BENZOFURAN

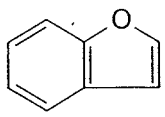
1. Exposure Data

1.1 Chemical and physical data

1.1.1 Nomenclature

Chem. Abstr. Serv. Reg. No.: 271-89-6
Chem. Abstr. Name: Benzofuran
IUPAC Systematic Name: Benzofuran
Synonyms: Benzo[*b*]furan; 2,3-benzofuran; benzofurfuran; 2,3-benzofurfuran; coumarone; cumarone; 1-oxindene

1.1.2 Structural and molecular formulae and relative molecular mass



C_8H_6O Relative molecular mass: 118.14

1.1.3 Chemical and physical properties of the pure substance

(*a*) *Description*: Clear, yellowish, oily liquid with an aromatic odour (Budavari, 1989; Henley Chemicals, Inc., 1990)

(*b*) *Boiling-point*: 174 °C (Lide, 1993)

(*c*) *Melting-point*: < –18 °C (Lide, 1993)

(*d*) *Density*: 1.0913 at 25 °C (Lide, 1993)

(*e*) *Spectroscopy data*: Infrared (prism [3739]; grating [33 363]), ultraviolet [20 800], nuclear magnetic resonance (proton [19 610]; C-13 [576]) and mass [448] spectral data have been reported (Sadtler Research Laboratories, 1980; Weast & Astle, 1985).

(*f*) *Solubility*: Insoluble in water and aqueous alkaline solutions; soluble in benzene, petroleum ether, diethyl ether and ethanol (Budavari, 1989; Lide, 1993)

(*g*) *Volatility*: Vapour pressure, 0.44 mm Hg [0.06 kPa] at 25 °C (Chao *et al.*, 1983)

(*h*) *Stability*: Polymerizes at elevated temperatures or upon contact with acids (Budavari, 1989; Henley Chemicals, Inc., 1990)

(*i*) *Octanol:water partition coefficient (P)*: log P, 2.67 (Hansch *et al.*, 1995)

(*j*) *Conversion factor*: $mg/m^3 = 4.83 \times ppm$[1]

1.1.4 Technical products and impurities

Benzofuran is available commercially at a minimal purity of 99% (Henley Chemicals, Inc., 1990). Trade names for benzofuran include AT 33852 and R 7204.

1.1.5 Analysis

Benzofuran has been determined in air samples after collection on Tenax or Chromosorb, thermal desorption and high-resolution gas chromatography/mass spectrometry. It has been concentrated from water samples by the purge-and-trap method or by extraction with dichloromethane. It has also been extracted from particulate samples with dichloromethane (Ferretti & Flanagan, 1971; Erikson & Pellizzari, 1978; Pellizzari *et al.*, 1979; Hunt *et al.*, 1982; Rostad *et al.*, 1985; Juttner, 1986; van Netten *et al.*, 1988).

Benzofuran has been detected, but not quantified, in samples of blood and breast milk by purging them with an inert gas at an elevated temperature, trapping on Tenax, thermal desorption and high-resolution gas chromatography/mass spectrometry (Anderson & Harland, 1980; Pellizzari *et al.*, 1982).

1.2 Production and use

1.2.1 Production

Benzofuran is a constituent of coal-tar (see IARC, 1987a) and can be isolated from coal-tar oils. It is produced by three companies in China, one in Armenia and one in Switzerland (Chemical Information Services, Inc., 1994).

1.2.2 Use

Benzofuran derived from the crude, heavy solvent naphtha fraction of coal-tar light oil, obtained as a by-product in the coking of bituminous coal (see IARC, 1987b), is used in the manufacture of coumarone–indene resin (Budavari, 1989). The fraction of coal-tar oil that distils at 167–184 °C contains small quantities (probably < 10%) of benzofuran and about 30% indene, indan, substituted benzenes and related compounds. Polymerization is initiated by addition of an acid catalyst such as boron trifluoride or sulfuric acid (United States Agency for Toxic Substances and Disease Registry, 1992).

Coumarone–indene resins harden when heated and have been used to make floor tiles and other products. They are also used as a coating on grapefruit, lemons, limes, oranges, tangelos and tangerines and in the production of corrosion-resistant paints and varnishes, in water-resistant coatings on paper products and fabrics and as adhesives in food containers (United States Agency for Toxic Substances and Disease Registry, 1992).

