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Paraquat

DESIGNATIONS

CAS No.: 1910-42-5; 4685-14-7 (Paraquat dichloride)
Registry names: Paraquat
Chemical name: 1,1'-Dimethyl-(4,4'-bipyridinium) cation
Synonyms, Trade names: 1,1'-Dimethyl-(4,4'-bipyridinium) [dichloride], N,N'-dimethyl-4,4'-bipyridinium chloride, methylviologen, Gramoxone, Gramoxon, Terraklene, Weedol, Dextrone X and many others
Chemical name (German): Paraquat [Dichlorid];1,1'-Dimethyl-(4,4'-bipyridinium) [Dichlorid]
Chemical names (French): [Dichlorure de] paraquat, [dichlorure de] 1,1'-dimthyl-(4,4'-dipyridinium)
Appearance: pure paraquat salt is a white, crystalline, odourless powder; the technical product has a yellowish appearance.

BASIC CHEMICAL AND PHYSICAL DATA

Note:	All data refer to the dichloride.
Empirical formula:	$C_{12}H_{14}N_2$ [$C_{12}H_{14}Cl_2N_2$]
Rel. molecular mass:	257.2 g

Density:	1.25 g/cm^3 at 20C
Relative gas density:	8.88
Boiling point:	decomposition
Melting point:	above 300C decomposition
Vapour pressure:	very low (<10^{-3} Pa at 20C; also 10^{-5} Pa at 20C cited)
Ignition temperature:	(may be marketed in flammable mixtures)
Solvolysis/solubility:	in water 700 g/l at 20C; soluble in alcohol; insoluble in organic solvents
Conversion factors:	1 ppm = 10.7 mg/m^3
	1 mg/m^3 = 0.094 ppm

ORIGIN AND USE

Usage:

Paraquat is a non-selective contact herbicide used in particular in the cultivation of fruit and vines to combat weeds directly before cultivating useful plants. The sulphate or chloride is normally used. There is a ban in Germany on substances which have only paraquat as active substance for treating plants.

Origin/derivation:

Paraquat is produced synthetically. There are no known natural sources. Paraquat is part of the bipyridinium derivative group. Two technical products are manufactured: 1,1'-dimethyl-4,4'-bipyridinium dichloride and 1,1'-dimethyl-4,4'-bipyridinium dimethyl sulphate. The product is synthesised from pyridine, by treatment with sodium in liquid ammonia, followed by oxidation to form 4,4'-bipyridine, and subsequent methylation.

Production figures:

Paraquat is produced in a number of countries (e.g. People's Republic of China, Taiwan, Italy, Great Britain, USA). It is applied in more than 130 countries (normally as paraquat dichloride, in the (former) USSR as paraquat dimethyl phosphate). Production figures are not available (WHO, 1984).

Toxicity

Humans:	DTA 0.008 mg/kg	acc. DFG, 1985
Mammals:		
Mouse:	LD_{50} 100-120 mg/kg, oral	acc. DVGW, 1988
Mouse:	LD_{50} 62 mg/kg, dermal	acc. WHO, 1984
Rat:	LD_{50} 100-150 mg/kg, oral	acc. DVGW, 1988
Rat:	LD_{50} 80-90 mg/kg, dermal	acc. DVGW, 1988
Rat:	LC_{50} 1-10 mg/m^3, inhalation	acc. WHO, 1984

Dog:	LD_{50} 25-50 mg/kg, oral	acc. DVGW, 1988
Cat:	LD_{50} 30-50 mg/kg, oral	acc. DVGW, 1988
Rabbit:	LD_{50} 120-130 mg/kg, oral	acc. DVGW, 1988
Rabbit:	LD_{50} 236-500 mg/kg, dermal	acc. WHO, 1984
Guinea pig:	LD_{50} 20-40 mg/kg, oral	acc. DVGW, 1988
Guinea pig:	LD_{50} 319 mg/kg, dermal	acc. WHO, 1984
Guinea pig:	LC_{50} 4 mg/m^3, inhalation	acc. WHO, 1984
Monkey:	LD_{50} 50 mg/kg, oral	acc. WHO, 1984
Aquatic organisms:		
Guppy:	LC_{50} 21.8-46.4 mg/l (96h)	acc. DVGW, 1988
Sun perch:	LC_{50} 100 mg/l (48h)	acc. DVGW, 1988
Sun perch:	LC_{50} 12 mg/l (96h)	acc. DVGW, 1988
Trout:	LC_{50} 4.5-32 mg/l (96h)	acc. DVGW, 1988

Trout:	LC_{50} 4.5-32 mg/l (96h)	acc. DVGW, 1988
Crawfish:	LC_{50} 11 mg/l (96h)	acc. DVGW, 1988

Characteristic effects:

Humans/mammals: **Paraquat is toxic for humans and damages the kidneys, liver and lungs. In aqueous form the herbicide has a caustic effect on the skin, mucous membranes and conjunctiva; it is absorbed through the skin. There is also good absorption of paraquat via the lungs where the substance is stored. However, resorption is usually minimal (5% of the amount absorbed) (DVGW, 1988). Metabolisation in the body is likewise very limited; most of the substance is excreted without undergoing change.**

Animal experiments have not revealed any increase in the tumour rate due to paraquat. Genetic toxicity and teratogenic effects have been substantiated with certain species of animal.

Plants: **Paraquat is absorbed by plant leaves only from the aqueous solutions of its salts. Absorption takes place more readily and more effectively in the dark than in daylight. It is transported with the perspiration flow in the xylem. Phytotoxicity is only encountered in daylight and with sufficient oxygen content. There is a sustained**

ENVIRONMENTAL BEHAVIOUR

Water:

Paraquat is adsorbed on suspended matter and on sediment in water or absorbed by plants. The herbicide finds its way into the water either following direct usage or by erosion from neighbouring areas. If paraquat is not subject to sorption, it is rapidly degraded by microorganisms and thus no longer effective. Because of this, there is only a low risk of groundwater pollution.

Air:

Small quantities of paraquat are released into the air as a function of the type of application (as spray or mixed with liquid). The crucial factor is, however, whether paraquat is inhaled during application or resorbed through the skin. Passage through the skin represents the principal way of assimilation. The half-life in air is reported between a period of several hours up to 64 days.

Soil:

Paraquat is subject to considerable sorption in clay soils. In topsoils with a high content of organic matter, it is more or less immobile and then it may not be absorbed by plants. Depending on the type of soil, paraquat remains in the uppermost soil horizon. Because of the high sorption rate, there is no elution by seepage water and no metabolisation by microorganisms.

Half-life:

When used in water, paraquat could not be detected after 1-4 days; residues were still found in sludge after more than 400 days. The half-life in sandy clays is about 7 years.

Degradation, decomposition products:

Photochemical degradation results in less toxic decomposition products. Biological degradation in the soil leads to rapid decline of the amount applied, but also to a reduction in the population density of the microorganisms.

Food chain:

No accumulation by way of food chains.

ENVIRONMENTAL STANDARDS

Medium/acceptor	Sector	Country/organ.	Status	Value	Cat.	Remarks	Source
Water:	Drinkw	D	L	0.1 g/l			acc. DVGW, 1988
	Drinkw	EC	L	0.1 g/l			acc. DVGW, 1988

	Surface	EC	L	0.001 mg/l		1)	acc. DVGW, 1988
	Surface	EC	L	0.0025 mg/l		2)	acc. DVGW, 1988
	Surface	EC	L	0.005 mg/l		3)	acc. DVGW, 1988
Air:	Workp	BG	(L)	0.01 mg/m^3			acc. WHO, 1984
	Workp	D	L	0.1 mg/m^3	MAK		acc. DFG, 1994
	Workp	H	(L)	0.02 mg/m^3			acc. WHO, 1984
	Workp	USA	(L)	0.1 mg/m^3	TWA		ACGIH, 1986

Notes:
The use of paraquat in the cultivation of cereals is banned in the Federal Republic of Germany (Order Governing Use of Pesticides, as at 1988).

1) Limit value for physical treatment and sterilisation of drinking water

2) Limit value for physical and chemical treatment/sterilisation of drinking water

3) Limit value for physical and refined chemical treatment of drinking water

Assessment/comments

Paraquat is a strong contact herbicide; inhalation and skin contact should be avoided when using it. Use of the substance is not recommended because of the high toxicity for humans and animals. This recommendation is further strengthened by the high persistence in soil.

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Parathion

DESIGNATIONS

CAS No.: **56-38-2**
Registry name: **Parathion**
Chemical name: **O,O-Diethyl-O-4-nitrophenyl-thiophosphate**
Synonyms, Trade names: **Parathion-ethyl, O,O-Diethyl-O-4-nitrophenyl-phosphorothioate, E 605, Eftol, Folidol**
Chemical name (German): **Parathion, Ethyl-Parathion**
Chemical name (French): **Parathion**
Appearance: **yellowish to dark brown liquid with garlic odour**

BASIC CHEMICAL AND PHYSICAL DATA

Empirical formula:	$C_{10}H_{14}NO_5PS$
Rel. molecular mass:	291.27 g
Density:	1.265 g/cm^3

Boiling point:	375C (above 160C, parathion isomerises slowly to form O,S-Diethyl-O-4-nitrophenyl-thiophosphate which is less stable and less effective)
Melting point:	6.1C
Vapour pressure:	5 x 10^{-3} Pa
Flash point:	> 120C
Ignition temperature:	(may be marketed in flammable mixtures)
Solvolysis/solubility:	in water: 24 mg/l at 25C soluble in most organic solvents: in dichloromethane, 2-propanol, toluene > 200 g/l; in n-hexane 50-100 g/l; very slightly soluble in kerosene and mineral oil
Conversion factors:	1 mg/m^3 = 0.083 ppm 1 ppm = 12.106 mg/m^3

ORIGIN AND USE

Usage:

Parathion is a broad-spectrum insecticide which acts as a contact, feed or respiratory poison. It is widely used against biting and sucking insects in agriculture, fruit-, vegetable- and winegrowing as well as against mites, beetles and caterpillars. It is usually applied as a spray (emulsion: 500 g/l; oil: 10%).

Origin/derivation:

Emissions are mainly caused by the production and the use of parathion.

Toxicity

Humans:	LD_{50} 3-5 mg/kg, oral (estimated)	acc. PERKOW, 1992
	LD 5-15 mg/kg (pure subst.), oral	acc. UBA, 1986
Mammals:		
Rat	LD_{50} 3.6-13 mg/kg, oral	acc. PERKOW, 1992
	LD_{50} 6.8-21 mg/kg, dermal	acc. PERKOW, 1992
	LC_{50} 0.05 mg/l (4h), inhalation	acc. PERKOW, 1992
	NOEL 10 mg/kg feed (2a)	acc. PERKOW, 1992
	TDLo 0.36 mg/kg (2.-22. day of pregnance), oral	acc. UBA, 1986
Mouse	LD_{50} 12.8-25 mg/kg, oral	acc. PERKOW, 1992
Guinea pig	LD_{50} 16-32 mg/kg, oral	acc. PERKOW, 1992
Insects:		

Bees	LD$_{50}$ 0.11 mg/bee, contact	acc. PERKOW, 1992
	LD$_{50}$ 0.28 mg/bee, oral	acc. PERKOW, 1992
Aquatic organisms:		
Rainbow trout	LC$_{50}$ 1.43 mg/l (96 h)	acc. PERKOW, 1992
Perch	LC$_{50}$ 0.4 mg/l (96 h)	acc. PERKOW, 1992
Goldfish	LC$_{50}$ 1.83 mg/l (96 h)	acc. PERKOW, 1992
Golden orfe	LC$_{50}$ 0.57 mg/l (96 h)	acc. PERKOW, 1992
	LC$_{0}$ 0.26 mg/l, (96h)	acc. HOMMEL, 1993
	LC$_{50}$ 0.48 mg/l, (96h)	acc. HOMMEL, 1993
	LC$_{100}$ 1.2 mg/l, (96h)	acc. HOMMEL, 1993

Characteristic effects:

***Humans/mammals:* Human poisoning can result from oral intake, inhalation or dermal exposure. Parathion is readily adsorbed and distributed in the organism. It irreversibly inhibits the acetylcholinesterase enzyme and thus disrupts the normal functioning of the central nervous system. Typical symptoms of acute poisoning are headache, sweating and faintness followed by impaired vision, gastrointestinal disorders, shortness of breath, tremors,**

convulsions, unconsciousness, pulmonary paralysis and finally cardiac arrest. These symptoms may also appear after a delay of several hours [UBA, 1986].

Plants: **Tolerance is generally good. Some strains of apples, cucumbers and tomatoes are sensitive to overfeeding.**

ENVIRONMENTAL BEHAVIOUR

Water:

The half life in aqueous solutions is strongly dependent on the pH. At low pH, hydrolysis is very slow but in a neutral and especially in an alkaline environment, it takes place much faster. In addition, the hydrolysis rate rises with increasing temperature [KOCH, 1989].

pH	temperature	half-life
1-5	0C	3000 d
	20C	690 d
	30C	180 d
8	20C	99 d

In experiments carried out in a sealed glass jar (initial concentration: 10 mg/l) in sunlight and under artificial fluorescent light, residues of 50% have been detected after 1 week. After 4 weeks, residues of less then 5% have been detected and after 8 weeks no residues could be detected [VERSCHUEREN, 1983].

Soil:

The data on the persistence of parathion in soil are varying: the persistence of organophosphorus insecticides is generally low. The half-life of parathion is about 3-6 months [ULLMANN, 1989].

After 3 weeks, residues of 5% and after 15 weeks residues of 3.2% have been detected in sandy-loamy soil. In organic soil, residues of 5% have been found after 10 weeks. Residues are detectable up to 16 years following the application [PERKOW, 1992; VERSCHUEREN, 1983].

Degradation, decomposition products:

In the organism of mammals, parathion is oxidised forming the more toxic paraoxone, and hydrolysed forming nitrophenol and diethyl phosphate. It is excreted relatively fast mainly via urine (86-93%) [PERKOW, 1992].

ENVIRONMENTAL STANDARDS

Medium/ acceptor	Sector	Country/organ.	Status	Value	Cat.	Remarks	Source
Water:	Drinkw	D	L	0.1 mg/l		single substance	acc. KOCH, 1989
	Drinkw	D	L	0.5 mg/l		sum of pesticides	acc. KOCH, 1989
	Drinkw	SU	L	0.3 mg/l			acc. KOCH, 1989
	Surface	EC	G	1 mg/l	1)	physical treatment	acc. LAU-BW, 1989
	Surface	EC	G	2.5 mg/l	1)	physical / chemical treatment	acc. LAU-BW, 1989

	Surface	EC	G	5 mg/l	1)	physical / intensified chemical treatment	acc. LAU-BW, 1989
Air:	Workp	D	L	0.1 mg/m^3	MAK	Skin	acc. AUER TECHNIKUM, 1988
	Workp	D	L	500 mg/l	BAT	2)	acc. AUER TECHNIKUM, 1988
	Workp	SU	(L)	0.05 mg/m^3	PDK	Skin	acc. AUER TECHNIKUM, 1988
	Workp	USA	(L)	0.1 mg/m^3	TWA	Skin	acc. AUER TECHNIKUM, 1988
	Workp	USA	(L)	0.3 mg/m^3	STEL	Skin	acc. UBA, 1986

1)Quality requirements for the preparation of drinking water from surface water.
2) parameter: p-nitrophenol plus acetylcholinesterase in blood

Assessment/comments

Parathion is only moderately persistent in the environment and does not accumulate in the pedosphere or in the biosphere. On the other hand, it lacks sensitivity and is highly toxic to bees, beneficial parasites, fish, mammals and humans.

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Phenol

DESIGNATIONS

CAS No.: 108-95-2
Registry name: Phenol
Chemical name: Phenol
Synonyms, Trade names: Carbolic acid, hydroxybenzene, monohydroxybenzene, oxybenzene, phenic acid, phenyl hydrate, phenyl hydroxide, phenyl acid
Chemical name (German): Phenol, Karbolsure, Hydroxybenzol
Chemical names (French): Phnol, acide carbolique, acide phnique, benznol, phnol ordinaire
Appearance: colourless/whitish red substance or colourless melt; sweetish odour

BASIC CHEMICAL AND PHYSICAL DATA

Empirical formula:	C_6H_6O
Rel. molecular mass:	94.11 g
Density:	1.07 g/cm^3 at 20C

Relative gas density:	3.24
Boiling point:	181.75C
Melting point:	40.8C
Vapour pressure:	0.2 hPa at 20C; 3.5 hPa at 50C; 54 hPa at 100 C
Flash point:	82C
Ignition temperature:	595C
Explosion limit:	1.3 - 9.5 Vol%
Odour threshold:	0.18 mg/m^3 = 0.046 ppm
Solvolysis/solubility:	in water: 82 g/l
	readily soluble in alcohol, ether, chloroform, fats and ethereal oils
Conversion factors:	1 ppm = 3.91 mg/m^3
	1 mg/m^3 = 0.26 ppm

ORIGIN AND USE

Usage:

Phenol is used to make synthetic resins, dyes, pharmaceuticals, pesticides, synthetic tanning agents, perfumes, lubricating oils and solvents.

Origin/derivation:

In the phenols group, cresols and the parent compound itself are the most important compounds as well as thymol, naphthols, phenolphthalein, trichlorophenol and pentachlorophenol. Natural compounds such as pyrocatechol, guaiacol and their derivatives are not toxic. A well-known pyrocatechol derivative is adrenaline. Phenol naturally occurs in pine wood and pine needles, in the urine of herbivores (phenol sulphate) and in coal tar. Monohydric phenols provide numerous natural scents (e.g. vanillin, thymol, carvacrol, zingiverone (in ginger), salicylaldehyde). Amongst the synthetic multivalent phenols hexachlorophene is particularly toxic.

Phenol is obtained from the distillation of coal tar (according to RMPP, (1983) 1 t of coal gives approx.0.25 kg of phenol). Synthetic production has however become predominant and involves the decomposition of cumene hydroperoxide with acetone forming as by-product. Some use is still made of the preparation from benzene using benzene sulphonic acid or chlorobenzene.

Emissions are produced by the incomplete combustion of gasoline and coal tar, in the waste water from coking plants and as metabolites in the photolysis of benzene and chlorobenzene.

Production figures:

Annual production (worldwide):	3 million t/a	(RIPPEN, 1989)
Annual production (D):	250,000 t/a	(RIPPEN, 1989)
Annual production (USA, 1988):	1,600,000 t/a	(RIPPEN, 1989)

Toxicity

Humans:	1 g can be fatal	acc. RIPPEN, 1989
Mammals:		
Rat:	LD_{50} 414-530 mg/kg, oral	acc. RIPPEN, 1989
Rat:	LD_{50} 670 mg/kg, dermal	acc. RIPPEN, 1989
Rabbit:	LD_{50} 400-600 mg/kg, oral	acc. RIPPEN, 1989
Rabbit:	LD_{50} 850 mg/kg, dermal	acc. RIPPEN, 1989
Cat:	LD_{50} 100 mg/kg, oral	acc. RIPPEN, 1989
Dog:	LD_{50} 500 mg/kg, oral	acc. RIPPEN, 1989
Aquatic organisms:		
Pimephales promelas:	LC_{50} 24-68 mg/l	acc. RIPPEN, 1989
Leuciscus idus melanotus:	LC_{50} 25 mg/l (48h)	acc. RIPPEN, 1989
Lepomis macrochirus:	LC_{50} 24 mg/l (96h)	acc. RIPPEN, 1989

Daphnia:	LC_{50} 12 mg/l (48h)	acc. RIPPEN, 1989
Scenedesmus quadricauda:	EC_0 7.5-40 mg/l	acc. RIPPEN, 1989
Microcystis aeruginosa:	EC_0 4.6 mg/l	acc. RIPPEN, 1989

Toxicity data for various phenol compounds can be found in DFG, 1982, volume II: phenols.

Characteristic effects:

***Humans/mammals:* Vapours and liquids are toxic and easily absorbed through the skin. Once inhaled, vapours corrode the respiratory tract and the lungs. Severe burns result from the liquid coming into contact with skin and eyes (phenol is a powerful protoplasmic poison). Long-term exposure paralyzes the central nervous system and damages the kidneys and the lungs. Paralysis may cause death. Accompanying symptoms are headaches, tinnitus, dizziness, stomach and intestinal irritations, drowsiness, collapse, poisoning, loss of consciousness, irregular breathing, apnoea, heart failure and in some cases spasms. HORN (1989) classes phenol as having a teratogenic and carcinogenic effect. According to the Ames-test, phenol has no mutagenic potential.**

Damage caused by oral intake is usually prevented by the alarming odour and taste (Refer also to "cresol" and "chlorophenol" information sheets)

***Plants:* Passive permeability impaired; growth inhibited.**

ENVIRONMENTAL BEHAVIOUR

Water:
Phenol is heavier than water and sinks to the bottom. It dissolves slowly and continues to form toxic solutions even when diluted. Because of its considerable toxicity in water, phenol is listed in water hazard class 2 in

Germany.

Air:
Vapours are heavier than air and form explosive mixtures when exposed to heat. The oxidation of phenol in air is accelerated by light or impurities with a catalytic effect.

