

TRIS(2-CHLOROETHYL) PHOSPHATE

1. Chemical and Physical Data

1.1 Synonyms

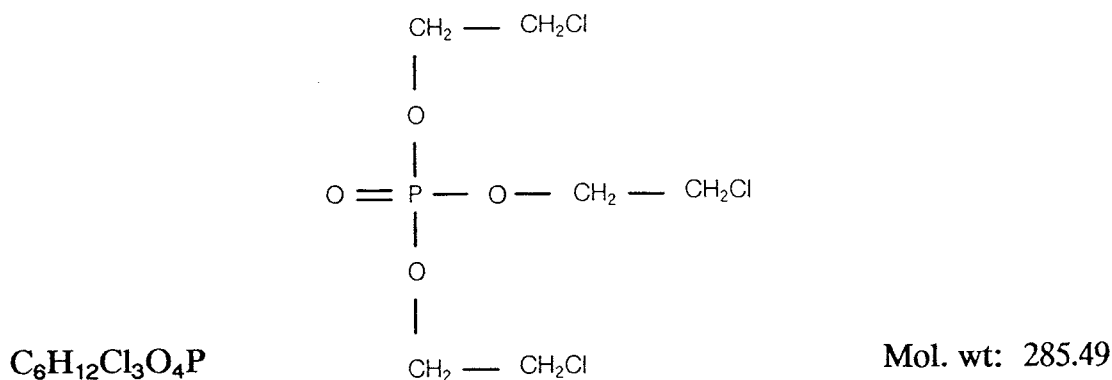
Chem. Abstr. Services Reg. No.: 115-96-8

Chem. Abstr. Name: Tris(2-chloroethyl) phosphate

IUPAC Systematic Name: Tris(2-chloroethyl) phosphate

Synonyms: Phosphoric acid, tris(2-chloroethyl) ester; TCEP; tri(chloroethyl) phosphate; tri(β -chloroethyl) phosphate; tri(2-chloroethyl) phosphate; tris(2-chloroethyl) orthophosphate; tris(chloroethyl) phosphate; tris(β -chloroethyl) phosphate

1.2 Structural and molecular formulae and molecular weight



1.3 Chemical and physical properties of the pure substance

- (a) *Description:* Clear, colourless liquid with a slight odour (Lefaux, 1968; Hawley, 1981)
- (b) *Boiling-point:* 330°C (Aldrich Chemical Co., 1988)
- (c) *Melting-point:* -55°C (Clayton & Clayton, 1981)
- (d) *Density:* 1.425 at 20°C (Clayton & Clayton 1981; Hawley, 1981)
- (e) *Spectroscopy data:* Mass (Chemical Information Systems, 1988), infrared (prism, Sadtler [6850], Aldrich [556E]; prism-FT [926C]; grating [33388]) and nuclear

magnetic resonance (proton, Sadtler [10547], Aldrich [876D]; C-13 [1036]) spectral data have been reported (Sadtler Research Laboratories, 1980; Pouchert, 1981, 1983, 1985).

- (f) *Solubility*: Very slightly soluble in water (0.7 wt %) and aliphatic hydrocarbons; soluble in alcohols, esters, ketones and aromatic hydrocarbons (Lefaux, 1968; Clayton & Clayton, 1981)
- (g) *Volatility*: Vapour pressure, < 10 mm Hg at 25°C (Akzo Chemicals, 1982)
- (h) *Flash-point*: 216°C (Hawley, 1981)
- (i) *Stability*: Thermally stable at temperatures below 150°C (Akzo Chemicals, 1982)
- (j) *Reactivity*: When heated to decomposition, carbon monoxide, hydrogen chloride, phosphorus oxides, phosphine and/or phosgene may be released (Morton Thiokol/Alfa Products Division, 1981; Aldrich Chemical Co., 1988).
- (k) *Refractive index*: 1.4721 (20°C) (Hawley, 1981)
- (l) *Viscosity*: 45 cp (20°C) (Lefaux, 1968)
- (m) *Octanol/water partition coefficient (P)*: log P, 1.7 (US Environmental Protection Agency, 1988)
- (n) *Conversion factor*: $\text{mg/m}^3 = 11.6 \times \text{ppm}^1$

