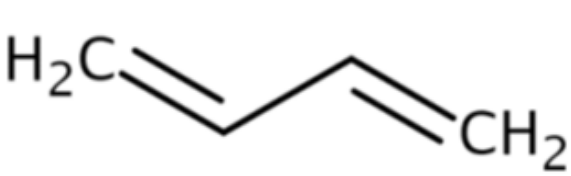
United States
Environmental Protection Agency

November 2024
Office of Chemical Safety and
Pollution Prevention

Data Quality Evaluation and Data Extraction Information for Environmental Fate and Transport for 1,3-Butadiene

Systematic Review Support Document for the Draft Risk Evaluation

CASRN: 106-99-0



November 2024

This supplemental file contains information regarding the data extraction and evaluation results for data sources that were considered for the *Draft Risk Evaluation for 1,3-Butadiene* that underwent systematic review. EPA used the TSCA systematic review process described in the *Draft Systematic Review Protocol Supporting TSCA Risk Evaluations for Chemical Substances* (also referred to as the '2021 Draft Systematic Review Protocol'). The systematic review steps are further described in the *Draft Risk Evaluation for 1,3-Butadiene - Systematic Review Protocol*. EPA conducted data extractions and data quality evaluations based on author-reported descriptions and results; additional analyses (*e.g.*, statistical analyses) potentially conducted by EPA are not contained in this supplemental file. Additionally, the overall quality determination (OQD) for each reference represents the data as a whole for each study, and not for individual metric domains within a study.

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Study Citation:	Andersson, Y., Ljungström, E. (1989). Gas phase reaction of the NO3 radical with organic compounds in the dark. Atmospheric Environment (1967) 23(5):1153-1155.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	5675250

EXTRACTION

Parameter	**Data**
CASRN and Test Material	Not Reported; 1,3-butadiene
Confidentiality, Type, Guideline	No; experimental; other: Non-guideline: gas-phase reaction with NO3 radical in the dark
Solvent, Reactivity, Storage, Stability	NR; NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR; NR Notes: NR
Duration and Test Temperature	ca. 28 minutes; 296±1K
Light Source, Intensity, and additional light details	not reported; not reported; not reported
Source Wavelength Lower and Upper	not reported; not reported
Test Details and Control	Conducted in N2 atmosphere at standard pressure; N2O5 used as source for NO3 radicals; experimental set-up described previously; not reported
Initial Concentration, Reference Compound	ca. 1.7x10^15 molecule/cm3; not reported
Substance Wavelength Lower and Upper	not reported; not reported
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	not reported; not reported; not reported
Indirect Type Results, Indirect Rate Constant Lower and Upper	NO3 radical rate constant (cm3/molecule sec); rate constant k dependent on k2/k-2 (K2); k = 5.6±0.8x10^-14 (K2 value at 296K from Malko and Troe 1982); k = 4.4x10^-14 (K2 value at 298K = 1.87x10^-11 cm3/molecule); k = 5.2x10^-14 (K2 value at 298K = 2.2x10^-11 cm3/molecule); k = 7.9x10^-14 (K2 at 298K = 3.35x10^-11 cm3/molecule)
Method Details Results and Products Details Results	IR spectra recorded using FTIR spectrometer; not reported
Parameter Value and Parameter Results	test material concentrations; Approximate rate constant k4 was estimated from the slope of plotting ln([org]0/[org]t) vs (k-2[N2O5]t)/(k2[NO2]t)+k4[org]t)t; k4 was fit by least squares to observed N2O5 and org concentrations over time.
Reference Substance Results, Percent Degradation Results and Standard Deviation Results	not reported; not reported; indicated error reported = two standard deviations
Results Remarks, Sample time Results, Results Details	not reported; not reported; not reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was identified.
	Metric 2:	Test Substance Purity	Low	The source and purity were not reported.
Domain 2: Test Design				
	Metric 3:	Study Controls	Low	Controls were not included.

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Study Citation:	Andersson, Y., Ljungström, E. (1989). Gas phase reaction of the NO3 radical with organic compounds in the dark. Atmospheric Environment (1967) 23(5):1153-1155.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	5675250

		EVALUATION		
Domain		Metric	Rating	Comments
	Metric 4:	Test Substance Stability	Medium	The test substance stability, homogeneity, preparation or storage conditions were not reported.
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	High	The test method was suitable.
	Metric 6:	Testing Conditions	High	Testing conditions were reported.
	Metric 7:	Testing Consistency	N/A	This metric is not applicable to this study type.
	Metric 8:	System Type and Design	Medium	Some detail was omitted regarding the system set up; additional information may be found in cited work.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	This metric is not applicable to this study type.
	Metric 10:	Sampling Methods	N/A	This metric is not applicable to this study type.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	High	The outcome assessment methodology addressed the intended outcome of interest.
	Metric 12:	Test Substance Purity	N/A	This metric is not applicable to this study type.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	N/A	This metric is not applicable to this study type.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	This metric is not applicable to this study type.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Medium	Analytical details were not reported.
	Metric 16:	Statistical Methods and Kinetic Calculations	High	Calculations were described.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	High	Reported values were reasonable.
	Metric 18:	QSAR Models	N/A	This metric is not applicable to this study type.

Overall Quality Determination — High

Study Citation:	EC, (2002). Summary risk assessment report for 1,3-butadiene.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	7348613

EXTRACTION

Parameter	**Data**
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, Guideline	no; estimated; other: not reported
Solvent, Reactivity, Storage, Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, Purity	Not Reported; Not Reported; Not Reported; Not Reported
Duration and Test Temperature	Not Reported; Not Reported
Light Source, Intensity, and additional light details	Not Reported; Not Reported; Not Reported
Source Wavelength Lower and Upper	Not Reported; Not Reported
Test Details and Control	Not Reported; Not Reported
Initial Concentration, Reference Compound	Not Reported Not Reported; Not Reported
Substance Wavelength Lower and Upper	Not Reported; Not Reported
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	Not Reported; Not Reported; Not Reported
Indirect Type Results, Indirect Rate Constant Lower and Upper	Reaction with Ozone; half-life = 1.9 days; Not Reported; Not Reported
Method Details Results and Products Details Results	Not Reported; Not Reported
Parameter Value and Parameter Results	Not Reported; Not Reported
Reference Substance Results, Percent Degradation Results and Standard Deviation Results	Not Reported; Not Reported; Not Reported
Results Remarks, Sample time Results, Results Details	Not Reported; Not Reported; Not Reported

EVALUATION

Domain	Metric	Rating	Comments
Domain 1: Test Substance			
Metric 1:	Test Substance Identity	High	The test substance was identified.
Metric 2:	Test Substance Purity	Low	The test substance source was not reported; no citation for data.
Domain 2: Test Design			
Metric 3:	Study Controls	Low	Details were not included; no citation reported.
Metric 4:	Test Substance Stability	Low	Details were not included; no citation reported.
Domain 3: Test Conditions			
Metric 5:	Test Method Suitability	Low	Details were not included; no citation reported.

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Study Citation:	EC, (2002). Summary risk assessment report for 1,3-butadiene.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	7348613

Domain	Metric		EVALUATION Rating	Comments
	Metric 6:	Testing Conditions	Low	Details were not included; no citation reported.
	Metric 7:	Testing Consistency	N/A	Estimated value from secondary source with no citation.
	Metric 8:	System Type and Design	N/A	Estimated value from secondary source with no citation.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	Not applicable to the study.
	Metric 10:	Sampling Methods	N/A	Not applicable to the study.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	Low	No methodology was reported; no citation.
	Metric 12:	Test Substance Purity	N/A	The metric is not applicable to the study.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	N/A	Estimated value from secondary source with no citation.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	This metric does not apply to this study type.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Low	Estimated value from secondary source with no citation.
	Metric 16:	Statistical Methods and Kinetic Calculations	Low	Estimated value from secondary source with no citation.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Low	Due to limited information, evaluation of the reasonableness of the study results was not possible.
	Metric 18:	QSAR Models	N/A	A QSAR model was not reported.

Overall Quality Determination Low

* Related References: no references citedData also found in Pubchem entry (cites NIST; NIST Chemistry WebBook. 1,3-Butadiene (106-99-0). NIST Standard Reference and Gas Kinetics Databases, 2013 Release. Washington, DC: US Sec Commerce. Available, as of Mar 9, 2015)

Study Citation:	EC, (2002). Summary risk assessment report for 1,3-butadiene.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	7348613

EXTRACTION

Parameter	Data
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, Guideline	no; estimated; other: not reported
Solvent, Reactivity, Storage, Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, Purity	Not Reported; Not Reported; Not Reported; Not Reported
Duration and Test Temperature	Not Reported; Not Reported
Light Source, Intensity, and additional light details	Not Reported; Not Reported; Not Reported
Source Wavelength Lower and Upper	Not Reported; Not Reported
Test Details and Control	Not Reported; Not Reported
Initial Concentration, Reference Compound	Not Reported Not Reported; Not Reported
Substance Wavelength Lower and Upper	Not Reported; Not Reported
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	Not Reported; Not Reported; Not Reported
Indirect Type Results, Indirect Rate Constant Lower and Upper	Reaction with hydroxyl radicals; half-life = 5.8 hours; Not Reported; Not Reported
Method Details Results and Products Details Results	Not Reported; Not Reported
Parameter Value and Parameter Results	Not Reported; Not Reported
Reference Substance Results, Percent Degradation Results and Standard Deviation Results	Not Reported; Not Reported; Not Reported
Results Remarks, Sample time Results, Results Details	Not Reported; Not Reported; Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was identified.
	Metric 2:	Test Substance Purity	Low	The test substance source was not reported; no citation for data.
Domain 2: Test Design				
	Metric 3:	Study Controls	Low	Details were not included; no citation reported.
	Metric 4:	Test Substance Stability	Low	Details were not included; no citation reported.
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	Low	Details were not included; no citation reported.
	Metric 6:	Testing Conditions	Low	Details were not included; no citation reported.
	Metric 7:	Testing Consistency	N/A	Estimated value from secondary source with no citation.

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Study Citation:	EC, (2002). Summary risk assessment report for 1,3-butadiene.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	7348613

Domain		Metric	EVALUATION Rating	Comments
	Metric 8:	System Type and Design	N/A	Estimated value from secondary source with no citation.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	Not applicable to the study.
	Metric 10:	Sampling Methods	N/A	Not applicable to the study.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	Low	No methodology was reported; no citation.
	Metric 12:	Test Substance Purity	N/A	The metric is not applicable to the study.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	N/A	Estimated value from secondary source with no citation.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	This metric does not apply to this study type.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Low	Estimated value from secondary source with no citation.
	Metric 16:	Statistical Methods and Kinetic Calculations	Low	Estimated value from secondary source with no citation.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Low	Due to limited information, evaluation of the reasonableness of the study results was not possible.
	Metric 18:	QSAR Models	N/A	A QSAR model was not reported.

Overall Quality Determination Low

* Related References: no references citedData also found in Pubchem entry (cites NIST; NIST Chemistry WebBook. 1,3-Butadiene (106-99-0). NIST Standard Reference and Gas Kinetics Databases, 2013 Release. Washington, DC: US Sec Commerce. Available, as of Mar 9, 2015)

Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	5155560

EXTRACTION

Parameter	**Data**
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, Type, Guideline	no; experimental; other: not specified
Solvent, Reactivity, Storage, Stability	NR; NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR; NR Notes: NR
Duration and Test Temperature	NR; 25 C
Light Source, Intensity, and additional light details	NR; NR; NR
Source Wavelength Lower and Upper	NR; NR
Test Details and Control	NR; NR
Initial Concentration, Reference Compound	NR NR; NR
Substance Wavelength Lower and Upper	NR; NR
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	NR; Not Reported; NR
Indirect Type Results, Indirect Rate Constant Lower and Upper	Second order rate constant for reaction with OH radicals; k=6.68E-11 cm^3/molecule*sec; NR
Method Details Results and Products Details Results	NR; NR
Parameter Value and Parameter Results	NR; NR
Reference Substance Results, Percent Degradation Results and Standard Deviation Results	NR; NR; NR
Results Remarks, Sample time Results, Results Details	NR; NR; NR

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was identified definitively.
	Metric 2:	Test Substance Purity	Medium	Test substance source and purity were not reported; more details may be in the source cited.
Domain 2: Test Design				
	Metric 3:	Study Controls	Medium	No concurrent control group details reported; more details may be in the source cited.
	Metric 4:	Test Substance Stability	Medium	Test substance stability, homogeneity, preparation, and storage conditions were not reported; more details may be in the source cited.

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Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	5155560

Domain		Metric	EVALUATION Rating	Comments
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	Medium	Test method not reported; ; more details may be in the source cited.
	Metric 6:	Testing Conditions	Medium	Testing conditions not reported; more details may be in the source cited.
	Metric 7:	Testing Consistency	Medium	Details on this metric were not reported; more details may be in the source cited
	Metric 8:	System Type and Design	Medium	System type and design not reported; more details may be in the source cited.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	This metric does not apply to this study type.
	Metric 10:	Sampling Methods	N/A	This metric does not apply to this study type
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	Medium	The outcome was reasonable; more details may be in the source cited.
	Metric 12:	Test Substance Purity	Medium	Sampling details not reported; more details may be in the source cited.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	Medium	Confounding variables not reported; more details may be in the source cited.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	This metric does not apply to this study type.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Medium	Analytical method was not reported; more details may be in the source cited
	Metric 16:	Statistical Methods and Kinetic Calculations	Medium	Statistical method was not reported; more details may be in the source cited.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Medium	Values seem appropriate; more details may be in the source cited.
	Metric 18:	QSAR Models	N/A	A QSAR model was not reported.

Overall Quality Determination — Medium

* Related References: Cites secondary source Atkinson1985 [HERO ID 38261]

Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	5155560

EXTRACTION

Parameter	Data
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, Type, Guideline	no; experimental; other: not specified
Solvent, Reactivity, Storage, Stability	NR; NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR; NR Notes: NR
Duration and Test Temperature	NR; NR
Light Source, Intensity, and additional light details	NR; NR; NR
Source Wavelength Lower and Upper	NR; NR
Test Details and Control	NR; NR
Initial Concentration, Reference Compound	NR NR; NR
Substance Wavelength Lower and Upper	NR; NR
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	NR; Not Reported; NR
Indirect Type Results, Indirect Rate Constant Lower and Upper	Second order rate constant for reaction with ozone; k=6.1E-18 cm^3/molecule*sec; NR
Method Details Results and Products Details Results	NR; NR
Parameter Value and Parameter Results	1.9 days; Half-life for reaction with atmospheric ozone
Reference Substance Results, Percent Degradation Results and Standard Deviation Results	NR; NR; NR
Results Remarks, Sample time Results, Results Details	NR; NR; NR

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was identified definitively.
	Metric 2:	Test Substance Purity	Medium	Test substance source and purity were not reported; more details may be in the source cited.
Domain 2: Test Design				
	Metric 3:	Study Controls	Medium	No concurrent control group details reported; more details may be in the source cited.
	Metric 4:	Test Substance Stability	Medium	Test substance stability, homogeneity, preparation, and storage conditions were not reported; more details may be in the source cited.
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	Medium	Test method not reported; ; more details may be in the source cited.

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Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	5155560

Domain		Metric	EVALUATION Rating	Comments
	Metric 6:	Testing Conditions	Medium	Testing conditions not reported; more details may be in the source cited.
	Metric 7:	Testing Consistency	Medium	Details on this metric were not reported; more details may be in the source cited
	Metric 8:	System Type and Design	Medium	System type and design not reported; more details may be in the source cited.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	This metric does not apply to this study type.
	Metric 10:	Sampling Methods	N/A	This metric does not apply to this study type
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	Medium	The outcome was reasonable; more details may be in the source cited.
	Metric 12:	Test Substance Purity	Medium	Sampling details not reported; more details may be in the source cited.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	Medium	Confounding variables not reported; more details may be in the source cited.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	This metric does not apply to this study type.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Medium	Analytical method was not reported; more details may be in the source cited
	Metric 16:	Statistical Methods and Kinetic Calculations	Medium	Statistical method was not reported; more details may be in the source cited.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Medium	Values seem appropriate; more details may be in the source cited.
	Metric 18:	QSAR Models	N/A	A QSAR model was not reported.

Overall Quality Determination **Medium**

* Related References: Cites secondary source Klopffer et al. 1988 [HERO ID 1939717]

Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	5155560

EXTRACTION

Parameter	Data
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, Type, Guideline	no; experimental; other: not specified
Solvent, Reactivity, Storage, Stability	NR; NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR; NR Notes: NR
Duration and Test Temperature	NR; 295 K
Light Source, Intensity, and additional light details	NR; NR; NR
Source Wavelength Lower and Upper	NR; NR
Test Details and Control	NR; NR
Initial Concentration, Reference Compound	NR NR; NR
Substance Wavelength Lower and Upper	NR; NR
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	NR; Not Reported; NR
Indirect Type Results, Indirect Rate Constant Lower and Upper	Second order rate constant for reaction with NO3 radicals; k=5.34E-13 cm^3/molecule*sec; NR
Method Details Results and Products Details Results	NR; NR
Parameter Value and Parameter Results	NR; NR
Reference Substance Results, Percent Degradation Results and Standard Deviation Results	NR; NR; NR
Results Remarks, Sample time Results, Results Details	NR; NR; NR

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was identified definitively.
	Metric 2:	Test Substance Purity	Medium	Test substance source and purity were not reported; more details may be in the source cited.
Domain 2: Test Design				
	Metric 3:	Study Controls	Medium	No concurrent control group details reported; more details may be in the source cited.
	Metric 4:	Test Substance Stability	Medium	Test substance stability, homogeneity, preparation, and storage conditions were not reported; more details may be in the source cited.
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	Medium	Test method not reported; ; more details may be in the source cited.

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Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	5155560

Domain		Metric	EVALUATION Rating	Comments
	Metric 6:	Testing Conditions	Medium	Testing conditions not reported; more details may be in the source cited.
	Metric 7:	Testing Consistency	Medium	Details on this metric were not reported; more details may be in the source cited
	Metric 8:	System Type and Design	Medium	System type and design not reported; more details may be in the source cited.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	This metric does not apply to this study type.
	Metric 10:	Sampling Methods	N/A	This metric does not apply to this study type
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	Medium	The outcome was reasonable; more details may be in the source cited.
	Metric 12:	Test Substance Purity	Medium	Sampling details not reported; more details may be in the source cited.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	Medium	Confounding variables not reported; more details may be in the source cited.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	This metric does not apply to this study type.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Medium	Analytical method was not reported; more details may be in the source cited
	Metric 16:	Statistical Methods and Kinetic Calculations	Medium	Statistical method was not reported; more details may be in the source cited.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Medium	Values seem appropriate; more details may be in the source cited.
	Metric 18:	QSAR Models	N/A	A QSAR model was not reported.

Overall Quality Determination **Medium**

* Related References: Cites secondary source Atkinson and Carter 1984 [HERO ID 38267]

Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	5155560

EXTRACTION

Parameter	Data
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, Type, Guideline	no; experimental; other: not specified
Solvent, Reactivity, Storage, Stability	NR; NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR; NR Notes: NR
Duration and Test Temperature	NR; 298 +/- 2 K
Light Source, Intensity, and additional light details	NR; NR; NR
Source Wavelength Lower and Upper	NR; NR
Test Details and Control	Environmental chamber under simulated atmospheric conditions; NO present at 0.11-2.4 ppm; NR
Initial Concentration, Reference Compound	0.5, 1.0, 2.0 ppm; NR
Substance Wavelength Lower and Upper	NR; NR
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	NR; NR; NR
Indirect Type Results, Indirect Rate Constant Lower and Upper	NR; NR; NR
Method Details Results and Products Details Results	NR; NR
Parameter Value and Parameter Results	NR; NR
Reference Substance Results, Percent Degradation Results and Standard Deviation Results	NR; NR; NR
Results Remarks, Sample time Results, Results Details	NR; NR; Acrolein and NO2 identified as primary stable photoproducts.

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was identified definitively.
	Metric 2:	Test Substance Purity	Medium	Test substance source and purity were not reported; more details may be in the source cited.
Domain 2: Test Design				
	Metric 3:	Study Controls	Medium	No concurrent control group details reported; more details may be in the source cited.
	Metric 4:	Test Substance Stability	Medium	Test substance stability, homogeneity, preparation, and storage conditions were not reported; more details may be in the source cited.
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	Medium	Test method not reported; ; more details may be in the source cited.

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Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	5155560

Domain		Metric	EVALUATION Rating	Comments
	Metric 6:	Testing Conditions	Medium	Testing conditions not reported; more details may be in the source cited.
	Metric 7:	Testing Consistency	Medium	Details on this metric were not reported; more details may be in the source cited
	Metric 8:	System Type and Design	Medium	System type and design not reported; more details may be in the source cited.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	This metric does not apply to this study type.
	Metric 10:	Sampling Methods	N/A	This metric does not apply to this study type
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	Medium	The outcome was reasonable; more details may be in the source cited.
	Metric 12:	Test Substance Purity	Medium	Sampling details not reported; more details may be in the source cited.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	Medium	Confounding variables not reported; more details may be in the source cited.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	This metric does not apply to this study type.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Medium	Analytical method was not reported; more details may be in the source cited
	Metric 16:	Statistical Methods and Kinetic Calculations	Medium	Statistical method was not reported; more details may be in the source cited.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Medium	Values seem appropriate; more details may be in the source cited.
	Metric 18:	QSAR Models	N/A	A QSAR model was not reported.