Soil:
There is only limited accumulation because of the microbial degradation in the soil (aerobic or anaerobic). The accumulation level depends on the presence of clay minerals (great affinity with aluminium oxide).

Degradation, decomposition products:
The biological degradability of natural phenols is generally very good with the result that there is scarcely any accumulation in plants or animals. Aerobic bacterial degradation involves complete breakdown to carbon dioxide. Condensation to humic acids may be found in soil. The degradability of synthetic phenols is less pronounced as many phenols are toxic to microorganisms. Toxicity increases with the number of chlorine or nitrogen atoms in the phenols. "Pentachlorophenol" is thus the most toxic compound of the chlorophenol group and trinitrophenol (picric acid) is the most poisonous compound within the nitrophenol group.

There is roughly 90% degradation in surface water in approx. 7 days (standing water); the same rate is achieved in soil in roughly 1 day depending on microflora and concentration (RIPPEN, 1989); complete degradation in earthy suspensions takes more than two days.

Phenol metabolites can also be extremely toxic: Incomplete combustion of 2,4,5-trichlorophenol may cause the formation of TCDD (dioxin). Biodegradation generally produces acetic acid and CO_2 by way of pyrocatechol, o-quinone and dicarboxylic acids (RIPPEN, 1982).

Phenol is excreted from the organism with the urine after oxidation or conjugation with sulphuric or gluconic acid.

Food chain:

There is only little accumulation in foodstuffs. Smokers are at risk since cigarette smoke contains phenols. The presence of phenol in groundwater causes polluted drinking water which may not be used because of its evil taste.

ENVIRONMENTAL STANDARDS

Medium/acceptor	Sector	Country/organ.	Status	Value	Cat.	Remarks	Source
Water:	Drinkw	EC	(L)	0.0005 g/m^3		Maximum concentration	acc. LAU-BW, 1989
	Drinkw	USA		0.001 mg/l		In State of Illinois	acc. WAITE, 1984
	Drinkw	USA		0.02 mg/l		In State of Iowa	acc. WAITE, 1984
	Surface	D	G	0.005 g/m^3		4)	acc. LAU-BW, 1989
	Surface	D	G	0.01 g/m^3		5)	acc. LAU-BW, 1989
	Groundw	NL	G	0.2 μ g/l		Reference	acc. TERRA TECH, 6/94
	Groundw	NL	L	2000 μ g/l		Intervention	acc. TERRA TECH, 6/94
	Waste	CH	(L)	0.005		6)	acc. LAU-BW,

	water			g/m^3			1989
	Waste water	CH	(L)	0.05-0.20 g/m^3		7)	acc. LAU-BW, 1989
	Waste water	D	G	100 g/m^3		Guideline8)	acc. LAU-BW, 1989
Soil:		GB	G	0-0.1 mg/kg		Not contaminated	acc. LAU-BW, 1989
		GB	G	5-50 mg/kg		Contaminated soil	acc. LAU-BW, 1989
		GB	G	> 250 mg/kg		Heavily contaminated	acc. LAU-BW, 1989
		NL	G	0.05 mg/kg		Reference	acc. TERRA TECH, 6/94
		NL	L	40 mg/kg		Intervention	acc. TERRA TECH, 6/94
Air:	Emiss.	D	L	20 mg/m^3		mass flow > 0.1 kg/h	acc. TA Luft, 1986
		BG	(L)	0.01 mg/m^3		30 min, 24 h8) 9)	acc. STERN, 1986
		CS				30 min, 24 h	acc. STERN, 1986
			(L)	0.1 mg/m^3			

	D	L	0.2 mg/m^3	MIK	Long-time value	acc. BAUM, 1988
	D	L	0.6 mg/m^3	MIK	Short-time value	acc. BAUM, 1988
	DDR	(L)	0.01 mg/m^3		Short-time value	acc. HORN, 1989
	DDR	(L)	0.003 mg/m^3		Long-time value	acc. HORN, 1989
	H	(L)	0.01 mg/m^3		30 min, 24 h8) 9)	acc. STERN, 1986
	H	(L)	0.6 mg/m^3		30 min10)	acc. STERN, 1986
	IL	(L)	0.02 mg/m^3		20 min	acc. STERN, 1986
	IL	(L)	0.01 mg/m^3		24 h	acc. STERN, 1986
	RO	(L)	0.1 mg/m^3		30 min	acc. STERN, 1986
	RO	(L)	0.03 mg/m^3		24 h	acc. STERN, 1986
	SU	(L)	0.01 mg/m^3		30 min, 24 h8) 9)	acc. STERN, 1986

		TJ	(L)	0.02 mg/m^3		60 min	acc. STERN, 1986
	Workp	D	L	19 mg/m^3	MAK		DFG, 1989
	Workp	DDR	L	20 mg/m^3			acc. HORN, 1989
	Workp	SU	(L)	0.3 mg/m^3	PDK		acc. SORBE, 1989
	Workp	USA	(L)	19 mg/m^3	TWA		ACGIH, 1986
	Workp	USA	(L)	38 mg/m^3	STEL		ACGIH, 1986

Notes:

1) Assessment value for soil and groundwater contamination, A value = no impact

2) Assessment value for soil and groundwater contamination, B value = further investigations necessary

3) Assessment value for soil and groundwater contamination, C value = rehabilitation needed

4) Impact limit up to which drinking water can be produced solely by natural methods

5) Impact limit up to which drinking water can be produced using currently tried and tested chemical/physical methods

6) "Swiss quality goal" used as basis for assessing surface water and drinking water supply

7) Limit value for introduction of sewage into flowing water

8) Guideline for requirements to be satisfied by sewage introduced into public sewage systems in Baden-Wrttemberg

9) Areas in need of protection

10) Areas in need of special protection

11) 0ther areas not in need of special protection

Comparison/reference values

Medium/origin	**Country**	**Value**	**Source**
Water:			
Sewage treatment plant (inflow/discharge)	D, USA	2-20 ppb	acc. RIPPEN, 1989
River water	USA	10-100 ppb	acc. RIPPEN, 1989
Surface water (1977)	J	< 10 ppb (n=9)	acc. RIPPEN, 1989
Danube (1972)	D	0.01-1 ppb	acc. RIPPEN, 1989
Drinking water	D	6-20 ppt	acc. RIPPEN, 1989
Soil/sediment:			
Sediment (1977)	J	30-40 ppb (n=3)	acc. RIPPEN, 1989
Air:			
Outdoor concentration	DDR	12 g/m^3	acc. HORN, 1989
City (1979)	J	0.5-1.0 ppb	acc. RIPPEN, 1989

City (1973)	USA	15-91 ppt	acc. RIPPEN, 1989
Paris (1977), (n=7)	F	0.17-2.1 ppb (2h values)	acc. RIPPEN, 1989
Motor vehicle emissions		1.3-1.5 ppm	acc. RIPPEN, 1989
Tobacco smoke		300-500 ppm	acc. RIPPEN, 1989
Humans:			
Excretion, urine:		0.02-6.6 mg/kg/d	acc. RIPPEN, 1989

Assessment/comments

There is urgent need for reduced emissions since synthetic phenols are more toxic than natural phenols. The risk of skin contact and inhalation when handling phenol needs particular attention.

(Refer also to "chlorophenols" and "cresols" information sheets).

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Polychlorinated biphenyls

DESIGNATIONS

CAS No.: **1336-36-3**
Registry name: **Polychlorinated biphenyls**
Chemical name: **Polychlorinated biphenyls**
Synonyms, Trade names: **PCB, Apirolio, Aroclor, Ascarele, Clophen, Delor, Fenclor, Inerteen, Kanechlor, Phenoclor, Pyralene, Pyranol, Pyroclor, Sovtol and many others**
Chemical name (German): **Polychlorierte Biphenyle**
Chemical name (French): **Polychlorure de biphnyle**
Appearance: **The pure mono- and dichlorobiphenyls are colourless crystalline compounds; PCBs with more than 3 chlorine atoms are colourless liquids with moderate to high viscosity. All industrial mixtures are liquids.**

Note: **The group of polychlorinated biphenyls consists of 209 isomeric and homologous compounds.**

BASIC CHEMICAL AND PHYSICAL DATA

Empirical formula:	$C_{12}H_{10-n}Cl_n$ n=1-10, mainly n=2-7
Rel. molecular mass:	189-499 g
Density:	1.2-1.6 g/cm^3
Boiling point:	320-420C
Vapour pressure:	0.2-133 x 10^{-3} Pa

Solvolysis/solubility:	only slightly soluble in water soluble in most organic solvents and in fat
Note:	Polychlorinated biphenyls have a low vapour pressure, high viscosity, minimal water solubility, high dielectric constant, high thermal stability and resistance to chemicals.

Note:
Polychlorinated biphenyls have a low vapour pressure, high viscosity, minimal water solubility, high dielectric constant, high thermal stability and resistance to chemicals.

ORIGIN AND USE

Usage:
PCBs are used as coolants and insulating materials, transformer oils and hydraulic fluids, as plasticisers for synthetics and as impregnation agents for wood and paper. They possess almost ideal properties for electrical purposes and are likewise highly resistant to ageing.

In the European Community, the use of PCBs has been restricted to *closed systems* by regulation in 1976. In the USA the production of PCBs has been prohibited since 1977, in Germany since 1983.

Origin/derivation:
The chlorination of biphenyls with iron and iron chloride acting as catalysts produces an isomeric mixture which is subsequently distilled.

Production figures:

D (1980):	7,400 t	(BMI, 1985)
D (since 1983):	no production	(BMI, 1985)
France (1980)	6,500 t	(LORENZ & NEUMEIER, 1983)
Spain (1980):	1,250 t	(LORENZ & NEUMEIER, 1983)

Toxicity

Mammals:		
General:	TDLo 325 mg/kg	acc. UBA, 1986
Aquatic organisms:		
Rainbow trout:	LC_{50} 2 mg/l (96 h)	acc. UBA, 1986
Micropterus salmoides:	LC_{50} 2.3 mg/l (96 h)	acc. UBA, 1986
American minnow:	LC_{50} 7.7-300 mg/l (96 h)	acc. UBA, 1986
Catfish:	LC_{50} 8.7-139 mg/l (30 d)	acc. UBA, 1986
Blue perch:	LC_{50} 84-400 mg/l (30 d)	acc. UBA, 1986
Gammarus spec.:	LC_{50}/EC_{50} 10-73 mg/l	acc. UBA, 1986

Green algae:	0.1-300 mg/l inhibited growth	acc. UBA, 1986

Characteristic effects:

Humans/mammals: **The toxicological effects of PCBs on humans still have to be fully established. The Chemicals Law in the Federal Republic of Germany classes PCBs as being of low toxicity despite their proven carcinogenic and teratogenic effects in animal experiments (supposed to be carcinogenic for humans). As a general rule, the toxicity level increases with the chlorine content; the same effect is produced by the oxidation products of PCB which may be far more toxic than PCB itself. The risk of poisoning due to inhalation is normally slight on account of the low vapour pressure. On the other hand, skin contact and oral intake can have serious consequences. The main points of attack are the liver and the enzyme system. The usual symptoms of chronic poisoning are nausea, vomiting, weight loss, oedemas and pains in the lower abdomen; if the liver is seriously damaged, coma or even death may result.**

Plants: **PCB reduces the cell division rate and the CO_2 fixing of algae. There is overall inhibition of growth. Population shifts are encountered with concentrations greater than 0.1 μ g/l (phytoplankton and invertebrates) [LORENZ & NEUMEIER, 1983].**

ENVIRONMENTAL BEHAVIOUR

Water:
PCBs ingress into surface water from various sources and by precipitation from the atmosphere.

Air:
PCBs are released into the atmosphere by evaporation, favoured by higher temperatures. They condense on aerosol particles and are thus widely spread. The evaporation rate for soil - as a function of soil texture - is greater than for water.

Soil:

Accumulation in humus layer with little mobility; following sorption, mobility by way of vapour phase. There is very little degradation; the persistence increases with the degree of chlorination.

Degradation, decomposition products:

Degradation due to hydrolysis is not to be expected since PCBs are stable even in the presence of strong alkalis and acids. Oxidative degradation involves considerable energy. Biotic degradation by microorganisms only occurs under aerobic conditions. Adsorption and/or transition to anaerobic areas totally inhibits degradation in soil. Mineralisation is possible under strong UV radiation.

Metabolites are hydroxy compounds, metafission products and chlorobenzenes. The degradation process ends in CO_2 and HCl.

Food chain:

Some 25% of the PCBs assimilated by humans are taken in by inhalation and 75% through foodstuffs (UBA, 1986). Animal products are the main source, with fish supplying between 4 and 5% of the amount absorbed. The intake with drinking water is minimal.

PCB is stored in fatty tissue, milk and the liver.

ENVIRONMENTAL STANDARDS

Medium/acceptor	**Sector**	**Country/organ.**	**Status**	**Value**	**Cat.**	**Remarks**	**Source**
Water	Surface	D	(G)	0.014 mg/l		Freshwater	acc. UBA, 1986
Air:	Refer to information sheets 164-166 as regards environmental standards for air						

Foodstuffs:		CDN	G	0.2-1.0 pg/(kgd)	ADI		acc. CRINE, 1988
		NL	G	4 pg/(kgd)	ADI		acc. CRINE, 1988
		USA	G	0.06 pg/(kgd)	ADI	EPA	acc. CRINE, 1988

The production of polychlorinated biphenyls has been banned in the USA since 1979; the use of concentrations > 500 mg/kg for transformers and electromagnets has been banned since 1985 (LORENZ & NEUMEIER, 1983).

Comparison/reference values

Medium/origin	**Value**	**Source**
Air	5-30 ng/m^3	acc. BMI, 1985
Air	0.1-20 ng/m^3	acc. PEARSON, 1982
Water:		
Rain/snow	0.1-200 ng/l	acc. PEARSON, 1982
Seawater	0.25-100 ng/l	acc. PEARSON, 1982
Surface water	0.1-3000 ng/l	acc. PEARSON, 1982
Soil/sediment	1-1000 mg/kg	acc. PEARSON, 1982
Soil	0.05-0.1 mg/kg	acc. BMI, 1985

Sludge	1-100 mg/kg	acc. PEARSON, 1982
Plankton	0.01-2 mg/kg	acc. PEARSON, 1982
Fish	0.01-25 mg/kg	acc. PEARSON, 1982
Birds	0.1-1000 mg/kg	acc. PEARSON, 1982
Aquatic mammals/amphibious creatures	0.1-1000 mg/kg	acc. PEARSON, 1982
Human beings (fatty tissue)	0.1-10 mg/kg	acc. PEARSON, 1982

Assessment/comments

PCBs are characterised by a high persistence and widespread use. Disposal is particularly problematic. Thermal decomposition in waste incineration plants at insufficient temperatures can cause considerable amounts of polychlorinated dibenzo-p-dioxins to escape into the environment. In addition, the question whether PCBs can be completely decomposed at high temperature remains to be fully clarified. Therefore, the use of PCBs must be restricted or limited to utilisation in *closed systems*. Sufficient substitute materials are already available.

Special sources: **HUTZINGER, SAFE & ZITKO (1974); CRINE (1988).**

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Polycyclic aromatic hydrocarbons

DESIGNATIONS

CAS No.:
Registry name: Polycyclic aromatic hydrocarbons
Chemical name: Polycyclic aromatic hydrocarbons
Synonyms, Trade names: PAH
Chemical name (German): Polyzyklische aromatische Kohlenwasserstoffe, PAK
Chemical name (French): Hydrocarbures aromatiques polycycliques, HAP
Appearance:

Note: Collective name for aromatic compounds with condensed cyclic systems. As benzo[a]pyrene is the most investigated PAH and representative of the effects caused by compounds of this group, environmental impacts caused by PAHs are often expressed in terms of equivalents of benzo[a]pyrene.

CAS No.: 50-32-8
Chemical name: Benzo[a]pyrene
Synonyms, Trade names: Benzo[def]chrysene; 1,2-Benzpyrene; 3,4-Benzpyrene; BaP; BAP
Chemical name (German): Benzo[a]pyren
Chemical name (French): Benzo[a]pyrne
Appearance: yellowish crystals

BASIC CHEMICAL AND PHYSICAL DATA

Empirical formula:	$C_{20}H_{12}$
Rel. molecular mass:	252.3

Density:	1.282 g/cm^3 (chips); 1.351 g/cm^3 (needles)
Melting point:	178C
Vapour pressure:	0.7 x 10^{-6} Pa at 20-25C
Solvolysis/solubility:	in water: 4.5 x 10^{-6} g/l at 15-30C

ORIGIN AND USE

Origin/usage:

PAHs are natural components of organic raw materials and in particular crude oils; produced by pyrolysis of organic substances.

Some examples of benzo[a]pyrene content:

Coal tar	0.65%
Road tar	0.51-1%
Pitches	1.25% (max. value)
Impregnating oils	0.045-0.35%
Engine oil (fresh)	0.008-0.27 mg/kg

Engine oil (used)	5.2-35 mg/kg
Diesel oil	0.026 mg/l
Fuel	0.09-8.3 mg/kg
Crude oil (Kuwait)	2.8 mg/kg
Crude oil (Libya)	1.32 mg/l
Crude oil (Venezuela)	1.66 mg/l
Crude oil (Persian Gulf)	0.40 mg/l

Production figures:

Only a few compounds from this group such as anthracene ((ρ) dyes), carbazole ((ρ) dyes, insecticides) and pyrene ((ρ) dyes) are extracted commercially. There is no commercial use of benzo[a]pyrene, except as analytical standard.

Emissions:

Emissions of benzo[a]pyrene due to combustion of fossil fuels:

Coal-fired heating	100 μ g/m^3
Coking oven	13-35 μ g/m^3

Waste incineration	11 μ g/m^3
Diesel exhausts	5 μ g/m^3
Coal-fired power station	0.3 μ g/m^3
Gas-fired power station	0.1 μ g/m^3
Motor vehicle emissions	1-48 μ g/l burned fuel

Emission contribution of different sources to the total emission (D 1981, estimated):

Brown-coal briquets	37%
Coke production	31%
Hard-coal briquets	14%
Car traffic	13%
Gas and gas flame coal	5%
Oil heating	0.1%
Anthracite	0.1%

Note:

Data from various sources; all quoted from RIPPEN, 1989.

Toxicity

Insects:	
Cricket (Acheta domesticus)	LC_{50} >15 mg/g, oral
Aquatic organisms:	
Saltwater fish (Leuresthes tenius)	EC_0 0.024 mg/l (14 d, hatching rate, embryonic development, growth)
Rainbow trout	EC_0 <50 mg/kg food (18 months, formation of tumour)
Chaetopodae	LC_{50} >1 mg/l (96 h)
Water flea (Daphnia pulex)	LC_{50} 0.005 mg/l (96 h)
Other organisms:	
Earthworm	LC_{50} >1mg/cm^2 (48 h)
Plants:	

Various cultivated plants	13 mg/l in nutrient medium (suspension cultures, no effect on growth)
Wheat germ plants	2.5 mg/l (initial solution, plants waste away)

***Note:* Data refer to benzo[a]pyrene. There are only few data available on toxic effects of single PAHs.**
All data as per RIPPEN, 1989

Characteristic effects:

***Humans/mammals:* A number of PAHs turned out to be carcinogenic in animal experiments, some even have mutagenic effects. The carcinogenic effect of benzo[a]pyrene has been clearly substantiated.**

ENVIRONMENTAL BEHAVIOUR

Water:
In brackish water and seawater 71 - 75 % adsorption after 3 h on particles, in particular phytoplankton and bacteria. Rapid reaction with chlorine and ozone. Photochemical transformation in water.

Degradation, decomposition products, half-life:
The data on the degradation of benzo[a]pyrene in surface water vary significantly thus not allowing any general statement. As to the microbial transformation of benzo[a]pyrene in sediment, durations of 8 weeks at higher concentrations and of more than two years at moderate to low concentrations may be found. In addition, half-lives of up to 10 years are quoted for the degradation of benzo[a]pyrene in sediment. The values for the degradation in soil likewise differ significantly between 2 days and 2 years depending on e.g. the type of soil, the microorganism species present in the soil and the degree of contamination. As a general rule, small concentrations are transformed more slowly than high concentrations [acc. RIPPEN, 1989 / KOCH, 1989].

Most important metabolites: 3-hydroxybenzo[a]pyrene and 9-hydroxybenzo[a]pyrene.