1.4 Technical products and impurities

Trade names: Celanese celluflex CEF; Celluflex CEF; 3CF; CLP; Disflamoll TCA; Fyrol CEF; Fyrol CF; Genomoll P; Nix 3CF; Nix Flame Retardant 3CF

Tris(2-chloroethyl) phosphate is available with a purity of 97% (Morton Thiokol/Alfa Products Division, 1981; Aldrich Chemical Co., 1988). One commercial product contains 10.8 wt% phosphorus, 36.7 wt% chlorine and a maximum of 0.10 wt% water (Akzo Chemicals, 1980).

2. Production, Use, Occurrence and Analysis

2.1 Production and use

(a) Production

Tris(2-chloroethyl) phosphate is produced by the reaction of phosphorus oxychloride with ethylene oxide (see IARC, 1985) or ethylene chlorohydrin (Weil, 1980; Anon., 1985).

¹Calculated from: $\text{mg/m}^3 = (\text{molecular weight}/24.45) \times \text{ppm}$, assuming standard temperature (25°C) and pressure (760 mm Hg)

It is available from five manufacturers in the USA, five in Japan and two in France. Total production by the major manufacturers in Japan was approximately 1100 tonnes in 1984 and 1200 tonnes in 1985 (Anon., 1985, 1986). No other data on production were available to the Working Group.

(b) *Use*

Tris(2-chloroethyl) phosphate combines the flame-retarding properties of chlorine and phosphorus compounds. It is used in the manufacture of polyester resins, polyacrylates, polyurethanes and cellulose derivatives, especially materials based on ethyl cellulose, nitrocellulose and cellulose acetate (Lefaux, 1968; Hawley, 1981). This compound is used as a flame-retardant additive for flexible and rigid polyurethane and polyisocyanate foams, carpet backing, paints and lacquers, epoxy, phenolic and amino resins, and wood-resin composites such as particle boards. When blended with binders such as vinyl or acrylic emulsions, it may also be used to coat the backs of upholstery (Weil, 1980). The major use appears to be in foams, such as the flexible foams used in automobiles and furniture and rigid foams for building insulation (US Environmental Protection Agency, 1988). In Japan, about 90-95% is reportedly utilized in urethane and polyvinyl chloride resin additives (Anon., 1986). Direct application to or use in formulations to be applied to fabrics intended for apparel use is not recommended (Akzo Chemicals, 1980).

(c) *Regulatory status and guidelines*

No regulatory standard or guideline has been established for tris(2-chloroethyl) phosphate.

2.2 Occurrence

(a) *Natural occurrence*

Tris(2-chloroethyl) phosphate is not known to occur as a natural product.

(b) *Occupational exposure*

No data were available to the Working Group.

(c) *Air*

Tris(2-chloroethyl) phosphate was detected at concentrations of 2-5 ng/m³ in ambient air at Kitakyushu, Japan (Haraguchi *et al.*, 1985).

(d) *Water and sediments*

Tris(2-chloroethyl) phosphate has been detected in river water, seawater and sediment, presumably as an environmental pollutant from industrial and domestic wastewater. Nationwide surveys conducted in Japan in 1977 and 1978 by the Environmental Agency did not indicate the presence of tris(2-chloroethyl) phosphate in water or sediment from river estuaries or the sea; it was detected only at a level of 90 ng/l in a sample of sea-water. In a survey around Kitakyushu in 1980, however, tris(2-chloroethyl) phosphate was identified at levels of

17-347 ng/l in river water, 10-60 ng/l in sea-water and 13-28 ng/g in sediment (Ishikawa *et al.*, 1985a). Tris(2-chloroethyl) phosphate was also detected in river water and sewage sludge from the Okayama area (Kenmochi *et al.*, 1981).