Overall Quality Determination **Medium**

* Related References: Cites secondary source Maldotti et al 1980 [HERO ID 5747014].

Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	5155560

EXTRACTION

Parameter	Data
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, Type, Guideline	no; experimental; other: not specified
Solvent, Reactivity, Storage, Stability	NR; NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR; NR Notes: NR
Duration and Test Temperature	NR; 305 K
Light Source, Intensity, and additional light details	NR; NR; NR
Source Wavelength Lower and Upper	NR; NR
Test Details and Control	NR; NR
Initial Concentration, Reference Compound	NR NR; NR
Substance Wavelength Lower and Upper	NR; NR
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	NR; NR; NR
Indirect Type Results, Indirect Rate Constant Lower and Upper	Second order rate constant for reaction with OH radicals; kOH=6.79E-11 cm^3/molecule*sec; NR
Method Details Results and Products Details Results	NR; relative to n-butane (k=2.69E-12 cm^3/ molecules* s
Parameter Value and Parameter Results	NR; NR
Reference Substance Results, Percent Degradation Results and Standard Deviation Results	NR; NR; NR
Results Remarks, Sample time Results, Results Details	NR; NR; NR

EVALUATION

Domain	Metric	Rating	Comments
Domain 1: Test Substance			
Metric 1:	Test Substance Identity	High	The test substance was identified definitively.
Metric 2:	Test Substance Purity	Medium	Test substance source and purity were not reported; more details may be in the source cited.
Domain 2: Test Design			
Metric 3:	Study Controls	Medium	No concurrent control group details reported; more details may be in the source cited.
Metric 4:	Test Substance Stability	Medium	Test substance stability, homogeneity, preparation, and storage conditions were not reported; more details may be in the source cited.
Domain 3: Test Conditions			
Metric 5:	Test Method Suitability	Medium	Test method not reported; ; more details may be in the source cited.

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Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	5155560

Domain		Metric	EVALUATION Rating	Comments
	Metric 6:	Testing Conditions	Medium	Testing conditions not reported; more details may be in the source cited.
	Metric 7:	Testing Consistency	Medium	Details on this metric were not reported; more details may be in the source cited
	Metric 8:	System Type and Design	Medium	System type and design not reported; more details may be in the source cited.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	This metric does not apply to this study type.
	Metric 10:	Sampling Methods	N/A	This metric does not apply to this study type
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	Medium	The outcome was reasonable; more details may be in the source cited.
	Metric 12:	Test Substance Purity	Medium	Sampling details not reported; more details may be in the source cited.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	Medium	Confounding variables not reported; more details may be in the source cited.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	This metric does not apply to this study type.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Medium	Analytical method was not reported; more details may be in the source cited
	Metric 16:	Statistical Methods and Kinetic Calculations	Medium	Statistical method was not reported; more details may be in the source cited.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Medium	Values seem appropriate; more details may be in the source cited.
	Metric 18:	QSAR Models	N/A	A QSAR model was not reported.

Overall Quality Determination — Medium

* Related References: Cites secondary source Lloyd et al., 1976 [HERO ID 8541109]

Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	5155560

EXTRACTION

Parameter	Data
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, Type, Guideline	no; experimental; other: not specified
Solvent, Reactivity, Storage, Stability	NR; NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR; NR Notes: NR
Duration and Test Temperature	NR; 299.5 K
Light Source, Intensity, and additional light details	NR; NR; NR
Source Wavelength Lower and Upper	NR; NR
Test Details and Control	NR; NR
Initial Concentration, Reference Compound	NR NR; NR
Substance Wavelength Lower and Upper	NR; NR
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	NR; NR; NR
Indirect Type Results, Indirect Rate Constant Lower and Upper	Second order rate constant for reaction with OH radicals; kOH=6.85E-11 cm^3/molecule*sec; NR
Method Details Results and Products Details Results	NR; absolute rate method
Parameter Value and Parameter Results	NR; NR
Reference Substance Results, Percent Degradation Results and Standard Deviation Results	NR; NR; NR
Results Remarks, Sample time Results, Results Details	NR; NR; NR

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was identified definitively.
	Metric 2:	Test Substance Purity	Medium	Test substance source and purity were not reported; more details may be in the source cited.
Domain 2: Test Design				
	Metric 3:	Study Controls	Medium	No concurrent control group details reported; more details may be in the source cited.
	Metric 4:	Test Substance Stability	Medium	Test substance stability, homogeneity, preparation, and storage conditions were not reported; more details may be in the source cited.
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	Medium	Test method not reported; ; more details may be in the source cited.

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Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	5155560

Domain		Metric	EVALUATION Rating	Comments
	Metric 6:	Testing Conditions	Medium	Testing conditions not reported; more details may be in the source cited.
	Metric 7:	Testing Consistency	Medium	Details on this metric were not reported; more details may be in the source cited
	Metric 8:	System Type and Design	Medium	System type and design not reported; more details may be in the source cited.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	This metric does not apply to this study type.
	Metric 10:	Sampling Methods	N/A	This metric does not apply to this study type
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	Medium	The outcome was reasonable; more details may be in the source cited.
	Metric 12:	Test Substance Purity	Medium	Sampling details not reported; more details may be in the source cited.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	Medium	Confounding variables not reported; more details may be in the source cited.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	This metric does not apply to this study type.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Medium	Analytical method was not reported; more details may be in the source cited
	Metric 16:	Statistical Methods and Kinetic Calculations	Medium	Statistical method was not reported; more details may be in the source cited.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Medium	Values seem appropriate; more details may be in the source cited.
	Metric 18:	QSAR Models	N/A	A QSAR model was not reported.

Overall Quality Determination **Medium**

* Related References: Cites secondary source Atkinson R, Perry RA, Pitts JN Jr. (1977). J Chem Phys. 67; 3170 [Not in HERO at the time of extraction]

Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	5155560

EXTRACTION

Parameter	**Data**
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, Type, Guideline	no; experimental; other: not specified
Solvent, Reactivity, Storage, Stability	NR; NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR; NR Notes: NR
Duration and Test Temperature	NR; ~300 K
Light Source, Intensity, and additional light details	NR; NR; NR
Source Wavelength Lower and Upper	NR; NR
Test Details and Control	NR; NR
Initial Concentration, Reference Compound	NR NR; NR
Substance Wavelength Lower and Upper	NR; NR
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	NR; NR; NR
Indirect Type Results, Indirect Rate Constant Lower and Upper	Second order rate constant for reaction with OH radicals; kOH=6.51E-11 cm^3/molecule*sec; NR
Method Details Results and Products Details Results	NR; relative to ethene (k=8.45E-12 cm^3/molecule*sec
Parameter Value and Parameter Results	NR; NR
Reference Substance Results, Percent Degradation Results and Standard Deviation Results	NR; NR; NR
Results Remarks, Sample time Results, Results Details	NR; NR; NR

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was identified definitively.
	Metric 2:	Test Substance Purity	Medium	Test substance source and purity were not reported; more details may be in the source cited.
Domain 2: Test Design				
	Metric 3:	Study Controls	Medium	No concurrent control group details reported; more details may be in the source cited.
	Metric 4:	Test Substance Stability	Medium	Test substance stability, homogeneity, preparation, and storage conditions were not reported; more details may be in the source cited.
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	Medium	Test method not reported; ; more details may be in the source cited.

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Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	5155560

Domain		Metric	EVALUATION Rating	Comments
	Metric 6:	Testing Conditions	Medium	Testing conditions not reported; more details may be in the source cited.
	Metric 7:	Testing Consistency	Medium	Details on this metric were not reported; more details may be in the source cited
	Metric 8:	System Type and Design	Medium	System type and design not reported; more details may be in the source cited.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	This metric does not apply to this study type.
	Metric 10:	Sampling Methods	N/A	This metric does not apply to this study type
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	Medium	The outcome was reasonable; more details may be in the source cited.
	Metric 12:	Test Substance Purity	Medium	Sampling details not reported; more details may be in the source cited.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	Medium	Confounding variables not reported; more details may be in the source cited.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	This metric does not apply to this study type.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Medium	Analytical method was not reported; more details may be in the source cited
	Metric 16:	Statistical Methods and Kinetic Calculations	Medium	Statistical method was not reported; more details may be in the source cited.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Medium	Values seem appropriate; more details may be in the source cited.
	Metric 18:	QSAR Models	N/A	A QSAR model was not reported.

Overall Quality Determination Medium

* Related References: Cites secondary source Barnes I, Bastian V, Becker KH, Fink EH, Zabel F (1982). Reactivity studies of organic substances towardshydroxyl radicals under atmospheric conditions. Atmos Environ. 16; 545-550. [Not in HERO at the time of extraction] and Atkinson, 1985 [HERO ID 38261].

Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	5155560

EXTRACTION

Parameter	Data
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, Type, Guideline	no; experimental; other: not specified
Solvent, Reactivity, Storage, Stability	NR; NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR; NR Notes: NR
Duration and Test Temperature	NR; 297 K
Light Source, Intensity, and additional light details	NR; NR; NR
Source Wavelength Lower and Upper	NR; NR
Test Details and Control	NR; NR
Initial Concentration, Reference Compound	NR NR; NR
Substance Wavelength Lower and Upper	NR; NR
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	NR; NR; NR
Indirect Type Results, Indirect Rate Constant Lower and Upper	Second order rate constant for reaction with OH radicals; kOH=6.16E-11 cm^3/molecule*sec; kOH=6.88E-11 cm^3/molecule*sec
Method Details Results and Products Details Results	NR; relative to propene (k=2.65E-11 cm^3/molecule*sec and 2-methyl-2-butene (k=8.72E-11 cm^3/molecule*sec
Parameter Value and Parameter Results	NR; NR
Reference Substance Results, Percent Degradation Results and Standard Deviation Results	NR; NR; NR
Results Remarks, Sample time Results, Results Details	NR; NR; NR

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was identified definitively.
	Metric 2:	Test Substance Purity	Medium	Test substance source and purity were not reported; more details may be in the source cited.
Domain 2: Test Design				
	Metric 3:	Study Controls	Medium	No concurrent control group details reported; more details may be in the source cited.
	Metric 4:	Test Substance Stability	Medium	Test substance stability, homogeneity, preparation, and storage conditions were not reported; more details may be in the source cited.
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	Medium	Test method not reported; ; more details may be in the source cited.

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Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.
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Domain		Metric	EVALUATION Rating	Comments
	Metric 6:	Testing Conditions	Medium	Testing conditions not reported; more details may be in the source cited.
	Metric 7:	Testing Consistency	Medium	Details on this metric were not reported; more details may be in the source cited
	Metric 8:	System Type and Design	Medium	System type and design not reported; more details may be in the source cited.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	This metric does not apply to this study type.
	Metric 10:	Sampling Methods	N/A	This metric does not apply to this study type
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	Medium	The outcome was reasonable; more details may be in the source cited.
	Metric 12:	Test Substance Purity	Medium	Sampling details not reported; more details may be in the source cited.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	Medium	Confounding variables not reported; more details may be in the source cited.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	This metric does not apply to this study type.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Medium	Analytical method was not reported; more details may be in the source cited
	Metric 16:	Statistical Methods and Kinetic Calculations	Medium	Statistical method was not reported; more details may be in the source cited.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Medium	Values seem appropriate; more details may be in the source cited.
	Metric 18:	QSAR Models	N/A	A QSAR model was not reported.

Overall Quality Determination Medium

* Related References: Cites secondary source Ohta T (1983). J Phys Chem. 87; 1209 [Not in HERO at the time of extraction] and Atkinson 1985 [HERO ID 38261]

Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	5155560

EXTRACTION

Parameter	Data
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, Type, Guideline	no; experimental; other: not specified
Solvent, Reactivity, Storage, Stability	NR; NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR; NR Notes: NR
Duration and Test Temperature	NR; 295 K
Light Source, Intensity, and additional light details	NR; NR; NR
Source Wavelength Lower and Upper	NR; NR
Test Details and Control	NR; NR
Initial Concentration, Reference Compound	NR NR; NR
Substance Wavelength Lower and Upper	NR; NR
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	NR; NR; NR
Indirect Type Results, Indirect Rate Constant Lower and Upper	Second order rate constant for reaction with OH radicals; kOH=6.65E-11 cm^3/molecule*sec; Not Reported
Method Details Results and Products Details Results	NR; relative to propene (k=2.68E-11 cm^3/molecule*sec
Parameter Value and Parameter Results	NR; NR
Reference Substance Results, Percent Degradation Results and Standard Deviation Results	NR; NR; NR
Results Remarks, Sample time Results, Results Details	NR; NR; NR

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was identified definitively.
	Metric 2:	Test Substance Purity	Medium	Test substance source and purity were not reported; more details may be in the source cited.
Domain 2: Test Design				
	Metric 3:	Study Controls	Medium	No concurrent control group details reported; more details may be in the source cited.
	Metric 4:	Test Substance Stability	Medium	Test substance stability, homogeneity, preparation, and storage conditions were not reported; more details may be in the source cited.
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	Medium	Test method not reported; ; more details may be in the source cited.

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Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.
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Domain		Metric	EVALUATION Rating	Comments
	Metric 6:	Testing Conditions	Medium	Testing conditions not reported; more details may be in the source cited.
	Metric 7:	Testing Consistency	Medium	Details on this metric were not reported; more details may be in the source cited
	Metric 8:	System Type and Design	Medium	System type and design not reported; more details may be in the source cited.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	This metric does not apply to this study type.
	Metric 10:	Sampling Methods	N/A	This metric does not apply to this study type
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	Medium	The outcome was reasonable; more details may be in the source cited.
	Metric 12:	Test Substance Purity	Medium	Sampling details not reported; more details may be in the source cited.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	Medium	Confounding variables not reported; more details may be in the source cited.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	This metric does not apply to this study type.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Medium	Analytical method was not reported; more details may be in the source cited
	Metric 16:	Statistical Methods and Kinetic Calculations	Medium	Statistical method was not reported; more details may be in the source cited.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Medium	Values seem appropriate; more details may be in the source cited.
	Metric 18:	QSAR Models	N/A	A QSAR model was not reported.

Overall Quality Determination **Medium**

* Related References: Cites secondary source Atkinson and Aschmann 1984 [HERO ID 8521463]

Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	5155560

EXTRACTION

Parameter	Data
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, Type, Guideline	no; experimental; other: not specified
Solvent, Reactivity, Storage, Stability	NR; NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR; NR Notes: NR
Duration and Test Temperature	NR; 295 K
Light Source, Intensity, and additional light details	NR; NR; NR
Source Wavelength Lower and Upper	NR; NR
Test Details and Control	NR; NR
Initial Concentration, Reference Compound	NR NR; NR
Substance Wavelength Lower and Upper	NR; NR
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	NR; NR; NR
Indirect Type Results, Indirect Rate Constant Lower and Upper	Second order rate constant for reaction with OH radicals; kOH=6.1E-11 cm^3/molecule*sec; kOH=6.8E-11 cm^3/molecule*sec
Method Details Results and Products Details Results	NR; NR
Parameter Value and Parameter Results	NR; NR
Reference Substance Results, Percent Degradation Results and Standard Deviation Results	NR; NR; NR
Results Remarks, Sample time Results, Results Details	NR; NR; NR

EVALUATION

Domain	Metric	Rating	Comments
Domain 1: Test Substance			
Metric 1:	Test Substance Identity	High	The test substance was identified definitively.
Metric 2:	Test Substance Purity	Medium	Test substance source and purity were not reported; more details may be in the source cited.
Domain 2: Test Design			
Metric 3:	Study Controls	Medium	No concurrent control group details reported; more details may be in the source cited.
Metric 4:	Test Substance Stability	Medium	Test substance stability, homogeneity, preparation, and storage conditions were not reported; more details may be in the source cited.
Domain 3: Test Conditions			
Metric 5:	Test Method Suitability	Medium	Test method not reported; ; more details may be in the source cited.

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Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	5155560

Domain		Metric	EVALUATION Rating	Comments
	Metric 6:	Testing Conditions	Medium	Testing conditions not reported; more details may be in the source cited.
	Metric 7:	Testing Consistency	Medium	Details on this metric were not reported; more details may be in the source cited
	Metric 8:	System Type and Design	Medium	System type and design not reported; more details may be in the source cited.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	This metric does not apply to this study type.
	Metric 10:	Sampling Methods	N/A	This metric does not apply to this study type
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	Medium	The outcome was reasonable; more details may be in the source cited.
	Metric 12:	Test Substance Purity	Medium	Sampling details not reported; more details may be in the source cited.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	Medium	Confounding variables not reported; more details may be in the source cited.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	This metric does not apply to this study type.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Medium	Analytical method was not reported; more details may be in the source cited
	Metric 16:	Statistical Methods and Kinetic Calculations	Medium	Statistical method was not reported; more details may be in the source cited.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Medium	Values seem appropriate; more details may be in the source cited.
	Metric 18:	QSAR Models	N/A	A QSAR model was not reported.

Overall Quality Determination Medium

* Related References: Cites secondary source Becker KH, Biehl HM, Bruckman P et al. (1984). Methods of the ecotoxicological evaluation of chemicals.Photochemical degradation in the gas phase. Volume 6: OH reaction rate constants and tropospheric lifetimes ofselected environmental chemicals. Report 1980-1983. Kernforschungsanlage Jülich GmbH, November 1983. [Not in HERO at the time of extraction]

Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	5155560

EXTRACTION

Parameter	Data
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, Type, Guideline	no; experimental; other: not specified
Solvent, Reactivity, Storage, Stability	NR; NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR; NR Notes: NR
Duration and Test Temperature	NR; NR
Light Source, Intensity, and additional light details	NR; NR; NR
Source Wavelength Lower and Upper	NR; NR
Test Details and Control	NR; NR
Initial Concentration, Reference Compound	NR NR; NR
Substance Wavelength Lower and Upper	NR; NR
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	NR; NR; NR
Indirect Type Results, Indirect Rate Constant Lower and Upper	Second order rate constant for reaction with OH radicals; kOH=6.85E-11 cm^3/molecule*sec; Not Reported
Method Details Results and Products Details Results	NR; NR
Parameter Value and Parameter Results	NR; NR
Reference Substance Results, Percent Degradation Results and Standard Deviation Results	NR; NR; NR
Results Remarks, Sample time Results, Results Details	NR; NR; NR

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was identified definitively.
	Metric 2:	Test Substance Purity	Medium	Test substance source and purity were not reported; more details may be in the source cited.
Domain 2: Test Design				
	Metric 3:	Study Controls	Medium	No concurrent control group details reported; more details may be in the source cited.
	Metric 4:	Test Substance Stability	Medium	Test substance stability, homogeneity, preparation, and storage conditions were not reported; more details may be in the source cited.
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	Medium	Test method not reported; ; more details may be in the source cited.

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Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.
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HERO ID:	5155560

Domain		Metric	EVALUATION Rating	Comments
	Metric 6:	Testing Conditions	Medium	Testing conditions not reported; more details may be in the source cited.
	Metric 7:	Testing Consistency	Medium	Details on this metric were not reported; more details may be in the source cited
	Metric 8:	System Type and Design	Medium	System type and design not reported; more details may be in the source cited.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	This metric does not apply to this study type.
	Metric 10:	Sampling Methods	N/A	This metric does not apply to this study type
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	Medium	The outcome was reasonable; more details may be in the source cited.
	Metric 12:	Test Substance Purity	Medium	Sampling details not reported; more details may be in the source cited.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	Medium	Confounding variables not reported; more details may be in the source cited.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	This metric does not apply to this study type.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Medium	Analytical method was not reported; more details may be in the source cited
	Metric 16:	Statistical Methods and Kinetic Calculations	Medium	Statistical method was not reported; more details may be in the source cited.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Medium	Values seem appropriate; more details may be in the source cited.
	Metric 18:	QSAR Models	N/A	A QSAR model was not reported.