ENVIRONMENTAL STANDARDS

Medium/acceptor	Sector	Country/organ.	Status	Value	Cat.	Remarks	Source
Water:	Drinkw	A	(L)	0.2 g/l		BaP + 5 other substances	acc. RIPPEN, 1989
	Drinkw	D	L	0.2 g/l		BaP + 5 other substances	acc. RIPPEN, 1989
	Drinkw	EC	G	0.2 g/l		BaP + 5 other substances	acc. RIPPEN, 1989
	Drinkw	SU	(L)	0.005 g/l			acc. RIPPEN, 1989
	Drinkw	WHO	G	0.2 g/l		BaP + 5 other substances	acc. RIPPEN, 1989
	Groundw	D(HH)	G	0.2 g/l		Closer investigation	acc. LAU-BW, 1989
	Groundw	D(HH)	G	1 g/l		Rehabilitation investigation	acc. LAU-BW, 1989
	Groundw	NL	G	0.1 g/l		Reference, Naphthalene	acc. TERRA TECH 6/94
			L	70 g/l		Intervention,	acc. TERRA

Groundw	NL				Naphthalene	TECH 6/94
Groundw	NL	G	0.02 g/l		Reference, Anthracene + Phenanthrene	acc. TERRA TECH 6/94
Groundw	NL	L	5 g/l		Intervention, Anthracene + Phenanthrene	acc. TERRA TECH 6/94
Groundw	NL	G	0.005 g/l		Reference, Fluoranthene	acc. TERRA TECH 6/94
Groundw	NL	L	1 g/l		Intervention, Fluoranthene	acc. TERRA TECH 6/94
Groundw	NL	G	0.002 g/l		Reference, Benzo[a]anthracene	acc. TERRA TECH 6/94
Groundw	NL	L	0.5 g/l		Intervention, Benzo[a]anthracene	acc. TERRA TECH 6/94
Groundw	NL	G	0.002 g/l		Reference, Chrysene	acc. TERRA TECH 6/94
Groundw	NL	L	0.05 g/l		Intervention, Chrysene	acc. TERRA TECH 6/94
Groundw	NL	G	0.001 g/l		Reference, BaP	acc. TERRA TECH 6/94
Groundw	NL	L	0.05 g/l		Intervention, BaP	acc. TERRA

							TECH 6/94
	Groundw	NL	G	0.0002 g/l		Reference, Benzo[ghi]perylene	acc. TERRA TECH 6/94
	Groundw	NL	L	0.05 g/l		Intervention, Benzo[ghi]perylene	acc. TERRA TECH 6/94
	Groundw	NL	G	0.001 g/l		Reference, Benzo[k]fluoranthene	acc. TERRA TECH 6/94
	Groundw	NL	L	0.05 g/l		Intervention, Benzo[k]fluoranthene	acc. TERRA TECH 6/94
	Groundw	NL	G	0.0004 g/l		Reference, Indeno[1,2,3-cd]pyrene	acc. TERRA TECH 6/94
	Groundw	NL	L	0.05 g/l		Intervention, Indeno[1,2,3-cd]pyrene	acc. TERRA TECH 6/94
Soil:		NL	G	1 mg/kg DM		Reference, PAHs	acc. TERRA TECH 6/94
		NL	L	40 mg/kg DM		Intervention, PAHs	acc. TERRA TECH 6/94
Air:	**Emiss.**	**D**	**L**	**0.1 mg/m^3**		**mass flow > 0.5 g/h**	**acc. TA Luft, 1986**

Note:

1) Baden-Wrttemberg Regional Environment Office

Comparison/reference values

Medium/origin	**Country**	**Value**
Water:		
Rhine (Karlsruhe, Cologne, Leibheim)	D	<1-13 ng/l (aqueous phase)
Rhine (locations see above 1977-79)	D	<1-82 ng/l (suspensions)
Wupper (mouth, 1984)	D	690 ng/l (max. value)
Lake Constance (Sipplingen, 1977-79)	D	<1-3 ng/l (aqueous phase)
Lake Constance (Sipplingen, 1977-79)	D	<1-4 ng/l (suspensions)
North Sea (various locations, 1980)	D	<0.02-0.56 ng/l (n=8)
Groundwater (non-contaminated)	NL	<5 ng/l (n=8)
Groundwater (contaminated)	NL	1,000 ng/l
Groundwater (contaminated)	USA	13 µg/l (max. value)
Drinking water (Helsinki, 1980)	SF	0.05 ng/l
Drinking water	N	<0.05 ng/l
Drinking water (1984-1986)	D	<50-<120 ng/l (n=598)
Sediment:		

Rhine (km 639, 1982/83)	D	1.25 mg/kg
Wupper	D	2 mg/kg (mean)
Lake Constance	D/CH	1-1,620 mg/kg
North Sea (various locations)		0.15-460 mg/kg (impacted and non-impacted)
Adriatic		0.4-13 mg/kg (n=24)
Soil:		
Forest soil (various locations)	D	1.5-4 mg/kg DM
Various contaminated soils	D	1-32 mg/kg
Soil covering (Solling)	D	110-360 μg/kg
Soils away from industry		15-18 μg/kg (average)
Soils close to industry		200-500 μg/kg DM (average)
Air:		
Urban air (Berlin, smog, 1980-82)	D	8-92 ng/m^3 (n=546)
Slightly polluted areas (1981)	D	1.3-1.4 ng/m^3 (n=208)
Non-polluted areas (1981)	D	<0.11-0.52 ng/m^3 (n=3)
Urban precipitation (1979/80)	D	1.8-3.6 ng/m^3 (annual average)

Urban precipitation (1979/80)	D	0.30-15 ng/m^3 (monthly average)
Rainwater (Los Angeles, 1982)	USA	<2-115 ng/l
Fog (Northern Franconian Forest, 1983)	D	260-880 ng/l (n=3)
Dust (Ruhr area, 1970-75)	D	50-100 ng/l
Workplace (bitumen)	CND	0.04-43 mg/m^3 (roofing, road construction)
Indoor air (smoke-filled)		22 ng/m^3
Aquatic animals:		
Various molluscs	Greenland	18-60 µg/kg
Various molluscs	I	2-540 µg/kg
Sole (non-contaminated, contaminated)	USA	30 and 570 µg/kg DS

Note:
All data refer to benzo[a]pyrene and are taken from RIPPEN, 1989. This work contains a large number of further investigation results including many relating to the benzo[a]pyrene content of plants and foodstuffs.

Assessment/comments

Although benzo[a]pyrene is a carcinogenic atmospheric pollutant, there are scarcely any limit values and environmental standards. In view of the fact that benzo[a]pyrene is incorporated by humans from different sources, it must be ensured that foodstuffs and drinking water are not polluted in any way by this substance.

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Pyridine

DESIGNATIONS

CAS No.: 110-86-1
Registry name: Pyridine
Chemical name: Pyridine
Synonyms, Trade names: Pyridinum, azine, azabenzene
Chemical name (German): Pyridin, Pyridinum
Chemical name (French): Pyridine
Appearance: colourless liquid with nauseating odour

BASIC CHEMICAL AND PHYSICAL DATA

Empirical formula:	C_5H_5N

Rel. molecular mass:	79.10 g
Density:	0.9819 g/cm^3
Relative gas density:	2.73
Boiling point:	115.5C
Melting point:	-41.8C
Vapour pressure:	20.5 hPa at 20C
Flash point:	17C
Ignition temperature:	550C
Explosion limits:	1.7-10.6 vol% (56-350 g/m^3)
Odour threshold:	0.02 ppm (in air)
Solvolysis/solubility:	unlimited in water, readily soluble in alcohols, ethers, oils and benzene
Conversion factors:	1 mg/m^3 = 0.304 ppm
	1 ppm = 3.288 mg/m^3

ORIGIN AND USE

Usage:
Technical pyridine is mixed with picolines and other substances. It is used as denaturant for ethanol, as a solvent in laboratories as well as for organic salts and chemicals in industry. Pyridine is a constituent in the synthesis of a large number of medical drugs, alkaloids, dyes, disinfectants, herbicides and insecticides.

Origin/derivation:
Pyridine is contained in bone, coal and low-temperature tar, in various types of pyrogenic oil, in oils obtained from bituminous slate and in coffee oil. Technical pyridine is obtained from coal tar by washing with diluted sulphuric acid; subsequent separation involves alkalis.

Production figures:
Worldwide 1989 = 26,000 t/a (ULLMANN, 1993)

Toxicity

Humans:	LD 15 g	
Mammals:		
Mouse	LD_{50} 891 mg/kg	acc. UBA, 1986
Rat	LD_{50} 866 mg/kg	acc. UBA, 1986
Rat	LC_{50} 4,000 ppm, 4 h, inhalation	acc. UBA, 1986

Aquatic organisms:		
Fish	LC 15 mg/l	acc. HOMMEL, 1993
Daphnia	LC_0 70 mg/l	acc. HOMMEL, 1993
Daphnia	LC_{50} 240 mg/l	acc. HOMMEL, 1993
Daphnia	LC_{100} 910 mg/l	acc. HOMMEL, 1993

Characteristic effects:

Humans/mammals: **Pyridine is a nerve toxin and local irritant particularly for the eyes and mucous membranes. Typical symptoms of poisoning are dizziness, headaches, drowsiness, vomiting, reddening of skin and paralysis of nerves in head. Adverse effects in mammals follow long-term exposure: the ammonia metabolism in the brain, the liver and the kidneys is inhibited.**

ENVIRONMENTAL BEHAVIOUR

Water:
Dissolves completely in water and forms toxic mixtures even when considerably diluted. In warm climates, explosive mixtures may form with air above the water's surface. Continuous pyridine immissions may increase the metabolism of the microflora. However, concentrations from 0.5 mg/l are already sufficient to suppress nitrification and ammonification processes. Oxidation processes are noticeably reduced by 5 mg/l. The compound is stable in water since there is no hydrolysis.

Air:

Toxic, combustible liquid which readily evaporates to form flammable vapours which are denser than air.

Soil:

Pyridine is highly mobile. Combined applications of pyridine and phenol enhance the stability of pyridine in soil. Initial inhibition of bacterial growth is followed by adaptation both in soil and in aquatic systems. Concentrations of 750 mg/kg in soil have disappeared after 4 months.

Degradation, decomposition products, half-life;

Following resorption, pyridine is rapidly distributed in the body. Metabolic degradation takes place primarily as a result of methylisation and oxidation involving the pair of free electrons of the nitrogen atom. N-oxymethyl pyridine has been identified as a metabolite. In addition, the substance is quickly excreted: concentrations of 0.4 g/kg body weight are completely excreted within three days.

ENVIRONMENTAL STANDARDS

Medium/acceptor	Sector	Country/organ.	Status	Value	Cat.	Remarks	Source
Water:	Drinkw	SU	G	0.2 mg/l			acc. KOCH, 1989
	Groundw	D(HH)	G	0.01 mg/l		Investigation	acc. LAU-BW, 1989
	Groundw	D(HH)	G	0.03 mg/l		Rehabilitation	acc. LAU-BW, 1989
	Waste water	SU	G	1 mg/l			acc. KOCH, 1989
	Fish breeding	SU	G	0.01 mg/l			acc. KOCH, 1989
				0.1 mg/kg			

Soil:		NL	G	0.1 mg/kg AD		Reference	acc. TERRA TECH, 6/94
		NL	L	1 mg/kg AD		Intervention	acc. TERRA TECH, 6/94
Air:	Emiss.	D	L	20 ml/m^3		mass flow > 0.1 kg/h	acc. TA Luft, 1986
	Workp	D	L	5 ml/m^3	MAK	Peak limit II, 1	DFG, 1989
	Workp	D	L	15 mg/m^3	MAK		DFG, 1989
	Workp	D	L	0.2 ml/m^3	MIK	1) A	acc. BAUM, 1988
	Workp	D	L	0.7 mg/m^3	MIK	1) A	acc. BAUM, 1988
	Workp	D	L	0.6 mg/m^3	MIK	2) B	acc. BAUM, 1988
	Workp	D	L	2.1 mg/m^3	MIK	2) B	acc. BAUM, 1988
	Workp	USA	(L)	15 mg/m^3	TWA		acc. SORBE, 1986
	Workp	USA	(L)	5 ml/m^3	TWA		acc. SORBE, 1986
	Workp	USA	(L)	30 mg/m^3	STEL		acc. SORBE, 1986
	Workp	USA	(L)	10 ml/m^3	STEL		acc. SORBE, 1986
			(L)				

	Workp	SU	(L)	1.5 ml/m^3			acc. SORBE, 1986
	Workp	SU	(L)	5.mg/m^3			acc. SORBE, 1986

Notes:

1) For drinking water treatment in each case: A = impact limits up to which drinking water can be produced solely by way of natural methods

2) For drinking water treatment in each case: B = impact limits up to which drinking water can be produced with the aid of currently tried and tested chemical/physical methods

Assessment/comments

Pyridine is considerably mobile and subject to high dispersion in the hydrosphere, pedosphere and atmosphere due to its water solubility and volatility and the only slight tendency towards bioaccumulation and accumulation in soil. Pyridine must not be dumped. Residues must be burnt in chemical incineration plants. The substance is hazardous to water.

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Sulphur dioxide

DESIGNATIONS

CAS No.: **7446-09-5**
Registry name: **Sulphur dioxide**
Chemical name: **Sulphur dioxide**
Synonyms, Trade names: **Sulphur(IV)oxide, sulphur oxide, sulphurous acid anhydride, sulphurous anhydride**
Chemical name (German): **Schwefeldioxid**
Chemical name (French): **Dioxyde de sulfure**
Appearance: **colourless, non-combustible, pungent gas with odour similar to burning sulphur; vinegar-like odour when diluted**

BASIC CHEMICAL AND PHYSICAL DATA

Empirical formula:	SO_2
Rel. molecular mass:	64.06 g
Density:	1.46 g/cm^3 at -10C (liquid); 2.93 g/l at 20C (gas)
Relative gas density:	2.26
Boiling point:	-10C
Melting point:	-75.5C
Vapour pressure:	331 kPa at 20C, 462 kPa at 30C, 842 kPa at 50C

Odour threshold:	0.3 - 1 ppm (in air)	
Solvolysis/solubility:	in water:	112.7 g/l at 20C (1013 mbar);
		228.3 g/l at 0C (1013 mbar);
	readily soluble in alcohol, benzene, acetone, carbon tetrachloride;	
	fully miscible with ether, carbon disulphide, chloroform, glycol	
Conversion factors:	1 ppm = 0.376 mg/m^3	
	1 mg/m^3 = 2.663 ppm	

ORIGIN AND USE

Usage:

There are many uses of sulphur dioxide. It is used e.g. as a reducing agent in metallurgy, as a coolant in the refrigeration industry, as a disinfectant and bleach, in the preservation of foodstuffs, for dechlorination and as a fumigant. Sulphur dioxide is one of the most important compounds in the chemical industry. 98% of technical SO_2 is used in the production of sulphur trioxide as a precursor of sulphuric acid.

Origin/derivation:

Sulphur dioxide is released naturally into the atmosphere from volcanoes and combustion processes. The anthropogenic impact on the environment primarily results from the combustion of sulphurous fossil fuels (e.g. coal, oil, natural gas) in power and heating plants, in industry, in household use and in traffic. The technical

product is made from elemental sulphur, pyrite, sulphide ores of non-ferrous metals, gypsum, anhydrite and flue gases (ULLMANN, 1994 for processes involved).

Production figures:

- excluded production from elemental sulphur and pyrites in 1,000 t of sulphur (1982):

Worldwide:	5,820
Soviet Union:	1,700
United States:	1,380
Japan:	1,370

- production from pyrites in 1,000 t of sulphur (1975):

Worldwide: 11,000

- production from metal ores and sulphur in 1,000 t of sulphur (1992):

Worldwide: 20,000

(all data from ULLMANN, 1994)

Emission figures (estimated):

Total emissions in Germany in 1986 were calculated at 2.3 x 10^6 tons approximately. Natural emissions in 1982

have been estimated at 750 x 10^6 t worldwide, whereas anthropogenic emissions amounted to about 100 x 10^6 t (RMPP, 1988).

Toxicity

Humans:	25 g/m^3 (annual average)	increased frequency of diseases of lower respiratory tract (acc. UN-ECE, 1984)
	225 g/m^3 (annual average)	increased frequency of respiratory symptoms; reduced pulmonary function in
		5 year olds (acc. UN-ECE, 1984)
	200 g/m^3 (daily max., 30 min)	significant increase in pseudocroup in children (acc. AFRL, 1987)
	200 g/m^3 (24 h values)	increased mortality amongst elderly people (acc. AFRL, 1987)
	1.3 mg/m^3 (40 min)	constriction of the respiratory tract amongst people suffering from asthma (acc. AFRL, 1987)
	53.3 mg/m^3 (10-30 min)	severe, extremely unpleasant irritation symptoms (acc. DFG, 1988)
	133.2 mg/m^3 (60 min)	severe irritation of mucous membranes, pulmonary haemorrhage and oedema,

		laryngospasm with danger of asphyxiation (acc. DFG, 1988)

Mammals:		
Mouse:	LC_{50} 346 mg/m^3 (24 h)	acc. DFG, 1988
Mouse:	LC 1,598 mg/m^3 (5 h)	acc. DFG, 1988
Mouse:	LC 2,130 mg/m^3 (20 min)	acc. DFG, 1988
Rabbit:	LC_{50} 679 mg/m^3 (24 h)	acc. DFG, 1988
Rabbit:	LC (after 7 d) 2130 mg/m^3 (1 h)	acc. DFG, 1988
Hamster:	LC 1,065 mg/m^3 (6 h)	acc. DFG, 1988
Guinea pig:	LC_{50} 1,076 mg/m^3 (24 h)	acc. DFG, 1988
Insects:	LC 2 vol% (6 h)	acc. RMPP, 1988
Flora:		
Various species	>20 g/m^3 (annual average, visible damage)	acc. AFRL, 1987

Fir	30-40 g/m^3 (annual average, damage)	acc. VDI, 1978
Fir	50-70 g/m^3 (annual average, severe damage)	acc. VDI, 1978
Cultivated plants	50 g/m^3 (90 d, damage)	acc. DFG, 1988
Pines (Ruhr area)	>80 g/m^3 (average, vegetation period, initial damage)	acc. VDI, 1978
Various species	2.7-5.5 mg/m^3 (a few hours, acute damage)1)	acc. ULLMANN, 1984

Sensitivity of higher plants (UBA, 1980):

very sensitive:	Bean	Blackcurrant	Sweet pea	Walnut
	Douglas fir	Clover	Spinach	
	Pea	Lupin	Gooseberry	
	Fir	Lucerne	Pine	
sensitive:	Linden	Pine	Oats	Bean
	Copper beech	Weymouth pine	Rye	Rape
	Apple	Larch	Wheat	

	Hazelnut	Barley	Lettuce	
less sensitive:	Maple	Potato	Plane	Tomato
	Beech	Cabbage	Plum family	Juniper
	Yew	Leek	Rhododendron	Willow
	Oak	Arborvitae	Robinia	Vine
	Strawberry	Maize	Turnip	
	Aldo	Carrot	False cypress	
	Lilac	Poplar	Black pine	

***Note:* 1) Leaf necrosis, inhibited photosynthesis**

Characteristic effects:

***Humans/mammals:* Keratitis, breathing difficulties, inflammation of respiratory organs and irritation of eyes due to the formation of sulphurous acid on the moist mucous membranes. Disturbances of consciousness, pulmonary oedema, bronchitis, heart failure and circulatory collapse. Similar effects with sulphur trioxide (SO_3)**

***Plants:* Visible damage to parts of plants above ground level due to direct action: SO_2 enters the leaves via the stomata. It physiologically and biochemically impairs the photosynthesis, the respiration and the transpiration due**

to its detrimental effect on the pore aperture mechanism. Indirect damage is above all due to soil acidification (damage to mycorrhiza) and results in stunted growth.

ENVIRONMENTAL BEHAVIOUR

Water:

Sulphur dioxide ingresses into surface water and groundwater through dry and wet deposition. The aqueous solution reacts as a strong acid. In Germany, SO_2 is classed as hazardous to water as are sulphuric acid and sulphurous acid.

Air:

Sulphur dioxide binds moisture from the air and forms aerosols of sulphuric and sulphurous acid which are deposited as acid rain. The aerosol formation and its dwell time in air depend on the meteorological conditions and on the presence of catalytic impurities in the air. The average dwell time in the atmosphere is approx. 3 - 5 days. Thus, sulphur dioxide may also be transported over long distances.

Soil:

Dry and wet depositions from the atmosphere are the major sources of sulphate accumulation in soil. Dry deposition particles chiefly consist of $(NH_4)_2SO_4$, $(NH_4)_3H(SO_4)_2$, $CaSO_4$, $MgSO_4$ with a small percentage of organic sulphur compounds.

SO_2 and its transformation products are the major sources of soil acidification, particularly if the buffer system of the soil is incapable of neutralising the acid which is either directly deposited or produced by the conversion of solid sulphates. The damage is not substance-specific. Almost all reactions in soil depend on the pH: Both the desorption of numerous substances with adverse effects as well as the leaching of nutrients increase with the acidification of the soil.

Degradation, decomposition products, half-life:

As described above (see *Air*, *Soil*), sulphur dioxide is readily oxidised and very reactive. Sulphuric and sulphurous acid are the most important reaction products relevant to the environment.

Synergisms/antagonisms:
Numerous experiments have been performed in this field generally under standardised conditions. It is however not possible to provide quantitative information relating to natural circumstances on account of the complexity of the factors involved and the courses of action concerned. Nonetheless, it is certain that the effect of SO_2 is more than additively enhanced in combination with other pollutant gases such as NO_x or HF.