Factory and domestic wastewater effluents in Kitakyushu, Japan, contained detectable levels of tris(2-chloroethyl) phosphate (detection limit, 30 ng/l). Concentrations of 83-87 ng/l were measured in effluents from two food factories, 43-740 ng/l at eight chemical factories, 170-14 000 ng/l at two steel factories, 45-11 000 ng/l at six other industrial sites, 40-560 ng/l at eight residences, 500-1200 ng/l at five sewage treatment plants and 51 ng/l in one metal processing plant. Although high levels were found in two factory effluents, the concentrations were not much higher than those in river water (17-350 ng/l; limit of detection, 10 ng/l), indicating that the pollution was due to a combination of municipal and industrial wastewater sources (Ishikawa *et al.*, 1985b).

Tris(2-chloroethyl) phosphate was detected in water from the River Rhine in the Netherlands at 1 µg/l in 1979 (Zoeteman *et al.*, 1980) and at 0.16-0.35 µg/l in 1986 (Brauch & Kühn, 1988). It was found at levels up to 5.5 µg/l in raw water samples from Trent, Torksey and Elsham, UK, in 1979-80 (Burchill *et al.*, 1983). The compound was also found in the River Waal at Brakel, The Netherlands, in 1974 (Meijers & van der Leer, 1976).

Tris(2-chloroethyl) phosphate was identified at a mean level of 0.57 µg/l in groundwater from two wells adjacent to a municipal wastewater infiltration system at Fort Devens, MA, USA, near Boston (Bedient *et al.*, 1983).

Tris(2-chloroethyl) phosphate has been identified in drinking-water throughout the world. It was found in one of 14 samples of drinking-water collected in 1976 in the UK (Fielding *et al.*, 1981); at 2.0-60.5 ng/l (mean, 17.4 ng/l) in drinking-water collected over a one-year period in Japan (Adachi *et al.*, 1984); at 0.3-9.2 ng/l in six eastern Ontario, Canada, treatment plants in 1978 (LeBel *et al.*, 1981); at 0.2-52 ng/l in 22 of 29 Canadian municipalities in 1979 (Williams & LeBel, 1981); at 0.3-13.8 ng/l in 11 of 12 Great Lakes municipalities in 1980 (Williams *et al.*, 1982); and at 3-9.6 ng/l in 1982 and 1983 in four of five Great Lakes areas (LeBel *et al.*, 1987).

(e) *Animal tissues*

Tris(2-chloroethyl) phosphate was identified at levels of < 0.005-0.019 µg/g in fish and shellfish captured in the Okayama, Japan, area (Kenmochi *et al.*, 1981).

2.3 Analysis

Selected methods for the analysis of tris(2-chloroethyl) phosphate are presented in Table 1.

Table 1. Methods for the analysis of tris(2-chloroethyl) phosphate

Sample matrix	Sample preparation	Assay procedure ^a	Limit of detection	References
Air	Sample on glass-fibre filter or XAD-7 resin; prefractionate on silica gel column	GC/NPD	0.04-0.1 ng	Haraguchi <i>et al.</i> (1985)
Water	Extract with dichloromethane; dry (anhydrous sodium sulfate); concentrate	GC/MS	10 ng/l	Ishikawa <i>et al.</i> (1985a); Ishikawa & Baba (1988)
	Extract with dichloromethane	GC/FPD	2 ng/l	Burchill <i>et al.</i> (1983)
Drinking-water	Adsorb on XAD resin cartridge; extract with dichloromethane; dry (anhydrous sodium sulfate); concentrate	GC/NPD	0.3 ng/l	LeBel <i>et al.</i> (1981)
	Adsorb on XAD resin cartridge; elute with acetone/hexane; dry (anhydrous sodium sulfate); concentrate; extract (dichloromethane)	GC/MS and GC/NPD	0.1 ng/l	LeBel <i>et al.</i> (1987)
Sediment	Extract with acetone; filter; add filtrate to purified water; extract with dichloromethane; dry (anhydrous sodium sulfate); concentrate	GC/MS	5 ng/g	Ishikawa <i>et al.</i> (1985a)
Sea-water, fish, sea sediment	Extract with acetonitrile and dichloromethane; adsorb; extract on activated charcoal column; extract with sulfuric acid; wash with sodium hydroxide; purify by Florisil chromatography	GC/MS	1-5 ng/g (fish)	Kenmotsu <i>et al.</i> (1980)
		GC/FPD		

