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Determination of toxicity of a gas or gas mixture

Détermination de la toxicité d'un gaz ou d'un mélange de gaz

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Foreword

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The main task of technical committees is to prepare International Standards. Draft International Standards adopted by the technical committees are circulated to the member bodies for voting. Publication as an International Standard requires approval by at least 75 % of the member bodies casting a vote.

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ISO 10298 was prepared by Technical Committee ISO/TC 58, *Gas cylinders*, Subcommittee SC 2, *Cylinder fittings*.

This second edition cancels and replaces the first edition (ISO 10298:1995), which has been technically revised.

Introduction

ISO 5145 "*Cylinder valve outlets for gases and gas mixtures — Selection and dimensioning*" and similar standards establish practical criteria for the determination of outlet connections of cylinder valves. These criteria are based on certain physical and chemical properties of the gases, in particular, the acute toxicity of the gases.

One of the difficulties in the application of ISO 5145 resides in the fact that, in the case of single components, there are abundant data in the literature (although differences may be found, depending upon the test methods employed), but in the case of gas mixtures, data in the literature are often incomplete or even non-existent.

The aim of this International Standard is to eliminate the ambiguities in the case of differences in the literature, to supplement existing data and to give a calculation method for gas mixtures.

Since the publication of the first edition of ISO 10298, this International Standard has been used for other purposes than the selection of cylinder valve outlets, e.g. providing toxicity data for the classification of gas and gas mixtures according to the international transport regulations and dangerous substances regulations, which since 2003 is under the umbrella of the Globally Harmonized System (GHS).

Determination of toxicity of a gas or gas mixture

1 Scope

This International Standard lists the best available acute-toxicity data of gases from the literature to allow the classification of gases and gas mixtures.

2 Terms and definitions

For the purposes of this document, the following terms and definitions apply.

2.1
lethal concentration 50
LC_{50}
concentration of a gas (or a gas mixture) in air administered by a single exposure during a short period of time (24 h or less) to a group of young adult albino rats (males and females) which leads to the death of half of the animals in at least 14 days

2.2
toxicity level
level of toxicity of gases and gas mixtures

NOTE 1 In ISO 5145, the toxicity level is divided into three groups:

— Subdivision 1: non toxic [LC_{50} > 5 000 ppm (volume fraction)]

— Subdivision 2: toxic [200 ppm (volume fraction) < $LC_{50} \leqslant$ 5 000 ppm (volume fraction)]

— Subdivision 3: very toxic [$LC_{50} \leqslant$ 200 ppm (volume fraction)]

where

LC_{50} values	correspond to 1 h exposure to gas;
ppm (volume fraction)	indicates parts per million, by volume.

NOTE 2 In the GHS, the inhalation toxicity levels are:

Category 1: Fatal if inhaled	0 ppm < $LC_{50} \leqslant$ 100 ppm (volume fraction)
Category 2: Fatal if inhaled	100 ppm (volume fraction) < $LC_{50} \leqslant$ 500 ppm (volume fraction)
Category 3: Toxic if inhaled	500 ppm (volume fraction) < $LC_{50} \leqslant$ 2 500 ppm (volume fraction)
Category 4: Harmful if inhaled	2 500 ppm (volume fraction) < $LC_{50} \leqslant$ 20 000 ppm (volume fraction)

NOTE 3 In GHS, the LC_{50} values correspond to 4 h exposure. Consequently, the LC_{50} values given in Annex A (see 3.2.2) need to be divided by 2 (i.e. $\sqrt{4/1}$). The reasoning behind the division by 2 is given in Clause B.2.

3 Determination of toxicity

3.1 General

Toxicity may be determined through a test method (3.2) for gas mixtures where the data for the components exist, or through a calculation method (3.3).

For reasons of animal welfare, inhalation toxicity tests geared only for the classification of gas mixtures should be avoided if the toxicity of each of the components is available. In this case, toxicity is determined in accordance with 3.3.

3.2 Test method

3.2.1 Test procedure

When new toxicity data is being considered for inclusion in this International Standard, an internationally recognized test method such as OECD TG 403[43] should be used.

3.2.2 Results for pure gases

The toxicity of pure gases is listed in Annex A, in which LC_{50} values correspond to 1 h exposure. Some of these values have been estimated in accordance with Annex B.

3.3 Calculation method

The LC_{50} value of a gas mixture is calculated using the following equation:

$$LC_{50} = \frac{1}{\sum_i \frac{C_i}{LC_{50}}}$$

where

C_i is the mole fraction of the ith toxic component present in the gas mixture;

LC_{50i} is the lethal concentration of the ith toxic component [$LC_{50} < 5\,000$ ppm (by volume)].

After the LC_{50} of the gas mixture has been calculated, this mixture is classified in accordance with 2.2.

