IMMEDIATELY DANGEROUS TO LIFE OR HEALTH (IDLH) VALUE PROFILE

FOR

CHLORINE PENTAFLUORIDE [CAS NO. 13637-63-3]

AND

BROMINE PENTAFLUORIDE [CAS NO. 7789-30-2]

Department of Health and Human Services
Centers for Disease Control and Prevention
National Institute for Occupational Safety and Health

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Foreword

Chemicals are a ubiquitous component of the modern workplace. Occupational exposures to chemicals have the potential to adversely affect the health and lives of workers. Acute or short-term exposures to high concentrations of some airborne chemicals have the ability to quickly overwhelm workers, resulting in a spectrum of undesirable health outcomes that may inhibit the ability to escape from the exposure environment (e.g., irritation of the eyes and respiratory tract or cognitive impairment), cause severe irreversible effects (e.g., damage to the respiratory tract or reproductive toxicity), and in extreme cases, cause death. Airborne concentrations of chemicals capable of causing such adverse health effects or of impeding escape from high-risk conditions may arise from a variety of non-routine workplace situations , including special work procedures (e.g., in confined spaces), industrial accidents (e.g., chemical spills or explosions), and chemical releases into the community (e.g., during transportation incidents or other uncontrolled-release scenarios).

The "immediately dangerous to life or health air concentration values (IDLH values)" developed by the National Institute for Occupational Safety and Health (NIOSH) characterize these high-risk exposure concentrations and conditions [NIOSH 2013]. IDLH values are based on a 30-minute exposure duration and have traditionally served as a key component of the decision logic for the selection of respiratory protection devices [NIOSH 2004]. Occupational health professionals have employed these values beyond their initial purpose as a component of the NIOSH Respirator Selection Logic to assist in developing Risk Management Plans for non-routine work practices governing operations in high-risk environments (e.g., confined spaces) and the development of Emergency Preparedness Plans.

The approach used to derive IDLH values for high priority chemicals is outlined in the NIOSH Current Intelligence Bulletin (CIB) 66: Derivation of Immediately Dangerous to Life or Health Values [NIOSH 2013]. CIB 66 provides 1) an update on the scientific basis and risk assessment methodology used to derive IDLH values, 2) the rationale and derivation process for IDLH values, and 3) a demonstration of the derivation of scientifically credible IDLH values using available data resources.

The purpose of this technical report is to present the IDLH values for chlorine pentafluoride (CAS # 13637-63-3) and bromine pentafluoride (CAS #7789-30-2). The scientific basis, toxicologic data and risk assessment approach used to derive the IDLH value are summarized to ensure transparency and scientific credibility.

John Howard, M.D.
Director
National Institute for Occupational Safety and Health
Centers for Disease Control and Prevention

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Abbreviations

ACGIH	American Conference of Governmental Industrial Hygienists
AEGL	Acute Exposure Guideline Levels
AIHA	American Industrial Hygiene Association
BMC	benchmark concentration
BMCL	benchmark concentration lower confidence limit
BrF_5	bromine pentafluoride
C°	Celsius
C	ceiling
CAS	chemical abstract service
ClF_5	chlorine pentafluoride
ERPG	Emergency Response Planning Guidelines
IDLH	immediately dangerous to life or health
LC_{50}	median lethal concentration
LC_{Lo}	lowest concentration of a chemical that caused death in humans or animals
LEL	lower explosive limit
LOAEL	lowest observed adverse effect level
mg/m^3	milligram(s) per cubic meter
mmHg	millimeter(s) of mercury
NAC	National Advisory Committee
NAS	National Academy of Sciences
NIOSH	National Institute for Occupational Safety and Health
NOAEL	no observed adverse effect level
OSHA	Occupational Safety and Health Administration
PEL	permissible exposure limit
ppm	parts per million
RD_{50}	concentration of a chemical in the air that is estimated to cause a 50% decrease in the respiratory rate
REL	recommend exposure limit
SCP	Standard Completion Program
STEL	short term exposure limit
TLV	threshold limit value
TWA	time weighted average
UEL	upper explosive limit
WEEL	workplace environmental exposure level

Glossary

Acute Exposure: Exposure by the oral, dermal, or inhalation route for 24 hours or less.

Acute Exposure Guideline Levels (AEGLs): Threshold exposure limits for the general public applicable to emergency exposure periods ranging from 10 minutes to 8 hours. AEGL-1, AEGL 2, and AEGL-3 are developed for five exposure periods (10 and 30 minutes, 1 hour, 4 hours, and 8 hours) and are distinguished by varying degrees of severity of toxic effects ranging from transient, reversible effects to life-threatening effects [NAS 2001]. AEGLs are intended to be guideline levels used during rare events or single once-in-a-lifetime exposures to airborne concentrations of acutely toxic, high-priority chemicals [NAS 2001]. The threshold exposure limits are designed to protect the general population, including the elderly, children or other potentially sensitive groups that are generally not considered in the development of workplace exposure recommendations (additional information available at http://www.epa.gov/oppt/aegl/).