ENVIRONMENTAL STANDARDS

Medium/acceptor	Sector	Country/organ.	Status	Value	Cat.	Remarks	Source
Air:		CDN	(L)	0.06 mg/m^3			acc. DORNIER, 1984
		CDN	(L)	0.06 mg/m^3		annual-average	acc. DORNIER, 1984
		CDN	(L)	0.3 mg/m^3		24 h	acc. DORNIER, 1984
		CDN	(L)	0.9 mg/m^3		1 h	acc. DORNIER, 1984
		CH	(L)	0.03 mg/m^3		annual-average	acc. WEIDNER, 1986
							acc. DORNIER,

	CH	(L)	0.4 mg/m^3		24 h	1984
	CH	(L)	0.26 mg/m^3		1 month	acc. DORNIER, 1984
	CH	(L)	0.7 mg/m^3		2 h	acc. DORNIER, 1984
	CS	(L)	0.15 mg/m^3		24 h	acc. DORNIER, 1984
	CS	(L)	0.5 mg/m^3		30 min	acc. CES, 1985
	D	L	0.14 mg/m^3	IW1	1 y arith. mean	acc. TA Luft, 1986
	D	L	0.40 mg/m^3	IW2	1 y 4)	acc. TA Luft, 1986
	D	L	1 mg/m^3	MIK	30 min	acc. BAUM, 1988
	D	L	0.3 mg/m^3	MIK	24 h	acc. BAUM, 1988
	D	L	0.1 mg/m^3	MIK	1 y	acc. BAUM, 1988
	D	G	0.05-0.06 mg/m^3	Precautions for low pollution		UBA, 1989

				areas		
	DDR	(L)	0.15 mg/m^3		24 h	acc. DORNIER, 1984
	DDR	(L)	0.5 mg/m^3		30 min	acc. DORNIER, 1984
	DK	(L)	0.14 mg/m^3		1 y	acc. WEIDNER, 1986
	E	(L)	0.065		1 y	acc. WEIDNER, 1986
	EC	G	0.1- 0.15 mg/m^3		24 h	EC, 1980
	EC	G	0.04-0.06 mg/m^3		1 y	EC, 1980
	EC	G	0.08 mg/m^3		1 y > 40$^{3)}$	EC, 1980
	EC	G	0.12 mg/m^3		1 y <= 40$^{3)}$	EC, 1980
	EC	G	0.13 mg/m^3		1 d$_{winter}$ > 60$^{3)}$	EC, 1980

		EC	G	0.18 mg/m^3		1 d$_{\text{winter}}$ <= 60 3)	EC, 1980
		EC	G	0.25 mg/m^3		1 y > 150 3)4)	EC, 1980
		EC	G	0.35 mg/m^3		1 y <= 150 3)4)	EC, 1980
		F	(L)	as EC		1 y	acc. WEIDNER, 1986
		GB	(L)	as EC		1 y	acc. WEIDNER, 1986
		GR	(L)	as EC		1 y	acc. WEIDNER, 1986
		H	(L)	1.15 mg/m^3		24 h protected areas	acc. DORNIER, 1984
		H	(L)	1 mg/m^3		30 min protected areas	acc. DORNIER, 1984
		H	(L)	0.5 mg/m^3		24 h specially protected	acc. DORNIER, 1984

					areas	
	H	(L)	0.5 mg/m^3		30 min specially protected areas	acc. DORNIER, 1984
	I	(L)	as EC		1 y	acc. WEIDNER, 1986
	I	(L)	0.38 mg/m^3		24 h	acc. DORNIER, 1984
	I	(L)	0.75 mg/m^3		30 min	acc. DORNIER, 1984
	IL	(L)	0.26 mg/m^3		24 h	acc. DORNIER, 1984
	IL	(L)	0.78 mg/m^3		30 min	acc. DORNIER, 1984
	IRL	(L)	as EC		1 y	acc. WEIDNER, 1986
	J	(L)	0.11 mg/m^3		24 h/1 y	acc. DORNIER, 1984
		(L)	0.29			acc. DORNIER,

	J	(L)	mg/m^3		1 h	1984
	COL	(L)	0.07 mg/m^3		1 y	acc. DORNIER, 1984
	L	(L)	as EC		1 y	acc. WEIDNER, 1986
	N	(L)	0.025-0.06 mg/m^3		1 y	acc. WEIDNER, 1986
	N	(L)	0.2 mg/m^3 (+2%)		24 h	acc. DORNIER, 1984
	N	(L)	0.4 mg/m^3 +2%		1 h	acc. DORNIER, 1984
	NL	G	0.075 mg/m^3		1 y 50% of 24 h av.	acc. WEIDNER,1986
	NL	G	0.20 mg/m^3		1 y 95% of 24 h av.	acc. UBA, 1980
	NL	G	0.25 mg/m^3		1 y 98% of 24 h av.	acc. WEIDNER,1986
	NL		0.15 mg/m^3		1 y	acc. DORNIER, 1984

		NL		$0.3\ mg/m^3$ (+2%)		24 h +2%	acc. DORNIER, 1984
		NL		$0.5\ mg/m^3$		24 h +0.3%; 1 d/y	acc. DORNIER, 1984
		PL		$0.075\ mg/m^3$		24 h specially protected areas	acc. DORNIER, 1984
		PL		$0.25\ mg/m^3$		20 min specially protected areas	acc. DORNIER, 1984
	Emiss.	D	L	$0.5\ mg/m^3$		mass flow > 5 kg/h5)	acc. TA Luft, 1986
	Workp	D	L	$5\ mg/m^3$		MAK	acc. DFG, 1994
		PL		$0.35\ mg/m^3$		24 h protected areas	acc. DORNIER, 1984
		PL		$0.9\ mg/m^3$		20 min protected areas	acc. DORNIER, 1984

	RU		0.25 mg/m^3		24 h	acc. DORNIER, 1984
	RU		0.75 mg/m^3		20 min	acc. DORNIER, 1984
	S		0.06 mg/m^3		1 y	acc. DORNIER, 1984
	S		0.75 mg/m^3		1 h	acc. DORNIER, 1984
	S		0.10 mg/m^3		Oct. to March	acc. DORNIER, 1984
	S		0.30 mg/m^3		24 h	acc. DORNIER, 1984
	SF	(L)	0.04 mg/m^3		1 y	acc. WEIDNER, 1986
	SF	(L)	0.25 mg/m^3		24 h	acc. DORNIER, 1984
	SF	(L)	0.7 mg/m^3		30 min	acc. DORNIER, 1984
		(L)	0.05		24 h resid.	acc. DORNIER,

	SU		mg/m^3		Areas	1984
	SU	(L)	0.5 mg/m^3		30 min resid. Areas	acc. DORNIER, 1984
	TU	(L)	0.15 mg/m^3		24 h resid. Areas	acc. DORNIER, 1984
	TU	G	0.30 mg/m^3		24 h industrial areas	acc. DORNIER, 1984
	USA	(L)	2 ppm	TWA		acc. ACGIH, 1986
	USA	(L)	5 mg/m^3	TWA		acc. ACGIH, 1986
	USA	(L)	5 ppm	STEL		acc. ACGIH, 1986
	USA	(L)	10 mg/m^3	STEL		acc. ACGIH, 1986
	WHO	G	0.1-0.15 mg/m^3		24h1)	WHO, 1979
	WHO	G	0.04-0.06 mg/m^3		1 y	WHO, 1979
	WHO	G	0.5 mg/m^3		10 min2)	WHO, 1987
		G	0.35			

		WHO		mg/m^3		1 h$^{2)}$	WHO, 1987
		WHO	G	0.125 mg/m^3		24 h$^{2)}$	WHO, 1987
		WHO	G	0.05 mg/m^3		1 y$^{2)}$	WHO, 1987
		YU	(L)	0.15 mg/m^3		24 h	acc. DORNIER, 1984
		YU	(L)	0.5 mg/m^3		30 min	acc. DORNIER, 1984
Water:		D	G	WGK 1			acc. ROTH, 1989

Notes:

1) **Mean value, max. 7 exceedings per annum**

2) **Recommendations for Europe**

3) **Given suspended-dust content (in g/m^3); median values**

4) **98% value of cumulative frequency of all daily mean values in year**

5) **SO_2 and SO_3, stated as SO_2**

VALUES STIPULATED IN REGIONAL SMOG ORDERS IN GERMANY

State	*Advance warning*	*Stage 1*	*Stage 2*

B1)	SO_2 + 1.3 x Suspended dust > 1.1 mg/m3 or SO_2 > 0.60 mg/m3	SO_2 + 1.3 x Suspended dust > 1.4 mg/m3 or SO_2 > 1.20 mg/m3	SO_2 + 1.3 x Suspended dust >1.7 mg/m3 or SO_2 > 1.80 mg/m3
B2)		SO_2 + 1.3 x Suspended dust > 1.1 mg/m3	SO_2 + 1.3 x Suspended dust >1.4 mg/m3
HH3)	SO_2 + 2.0 x Suspended dust > 1.1 mg/m3 or SO_2 > 0.60 mg/m3	SO_2 + 2.0 x Suspended dust > 1.4 mg/m3 or SO_2 > 1.20 mg/m3	SO_2 + 2.0 x Suspended dust >1.7 mg/m3 or SO_2 > 1.80 mg/m3
HH4)		SO_2 + 2.0 x Suspended dust > 1.1 mg/m3	SO_2 + 2.0 x Suspended dust >1.4 mg/m3

Lower Saxony 5); North-Rhine Westphalia; Hesse; Rhineland Palatinate; Saarland 5); Baden-Wrttemberg and Bavaria 5): all values as for Hamburg (HH); Federal States marked with superscripts have different methods of determining the limit values (refer to appropriate notes).

Notes:

1.3 x or 2.0 x = factors by which the suspended dust is multiplied

1) Berlin: averaged over 21 h and in last 3 h

2) Berlin: continuously over 72 h (mean values over 21 h)

3) Hamburg: averaged over 24 h and in last 3 h

4) Hamburg: continuously over 72 h (mean values over 24 h)

5) Averaged over 24 h / continuously over 72 h (mean values over 24 h)

Comparison/reference values

The annual average in Germany is between 0.01 and 0.08 mg/m^3. Because of favourable meteorological conditions, the flat lands of Northern Germany only reveal an annual average of 0.01 - 0.02 mg/m^3. Similar values are found in the hilly region of Southern Germany and in the Alps. Higher values - between 0.06 and 0.08 mg/m^3 - are found in conurbations such as the Ruhr and Rhine/Main areas or in Berlin. On the eastern boundaries of Germany, emissions from regional sources (primarily from Poland and Czechoslovakia) make a considerable contribution to the SO_2 concentration in these areas. Occasionally, the concentration in these rural areas reaches up to 2 mg/m^3 and thus attains the alarm levels stipulated in the Regional Smog Orders [UBA, 1989].

Approximate values for mean SO_2 immissions (annual averages) [SRU, 1988]:

"Clean-air zones"	0.005 mg/m^3
Rural areas	0.005 - 0.04 mg/m^3
Conurbations	0.03 - 0.1 mg/m^3

Urban areas	0.14 mg/m^3

The typical short-term impact (98 percentile of half-hour values) in conurbations is between 0.2 and 0.3 mg/m^3. In the most polluted areas, individual stations recorded values of 1.2 mg/m^3 (Bottrop, 1982) and even 1.7 mg/m^3 (Lnen-Brambauer, 1981).

Assessment/comments

The laboratory animals used to date for toxicity experiments are obviously far less sensitive to sulphur dioxide than humans. The most sensitive animal species (guinea pig) withstands - even over long periods - concentrations which are already intolerable to humans in the short term (DFG, 1988).

Sulphur dioxide is one of the chemicals for which there is a wealth of legislation. Limit and approximate values with differing points of reference are available from numerous countries. In comparison to the values for numerous other substances, the figures for SO_2 are subject to relatively rapid change.

When comparing the extensive range of values available, it is important to take account of the method of calculation (median, arithmetic mean, time frame, percentile etc.). The listed values for the Netherlands and the EC are good examples.

UBA (1980) compares technical installations, provides information on the sulphur content of raw materials from various countries and outlines different scenarios.

We have to distinguish between SO_2 produced for industrial processes (e.g. production of sulphuric acid) and SO_2 which is emitted. Although most of the SO_2 is of natural origin, care should be taken to reduce the emissions caused by humans, especially those from combustion processes.

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Tetrachloroethene

DESIGNATIONS

CAS No.: 127-18-4
Registry name: Tetrachloroethene
Chemical name: Tetrachloroethene
Synonyms, Trade names: Perchloroethene, PER, ethylene tetrachloride, 1,1,2,2-tetrachloroethene, Cecolin 2, Dekapir 2, Digrisol, Dow-Per, Drosol, Dynaper, Etilin, Peran, Perawin, Perclone, Sirius 2, Tetralex, Tetralina, Ankliostin, Didakene, Nema, Perc and many others
Chemical name (German): Tetrachlorethen, Perchlorethylen
Chemical name (French): Tetrachlorothne, perchlorthne
Appearance: colourless liquid with chloroform-like odour, vapour is much denser than air

BASIC CHEMICAL AND PHYSICAL DATA

Empirical formula:	C_2Cl_4
Rel. molecular mass:	165.83 g

Density:	1.624 g/cm^3 at 20C
Relative gas density:	5.73
Boiling point:	121.1C
Melting point:	-23C
Vapour pressure:	18.9 hPa at 20C; 32 hPa at 30C; 84 hPa at 50C
Flash point:	none
Odour threshold:	0.3-5 mg/l in water
	4.7-70 ppmv in air
Solvolysis/solubility:	in water: 129 mg/l
	readily soluble in organic solvents
Conversion factors:	1 ppm = 6.89 mg/m^3
	1 mg/m^3 = 0.145 ppm

ORIGIN AND USE

Usage:

Tetrachloroethene is a useful solvent. According to BGA (1988), 35% of the amount produced is used to degrease metal surfaces and 50% in dry cleaning establishments. LAI (1988) estimates that 60-65% are used for the treatment of metal surfaces and 20% in dry cleaning establishments. Stabilisers with widely differing chemical compositions are added to reduce the vapour pressure. Important products are e.g. contact adhesives, degreasing agents, wax removers, shoe polishes, garden pesticides, upholstery cleaners and carpet cleaners. In most products, tetrachloroethene has been replaced by other less toxic solvents.

Origin/derivation:

Tetrachloroethene is produced by oxyhydrochlorination, perchlorination and dehydrochlorination of hydrocarbons or chlorinated hydrocarbons.

Production figures:

Worldwide	1978-80	1,100,000 t	(RIPPEN, 1989)
Worldwide	1985	650,000 t	(ULLMANN, 1986)
EC	1980	< 500,000 t	(BGA, 1988)
USA	1977	304,000 t	(BGA, 1988)
USA	1985	220,000 t	(ULLMANN, 1986)
D	1979	113,000 t	(BMI, 1985)
D	1985	110,000 t	(ULLMANN, 1986)

D	1986	75,000 t	(LAI, 1988)
Japan	1973	57,000 t	(RIPPEN, 1989)
France	1981	26,000 t	(RIPPEN, 1989)
Mexico (Import)	1984	15,000 t	(RIPPEN, 1989)
Sweden	1977	5,300 t	(RIPPEN, 1989)

Toxicity

Humans:	LD_0 140 mg/m^3 (1.3 or 7.5 h/d for 5 d/w)	acc. WHO, 1984
Mammals:		
Mouse:	LD_{50} 8,000-11,000 mg/m^3, oral	acc. VERSCHUEREN, 1983
Mouse:	LC_{100} 135,000 mg/m^3 (2 h)	acc. MALTONI et al., 1986
Mouse:	LC_{50} 332,200 mg/m^3 (0,5 h)	acc. MALTONI et al., 1986
Rat:	NEL 475 mg/m^3, inhalation (8 h/d for 5 d/w)	acc. VERSCHUEREN, 1983

Rat:	LD_{50} > 5,000 mg/kg, oral	acc. VERSCHUEREN, 1983
Rat:	LD_{50} 13,000 mg/kg, oral (6 h)	acc. WHO, 1984
Rat:	LC_{100} 20,000 ppm, inhalation (0,4 h)	acc. MALTONI et al., 1986
Rat:	LC_{100} 2,500 ppm, inhalation (7 h)	acc. MALTONI et al., 1986
Rabbit:	LD $_{20}$,000 ppm, inhalation (2 h)	acc. MALTONI et al., 1986
Guinea pig:	LC_{100} 37,000 ppm, inhalation (0,67 h)	acc. MALTONI et al., 1986
Cat:	LCL_{0} 6,074 ppm, inhalation (2 h)	acc. MALTONI et al., 1986
Aquatic organisms:		
Water flea:	LC_{50} 18 mg/l (48 h)	acc. WHO, 1984
Water flea:	NEL 10 mg/l (48 h)	acc. WHO, 1984
American minnow:	LC_{50} 23.5 ng/l (24 h)	acc. VERSCHUEREN, 1983
Blue perch:	LC_{50} 46 mg/l (24 h)	acc. WHO, 1984
Blue perch:	LC_{50} 13 mg/l (96 h)	acc. WHO, 1984

Characteristic effects:

Humans/mammals: **Tetrachloroethene is resorbed through the skin because of its fat-dissolving properties. Concentrations above 680 mg/m^3 irritate the eyes and the respiratory tract, concentrations of 4,000-6,000 mg/m^3 during 45 minutes cause numbness. The substance acts on the central nervous system and produces headaches, dizziness and nausea. Inhalation often results in delayed neurological damage.**

Both, the WHO and the German Research Foundation (DFG) have classified tetrachloroethene as a substance suspected of carcinogenic potential. A few experiments with yeast cells have also revealed mutagenic effects. There is no proof of teratogenity or fetal toxicity yet.

ENVIRONMENTAL BEHAVIOUR

Water:

Tetrachloroethene sinks in water because of its poor water solubility and its high density. Thus, it may accumulate in groundwater and surface water. Tetrachloroethene is classed as very hazardous to water (in Germany: water hazard class 3). It is toxic to aquatic organisms and decomposes slowly to form trichloroacetic acid and hydrochloric acid. Degradation by microorganisms has been observed (from sequential dehydrochlorination up to mineralisation). Tetrachloroethene finds its way into the water cycle via industrial waste water.

Air:

Because of its high vapour pressure, about 80-90% of the substance ingresses into the atmosphere where it is ubiquitously distributed. Tetrachloroethene may be degraded by photolysis and is probably involved in the depletion of the ozone layer. Exchange takes place between air and water with the transition into the atmosphere being the most common path.

Soil:

The accumulation of tetrachloroethene in soil is dependent on the grain size and the water and humus content.

Biological degradation takes place in soil. High concentrations are to be found in the immediate vicinity of emission sources.

Half-life:
The half-life for hydrolysis in aerated water is between 9 months and 6 years (UBA, 1986). In the troposphere, half-life amounts to approx. 12 weeks or, if photodegradation takes place, up to 8 weeks (UBA, 1986 and MALTONI et al., 1986). The persistence in water-unsaturated soils is 2-18 months (DVGW, 1985).

Degradation, decomposition products:
Degradation in soil takes place via methanogenic, anaerobic microorganisms (UBA, 1986). In the troposphere, the substance is decomposed by photo-oxidation to form carbon dioxide and hydrochloric acid. In water, trichloroacetic and hydrochloric acid are formed (BGA, 1985). Other decomposition products are phosgene ($COCl_2$), di- and trichloroacetyl chloride. The liver degrades tetrachloroethene in the human body.

Food chain:
There is a moderate accumulation of tetrachloroethene in fatty tissues.