Overall Quality Determination Medium

* Related References: Cites secondary source Funcke W (1979). Studie zur Erkennung des Zusammenhangs zwischen der Struktur einer chemischen Substanz undderen Anfaelligkeit fuer den Photoabbau. Forschungsbericht 10702003, Umweltbundesamt, Berlin. Quoted in FrankR (1986). Zusammenstellung einer Liste von kOH-Reaktionsgeschwindigkeitskonstanten aus Originalveroeffentlichungen fuer einzelne chemikalien und Bewertung des Verhaltens dieser Stoffe in der Troposphaere,Batelle-Institut, Frankfurt A. M., 11-12[Not in HERO at the time of extraction]

Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	5155560

EXTRACTION

Parameter	Data
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, Type, Guideline	no; experimental; other: not specified
Solvent, Reactivity, Storage, Stability	NR; NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR; NR Notes: NR
Duration and Test Temperature	NR; NR
Light Source, Intensity, and additional light details	NR; NR; NR
Source Wavelength Lower and Upper	NR; NR
Test Details and Control	NR; NR
Initial Concentration, Reference Compound	NR NR; NR
Substance Wavelength Lower and Upper	NR; NR
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	NR; NR; NR
Indirect Type Results, Indirect Rate Constant Lower and Upper	Second order rate constant for reaction with ozone; k=8.1E-18 cm^3/molecule*sec; k=8.4E-18 cm^3/molecule*sec
Method Details Results and Products Details Results	NR; NR
Parameter Value and Parameter Results	NR; NR
Reference Substance Results, Percent Degradation Results and Standard Deviation Results	NR; NR; NR
Results Remarks, Sample time Results, Results Details	NR; NR; NR

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was identified definitively.
	Metric 2:	Test Substance Purity	Medium	Test substance source and purity were not reported; more details may be in the source cited.
Domain 2: Test Design				
	Metric 3:	Study Controls	Medium	No concurrent control group details reported; more details may be in the source cited.
	Metric 4:	Test Substance Stability	Medium	Test substance stability, homogeneity, preparation, and storage conditions were not reported; more details may be in the source cited.
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	Medium	Test method not reported; ; more details may be in the source cited.

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Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	5155560

Domain		Metric	EVALUATION Rating	Comments
	Metric 6:	Testing Conditions	Medium	Testing conditions not reported; more details may be in the source cited.
	Metric 7:	Testing Consistency	Medium	Details on this metric were not reported; more details may be in the source cited
	Metric 8:	System Type and Design	Medium	System type and design not reported; more details may be in the source cited.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	This metric does not apply to this study type.
	Metric 10:	Sampling Methods	N/A	This metric does not apply to this study type
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	Medium	The outcome was reasonable; more details may be in the source cited.
	Metric 12:	Test Substance Purity	Medium	Sampling details not reported; more details may be in the source cited.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	Medium	Confounding variables not reported; more details may be in the source cited.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	This metric does not apply to this study type.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Medium	Analytical method was not reported; more details may be in the source cited
	Metric 16:	Statistical Methods and Kinetic Calculations	Medium	Statistical method was not reported; more details may be in the source cited.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Medium	Values seem appropriate; more details may be in the source cited.
	Metric 18:	QSAR Models	N/A	A QSAR model was not reported.

Overall Quality Determination — Medium

* Related References: Cites secondary source Atkinson and Carter (1984) [HERO ID 38267]

Study Citation:	Ghosh, B., Bugarin, A., Connell, B. T., North, S. W. (2010). OH radical initiated oxidation of 1,3-butadiene: isomeric selective study of the dominant addition channel. Journal of Physical Chemistry A 114(16):5299-5305.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	860294

EXTRACTION

Parameter	Data
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, Guideline	none; experimental; other: non-guideline: OH radical oxidation in the presence of O2 and NO via laser photolysis
Solvent, Reactivity, Storage, Stability	NA; NA; NA; NA
Radiolabel, Source, State, Purity	NA; Isomeric selective study starting with photodissociation (at 248 nm) of 2-iodo-but-3-en-1-ol which results in the hydroxy alkyl radical, OH-butadiene, the major addition product; 1-hydroxy-2-iodo-3-butene: colorless oil; NR Notes: 1-hydroxy-2-iodo-3-butene was synthesized from 57% hydroiodic acid and butadiene monoxide in water
Duration and Test Temperature	not specified; 298±3K
Light Source, Intensity, and additional light details	XE10 excimer laser (GAM Laser); not specified; not specified
Source Wavelength Lower and Upper	282 nm; 287 nm
Test Details and Control	NO concentration: 3.2E14 to 1.9E15 molecules/cm3; O2 concentration 6.5E15 to 6.5E16 molecules/cm3; not specified
Initial Concentration, Reference Compound	NA Not Reported; not reported
Substance Wavelength Lower and Upper	not specified; not specified
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	not specified; not specified; not specified
Indirect Type Results, Indirect Rate Constant Lower and Upper	Not Reported; Rate constant for the addition of O2 to the hydroxy alkyl radical: 7.0E-13 cm3/sec; Rate constant for the addition of NO to the hydroxy peroxy radical: 1.5E-11 cm3/sec
Method Details Results and Products Details Results	Analysis of time dependent OH/OD signals using laser photolysis-laser induced fluorescence (LP-LIF) method; isotopic cycling experiments conducted; end product yields: 7% organic nitrate (predicted, not directly measured), 63±10% acrolein, 21±9% 4-hydroxy-2-butenal, 9% 3-butenal, 63±10% HCHO
Parameter Value and Parameter Results	not reported; not reported
Reference Substance Results, Percent Degradation Results and Standard Deviation Results	not reported; not reported; not reported
Results Remarks, Sample time Results, Results Details	Quantification of the branching between the E- and Z-isomers: the upper limit for E-isomer branching of the δ-hydroxy alkoxy radical was found to be 13±5%; not reported; not reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was identified.
	Metric 2:	Test Substance Purity	High	The source the test substance was reported.
Domain 2: Test Design				
	Metric 3:	Study Controls	N/A	The study did not require concurrent control groups.

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Study Citation:	Ghosh, B., Bugarin, A., Connell, B. T., North, S. W. (2010). OH radical initiated oxidation of 1,3-butadiene: isomeric selective study of the dominant addition channel. Journal of Physical Chemistry A 114(16):5299-5305.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	860294

		EVALUATION		
Domain	Metric		Rating	Comments
	Metric 4:	Test Substance Stability	High	The test substance preparation conditions were reported.
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	High	The test method was suitable for the test substance.
	Metric 6:	Testing Conditions	High	Testing conditions were reported.
	Metric 7:	Testing Consistency	High	Test conditions were consistent.
	Metric 8:	System Type and Design	High	The system type and design were appropriate.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	The metric is not applicable to the study.
	Metric 10:	Sampling Methods	N/A	The metric is not applicable to the study.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	Medium	There were minor differences between the assessment methodology and the intended outcome assessment.
	Metric 12:	Test Substance Purity	High	The study reported the use of sampling methods that address the outcome of interest.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	N/A	The metric is not applicable.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	The metric is not applicable.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	High	Data reporting was appropriate.
	Metric 16:	Statistical Methods and Kinetic Calculations	Low	Statistical analysis and kinetic calculations were not described clearly.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	High	The study results were reasonable.
	Metric 18:	QSAR Models	N/A	A QSAR model was not reported.

Overall Quality Determination — High

Study Citation:	Greenwald, E. E., Park, J., Anderson, K. C., Kim, H., Reich, B. J., Miller, S. A., Zhang, R., North, S. W. (2005). The OH-initiated oxidation of 1,3-butadiene in the presence of O2 and NO: a photolytic route to study isomeric selective reactivity. DUPE - Journal of Physical Chemistry A 109(35):7915-7922.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	5696791

EXTRACTION

Parameter	Data
CASRN and Test Material	Not Reported; 3-Buten-2-ol, 1-radical ion
Confidentiality, Type, Guideline	No; calculations; other: Non-guideline: RRKM/ME calculations correlated with experimental data
Solvent, Reactivity, Storage, Stability	NA; NA; NA; NA
Radiolabel, Source, State, Purity	deuteration of the -OH group; test material was generated via photolysis of 1% 1-iodo-3-butene-2-ol in He (1 atm) (both non-deuterated and monodeuterated); Gas; NR Notes: 3-Buten-2-ol, 1-radical ion is the theoretical minor addition product of OH radical to 1,3-butadiene; to produce this radical ion as a major photolysis product, it was generated from photolysis of 1-iodo-3-butene-2-ol
Duration and Test Temperature	Pulsed; 298K (760 Torr)
Light Source, Intensity, and additional light details	unfocused 266 nm beam from an Nd: YAG laser (Spectra Physics GCR-150-10); Not reported; The repetition rate of the lasers was set at 10 Hz and the delay between photolysis and probe lasers was controlled by a digital delay/ pulse generator
Source Wavelength Lower and Upper	266 nm; Not reported
Test Details and Control	Laser photolysis/laser-induced fluorescence (LP/LIF) experiments used to produce activated adduct formed via OH addition to 1,3-butadiene; photodissociation dynamics via velocity-map imaging of 1-iodo-3-buten-2-ol were used for analysis via quantum chemical calculations using Gaussian 0341 software to provide all relevant energetics, geometries, and frequencies to obtain state counts as a function of energy for the OH-butadiene adduct radical cyclic isomerization reaction. Using RRKM theory coupled with master equation (ME) formalism reaction rate constants were calculated including branching ratios among isomers and further into the dissociative channel resulting in 1,3-butadiene and OH.; NA
Initial Concentration, Reference Compound	NA NA; Not reported
Substance Wavelength Lower and Upper	NA; NA
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	Not reported; Not reported; Not reported
Indirect Type Results, Indirect Rate Constant Lower and Upper	distribution of hydroxyalkyl radicals: 70% beta, 30% alpha; radical rate constant for D-abstraction from alpha radical: CH2CHCH2CHOD + O2 -> CH2CHCH2CHO + DO2, k = 3.3x10^-11 molecules/cm3 sec; Not reported
Method Details Results and Products Details Results	Not reported; Not Reported
Parameter Value and Parameter Results	Not reported; Not reported
Reference Substance Results, Percent Degradation Results and Standard Deviation Results	Not reported; Not reported; Not reported
Results Remarks, Sample time Results, Results Details	cyclic isomerization of beta-hydroxyalkyl radical to alpha-hydroxyalkyl radical was evident; Not reported; Not reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	Medium	The test substance was identified; however, the test substance was not specifically 1,3-butadiene.
	Metric 2:	Test Substance Purity	N/A	The test substance was generated photolytically as part of the experiment.

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Study Citation:	Greenwald, E. E., Park, J., Anderson, K. C., Kim, H., Reich, B. J., Miller, S. A., Zhang, R., North, S. W. (2005). The OH-initiated oxidation of 1,3-butadiene in the presence of O2 and NO: a photolytic route to study isomeric selective reactivity. DUPE - Journal of Physical Chemistry A 109(35):7915-7922.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	5696791

			EVALUATION	
Domain		Metric	Rating	Comments
Domain 2: Test Design				
	Metric 3:	Study Controls	N/A	The metric is not applicable to this type of study.
	Metric 4:	Test Substance Stability	N/A	The metric is not applicable to this type of study.
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	Low	Non-standard method evaluating transformation product; UV photolysis of iodohydrins.
	Metric 6:	Testing Conditions	High	Testing conditions were monitored, reported, and appropriate for the method.
	Metric 7:	Testing Consistency	N/A	The metric is not applicable to this type of study.
	Metric 8:	System Type and Design	N/A	The metric is not applicable to this type of study.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	The metric is not applicable to this type of study.
	Metric 10:	Sampling Methods	N/A	The metric is not applicable to this type of study.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	Low	The outcome assessment methodology did not specifically address the intended outcome of interest; however, OH rate constant for a transformation product was reported.
	Metric 12:	Test Substance Purity	N/A	The metric is not applicable to this type of study.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	N/A	The metric is not applicable to this type of study.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	The metric is not applicable to this type of study.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	High	Data reporting was appropriate.
	Metric 16:	Statistical Methods and Kinetic Calculations	High	Methods for kinetic calculations were described.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Low	Reported values were reasonable; however, not specific to the target chemical.
	Metric 18:	QSAR Models	High	Model calculations were described.

Overall Quality Determination Low

Study Citation:	Howard, P. H., Boethling, R. S., Jarvis, W. F., Meylan, W. M., Michalenko, E. M. (1991). Handbook of environmental degradation rates: 1,3-butadiene. :380-381.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	11779754

EXTRACTION

Parameter	**Data**
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, Guideline	No; calculation; None
Solvent, Reactivity, Storage, Stability	NR; NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR; NR Notes: NR
Duration and Test Temperature	NR; NR
Light Source, Intensity, and additional light details	NR; NR; NR
Source Wavelength Lower and Upper	NR; NR
Test Details and Control	NR; NR
Initial Concentration, Reference Compound	NR NR; NR
Substance Wavelength Lower and Upper	NR; NR
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	NR; NR; NR
Indirect Type Results, Indirect Rate Constant Lower and Upper	NR; NR; NR
Method Details Results and Products Details Results	NR; NR
Parameter Value and Parameter Results	NR; NR
Reference Substance Results, Percent Degradation Results and Standard Deviation Results	NR; NR; NR
Results Remarks, Sample time Results, Results Details	Half-lives in air = 0.76-7.8 hours (0.03 days-0.32 days). Based on measured photooxidation rate constant in air.; NR; NR

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was identified definitively.
	Metric 2:	Test Substance Purity	Medium	The source and purity of the test substance were not reported; however, the omissions were not likely to have a substantial impact on the study results.
Domain 2: Test Design				
	Metric 3:	Study Controls	Medium	Study controls were not reported and may affect the study results; however, the data are from a trusted secondary source.

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Study Citation:	Howard, P. H., Boethling, R. S., Jarvis, W. F., Meylan, W. M., Michalenko, E. M. (1991). Handbook of environmental degradation rates: 1,3-butadiene. :380-381.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	11779754

			EVALUATION	
Domain		Metric	Rating	Comments
	Metric 4:	Test Substance Stability	Medium	The test substance stability, homogeneity, preparation or storage conditions were not reported; however, these factors were not likely to influence the test substance or were not likely to have a substantial impact on study results.
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	Medium	The test method was not reported; however, the data is from a trusted secondary source with reference to the source the calculation was based on.
	Metric 6:	Testing Conditions	Medium	Testing conditions were not reported; however, the data are from a trusted secondary source.
	Metric 7:	Testing Consistency	Medium	Testing conditions were not reported; however, the data are from a trusted secondary source.
	Metric 8:	System Type and Design	Medium	Equilibrium was not reported; however, the data are from a trusted secondary source.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	This metric does not apply to this study type.
	Metric 10:	Sampling Methods	N/A	This metric does not apply to this study type.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	High	The outcome of interest was reported.
	Metric 12:	Test Substance Purity	Medium	The sampling method was not reported; however, the data are from a trusted secondary source.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	Medium	Sources of variability and uncertainty in the measurements were not reported; however, the omissions were not likely to have a substantial impact on study results.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	This metric does not apply to this study type.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Medium	Data reporting was limited, the analytical method was not reported; however, the information is presented in a trusted secondary source.
	Metric 16:	Statistical Methods and Kinetic Calculations	Medium	Kinetic and calculation details were not reported; however, the information is presented in a trusted secondary source.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Low	Due to limited information, evaluation of the reasonableness of the study results was not possible.
	Metric 18:	QSAR Models	N/A	This metric does not apply to this study type.

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Study Citation:	Howard, P. H., Boethling, R. S., Jarvis, W. F., Meylan, W. M., Michalenko, E. M. (1991). Handbook of environmental degradation rates: 1,3-butadiene. :380-381.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	11779754

EVALUATION

Domain	Metric	Rating	Comments
Overall Quality Determination		**Medium**	

* Related References: Atkinson, R 1985; Atkinson, R and Carter, WPL 1984; Atkinson, R et al 1984A

Study Citation:	Howard, P. H., Boethling, R. S., Jarvis, W. F., Meylan, W. M., Michalenko, E. M. (1991). Handbook of environmental degradation rates: 1,3-butadiene. :380-381.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	11779754

EXTRACTION

Parameter	Data
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, Guideline	No; calculation; None
Solvent, Reactivity, Storage, Stability	NR; NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR; NR Notes: NR
Duration and Test Temperature	NR; NR
Light Source, Intensity, and additional light details	NR; NR; NR
Source Wavelength Lower and Upper	NR; NR
Test Details and Control	NR; NR
Initial Concentration, Reference Compound	NR NR; NR
Substance Wavelength Lower and Upper	NR; NR
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	NR; Indirect half-life = 0.76 hours (0.03 days); Indirect half-life = 7.8 hours (0.32 days)
Indirect Type Results, Indirect Rate Constant Lower and Upper	NR; NR; NR
Method Details Results and Products Details Results	NR; NR
Parameter Value and Parameter Results	NR; NR
Reference Substance Results, Percent Degradation Results and Standard Deviation Results	NR; NR; NR
Results Remarks, Sample time Results, Results Details	Based on measured photooxidation rate constant in air with hydroxyl radicals, ozone, and nitrate radicals.; NR; NR

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was identified definitively.
	Metric 2:	Test Substance Purity	Medium	The source and purity of the test substance were not reported; however, the omissions were not likely to have a substantial impact on the study results.
Domain 2: Test Design				
	Metric 3:	Study Controls	Medium	Study controls were not reported and may affect the study results; however, the data are from a trusted secondary source.
	Metric 4:	Test Substance Stability	Medium	The test substance stability, homogeneity, preparation or storage conditions were not reported; however, these factors were not likely to influence the test substance or were not likely to have a substantial impact on study results.

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Study Citation:	Howard, P. H., Boethling, R. S., Jarvis, W. F., Meylan, W. M., Michalenko, E. M. (1991). Handbook of environmental degradation rates: 1,3-butadiene. :380-381.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	11779754

Domain	Metric	EVALUATION Rating	Comments
Domain 3: Test Conditions			
	Metric 5: Test Method Suitability	Medium	The test method was not reported; however, the data is from a trusted secondary source with reference to the source the calculation was based on.
	Metric 6: Testing Conditions	Medium	Testing conditions were not reported; however, the data are from a trusted secondary source.
	Metric 7: Testing Consistency	Medium	Testing conditions were not reported; however, the data are from a trusted secondary source.
	Metric 8: System Type and Design	Medium	Equilibrium was not reported; however, the data are from a trusted secondary source.
Domain 4: Test Organisms			
	Metric 9: Outcome Assessment Methodology	N/A	This metric does not apply to this study type.
	Metric 10: Sampling Methods	N/A	This metric does not apply to this study type.
Domain 5: Outcome Assessment			
	Metric 11: Test Substance Identity	High	The outcome of interest was reported.
	Metric 12: Test Substance Purity	Medium	The sampling method was not reported; however, the data are from a trusted secondary source.
Domain 6: Confounding/Variable Control			
	Metric 13: Confounding Variables	Medium	Sources of variability and uncertainty in the measurements were not reported; however, the omissions were not likely to have a substantial impact on study results.
	Metric 14: Health Outcomes Unrelated to Exposure	N/A	This metric does not apply to this study type.
Domain 7: Data Presentation and Analysis			
	Metric 15: Data Reporting	Medium	Data reporting was limited, the analytical method was not reported; however, the information is presented in a trusted secondary source.
	Metric 16: Statistical Methods and Kinetic Calculations	Medium	Kinetic and calculation details were not reported; however, the information is presented in a trusted secondary source.
Domain 8: Other			
	Metric 17: Verification or Plausibility of Results	Low	Due to limited information, evaluation of the reasonableness of the study results was not possible.
	Metric 18: QSAR Models	N/A	This metric does not apply to this study type.

Overall Quality Determination — Medium

* Related References: Atkinson, R 1985; Atkinson, R and Carter, WPL 1984; Atkinson, R et al 1984A

Study Citation:	Jenkin, M. E., Boyd, A. A., Lesclaux, R. (1998). Peroxy radical kinetics resulting from the OH-Initiated oxidation of 1,3-butadiene, 2,3-dimethyl-1,3-butadiene and isoprene. Journal of Atmospheric Chemistry 29(3):267-298.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	1696190

EXTRACTION

Parameter	Data
CASRN and Test Material	Not Reported; 1,3-butadiene
Confidentiality, Type, Guideline	No; experimental; other: Non-guideline: laser flash photolysis/UV absorption spectrometry for peroxy radical permutation reactions from OH-initiated oxidation of 1,3-butadiene
Solvent, Reactivity, Storage, Stability	NR; NR; NR; NR
Radiolabel, Source, State, Purity	NR; Aldrich; NR; >99% Notes: NR
Duration and Test Temperature	Not Reported; 298K (760 Torr)
Light Source, Intensity, and additional light details	OH radicals were generated by the KrF excimer laser photolysis of H2O2; Not Reported; Not Reported
Source Wavelength Lower and Upper	248 nm; Not Reported
Test Details and Control	Not Reported; no absorption signals were detected at 270 nm in the absence of H2O2, indicating no absorbing species were formed from direct diene photolysis
Initial Concentration, Reference Compound	9.0-26 10E16 molecule/cm3; Ethene
Substance Wavelength Lower and Upper	Absorption-time profiles from the photolysis of the H2O2/diene/O2 mixtures recorded at 270-280 nm; Not Reported
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	Not Reported; Not Reported; Not Reported
Indirect Type Results, Indirect Rate Constant Lower and Upper	OH + 1,3-butadiene (+O2); OH + diene rate coefficients taken from reviews of Atkinson (1989; 1994); 6.66E-11 x 0.134 Rate coefficient x branching ratio (cm3/molecule sec); 6.66E-11 x 0.866 x 0.75 Rate coefficient x branching ratio (cm3/molecule sec)
Method Details Results and Products Details Results	Quantitative absorption-time profiles were simulated using the FACSIMILE program and modeling of peroxy radicals via their permutation reactions and reactions with HO2 (and CH3O2, where appropriate).; Not Reported
Parameter Value and Parameter Results	Not Reported; Not Reported
Reference Substance Results, Percent Degradation Results and Standard Deviation Results	Test system was run with ethene, results verified tje laser photolysis apparatuswas correctly aligned and functioning well; Not Reported; Not Reported
Results Remarks, Sample time Results, Results Details	Not Reported; Not Reported; Not Reported

EVALUATION

Domain	Metric	Rating	Comments
Domain 1: Test Substance			
Metric 1:	Test Substance Identity	High	The test substance was identified.
Metric 2:	Test Substance Purity	High	The source and purity of the test substance were reported.
Domain 2: Test Design			
Metric 3:	Study Controls	Medium	Qualitative control results were reported.