Acute Reference Concentration (RfC): An estimate (with uncertainty spanning perhaps an order of magnitude) of a continuous inhalation exposure for an acute duration (24 hours or less) of the human population (including sensitive subgroups) that is likely to be without an appreciable risk of deleterious effects during a lifetime. It can be derived from a NOAEL, LOAEL, or benchmark concentration, with uncertainty factors (UFs) generally applied to reflect limitations of the data used. Generally used in USEPA noncancer health assessments [USEPA 2014].

Acute Toxicity: Any poisonous effect produced within a short period of time following an exposure, usually 24 to 96 hours.

Adverse Effect: A substance-related biochemical change, functional impairment, or pathologic lesion that affects the performance of an organ or system or alters the ability to respond to additional environmental challenges.

Benchmark Dose/Concentration (BMD/BMC): A dose or concentration that produces a predetermined change in response rate of an effect (called the benchmark response, or BMR) compared to background [USEPA 2014] (additional information available at http://www.epa.gov/ncea/bmds/).

Benchmark Response (BMR): A predetermined change in response rate of an effect. Common defaults for the BMR are 10% or 5%, reflecting study design, data variability, and sensitivity limits used.

BMCL: A statistical lower confidence limit on the concentration at the BMC [USEPA 2014].

Bolus Exposure: A single, relatively large dose.

Ceiling Value ("C"): U.S. term in occupational exposure indicating the airborne concentration of a potentially toxic substance that should never be exceeded in a worker's breathing zone.

Chronic Exposure: Repeated exposure for an extended period of time. Typically exposures are more than approximately 10% of life span for humans and >90 days to 2 years for laboratory species.

Critical Study: The study that contributes most significantly to the qualitative and quantitative assessment of risk [USEPA 2014].

Dose: The amount of a substance available for interactions with metabolic processes or biologically significant receptors after crossing the outer boundary of an organism [USEPA 2014].

ECt_{50}: A combination of the effective concentration of a substance in the air and the exposure duration that is predicted to cause an effect in 50% (one half) of the experimental test subjects.

Emergency Response Planning Guidelines (ERPGs): Maximum airborne concentrations below which nearly all individuals can be exposed without experiencing health effects for 1-hour exposure. ERPGs are presented in a tiered fashion with health effects ranging from mild or transient to serious, irreversible, or life threatening (depending on the tier). ERPGs are developed by the American Industrial Hygiene Association [AIHA 2006].

Endpoint: An observable or measurable biological event or sign of toxicity ranging from biomarkers of initial response to gross manifestations of clinical toxicity.

Exposure: Contact made between a chemical, physical, or biological agent and the outer boundary of an organism. Exposure is quantified as the amount of an agent available at the exchange boundaries of the organism (e.g., skin, lungs, gut).

Extrapolation: An estimate of the response at a point outside the range of the experimental data, generally through the use of a mathematical model, although qualitative extrapolation may also be conducted. The model may then be used to extrapolate to response levels that cannot be directly observed.

Hazard: A potential source of harm. Hazard is distinguished from risk, which is the probability of harm under specific exposure conditions.

Immediately Dangerous to Life or Health (IDLH) condition: A situation that poses a threat of exposure to airborne contaminants when that exposure is likely to cause death or immediate or delayed permanent adverse health effects or prevent escape from such an environment [NIOSH 2004, 2013].

IDLH value: A maximum (airborne concentration) level above which only a highly reliable breathing apparatus providing maximum worker protection is permitted [NIOSH 2004, 2013]. IDLH values are based on a 30-minute exposure duration.

LC_{01}: The statistically determined concentration of a substance in the air that is estimated to cause death in 1% of the test animals.

LC_{50}: The statistically determined concentration of a substance in the air that is estimated to cause death in 50% (one half) of the test animals; median lethal concentration.

LC_{LO}: The lowest lethal concentration of a substance in the air reported to cause death, usually for a small percentage of the test animals.

LD_{50}: The statistically determined lethal dose of a substance that is estimated to cause death in 50% (one half) of the test animals; median lethal concentration.

LD_{LO}: The lowest dose of a substance that causes death, usually for a small percentage of the test animals.

LEL: The minimum concentration of a gas or vapor in air, below which propagation of a flame does not occur in the presence of an ignition source.