^aAbbreviations: GC/NPD, gas chromatography/nitrogen phosphorus detection; GC/MS, gas chromatography/mass spectrometry; GC/FPD, gas chromatography/flame photometric detection

3. Biological Data Relevant to the Evaluation of Carcinogenic Risk to Humans

3.1 Carcinogenicity studies in animals¹

Skin application

Mouse: Groups of 35 female Swiss mice, nine weeks of age, received skin applications of tris(2-chloroethyl) phosphate (Genomoll P) [purity unspecified] in acetone to examine its initiating potential. One group of mice received a single application of 71 mg/mouse Genomoll P followed by applications of 1 µg/mouse tetradecanoyl phorbol acetate (TPA) twice a week for 78 weeks. A control group was treated with TPA alone. The incidence of squamous-cell papillomas of the skin was 17/33 (52%) Genomoll P plus TPA-treated animals and 12/28 (43%) TPA-treated mice; squamous-cell carcinomas of the skin developed in 2/33 Genomoll P plus TPA-treated animals but in none of the TPA-treated controls. The incidences of lung adenomas were 7/33 and 5/28 in Genomoll P plus TPA-treated and in TPA-treated groups, respectively (Sala *et al.*, 1982). [The Working Group noted that the promoting activity and complete carcinogenicity of Genomoll P could not be evaluated because of the lack of controls.]

3.2 Other relevant data

(a) *Experimental systems*

(i) *Absorption, distribution, excretion and metabolism*

No data were available to the Working Group.

(ii) *Toxic effects*

Acute oral LD₅₀s for tris(2-chloroethyl) phosphate have been reported to be 1230 for rats [sex unspecified] and 501 mg/kg bw for male rats; LD₅₀s for female rats were reported to be 794, 501 and 430 mg/kg bw with three different lots of the chemical (Ulsamer *et al.*, 1980).

Neurotoxic effects of tris(2-chloroethyl) phosphate have been reported in rats (Smith, 1936) and hens (Sprague *et al.*, 1981).

Tris(2-chloroethyl) phosphate did not react with DNA *in vitro* (Lown *et al.*, 1980).

(iii) *Effects on reproduction and prenatal toxicity*

Wistar rats were given 50, 100 or 200 mg/kg bw tris(2-chloroethyl) phosphate suspended in olive oil by gavage on days 7-15 of gestation. No change in maternal body weight gain, food

¹The Working Group was aware of studies in progress by oral administration in mice and rats and by skin application in mice (IARC, 1988).

consumption or general appearance was found in the low- and mid-dose groups, but in the high-dose group, maternal food consumption was markedly suppressed; piloerection and general weakness occurred, and 7/30 dams died. On day 20 of gestation, no increase in fetal deaths or in malformations attributable to treatment was observed in any group, but there was some increase in the incidence of cervical and lumbar ribs in the high-dose group. [The Working group noted that this result may have been related to maternal toxicity.] Postnatal examination revealed normal development in the offspring of all groups; no disorder attributable to treatment was observed on morphological examination, and no effect on functional behaviour was seen (Kawashima *et al.*, 1983).

(iv) *Genetic and related effects* (see Appendix 1)

Tris(2-chloroethyl) phosphate was not mutagenic to several strains of *Salmonella typhimurium* in the presence or absence of an exogenous metabolic system from livers of untreated rats or from rats or Syrian hamsters treated with Aroclor 1254 (Prival *et al.*, 1977; Haworth *et al.*, 1983). In contrast, tris(2-chloroethyl) phosphate produced a dose-related increase in mutations (with a maximal 7.6-fold increase in the number of revertants over that in controls at 10 $\mu\text{mol}/\text{plate}$) in *S. typhimurium* TA1535 in the presence but not in the absence of an exogenous metabolic system from the livers of rats treated with Kanechlor 500. The same doses produced a dose-related increase in mutations in *S. typhimurium* TA100, with a maximal 1.8-fold increase in the number of revertants at 10 $\mu\text{mol}/\text{plate}$ (Nakamura *et al.*, 1979).