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Study Citation:	Jenkin, M. E., Boyd, A. A., Lesclaux, R. (1998). Peroxy radical kinetics resulting from the OH-Initiated oxidation of 1,3-butadiene, 2,3-dimethyl-1,3-butadiene and isoprene. Journal of Atmospheric Chemistry 29(3):267-298.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	1696190

		EVALUATION		
Domain		Metric	Rating	Comments
	Metric 4:	Test Substance Stability	Medium	The test substance stability, homogeneity, preparation or storage conditions were not reported; however, these factors were not likely to influence the test substance or were not likely to have a substantial impact on study results.
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	High	The test method was suitable for the test substance.
	Metric 6:	Testing Conditions	High	Conditions were reported.
	Metric 7:	Testing Consistency	N/A	The metric is not applicable to this study.
	Metric 8:	System Type and Design	High	The system was appropriate.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	The metric is not applicable to this study.
	Metric 10:	Sampling Methods	N/A	The metric is not applicable to this study.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	Uninformative	Rate constant for intended outcome of interest is from another source and was not measured in this study.
	Metric 12:	Test Substance Purity	N/A	The metric is not applicable to this study.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	N/A	The metric is not applicable to this study.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	The metric is not applicable to this study.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Low	Analytical details were omitted.
	Metric 16:	Statistical Methods and Kinetic Calculations	N/A	The metric is not applicable to the study.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Uninformative	Results for outcome of interest are from a secondary source.
	Metric 18:	QSAR Models	N/A	The metric is not applicable to this study.

Overall Quality Determination — Uninformative

Study Citation:	Khaled, F., Giri, B. R., Liu, D., Assaf, E., Fittschen, C., Farooq, A. (2019). Insights into the Reactions of Hydroxyl Radical with Diolefins from Atmospheric to Combustion Environments. Journal of Physical Chemistry A 123(11):2261-2271.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	5618698

EXTRACTION

Parameter	Data
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, Guideline	None; Experimental; other: Hydroxyl radical reactions
Solvent, Reactivity, Storage, Stability	NR; NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR; 99%
Duration and Test Temperature	ca. 1.5 m-seconds; 294-438 K at 53 mbar (approximately); 881-1348 K at 1-2.5 bar approximately
Light Source, Intensity, and additional light details	Excimer laser; measured but not reported; Lambda Physik LPX 201, operating at a repetition rate of 1 Hz and a laser fluence of ~70 mJ/cm2
Source Wavelength Lower and Upper	248 nm for low temperature studies; 308 nm
Test Details and Control	laser flash photolysis and laser-inducedfluorescence (LPFR/LIF) for lower temperature studies and shock tube and UV laser-absorption (ST/LA) for higher temperature studies that are not environmentally relevant; TBHP in argon (ST/LA technique); He/H2O2 mixture (LPFR/LIF technique)
Initial Concentration, Reference Compound	15 ppm 70 ppm; Not reported
Substance Wavelength Lower and Upper	Not reported; Not reported
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	Not reported; Not reported; Not reported
Indirect Type Results, Indirect Rate Constant Lower and Upper	Not reported; Not reported; Not reported
Method Details Results and Products Details Results	Not reported; Not reported
Parameter Value and Parameter Results	rate coefficients for the reaction of hydroxyl radicals; 7.96-4.86E-11 cm3/molecule second at 294-438 K
Reference Substance Results, Percent Degradation Results and Standard Deviation Results	Not reported; Not reported; Not reported
Results Remarks, Sample time Results, Results Details	Not reported; Not reported; Not reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was identified by chemical name.
	Metric 2:	Test Substance Purity	High	The test substance source and purity were reported.
Domain 2: Test Design				
	Metric 3:	Study Controls	High	A control experiment was reported.
	Metric 4:	Test Substance Stability	Medium	The test substance stability, homogeneity, preparation, and storage conditions were not reported.

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Study Citation:	Khaled, F., Giri, B. R., Liu, D., Assaf, E., Fittschen, C., Farooq, A. (2019). Insights into the Reactions of Hydroxyl Radical with Diolefins from Atmospheric to Combustion Environments. Journal of Physical Chemistry A 123(11):2261-2271.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	5618698

			EVALUATION	
Domain		Metric	Rating	Comments
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	High	The test method was suitable for the test substance.
	Metric 6:	Testing Conditions	Medium	Some details were omitted regarding testing conditions; however, this was not likely to have influenced the interpretation of the results.
	Metric 7:	Testing Consistency	High	This metric met the criteria for high confidence as expected for this type of study.
	Metric 8:	System Type and Design	High	This metric met the criteria for high confidence as expected for this type of study.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	The metric is not applicable to this study type.
	Metric 10:	Sampling Methods	N/A	The metric is not applicable to this study type.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	High	The outcome assessment methodology addressed the outcomes of interest.
	Metric 12:	Test Substance Purity	Medium	Details regarding sampling methods were not fully reported; however, the omissions were not likely to have a substantial impact on results.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	N/A	No confounding variables were noted.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	The metric is not applicable to this study type.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Medium	Some experimental data and half-life data was not reported.
	Metric 16:	Statistical Methods and Kinetic Calculations	Medium	The kinetic calculations were not described in detail but are assumed to be adequate.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	High	The study results were reasonable.
	Metric 18:	QSAR Models	N/A	The metric is not applicable to this study type.

Overall Quality Determination — High

Study Citation:	Klamt, A. (1993). Estimation of gas-phase hydroxyl radical rate constants of organic compounds from molecular orbital calculations. Chemosphere 26(7):1273-1289.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	660158

EXTRACTION

Parameter	Data
CASRN and Test Material	106-99-0; Structural Estimation
Confidentiality, Type, Guideline	None; QSAR; other: Estimation of gas-phase hydroxyl radical rate constants using molecular orbital calculations
Solvent, Reactivity, Storage, Stability	NA; NA; NA; NA
Radiolabel, Source, State, Purity	NA; NA; NA; NA Notes: Estimation based on functional groups in chemical
Duration and Test Temperature	Not reported; Not reported
Light Source, Intensity, and additional light details	Not reported; Not reported; Not reported
Source Wavelength Lower and Upper	Not reported; Not reported
Test Details and Control	OH rate constants determined using quantitative relationships between MO-based descriptors for electronic properties of reaction sites and rate constants for OH-radical reaction mechanisms.; Not reported
Initial Concentration, Reference Compound	Not reported Not reported; Experimental data for comparison
Substance Wavelength Lower and Upper	Not reported; Not reported
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	Not reported; Not reported; Not reported
Indirect Type Results, Indirect Rate Constant Lower and Upper	Hydroxyl radical rate constant; 83.4; Not reported
Method Details Results and Products Details Results	Rate constant for OH radical addition to olefinic carbon-carbon double bonds (sp2-carbon atoms); Not reported
Parameter Value and Parameter Results	Not reported; Rate constant units: 10E-12 cm3/molecule/s
Reference Substance Results, Percent Degradation Results and Standard Deviation Results	66.9; Not reported; s = 0.28; r-squared = 0.954
Results Remarks, Sample time Results, Results Details	Not reported; Not reported; Not reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was definitively identified.
	Metric 2:	Test Substance Purity	N/A	The metric is not applicable to this study type.
Domain 2: Test Design				
	Metric 3:	Study Controls	N/A	The metric is not applicable to this study type.
	Metric 4:	Test Substance Stability	N/A	The metric is not applicable to this study type.

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Study Citation:	Klamt, A. (1993). Estimation of gas-phase hydroxyl radical rate constants of organic compounds from molecular orbital calculations. Chemosphere 26(7):1273-1289.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	660158

		EVALUATION		
Domain	Metric		Rating	Comments
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	N/A	The metric is not applicable to this study type.
	Metric 6:	Testing Conditions	N/A	The metric is not applicable to this study type.
	Metric 7:	Testing Consistency	N/A	The metric is not applicable to this study type.
	Metric 8:	System Type and Design	High	This metric met the criteria for high confidence as expected for this type of study.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	The metric is not applicable to this study type.
	Metric 10:	Sampling Methods	N/A	The metric is not applicable to this study type.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	High	The outcome assessment methodology addressed or reported the intended outcome of interest.
	Metric 12:	Test Substance Purity	N/A	The metric is not applicable to this study type.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	N/A	The metric is not applicable to this study type.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	The metric is not applicable to this study type.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	High	This metric met the criteria for high confidence as expected for this type of study.
	Metric 16:	Statistical Methods and Kinetic Calculations	High	Statistical analysis reported and acceptable.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	High	The study results were reasonable.
	Metric 18:	QSAR Models	High	The QSAR model had a defined, unambiguous endpoint and parameters of model performance were reported.

Overall Quality Determination High

Study Citation:	Liu, X., Jeffries, H. E., Sexton, K. G. (1999). Hydroxyl radical and ozone initiated photochemical reactions of 1,3-butadiene. Atmospheric Environment 33(18):3005-3022.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	598253

EXTRACTION

Parameter	**Data**
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, Guideline	None; Experimental; other: Mechanistic study of the reactions of 1,3-butadiene with hydroxy radicals and ozone in the presence of nitrogen oxides
Solvent, Reactivity, Storage, Stability	NR; NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR; 99%
Duration and Test Temperature	ca. 10 hours; 25°C (indoor experiment)
Light Source, Intensity, and additional light details	Natural light; day Sept 19, 1997, night Oct 7, 1997; UVA340, F40BL black and Vitalite full spectrum lamps (indoor experiment); Not reported; Not reported
Source Wavelength Lower and Upper	Not reported; Not reported
Test Details and Control	Ozone was injected during the experiment at a constant rate of 0.33 ppm/h.; Not reported
Initial Concentration, Reference Compound	10 ppm Not reported; Not reported
Substance Wavelength Lower and Upper	Not reported; Not reported
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	Not reported; Not reported; Not reported
Indirect Type Results, Indirect Rate Constant Lower and Upper	Not reported; Not reported; Not reported
Method Details Results and Products Details Results	Analytical derivative method (O-(2,3,4,5,6-pentfluorobenzyl)-hydroxylamine (PFBHA) coupled with gas chromatography (GC)/ion trap mass spectrometry (MS) separation and detection; Transformation products: 1,3-butadiene monoxide, 1,3-butadiene diepoxide, furan, glycolaldehyde, glycidaldehyde, glyoxal, malonaldehyde, butendial, C4 unsaturated hydroxy carbonyl, hydroxy acetone, glycidaldehyde, 3-hydroxypropanaldehyde, formaldehyde, acetaldehyde, acrolein, methylglyoxal, 2,3-butadione
Parameter Value and Parameter Results	Not reported; Not reported
Reference Substance Results, Percent Degradation Results and Standard Deviation Results	Not reported; Not reported; Not reported
Results Remarks, Sample time Results, Results Details	Not reported; Not reported; Indoor experiments of OH-initiated photodegradation resulted in the same outcome.

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was definitively identified.
	Metric 2:	Test Substance Purity	High	The test substance purity was reported. The test substance source was not reported.
Domain 2: Test Design				
	Metric 3:	Study Controls	Medium	Some concurrent control group details were not included; however, the lack of data was not likely to have a substantial impact on study results.

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Study Citation:	Liu, X., Jeffries, H. E., Sexton, K. G. (1999). Hydroxyl radical and ozone initiated photochemical reactions of 1,3-butadiene. Atmospheric Environment 33(18):3005-3022.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	598253

			EVALUATION	
Domain		Metric	Rating	Comments
	Metric 4:	Test Substance Stability	Medium	The test substance stability, homogeneity, preparation or storage conditions were not reported; however, these factors were not likely to influence the test substance or were not likely to have a substantial impact on study results.
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	High	This metric met the criteria for high confidence as expected for this type of study.
	Metric 6:	Testing Conditions	High	This metric met the criteria for high confidence as expected for this type of study.
	Metric 7:	Testing Consistency	High	This metric met the criteria for high confidence as expected for this type of study.
	Metric 8:	System Type and Design	High	This metric met the criteria for high confidence as expected for this type of study.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	The metric is not applicable to this study type.
	Metric 10:	Sampling Methods	N/A	The metric is not applicable to this study type.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	Low	Quantitative data not reported for photodegradation rates or formation of transformation products.
	Metric 12:	Test Substance Purity	High	This metric met the criteria for high confidence as expected for this type of study.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	N/A	No confounding variables were noted.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	The metric is not applicable to this study type.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Low	Degradation of test substance shown; however, quantitative data not reported for photodegradation rates or formation of transformation products.
	Metric 16:	Statistical Methods and Kinetic Calculations	Low	Data presented in figures as concentration over a time series.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	High	The transformation products identified were reasonable.
	Metric 18:	QSAR Models	N/A	The metric is not applicable to this study type.

Overall Quality Determination Low

Study Citation:	Orlando, J. J., Tyndall, G. S., Apel, E. C., Riemer, D. D., Paulson, S. E. (2003). Rate coefficients and mechanisms of the reaction of Cl-atoms with a series of unsaturated hydrocarbons under atmospheric conditions. International Journal of Chemical Kinetics 35(8):334-353.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	3254900

EXTRACTION

Parameter	**Data**
CASRN and Test Material	Not Reported; 1,3-butadiene
Confidentiality, Type, Guideline	No; experimental; other: Non-guideline: photolysis of mixtures and reaction of Cl2 with 1,3-butadiene
Solvent, Reactivity, Storage, Stability	NR; NR; NR; NR
Radiolabel, Source, State, Purity	NR; Aldrich; NR; ≥99% Notes: NR
Duration and Test Temperature	Not reported; 296K (700 Torr)
Light Source, Intensity, and additional light details	Xe-arc lamp; Not reported; Not reported
Source Wavelength Lower and Upper	235 nm; 400 nm
Test Details and Control	Cl2 = 1.1–3.1E15 molecule/cm3; reaction vessel: stainless steel environmental chambers; Not reported
Initial Concentration, Reference Compound	ca. 2.8E15 molecule/cm3; Not reported
Substance Wavelength Lower and Upper	Not reported; Not reported
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	Not reported; Not reported; Not reported
Indirect Type Results, Indirect Rate Constant Lower and Upper	Not reported; Not reported; Not reported
Method Details Results and Products Details Results	FTIR and GC/MS; observed products: CH2O 7±1%, HCOCl 3±1%, and acrolein ca. 3%; other lab sorptions were observed but not specifically identified, likely end products: chlorinated methyl vinyl ketone, HC(O)Cl, acrolein, 2-chloro-3-butenal, 4-chlorocrotonaldehyde, CH2O, CO, and CO2
Parameter Value and Parameter Results	Not reported; Not reported
Reference Substance Results, Percent Degradation Results and Standard Deviation Results	Not reported; Not reported; Not reported
Results Remarks, Sample time Results, Results Details	Not reported; Not reported; Study results for 1,3-butadiene were not quantitative

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was identified.
	Metric 2:	Test Substance Purity	High	The source and purity of the test substance were reported.
Domain 2: Test Design				
	Metric 3:	Study Controls	Low	No controls were reported.

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Study Citation:	Orlando, J. J., Tyndall, G. S., Apel, E. C., Riemer, D. D., Paulson, S. E. (2003). Rate coefficients and mechanisms of the reaction of Cl-atoms with a series of unsaturated hydrocarbons under atmospheric conditions. International Journal of Chemical Kinetics 35(8):334-353.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	3254900

			EVALUATION	
Domain		Metric	Rating	Comments
	Metric 4:	Test Substance Stability	Medium	The test substance stability, homogeneity, preparation or storage conditions were not reported; however, these factors were not likely to influence the test substance or were not likely to have a substantial impact on study results.
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	High	The test method was suitable.
	Metric 6:	Testing Conditions	High	Test conditions were reported.
	Metric 7:	Testing Consistency	N/A	The metric is not applicable to this study type.
	Metric 8:	System Type and Design	High	The system was appropriate.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	The metric is not applicable to this study type.
	Metric 10:	Sampling Methods	N/A	The metric is not applicable to this study type.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	Low	Quantitative rate results were not reported.
	Metric 12:	Test Substance Purity	N/A	The metric is not applicable to this study type.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	N/A	The metric is not applicable to this study type.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	The metric is not applicable to this study type.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Low	Limited detail regarding analytical method; percent recovery or mass balance were not reported.
	Metric 16:	Statistical Methods and Kinetic Calculations	N/A	The metric is not applicable to this study.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Low	Quantitative rate results were not reported; however, transformation products were reported.
	Metric 18:	QSAR Models	N/A	The metric is not applicable to this study type.

Overall Quality Determination — Medium

Study Citation:	Parsons, T. B., Wilkins, G. E. (1976). Biological effects and environmental aspects of 1,3-butadiene.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	5589165

EXTRACTION

Parameter	**Data**
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, Type, Guideline	no; experimental; other: not specified
Solvent, Reactivity, Storage, Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, Purity	Not Reported; Not Reported; Not Reported; Not Reported
Duration and Test Temperature	24 hr; 45-50°F
Light Source, Intensity, and additional light details	not specified; UV irradiation; Not Reported; Not Reported
Source Wavelength Lower and Upper	Not Reported; Not Reported
Test Details and Control	Air sample collected for irradiation: Ambient air, 12/22/65, 7:40-8:00 PST, light haze; Not Reported
Initial Concentration, Reference Compound	9.0 ppb; Not Reported
Substance Wavelength Lower and Upper	Not Reported; Not Reported
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	Not Reported; Not Reported; Not Reported
Indirect Type Results, Indirect Rate Constant Lower and Upper	Not Reported; Not Reported; Not Reported
Method Details Results and Products Details Results	Not Reported; Not Reported
Parameter Value and Parameter Results	0 ppb; Concentration of butadiene after 24 hr UV Irradiation
Reference Substance Results, Percent Degradation Results and Standard Deviation Results	Not Reported; Not Reported; Not Reported
Results Remarks, Sample time Results, Results Details	Not Reported; Not Reported; Not Reported

EVALUATION

Domain	Metric	Rating	Comments
Domain 1: Test Substance			
Metric 1:	Test Substance Identity	High	The test substance was identified by name.
Metric 2:	Test Substance Purity	Medium	The test substance source and purity were not reported.
Domain 2: Test Design			
Metric 3:	Study Controls	Medium	Concurrent control group details were not reported in the secondary source.
Metric 4:	Test Substance Stability	Medium	Test substance stability, homogeneity, preparation, and storage conditions were not reported in the secondary source.
Domain 3: Test Conditions			

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Study Citation:	Parsons, T. B., Wilkins, G. E. (1976). Biological effects and environmental aspects of 1,3-butadiene.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	5589165

			EVALUATION	
Domain		Metric	Rating	Comments
	Metric 5:	Test Method Suitability	Medium	Test method details were not reported in the secondary source.
	Metric 6:	Testing Conditions	Medium	Testing conditions are unknown but are likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
	Metric 7:	Testing Consistency	Medium	Testing consistency is unknown but are likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
	Metric 8:	System Type and Design	N/A	Rating of this factor is not applicable to this kind of information.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 10:	Sampling Methods	N/A	Rating of this factor is not applicable to this kind of information.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	Medium	The outcome assessment methodology is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
	Metric 12:	Test Substance Purity	Medium	Sampling methodology is unknown is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	Medium	Sources of variability and uncertainty were not reported in the secondary source.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	Rating of this factor is not applicable to this kind of information.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Medium	Limited data is reported in the secondary source but study data are likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
	Metric 16:	Statistical Methods and Kinetic Calculations	N/A	No statistical methods or kinetic calculations were reported in the secondary source.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Medium	The results are reasonable based on the data's inclusion in a peer- reviewed/recognized database or other secondary source.
	Metric 18:	QSAR Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination Medium

* Related References: Cited from Stephens, Edgar R. and Frank R. Burleson, "Analysis of the Atmosphere for Light Hydrocarbons", J. APCA 17 (33), 147-53 (1967). [HERO ID 15208]

Study Citation:	Parsons, T. B., Wilkins, G. E. (1976). Biological effects and environmental aspects of 1,3-butadiene.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	5589165