Lethality: Pertaining to or causing death; fatal; referring to the deaths resulting from acute toxicity studies. May also be used in lethality threshold to describe the point of sufficient substance concentration to begin to cause death.

Lowest Observed Adverse Effect Level (LOAEL): The lowest tested dose or concentration of a substance that has been reported to cause harmful (adverse) health effects in people or animals.

Mode of Action: The sequence of significant events and processes that describes how a substance causes a toxic outcome. Mode of action is distinguished from the more detailed mechanism of action, which implies a more detailed understanding on a molecular level.

No Observed Adverse Effect Level (NOAEL): The highest tested dose or concentration of a substance that has been reported to cause no harmful (adverse) health effects in people or animals.

Occupational Exposure Limit (OEL): Workplace exposure recommendations developed by governmental agencies and non-governmental organizations. OELs are intended to represent the maximum airborne concentrations of a chemical substance below which workplace exposures should not cause adverse health effects. OELs may apply to ceiling, short-term (STELs), or time-weighted average (TWA) limits.

Peak Concentration: Highest concentration of a substance recorded during a certain period of observation.

Permissible Exposure Limit (PEL): Occupational exposure limits developed by OSHA (29 CFR 1910.1000) or MSHA (30 CFR 57.5001) for allowable occupational airborne exposure concentrations. PELs are legally enforceable and may be designated as ceiling, STEL, or TWA limits.

Point of Departure (POD): The point on the dose–response curve from which dose extrapolation is initiated. This point can be the lower bound on dose for an estimated incidence or a change in response level from a concentration-response model (BMC), or it can be a NOAEL or LOAEL for an observed effect selected from a dose evaluated in a health effects or toxicology study.

RD_{50}: The statistically determined concentration of a substance in the air that is estimated to cause a 50% (one half) decrease in the respiratory rate.

Recommended Exposure Limit (REL): Recommended maximum exposure limit to prevent adverse health effects based on human and animal studies and established for occupational (up to 10-hour shift, 40-hour week) inhalation exposure by NIOSH. RELs may be designated as ceiling, STEL, or TWA limits.

Short-Term Exposure Limit (STEL): A worker's 15-minute time-weighted average exposure concentration that shall not be exceeded at any time during a work day.

Target Organ: Organ in which the toxic injury manifests in terms of dysfunction or overt disease.

Threshold Limit Values (TLVs®): Recommended guidelines for occupational exposure to airborne contaminants, published by the American Conference of Governmental Industrial Hygienists (ACGIH). TLVs refer to airborne concentrations of chemical substances and represent conditions under which it is believed that nearly all workers may be repeatedly exposed, day after day, over a working lifetime, without adverse effects. TLVs may be designated as ceiling, short-term (STELs), or 8-hr TWA limits.

Time-Weighted Average (TWA): A worker's 8-hour (or up to 10-hour) time-weighted average exposure concentration that shall not be exceeded during an 8-hour (or up to 10-hour) work shift of a 40-hour week. The average concentration is weighted to take into account the duration of different exposure concentrations.

Toxicity: The degree to which a substance is able to cause an adverse effect on an exposed organism.

Uncertainty Factors (UFs): Mathematical adjustments applied to the POD when developing IDLH values. The UFs for IDLH value derivation are determined by considering the study and effect used for the POD, with further modification based on the overall database.

Workplace Environmental Exposure Levels (WEELs): Exposure levels developed by the American Industrial Hygiene Association (AIHA) that provide guidance for protecting most workers from adverse health effects related to occupational chemical exposures expressed as a TWA or ceiling limit.

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Education and Information Division

Devin Baker, M.Ed.
Charles L. Geraci, Ph.D.
Thomas J. Lentz, Ph.D.
Richard Niemeier, Ph.D.
Chris Sofge, Ph.D.

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Michael S. Bisesi, Ph.D., R.E.H.S., C.I.H., Senior Associate Dean for Academic Affairs; Director, Center for Public Health Practice; Interim Chair & Associate Professor, Division of Environmental Health Science, College of Public Health, Ohio State University

Mary A. Fox, Ph.D., Assistant Professor; Co-Director, Risk Sciences and Public Policy Institute; Department of Health Policy and Management, Bloomberg School of Public Health, Johns Hopkins University

Richard B. Schlesinger, Ph.D., Fellow A.T.S., Senior Associate Dean for Academic Affairs and Research Professor of Biology, Dyson College of Arts and Sciences, Pace University

1.0 Chlorine Pentafluoride

1.1 Introduction

1.1.1 Overview of the IDLH Value for Chlorine Pentafluoride

IDLH Value: 1.7 ppm

Basis for IDLH Value: The IDLH value for chlorine pentafluoride is based on a 10-minute mouse LOAEL of 30 ppm associated with severe respiratory irritation in multiple species, which represents potentially escape-impairing effects [MacEwen and Vernot 1972]. Duration adjustment yielded a 30-minute equivalent of 17.3 ppm. Application of a composite uncertainty factor of 10 to account for extrapolation from an escape-impairing effect, interspecies differences and human variability results an IDLH value for chlorine pentafluoride of **1.7 ppm**.