ENVIRONMENTAL STANDARDS

Medium/ acceptor	Sector	Country/organ.	Status	Value	Cat.	Remarks	Source
Water:	Drinkw	D	L	0.01 mg/l			acc. TVO, 1990
	Drinkw	EC	G	0.001 g/m^3			acc. LAU-BW, 1989
	Drinkw	WHO	G	10 g/l			acc. WHO, 1984
	Surface	USA		20 g/l			acc. WHO, 1987

	Waste water	CH	L	0.05 g/m^3		For drinking water	acc. LAU-BW, 1989
	Waste water	D	L	5 g/m^3		At point of discharge	acc. ROTH, 1989
Air:		D	L	35 mg/m^3	MIK	Long-time value	acc. BAUM, 1988
		D	L	110 mg/m^3	MIK	Short-time value 2)	acc. BAUM, 1988
		D	L	100 mg/m^3		1)	acc. KHN & BIRETT, 1988
		D	G	5 mg/m^3		3)	acc. BGA, 1988
		DDR	L	0.5 mg/m^3		Short-time value	acc. HORN, 1989
		DDR	L	0.06 mg/m^3		Long-time value	acc. HORN, 1989
		WHO	G	5 mg/m^3		24 h guide value	acc. LAU-BW, 1989
		WHO	G	8 mg/m^3		30 min	acc. LAU-BW, 1989
	Emiss.	D	L	0.1 g/m^3		mass flow > 2 kg/h	acc. TA Luft, 1986
	Workp	A	(L)	260 mg/m^3		Long-time value	acc. MALTONI et al., 1986

Workp	AUS	(L)	670 mg/m^3		Long-time value	acc. WHO, 1987
Workp	B	(L)	670 mg/m^3		Long-time value	acc. WHO, 1987
Workp	BG	(L)	10 mg/m^3			acc. MALTONI et al., 1986
Workp	BR	(L)	525 mg/m^3		48 h/w	acc. WHO, 1987
Workp	CH	(L)	345 mg/m^3		Long-time value, skin	acc. WHO, 1987
Workp	CS	(L)	250 mg/m^3		4)	acc. WHO, 1984
Workp	CS	(L)	1,250 mg/m^3		Short-time value	acc. WHO, 1984
Workp	D	L	345 mg/m^3		TRK (IIIB)	DFG, 1989
Workp	DDR	(L)	300 mg/m^3		Long-time value	acc. HORN, 1989
Workp	DDR	(L)	900 mg/m^3		Short-time value	acc. HORN, 1989
Workp	E	(L)	110 mg/m^3		Long-time value	acc. MALTONI et al., 1986
Workp	ET	(L)	267 mg/m^3		Long-time value	acc. MALTONI et al., 1986
Workp	F	(L)	405 mg/m^3		Long-time value	acc. MALTONI et al., 1986

Workp	F	(L)	1,080 mg/m^3		4)	acc. MALTONI et al., 1986
Workp	GB	(L)	678 mg/m^3		Long-time value	acc. WHO, 1987
Workp	GB	(L)	1,000 mg/m^3		10 min	acc. WHO, 1987
Workp	H	(L)	10 mg/m^3		Long-time value	acc. WHO, 1987
Workp	H	(L)	50 mg/m^3		30 min	acc. WHO, 1987
Workp	I	(L)	400 mg/m^3		Long-time value	acc. MALTONI et al.,1986
Workp	I	(L)	1,000 mg/m^3		Skin	acc. MALTONI et al.,1986
Workp	J	(L)	268 mg/m^3		Long-time value	acc. MALTONI et al.,1986
Workp	J	(L)	345 mg/m^3		4)	acc. WHO, 1987
Workp	NL	(L)	190 mg/m^3		Long-time value	acc. MALTONI et al.,1986
Workp	NL	(L)	240 mg/m^3		Long-time value, skin	acc. WHO, 1987
Workp	PL	(L)	60 mg/m^3		4)	acc. WHO, 1987

	Workp	RO	(L)	400 mg/m^3		Long-time value	acc. WHO, 1987
	Workp	RO	(L)	500 mg/m^3		4)	acc. WHO, 1987
	Workp	S	(L)	140 mg/m^3		1 day	acc. WHO, 1987
	Workp	S	(L)	350 mg/m^3		15 min	acc. WHO, 1987
	Workp	SF	(L)	335 mg/m^3			acc. WHO, 1987
	Workp	SU	(L)	10 mg/m^3		4)	acc. MALTONI et al.,1986
	Workp	USA	(L)	335 mg/m^3	TWA		ACGIH, 1986
	Workp	USA	(L)	1,340 mg/m^3	STEL	15 min	ACGIH, 1986
	Workp	YU	(L)	10 mg/m^3		Long-time value	acc. WHO, 1987
	Workp	YU	(L)	200 mg/m^3		Long-time value	acc. MALTONI et al.,1986
	Workp	D	L	100 g/dl	BAT	Blood	DFG, 1989
	Workp	D	L	9.5 ml/m^3	BAT	Alveolar air	DFG, 1989
		D	L	1 mg/kg			acc. BGA, 1988

Foodstuffs:		D	L	0.1 mg/kg			acc. UMWELT, 1989
		D	L	0.2 mg/kg		5)	acc. UMWELT, 1989
Cosmetics:		D	L	0 mg/kg		Ban	acc. DVGW, 1985
		EC	L	0 mg/kg		Ban	acc. WHO, 1984

Notes:

1) **With mass flow of 2 kg/h and more**

2) **With in 4 hours with max. 30 min. overshoot**

3) **Indoor air**

4) **Maximum value**

5) **Cumulative value for several solvents in one foodstuff**

Comparison/reference values

Medium/origin	**Country**	**Value**	**Source**
Surface water			

Rhine (Basle, 1982):	D	0.18-1.73 g/l	acc. DVGW, 1985
Rhine (Karlsruhe, 1982):	D	0.2-1.39 g/l	acc. DVGW, 1985
Rhine (Wiesbaden, 1983):	D	0.14-4.1 g/l	acc. DVGW, 1985
Rhine (Cologne, 1983):	D	0.16-0.63 g/l	acc. DVGW, 1985
Main (Frankfurt, 1979):	D	0.35-2.8 g/l	acc. DVGW, 1985
Ruhr (Witten, 1983):	D	0.1-0.6 g/l	acc. DVGW, 1985
Elbe (1982/83):	D	0.2-9.3 g/l	acc. UBA, 1986
Weser (1982/83):	D	0.5-1 g/l	acc. UBA, 1986
Danube (1983-1985):	D	0.1-2.8 g/l	acc. UBA, 1986
Drinking water:			
Wiesbaden (1980)	D	< 1.8 g/l	acc. DVGW, 1985
Taunus (1980)	D	< 10.5 g/l	acc. DVGW, 1985
Medmenham (1981)	GB	< 0.01 g/l	acc. DVGW, 1985
5 cities (1977)	J	0.2-0.6 g/l	acc. DVGW, 1985
22 cities (1977)	USA	< 2 g/l	acc. DVGW, 1985
Gothenburg (1978)	S	< 0.008 g/l	acc. DVGW, 1985
Sediment:			

Rhine: (Hitdorf, 1982)	D	4 g/kg	acc. DVGW, 1985
Ruhr: (1972-1981)	D	4-36 g/kg	acc. DGVW, 1985

Assessment/comments

According to the Chemicals Law, tetrachloroethene is classed as non-toxic in Germany, but the risk of cancer has not yet been ruled out. Due to the various sources of contamination, chronic exposure of employees to concentrations which may cause adverse effects is frequent.

Assessment is made more difficult because of the variety of stabilisers which are added to technical tetrachloroethene. Some of the reactive hydrocarbons contained in the stabiliser mixtures such as epichlorohydrin and 1,4-dioxane are suspected of being carcinogenic. The contamination of groundwater and drinking water is of major concern as tetrachloroethene is only slowly degraded in groundwater.

Therefore, the usage of tetrachloroethene should be considerably restricted, production plants should be converted into closed systems and provided with solvent-recovery systems. Whenever it is necessary to work on open systems (e.g. servicing, repairs), these have to be cooled down previously, and respiratory protection must be worn.

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Thallium

DESIGNATIONS

CAS No.: **7440-28-0**
Registry name: **Thallium**
Chemical name: **Thallium**
Synonyms, Trade names: **Thallium**
Chemical name (German): **Thallium**
Chemical name (French): **Thallium**
Appearance: **very similar to lead: soft and ductile heavy metal; shiny white at fresh cuts turning blue-grey; (alpha-thallium has a hexagonal crystalline structure and is converted at temperatures above 232C into beta-thallium with cubic structure)**

BASIC CHEMICAL AND PHYSICAL DATA

Chemical symbol: **Tl**
Rel. atomic mass: **204.37 g**
Density: **11.85 g/cm^3**
Boiling point: **1457C**
Melting point: **303C**
Vapour pressure: **0.013 Pa at 473C**
Solvolysis/solubility: **in water: virtually insoluble (forming hydroxides in air saturated water); thallium sulphate: 48.7g/l insoluble in lyes, soluble in diluted nitric acid and alcohol**

ORIGIN AND USE

Usage:

Together with sulphur and arsenic, thallium is used to produce low-melting glass (around 150C). Adding thallium to other metals increases their resistance to deformation and corrosion. The substance is used in the semiconductor

industry in photocells and as an activator for light-sensitive crystals. Thallium sulphate (which used to be an important rat poison) is hardly ever produced today because of its high toxicity.

Important thallium compounds:

- **thallium sulphate (Tl_2SO_4) - very toxic**
- **sodium thallide (NaTl);**
- **thallium(I) alkoxides.**

Origin/derivation:

Thallium makes up approx. 10^{-4}% of the Earth's crust (61st position in element frequency table). It is found as an accompanying metal in zinc, copper, iron and lead ores. All thallium minerals such as lorandite, vrbite and crookesite are extremely rare. Roasted pyrites used to produce cement may contain considerable quantities of thallium (KEMPER, 1987).

Production:
Worldwide production < 100 t/a; the substance is manufactured in the USA, Russia, Belgium and Germany (BREUER, 1981). According to ZARTNER-NYILAS et al. (1983), the worldwide production of thallium and its compounds amounts to approximately 20 t/a.

Toxicity

Humans:	LD 8-10 mg/kg	acc. ZARTNER-NYILAS et al., 1983
	220 g/(kgd) 1)	acc. ZARTNER-NYILAS et al., 1983
	15.4 g 2)	acc. ZARTNER-NYILAS et al., 1983

Plants:			
Various species	20-30 mg/kg	Lower yield	BAFEF, 1987
Young barley	11-45 mg/kg	Lower yield	BAFEF, 1987

Notes:

1) Smallest toxic dose referenced to entire life

2) Tolerable daily thallium absorption from air, water, foodstuffs

Characteristic effects:

Humans/mammals: **Thallium is assimilated by humans via the food chain, respiration and by skin resorption. It is distributed throughout the entire body through the bloodstream and mainly accumulates in the liver, kidneys, intestinal wall and muscle tissue. Additional accumulation takes place in the bones, skin, sweat glands, sebaceous glands, nails, hair and in the entire nervous system. Moreover, thallium passes through the placenta of pregnant women and can thus harm unborn children. The substance is excreted with urine and stool, as well as in small quantities via hair, sweat, tears, saliva and mother's milk (ZARTNER-NYILAS et al., 1983). Thallium and its compounds are very toxic. Symptoms are hair loss, cataracts, degeneration of the nerves, impaired vision, inhibited growth, neuralgia and psychosis. Accumulation takes place in the skin and hair.**

Plants: **Just like several other heavy metals, thallium is absorbed by plants via the roots and thus accumulates in the leaf tissue as well as in other parts of the plant. Phytotoxic effects may occur. The damage pattern, which involves chlorosis of the leaves as well as intercostal necrosis and/or necrosis around the edges, does however vary**

in terms of intensity and extent from plant to plant. The type/species-specific resistance is particularly apparent. Plants with a hard surface are usually subject to less damage than plants with soft, pilose surfaces (ZARTNER-NYILAS et al., 1983).

ENVIRONMENTAL BEHAVIOUR

Water:
Like other heavy metals, thallium accumulates in sediment.

Soil:
Very little is known to date about the persistence of thallium in soil. Even thallium sulphate is washed out only to a slight extent. The low thallium content in groundwater - even in the immediate vicinity of emission sources - underlines that soils are an important sink for thallium.

Food chain:
Certain plant species (e.g. curly kale) considerably accumulate thallium from the soil. The accumulation proceeds in the food chain.

ENVIRONMENTAL STANDARDS

Medium/ acceptor	**Sector**	**Country/organ.**	**Status**	**Value**	**Cat.**	**Remarks**	**Source**
Water:	Marine	USA		0.01 mg/l (max.)		Hazard threshold	EPA, 1973
	Marine	USA		0.05 mg/l (max.)		Minimal risk	EPA, 1973
			G	1 mg/kg			

Soil:		D	G	1 mg/kg			KLOKE, 1980
		CH	G	1 mg/kg	VSBO		acc. LAU-BW, 1989
Air:		D	L	$0.01 mg/m^2d$	IW1	$24 h^{1)}$	TA-Luft, 1986
	Emiss.	D	L	$0.2 mg/m^3$		mass flow > 1 g/h	acc. TA Luft, 1986
	Workp	Aus	(L)	$0.1 mg/m^3$		Soluble compounds	acc. MERIAN, 1984
	Workp	B	(L)	$0.1 mg/m^3$		Soluble compounds	acc. MERIAN, 1984
	Workp	D	L	$0.1 mg/m^3$	MAK	Total dust	DFG, 1988
	Workp	CH	(L)	$0.1 mg/m^3$		Soluble compounds	acc. MERIAN, 1984
	Workp	NL	(L)	$0.1 mg/m^3$		Soluble compounds	acc. MERIAN, 1984
	Workp	PL	(L)	$0.1 mg/m^3$		Soluble compounds	acc. MERIAN, 1984
	Workp	RO	(L)	$0.05 mg/m^3$		Short-time, soluble compounds	acc. MERIAN, 1984
			(L)	$0.1 mg/m^3$			

	Workp	SF	(L)	0.1 mg/m^3		Soluble compounds	acc. MERIAN, 1984
	Workp	SU	(L)	0.01 mg/m^3		1967	acc. ACGIH, 1982
	Workp	YU	(L)	0.1 mg/m^3		Soluble compounds	acc. MERIAN, 1984
Plants:		D	G	0.25 mg/kg			acc. BAFEF, 1987
Foodstuffs:		D	G	0.25 mg/kg			acc. BAFEF, 1987

Note:

1) Tl and its organic compounds within dust sediments, stated as Tl

Comparison/reference values

Medium/origin	**Country**	**Value**	**Source**
Water:			
Rhine (km 865)		0.5-2.5 g/l	acc. ZARTNER-NYILAS et al., 1983
Soil:			
Various soils (normal)		<0.5 mg/kg	
Various soils (frequent)		0.01-0.5 mg/kg	acc. KLOKE, 1980

Plants:		0.01-0.5 mg/kg	

Assessment/comments

On the basis of the data available at present, the risk to the public from increased thallium exposure is slight. Local dust depositions from thallium-emitting industries (e.g. cement) have seldom given an indication of human health hazards. One case of remarkable thallium emissions from the cement industry is known in Germany. Animals and plants do however reveal regional damage. There is little information available on the chronic effects of thallium in humans as an environmental pollutant. Opinions differ on the subject of mutagenity, teratogenity and carcinogenity.

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Toluene

DESIGNATIONS

CAS No.: 108-88-3
Registry name: Toluene
Chemical name: Toluene
Synonyms, Trade names: Toluene, methylbenzene, phenylmethane, methacide
Chemical name (German): Toluol, Methylbenzol, Toluen

Chemical name (French): **Tolune, methylbenzne**
Appearance: **colourless liquid with benzene-like odour**

BASIC CHEMICAL AND PHYSICAL DATA

Empirical formula:	C_7H_8
Rel. molecular mass:	92.15 g
Density:	0.867 g/cm^3 at 20C
Relative gas density:	3.18
Boiling point:	110.6C
Melting point:	-95C
Vapour pressure:	28 hPa at 20C, 45 hPa at 30C, 109 hPa at 50C
Flash point:	6C
Ignition temperature:	535C
Explosion limits:	1.2-7 vol%
Odour threshold:	0.2 ppm

Solvolysis/solubility:	in water: 0.53 g/l at 20-25C
	in seawater: 0.38 g/l
	unlimited in chloroform, acetone, ether
Conversion factors:	1 ppm = 3.83 mg/m^3
	1 mg/m^3 = 0.261 ppm

ORIGIN AND USE

Usage:
Toluene is a parent substance in the manufacture of benzene derivatives, caprolactam, saccharine, pharmaceuticals, dyes, perfumes, TNT and detergents. It is used in fuels (anti-knock additive) and as a solvent for paints and coatings, rubber, resins, thinners in nitrocellulose lacquers and adhesives. It serves as a raw material in the manufacture of phenol (predominantly in Western Europe), benzene, cresol (chiefly Japan) and a wide range of other substances.

Origin/derivation:
Natural sources: in coal tar and mineral oils; produced in the combustion of natural resins (e.g. forest fires).

Production figures:
Estimates of worldwide production vary between 6.5 and more than 10 million t/a.

Federal Republic of Germany (1984)	358,000 t

Canada (1984)	430,000 t
France (1984)	39,000 t
Italy (1984)	312,000 t
Japan (1984)	784,000 t
Mexico (1984)	216,000 t
Taiwan (1984)	169,000 t
USA (1984)	2,390,000 t

Emission figures (estimated):
Various estimates vary between 6 and 8 million t/a. The proportional emissions were calculated as follows for a total of 6.2 million t:

Losses into sea	500,000 t/a
Losses into air from refineries	2,500,000 t/a
Evaporation of fuels	50,000 t/a
Exhaust fumes from motor vehicles	2,000,000 t/a

Solvent losses	1,000,000 t/a
Chemical industry losses	100,000 t/a

Toxicity

Humans:	LD 50-500 mg/kg	
	TCLo 0.77 mg/l, inhalation	
	>2.9 mg/l, inhalation	damage to central nervous system
	50-100 ppm	fatigue, headaches
	200 ppm	slight irritation of throat and eyes
	100-300 ppm (8 h)	slight signs of lack of coordination
	300-800 ppm (8 h)	distinct signs of lack of coordination
	>4,000 ppm (1 h)	loss of consciousness, fatal over a lengthy period
	10,000-30,000 ppm	loss of consciousness after several minutes,

		fatal over lengthy period
Mammals:		
Rat	LD_{50} 5,000-7,000 mg/kg, oral	
Rat (new born)	LD_{50} 870 mg/kg, oral	
Rat	NOEL >590 mg/kg and d, oral (193 d)	
Mouse	LC_{50} 20 mg/l (8 h)	
Aquatic organisms:		
Freshwater fish	LC_{50} 13-240 mg/l (96 h)	
Golden orfe	LC_{50} 70 mg/l	
Salmon	LC_{50} 6.4-8.1 mg/l (96 h)	
Molluscs	LC_{50} 24-74 mg/l (24 h)	
Water flea (Daphnia magna)	EC_{50} 11.5-310 mg/l (48 h)	
Green algae	EC_{50} 134-210 mg/l (reduction of	

	photosynthesis)	
Blue algae	10 mg/l (96 h, 75% reduction of photosynthesis)	
Plants:		
Corn, soja	200-20,000 ppm in soil toxic	
Carrots, tomatoes, barley	3 ppm (0.5 h) in air toxic	

Note:
The data cited from various sources; all quoted in RIPPEN, 1989.

Characteristic effects:

Humans/mammals: **Inhalation (100 ppm) causes headaches, dizziness, irritation of eyes and nose. Long-term exposure impairs the central nervous system, alters the blood count and causes other chronic effects. Chromosome damage was established in rats. The investigation of employees exposed to toluene revealed controversial results. Toluene itself is not known to be carcinogenic, but other components in a solvent mixture may be carcinogenic. Rats and mice revealed abnormal skeletons and reduced fetal weight with mice likewise being subject to increased embryonic mortality.**

Synerg./antagon.:

- **reduction of metabolism in rats with benzene, trichloroethylene or styrene;**
- **enhancement of toxic effect of acetylsalicylic acid (in particular deformities and anomalies in embryo);**

- likelihood of increased chromosome damage in smokers exposed to toluene;
- attenuation of various toxic effects of benzene in mice;
- increase in skin cancer induced by 7,12-dimethyl-benz[b]anthracene.

ENVIRONMENTAL BEHAVIOUR

Water:

Toluene is hazardous to water. Because of its volatility, it is partly released into the atmosphere, but its solubility in water is sufficient to cause surface water and groundwater pollution problems.

Air:

The majority of the toluene which impacts the environment enters the atmosphere because of its high vapour pressure. Degradation is rather effective with the result that neither wet nor dry deposition causes large quantities to return to the Earth's surface.

Soil:

Adsorption takes place primarily on organic matter and clay particles. The adsorption capacity increases with decreasing pH value. If not spilled in large quantities, toluene which enters the soil passes into the atmosphere or is subject to chemical transformation and biodegradation.

Degradation, decomposition products, half-life:

The estimated mean half-life in air is about 60 h (reaction with $^{\cdot}OH$). The dwell time in summer in northern climates is approx. 4 days in contrast to several months in winter. In the tropics, the figure is between several days and several weeks irrespective of the time of year.

Laboratory experiments have shown that toluene escapes into the atmosphere with a half-life of 5 h from a uniformly mixed body of water with a depth of 1 m.

Some 20% of the dose absorbed by rats, rabbits and humans is exhaled. Approx. 80% is metabolised mainly into benzoic acid (via benzyl alcohol / benzaldehyde) with small quantities being converted into cresols.

Food chain:

Accumulation by way of the food chain is highly improbable since toluene is only slightly persistent and highly volatile.