EXTRACTION

Parameter	Data
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, Type, Guideline	no; experimental; other: not specified; photooxidation
Solvent, Reactivity, Storage, Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, Purity	Not Reported; Not Reported; Not Reported; Not Reported
Duration and Test Temperature	not reported; 79°F
Light Source, Intensity, and additional light details	not reported; not reported; not reported
Source Wavelength Lower and Upper	not reported; not reported
Test Details and Control	In a long-path infrared spectrometer mixtures of N2, O2, NO, NO2, and butadiene were irradiated and formation of NO2 was monitored.; not reported
Initial Concentration, Reference Compound	not reported; not reported
Substance Wavelength Lower and Upper	not reported; not reported
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	not reported; not reported; not reported
Indirect Type Results, Indirect Rate Constant Lower and Upper	not reported; not reported; not reported
Method Details Results and Products Details Results	not reported; not reported
Parameter Value and Parameter Results	4.3 ppb/min; NO photooxidation rate in the presence of butadiene
Reference Substance Results, Percent Degradation Results and Standard Deviation Results	not reported; not reported; not reported
Results Remarks, Sample time Results, Results Details	not reported; not reported; not reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was identified by name.
	Metric 2:	Test Substance Purity	Medium	The test substance source and purity were not reported; additional details may be in source cited.
Domain 2: Test Design				
	Metric 3:	Study Controls	Medium	Concurrent control group details were not reported in the secondary source.
	Metric 4:	Test Substance Stability	Medium	Test substance stability, homogeneity, preparation, and storage conditions were not reported in the secondary source.
Domain 3: Test Conditions				

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Study Citation:	Parsons, T. B., Wilkins, G. E. (1976). Biological effects and environmental aspects of 1,3-butadiene.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	5589165

Domain	Metric		EVALUATION Rating	Comments
	Metric 5:	Test Method Suitability	Medium	Test method details were not reported in the secondary source.
	Metric 6:	Testing Conditions	Medium	Testing conditions are unknown but are likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
	Metric 7:	Testing Consistency	Medium	Testing consistency is unknown but are likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
	Metric 8:	System Type and Design	N/A	Rating of this factor is not applicable to this kind of information.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 10:	Sampling Methods	N/A	Rating of this factor is not applicable to this kind of information.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	Medium	The outcome assessment methodology is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
	Metric 12:	Test Substance Purity	Medium	Sampling methodology is unknown is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	Medium	Sources of variability and uncertainty were not reported in the secondary source.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	Rating of this factor is not applicable to this kind of information.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Medium	Limited data is reported in the secondary source but study data are likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
	Metric 16:	Statistical Methods and Kinetic Calculations	Medium	No statistical methods or kinetic calculations were reported in the secondary source.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Medium	The results are reasonable based on the data's inclusion in a peer- reviewed/recognized database or other secondary source.
	Metric 18:	QSAR Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination Medium

* Related References: Cited from Glasson, William A. and Charles S. Tuesday, "Hydrocarbon Reactivitiesin the Atmospheric Photooxidation of Nitric Oxide",. Env. Sci.Technol. 4 (11), 916-24 (1970b). [HERO ID 14872]

Study Citation:	Parsons, T. B., Wilkins, G. E. (1976). Biological effects and environmental aspects of 1,3-butadiene.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	5589165

EXTRACTION

Parameter	**Data**
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, Type, Guideline	no; experimental; other: not specified; photooxidation
Solvent, Reactivity, Storage, Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, Purity	Not Reported; Not Reported; Not Reported; Not Reported
Duration and Test Temperature	Not Reported; 29°C
Light Source, Intensity, and additional light details	Not Reported; Not Reported; Not Reported
Source Wavelength Lower and Upper	Not Reported; Not Reported
Test Details and Control	Not Reported; Not Reported
Initial Concentration, Reference Compound	Not Reported Not Reported; Not Reported
Substance Wavelength Lower and Upper	Not Reported; Not Reported
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	Not Reported; Not Reported; Not Reported
Indirect Type Results, Indirect Rate Constant Lower and Upper	Not Reported; Not Reported; Not Reported
Method Details Results and Products Details Results	Not Reported; Not Reported
Parameter Value and Parameter Results	0.44x10^-3/ppm min; Rate constant for NO thermal oxidation
Reference Substance Results, Percent Degradation Results and Standard Deviation Results	Not Reported; Not Reported; Not Reported
Results Remarks, Sample time Results, Results Details	Acrolein and formaldehyde were identified as NO-butadiene reaction products.; Not Reported; Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was identified by name.
	Metric 2:	Test Substance Purity	Medium	The test substance source and purity were not reported in this secondary source.
Domain 2: Test Design				
	Metric 3:	Study Controls	Medium	Concurrent control group details were not reported in the secondary source.
	Metric 4:	Test Substance Stability	Medium	Test substance stability, homogeneity, preparation, and storage conditions were not reported in the secondary source.
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	Medium	Test method details were not reported in the secondary source.

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Study Citation:	Parsons, T. B., Wilkins, G. E. (1976). Biological effects and environmental aspects of 1,3-butadiene.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	5589165

Domain		Metric	EVALUATION Rating	Comments
	Metric 6:	Testing Conditions	Medium	Testing conditions are unknown but are likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
	Metric 7:	Testing Consistency	Medium	Testing consistency is unknown but are likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
	Metric 8:	System Type and Design	N/A	Rating of this factor is not applicable to this kind of information.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 10:	Sampling Methods	N/A	Rating of this factor is not applicable to this kind of information.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	Medium	The outcome assessment methodology is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
	Metric 12:	Test Substance Purity	Medium	Sampling methodology is unknown is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	Medium	Sources of variability and uncertainty were not reported in the secondary source.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	Rating of this factor is not applicable to this kind of information.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Medium	Limited data is reported in the secondary source but study data are likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
	Metric 16:	Statistical Methods and Kinetic Calculations	N/A	No statistical methods or kinetic calculations were reported in the secondary source.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Medium	The results are reasonable based on the data's inclusion in a peer- reviewed/recognized database or other secondary source.
	Metric 18:	QSAR Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination Medium

* Related References: Cited from Glasson, William A. and Charles S. Tuesday, "Atmospheric Thermal Oxidation of Nitric Oxide in the Presence of Dienes", Env. Sci. Technol. 4 (9) , 752-57 (1970a).

Study Citation:	Parsons, T. B., Wilkins, G. E. (1976). Biological effects and environmental aspects of 1,3-butadiene.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	5589165

EXTRACTION

Parameter	Data
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, Type, Guideline	no; experimental; other: not specified
Solvent, Reactivity, Storage, Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, Purity	Not Reported; Not Reported; Not Reported; Not Reported
Duration and Test Temperature	Not Reported; Not Reported
Light Source, Intensity, and additional light details	Not Reported; Not Reported; Not Reported
Source Wavelength Lower and Upper	Not Reported; Not Reported
Test Details and Control	Not Reported; Not Reported
Initial Concentration, Reference Compound	Not Reported Not Reported; Not Reported
Substance Wavelength Lower and Upper	Not Reported; Not Reported
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	Not Reported; Not Reported; Not Reported
Indirect Type Results, Indirect Rate Constant Lower and Upper	Not Reported; Not Reported; Not Reported
Method Details Results and Products Details Results	Rate of decrease of NO2 concentrations in the butadiene-air mixture was measured; Not Reported
Parameter Value and Parameter Results	0.4x10^-4/ppm min; Rate constant for NO2-butadiene reaction
Reference Substance Results, Percent Degradation Results and Standard Deviation Results	Not Reported; Not Reported; Not Reported
Results Remarks, Sample time Results, Results Details	Not Reported; Not Reported; Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was identified by name.
	Metric 2:	Test Substance Purity	Medium	The test substance source and purity were not reported.
Domain 2: Test Design				
	Metric 3:	Study Controls	Medium	Concurrent control group details were not reported in the secondary source.
	Metric 4:	Test Substance Stability	Medium	Test substance stability, homogeneity, preparation, and storage conditions were not reported in the secondary source.
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	Medium	Test method details were not reported in the secondary source.

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Study Citation:	Parsons, T. B., Wilkins, G. E. (1976). Biological effects and environmental aspects of 1,3-butadiene.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	5589165

Domain	Metric		EVALUATION Rating	Comments
	Metric 6:	Testing Conditions	Medium	Testing conditions are unknown but are likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
	Metric 7:	Testing Consistency	Medium	Testing consistency is unknown but are likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
	Metric 8:	System Type and Design	N/A	Rating of this factor is not applicable to this kind of information.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 10:	Sampling Methods	N/A	Rating of this factor is not applicable to this kind of information.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	Medium	The outcome assessment methodology is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
	Metric 12:	Test Substance Purity	Medium	Sampling methodology is unknown is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	Medium	Sources of variability and uncertainty were not reported in the secondary source.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	Rating of this factor is not applicable to this kind of information.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Medium	Limited data is reported in the secondary source but study data are likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
	Metric 16:	Statistical Methods and Kinetic Calculations	N/A	No statistical methods or kinetic calculations were reported in the secondary source.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Medium	The results are reasonable based on the data's inclusion in a peer- reviewed/recognized database or other secondary source.
	Metric 18:	QSAR Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination Medium

* Related References: Cited from Glasson, William A. and Charles s. Tuesday, "Atmospheric Thermal Oxidation of Nitric Oxide in the Presence of Dienes", Env.Sci. Technol. 4 (9) , 752-57 (1970a).

Study Citation:	Parsons, T. B., Wilkins, G. E. (1976). Biological effects and environmental aspects of 1,3-butadiene.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	5589165

EXTRACTION

Parameter	Data
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, Type, Guideline	no; experimental; other: not specified
Solvent, Reactivity, Storage, Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, Purity	Not Reported; Not Reported; Not Reported; Not Reported
Duration and Test Temperature	24 hr; 40-45°F
Light Source, Intensity, and additional light details	Not Reported; Not Reported; Not Reported
Source Wavelength Lower and Upper	Not Reported; Not Reported
Test Details and Control	Air sample collected for irradiation: Ambient air, 3/10/66, 8:05-8:25 PST, moderate haze; Control measured under same conditions in the dark. Starting concentration: 2.0 ppb; after 24 hr in dark: 2.0 ppb
Initial Concentration, Reference Compound	2.4 ppb; Not Reported
Substance Wavelength Lower and Upper	Not Reported; Not Reported
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	Not Reported; Not Reported; Not Reported
Indirect Type Results, Indirect Rate Constant Lower and Upper	Not Reported; Not Reported; Not Reported
Method Details Results and Products Details Results	Not Reported; Not Reported
Parameter Value and Parameter Results	0 ppb; Concentration of butadiene after 24 hr UV Irradiation
Reference Substance Results, Percent Degradation Results and Standard Deviation Results	Not Reported; Not Reported; Not Reported
Results Remarks, Sample time Results, Results Details	Not Reported; Not Reported; Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was identified by name.
	Metric 2:	Test Substance Purity	Medium	The test substance source and purity were not reported.
Domain 2: Test Design				
	Metric 3:	Study Controls	Medium	Concurrent control group details were not reported in the secondary source.
	Metric 4:	Test Substance Stability	Medium	Test substance stability, homogeneity, preparation, and storage conditions were not reported in the secondary source.
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	Medium	Test method details were not reported in the secondary source.

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Study Citation:	Parsons, T. B., Wilkins, G. E. (1976). Biological effects and environmental aspects of 1,3-butadiene.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	5589165

Domain		Metric	EVALUATION Rating	Comments
	Metric 6:	Testing Conditions	Medium	Testing conditions are unknown but are likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
	Metric 7:	Testing Consistency	Medium	Testing consistency is unknown but are likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
	Metric 8:	System Type and Design	N/A	Rating of this factor is not applicable to this kind of information.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 10:	Sampling Methods	N/A	Rating of this factor is not applicable to this kind of information.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	Medium	The outcome assessment methodology is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
	Metric 12:	Test Substance Purity	Medium	Sampling methodology is unknown is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	Medium	Sources of variability and uncertainty were not reported in the secondary source.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	Rating of this factor is not applicable to this kind of information.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Medium	Limited data is reported in the secondary source but study data are likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
	Metric 16:	Statistical Methods and Kinetic Calculations	N/A	No statistical methods or kinetic calculations were reported in the secondary source.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Medium	The results are reasonable based on the data's inclusion in a peer- reviewed/recognized database or other secondary source.
	Metric 18:	QSAR Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination Medium

* Related References: Cited from Stephens, Edgar R. and Frank R. Burleson, "Analysis of theAtmosphere for Light Hydrocarbons", J. APCA 17 (33), 147-53(1967). [HERO ID 15208]

Study Citation:	Parsons, T. B., Wilkins, G. E. (1976). Biological effects and environmental aspects of 1,3-butadiene.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	5589165

EXTRACTION

Parameter	Data
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, Type, Guideline	no; experimental; other: not specified
Solvent, Reactivity, Storage, Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, Purity	Not Reported; Not Reported; Not Reported; Not Reported
Duration and Test Temperature	24 hr; 55-60°F
Light Source, Intensity, and additional light details	not specified; UV irradiation; Not Reported; Not Reported
Source Wavelength Lower and Upper	Not Reported; Not Reported
Test Details and Control	Air sample collected for irradiation: Ambient air, 3/10/66, 7:50-8:00 PST, heavy haze; Control measured under same conditions in the dark. Starting concentration: 2.8 ppb; after 24 hr in dark; 2.6 ppb
Initial Concentration, Reference Compound	2.6 ppb; Not Reported
Substance Wavelength Lower and Upper	Not Reported; Not Reported
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	Not Reported; Not Reported; Not Reported
Indirect Type Results, Indirect Rate Constant Lower and Upper	Not Reported; Not Reported; Not Reported
Method Details Results and Products Details Results	Not Reported; Not Reported
Parameter Value and Parameter Results	0 ppb; Concentration of butadiene after 24 hr UV Irradiation
Reference Substance Results, Percent Degradation Results and Standard Deviation Results	Not Reported; Not Reported; Not Reported
Results Remarks, Sample time Results, Results Details	Not Reported; Not Reported; Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was identified by name.
	Metric 2:	Test Substance Purity	Medium	The test substance source and purity were not reported.
Domain 2: Test Design				
	Metric 3:	Study Controls	Medium	Concurrent control group details were not reported in the secondary source.
	Metric 4:	Test Substance Stability	Medium	Test substance stability, homogeneity, preparation, and storage conditions were not reported in the secondary source.
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	Medium	Test method details were not reported in the secondary source.

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Study Citation:	Parsons, T. B., Wilkins, G. E. (1976). Biological effects and environmental aspects of 1,3-butadiene.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	5589165

Domain	Metric		EVALUATION Rating	Comments
	Metric 6:	Testing Conditions	Medium	Testing conditions are unknown but are likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
	Metric 7:	Testing Consistency	Medium	Testing consistency is unknown but are likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
	Metric 8:	System Type and Design	N/A	Rating of this factor is not applicable to this kind of information.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 10:	Sampling Methods	N/A	Rating of this factor is not applicable to this kind of information.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	Medium	The outcome assessment methodology is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
	Metric 12:	Test Substance Purity	Medium	Sampling methodology is unknown is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	Medium	Sources of variability and uncertainty were not reported in the secondary source.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	Rating of this factor is not applicable to this kind of information.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Medium	Limited data is reported in the secondary source but study data are likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
	Metric 16:	Statistical Methods and Kinetic Calculations	N/A	No statistical methods or kinetic calculations were reported in the secondary source.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Medium	The results are reasonable based on the data's inclusion in a peer- reviewed/recognized database or other secondary source.
	Metric 18:	QSAR Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination Medium

* Related References: Cited from Stephens, Edgar R. and Frank R. Burleson, "Analysis of theAtmosphere for Light Hydrocarbons", J. APCA 17 (33), 147-53(1967). [HERO ID 15208]

Study Citation:	Sexton, K. G., Doyle, M. L., Jeffries, H. E., Ebersviller, S. (2007). Development and testing of a chemical mechanism for atmospheric photochemical transformations of 1,3-butadiene. Chemico-Biological Interactions 166(1-3):156-162.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	618974

EXTRACTION

Parameter	Data
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, Guideline	None; Experimental; other: Mechanistic study of the reactions of 1,3-butadiene with OH, NO3 and O3
Solvent, Reactivity, Storage, Stability	NR; NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR; NR
Duration and Test Temperature	19 hours; 60-100, 38-79, 65-95°F
Light Source, Intensity, and additional light details	Natural sunlight; Not reported; 0.5, 0.7, 0.4 Langley's
Source Wavelength Lower and Upper	Not applicable; Not applicable
Test Details and Control	3 chamber experiments on 5/20/98, 5/20/2005, 9/17/97. % humidity: 46-55, 35-45, 54-57. Air samples from both hydroxyl- and ozone-initiated of photooxidized 1,2-butadiene were analyzed; Not reported
Initial Concentration, Reference Compound	1.513, 1.996, 1.120 ppm; Not applicable
Substance Wavelength Lower and Upper	Not applicable; Not applicable
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	Not reported; Not applicable; Not applicable
Indirect Type Results, Indirect Rate Constant Lower and Upper	Not applicable; Not applicable; Not applicable
Method Details Results and Products Details Results	Analyzed by derivatization with O-(2,3,4,5,6-pentafluorobenzyl)-hydroxylamine; GC-MS; Major products: acrolein, formaldehyde, furan, 1,3-butadiene monoxide and an organic nitrate
Parameter Value and Parameter Results	0.468, 0.495, 0.686; 0.258, 0.074, 0.097; ppm NO; NO2 formation
Reference Substance Results, Percent Degradation Results and Standard Deviation Results	Not applicable; Not applicable; Not applicable
Results Remarks, Sample time Results, Results Details	Primary reactions of 1,3-butadiene with OH, NO3 and O3 were represented; 10, 6.8, 9 hours; Univ NC outdoor smog chamber

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	Medium	The test substance was identified by trade name or other internal designation, but characterization details were omitted that could affect interpretation of study results; however, the omission was not likely to have a substantial impact on the study results.
	Metric 2:	Test Substance Purity	Medium	The test substance source was not reported and the test substance purity was not reported; however, the omissions or identified impurities were not likely to have a substantial impact on the study results.
Domain 2: Test Design				

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Study Citation:	Sexton, K. G., Doyle, M. L., Jeffries, H. E., Ebersviller, S. (2007). Development and testing of a chemical mechanism for atmospheric photochemical transformations of 1,3-butadiene. Chemico-Biological Interactions 166(1-3):156-162.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	618974

		EVALUATION		
Domain		Metric	Rating	Comments
	Metric 3:	Study Controls	N/A	The metric is not applicable to this study type.
	Metric 4:	Test Substance Stability	Medium	The test substance stability, homogeneity, preparation or storage conditions were not reported; however, these factors were not likely to influence the test substance or were not likely to have a substantial impact on study results.
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	High	The test method was suitable for the test substance.
	Metric 6:	Testing Conditions	High	Testing conditions were monitored, reported, and appropriate for the method.
	Metric 7:	Testing Consistency	High	The conditions of the exposure were documented.
	Metric 8:	System Type and Design	High	The system type and design were capable of appropriately maintaining substance concentrations.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	The metric is not applicable to this study type.
	Metric 10:	Sampling Methods	N/A	The metric is not applicable to this study type.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	High	The outcome assessment methodology addressed or reported the intended outcome of interest.
	Metric 12:	Test Substance Purity	High	The study reported the use of sampling methods that address the outcome(s) of interest, and used widely accepted methods/approaches for the chemical and media being analyzed and no notable uncertainties or limitations were expected to influence results.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	N/A	No confounding variables were noted.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	The metric is not applicable to this study type.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Medium	The target chemical and transformation product(s) concentrations, extraction efficiency, percent recovery, or mass balance were not reported; however, these omissions were not likely to have a substantial impact on study results.
	Metric 16:	Statistical Methods and Kinetic Calculations	High	Statistical methods or kinetic calculations were clearly described and address the dataset.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	High	Reported values were within expected range as defined by reference substance.
	Metric 18:	QSAR Models	N/A	The metric is not applicable to this study type.