1.1.2 Purpose

This *IDLH Profile* presents (1) a brief summary of technical data associated with acute inhalation exposures to chlorine pentafluoride and (2) the rationale behind the Immediately Dangerous to Life or Health (IDLH) value for chlorine pentafluoride. IDLH values are developed based on the scientific rationale and logic outlined in the NIOSH Current Intelligence Bulletin (CIB) 66: Derivation of Immediately Dangerous to Life or Health (IDLH) values [NIOSH 2013]. As described in CIB 66, NIOSH performs in-depth literature searches to ensure that all relevant data from human and animal studies with acute exposures to the substance are identified. Information included in CIB 66 on the literature search includes pertinent databases, key terms, and guides for evaluating data quality and relevance for the establishment of an IDLH value. The information that is identified in the in-depth literature search is evaluated with general considerations that include description of studies (i.e., species, study protocol, exposure concentration and duration), health endpoint evaluated, and critical effect levels (e.g., NOAELs, LOAELs, LC_{50} values). For chlorine pentafluoride, the in-depth literature search was conducted through February 2014.

1.1.3 General Substance Information

Chemical: Chlorine pentafluoride (ClF_5)*

CAS No: 13637-63-3

Synonyms: Chlorine fluoride

Chemical category: Inorganic fluorine compounds; Inorganic chlorine compounds; Inorganic gases[†]

Structural formula:

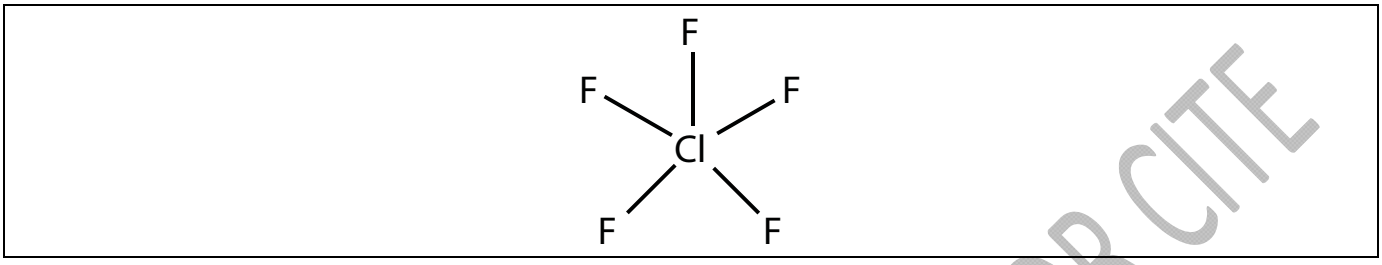

Table 1 highlights selected physiochemical properties of chlorine pentafluoride relevant to IDLH conditions. Table 2 provides alternative exposure guidelines for chlorine pentafluoride. Table 3 summarizes the Acute Exposure Guidelines Level (AEGL) values for chlorine pentafluoride.

Table 1: Physiochemical Properties of Chlorine Pentafluoride

Property	Value
Molecular weight	130.45[†]
Chemical formula	ClF_5
Description	Colorless or yellow gas
Odor	Suffocating, pungent
Odor Threshold	Not available
UEL	Not available
LEL	Not available
Vapor pressure	3.4 bar at 20°C
Flash point	Noncombustible[†]
Ignition temperature	Noncombustible[†]
Solubility	Hydrolysis[†]

Abbreviation: °C – Celsius; °F – Fahrenheit; mmHg – millimeter mercury; LEL – lower explosive limit; UEL – upper explosive limit
[*] AEGL [2010a]; [†] IFA [2014]

Table 2: Alternative Exposure Guidelines for Chlorine Pentafluoride

Organization	Value
Original (SCP) IDLH value	None
NIOSH REL	Not available
OSHA PEL [2011]	Not available
ACGIH TLV [2014]	Not available
AIHA ERPG [2010]	Not available
AIHA WEEL [2010]	Not available

Abbreviation: ACGIH – American Conference of Governmental Industrial Hygienists; AIHA – American Industrial Hygiene Association; ERPG – Emergency Response Preparedness Guidelines; IDLH – immediately dangerous to life or health; NIOSH – National Institute for Occupational Safety and Health; OSHA – Occupational Safety and Health Administration; PEL – permissible exposure limit; REL – recommended exposure limit; SCP – Standard Completion Program; WEEL – workplace environmental exposure level

