissue, skeletal) in any treated group compared to controls: 5/12 litters (85 pups), 1/13 litters (84 pups), 3/13 litters (83 pups) and 5/13 litters (82 pups examined) in 0, 10, 25, and 50mg/kg/day, respectively. In the 50mg/kg/day group, one occurrence of atlas-occipital anomaly and one occurrence of enlarged heart with great vessel anomaly, were observed in 2 separate litters. Scoliosis was present in all groups including control, with slightly higher incidence in the 50mg/kg/day group., but incidences were within the range of historical control data for this laboratory. Fetuses and litters with genetic or developmental variations were comparable in all groups.</p> <p>Rerun tower overhead did not produce a teratogenic response in pregnant New Zealand White rabbits when administered orally in corn oil vehicle at dose levels of 10, 25 and 50mg/kg/day. With the exception of one 50mg/kg/day female that aborted, minimal maternal toxicity was observed at any dose level.</p>
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<p><u>Data Quality</u> <i>Reliabilities</i></p> <p><u>References</u></p> <p><u>Other</u> <i>Last changed</i></p>	<p>2. Reliable with restrictions. Analysis of test article concentration in corn oil vehicle was not performed.</p> <p>Schardein, J.L. 1981. Teratology study in rabbits: Rerun tower overheads (MRTC-171-79) IRDC #450-011. International Research and Development Corp., Mattawan, MI. for Mobil Petrochemicals Division, Edison, NJ</p> <p>2/28/2002 (Prepared by a contractor to the Olefins Panel)</p>
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