NOTE Synergistic effects[1)] have not been considered in the above, due to a lack of scientific data.

1) For example, LEVIN, B.C. *et al*. Toxicological interactions between carbon monoxide and carbon dioxide. *Toxicol.*, **47**, 1987, pp. 135-164.

Annex A
(informative)

LC_{50} values for toxic gases and toxic vapours used in gas mixtures

Table A.1 lists for each gas the LC_{50} values and the literature references.

Table A.2 lists for each vapour the LC_{50} values and the literature references.

Table A.3 specifies the criteria for oxidizing gases.

Table A.1— List of toxic gases with their LC_{50} values and literature sources

Gases Common name	**CAS[a] No.**	**UN No.**	LC_{50}[b]/1 h ppm **(volume fraction)**	**Remarks**	**Literature reference** (see the Bibliography)
Ammonia	7664-41-7	1005	7 338		[1]
Arsine	7784-42-1	2188	178		[62]
Arsenic pentafluoride	7784-36-3	3308	178	By analogy with arsine	
Boron trichloride	10294-34-5	1741	2 541		[1]
Boron trifluoride	7637-07-2	1008	864		[44]
Bromine chloride	13863-41-7	2901	290	Estimated from chlorine	
Carbon monoxide	630-08-0	1016	3 760	Time-adjusted	[6]
Carbonyl fluoride	353-50-4	2417	360		[5]
Carbonyl sulfide	463-58-1	2204	1 700	Time-adjusted	[7]
Chlorine	7782-50-5	1017	293		[1]
Chlorine pentafluoride	13637-63-3	2548	122		[8]
Chlorine trifluoride	7790-91-2	1749	299		[8]
Chlorotrifluoroethylene	79-38-9	1082	2 000	Time-adjusted	[10]
Chloromethane	74-87-3	1063	5 133		[54]
Cyanogen	460-19-5	1026	350		[11]
Cyclopropane	75-19-4	1027	220 000	“Non toxic” – LC_{LO}[c] – Mouse – Time-adjusted	
Cyanogen chloride	506-77-4	1589	80	Time-adjusted	[12]
Deuterium chloride	7698-05-7	1789	3 120		
Deuterium selenide	13536-95-3	2202	51	Same as hydrogen selenide	
Deuterium sulfide	13536-94-2	1053	710	Similar to hydrogen sulfide	
Diborane	19287-45-7	1911	80	Time-adjusted	[13]
Dichlorosilane	4109-96-0	2189	314		[52]
Dimethylamine	124-40-3	1032	5 290	Time-adjusted	[67]
Dinitrogen trioxide	10544-73-7	2421	57	Calculated from decomposition into NO_2	
Ethylene oxide	75-21-8	1040	2 900	Time-adjusted	[18]
Fluorine	7782-41-4	1045	185		[19]
Germane	7782-65-2	2192	620		[55]
Hexafluoroacetone	684-16-2	2420	470	Time-adjusted	[56]
Hydrogen bromide	10035-10-6	1048	2 860		[51]
Hydrogen chloride	7647-01-0	1050	2 810		[45]

Table A.1 (*continued*)