Table 3: AEGL Values for Chlorine Pentafluoride

Classification	10-min	30-min	1-hour	4-hour	8-hour	Endpoint [reference]
AEGL-1	0.3 ppm 1.6 mg/m^3	0.3 ppm 1.6 mg/m^3	0.3 ppm 1.6 mg/m^3	NR	NR	No observed irritation - rat [MacEwen and Vernot 1973]
AEGL-2	3.0 ppm 16.0 mg/m^3	2.0 ppm 10.1 mg/m^3	1.0 ppm 5.3 mg/m^3	0.48 ppm 2.6 mg/m^3	0.33 ppm 1.8 mg/m^3	Sensory irritation, mild lung congestion – monkey, dog, rat, and mouse [MacEwen and Vernot 1972; 1973]
AEGL-3	21.0 ppm 112.0 mg/m^3	12.0 ppm 64.0 mg/m^3	8.0 ppm 42.7 mg/m^3	3.9 ppm 20.8 mg/m^3	2.7 ppm 14.4 mg/m^3	Highest 1-hour non-lethal concentration in rats [Darmer et al. 1972]

Abbreviation: AEGL – acute exposure guideline levels; mg/m^3 – milligrams per cubic meter; min – minute; NR – not recommended due to inadequate data; ppm – parts per million
*__References__: NAS [2010a]

1.2 Animal Toxicity Data

Chlorine pentafluoride penetrates the lungs, causing edema and destruction of lung tissue at lethal concentrations leading to pneumonia. It is also a potent irritant of the eyes and respiratory tract at non-lethal concentrations [Darmer et al. 1972; MacEwen and Vernot 1972, 1973]. Darmer et al. [1972] reported signs of moderate irritation (lacrimation, sneezing, and salivation) at the lowest concentrations tested for dogs and monkeys at 30 minutes, 102 ppm for dogs (one death at this level) and 198 ppm for monkeys (no deaths at this level).

MacEwen and Vernot [1972] exposed rats, mice, and monkeys to 10, 20, or 30 ppm for 60, 30, or 10 minutes, respectively. Lacrimation was observed in rats and mice, and rats also experienced salivation in all exposure groups. In monkeys, lacrimation and nausea were observed in all the exposure groups almost immediately after onset of exposure; all exposure groups also experienced transient depression of weight gain when observed for 28 days after exposure. Monkeys exposed to 10 ppm for 60 minutes exhibited congested lungs; however, no gross lung lesions were observed in monkeys exposed to 30 ppm for 10 minutes.

MacEwen and Vernot [1973] followed up with another study exposing mice, monkeys and dogs to 5, 10, or 30 ppm for 60, 30, or 10 minutes, respectively. Immediate salivation, eye irritation, lacrimation, and rhinorrhea were observed in all species with the most severe irritation in the 30 ppm dose group, but no gross lung lesions were seen in any of the exposure groups. These effects were judged not to be of sufficient severity to be escape impairing. In addition, rats were exposed to 3, 7, or 30 ppm for 10 minutes. Slight eye irritation was noted in rats exposed to 7 ppm for 10 minutes, but there was no eye irritation in rats exposed to 3 ppm for 10 minutes [MacEwen and Vernot 1973].

Table 4 summarizes the LC data identified in animal studies and provides 30-minute equivalent derived values for chlorine pentafluoride. Table 5 provides non-lethal data reported in animal studies with 30-minute equivalent derived values. Information in these tables includes species of test animals, toxicological metrics (i.e., LC, NOAEL, LOAEL), adjusted 30-minute concentration, and the justification for the composite uncertainty factors applied to calculate the derived values.

Table 4: Lethal Concentration Data for Chlorine Pentafluoride

Reference	Species	LC_{50} (ppm)	LC_{10} (ppm)	Time (min)	Adjusted 30-min Concentration* (ppm)	Composite Uncertainty Factor	Derived Value (ppm)†
Darmer et al. [1972]	Dog	156	--	30	156	30‡	5.2
Darmer et al. [1972]	Monkey	218	--	30	218	30‡	7.3
Darmer et al. [1972]	Mouse	105	--	30	105	30‡	3.5
Darmer et al. [1972]	Rat	194	--	30	194	30‡	6.5
Weinberg and Goldhamer [1967]	Rat	--	200	10	115	10±	12

Abbreviation: LC – lethal concentration; LC_{10} – concentration estimated to cause a 10% mortality rate; LC_{50} – median lethal concentration; LC_{Lo} – lowest concentration of a chemical that caused death in humans or animals; min – minute; ppm – parts per million

*For exposures other than 30 minutes the ten Berge et al. [1986] relationship is used for adjustment ($C^n \times t = k$); NAS [2010a] empirically estimated a n value of 1.9 that was used for extrapolating from all exposure times.