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[1] Calculated from: mg/m^3 = (relative molecular mass/24.45) × ppm, assuming normal temperature (25 °C) and pressure (101 kPa)

1.3 Occurrence

1.3.1 Natural occurrence

Benzofuran is not known to occur as a natural product.

1.3.2 Occupational exposure

No data were available to the Working Group, although occupational exposure to benzofuran may occur in several industries, including coke production and coal gasification facilities (see IARC, 1987c) and the polymerization process used to produce coumarone–indene resin. Benzofuran was not found in two surveys in the United States of America (United States National Institute for Occupational Safety and Health, 1994).

The naphtha fraction of coal-tar was included among the occupational hazards associated with coal gasification (United States National Institute for Occupational Safety and Health, 1978). Individuals occupationally exposed to coal-tars, including road-pavement workers, or to the naphtha fraction of coal-tar distillate are potentially exposed to benzofuran (United States Agency for Toxic Substances and Disease Registry, 1992). In a study of laser cutting of fibre-reinforced plastics, benzofuran was produced at a rate of 0.03–0.25 mg/g, the highest levels occurring during the cutting of epoxy resins reinforced with aramide fibres (Busch *et al.*, 1989; Levsen *et al.*, 1991).

1.3.3 Air

Benzofuran may be released into the environment during the production and use of benzofuran-containing products and in coke production, coal gasification and oil-shale facilities (see IARC, 1987d). Coke oven emissions were composed on average of 0.29% benzofuran (Kirton *et al.*, 1991). Benzofuran was also detected in emissions from a Swedish floor finish used on domestic flooring (van Netten *et al.*, 1988), in emissions from the pyrolysis of silk (Junk & Ford, 1980), in combustor flue gas emissions from fluidized-bed coal combustion at a concentration of 900 ng/g (Hunt *et al.*, 1982) and from burning scrap tyres at a rate of 25 mg/kg tyre (Lemieux & Ryan, 1993).

Exhaust produced by an automobile burning simple hydrocarbon fuels contained benzofuran at concentrations of < 0.1–2.8 ppm [0.48–13.5 mg/m^3] (Seizinger & Dimitriades, 1972), but an analysis of air in a highway tunnel used by both diesel- and gasoline-powered vehicles showed no benzofuran (Hampton *et al.*, 1982). Residential burning of brown-coal briquets led to an estimated emission factor of 6.85 mg/kg benzofuran. The estimated total amount of benzofuran emitted in the city of Leipzig, Germany, was 2220 kg/year (Engewald *et al.*, 1993). Benzofuran was detected but not quantified in one of 10 samples of ambient air taken in an industrial area in the Kanawha Valley, West Virginia, United States (Erickson & Pellizzari, 1978); it was also detected among pollutants in the air of the southern Black Forest in Germany (Juttner, 1986). Benzofuran was identified as a minor component of smoke condensates of cottonwood in an experimental setting (Edye & Richards, 1991).

1.3.4 Water

Benzofuran was detected in the effluents from a coal gasification facility at concentrations of 6–267 ppb [μg/L], but it was not detected (detection limit, 0.1 ppb) in effluents from oil-shale processing facilities (Pellizzari *et al.*, 1979). It was also detected in one of 18 wastewater concentrates and at a concentration of 770 ppb in a groundwater sample, but not in surface water samples, taken at a hazardous waste site in the United States (United States Agency for Toxic Substances and Disease Registry, 1992). It was detected in contaminated groundwater at a coal-tar distillation and wood-preserving facility in Minnesota, United States (Rostad *et al.*, 1985).

1.3.5 Soil

Benzofuran was found at a concentration of 60 ppb [μg/kg] in one soil and sediment sample taken at a hazardous waste site in the United States (United States Agency for Toxic Substances and Disease Registry, 1992).