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Study Citation:	Sexton, K. G., Doyle, M. L., Jeffries, H. E., Ebersviller, S. (2007). Development and testing of a chemical mechanism for atmospheric photochemical transformations of 1,3-butadiene. Chemico-Biological Interactions 166(1-3):156-162.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	618974

		EVALUATION	
Domain	Metric	Rating	Comments
Overall Quality Determination		**High**	

Study Citation:	Tuazon, E. C., Alvarado, A., Aschmann, S. M., Atkinson, R., Arey, J. (1999). Products of the gas-phase reactions of 1,3-butadiene with OH and NO3 radicals. Environmental Science & Technology 33(20):3586-3595.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	1742345

EXTRACTION

Parameter	Data
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, Guideline	None; Experimental, OH radical, products reported, % loss degradation reported; None
Solvent, Reactivity, Storage, Stability	NA; NR; NR; NR
Radiolabel, Source, State, Purity	NA; Aldrich Chemical Co.; NR; >/= 99.0%
Duration and Test Temperature	2-7 min; 298 ± 2 K
Light Source, Intensity, and additional light details	Two parallel banks of black lamps; NR; 20% maximum light intensity used; NR
Source Wavelength Lower and Upper	300; NR
Test Details and Control	OH radicals generated by photolysis of methyl nitrite; NR
Initial Concentration, Reference Compound	5.7 - 6.2E10^13 molecule/cm^3; NR
Substance Wavelength Lower and Upper	NR; NR
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	Not Reported; NR; NR
Indirect Type Results, Indirect Rate Constant Lower and Upper	OH radical (in the presence of NO); NR; NR
Method Details Results and Products Details Results	7500 L Teflon chamber at ~5% relative humidity, samples analyzed by GC-FID; Acrolein (0.55 Â± 0.05), HCHO (0.62 Â± 0.05), Furan (0.03 - 0.04), organic nitrates (0.07 Â± 0.03)
Parameter Value and Parameter Results	Not Reported; Not Reported
Reference Substance Results, Percent Degradation Results and Standard Deviation Results	Not Reported; 53%; NR
Results Remarks, Sample time Results, Results Details	Not Reported; 6.5 min; Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was identified by name.
	Metric 2:	Test Substance Purity	High	The test substance source and purity were reported.
Domain 2: Test Design				
	Metric 3:	Study Controls	Medium	Dark controls were not explicitly included.
	Metric 4:	Test Substance Stability	Medium	Minimal details on test substance preparation and no details on storage were reported.
Domain 3: Test Conditions				

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Study Citation:	Tuazon, E. C., Alvarado, A., Aschmann, S. M., Atkinson, R., Arey, J. (1999). Products of the gas-phase reactions of 1,3-butadiene with OH and NO3 radicals. Environmental Science & Technology 33(20):3586-3595.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	1742345

			EVALUATION	
Domain		Metric	Rating	Comments
	Metric 5:	Test Method Suitability	High	The test method was suitable for the test substance.
	Metric 6:	Testing Conditions	Low	Minimal details on test set up and apparatus were reporetd.
	Metric 7:	Testing Consistency	Medium	Test conditions were presumably consistent throughout the study and between study groups.
	Metric 8:	System Type and Design	N/A	Not applicable.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	Not applicable.
	Metric 10:	Sampling Methods	N/A	Not applicable.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	Medium	The outcome assessment methodology was appropriate for determining overall loss and products. Rates were not determined.
	Metric 12:	Test Substance Purity	High	Sampling methods were described and appropriate, frequency was acceptable for the reported endpoints.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	High	Uncertainty in measurements and variability were explicitly addressed through appropriate statistical methods.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	Not applicable.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Medium	The analytical method was appropriate; extraction efficiency and limits of detection were not reported. Product detection units were not reported.
	Metric 16:	Statistical Methods and Kinetic Calculations	N/A	Statistical and kinetic calculations were not conducted.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Low	The results deviated significantly from previously reported product yields.
	Metric 18:	QSAR Models	N/A	Not applicable.

Overall Quality Determination Medium

Study Citation:	Tuazon, E. C., Alvarado, A., Aschmann, S. M., Atkinson, R., Arey, J. (1999). Products of the gas-phase reactions of 1,3-butadiene with OH and NO3 radicals. Environmental Science & Technology 33(20):3586-3595.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	1742345

EXTRACTION

Parameter	**Data**
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, Guideline	None; Experimental, NO3 radical, products reported, % loss degradation reported; None
Solvent, Reactivity, Storage, Stability	NA; NR; NR; NR
Radiolabel, Source, State, Purity	NA; Aldrich Chemical Co.; NR; >/= 99.0%
Duration and Test Temperature	NR; 298 ± 2 K
Light Source, Intensity, and additional light details	Two parallel banks of black lamps; NR; 20% maximum light intensity used; NR
Source Wavelength Lower and Upper	300; NR
Test Details and Control	NO3 radicals generated by thermal decomposition of N2O5; NR
Initial Concentration, Reference Compound	5.7 - 6.0E10^13 molecule/cm^3; NR
Substance Wavelength Lower and Upper	NR; NR
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	Not Reported; NR; NR
Indirect Type Results, Indirect Rate Constant Lower and Upper	NO3 radicals; NR; NR
Method Details Results and Products Details Results	7500 L Teflon chamber at ~5% relative humidity, samples analyzed by GC-FID; Ratio: Acrolein (0.045), HCHO (0.065), furan (0.014), organic nitrates (0.63 Â± 0.15), and R(ONO2)(OONO2) species (0.08 â€“ 0.16)
Parameter Value and Parameter Results	Not Reported; Not Reported
Reference Substance Results, Percent Degradation Results and Standard Deviation Results	Not Reported; NR; NR
Results Remarks, Sample time Results, Results Details	Not Reported; NR; Not Reported

EVALUATION

Domain	Metric	Rating	Comments
Domain 1: Test Substance			
Metric 1:	Test Substance Identity	High	The test substance was identified by name.
Metric 2:	Test Substance Purity	High	The test substance source and purity were reported.
Domain 2: Test Design			
Metric 3:	Study Controls	Medium	Dark controls were not explicitly included.
Metric 4:	Test Substance Stability	Medium	Minimal details on test substance preparation and no details on storage were reported.
Domain 3: Test Conditions			
Metric 5:	Test Method Suitability	High	The test method was suitable for the test substance.
Metric 6:	Testing Conditions	Low	Minimal details on test set up and apparatus were reporetd.

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Study Citation:	Tuazon, E. C., Alvarado, A., Aschmann, S. M., Atkinson, R., Arey, J. (1999). Products of the gas-phase reactions of 1,3-butadiene with OH and NO3 radicals. Environmental Science & Technology 33(20):3586-3595.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	1742345

			EVALUATION	
Domain		Metric	Rating	Comments
	Metric 7:	Testing Consistency	Medium	Test conditions were presumably consistent throughout the study and between study groups.
	Metric 8:	System Type and Design	N/A	Not applicable.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	Not applicable.
	Metric 10:	Sampling Methods	N/A	Not applicable.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	Medium	The outcome assessment methodology was appropriate for determining overall loss and products. Rates were not determined.
	Metric 12:	Test Substance Purity	High	Sampling methods were described and appropriate, frequency was acceptable for the reported endpoints.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	High	Uncertainty in measurements and variability were explicitly addressed through appropriate statistical methods.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	Not applicable.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Medium	The analytical method was appropriate; extraction efficiency and limits of detection were not reported. Product detection units were not reported.
	Metric 16:	Statistical Methods and Kinetic Calculations	N/A	Statistical and kinetic calculations were not conducted.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Low	The results deviated significantly from previously reported product yields for most products except organic nitrates.
	Metric 18:	QSAR Models	N/A	Not applicable.

Overall Quality Determination Medium

Study Citation:	U.S. EPA, (1989). Health and environmental effects document for 1,3-butadiene.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	3454

EXTRACTION

Parameter	**Data**
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, Type, Guideline	Not Reported; Not Reported; Not Reported
Solvent, Reactivity, Storage, Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, Purity	Not Reported; Not Reported; Not Reported; Not Reported
Duration and Test Temperature	Not Reported; 25 deg C
Light Source, Intensity, and additional light details	Not Reported; Not Reported; Not Reported
Source Wavelength Lower and Upper	Not Reported; Not Reported
Test Details and Control	Not Reported; Not Reported
Initial Concentration, Reference Compound	Not Reported Not Reported; Not Reported
Substance Wavelength Lower and Upper	Not Reported; Not Reported
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	Not Reported; Not Reported; Not Reported
Indirect Type Results, Indirect Rate Constant Lower and Upper	Not Reported; Not Reported; Not Reported
Method Details Results and Products Details Results	Not Reported; Not Reported
Parameter Value and Parameter Results	Not Reported; Not Reported
Reference Substance Results, Percent Degradation Results and Standard Deviation Results	Not Reported; Not Reported; Not Reported
Results Remarks, Sample time Results, Results Details	Not Reported; Not Reported; Degradation product from reaction with ozone: Acrolein

EVALUATION

Domain	Metric	Rating	Comments
Domain 1: Test Substance			
Metric 1:	Test Substance Identity	High	The test substance was identified.
Metric 2:	Test Substance Purity	N/A	This metric is not applicable to this study type.
Domain 2: Test Design			
Metric 3:	Study Controls	N/A	This metric is not applicable to this study type.
Metric 4:	Test Substance Stability	N/A	This metric is not applicable to this study type.
Domain 3: Test Conditions			
Metric 5:	Test Method Suitability	N/A	This metric is not applicable to this study type.

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Study Citation:	U.S. EPA, (1989). Health and environmental effects document for 1,3-butadiene.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	3454

Domain		Metric	EVALUATION Rating	Comments
	Metric 6:	Testing Conditions	N/A	This metric is not applicable to this study type.
	Metric 7:	Testing Consistency	N/A	This metric is not applicable to this study type.
	Metric 8:	System Type and Design	N/A	This metric is not applicable to this study type.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	This metric is not applicable to this study type.
	Metric 10:	Sampling Methods	N/A	This metric is not applicable to this study type.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	N/A	This metric is not applicable to this study type.
	Metric 12:	Test Substance Purity	N/A	This metric is not applicable to this study type.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	N/A	This metric is not applicable to this study type.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	This metric is not applicable to this study type.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	N/A	This metric is not applicable to this study type.
	Metric 16:	Statistical Methods and Kinetic Calculations	N/A	This metric is not applicable to this study type.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	N/A	This metric is not applicable to this study type.
	Metric 18:	QSAR Models	N/A	This metric is not applicable to this study type.

Overall Quality Determination High

Study Citation:	U.S. EPA, (1989). Health and environmental effects document for 1,3-butadiene.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	3454

EXTRACTION

Parameter	Data
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, Type, Guideline	Not Reported; Not Reported; Not Reported
Solvent, Reactivity, Storage, Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, Purity	Not Reported; Not Reported; Not Reported; Not Reported
Duration and Test Temperature	Not Reported; 25 deg C
Light Source, Intensity, and additional light details	Not Reported; Not Reported; Not Reported
Source Wavelength Lower and Upper	Not Reported; Not Reported
Test Details and Control	Not Reported; Not Reported
Initial Concentration, Reference Compound	Not Reported Not Reported; Not Reported
Substance Wavelength Lower and Upper	Not Reported; Not Reported
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	Not Reported; Not Reported; Not Reported
Indirect Type Results, Indirect Rate Constant Lower and Upper	Not Reported; Not Reported; Not Reported
Method Details Results and Products Details Results	Not Reported; Not Reported
Parameter Value and Parameter Results	Not Reported; Not Reported
Reference Substance Results, Percent Degradation Results and Standard Deviation Results	Not Reported; Not Reported; Not Reported
Results Remarks, Sample time Results, Results Details	Not Reported; Not Reported; Degradation product from reaction with ozone: Acrolein

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was identified.
	Metric 2:	Test Substance Purity	N/A	This metric is not applicable to this study type.
Domain 2: Test Design				
	Metric 3:	Study Controls	N/A	This metric is not applicable to this study type.
	Metric 4:	Test Substance Stability	N/A	This metric is not applicable to this study type.
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	N/A	This metric is not applicable to this study type.
	Metric 6:	Testing Conditions	N/A	This metric is not applicable to this study type.
	Metric 7:	Testing Consistency	N/A	This metric is not applicable to this study type.

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Study Citation:	U.S. EPA, (1989). Health and environmental effects document for 1,3-butadiene.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	3454

			EVALUATION	
Domain		Metric	Rating	Comments
	Metric 8:	System Type and Design	N/A	This metric is not applicable to this study type.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	This metric is not applicable to this study type.
	Metric 10:	Sampling Methods	N/A	This metric is not applicable to this study type.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	N/A	This metric is not applicable to this study type.
	Metric 12:	Test Substance Purity	N/A	This metric is not applicable to this study type.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	N/A	This metric is not applicable to this study type.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	This metric is not applicable to this study type.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	N/A	This metric is not applicable to this study type.
	Metric 16:	Statistical Methods and Kinetic Calculations	N/A	This metric is not applicable to this study type.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	High	The reported values were consistent with related physical chemical properties.
	Metric 18:	QSAR Models	N/A	This metric is not applicable to this study type.

Overall Quality Determination High

Study Citation:	Vimal, D. (2008). Laboratory investigations of the hydroxyl radical-initiated oxidation of atmospheric volatile organic compounds. ProQuest Dissertations and Theses Doctoral Dissertation:213.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	5699949

EXTRACTION

Parameter	Data
CASRN and Test Material	Not Reported; 1,3-Butadiene
Confidentiality, Type, Guideline	No; experimental; other: Gas-phase reaction of OH radical and 1,3-butadiene using a discharge flow technique
Solvent, Reactivity, Storage, Stability	NR; NR; NR; NR
Radiolabel, Source, State, Purity	NR; Sigma-Aldrich; Not Reported; 99% Notes: Reagent mixtures prepared as 0.08-0.4% 1,3-butadiene)
Duration and Test Temperature	Not Reported; 263 - 423 K (reaction temperatures controlled and monitored); total pressures 1-6 Torr
Light Source, Intensity, and additional light details	OH radicals were produced by the F + H2O OH + HF reaction or the H + NO2 OH + NO reaction.; not applicable; Flow tube reactor with photomultiplier using National Instruments LabView hardware/software environment user interface Ctrdaq_e.vi designed by Dr. Drew L'Esperance. Reactor: jacketed 1 m long, 2.54 cm diameter pyrex glass tube connected to a Haolocarbon wax coated aluminum detection chamber evacuated by a mechanical pump (average velocity: ca. 10 m/s)
Source Wavelength Lower and Upper	not applicable; not applicable
Test Details and Control	OH concentrations below 3E11 molecules/cm3; experiments were performed with either resonance fluorescence or laser induced fluorescence detection of the OH radicals; laser-induced fluorescence detection of OH: minimum detectable OH concentration of approximately 2E7 molecules cm-3 (S/N=1; 10 s integration time); resonance fluorescence detection of OH: minimum detectable OH concentration of approximately 1E9 molecules cm-3 (background signal 300-400 counts/s, S/N=1; 10 s integration time); not reported
Initial Concentration, Reference Compound	Test concentrations ranged from 1.16 to 44.57 10^11 cm-3; Not reported
Substance Wavelength Lower and Upper	not reported; not reported
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	not reported; Not Reported; Not Reported
Indirect Type Results, Indirect Rate Constant Lower and Upper	bimolecular rate constant k^II OH + 1,3-Butadiene (10^-11 cm3 molecule-1 s-1); 3.15±0.28 (at 423K); 8.57±0.42 (at 263K)
Method Details Results and Products Details Results	Pseudo-first-order decay rates: slope of log OH fluorescence signal versus reaction distance for given reagent concentration under plug flow approximation; first-order decay rates were corrected for axial diffusion and OH loss; bimolecular rate constants (k1^II) at variable pressures and temperatures calculated from weighted linear least-squares fit of k^I versus 1,3-butadiene concentration.; Based on results evaluating the isotopic effect, indicates that OH addition dominates the mechanism for photooxidation of 1,3-butadiene and H-abstraction is not occurring at a significant rate under these experimental conditions
Parameter Value and Parameter Results	Not Reported; Not Reported
Reference Substance Results, Percent Degradation Results and Standard Deviation Results	kinetic isotope effect at a temperature of 363 K and pressure of 1 Torr (kII(D) = (4.79 ± 0.4) × 10-11 cm3 molecule-1 s-1; kII(H) = (4.75 ± 0.3) × 10-11 cm3 molecule-1 s-1); OH + 1,3-butadiene-d6 at 300K (1,3-butadiene-d6: 2.2-14.24x10^11 cm-3) k^II = 6.94±0.38x10^-11 cm3 molecule-1 s-1 (value based on 15 experiments); not reported; reported with values: ± uncertainties represent 2 standard deviations
Results Remarks, Sample time Results, Results Details	Arrhenius expression: kII (T) = (7.23 ± 1.2) × 10-12 exp((664 ± 49/T)) cm3 molecule-1 s-1; Not Reported; At 283K (1,3-butadiene: 1.53-16.89x10^11 cm-3) k^II = 7.68±0.30x10^-11 cm3 molecule-1 s-1 (value based on 13 experiments) At 300K, 2 Torr (1,3-butadiene: 2.24-20.81x10^11 cm-3) k^II = 6.96±0.68x10^-11 cm3 molecule-1 s-1 (value based on 17 experiments) At 300K, 3 Torr (1,3-butadiene: 1.91-24.21x10^11 cm-3) k^II = 7.01±0.45x10^-11 cm3 molecule-1 s-1 (value based on 16 experiments) At 300K, 5 Torr (1,3-butadiene: 2.41-24.7x10^11 cm-3) k^II = 6.99±0.28x10^-11 cm3 molecule-1 s-1 (value based on 54 experiments)

EVALUATION

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Study Citation:	Vimal, D. (2008). Laboratory investigations of the hydroxyl radical-initiated oxidation of atmospheric volatile organic compounds. ProQuest Dissertations and Theses Doctoral Dissertation:213.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	5699949

EVALUATION

Domain	Metric		Rating	Comments
Domain	Metric		Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was identified clearly.
	Metric 2:	Test Substance Purity	High	The source and purity of the test substance were reported.
Domain 2: Test Design				
	Metric 3:	Study Controls	High	Blanks were run and accounted for in the data.
	Metric 4:	Test Substance Stability	High	The test substance preparation was reported.
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	High	The test method was suitable.
	Metric 6:	Testing Conditions	High	Testing conditions were monitored, reported, and appropriate for the method.
	Metric 7:	Testing Consistency	Medium	Variable [He], [1,3-butadiene], and number of experiments run at several temperatures.
	Metric 8:	System Type and Design	High	The system type and design were appropriate.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	This metric is not applicable to the study type.
	Metric 10:	Sampling Methods	N/A	This metric is not applicable to the study type.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	High	The outcome assessment methodology addressed the intended outcome of interest.
	Metric 12:	Test Substance Purity	N/A	This metric is not applicable to this study type.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	High	Reported variability or uncertainty was not likely to influence the outcome assessment.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	This metric is not applicable to the study type.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	High	Data reporting was appropriate.
	Metric 16:	Statistical Methods and Kinetic Calculations	High	Kinetic calculations were described and address the data.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	High	The study results were reasonable and compared to previously reported literature values.
	Metric 18:	QSAR Models	N/A	This metric is not applicable to the study type.

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Study Citation:	Vimal, D. (2008). Laboratory investigations of the hydroxyl radical-initiated oxidation of atmospheric volatile organic compounds. ProQuest Dissertations and Theses Doctoral Dissertation:213.
OECD Harmonized Template:	Photolysis in Air
HERO ID:	5699949

EVALUATION

Domain	Metric	Rating	Comments
Overall Quality Determination		**High**	

Study Citation:	NCBI, (2020). PubChem database: compound summary: 1,3-butadiene.
OECD Harmonized Template:	Hydrolysis
HERO ID:	6628926

EXTRACTION

Parameter	**Data**
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, Guideline	none; not specified; Not Reported: not specified
Solvent, Reactivity, Storage, Stability	NR; NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR; NR Notes: NR
Buffer, Test Temperature, Number of Replicates	NR; NR; NR
Positive Controls and Negative Controls	Positive: NR; Negative: NR
pH and Duration	NR; NR
Sampling Frequency and Test Setup	NR; NR
Concentration	Not Reported
Analytical Method, Analytical Details, and Statistics	NR; NR; NR
Transformation Products	NR
Reference Substance and Reference Substance Results	NR; NR
Percent Recovery, Hydrolysis Rate Constant, and Half-life	NR; NR; NR
Results Remarks	Not expected to undergo hydrolysis in the environment due to a lack of hydrolyzable functional groups

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was identified.
	Metric 2:	Test Substance Purity	Medium	Details regarding this metric were not reported in this secondary source.
Domain 2: Test Design				
	Metric 3:	Study Controls	Medium	Details regarding this metric were not reported in this secondary source.
	Metric 4:	Test Substance Stability	Medium	Details regarding this metric were not reported in this secondary source.
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	Medium	Details regarding this metric were not reported in this secondary source.
	Metric 6:	Testing Conditions	Medium	Details regarding this metric were not reported in this secondary source.
	Metric 7:	Testing Consistency	Medium	Details regarding this metric were not reported in this secondary source.
	Metric 8:	System Type and Design	Medium	Details regarding this metric were not reported in this secondary source.
Domain 4: Test Organisms				

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Study Citation:	NCBI, (2020). PubChem database: compound summary: 1,3-butadiene.
OECD Harmonized Template:	Hydrolysis
HERO ID:	6628926

		EVALUATION		
Domain		Metric	Rating	Comments
	Metric 9:	Outcome Assessment Methodology	N/A	The metric is not applicable to the study.
	Metric 10:	Sampling Methods	N/A	The metric is not applicable to the study.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	Medium	Details regarding this metric were not reported in this secondary source.
	Metric 12:	Test Substance Purity	Medium	Details regarding this metric were not reported in this secondary source.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	Medium	Details regarding this metric were not reported in this secondary source.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	The metric is not applicable to the study.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Medium	Details regarding this metric were not reported in this secondary source.
	Metric 16:	Statistical Methods and Kinetic Calculations	Medium	Details regarding this metric were not reported in this secondary source.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Low	Results were limited to a qualitative assessment.
	Metric 18:	QSAR Models	N/A	The metric is not applicable to the study.