†The derived value is the result of the adjusted 30-minute LC value divided by the composite uncertainty factor.

‡Composite uncertainty factor to account for adjustment of LC_{50} values to LC_{01} values, use of lethal concentration threshold in animals, interspecies differences and human variability.

±Composite uncertainty factor to account for lethal concentration threshold in animals, interspecies differences and human variability.

Table 5: Non-lethal Concentration Data for Chlorine Pentafluoride

Reference	Species (reference)	NOAEL (ppm)	LOAEL (ppm)	Time (min)	Adjusted 30-min Concentration* (ppm)	Composite Uncertainty Factor	Derived Value (ppm)†
MacEwen and Vernot [1972]	Monkey, Dog, Mouse		10^	30	10	3‡	3.3
MacEwen and Vernot [1972]€	**Monkey, Dog, Mouse, Rat**		**30±**	**10**	**17.3**	**10+**	**1.7**
MacEwen and Vernot [1972]	Rat	3		10	1.7	3‡	00.6
MacEwen and Vernot [1972]	Rat		7**	10	4	3‡	1.3
MacEwen and Vernot [1972]	Rat		20††	30	20	3‡	6.7

Abbreviation: NOAEL – no observed adverse effect level; min – minute; LOAEL – lowest observed adverse effect level; ppm – parts per million

*For exposures other than 30 minutes the ten Berge et al. [1986] relationship is used for adjustment ($C^n \times t = k$); NAS [2010a] empirically estimated a n value of 1.9 that was used for extrapolating from all exposure times.

† The derived value is the result of the adjusted 30-min value divided by the composite uncertainty factor.

^Concentration associated with immediate salivation, eye irritation, lacrimation, and rhinorrhea in multiple species.

‡ Composite uncertainty factor assigned to account for interspecies differences and human variability.

€Identified study is the primary basis of the IDLH value for chlorine pentafluoride.

±Concentration associated with severe irritation in multiple species.

+ Composite uncertainty factor to account for adjusting from adjustment to an escape-impairing effect, interspecies differences and human variability.

**Concentration associated with slight irritation.

††Concentration associated with immediate salivation, eye irritation, lacrimation, and rhinorrhea.

1.3 Human Data

No human toxicity data were found, with the exception of a single case report. In this report, a researcher who had taken a single breath of 30 ppm chlorine pentafluoride in an exposure chamber while conducting an animal toxicity study [MacEwen and Vernot 1973], reported a mild "burning" of the lungs, mild nausea, an unpleasant taste in the mouth, and headache. The persistence of these symptoms was not reported [MacEwen and Vernot 1973].

1.4 Summary

In the absence of adequate human data, the IDLH value is based on potentially escape-impairing effects including severe respiratory irritation in multiple species [MacEwen and Vernot 1972]. Test animals (i.e., monkey, dog, mouse, and rat) exposed to chlorine pentafluoride at concentrations ranging from 10 to 30 ppm for durations up to 30 minutes experienced immediate salivation, eye irritation, lacrimation, rhinorrhea and respiratory irritation. More specifically, exposures to 30 ppm chlorine pentafluoride for 10 ppm was associated with severe respiratory irritation, which is considered escape-impairing. Duration adjusting yielded a 30-minute equivalent value of 17.3 ppm. Application of a composite uncertainty factor to account for adjusting from an escape-impairing effect, interspecies differences and human variability results in an IDLH value of **1.7 ppm** for chlorine pentafluoride.

2.0 Bromine Pentafluoride

2.1 Introduction

2.1.1 Overview of the IDLH Value for Bromine Pentafluoride

IDLH value: **3.5 ppm**

Basis for IDLH Value:

Data were inadequate to directly derive an IDLH value for bromine pentafluoride. For this reason, data from studies with chlorine pentafluoride were used to develop an IDLH value for bromine pentafluoride because their structures, reaction mechanisms, and potencies are similar. Therefore, deriving an IDLH value based on the toxicity data for chlorine pentafluoride is appropriately health-protective.

The IDLH value for bromine pentafluoride is based on the 10-minute mouse LOAEL associated with severe escape-impairing effects including respiratory irritation reported in multiple species exposed to 30 ppm chlorine pentafluoride [MacEwen and Vernot 1972]. Duration adjustment yielded a 30-minute equivalent of 17.3 ppm. Application of a composite uncertainty factor of 10 to account for extrapolation from an escape-impairing effect, interspecies differences and human variability results an IDLH value for bromine pentafluoride of **1.7 ppm**.