ENVIRONMENTAL STANDARDS

Medium/ acceptor	**Sector**	**Country/organ.**	**Status**	**Value**	**Cat.**	**Remarks**	**Source**
Water:	Drinkw	A	(L)	20 g/l			acc. RIPPEN, 1989
	Drinkw	SU	(L)	500 g/l			acc. RIPPEN, 1989
	Drinkw	USA	G	14.3 g/l			acc. RIPPEN, 1989
	Surface	USA	G	12.4 mg/l			acc. RIPPEN, 1989
	Surface	USA	G	2.3 mg/l		24 h average1)	acc. RIPPEN, 1989
	Surface	USA	G	5.2 mg/l		Peak value1)	acc. RIPPEN, 1989
	Seawater	USA	G	0.1 mg/l		24 h average2)	acc. RIPPEN, 1989
	Seawater	USA	G	0.23 mg/l		Peak value2)	acc. RIPPEN, 1989
	Groundw	D(HH)	G	15 g/l		Closer investigation	acc. DVGW, 1988

	Groundw	D(HH)	G	30 g/l		Rehabilitation investigation	acc. DVGW, 1988
	Groundw	NL	G	15 µg/l		Reference	acc. RIPPEN, 1989
	Groundw	NL	L	50 µg/l		Intervention	acc. RIPPEN, 1989
Soil:		NL	G	0.05 mg/kg		Reference	acc. TERRA TECH, 6/94
		NL	L	130 mg/kg		Intervention	acc. TERRA TECH, 6/94
Air:		BG	(L)	0.6 mg/m^3		20 min/24 h	acc. EPA, 1983
		DDR	(L)	2 mg/m^3		30 min	acc. EPA, 1983
		DDR	(L)	0.6 mg/m^3		24 h	acc. EPA, 1983
		Europe	G	8 mg/m^3		30 min	WHO, 1987
		Europe	G	1 mg/m^3		24 h	WHO, 1987
		SU	(L)	0.6 mg/m^3		20 min/24 h	acc. WHO, 1985
		YU	(L)	0.6		20 min/24 h	acc. EPA, 1983

			mg/m^3 3)			
	WHO	G	1 mg/m^3 3)		30 min	acc. SLOOFF, 1988
	WHO	G	8 mg/m^3		24 h	acc. SLOOFF, 1988
Emiss.	D	L	0.1 g/m^3		mass flow > 2 kg/h	acc. TA Luft, 1986
Workp	AUS	(L)	375 mg/m^3			acc. RIPPEN, 1989
Workp	B	(L)	375 mg/m^3			acc. RIPPEN, 1989
Workp	BG	(L)	50 mg/m^3			acc. RIPPEN, 1989
Workp	CH	(L)	380 mg/m^3			acc. RIPPEN, 1989
Workp	CS	(L)	800 mg/m^3		Short term	acc. RIPPEN, 1989
Workp	D	L	190 mg/m^3	MAK		DFG, 1994
Workp	DDR	(L)	200 mg/m^3			acc. RIPPEN, 1989
		(L)	50 mg/m^3			

Workp	H	(L)	30 mg/m			acc. RIPPEN, 1989
Workp	I	(L)	300 mg/m^3			acc. RIPPEN, 1989
Workp	IRL	(L)	375 mg/m^3			acc. RIPPEN, 1989
Workp	J	(L)	375 mg/m^3			acc. RIPPEN, 1989
Workp	NL	(L)	375 mg/m^3			acc. RIPPEN, 1989
Workp	PL	(L)	100 mg/m^3			acc. RIPPEN, 1989
Workp	RO	(L)	300 mg/m^3			acc. RIPPEN, 1989
Workp	S	(L)	375 mg/m^3			acc. RIPPEN, 1989
Workp	SF	(L)	750 mg/m^3			acc. RIPPEN, 1989
Workp	USA	(L)	375 mg/m^3	TWA		acc. RIPPEN, 1989

	Workp	USA	(L)	560 mg/m^3	STEL		acc. RIPPEN, 1989
	Workp	YU	(L)	200 mg/m^3			acc. RIPPEN, 1989
	Workp	D	L	170 g/dl	BAT	In blood	acc. DVGW, 1988
Foodstuffs:		USA	G	30 mg/d	ADI		acc. RIPPEN, 1989

Notes:

1) Protection of freshwater organisms
2) Protection of saltwater organisms
3) Protected areas

Comparison/reference values

Medium/origin	**Country**	**Value**	**Source**1)
Water:			
Surface water	GB	1.8-3.8 g/l	
Rhine (Basle-Duisburg, 1976)	D	0.7-1.9 g/l	
Gulf of Mexico2)		3-10 ng/l	

Gulf of Mexico3)		4-60 ng/l	
Groundwater (contaminated)	USA	0.01-0.1 g/l (n=8)	
Drinking water (5 cities)	USA	1.5-8,300 g/l (n=6 of 13)	
		0.1-19 g/l	
Sediment/soil:			
River Tees estuary	GB		
Sewage sludge	USA	1.2-6.4 g/kg NG (n=4)	
		1.4-705 mg/kg TG (n=12 of 13)	
Air:			
Northern hemisphere4) (1980-83)			
Southern hemisphere4) (1980-83)		10-210 pptv (mean values)	
Desert	Egypt	<5-90 pptv (mean values)	
Background impact	Brazil	0.22 ppbv (mean value)	
Background impact	Kenya	0.04-0.19 ppbv (n=6)	

Urban air	D	0.05-1.08 ppbv (n=13)	
Low pollution areas	D	0.52-27 ppbv	
Dump gas	D	1.3 ppbv	
Rainwater	GB	0.2-620 mg/m^3	
Rainwater	USA	43 g/l	
		0.9-220 ng/l	

Notes:

1) All data quoted as per RIPPEN, 1989
2) Background value
3) Under anthropogenic influence
4) Clean air

Assessment/comments

Toluene vapours are dangerous especially in confined areas such as cellars or sewage systems when they reach the explosion limit. Accumulation in the food chain is unlikely. The toxicity in aquatic organisms is moderate. Symptoms of poisoning are inhibited growth and reduced reproduction rates. Spilled toluene may cause groundwater pollution.

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1,1,1-trichloroethane

DESIGNATIONS

CAS No.: **71-55-6**
Registry name: **1,1,1-Trichloroethane**
Chemical name: **Ethane, 1,1,1-trichloro**
Synonyms, Trade names: **Methyl chloroform, Aerothene, TT, alpha-trichloroethane, Armaclean, Baltane, Champion Fluid, Chlorotene, Chlorothane NU, Chlorothene, Chlorten, Dowclene WR, Drivertan, Escothen, FO 178, Genklene, Inhibisol, K 31, Mecloran, methyltrichloromethane, NCI-CO4626, Solvethane, Telclair X 31, 1,1,1-tri, triethane, Vythene C, Wacker 3X1**
Chemical name (German): **1,1,1-Trichlorethan, Methylchloroform**
Chemical name (French): **Trichloro-1,1,1-thane, chlorethne, mthylchloroforme**
Appearance: **colourless liquid with sweet, ethereal odour**

BASIC CHEMICAL AND PHYSICAL DATA

Empirical formula:	$C_2H_3Cl_3$
Rel. molecular mass:	133.41

Density:	1.338 g/cm^3
Relative gas density:	4.55
Boiling point:	74.1C
Melting point:	-32.6C
Vapour pressure:	133 hPa at 20C; 200 hPa at 30C; 445 hPa at 50C
Ignition temperature:	537C
Explosion limits:	8.0 - 10.5 vol%
Odour threshold:	100 ppm
Solvolysis/solubility:	in water: 1.3 g/l; readily soluble in acetone, benzene, carbon tetrachloride, methanol, diethylether, carbon disulphide
Conversion factors:	1 ppm = 5.54 mg/m^3
	1 mg/m^3 = 0.183 ppm

ORIGIN AND USE

Usage:

According to BGA (1985) about 30% were used as solvents for hot degreasing of metals, 30% for cold degreasing of metals, 30% as solvents in dyes, putties, adhesives, engine cleaners, polishes, lubricants, shrinkdown films, protective coatings, insecticides and aerosols and 10% for miscellaneous purposes such as typewriter corrector fluid. Nowadays, the demand has decreased because of stringent regulations in many industrialised countries. This solvent has been replaced by other products in several applications. Stabilisers are always added to the marketed product. The German Order Governing Working Media (1980) classes 1,1,1-trichloroethane as hazardous to health.

Origin/derivation:

1,1,1-trichloroethane is not a natural product; it is produced industrially from 1,2-dichloroethane or ethane.

Production figures:

USA	1980	314,022 t	(ATRI, 1985)
EC	1978	123,000 t	(ATRI, 1985)
Japan	1980	86,000 t	(ATRI, 1985)
D	1978	35,000 t	(DVGW, 1985)
Worldwide	1984	450,000 t	(ULLMANN, 1986)

Toxicity

Mammals:		
Mouse:	LD_{50} 2,568-9,700 mg/kg, oral	acc. EPA, 1984
Rat:	LD_{50} 10,000 mg/kg (14 d)	acc. UBA, 1986
Rat:	LD_{50} 11,000-14,300 mg/kg, oral	acc. EPA, 1984
Rabbit:	LD_{50} 15,800 mg/kg, dermal	acc. EPA, 1984
Dog:	LD_{50} 4,140 mg/kg, intravenous	acc. EPA, 1984
Guinea pig:	LD_{50} 8,600 mg/kg, oral	acc. EPA, 1984
Aquatic organisms:		
Golden orfe:	LC_{0} 94 mg/l (48 h)	acc. UBA, 1986
Golden orfe:	LC_{50} 123 mg/l (48 h)	acc. UBA, 1986
Golden orfe:	LC_{100} 201 mg/l (48 h)	acc. UBA, 1986
American minnow:	LC_{50} 52.8-105 mg/l (96 h)	acc. UBA, 1986
Blue perch:	LC_{50} 69.7 mg/l (96 h)	acc. UBA, 1986

Water flea:	LC_0 2,275 mg/l (24 h)	acc. UBA, 1986
Water flea:	LC_{50} 530 mg/l (48 h)	acc. UBA, 1986
Water flea:	LC_{100} 2,384 mg/l (24 h)	acc. UBA, 1986
Blue algae:	EC_3 350 mg/l (7 d, pH=7)	acc. UBA, 1986
Green algae:	EC_3 430 mg/l (7 d, pH=7)	acc. UBA, 1986
Invertebrates:		
Pseudomonas putida:	EC_{10} > 100 mg/l (30 min)	acc. UBA, 1986
Pseudomonas putida:	EC_3 > 100 mg/l (16 h, pH=7)	acc. UBA, 1986
Uronema parduczi:	EC_5 > 1,040 mg/l (20 h, pH=6.8)	acc. UBA, 1986

Characteristic effects:

Humans/mammals: **The inhalation of 1,1,1-trichloroethane has a narcotic effect. In contrast to the comparable solvents trichloroethylene ("Tri") and tetrachloroethylene ("Per"), this substance is considerably less toxic. Like other chlorinated hydrocarbons, 1,1,1-trichloroethane may cause severe damages of the liver.**

The inhalation of large concentrations causes loss of consciousness, numbness, retarded reaction and respiratory

and circulatory paralysis with lethal consequences. The threshold concentration for the occurrence of paralysis in humans is 500 ppm; narcotic effects are observed at 1000 ppm (BGA, 1985). Due to the findings of American studies, 1,1,1-trichloroethane is suspected to cause malignant liver tumours.

In the Federal Republic of Germany, 1,1,1-trichloroethane is listed under pregnancy group C (no hazard of damage to embryos given compliance with MAK and BAT values).

ENVIRONMENTAL BEHAVIOUR

Water:
1,1,1-trichloroethane is heavier than water and thus sinks even in groundwater. It enters the biocycle via the water path. It is ubiquitously detected in surface water; increased concentrations have been observed in recent years in the sea.

Air:
90% of the entire production finally evaporates into the atmosphere and thus participates in the depletion of the ozone layer (DVGW, 1985).

Soil:
1,1,1-trichloroethane accumulates in water-unsaturated soils and in sewage sludge.

Half-life:
The half-life in water-unsaturated soils is more than 2 years. The tropospheric half-life is estimated at 5-10 years (UBA, 1986), with the estimated figure for seawater being 39 weeks, given pH = 8 and 10C (ATRI, 1985).

Degradation, decomposition products:
Degradation in the troposphere - according to ATRI (1985) some 15% of the total amount liberated - finally results by way of phosgene in CO_2 and HCl. The reaction with ozone depletes the ozone layer (0.4% by trichloroethane

(ATRI, 1985)). Recent investigations have revealed that 1,1,1-trichloroethane may be converted into the toxic 1,2-dichloroethene in the C-horizon (DVGW, 1985).

Food chain:

Roughly 79% of 1,1,1-trichloroethane is absorbed via respiration, 17% by way of foodstuffs and 4% in drinking water.

ENVIRONMENTAL STANDARDS

Medium/ acceptor	**Sector**	**Country/ organ.**	**Status**	**Value**	**Cat.**	**Remarks**	**Source**
Water:	Drinkw	D	L	0.01 mg/l		1)	acc. TVO, 1990
	Drinkw	EC	G	1 g/l		2)	acc. DVGW, 1985
	Groundw	D	G	25 g/l		1)	acc. UBA, 1986
Air:		D	L	90 mg/m^3	MIK	Short-time value	acc. BAUM, 1988
		D	L	30 mg/m^3	MIK	Long-time value	acc. BAUM, 1988
	Emiss.	D	L	0.1 g/m^3		mass flow > 2 kg/h	acc. TA Luft, 1986
	Workp	D	L	1,080 mg/m^3	MAK		DFG, 1989
	Workp	SU	(L)	20 mg/m^3	PDK		*acc. SORBE, 1986*

	Workp	USA	L	1,900 mg/m^3		Long-time value	ACGIH, 1986
	Workp	USA	L	2,450 mg/m^3		Short-time value	ACGIH, 1986
Foodstuffs:		D	L	0.1 mg/kg		3)	*acc. UMWELT, 1989*
		D	L	0.2 mg/kg		4)	*acc. UMWELT, 1989*

Notes:

1) Total concentration for 1,1,1-trichloroethane, dichloromethane, trichloroethylene and tetrachloroethylene

2) Sum total of org. chlorine compounds except pesticides

3) 0.1 mg/kg for one of the following substances in each case: tetrachloroethylene, trichloroethane or chloroform

4) As sum total of several solvents within a foodstuff product.

Comparison/reference values

Medium/origin	**Country**	**Value**	**Source**
Surface water:			
Rhine tributaries, 1978	D	0.1-20 g/l	acc. DVGW, 1985
Rhine: (Lobith, 1978)	D	0.01-0.67 g/l	acc. DVGW, 1985
Main: (Kostheim, 1978)	D	1.76-2.57 g/l	acc. DVGW, 1985
		max. 98 g/l	

Lower Main (1980)	D		acc. DVGW, 1985
Drinking water:			
Ried (1980)	D	max. 1.5 g/l	acc. DVGW, 1985
Mannheim (1980)	D	max. 2.5 g/l	acc. DVGW, 1985
Japan (5 cities, 1977)	J	max. 0.5 g/l	acc. DVGW, 1985
Vienna (1980)	A	0.11 g/l	acc. DVGW, 1985
Gothenburg (1978)	S	0.06 g/l	acc. DVGW, 1985
Air:			
Mean air concentration		0.1 g/m^3	acc. DVGW, 1985
Densely populated areas		0.5-1 g/m^3	acc. DVGW, 1985
Bremen (May-June 1980)	D	0.98 g/m^3 (n=15)	acc. ATRI, 1985
Bochum (June-Dec. 1978)	D	1.8 g/m^3	acc. ATRI, 1985
Niagara Falls and Buffalo	USA	3,600 ng/m^3	acc. ATRI, 1985
Sediment:			
		< 1 g/l	

Ruhr (1972-1981)	D		acc. DVGW, 1985
Sewage sludge	GB	0.02 mg/kg	acc. ATRI, 1985
Foodstuffs:			
Dairy products and fruit	D	max. 0.6 g/kg	acc. ATRI, 1985
Olive oil	E	10 g/kg	acc. ATRI, 1985
Beef, fat	GB	6 g/kg	acc. ATRI, 1985
Potatoes	GB	4 g/kg	acc. ATRI, 1985

Assessment/comments

Although 1,1,1-trichloroethane is less toxic than other chlorinated hydrocarbons, the substance cannot be used without restriction. Chronic exposure to low concentrations can cause malignant liver tumours. However, another difference between 1,1,1-trichloroethane and tri- or tetrachloroethylene is its higher stabiliser content which in turn may be harmful. Thus, a substance which is only slightly toxic in its pure form may be highly toxic because of its additives. Residues increasingly accumulate in groundwater as well as in the atmosphere.

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Trichloroethene

DESIGNATIONS

CAS No.: **79-01-6**
Registry name: **Trichloroethene**
Chemical name: **Ethene, trichloro**
Synonyms, Trade names: **Tri, ethene trichloride, trichloroethene, Chlorylen, Algylen, Benzinol, Circosolv, Lanadin, Perm-a-chlor, Triasol, Trichloran, Triclene, Trimar, Vitran and many others**
Chemical name (German): **Trichlorethen**
Chemical name (French): **Trichlorothne, thne trichlor**
Appearance: **colourless, volatile liquid with sweet odour reminiscent of chloroform, the gas is much denser than air.**

BASIC CHEMICAL AND PHYSICAL DATA

Empirical formula:	C_2HCl_3
Rel. molecular mass:	131.4 g
Density:	1.46 g/cm^3 at 20C
Relative gas density:	4.54
Boiling point:	86.7C
Melting point:	-73 to -87C

Vapour pressure:	77 hPa at 20C
Ignition temperature:	410C
Explosion limits:	7.9 - 41 Vol%
Odour threshold:	50 ppm in air
Solvolysis/solubility:	in water: 1.1 g/l at 20C; readily soluble in organic solvents
Conversion factors:	1 ppm = 5.46 mg/m^3
	1 mg/m^3 = 0.18 ppm

ORIGIN AND USE

Usage:
Trichloroethene is used for a wide range of applications. 75-80% of the worldwide trichloroethene production is used for degreasing in the metal and glass industry (DVGW, 1985). Because of its good solvent properties, it was formerly used in dry-cleaning facilities and for the extraction of natural substances (e.g. for decaffeinated coffee and for fruit juice extracts). It is also used as an intermediate product in the manufacture of chloroacetic acid and as a solvent for greases, oils, waxes, resins, rubber, paints, lacquers, cellulose ester and cellulose ether.

Origin/derivation:

Trichloroethene is an artificial compound; it is produced synthetically from 1,2-dichloroethane. Stabilisers are added to the marketed product.

Production figures:

Worldwide	1978-80	600,000 t	(RIPPEN, 1989)
EC	1984	200,000 t	(ULLMANN, 1986)
USA	1984	110,000 t	(ULLMANN, 1986)
Federal Republic of Germany	1984	30,400 t	(RIPPEN, 1989)
Japan	1984	80,000 t	(ULLMANN, 1986)

with a common annual decline of 5 - 7 % worldwide

Toxicity

Humans:	LD_{100} 150 g, dermal	acc. RIPPEN, 1989
	TCL_0 44 mg/l, inhalation (83 min)	acc. RIPPEN, 1989

Mammals:		
Rat:	LC_{50} 7,200 mg/kg, oral (14 d)	acc. RIPPEN, 1989
	LC_{50} 28-29 mg/kg, dermal	acc. RIPPEN, 1989
	NEL 400 mg/kg, oral (28 d)	acc. RIPPEN, 1989
Mouse:	LD_{50} 2,400 mg/kg, oral	acc. RIPPEN, 1989
	LC_{50} 45 mg/l, inhalation (4 h)	acc. RIPPEN, 1989
Rabbit:	LD 7,330 mg/kg	acc. DVGW, 1985
Cat:	LD 5,860 mg/kg	acc. DVGW, 1985
Dog:	LD_{50} 5,900 mg/kg	acc. DVGW, 1985
Aquatic organisms:		
	LC_{50} 120-150 mg/l (48 h)	acc. RIPPEN, 1989
American minnow:	LC_{50} 41-67 mg/l (96 h)	acc. RIPPEN, 1989
	EC_{50} 22 mg/l (96 h)	acc. RIPPEN, 1989
Blue perch:		acc. RIPPEN, 1989

	LC_{50} 41-45 mg/l (96 h)	
Water flea:	EC_{50} 21 mg/l (48 h)	acc. RIPPEN, 1989
Plants:		
Green algae:	EC_{50} 530 mg/l (24 h)	acc. RIPPEN, 1989

Characteristic effects:

Humans/mammals: Trichlorethene irritates the eyes and skin as well as having a narcotic effect; loss of consciousness occurs on inhaling an amount of more than 3 mg/kg weight. Loss of weight and nervous phenomena such as headaches, disturbance of consciousness, agitation and frenzy are the consequences of chronic absorption which damages the central nervous system (with female employees from more than 200 vppm; RIPPEN, 1989).

Trichloroethene likewise affects the heart, liver and kidneys. For a long time the substance was considered carcinogenic, but the current opinion is that the pure substance is not. The enhanced tumour rates in animal experiments were the result of stabilisers added to trichloroethene such as epichlorohydrin or epoxybutane. Experiments performed in the USA with pure trichloroethene have, however, revealed an increase in the number of tumours in two types of animal (UBA, 1986).

A direct degradation product has likewise proven to be injurious to humans: trichloroacetyldehydride forms in the body and has a mutagenic effect.

Plants: Trichloroethene inhibits cell reproduction and stunts growth. Slight yellowing of leaves is sometimes encountered.

ENVIRONMENTAL BEHAVIOUR

Water:

Trichloroethene is denser than water and sinks gradually to the bottom even in groundwater. Groundwater contamination may last for many decades. It is listed in water hazard class 3 (extremely hazardous) in Germany.