1.3.6 Other media

Benzofuran has not usually been found in foods, but it was one of the volatile constituents of freeze-dried whey powder subjected to accelerated browning (Ferreti & Flanagan, 1971). It was also detected in three samples of human milk (Pellizzari *et al.*, 1982) and in the blood of fire victims (Anderson & Harland, 1980). It is reportedly a constituent of cigarette smoke (Florin *et al.*, 1980; Curvall *et al.*, 1984; IARC, 1986; Schlotzhauer & Chortyk, 1987).

1.4 Regulations and guidelines

No guidelines or regulations have been reported for benzofuran (ILO, 1991).

2. Studies of Cancer in Humans

No data were available to the Working Group.

3. Studies of Cancer in Experimental Animals

Oral administration

Mouse: Groups of 50 male and 50 female B6C3F1 mice, seven to eight weeks of age, were administered benzofuran (purity, 99%) dissolved in corn oil at 0, 60 or 120 mg/kg bw (males) and 0, 120 or 240 mg/kg bw (females) by gavage on five days a week for 104 weeks. The numbers of male mice still alive at the end of the experiment were 33/50 controls, 20/50 at the low dose and 28/50 at the high dose; survival of treated females was significantly lower than that of controls ($p = 0.005$), with 37/50 controls, 19/50 at the low dose and 21/50 at the high dose still

alive at the end of the experiment. The incidences of hepatocellular adenomas were increased in treated animals: 4/49 male controls, 24/39 at the low dose ($p < 0.001$, incidental tumour test) and 34/48 at the high dose ($p < 0.001$); and 1/50 female controls, 22/48 at the low dose ($p < 0.001$) and 21/47 at the high dose ($p < 0.001$). The incidences of hepatoblastoma, which had not been observed in historical controls in the study laboratory, were increased in male animals: 0/49 male controls, 3/39 at the low dose ($p = 0.083$) and 18/48 at the high dose ($p < 0.001$); one hepatoblastoma was found in a female at the low dose and in two females at the high dose. The incidence of hepatocellular carcinomas was not increased in treated animals. Male mice had increased incidences of squamous-cell papillomas of the forestomach, which occurred in 2/49 controls, 7/39 at the low dose ($p = 0.018$) and 10/48 at the high dose ($p = 0.007$); and of squamous-cell carcinomas, seen in 0/49 controls, 4/39 at the low dose ($p = 0.05$) and 3/48 at the high dose. The combined incidences of forestomach papillomas and carcinomas in males were 2/49 controls, 11/39 at the low dose ($p = 0.001$) and 13/48 at the high dose ($p = 0.001$). Squamous-cell papillomas of the forestomach occurred in 2/50 female controls, 8/50 at the low dose ($p = 0.035$) and 5/50 at the high dose; the incidence of carcinomas of the forestomach was not increased in females. Treated animals had increased incidences of pulmonary alveolar–bronchiolar adenomas, which occurred in 4/49 male controls, 7/39 at the low dose and 15/48 at the high dose ($p = 0.003$); and in 1/50 female controls, 5/48 at the low dose ($p = 0.040$) and 13/47 at the high dose ($p < 0.001$). Females had an increased incidence of alveolar–bronchiolar carcinomas, seen in 1/50 controls, 4/48 at the low dose ($p = 0.038$) and 3/47 at the high dose. The frequency of epithelial hyperplasia of the forestomach was increased in all treated mice except males at the low dose. Bronchiolar epithelial hyperplasia was observed in all treated animals (United States National Toxicology Program, 1989).

Rat: Groups of 50 male and 50 female Fischer 344/N rats, six to seven weeks of age, were administered benzofuran (purity, 99%) dissolved in corn oil at doses of 0, 30 or 60 mg/kg bw (males) and 0, 60 or 120 mg/kg bw (females) by gavage on five days a week for 103 weeks. The numbers of animals that survived to the end of the study were 33/50 male controls, 12/50 at the low dose ($p < 0.001$) and 18/50 at the high dose ($p = 0.003$); and 27/50 female controls, 23/50 at the low dose and 25/50 at the high dose. Nephropathy was seen in almost all aged male rats, including controls, but was more severe in treated animals; nephropathy was more frequent and more severe in treated females. The incidences of renal-cell adenocarcinomas were increased in female, but not in male, rats, occurring in 0/50 controls, 1/50 at the low dose and 4/50 at the high dose ($p = 0.032$, incidental tumour test). This tumour is rare in female rats: the incidence in historical controls at the study laboratory was 1/149 and that in the United States National Toxicology Testing Program was 2/2094 (United States National Toxicology Program, 1989).