2.1.2 Purpose

This *IDLH Profile* presents (1) a brief summary of technical data associated with acute inhalation exposures to bromine pentafluoride and (2) the rationale behind the Immediately Dangerous to Life or Health (IDLH) value for bromine pentafluoride. IDLH values are developed based on the scientific rationale and logic outlined in the NIOSH Current Intelligence Bulletin (CIB) 66: Derivation of Immediately Dangerous to Life or Health (IDLH) values [NIOSH 2013]. As described in CIB 66, NIOSH performs in-depth literature searches to ensure that all relevant data from human and animal studies with acute exposures to the substance are identified. Information included in CIB 66 on the literature search includes pertinent databases, key terms, and guides for evaluating data quality and relevance for the establishment of an IDLH value. The information that is identified in the in-depth literature search is evaluated with general considerations that include description of studies (i.e., species, study protocol, exposure concentration and duration), health endpoint evaluated, and critical effect levels (e.g., NOAELs, LOAELs, LC_{50} values). For bromine pentafluoride, the in-depth literature search was conducted through February 2014.

2.1.3 General Substance Information

Chemical: Bromine pentafluoride (BrF_5)

CAS No: 7789-30-2

Synonyms: Bromine fluoride*

Chemical category: Inorganic fluoride compounds; inorganic bromine compounds†

Structural formula:

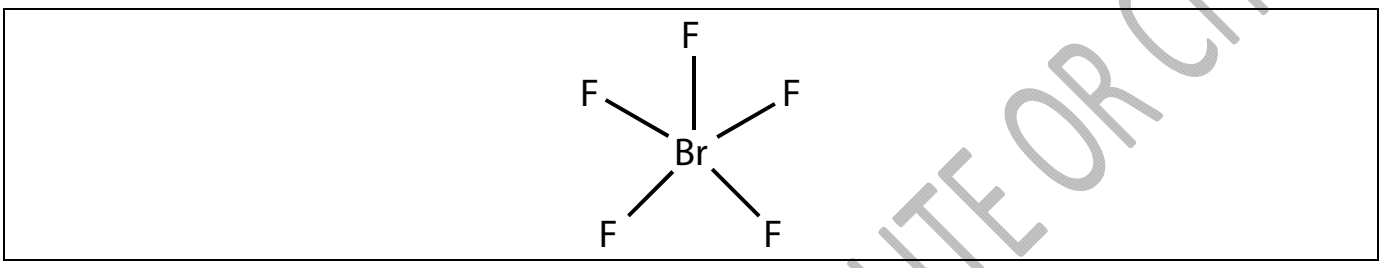

Table 5 highlights selected physiochemical properties of bromine pentafluoride relevant to IDLH conditions. Table 6 provides alternative exposure guidelines for bromine pentafluoride. Table 7 summarizes the Acute Exposure Guidelines Level (AEGL) values for bromine pentafluoride.

Table 5: Physiochemical Properties of Bromine Pentafluoride

Property	Value
Molecular weight	174.89‡
Chemical formula	BrF_5
Description	Colorless to pale yellow liquid
Odor	Pungent
Odor Threshold	Not available
UEL	Not available§
LEL	Not available§
Vapor pressure	328 mmHg at 20°C§
Flash point	Noncombustible‡
Ignition temperature	Noncombustible‡
Solubility	Decomposes in water†

Abbreviation: °C – Celsius; °F – Fahrenheit; mmHg – millimeter mercury; LEL – lower explosive limit; UEL – upper explosive limit
* NLM [2014]; † IFA [2014]; ‡ HSDB [2014];

Table 6: Alternative Exposure Guidelines for Bromine Pentafluoride

Organization	Value
Original (SCP) IDLH value	None
NIOSH REL	0.1 ppm (0.7 mg/m^3), TWA
OSHA PEL [2014]	0.1 ppm, TWA 8-hour
ACGIH TLV [2014]	0.1 ppm, TWA
AIHA ERPG [2010]	Not available
AIHA WEEL [2010]	Not available

Abbreviation: ACGIH – American Conference of Governmental Industrial Hygienists; AIHA – American Industrial Hygiene Association; ERPG – Emergency Response Preparedness Guidelines; IDLH – immediately dangerous to life or health; NIOSH – National Institute for Occupational Safety and Health; OSHA – Occupational Safety and Health Administration; PEL – permissible exposure limit; REL – recommended exposure limit; SCP – Standards Completion Program; TWA – time-weighted average; WEEL – workplace environment exposure level