Air:

Because of its volatility, large quantities of the substance produced (an estimated 50,000 t in 1979; DVGW, 1985) evaporate and are uniformly distributed in the atmosphere (ubiquitous). Exchange takes place between air and water. According to RIPPEN (1989), the substance makes a minor contribution to the formation of smog. It is washed out by precipitation and thus ingresses into surface water or groundwater.

Soil:

The substance accumulates in sediment; in sewage sludge, sometimes even to an extent which damages anaerobes.

Half-life:

The estimated dwell time in the atmosphere is roughly 1 week. If not evaporated, trichloroethene is persistent for 2-18 months in water-unsaturated soils. The half-life in seawater (pH 8 / 10C) is 39 weeks and 2.5 - 6 years in freshwater (RIPPEN, 1989). The half-life in darkness is 11 months. Trichloroethene is stable under normal conditions (pH 7 / 25C) (RIPPEN, 1989).

Degradation, decomposition products:

Trichloroethene is converted when exposed to light and heat in the atmosphere to phosgene, formyl chloride, acetyl chloride and finally to CO_2 and HCl. In water, it forms $CHCl_2COCl$. Hexachlorobenzene is formed at high temperatures; reaction with alkaline materials (e.g. mortar) to form dichloroacetylene. Anaerobic transformation to dichloroethene isomers and vinyl chloride takes place in contaminated groundwater, in anaerobic soil and on dumps. There is no transformation in sandy soils. There is degradation by adapted microorganisms.

Food chain:

Approx. 2-4% of the human intake of trichloroethene results from drinking water, 3-26% from foodstuffs and 70-95% from the air (UBA, 1986). Metabolism and accumulation take place in the bodily tissue.

ENVIRONMENTAL STANDARDS

Medium/ acceptor	Sector	Country/organ.	Status	Value	Cat.	Remarks	Source
Water:		CH	G	25 g/l		1)	acc. RIPPEN, 1989
	Drinkw	A	L	30 g/l		2)	acc. RIPPEN, 1989
	Drinkw	A		100 g/l		3)	acc. RIPPEN, 1989
	Drinkw	D	G	10 g/l	TVO	4)	acc. DVGW, 1985
	Drinkw	DDR	G	1 g/l			acc. RIPPEN, 1989
	Drinkw	EC	G	1 g/l		5)	acc. DVGW, 1985
	Drinkw	USA	G	75 g/l		6)	acc. RIPPEN, 1989
	Drinkw	WHO	G	30 g/l			acc. DVGW, 1985
	Surface	USA	G	27 g/l			acc. UBA, 1986
	Waste water	D	R	5 g/m^3		At point of discharge	acc. ROTH, 1989
Air:	Emiss.	D	L	0.1 g/m^3		mass flow > 2 kg/h	acc. TA Luft, 1986

Workp	D	L	270 mg/m^3	TRK	Kat. 3	DFG, 1994
Workp	DDR	L	750 mg/m^3	MAK_K		acc. HORN, 1989
Workp	DDR	L	250 mg/m^3	MAK_D		acc. HORN, 1989
Workp	SU	(L)	10 mg/m^3	PDK		acc. RIPPEN, 1989
Workp	USA	(L)	270 mg/m^3	TWA		acc. RIPPEN, 1989
Workp	USA	(L)	1,080 mg/m^3	STEL		ACGIH, 1986
	D	L	30 mg/m^3	MIK_K		acc. BAUM, 1988
	D	L	90 mg/m^3	MIK_D		acc. BAUM, 1988
	D	G	5 mg/m^3		1/2 h, VDI Guideline 2310	acc. LAU-BW, 1989
	DDR	L	4 mg/m^3	MIK_K		acc. HORN, 1989
	DDR	L	1 mg/m^3	MIK_D		acc. HORN, 1989
	WHO	G	1 mg/m^3		24 h	acc. LAU-BW, 1989
	D	L	500 g/dl	BAT	8)	DGE, 1989
	D	L	100 mg/l	BAT	9)	DFG, 1989

Foodstuffs:		D	L	0 mg/kg	LHmV		acc. UMWELT, 1989
		D	L	0.2 mg/kg	LHmV	10)	acc. UMWELT, 1989

Notes:

1) Provisional tolerance value (sum total of all chlorinated solvents)
2) Sum total of 14 halogenated hydrocarbons
3) Sum total of 14 halogenated hydrocarbons in less than 6 months
4) Sum total of trichloroethane, trichloroethene, tetrachloroethene and dichloromethane
5) Sum total of organic chlorine compounds except pesticides
6) With chronic exposure
7) Criterion for water quality
8) Parameter, trichloroethanol in whole blood
9) Parameter, trichloroacetic acid in urine
10) Cumulative value for several solvents in one item of food

COMPARISON/REFERENCE VALUES

Medium/origin	**Country**	**Value**	**Source**
Drinking water:			
Bremen (1980)	D	0.1 g/l	acc. DVGW, 1985

Mannheim (1980)	D	0.3 - 7.1 g/l	acc. DVGW, 1985
Taunus (1980)	D	<9.5 g/l	acc. DVGW, 1985
Great Britain (1981)	GB	0.24 g/l	acc. DVGW, 1985
Japan (1977)	J	0.2-0.9 g/l (5 cities)	acc. DVGW, 1985
USA (1977)	USA	0.1-0.5 g/l (5 cities)	acc. DVGW, 1985
Vienna 1984)	A	<3.5 g/l	acc. RIPPEN, 1989
Zurich (1977)	CH	0.005-0.105 g/l	acc. DVGW, 1985
Gothenburg	S	0.015 g/l	acc. DVGW, 1985
Surface water			
Rhine (Basle, 1982)	D	0.2-2.44 g/l	acc. DVGW, 1985
Rhine (Cologne, 1983)	D	0.06-0.81 g/l	acc. DVGW, 1985
Main (1980)	D	0.4-13 g/l	acc. DVGW, 1985
Lake Constance (1982)	D	0.01- 0.08 g/l	acc. DVGW, 1985
Liverpool Bay	GB	0.3 g/l	acc. RIPPEN, 1989
Niagara (1981)	USA	8 g/l (mean value)	acc. RIPPEN, 1989
Lake Ontario (1981)	CDN	13 g/l (mean value)	acc. RIPPEN, 1989
Gulf of Kavala	GR	0.26-2.80 ng/l	acc. RIPPEN, 1989

Switzerland (1981-83)	CH	<1.3 g/l (mean value)	acc. RIPPEN, 1989
Japan (1974)	J	5 g/l (mean value)	acc. RIPPEN, 1989
Gulf of Mexico, coast	MEX	10-50 ng/l	acc. RIPPEN, 1989
South Pacific (1981)		0.1-0.7 ng/l	acc. RIPPEN, 1989
Groundwater			
North Bremen (1985)	D	<100 g/l	acc. DVGW, 1985
Holland	NL	<1,000 g/l (mean value)	acc. RIPPEN, 1989
Holland, contaminated	NL	3,000 g/l	acc. RIPPEN, 1989
Great Britain	GB	<0.01 - 60 g/l	acc. RIPPEN, 1989
Minnesota	USA	0.2 - 6.8 g/l	acc. RIPPEN, 1989
Ohio, contaminated	USA	<6,000 g/l	acc. RIPPEN, 1989
Switzerland (1981-83)	CH	<15 g/l	acc. RIPPEN, 1989
Sediment/soil:			
Rhine (1978)	D	<300 g/kg	acc. DVGW, 1985
Rhine (Hitdorf) (1982)	D	<10 g/kg	acc. DVGW, 1985
Black Forest, west facing	D	8 - 30 g/m^3	acc. RIPPEN, 1989
Close to dry cleaning establishments	D	30 - 200 g/m^3	acc. RIPPEN, 1989

Sewage sludge (dry subst.)	USA	0.048 - 44 mg/kg	acc. RIPPEN, 1989
Air			
Northern hemisphere		87 ng/m^3	acc. RIPPEN, 1989
Southern hemisphere		8.2 ng/m^3	acc. RIPPEN, 1989
Arctic (1980-82)		22 - 220 ng/m^3	acc. RIPPEN, 1989
Frankfurt, city centre	D	2-46 g/m^3 (max.: 1,100)	acc. RIPPEN, 1989
Berlin (1977)	D	1-61 g/m^3	acc. RIPPEN, 1989
Japan (1979)	J	0.08-32 g/m^3	acc. RIPPEN, 1989
Sweden (city)	S	10 g/m^3	acc. RIPPEN, 1989
Mammals:			
Invertebrates		1-10 g/kg	acc. RIPPEN, 1989
Fish		0.5-100 g/kg	acc. RIPPEN, 1989
Waterfowl		1-100 g/kg	acc. RIPPEN, 1989
Mammals		1-10 g/kg	acc. RIPPEN, 1989
Humans (fat)		< 32 g/kg	acc. RIPPEN, 1989
Humans (total)		1 g/kg	acc. RIPPEN, 1989

Foodstuffs:			
Beverages	D	<0.1-8 g/kg	acc. RIPPEN, 1989
Solid food	D	0.1-64 g/kg	acc. RIPPEN, 1989

Assessment/comments

Because of the high toxicity in aquatic organisms, the US EPA recommends a general surface-water concentration of zero. As the risk of cancer due to the consumption of contaminated drinking water cannot be precluded, a quality value has been established for the sum of four similar chlorinated hydrocarbons. Despite an extremely broad span in various countries, this figure should not exceed 10 μ g/l for drinking water.

As trichloroethene is a typical contaminant for sewage water from cities and communities, it must be handled carefully to minimise emissions.

In the Nineties, several countries restricted the use of trichloroethene by law, so that gradually a replacement is taking place.

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2,4,5-trichlorophenoxy acetic acid

DESIGNATIONS

***CAS No.:* 93-76-5**
***Registry name:* 2,4,5-Trichlorophenoxy acetic acid**
***Chemical name:* Acetic acid, (2,4,5-trichlorophenoxy)**
***Synonyms, Trade names:* 2,4,5-T**
***Chemical name (German):* 2,4,5-Trichlorphenoxyessigsure, 2,4,5-T**
***Chemical name (French):* 2,4,5-trichlorophnoxy acide actique,**
***Appearance:* colourless to white, musty smelling crystals**

BASIC CHEMICAL AND PHYSICAL DATA

Empirical formula:	$C_8H_5Cl_3O_3$
Rel. molecular mass:	255.49 g
Density:	1.803 g/cm^3 at 20C
Boiling point:	above 200C decomposition
Melting point:	157-158C (acid); 113-115C (triethanolamine salt)
Vapour pressure:	0.7 x 10^{-6} Pa at 25C
Solvolysis/solubility:	in water: 280 mg/l at 25C
	in diethylether: 234 g/l;

	in toluene: 7.3 g/l;
	in xylene: 6.1 g/l;
	soluble in isopropyl alcohol;
	the alkali and amine salts of 2,4,5-T are readily soluble in water, whereas the esters are virtually insoluble in water but soluble in mineral oils

ORIGIN AND USE

Usage:
2,4,5-T is used in forestry and in agriculture as a systemic herbicide (for eradication of undergrowth etc.). The US military used it during the defoliation campaigns in Vietnam (mixture of 2,4,5-T and 2,4-D). These mixtures contained a significant amount of TCDD, which caused severe illnesses. 2,4,5-T as a salt or ester is generally applied in combination with other phenoxy acids. Its usage is restricted in Germany.

Origin/derivation:
2,4,5-T is produced synthetically by the reaction of 2,4,5-trichlorophenol, chloroacetic acid and sodium hydroxide. Lindane production residues are also useful for the 2,4,5-T synthesis.

The technical product contains 2.9% dichloromethoxyphenoxyacetic acid, 0.6% dichlorophenoxyacetic acid, 0.4% bis(2,4,5-trichlorophenoxy)acetic acid and < 0.5 mg/kg TCDD (dioxin). As of 1981, manufacturers guarantee a TCDD content of < 0.01 mg/kg (DFG, 1986). There are about 400 products which contain 2,4,5-T.

Production figures:

Worldwide (1992, estimated)	1,000 - 3,000 t	(RIPPEN, 1989)
USA (1968)	27,000 t	(RIPPEN, 1989)
USA (1979)	<1,000 t	(RIPPEN, 1989)
USA (1985)	banned	(RIPPEN, 1989)
D (1977)	1,800 t	(RIPPEN, 1989)
D (1984)	no further production	
EC (1980)	1,000 t	(RIPPEN, 1989)

Toxicity

Mammals:		
Rat:	LD_{50} 500 mg/kg, oral	acc. PERKOW, 1989
Rat:	LD_{50} >5000 mg/kg, dermal	acc. PERKOW, 1989
Rat:	LD_{50} 300-800 mg/m^3, oral	acc. RIPPEN, 1989

Rat:	LC_{50} 0.83 mg/l, inh. (4 h)	acc. RIPPEN, 1989
Mouse:	LD_{50} 389 mg/kg, oral	acc. RIPPEN, 1989
Dog:	LD_{50} 100 mg/kg, oral	acc. RIPPEN, 1989
Guinea pig:	LD_{50} 380 mg/kg, oral	acc. RIPPEN, 1989
Birds:		
Chicken:	LD_{50} 310 mg/kg, oral	acc. RIPPEN, 1989
Aquatic organisms:		
Rainbow trout:	LC_{50} 0.98 mg/l, semistat. (96 h)	acc. RIPPEN, 1989
Striped sawfish:	LC_{50} 15 mg/l (96 h)	acc. RIPPEN, 1989
Carp:	LC_{50} 0.87 mg/l (48 h)	acc. RIPPEN, 1989
Golden orfe:	LC_{50} 530 mg/l (48 h)	acc. RIPPEN, 1989
Plants:		

Cress seeds:	ED_{50} 0.02 ppm	acc. RIPPEN, 1989
Winter rye seeds:	ED_{50} 8.3 ppm (72h)	acc. RIPPEN, 1989

Note:
Comprehensive toxicity data for various species of animal can be found in DFG (1986).

Characteristic effects:

Humans/mammals: **2,4,5-T considerably irritates the eyes, and the skin. Skin resorption is likely. Chronic exposure causes impairment of the liver function, changes in behaviour and nerve damage. Chloracne is frequently encountered because of the contamination with chlorophenols and TCDD. The teratogenic effect is attributed to contamination with TCDD and not to the pure 2,4,5-T.**

The no-effect level in the most sensitive type of animal (mice) is 20 mg/kg (DFG, 1986).

2,4,5-T is found to be slightly mutagenic and teratogenic. There are not enough facts to definitely attest cancerogenic effects.

Plants: **2,4,5-T is an effective defoliant. Plants (and in particular dicotyledons) absorb 2,4,5-T through their leaves and metabolise the substance. Numerous metabolic processes are impaired. The direct effect sometimes takes the form of problems with passive permeability, but is also reflected by increased oxygen formation and greater growth. 2,4,5-T also acts as decoupler for the respiratory chain.**

ENVIRONMENTAL BEHAVIOUR

Water:
There is moderate sorption of 2,4,5-T on organic suspended matter and on sediments. It forms a film on the

water's surface and is photolytically decomposed. Residues may be leached into the groundwater.

Air:

In hot climates, a considerable amount of the quantity applied is subject to evaporation. In the atmosphere, 2,4,5-T is either subject to photolytic decomposition or washed out by precipitation. The estimated half-life is about 1 day.

Soil:

In soil, 2,4,5-T is either microbially degraded or it evaporates into the atmosphere. The majority of the herbicide remains in the topsoil (up to depths of 10 cm) due to the moderate mobility in soil. Considerable amounts are taken from the soil by plants.

Half-life:

More than 90% of the 2,4,5-T in soil is degraded within 70 days and 99% within one year (WEGLER, 1982). According to RIPPEN (1989), the "detoxification time" is, however, 270 days (extrapolated). A half-life in soil between 2 and 10 weeks is reported (DFG, 1986). In damp loam (application of 0.6 - 3.4 kg/ha) the substance can still be detected after 2-5 weeks. No further degradation takes place after 7 days in sewage treatment plants under aerobic conditions. The half-life in grass is 17 days.

Degradation, decomposition products:

Above 500C, the substance is thermally destroyed and TCDD is formed. In an acid milieu, it is stable. In soil, degradation is mainly due to microorganisms; degradation to form CO_2 is accelerated by humic substances and fulvic acids. 2,4,5-trichlorophenol forms in anaerobic sediments and during photolysis in the presence of humic substances. 2,4,5-T is transformed into chlorophenols, polyphenols, quinones and products similar to humic acids.

Combination effects:

Synergism with TCDD (> 1.5 ppm) is assumed (RIPPEN, 1989). Subcutaneous injections of lindane, phenobarbital or DDT over a period of several days accelerate the 2,4,5-T metabolism.

ENVIRONMENTAL STANDARDS

Medium/ acceptor	**Sector**	**Country/ organ.**	**Status**	**Value**	**Cat.**	**Remarks**	**Source**
Water:	Surface	EC	L	0.001 mg/l		1)	acc. DVGW, 1988
	Surface	EC	L	0.0025 mg/l		2)	acc. DVGW, 1988
	Surface	EC	L	0.005 mg/l		3)	acc. DVGW, 1988
	Drinkw	A		10 mg/l			acc. DVGW, 1988
	Drinkw	D	L	0.1 mg/l			acc. DVGW, 1988
	Drinkw	EC	L	0.1 mg/l			acc. DVGW, 1988
Air:	Workp	D	L	10 mg/m^3	MAK		acc. DFG, 1994
	Workp	USA	(L)	10 mg/m^3	TWA		acc. RIPPEN, 1989
Foodstuffs:		D	G	0.03 mg/kg.d	ADI	TCDD: <0.01 mg/kg.d	DFG, 1986
		D	L	2 mg/kg	4)	Forest fungi	acc. DVGW, 1988
		D	L	0.05 mg/kg	4)	Vegetable foodstuffs	acc. DVGW, 1988

Notes:

1) For drinking water treatment in each case: A1 for simple physical treatment and sterilisation

2) For drinking water treatment in each case: A2 for normal physical/chemical treatment and sterilisation

3) For drinking water treatment in each case: A3 for physical and refined chemical treatment, oxidation, adsorption and sterilisation

4) Order Governing Maximum Amounts of Pesticide, as at 1984

Usage banned in Italy since 1970; likewise in Holland, Norway, Sweden and the USA.

The TCDD level permitted in the Federal Republic of Germany must not exceed 0.005 mg/kg technical active substance (DFG, 1986).

The use of 2,4,5-T is restricted in Germany in the vicinity of surface water (Order Governing Use of Pesticides, as at 1986: use by aircraft and rail vehicles banned, as is utilisation on areas of open land not set aside for agriculture or gainful horticulture).

All 2,4,5-T formulations have been banned since 1985.

Comparison/reference values

Medium/origin	**Country**	**Value**	**Source**
Foodstuffs:			
Coot/muscle in contaminated areas		<1.34 ppm	acc. RIPPEN, 1989
Coot/fat in contaminated areas		<30 ppb	acc. RIPPEN, 1989
		0.1-30 ppm	

Foliage (n=37)	SF	0.1-30 ppm	acc. RIPPEN, 1989
Mushrooms (n=26)	SF	<0.02-1.8 ppm	acc. RIPPEN, 1989
Berries (n=32)	SF	0.07-15 ppm	acc. RIPPEN, 1989

Assessment/comments

The epidemiological investigations performed to date indicate only a minor risk of cancer and species-specific and dosage-dependent teratogenic effects in certain animals. These results cannot however be projected onto humans. To avoid TCDD formation, 2,4,5-T residues must not be incinerated. If applied as a herbicide, the drift of the fogs should be watched.

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Vanadium

DESIGNATIONS

CAS No.:	7440-62-2	1314-62-1

Registry name:	Vanadium	Vanadium pentoxide
Chemical name:	Vanadium	Vanadium pentoxide
Synonyms, Trade names:	Vanadium	Vanadium(V)oxide, divanadium pentoxide, vanadic acid anhydride, vanadic anhydride, vanadium pentaoxide
Chemical name German):	Vanadium	Vanadium pentoxid
Chemical name (French):	Vanadium	Pentoxyde de vanadium, anhydride vanadique, pentaoxyde de vanadium
Appearance:	steely grey, ductile metal	yellow to orange, crystalline powder or dark grey to brown lumps; odourless and tasteless

BASIC CHEMICAL AND PHYSICAL DATA

Empirical formula:	V	V_2O_5
Rel. molecular mass:	50.94 g	181.88 g
Density:	6.11 g/cm3 at 18.7C	3.357 g/cm3
Relative gas density:		
Boiling point:	3380C	1750C (decomposition)
Melting point:	1930C	690C

Flash point:		not combustible; promotes the combustion of other combustible substances
Solvolysis/solubility:	insoluble in water, hydrochloric and sulphuric acid as well as in alkali lye at normal temperature, soluble in hydrofluoric and nitric acid	0.005 g/l at 20C in water, soluble in concentrated acids and lyes

ORIGIN AND USE

Usage:

Roughly 90% of vanadium compounds are used as alloying elements (80% in the form of ferrous vanadium and 9% as non-ferrous compounds in the aerospace industry). The pure metal serves as jacket material for nuclear fuel elements. Further use is as a catalyst, especially V_2O_5 in the production of sulphuric acid.