Tris(2-chloroethyl) phosphate caused a dose-related (343-1000 $\mu\text{g}/\text{ml}$) increase in the incidence of sister chromatid exchange in the Chinese hamster V79 cell line. Doses up to 2 mg/ml did not induce mutation at the *hprt* locus in the same cell line. The compound induced dose-related (400-800 $\mu\text{g}/\text{ml}$) transformation in Syrian hamster embryo cells but only weakly transformed C3H 10T $\frac{1}{2}$ cells at 1.5 mg/ml. Equivocal results were obtained at 62.5-250 mg/kg bw in an assay for induction of micronuclei in Chinese hamsters *in vivo* (Sala *et al.*, 1982). It caused dominant lethal mutations in rats exposed by inhalation to 0.5 or 1.5 mg/m³ for four months (Shepel'skaia & Dyshginevich, 1981).

(b) *Humans*

No data were available to the Working Group.

3.3 Case reports and epidemiological studies of carcinogenicity to humans

No data were available to the Working Group.

4. Summary of Data Reported and Evaluation

4.1 Exposure data

Tris(2-chloroethyl) phosphate is used as a flame retardant in plastics, especially in flexible foams used in automobiles and furniture, and in rigid foams used for building insulation.

No data on occupational exposure levels were available. Tris(2-chloroethyl) phosphate has been detected in drinking-water, river water, sea water and sediments in various parts of the world.

4.2 Experimental carcinogenicity data

Tris(2-chloroethyl) phosphate was tested for initiating and promoting activity and for complete carcinogenicity in one strain of mice by skin application. No initiating activity was found; promoting activity and complete carcinogenicity could not be evaluated.

4.3 Human carcinogenicity data

No data were available to the Working Group.

4.4 Other relevant data

In single studies, tris(2-chloroethyl) phosphate gave equivocal results in a micro-nucleus test in Chinese hamsters *in vivo* and caused dominant lethal mutation in rats. It caused cell transformation and, in single studies, sister chromatid exchange but not mutation in rodent cells *in vitro*. It was not mutagenic to bacteria in the absence of an exogenous metabolic system but gave equivocal results in the presence of an exogenous metabolic system.

4.5 Evaluation¹

There is *inadequate evidence* for the carcinogenicity of tris(2-chloroethyl) phosphate in experimental animals.

No data were available from studies in humans on the carcinogenicity of tris(2-chloroethyl) phosphate.

Overall evaluation

Tris(2-chloroethyl) phosphate is *not classifiable as to its carcinogenicity to humans (Group 3)*.

5. References

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¹For description of the italicized terms and criteria for making the evaluation, see Preamble, pp. 25-29.

Summary table of genetic and related effects of tris(2-chloroethyl) phosphate

Nonmammalian systems												Mammalian systems																																					
Proka-ryotes		Lower eukaryotes				Plants			Insects			In vitro									In vivo																												
												Animal cells						Human cells			Animals			Humans																									
D	G	D	R	G	A	D	G	C	R	G	C	A	D	G	S	M	C	A	T	I	D	G	S	M	C	A	T	I	D	G	S	M	C	DL	A	D	S	M	C	A									
	?															- ¹	+ ¹																																

A, aneuploidy; C, chromosomal aberrations; D, DNA damage; DL, dominant lethal mutation; G, gene mutation; I, inhibition of intercellular communication; M, micronuclei; R, mitotic recombination and gene conversion; S, sister chromatid exchange; T, cell transformation

In completing the tables, the following symbols indicate the consensus of the Working Group with regard to the results for each endpoint:

- ? considered to be equivocal or inconclusive (e.g., there were contradictory results from different laboratories; there were confounding exposures; the results were equivocal)
- ¹ considered to be negative, but only one valid study was available to the Working Group
- +¹ considered to be positive, but only one valid study was available to the Working Group.
- + considered to be positive for the specific endpoint and level of biological complexity

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