Table 7: AEGL Values for Bromine Pentafluoride*

Classification	10-min	30-min	1-hour	4-hour	8-hour	Endpoint [reference]
AEGL-1	NR	NR	NR	NR	NR	No data
AEGL-2	3.0 ppm 21.5 mg/m^3	2.0 ppm 14.3 mg/m^3	1.0 ppm 7.2 mg/m^3	0.48 ppm 3.4 mg/m^3	0.33 ppm 2.4 mg/m^3	Based on analogy with chlorine pentafluoride
AEGL-3	79.0 ppm 565.1 mg/m^3	55.0 ppm 393.4 mg/m^3	33.0 ppm 236.0 mg/m^3	8.3 ppm 59.4 mg/m^3	4.2 ppm 30.0 mg/m^3	Highest non-lethal concentration in the rat [Dost et al. 1970]

Abbreviation: AEGL – acute exposure guideline levels; mg/m^3 – milligrams per cubic meter; min – minute; NR – not recommended due to insufficient data; ppm – parts per million
References: NAS [2010b]
*Values based on analogy with chlorine pentafluoride

2.2 Animal Toxicity Data

Bromine pentafluoride is corrosive to eyes, mucous membranes, respiratory tract and exposed skin. No deaths were reported in rats exposed to bromine pentafluoride at 500 ppm for 40 minutes, or to 1000 ppm for 20 minutes [Dost et al. 1968]. The impact of exposure scenario on toxicity appears to be large, at least in this exposure duration, since slightly longer durations resulted in very high lethality. Exposure to 500 ppm for 60 minutes resulted in 95% mortality, and 12/12 rats died after exposure to 1000 ppm for 25 minutes [Dost et al. 1968]. Because of the apparently large impact of exposure duration, with large implications of small differences in measurements or between studies, it would be useful to have additional supporting studies on bromine pentafluoride. In the absence of additional studies, these data were considered insufficient for derivation of an IDLH value.

The toxicity of halogen fluorides appears to be consistent with their relative reactivity. The mechanism of toxicity is the same as that of the other halogen causing localized irritation and tissue damage at the site of contact [AEGL 2010b]. In studies with rats, one found no lethality after exposure to 500 ppm bromine pentafluoride for 30 minutes [Dost et al. 1970], while Darmer et al. [1972] reported a 30-minute LC_{50} value of 194 ppm for chlorine pentafluoride. This suggests that bromine pentafluoride is less toxic than chlorine pentafluoride. Dost et al. [1970] also found similar signs of toxicity for chlorine trifluroide and bromine pentafluoride. There was however, a greater severity of respiratory tract damage following bromine pentafluoride exposure, but this may have been due to the somewhat higher concentrations tested for this chemical (e.g., 500 ppm vs. 400 ppm). Based on these considerations and the limited empirical data for bromine pentafluoride, this assessment uses chlorine pentafluoride as a surrogate.

LC_{50} data and information on nonlethal effects of chlorine pentafluoride are available in multiple species, with the results showing respiratory and ocular irritation, leading to edema and tissue destruction at lethal levels [Darmer et al. 1972; MacEwen and Vernot 1972, 1973]. In monkeys, dogs, rats and mice, sensory irritation and reversible mild lung congestion were observed following chlorine pentafluoride exposures to 30 ppm for 10 minutes, 20 ppm for 30 minutes or 10 ppm for 60 minutes [MacEwen and Vernot 1972, 1973]. Table 4 summarizes the LC data, while Table 5 summarizes non-lethal data, presented in animal studies and provides 30-minute equivalent derived values for chlorine pentafluoride.

2.3 Human Data

No human toxicity data were located.

2.4 Summary

Inadequate toxicity data were available for bromine pentafluoride. The data on chlorine pentafluoride are used to derive an IDLH value for bromine pentafluoride because their structures, reaction mechanisms, and potencies are similar. Therefore, deriving an IDLH value based on the toxicity data for chlorine pentafluoride is appropriately health-protective. In the absence of adequate human data, the IDLH value is based on potentially escape-impairing effects including severe respiratory irritation in multiple species [MacEwen and Vernot 1972]. Test animals (i.e., monkey, dog, mouse, and rat) exposed to chlorine pentafluoride at concentrations ranging from 10 to 30 ppm for durations up to 30 minutes experienced immediate salivation, eye irritation, lacrimation, rhinorrhea and respiratory irritation. More specifically, exposures to 30 ppm chlorine pentafluoride for 10 ppm was associated with severe respiratory irritation, which is considered escape-impairing. Duration adjusting yielded a 30-minute equivalent value of 17.3 ppm. Application of a composite uncertainty factor to account for adjusting from an escape-impairing effect, interspecies differences and human variability results in an IDLH value of **1.7 ppm** for chlorine pentafluoride.

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