Overall Quality Determination Medium

* Related References: Primary source cited: Capel PD, Larson SJ; Chemosphere 30: 1097- 1107 (1995)

Study Citation:	Howard, P. H., Boethling, R. S., Jarvis, W. F., Meylan, W. M., Michalenko, E. M. (1991). Handbook of environmental degradation rates: 1,3-butadiene. :380-381.
OECD Harmonized Template:	Photolysis in Water
HERO ID:	11779754

EXTRACTION

Parameter	Data
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, Guideline	no; calculation; EPA OTS 796.3700 (Direct Photolysis Rate in Water by Sunlight): NR
Solvent, Reactivity, Storage, Stability	NR; NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR; NR Notes: NR
Duration and Test Temperature	NR; NR
Light Source, Intensity, and additional light details	NR; NR; NR
Source Wavelength Lower and Upper	NR; NR
Test Details and Control	NR; NR
Initial Concentration and Reference Compound	NR NR; NR
Substance Wavelength Lower and Upper	NR; NR
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	NR; Indirect half-life = 1200 hours (50 days); Indirect half-life = 48000 hours (200 days)
Indirect Rate Constant Lower and Upper	NR; NR
Method Details Results and Products Details Results	NR; NR
Parameter Value and Parameter Results	NR; NR
Reference Compound, Reference Substance Results, Percent Degradation Results and Standard Deviation Results	NR; NR; NR; NR
Results Remarks, Sample time Results, Results Details	Based on measured hydroxyl radical rate constant in water; NR; NR

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test material was identified definitively.
	Metric 2:	Test Substance Purity	Medium	The source and purity of the test substance were not reported; however, the omissions were not likely to have a substantial impact on the study results.
Domain 2: Test Design				
	Metric 3:	Study Controls	Medium	Study controls were not reported and may affect the study results; however, the data are from a trusted secondary source.
	Metric 4:	Test Substance Stability	Medium	The test substance stability, homogeneity, preparation or storage conditions were not reported; however, these factors were not likely to influence the test substance or were not likely to have a substantial impact on study results.

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Study Citation:	Howard, P. H., Boethling, R. S., Jarvis, W. F., Meylan, W. M., Michalenko, E. M. (1991). Handbook of environmental degradation rates: 1,3-butadiene. :380-381.
OECD Harmonized Template:	Photolysis in Water
HERO ID:	11779754

Domain	Metric		EVALUATION Rating	Comments
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	Medium	The test method was not reported; however, the data is from a trusted secondary source with reference to the source the calculation was based on.
	Metric 6:	Testing Conditions	Medium	Testing conditions were not reported; however, the data are from a trusted secondary source.
	Metric 7:	Testing Consistency	Medium	Testing conditions were not reported; however, the data are from a trusted secondary source.
	Metric 8:	System Type and Design	Medium	Equilibrium was not reported; however, the data are from a trusted secondary source.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	This metric does not apply to this study type.
	Metric 10:	Sampling Methods	N/A	This metric does not apply to this study type.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	High	The outcome of interest was reported.
	Metric 12:	Test Substance Purity	Medium	The sampling method was not reported; however, the data are from a trusted secondary source.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	Medium	Sources of variability and uncertainty in the measurements were not reported; however, the omissions were not likely to have a substantial impact on study results.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	This metric does not apply to this study type.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Medium	Data reporting was limited, the analytical method was not reported; however, the information is presented in a trusted secondary source.
	Metric 16:	Statistical Methods and Kinetic Calculations	Medium	Kinetic and calculation details were not reported; however, the information is presented in a trusted secondary source.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Low	Due to limited information, evaluation of the reasonableness of the study results was not possible.
	Metric 18:	QSAR Models	N/A	This metric does not apply to this study type.

Overall Quality Determination — Medium

* Related References: Guesten, H et al 1981

Study Citation:	Howard, P. H., Boethling, R. S., Jarvis, W. F., Meylan, W. M., Michalenko, E. M. (1991). Handbook of environmental degradation rates: 1,3-butadiene. :380-381.
OECD Harmonized Template:	Biodegradation in Water
HERO ID:	11779754

EXTRACTION

Parameter	Data
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, EndPoint, Type, Guideline	No; Other; Calculation (scientific judgement); other: NR
Solvent, Reactivity, Storage, Stability	NR; NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR; NR Notes: NR
Blank and Control	NR; NR
Oxygen and Inoculum	Not specified; not specified: ground water
Duration, Parameter, System, and Sampling Frequency	NR; NR: NR; NR
pH Adjusted and pH	NR; NR
Concentration	NR NR - NR NR NR
Composition and Test Temperature	NR; NR
CEC, Water Aeration Dilution, Continuous Darkness, and Other Design	NR; NR; NR; NR
Results Details Method, Results per Degradation Parameter, and Direct Quantum Yield Results	NR; NR; NR
Results Value, Results Standard Deviation, Results Sample Time, and Results Reference Substance Compartments	NR; NR; NR; NR
Results Remarks and Results Details	Ground water half-life: 336 hours (14 days) - 1344 hours (8 weeks); scientific judgement based on estimated aqueous aerobic biodegradation half-lives.; NR
Results Mean Total Recovery and Results per Recovery	NR; NR

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was identified definitively.
	Metric 2:	Test Substance Purity	N/A	This metric is not applicable to the data type.
Domain 2: Test Design				
	Metric 3:	Study Controls	Low	Study controls were not reported and may affect the study results; however, the data are from a trusted secondary source.
	Metric 4:	Test Substance Stability	N/A	This metric is not applicable to the data type.

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Study Citation:	Howard, P. H., Boethling, R. S., Jarvis, W. F., Meylan, W. M., Michalenko, E. M. (1991). Handbook of environmental degradation rates: 1,3-butadiene. :380-381.
OECD Harmonized Template:	Biodegradation in Water
HERO ID:	11779754

			EVALUATION	
Domain		Metric	Rating	Comments
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	Low	The test method was not reported and citations were not provided.
	Metric 6:	Testing Conditions	Low	Testing conditions were not reported and citations were not provided.
	Metric 7:	Testing Consistency	N/A	This metric is not applicable to the data type.
	Metric 8:	System Type and Design	N/A	This metric is not applicable to the data type.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	The metric is not applicable to the data type.
	Metric 10:	Sampling Methods	N/A	This metric does not apply to this study type.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	Medium	The outcome of interest was reported; however, there was incomplete reporting of outcome assessment methods.
	Metric 12:	Test Substance Purity	N/A	This metric is not applicable to the data type.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	Low	Confounding variables were not discussed.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	This metric does not apply to this study type.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Low	Data reporting was limited, basis for scientific judgement and estimations were not reported; however, the information is presented in a trusted secondary source.
	Metric 16:	Statistical Methods and Kinetic Calculations	N/A	This metric does not apply to this study type.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Low	Due to limited information, evaluation of the reasonableness of the study results was not possible.
	Metric 18:	QSAR Models	N/A	This metric does not apply to this study type.

Overall Quality Determination — Low

Study Citation:	Howard, P. H., Boethling, R. S., Jarvis, W. F., Meylan, W. M., Michalenko, E. M. (1991). Handbook of environmental degradation rates: 1,3-butadiene. :380-381.
OECD Harmonized Template:	Biodegradation in Water
HERO ID:	11779754

EXTRACTION

Parameter	Data
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, EndPoint, Type, Guideline	No; Aqueous biodegradation; Calculation (scientific judgement); other: NR
Solvent, Reactivity, Storage, Stability	NR; NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR; NR Notes: NR
Blank and Control	NR; NR
Oxygen and Inoculum	Aerobic; not specified: unacclimated
Duration, Parameter, System, and Sampling Frequency	NR; NR: NR; NR
pH Adjusted and pH	NR; NR
Concentration	NR NR - NR NR NR
Composition and Test Temperature	NR; NR
CEC, Water Aeration Dilution, Continuous Darkness, and Other Design	NR; NR; NR; NR
Results Details Method, Results per Degradation Parameter, and Direct Quantum Yield Results	NR; NR; NR
Results Value, Results Standard Deviation, Results Sample Time, and Results Reference Substance Compartments	NR; NR; NR; NR
Results Remarks and Results Details	Aerobic half-life: 168 hours (7 days) - 672 hours (4 weeks) (Aqueous biodegradation); scientific judgement.; NR
Results Mean Total Recovery and Results per Recovery	NR; NR

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was identified definitively.
	Metric 2:	Test Substance Purity	Medium	The source and purity of the test substance were not reported; however, the omissions were not likely to have a substantial impact on the study results.
Domain 2: Test Design				
	Metric 3:	Study Controls	Low	Study controls were not reported and citations were not provided; however, the data are from a trusted secondary source.
	Metric 4:	Test Substance Stability	Low	The test substance stability, homogeneity, preparation or storage conditions were not reported and citations were not provided; however, the data are from a trusted secondary source.

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Study Citation:	Howard, P. H., Boethling, R. S., Jarvis, W. F., Meylan, W. M., Michalenko, E. M. (1991). Handbook of environmental degradation rates: 1,3-butadiene. :380-381.
OECD Harmonized Template:	Biodegradation in Water
HERO ID:	11779754

			EVALUATION	
Domain		Metric	Rating	Comments
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	Low	The test method was not reported and citations were not provided.
	Metric 6:	Testing Conditions	Low	Testing conditions were not reported and citations were not provided.
	Metric 7:	Testing Consistency	N/A	This metric does not apply to this data type.
	Metric 8:	System Type and Design	Low	Equilibrium was not reported; however, the data are from a trusted secondary source.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	Low	The inoculum and source were not reported and citations were not provided; however, the data are from a trusted secondary source.
	Metric 10:	Sampling Methods	N/A	This metric does not apply to this study type.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	Medium	The outcome of interest was reported; however, there was incomplete reporting of outcome assessment methods.
	Metric 12:	Test Substance Purity	Low	The sampling method was not reported and citations were not provided; however, the data are from a trusted secondary source.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	N/A	This metric does not apply to this study type.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	This metric does not apply to this study type.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Low	Data reporting was limited, basis for scientific judgement and estimations were not reported; however, the information is presented in a trusted secondary source.
	Metric 16:	Statistical Methods and Kinetic Calculations	N/A	This metric does not apply to this study type.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Low	Due to limited information, evaluation of the reasonableness of the study results was not possible.
	Metric 18:	QSAR Models	N/A	This metric does not apply to this study type.

Overall Quality Determination — Low

Study Citation:	Howard, P. H., Boethling, R. S., Jarvis, W. F., Meylan, W. M., Michalenko, E. M. (1991). Handbook of environmental degradation rates: 1,3-butadiene. :380-381.
OECD Harmonized Template:	Biodegradation in Water
HERO ID:	11779754

EXTRACTION

Parameter	Data
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, EndPoint, Type, Guideline	No; Other; Calculation (scientific judgement); other: NR
Solvent, Reactivity, Storage, Stability	NR; NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR; NR Notes: NR
Blank and Control	NR; NR
Oxygen and Inoculum	Not specified; other:: surface water
Duration, Parameter, System, and Sampling Frequency	NR; NR: NR; NR
pH Adjusted and pH	NR; NR
Concentration	NR NR - NR NR NR
Composition and Test Temperature	NR; NR
CEC, Water Aeration Dilution, Continuous Darkness, and Other Design	NR; NR; NR; NR
Results Details Method, Results per Degradation Parameter, and Direct Quantum Yield Results	NR; NR; NR
Results Value, Results Standard Deviation, Results Sample Time, and Results Reference Substance Compartments	NR; NR; NR; NR
Results Remarks and Results Details	Surface water half-life: 168 hours (7 days) - 672 hours (4 weeks); based on estimated aerobic biodegradation half-lives.; NR
Results Mean Total Recovery and Results per Recovery	NR; NR

EVALUATION

Domain	Metric	Rating	Comments
Domain 1: Test Substance			
Metric 1:	Test Substance Identity	High	The test substance was identified definitively.
Metric 2:	Test Substance Purity	N/A	This metric is not applicable to the data type.
Domain 2: Test Design			
Metric 3:	Study Controls	Low	Study controls were not reported and citations were not provided; however, the data are from a trusted secondary source.
Metric 4:	Test Substance Stability	N/A	This metric is not applicable to the data type.
Domain 3: Test Conditions			
Metric 5:	Test Method Suitability	Low	The test method was not reported and citations were not provided.
Metric 6:	Testing Conditions	Low	Testing conditions were not reported and citations were not provided.

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Study Citation:	Howard, P. H., Boethling, R. S., Jarvis, W. F., Meylan, W. M., Michalenko, E. M. (1991). Handbook of environmental degradation rates: 1,3-butadiene. :380-381.
OECD Harmonized Template:	Biodegradation in Water
HERO ID:	11779754

			EVALUATION	
Domain		Metric	Rating	Comments
	Metric 7:	Testing Consistency	N/A	This metric does not apply to this data type.
	Metric 8:	System Type and Design	N/A	This metric does not apply to this data type.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	The metric is not applicable to the data type.
	Metric 10:	Sampling Methods	N/A	This metric does not apply to this study type.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	Medium	The outcome of interest was reported; however, there was incomplete reporting of outcome assessment methods.
	Metric 12:	Test Substance Purity	N/A	The metric is not applicable to the data type.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	Low	Confounding variables were not discussed.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	This metric does not apply to this study type.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Medium	Data reporting was limited, basis for scientific judgement and estimations were not reported; however, the information is presented in a trusted secondary source.
	Metric 16:	Statistical Methods and Kinetic Calculations	N/A	This metric does not apply to this study type.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Low	Due to limited information, evaluation of the reasonableness of the study results was not possible.
	Metric 18:	QSAR Models	N/A	This metric does not apply to this study type.

Overall Quality Determination Medium

Study Citation:	Howard, P. H., Boethling, R. S., Jarvis, W. F., Meylan, W. M., Michalenko, E. M. (1991). Handbook of environmental degradation rates: 1,3-butadiene. :380-381.
OECD Harmonized Template:	Biodegradation in Water
HERO ID:	11779754

EXTRACTION

Parameter	Data
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, EndPoint, Type, Guideline	No; Aqueous biodegradation; Calculation (scientific judgement); other: NR
Solvent, Reactivity, Storage, Stability	NR; NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR; NR Notes: NR
Blank and Control	NR; NR
Oxygen and Inoculum	Anaerobic; not specified: unacclimated
Duration, Parameter, System, and Sampling Frequency	NR; NR: NR; NR
pH Adjusted and pH	NR; NR
Concentration	NR NR - NR NR NR
Composition and Test Temperature	NR; NR
CEC, Water Aeration Dilution, Continuous Darkness, and Other Design	NR; NR; NR; NR
Results Details Method, Results per Degradation Parameter, and Direct Quantum Yield Results	NR; NR; NR
Results Value, Results Standard Deviation, Results Sample Time, and Results Reference Substance Compartments	NR; NR; NR; NR
Results Remarks and Results Details	Anaerobic half-life: 672 hours (28 days) -2688 hours (16 weeks) (Aqueous biodegradation); scientific judgement based upon estimated aqueous aerobic biodegradation half-lives.; NR
Results Mean Total Recovery and Results per Recovery	NR; NR

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was identified definitively.
	Metric 2:	Test Substance Purity	Medium	The source and purity of the test substance were not reported; however, the omissions were not likely to have a substantial impact on the study results.
Domain 2: Test Design				
	Metric 3:	Study Controls	Low	Study controls were not reported and citations were not provided; however, the data are from a trusted secondary source.
	Metric 4:	Test Substance Stability	Low	The test substance stability, homogeneity, preparation or storage conditions were not reported and citations were not provided; however, the data are from a trusted secondary source.

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Study Citation:	Howard, P. H., Boethling, R. S., Jarvis, W. F., Meylan, W. M., Michalenko, E. M. (1991). Handbook of environmental degradation rates: 1,3-butadiene. :380-381.
OECD Harmonized Template:	Biodegradation in Water
HERO ID:	11779754

Domain	Metric		EVALUATION Rating	Comments
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	Low	The test method was not reported and citations were not provided; however, the data are from a trusted secondary source.
	Metric 6:	Testing Conditions	Low	Testing conditions were not reported and citations were not provided.
	Metric 7:	Testing Consistency	N/A	This metric does not apply to this data type.
	Metric 8:	System Type and Design	Low	Equilibrium was not established or reported; however, the data are from a trusted secondary source.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	Low	The inoculum and source were not reported and citations were not provided; however, the data are from a trusted secondary source.
	Metric 10:	Sampling Methods	N/A	This metric does not apply to this study type.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	Medium	The outcome of interest was reported; however, there was incomplete reporting of outcome assessment methods.
	Metric 12:	Test Substance Purity	Low	The sampling method was not reported and citations were not provided; however, the data are from a trusted secondary source.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	N/A	This metric does not apply to the data type.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	This metric does not apply to this study type.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Low	Data reporting was limited, basis for scientific judgement and estimations were not reported; however, the information is presented in a trusted secondary source.
	Metric 16:	Statistical Methods and Kinetic Calculations	N/A	This metric does not apply to this study type.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Low	Due to limited information, evaluation of the reasonableness of the study results was not possible.
	Metric 18:	QSAR Models	N/A	This metric does not apply to this study type.

Overall Quality Determination — Low

Study Citation:	NCBI, (2020). PubChem database: compound summary: 1,3-butadiene.
OECD Harmonized Template:	Biodegradation in Water
HERO ID:	6628926

EXTRACTION

Parameter	**Data**
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, EndPoint, Type, Guideline	None; other; Experimental; other
Solvent, Reactivity, Storage, Stability	NR; NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR; NR
Blank and Control	Not reported; Not reported
Oxygen and Inoculum	aerobic/anaerobic; not specified: Not reported
Duration, Parameter, System, and Sampling Frequency	Not reported; Not Reported: Not reported; Not reported
pH Adjusted and pH	Not Reported; Not reported
Concentration	Not Reported
Composition and Test Temperature	Aerobic waters/anaerobic waters; Not reported
CEC, Water Aeration Dilution, Continuous Darkness, and Other Design	Not reported; Not reported; Not Reported; Not reported
Results Details Method, Results per Degradation Parameter, and Direct Quantum Yield Results	Not reported; Aerobic biodegradation half-life; anaerobic biodegradation half-life; Not Reported
Results Value, Results Standard Deviation, Results Sample Time, and Results Reference Substance Compartments	7 days; 28 days; Not reported; Not reported; Not reported
Results Remarks and Results Details	Not reported; Not reported
Results Mean Total Recovery and Results per Recovery	Not reported; Not reported

EVALUATION

Domain	Metric	Rating	Comments
Domain 1: Test Substance			
Metric 1:	Test Substance Identity	High	The test substance was identified clearly.
Metric 2:	Test Substance Purity	Medium	Details regarding this metric were not reported in this secondary source.
Domain 2: Test Design			
Metric 3:	Study Controls	Medium	Limited data is presented in this secondary source.
Metric 4:	Test Substance Stability	Medium	Limited data is presented in this secondary source.
Domain 3: Test Conditions			
Metric 5:	Test Method Suitability	Medium	Limited data is presented in this secondary source.

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Study Citation:	NCBI, (2020). PubChem database: compound summary: 1,3-butadiene.
OECD Harmonized Template:	Biodegradation in Water
HERO ID:	6628926

Domain		Metric	EVALUATION Rating	Comments
	Metric 6:	Testing Conditions	Medium	Limited data is presented in this secondary source.
	Metric 7:	Testing Consistency	Medium	Limited data is presented in this secondary source.
	Metric 8:	System Type and Design	Medium	Limited data is presented in this secondary source.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	Low	Limited data is presented in this secondary source.
	Metric 10:	Sampling Methods	N/A	The metric is not applicable to this study type.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	N/A	The intended outcome is reported for the target substance.
	Metric 12:	Test Substance Purity	Medium	Limited data is presented in this secondary source.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	Medium	Limited data is presented in this secondary source.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	This metric is not applicable to this type of study.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Medium	Limited data is presented in this secondary source.
	Metric 16:	Statistical Methods and Kinetic Calculations	Medium	Limited data is presented in this secondary source.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Low	Due to limited information, evaluation of the reasonableness of the study results was not possible.
	Metric 18:	QSAR Models	N/A	This metric is not applicable to this type of study.