Gases Common name	**CAS[a] No.**	**UN No.**	LC_{50}[b]/1 h ppm **(volume fraction)**	**Remarks**	**Literature reference** (see the Bibliography)
Hydrogen iodide	10034-85-2	2197	2 860	By analogy with hydrogen bromide	
Hydrogen selenide	07783-07-5	2 202	51		[57]
Hydrogen sulfide	07783-06-4	1053	712		[1]
Hydrogen telluride	07783-09-7	3160	51	By analogy with hydrogen selenide	
Methyl bromide	74-83-9	1062	850	Time-adjusted	[23]
Methyl mercaptan	74-93-1	1064	1 350	Time-adjusted	[24]
Methyl vinyl ether (inhibited)	107-25-5	1087	>40 000	Unverified source at 64 000 ppm	
Monoethylamine	75-04-7	1036	16 000	Time-adjusted	[25]
Monomethylamine	74-89-5	1061	7 110		[46]
Mustard gas			4	LC_{LO} – Human – Time-adjusted	[17]
Nitrogen monoxide	10102-43-9	1070	115	Same as nitrogen dioxide	
Nitrogen dioxide	10102-44-0	1067	115		[28]
Nitrogen trifluoride	7783-54-2	2451	6 700		[48]
Nitrosyl chloride	2696-92-6	1069	35	Time-adjusted – LC_{LO} – cat	[29]
Oxygen difluoride	7783-41-7	2190	2,6		[8]
Ozone	10028-15-6		9	Time-adjusted	[30]
Phosgene	75-44-5	1076	5	Time-adjusted	[32]
Phosphine	7803-51-2	2199	20	Time-adjusted	[64]
Phosphorus pentafluoride	07647-19-0	2198	261	Derived from decomposition to HF	—
Phosphorus trifluoride	7783-55-3	3308	436	Derived from decomposition to HF	—
Selenium hexafluoride	7783-79-1	2194	50	Time-adjusted	[39]
Silane	7803-62-5	2203	19 000	Time-adjusted	[1]
Silicon tetrafluoride	7783-61-1	1859	922		[5]
Stibine	7803-52-3	2676	178	By analogy with arsine	—
Sulfur dioxide	7446-09-5	1079	2 520		[35]
Sulfur tetrafluoride	7783-60-0	2418	40		[36]
Sulfuryl fluoride	2699-79-8	2191	3 020		[1]
Tellurium hexafluoride	7783-80-4	2195	25	Time-adjusted	[39]
Tetrafluoroethylene	116-14-3	1081	2 000		
Trifluoroacetyl chloride	354-32-5	3057	10	Similar to trichloroacetyl chloride	
Trifluoroethylene	359-11-5	1954	2 000	Time-adjusted - Taken from chlorotrifluoroethylene	
Trimethylamine	75-50-3	1083	7 000	LC_{LO} – Time-adjusted	[66]
Tungsten hexafluoride	7783-82-6	2196	218	Derived from decomposition to HF	
Vinyl bromide (inhibited)	593-60-2	1085	> 40 000		
Vinyl chloride (inhibited)	75-01-4	1086	150 000		[47]
Vinyl fluoride (inhibited)	75-02-5	1860	> 40 000		

[a] CAS = Chemical Abstract System.

[b] See 3.2.2.

[c] LC_{LO} = lethal concentration low value.

Table A.2 — List of toxic liquefiable vapours with their LC_{50} values and literature sources

Vapours Common name	**CAS[a] No.**	**UN No.**	LC_{50}[b]/1 h ppm **(volume fraction)**	**Remarks**	**Literature reference** (see the Bibliography)
Antimony pentafluoride	7783-70-2	1732	30	Mouse	[2]
Arsenic trifluoride	7784-35-2	1556	178	By analogy with arsine	
Bis(trifluoromethyl) peroxide	927-84-4		10	Assumed (conservative)	
Boron tribromide	10294-33-4	2692	950	Derived from HBr with BF_3	
Bromine chloride	13863-41-7	2901	290	Estimated from chlorine	
Bromine pentafluoride	7789-30-2	1745	25	Time- and effect-adjusted	[4]
Bromine trifluoride	7787-71-5	1746	180	Estimated from F_2	
Bromoacetone	598-31-2	1569	260	By analogy with chloroacetone	
Deuterium fluoride	14333-26-7		1 100		
Dibromodifluoro-methane	1868-53-7	1941	27 000	LC_{LO} – Time-adjusted	
Dichloro(2-chlorovinyl) arsine			8	Extrapolated from intravenous injection	[14]
Diethylamine	109-89-7	1154	8 000	Time adjusted	[67]
Diethylzinc	557-20-0	1366	non-toxic	Assumed (conservative)	[15]
Diphosgene	503-38-8	1076	2	Derived from phosgene (conservative)	
Ethyldichloroarsine	598-14-1	1892	7	LC_{LO} – Human – Time-adjusted	[17]
Heptafluorobutyronitrile	375-00-8		10	Assumed (conservative)	
Hydrogen cyanide	74-90-8	1613	144	Time-adjusted	[59]
Hydrogen fluoride	7664-39-3	1052	1 307	Median value of 5 studies	[61]
Iodine pentafluoride	7783-66-6	2495	120	Similar to ClF_5	
Methylchlorosilane	993-00-0	2534	2 810	Adjusted for HCl equivalent	[53]
Methyldichloroarsine	593-89-5	1556	7	By analogy with ethyldichloroarsine	
Methyldichlorosilane	75-54-7	1242	1 785		[49]
Nickel carbonyl	13463-39-3	1259	20	Time-adjusted	[27]
Pentaborane	19624-22-7	1380	10	Time-adjusted	[31]
Pentafluorobutyronitrile	None listed		10		
Pentafluoropropionitrile	422-04-8		10	Assumed (conservative)	
Perchloryl fluoride	7616-94-6		770	Time-adjusted	[12]
Perfluorobut-2-ene	360-89-4		12 000	"Non toxic" – LC_{LO} – Time-adjusted	[2]
Phenylcarbylamine chloride	622-44-6	1672	5	By analogy with phosgene	—
Propylene oxide	75-56-9	1951	7 140	Time-adjusted	[60]
Silicon tetrachloride	10026-04-7	1818	1 312		[49]