Origin/derivation:

Vanadium is found throughout the world and makes up 0.015% of the Earth's crust. The largest natural deposits are found in South Africa (42.2%), Russia (39.2%) and China (12.7%). Depending on location, the geogenic concentration in water fluctuates between 0.2 and 100 μ g/l in freshwater and between 0.2 and 29 g/l in seawater. The ocean bed serves as a long-term sink. Natural deposits in coal and crude oil vary between 1 and 1500 mg/kg (WHO, 1987). It is estimated that some 65,000 t are released into the environment each year by natural emissions (volcanoes, etc.) and 200,000 t by human activities (chiefly in metalworking).

Production figures:

1979:	29,700 t	acc. DVGW, 1985

1981:	35,000 t	acc. WHO, 1987
1980-84:	34-46,000 t	acc. WHO, 1988
1984	33,300 t	acc. RMPP, 1988

The principal producers are Chile, Finland, Namibia, Norway, South Africa, Russia and the USA.

Toxicity

Vanadium pentoxide:		
Mouse	LD_{50} 23.4 mg/kg, oral	acc. WHO, 1988
Rat	LC_{50} 70 mg/m^3, inhalation	acc. WHO, 1988
Rat	LD 10 mg/kg, oral	acc. WHO, 1988
Cat	LC_{50} 500 mg/m^3, inhalation	acc. WHO, 1988
Rabbit	LC 205 mg/m^3, inhalation	acc. WHO, 1988
Ammonium vanadate:		

Mouse	LD$_{50}$ 10 mg/kg, oral	acc. WHO, 1988
Vanadium trichloride:		
Mouse	LD$_{50}$ 24 mg/kg, oral	acc. WHO, 1988
Vanadium dibromide:		
Mouse	LD$_{50}$ 88 mg/kg, oral	acc. WHO, 1988
Vanadium sulphate:		
Rat	LD 10 mg/kg, oral	acc. WHO, 1988
Rabbit	LD$_{50}$ 59.1 mg/kg, subcutaneous	acc. WHO, 1988
Guinea pig	LD 800 mg/kg, subcutaneous	acc. WHO, 1988
Guinea pig	LD$_{50}$ 560 mg/kg	acc. WHO, 1988

Characteristic effects:

***Humans/mammals:* Vanadium pentoxide irritates the skin and mucous membranes (0.1 mg/m^3 after 8 hours) and acts as a blood, liver and kidney poison. Symptoms of chronic exposure are bronchitis, pneumonia, anaemia, liver**

and kidney damage (concentrations of 0.1 - 0.4 mg/m^3 during 10 years may result in changes in the nasal mucous membranes, chronic bronchitis and discolouration of the tongue; acc. HORN, 1989). The effect depends on the particle size: aerosols > 5 μ m cannot penetrate the lungs. 40-60% are excreted via the kidneys after 1-3 days with 10-12% being excreted via the intestines. Vanadium pentoxide inhibits enzymes and prevents the synthesis of ascorbic and fatty acids in addition to affecting DNA (HORN, 1989).

ENVIRONMENTAL BEHAVIOUR

Water:

Vanadium compounds are denser than water and sink to the bottom. Vanadium pentoxide slowly dissolves in a large volume of water and forms toxic mixtures. Vanadium trichloride, vanadium tetrachloride and vanadium oxytrichloride react with water when exposed to heat to form toxic and irritating hydrochloric acid vapours which in turn form a white mist over the water surface.

Air:

The atmosphere represents a transport medium. Vanadium pentoxide is a reactive solid which promotes the combustion of other combustible substances. Vanadium trichloride forms toxic mixtures in air which decompose vigorously in contact with moisture and form corrosive hydrogen chloride. Decomposition to chlorine gas or hydrogen chloride gas occurs at high temperatures. Vanadium tetrachloride and vanadium oxytrichloride are corrosive, non-combustible liquids, which, when exposed to heat, likewise form corrosive mists made up of vanadium pentoxide, hydrogen chloride gas or hydrochloric acid. These are denser than air and creep along the ground. Vanadium tetrachloride reacts vigorously in water to form corrosive vanadium trichloride, vanadium oxytrichloride and hydrochloric acid.

Soil:

Vanadium compounds are geogenic and ubiquitous. Vanadium is an essential trace element whose compounds are absorbed by plants and incorporated into their growth process. Vanadium thus finds its way from the soil into the food chain.

Degradation, decomposition products, half-life:

When exposed to light and heat, most vanadium compounds decompose to form corrosive vapours or gases. Contact with water usually produces vigorous reactions in which corrosive vapours and gases are likewise formed.

Food chain:

Plants and animals incorporate vanadium as an essential trace element. The daily intake with foodstuffs is estimated at 100 μ g for humans with most of the vanadium being excreted again without resorption.

ENVIRONMENTAL STANDARDS

Medium/ acceptor	Sector	Country/organ.	Status	Value	Cat.	Remarks	Source
Water:	Surface	D	G	0.05 mg/l		For treatment	(DVGW, 1985)
	Irrigation	USA		10 mg/l		Short-time value	(DVGW, 1985)
Soil:		D	G	50 mg/kg			(KLOKE, 1988)
Air:	Emiss.	D	L	5 mg/m^3		mass flow > 25 g/h$^{1)}$	acc. TA Luft, 1986
		DDR	(L)	0.002 mg/m^3		V_2O_5, long-time value	acc. HORN et al., 1989
	Workp	AUS	(L)	0.05 mg/m^3		V_2O_5 (smoke)	acc. MERIAN, 1984
	Workp	B	(L)	0.05 mg/m^3		V_2O_5 (smoke)	acc. MERIAN, 1984
				0.05 mg/m^3			

Workp	D	L	0.05 mg/m	MAK	V_2O_5 (fine dust)	acc. BAUM, 1988
Workp	CH	(L)	0.1 mg/m^3		V_2O_5 (smoke)	acc. MERIAN, 1984
Workp	CS	(L)	0.1 mg/m^3		V_2O_5 (smoke), average	acc. MERIAN, 1984
Workp	CS	(L)	0.3 mg/m^3		V_2O_5 (smoke), short term	acc. MERIAN, 1984
Workp	CS	(L)	1.5 mg/m^3		Dust	acc. WHO, 1988
Workp	DDR	(L)	0.1 mg/m^3		V_2O_5 (smoke)	acc. HORN et al., 1989
Workp	DDR	(L)	0.5 mg/m^3		V2O5 (dust), short time	acc. HORN et al., 1989
Workp	DDR	(L)	0.002 mg/m^3		V_2O_5 (dust), long time	acc. HORN et al., 1989
Workp	H	(L)	0.1 mg/m^3		V_2O_5 (smoke)	acc. WHO, 1988
Workp	I	G	0.015 mg/m^3		V_2O_5 (smoke)	acc. MERIAN, 1984
Workp	J	(L)	0.1 mg/m^3		V_2O_5 (smoke)	acc. MERIAN, 1984
Workp	NL	(L)	0.05 mg/m^3		V_2O_5 (smoke)	acc. WHO, 1988
Workp	RO	(L)	0.1 mg/m^3		V_2O_5 (smoke),	acc. WHO, 1988

				0.1 mg/m		short time	
	Workp	S	(L)	0.5 mg/m^3		V_2O_5 (dusts)	acc. ACGIH, 1982
	Workp	S	(L)	0.05 mg/m^3		V_2O_5 (smoke)	acc. MERIAN, 1984
	Workp	SF	(L)	0.05 mg/m^3		V_2O_5 (smoke)	acc. MERIAN, 1984
	Workp	SU	(L)	0.002 mg/m^3		24 h, V_2O_5	acc. STERN, 1986
	Workp	SU	(L)	0.1 mg/m^3		V_2O_5 (smoke)	acc. MERIAN, 1984
	Workp	SU	(L)	0.5 mg/m^3		V_2O_3	acc. KETTNER, 1979
	Workp	USA	(L)	0.05 mg/m^3	TWA	V_2O_5 (smoke/ dusts)	acc. ACGIH, 1986
	Workp	YU	(L)	0.1 mg/m^3		V_2O_5 (smoke)	acc. WHO, 1988

Note:

Limit and approximate values generally exist for the sum total of all vanadium compounds and are given in V_2O_5

1) dustlike V and its compounds, stated as V

Comparison/reference values

Medium/origin	**Country**	**Value**	**Source**

Water:			
Lake Constance (berlingen, 1973-74)		1.1-1.9 g/l	acc. DVGW, 1985
Rhine (Mannheim, 1971-74)		0.9-11.6 g/l	acc. DVGW, 1985
Rhine (Mainz, 1971-74)		1.6- 3 g/l	acc. DVGW, 1985
Rhine (Wiesbaden, 1971-74)		0.1-10.3 g/l	acc. DVGW, 1985
Main (Ottendorf, 1971-73)		0.2-9.6 g/l	acc. DVGW, 1985
Main (Kostheim, 1971-73)		0.9-16 g/l	acc. DVGW, 1985
Ruhr (Echthausen, 1983)		0.2-1.2 g/l	acc. DVGW, 1985
Seawater		0.2-29 g/l	acc. DVGW, 1985
Drinking water (USA, 1962, 100 cities)		n.d.--70 g/l	acc. DVGW, 1985
Soil/sediment:			
Various soils (mean)		100 mg/kg	acc. DVGW, 1985
Various soils		1-680 mg/kg	acc. WHO, 1988
Coal (mean)		30 mg/kg	acc. DVGW, 1985
Oil (mean)		50 mg/kg	acc. DVGW, 1985
Air:			

South Pole		0.001-0.002 ng/m^3	acc. WHO, 1988
Rural areas	CDN	0.21-1.9 ng/m^3	acc. WHO, 1988
Outdoors		0.02-13 μ g/m^3 V_2O_5	acc. HORN, 1989
Animals:			
Molluscs		0.7 mg/kg	acc. WHO, 1988
Crustaceans		0.4 mg/kg	acc. WHO, 1988
Insects		0.15 mg/kg	acc. WHO, 1988
Fish		0.14 mg/kg	acc. WHO, 1988
Mammals		0.4 mg/kg	acc. WHO, 1988

Assessment/comments

There are still no clear-cut results on the effects of the majority of vanadium compounds. Therefore, attempts should be made to avoid any possible impacts caused by them.

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Vinyl chloride

DESIGNATIONS

CAS No.: 75-01-4
Registry name: Vinyl chloride
Chemical name: Chloroethene
Synonyms, Trade names: Monochloroethene, ethene monochloride, VC, VCM, Freon 1140
Chemical name (German): Vinylchlorid
Chemical name (French): Chlorure de vinyle
Appearance: colourless gas with slightly sweet odour; it is transported only in stabilised condition (using phenol and its derivatives) in pressurised cylinders.

BASIC CHEMICAL AND PHYSICAL DATA

Empirical formula:	C_2H_3Cl
Rel. molecular mass:	62.50 g
Density:	0.9106 g/cm^3 at 20C, 0.983 g/cm^3 at -20C (liquid)

Relative gas density:	2.16
Boiling point:	-13.4 to -14.0C
Melting point:	-153.8 to -160.0C
Vapour pressure:	3,300 hPa at 20C; 4,500 hPa at 30C; 7,800 hPa at 50C
Flash point:	-77 to -78C
Ignition temperature:	415C
Auto-ignition:	472C
Explosion limits:	3.8-31 vol%
Odour threshold:	4,000 ppm in air
Solvolysis/solubility:	in water: 1.1 g/l at 25C;
	soluble in oil, alcohol, chlorinated solvents and hydrocarbons;
	enhanced by silver and copper salts due to complexing
Conversion factors:	1 ppm = 2.60 mg/m^3

	1 mg/m^3 = 0.39 ppm

ORIGIN AND USE

Usage:

96-98% of vinyl chloride is used to make polyvinyl chloride (PVC) with the remaining 2-4% being utilised in the manufacture of specific chlorinated hydrocarbons such as 1,1,1-trichloroethane, 1,1,2-trichloroethane and vinylidene chloride. VC is used on a large scale to make polymers (ATRI, 1985). About 25% of the world's total chlorine production is required for the production of VC.

Origin/derivation:

Production is by way of the addition of hydrogen chloride to acetylene or by way of the decomposition of 1,2-dichloroethane with the formation of hydrogen chloride as a by-product. The polymer of vinyl chloride is polyvinyl chloride (PVC).

Production figures:

Worldwide 1985:	13,500,000 t	(ULLMANN, 1986)
Worldwide:	10,000,000 t	(RIPPEN, 1988)
EC 1977:	3,500,000 t	(RIPPEN, 1988)
USA 1987:	3,800,000 t	(RIPPEN, 1991)
Japan 1980:	1,656,000 t	(ATRI, 1985)

Germany 1988:	1,459,000 t	(RIPPEN, 1991)
France 1982:	1,150,000 t	(ATRI, 1985)
Italy 1977:	750,000 t	(RIPPEN, 1988)
Taiwan 1984:	492,000 t	(RIPPEN, 1991)
Canada 1982:	408,000 t	(ATRI, 1985)
Great Britain 1977:	405,000 t	(RIPPEN, 1988)
Mexico 1984:	132,000 t	(RIPPEN, 1991)

Toxicity

Mammals:		
Mouse:	TCLo 50 ppmv, 120 h intermitt.	acc. RIPPEN, 1991
Rat:	LD_{50} 500 mg/kg, oral	acc. RIPPEN, 1991
Rat:	TCLo$^{1)}$ 6,000 ppm	acc. RIPPEN, 1991

Rabbit:	TCLo 500 ppm, inhalation (7 h/d during 6 months)	acc. RIPPEN, 1991

Note:
1) Inhalation, 4h, 12th-18th day after conception

Characteristic effects:

Humans/mammals: **This flammable, toxic and narcotic gas irritates the eyes, the skin and the respiratory tract. Repeated exposure damages the liver, kidneys and spleen; malignant tumours may occur. Toxic concentrations in air may occur without producing an alarming odour. VC is definitely carcinogenic and teratogenic (deformities and skeletal changes on inhalation) as revealed both by animal experiments and human exposure.**

Thermal decomposition produces acidic gases which irritate the eyes, the nose and the throat.

ENVIRONMENTAL BEHAVIOUR

Water:
Vinyl chloride is persistent in water, if not evaporating. However, there are no known cases of damage to aquatic organisms (UBA, 1986). Accumulation in the aquatic food chain is unlikely (BUA, 1989).

Air:
On expansion, the pressurised gas forms cold mists which are denser than air. They evaporate easily and form toxic, explosive mixtures. Accumulation in the atmosphere is likely because of the physical and chemical properties of vinyl chloride.

Half-life:
Under normal environmental conditions, vinyl chloride is extremely persistent. Under anaerobic conditions its half-

life in soil is more than 2 years. Aerobic degradation in sewage treatment plants and surface water in an isolated bacteria culture with 20-120 mg/l requires at least 5 weeks (UBA, 1986). OH radicals reduce the half-life to 66 h. The hydrolytic half-life is less than 10 years (calculated, 25C) (RIPPEN, 1991). The half-life in the troposphere is eleven weeks (abiotic degradation) (ATRI, 1985). An average half-life between 2.2 and 2.7 days is reported by the BUA (1989).

Degradation, decomposition products:
Photochemical oxidation results in the formation of HCl, CO and formyl chloride as well as formaldehyde. There is no photolysis of 10 mg/l in water at 300 nm over 90 hours. Biotic mineralisation is extremely slow.

Combination effects:
Vinyl chloride reacts with acetylene, chlorine, fluorine, oxidising agents and peroxides with considerable amounts of heat being generated. Polymers are formed. Light, heat and hydrogen sulphide act as polymerisation initiators.

ENVIRONMENTAL STANDARDS

Medium/ acceptor	**Sector**	**Country/organ.**	**Status**	**Value**	**Cat.**	**Remarks**	**Source**
Water:	Drinkw	EC	G	1 g/l		1)	acc. RIPPEN, 1991
	Groundw	NL	G	0.01 μ g/l		Reference	acc. TERRA TECH, 6/94
	Groundw	NL	L	0.7 μ g/l		Intervention	acc. TERRA TECH, 6/94
	Waste water	USA	G	50 g/l		2)	acc. RIPPEN, 1991
Air:		DDR	L	0.6 mg/m^3	MIK$_K$		acc. HORN, 1989

		DDR	L	0.2 mg/m^3	MIK$_D$		acc. HORN, 1989
	Emiss.	D	L	5 mg/m^3		mass flow > 25 g/h	acc. TA Luft, 1986
	Workp	D	L	8 mg/m^3	TRK	3)	DFG, 1989
	Workp	D	L	5 mg/m^3	TRK	In other cases	DFG, 1989
	Workp	DDR	L	30 mg/m^3		Long and short-time value	acc. HORN, 1989
	Workp	SU	(L)	5 mg/m^3			acc. UBA, 1986
	Workp	USA	(L)	10 mg/m^3	TWA	4)	ACGIH, 1986
	Workp	USA	(L)	0.010 ppmv	TLV	5)	acc. RIPPEN, 1989
Foodstuffs:		D	L	0.05 ppm		Packaging	acc. RIPPEN, 1989

Notes:

1) **Sum of all chlorinated hydrocarbons except pesticides**

2) **4 day average for special synthetics industry, direct introduction**

3) **Applies to existing installations**

4) **Clearly carcinogenic**

5) **Ambient air, California**

Within the framework of the specifications governing the handling of carcinogens, there is a special regulation in Germany for vinyl chloride. Accordingly, the concentration in workplace air must not exceed 3 ppm, marking and mandatory investigation are regulated, personal protection equipment defined and cleaning measures described (VGB 113, 1982, Appendix, 1 vinyl chloride). Furthermore, the Appendix to the BAT list (DFG, 1989) describes the relationship between the substance concentration in workplace air and the substance/metabolite concentration in biological material (EKA values) for vinyl chloride as a carcinogenic substance. The following accordingly applies:

mg/m^3	thiodiglycolic acid
2.6	1.8
5.2	2.4
10	4.5
21	8.2
42	10.6

Air vinyl chloride Sample: urine at end of shift/end of exposure

The Order Governing Vinyl Chloride Consumer Goods (1983) in Germany bans the marketing of articles with a monomeric vinyl-chloride content of > 1 mg/kg. No risk from foodstuffs is assumed as long as the detectable monomeric vinyl-chloride level does not exceed 0.01 mg/kg.

On the basis of the Order Banning PCB (superseded regulations enforced since 1978 in 1990) vinyl chloride cannot be used in the Federal Republic of Germany as a propellant for aerosols.

Vinyl chloride is a substance hazardous to water for which approval must be granted in line with 19a of the WHG if they are to be conveyed in pipelines.

Comparison/reference values

Medium/origin	**Country**	**Value**	**Source**
Surface water:			
New Jersey, 1977-79	USA	max. 570 g/l	acc. RIPPEN, 1991
Rhine, 1982	D	< 200 ng/l	acc. RIPPEN, 1991
Rhine tributaries	D	<0.001-0.005 mg/l	acc. ATRI, 1985
Drinking water:			
113 cities	USA	0.05-0.18 g/l	acc. RIPPEN, 1991
100 cities, 1977	D	max. 1.7 g/l	acc. ATRI, 1985
Groundwater:			
New Jersey, 1977-79	USA	max. 9.5 g/l	acc. RIPPEN, 1991
Nassau County	USA	1.6-2.5 g/l	acc. RIPPEN, 1991
Sediment/soil:			
Los Angeles Bay, 1980/81	USA	<0.5 g/kg	acc. RIPPEN, 1991
Sewage sludge	USA	3-110 mg/kg	acc. RIPPEN, 1991
Air:			

Clean-air zones	D	6.6-24 g/m^3	acc. ATRI, 1985
Taunus	D	0.01 g/m^3	acc. ATRI, 1985
Frankfurt a.M.	D	21.8 g/m^3	acc. ATRI, 1985
Industrial estate, Marl	D	213 g/m^3	acc. ATRI, 1985
Production facilities, 1980	NL	3-70 ppm	acc. RIPPEN, 1991
Dump gas, 1980-83	USA	max. 2,000 ppm	acc. RIPPEN, 1991
Animals:			
Invertebrates, Los Angeles	USA	<0.3 g/kg	acc. RIPPEN, 1991
Fish, liver	USA	<0.3 g/kg	acc. RIPPEN, 1991
Foodstuffs:			
Cooking oil in PVC packaging		0.05-14.8 mg/kg	acc. ATRI, 1985
Butter/margarine in PVC packaging		0.05 mg/kg	acc. ATRI, 1985
Alcoholic beverages		0-2.1 mg/kg	acc. ATRI, 1985

Assessment/comments

The use of vinyl chloride must be avoided as far as possible because of its definite carcinogenic effect and its high

persistence. Waste incineration is inadequate since incomplete combustion produces highly toxic pollutants (e.g. hydrochloric acid and TCDD). Special sources: ATRI (1985); DRAFT (1988). Polyvinyl chloride (PVC) should be substituted by other (non-chlorinated) materials wherever possible.

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