Overall Quality Determination — Medium

* Related References: Primary source cited: Capel PD, Larson SJ; Chemosphere 30: 1097- 1107 (1995)

Study Citation:	NCBI, (2020). PubChem database: compound summary: 1,3-butadiene.
OECD Harmonized Template:	Biodegradation in Water
HERO ID:	6628926

EXTRACTION

Parameter	Data
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, EndPoint, Type, Guideline	None; ready biodegradability; Experimental; OECD Guideline 301 D (Ready Biodegradability: Closed Bottle Test): Similar to OECD 301D
Solvent, Reactivity, Storage, Stability	NR; NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR; NR
Blank and Control	Not reported; Not reported
Oxygen and Inoculum	aerobic; not specified: sludge inoculum at 1 drop/liter
Duration, Parameter, System, and Sampling Frequency	4 weeks; not specified: Not reported; Not reported
pH Adjusted and pH	Not Reported; Not reported
Concentration	2.06 - 4.95 mg/L
Composition and Test Temperature	Not reported; Not reported
CEC, Water Aeration Dilution, Continuous Darkness, and Other Design	Not reported; Not reported; Not Reported; Not reported
Results Details Method, Results per Degradation Parameter, and Direct Quantum Yield Results	Not reported; Theoretical BOD; Not Reported
Results Value, Results Standard Deviation, Results Sample Time, and Results Reference Substance Compartments	4%; Not reported; Not reported; Not reported
Results Remarks and Results Details	Not reported; Not reported
Results Mean Total Recovery and Results per Recovery	Not reported; Not reported

EVALUATION

Domain	Metric	Rating	Comments
Domain 1: Test Substance			
Metric 1:	Test Substance Identity	High	The test substance was identified clearly.
Metric 2:	Test Substance Purity	Medium	Details regarding this metric were not reported in this secondary source.
Domain 2: Test Design			
Metric 3:	Study Controls	Medium	Limited data is presented in this secondary source.
Metric 4:	Test Substance Stability	Medium	Limited data is presented in this secondary source.
Domain 3: Test Conditions			
Metric 5:	Test Method Suitability	High	Reported as similar to an OECD Guideline study.
Metric 6:	Testing Conditions	Medium	Limited data is presented in this secondary source.
Metric 7:	Testing Consistency	Medium	Limited data is presented in this secondary source.

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Study Citation:	NCBI, (2020). PubChem database: compound summary: 1,3-butadiene.
OECD Harmonized Template:	Biodegradation in Water
HERO ID:	6628926

		EVALUATION		
Domain		Metric	Rating	Comments
	Metric 8:	System Type and Design	High	Reported as similar to an OECD Guideline study.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	Medium	Reported as similar to an OECD Guideline study using a sludge inoculum.
	Metric 10:	Sampling Methods	N/A	The metric is not applicable to the study type.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	High	The intended outcome is reported for the target substance.
	Metric 12:	Test Substance Purity	Medium	Limited data is presented in this secondary source.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	Medium	Limited data is presented in this secondary source.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	This metric is not applicable to this type of study.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Medium	Limited data is presented in this secondary source.
	Metric 16:	Statistical Methods and Kinetic Calculations	Medium	Limited data is presented in this secondary source.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Medium	Due to limited information, evaluation of the reasonableness of the study results was not possible.
	Metric 18:	QSAR Models	N/A	This metric is not applicable to this type of study.

Overall Quality Determination — Medium

* Related References: NITE; Chemical Risk Information Platform (CHRIP). Biodegradation and Bioconcentration. Tokyo, Japan: Natl Inst Tech Eval. Available from, as of Mar 9, 2015: http://www.safe.nite.go.jp/english/db.html

Study Citation:	Howard, P. H., Boethling, R. S., Jarvis, W. F., Meylan, W. M., Michalenko, E. M. (1991). Handbook of environmental degradation rates: 1,3-butadiene. :380-381.
OECD Harmonized Template:	Biodegredation in Soil
HERO ID:	11779754

EXTRACTION

Parameter	Data
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, EndPoint, Type, Guideline	no; other; Calculation (scientific judgement); other: NR
Solvent, Reactivity, Storage, Stability	NR; NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR; NR Notes: NR
Oxygen, pH, and CEC	NR; NR; NR
Test Type, Test Temperature, and Test Details	not specified; NR; NR
Soil Type, Clay Silts and Organic Carbon, and Bulk Density	other; NR; NR
Soil Classification, Microbial Biomass, and Humidity	NR; NR: NR
Duration, Parameter, System, and Sampling Frequency	NR; NR; NR; NR
Control and Blank	NR; NR
Concentration	NR NR - NR NR NR
Analytical Method, Analytical Details, and Results Per Degredation Parameter	NR; NR; NR
Results Remarks	Half-life: 168-672 hours (7 days-4weeks) in soil; scientific judgement based upon estimated aqueous aerobic biodegradation half-lives.
Results Value, Standard Deviation Results, Sample Time Results, Reference Substance Results, and Referencs Substance Compartment Results	NR; NR; NR; NR; NR
Results Details	NR
Mean Total Recovery Results and Results Per Recovery	NR; NR

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test material was identified definitively.
	Metric 2:	Test Substance Purity	N/A	The metric is not applicable to the data type.
Domain 2: Test Design				
	Metric 3:	Study Controls	Low	Study controls were not reported and may affect the study results; however, the data are from a trusted secondary source.
	Metric 4:	Test Substance Stability	N/A	The metric is not applicable to the data type.

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Study Citation:	Howard, P. H., Boethling, R. S., Jarvis, W. F., Meylan, W. M., Michalenko, E. M. (1991). Handbook of environmental degradation rates: 1,3-butadiene. :380-381.
OECD Harmonized Template:	Biodegredation in Soil
HERO ID:	11779754

			EVALUATION	
Domain		Metric	Rating	Comments
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	Low	The test method was not reported and citations were not provided.
	Metric 6:	Testing Conditions	Low	The test conditions were not reported.
	Metric 7:	Testing Consistency	N/A	The metric is not applicable to the data type.
	Metric 8:	System Type and Design	N/A	The metric is not applicable to the data type.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	The metric is not applicable to the data type.
	Metric 10:	Sampling Methods	N/A	This metric does not apply to this study type.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	Medium	The outcome of interest was reported; however, there was incomplete reporting of out-come assessment methods.
	Metric 12:	Test Substance Purity	N/A	The metric is not applicable to the data type.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	Medium	Confounding variables were not reported.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	This metric does not apply to this study type.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Low	Data reporting was limited, basis for scientific judgement and estimations were not reported; however, the information is presented in a trusted secondary source.
	Metric 16:	Statistical Methods and Kinetic Calculations	N/A	This metric does not apply to this study type.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Low	Due to limited information, evaluation of the reasonableness of the study results was not possible.
	Metric 18:	QSAR Models	N/A	This metric does not apply to this study type.

Overall Quality Determination — Low

Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.
OECD Harmonized Template:	Miscellaneous
HERO ID:	5155560

EXTRACTION

Parameter	**Data**
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, Guideline	no; experimental; experimental
Solvent, Reactivity, Storage, Stability	NR; NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR; NR Notes: NR
Test Method Details, Test Condition Details, and Test Consistency Details	Oxidation of 1,3-butadiene with 27 strains of propane-utilising bacteria; Bacteria was incubated in a 50% 1,3-butadiene/50% oxygen atmosphere at 30C.; Not Reported
System Type Design	resting cell suspensions
Sampling Frequency and Sampling Details	Not Reported; Not Reported
Test Temperature	Not Reported
Results Details	Not Reported
Analytical Method and Analytical Details	Not Reported; Not Reported
Transformation Products, Statistics, and Kinetics	1,2-epoxybutene; Not Reported; Not Reported
Reference Substance and Reference Substance Results	Not Reported; Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was identified definitively
	Metric 2:	Test Substance Purity	Medium	Details regarding this metric were not reported; more details may be in the source cited.
Domain 2: Test Design				
	Metric 3:	Study Controls	Medium	Details regarding this metric were not reported; more details may be in the source cited.
	Metric 4:	Test Substance Stability	Medium	Details regarding this metric were not reported; more details may be in the source cited.
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	Medium	Details regarding this metric were not reported; more details may be in the source cited.
	Metric 6:	Testing Conditions	Medium	Details regarding this metric were not reported; more details may be in the source cited.
	Metric 7:	Testing Consistency	Medium	Details regarding this metric were not reported; more details may be in the source cited.
	Metric 8:	System Type and Design	Medium	Details regarding this metric were not reported; more details may be in the source cited.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	High	The test organism was reported; more details may be in the source cited.
	Metric 10:	Sampling Methods	N/A	This metric does not apply to this study type.

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Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.
OECD Harmonized Template:	Miscellaneous
HERO ID:	5155560

Domain	Metric		EVALUATION Rating	Comments
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	Medium	Details regarding this metric were not reported; more details may be in the source cited.
	Metric 12:	Test Substance Purity	Medium	Details regarding this metric were not reported; more details may be in the source cited.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	Medium	Details regarding this metric were not reported; more details may be in the source cited.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	This metric does not apply to this study type.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Medium	Details regarding this metric were not reported; more details may be in the source cited.
	Metric 16:	Statistical Methods and Kinetic Calculations	N/A	This metric does not apply to this study type
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Medium	Details regarding this metric were not reported; more details may be in the source cited.
	Metric 18:	QSAR Models	N/A	This metric does not apply to this study type.

Overall Quality Determination Medium

* Related References: Cited secondary source Hou CT, Patel R, Laskin AI, Barnabe N, Barist I (1983). Epoxidation of short-chain alkenes by resting-cellsuspensions of propane-grown bacteria. Appl Environ Microbiol. 46; 171-177. [Not in HERO at the time of extraction].

Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.
OECD Harmonized Template:	Miscellaneous
HERO ID:	5155560

EXTRACTION

Parameter	Data
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, Guideline	no; experimental; experimental
Solvent, Reactivity, Storage, Stability	NR; NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR; NR Notes: NR
Test Method Details, Test Condition Details, and Test Consistency Details	Not Reported; Culture of Norcardia that were isolated from soil were grown at 25C with 1,-butadiene present in the headspace by 10-15% by volume.; Not Reported
System Type Design	Not Reported
Sampling Frequency and Sampling Details	Not Reported; Not Reported
Test Temperature	Not Reported
Results Details	Not Reported
Analytical Method and Analytical Details	Not Reported; Not Reported
Transformation Products, Statistics, and Kinetics	Degrades by several steps to give carbon dioxide and acetate. The stepwise intermediates were thought to be monoepoxide, beta, gamma-unsaturated alpha-keto acid, acrylate, lactate, and pyruvate; Not Reported; Not Reported
Reference Substance and Reference Substance Results	Not Reported; Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was identified definitively
	Metric 2:	Test Substance Purity	Medium	Details regarding this metric were not reported; more details may be in the source cited.
Domain 2: Test Design				
	Metric 3:	Study Controls	Medium	Details regarding this metric were not reported; more details may be in the source cited.
	Metric 4:	Test Substance Stability	Medium	Details regarding this metric were not reported; more details may be in the source cited.
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	Medium	Details regarding this metric were not reported; more details may be in the source cited.
	Metric 6:	Testing Conditions	Medium	Details regarding this metric were not reported; more details may be in the source cited.
	Metric 7:	Testing Consistency	Medium	Details regarding this metric were not reported; more details may be in the source cited.
	Metric 8:	System Type and Design	Medium	Details regarding this metric were not reported; more details may be in the source cited.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	High	The test organism was reported; more details may be in the source cited.
	Metric 10:	Sampling Methods	N/A	This metric does not apply to this study type.

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Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.
OECD Harmonized Template:	Miscellaneous
HERO ID:	5155560

Domain	Metric		EVALUATION Rating	Comments
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	Medium	Details regarding this metric were not reported; more details may be in the source cited.
	Metric 12:	Test Substance Purity	Medium	Details regarding this metric were not reported; more details may be in the source cited.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	Medium	Details regarding this metric were not reported; more details may be in the source cited.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	This metric does not apply to this study type.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Medium	Details regarding this metric were not reported; more details may be in the source cited.
	Metric 16:	Statistical Methods and Kinetic Calculations	N/A	This metric does not apply to this study type
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Medium	Details regarding this metric were not reported; more details may be in the source cited.
	Metric 18:	QSAR Models	N/A	This metric does not apply to this study type.

Overall Quality Determination Medium

* Related References: Cited secondary source Watkinson and Somerville 1975 [HERO ID 5349224]

Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.
OECD Harmonized Template:	Miscellaneous
HERO ID:	5155560

EXTRACTION

Parameter	**Data**
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, Guideline	no; experimental; experimental
Solvent, Reactivity, Storage, Stability	NR; NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR; NR Notes: NR
Test Method Details, Test Condition Details, and Test Consistency Details	Oxidation of 1,3-butadiene with three strains of methane-utilising bacteria (Methylosinus trichosporium, methylococcus capsulantus, and methylobacterium organophilum.; Bacteria was grown in a 50% methane/50% air atmosphere and incubated in a 50% 1,3-butadiene/50% oxygen atmosphere at 30C.; Not Reported
System Type Design	resting cell suspensions
Sampling Frequency and Sampling Details	Not Reported; Not Reported
Test Temperature	Not Reported
Results Details	Not Reported
Analytical Method and Analytical Details	Not Reported; Not Reported
Transformation Products, Statistics, and Kinetics	1,2-epoxybutene; Not Reported; Not Reported
Reference Substance and Reference Substance Results	Not Reported; Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was identified definitively
	Metric 2:	Test Substance Purity	Medium	Details regarding this metric were not reported; more details may be in the source cited.
Domain 2: Test Design				
	Metric 3:	Study Controls	Medium	Details regarding this metric were not reported; more details may be in the source cited.
	Metric 4:	Test Substance Stability	Medium	Details regarding this metric were not reported; more details may be in the source cited.
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	Medium	Details regarding this metric were not reported; more details may be in the source cited.
	Metric 6:	Testing Conditions	Medium	Details regarding this metric were not reported; more details may be in the source cited.
	Metric 7:	Testing Consistency	Medium	Details regarding this metric were not reported; more details may be in the source cited.
	Metric 8:	System Type and Design	Medium	Details regarding this metric were not reported; more details may be in the source cited.
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	High	The test organism was reported; more details may be in the source cited.
	Metric 10:	Sampling Methods	N/A	This metric does not apply to this study type.
Domain 5: Outcome Assessment				

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Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.
OECD Harmonized Template:	Miscellaneous
HERO ID:	5155560

			EVALUATION	
Domain		Metric	Rating	Comments
	Metric 11:	Test Substance Identity	Medium	Details regarding this metric were not reported; more details may be in the source cited.
	Metric 12:	Test Substance Purity	Medium	Details regarding this metric were not reported; more details may be in the source cited.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	Medium	Details regarding this metric were not reported; more details may be in the source cited.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	This metric does not apply to this study type.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	Medium	Details regarding this metric were not reported; more details may be in the source cited.
	Metric 16:	Statistical Methods and Kinetic Calculations	N/A	This metric does not apply to this study type
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Medium	Details regarding this metric were not reported; more details may be in the source cited.
	Metric 18:	QSAR Models	N/A	This metric does not apply to this study type.

Overall Quality Determination — Medium

* Related References: Cited secondary source Hou et al (1979) [HERO ID 5349195]

Study Citation:	Zhao, Z., Husainy, S., Smith, G. D. (2011). Kinetics studies of the gas-phase reactions of NO3 radicals with series of 1-alkenes, dienes, cycloalkenes, alkenols, and alkenals. Journal of Physical Chemistry A 115(44):12161-12172.
OECD Harmonized Template:	Miscellaneous
HERO ID:	901429

EXTRACTION

Parameter	**Data**
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, Guideline	None; Experimental; Experimental
Solvent, Reactivity, Storage, Stability	Nitrogen carrier gas; NR; NR; NR
Radiolabel, Source, State, Purity	NA; TCI America; Gas; 99%
Test Method Details, Test Condition Details, and Test Consistency Details	Disappearance of test material and reference substance in gas-phase reaction with NO3 measured to determine rate; Atmospheric-pressure. Reaction times of 6.0 - 24 seconds; Test groups used the same method. NO3 concentrations 3E10 - 2E12 molecules/cm^3
System Type Design	Test material, reference compound, and N2 carrier gas in a glass flow tube with flow rate of 2.0 standard liters per min allowed to react with N2 carrying N2O5 (thermally dissociates to NO3) at a flow rate of 70 standard cubic centimeters per min
Sampling Frequency and Sampling Details	Not reported; Flow leaves the flow tube and to a 523 K 1/4 ” o.d., 4” long vaporizer tube (to minimize condensation), to sampling ion tube region of a stainless steel orifice 0.5 mm i.d.
Test Temperature	295 ± 2 K
Results Details	Rate of disappearance of the gas-phase test material via NO3 + test material –> products
Analytical Method and Analytical Details	Chemical ionization method with mass spectrometer; Ions generated by 210Po source, detected using Channeltron electron multiplier
Transformation Products, Statistics, and Kinetics	Not applicable; ±0.15 and ±0.07 E-13 cm^3 /molecule sec; Rate of disappearance KOC: 1.23 and 1.26 E-13 cm^3 /molecule sec Plot of ln (OC/[OC]0) vs ln([R]/[R]0) analyzed by linear least-squares fitting to obtain KOC / Kr ratio Where OC = test material; r = reference material
Reference Substance and Reference Substance Results	trans-2-butene; cyclopentene; trans 2-butene KOC / Kr = 0.310±0.038 cyclopentene KOC / Kr = 0.262 ± 0.012 Where Kr = rate of disappearance of the reference substance

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was definitively identified.
	Metric 2:	Test Substance Purity	High	The source and purity of the test substance was reported.
Domain 2: Test Design				
	Metric 3:	Study Controls	N/A	The metric is not applicable to this study type.
	Metric 4:	Test Substance Stability	High	The test substance preparation was reported and appropriate for the study.
Domain 3: Test Conditions				
	Metric 5:	Test Method Suitability	High	Test method was suitable for the test substance.
	Metric 6:	Testing Conditions	High	Test conditions were monitored and reported.
	Metric 7:	Testing Consistency	High	Test conditions were consistent across study groups.
	Metric 8:	System Type and Design	N/A	The metric is not applicable to this study type.

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Study Citation:	Zhao, Z., Husainy, S., Smith, G. D. (2011). Kinetics studies of the gas-phase reactions of NO3 radicals with series of 1-alkenes, dienes, cycloalkenes, alkenols, and alkenals. Journal of Physical Chemistry A 115(44):12161-12172.
OECD Harmonized Template:	Miscellaneous
HERO ID:	901429

Domain	Metric	Metric	EVALUATION Rating	Comments
Domain 4: Test Organisms				
	Metric 9:	Outcome Assessment Methodology	N/A	The metric is not applicable to this study type.
	Metric 10:	Sampling Methods	N/A	The metric is not applicable to this study type.
Domain 5: Outcome Assessment				
	Metric 11:	Test Substance Identity	High	The outcome assessment methodology addressed the intended outcomes of interest.
	Metric 12:	Test Substance Purity	High	Sampling methods addressed the outcomes of interest, used widely acceptable methods, and no notable uncertainties were expected to influence results.
Domain 6: Confounding/Variable Control				
	Metric 13:	Confounding Variables	High	Sources of variability and uncertainty in the measurements and statistical techniques between study groups were considered and accounted for in data evaluation.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	The metric is not applicable to this study type.
Domain 7: Data Presentation and Analysis				
	Metric 15:	Data Reporting	High	Analytical methods were suitable for detection and quantification of the target chemical and sufficient evidence was presented to confirm the parent compound disappearance was not due to other processes.
	Metric 16:	Statistical Methods and Kinetic Calculations	High	Statistical and kinetic calculations were described and appropriate for the datasets.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	High	The results were reasonable.
	Metric 18:	QSAR Models	N/A	The metric is not applicable to this study type.

Overall Quality Determination High

List of Abbreviations and Acronyms for Data Quality Evaluation and Extraction Tables

Term	Definition
BAF	Biaccumulation Factor
BCF	Bioconcentration Factor
BMF	Biomagnification Factor
BSAF	Biota-sediment Accumulation Factor
C	Concentration
CASRN	Chemical Abstract Service registry number
DOC	Dissolved Organic Carbon
dw	Dry weight
DW	Drinking Water
DWTP	Drinking Water Treatment Plant
EPA	Environmental Protection Agency
ESI	Electrospray Ionisation
FID	Flame Ionisation Detector
FPD	Flame Photometric Detector
GC	Gas Chromatography
g/L	Grams per Liter
HLC	Henry's Law Constant
HPLC	High-performance liquid chromatography
ISO	International Organization for Standardization
K_{oa}	Octanol-Air partition coefficient
K_{oc}	Organic carbon-water partition coefficient
K_{ow}	Octanol-Water partition coefficient
L/d	Liters per day
LOD	Limit of Detection
LOQ	Limit of Quantification
lw	Lipid weight
M	Molarity (mol/L = moles per Liter)
mL/min	Milliliters per minute
mM	Millimolar
MDL	Method Detection Limit
mg/kg	Milligrams per Kilogram
mg/L	Milligrams per Liter
mg/m^3	Milligrams per cubic meter
MRL	Method Reporting Limit
MS	Mass Spectrometry
n	Sample Size
N/A	Not applicable
ND	Non-Detection
ng/L	Nanograms per Liter

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Term	Definition
nm	Nanometers
NR	Not Reported
OECD	Organisation for Economic Co-operation and Development
· OH	Hydroxyl radical
OPE	Organophosphate Ester
pg/L	Picograms per Liter
ppm	parts per million
QSAR	Quantatative Structure Activity Relationship
RSD	Relative Standard Deviation
SI	Supplemental Information
SIM	Selected Ion Monitoring
SPE	Solid Phase Extraction
STP	Sewage Treatment Plant
TMF	Trophic Magnification Factor
TOC	Total Organic Carbon
TOF	Time of Flight
μg/L or μg/mL	micrograms per liter or per milliliter
UPLC	Ultra-performance liquid chromatography
US or USA	United States of America
UV (UV-Vis)	Ultra Violet (Visible)
ww	Wet Weight
WWTP	Wastewater Treatment Plant