4. Other Data Relevant to an Evaluation of Carcinogenicity and its Mechanisms

4.1 Absorption, distribution, metabolism and excretion

No data were available to the Working Group.

4.2 Toxic effects

4.2.1 Humans

No data were available to the Working Group.

4.2.2 Experimental systems

Groups of 10 male and 10 female Fischer 344/N rats and B6C3F1 mice were administered 0, 31, 63, 125, 250 or 500 mg/kg bw benzofuran (purity, 99%) in corn oil by gavage on five days per week for 13 weeks. Minimal centrilobular degeneration and necrosis of individual hepatocytes throughout the liver occurred in rats of each sex at the two highest doses and in males at 125 mg/kg bw. Severe nephropathy with foci of tubular regeneration and dilated tubules occurred in male rats at the two highest doses. Cytoplasmic vacuolization was observed in all animals at the highest dose. Of the mice, 7/10 males at the high dose died, and 7/10 males at 250 mg/kg bw had nephrosis, with tubular-cell necrosis, inflammation, fibrosis, regeneration and focal mineralization (United States National Toxicology Program, 1989).

Female CD-1 mice administered benzofuran at 5 mmol/kg bw [590 mg/kg bw] in corn oil by gavage for 10 days had liver microsomal P450 levels that were decreased by 70% in comparison with controls, 7-ethoxycoumarin *O*-deethylase activity increased by 150% and no significant changes in the activities of aniline hydroxylase and aminopyrine *N*-demethylase. Treatment also increased the activities of microsomal epoxide hydrolase (218% of the control level), UDP-glucuronosyl transferase (237% of control levels), cytosolic glutathione *S*-transferase (631% of control levels, with 1-chloro-2,4-dinitrobenzene as the substrate) and NADH-quinone reductase (230% of control levels) (Cha *et al.*, 1985). The same data were subsequently published elsewhere (Heine *et al.*, 1986).

4.3 Reproductive and prenatal effects

No data were available to the Working Group.

4.4 Genetic and related effects

4.4.1 Humans

No data were available to the Working Group

4.4.2 Experimental systems (see also Table 1 and Appendices 1 and 2)

Benzofuran was not mutagenic to *Salmonella typhimurium* when tested in either the standard plate incorporation assay or in a preincubation protocol in the presence or absence of an exogenous metabolic activation system.

Benzofuran induced gene mutation at the thymidine kinase locus of L5178Y mouse lymphoma cells in the absence of metabolic activation. It induced sister chromatid exchange and chromosomal aberrations in Chinese hamster ovary cells both in the presence and absence of metabolic activation.

Table 1. Genetic and related effects of benzofuran

Test system	Result[a]		Dose[b] (LED/HID)	Reference
	Without exogenous metabolic system	With exogenous metabolic system		
SA0, *Salmonella typhimurium* TA100, reverse mutation	–	–	350	Florin *et al.* (1980)
SA0, *Salmonella typhimurium* TA100, reverse mutation	–	–	0.00	Weill-Thevenet *et al.* (1981)
SA0, *Salmonella typhimurium* TA100, reverse mutation	–	–	385	US National Toxicology Program (1989)
SA5, *Salmonella typhimurium* TA1535, reverse mutation	–	–	350	Florin *et al.* (1980)
SA5, *Salmonella typhimurium* TA1535, reverse mutation	–	–	0.00	Weill-Thevenet *et al.* (1981)
SA5, *Salmonella typhimurium* TA1535, reverse mutation	–	–	385	US National Toxicology Program (1989)
SA7, *Salmonella typhimurium* TA1537, reverse mutation	–	–	350	Florin *et al.* (1980)
SA7, *Salmonella typhimurium* TA1537, reverse mutation	–	–	0.00	Weill-Thevenet *et al.* (1981)
SA7, *Salmonella typhimurium* TA1537, reverse mutation	–	–	385	US National Toxicology Program (1989)
SA8, *Salmonella typhimurium* TA1538, reverse mutation	–	–	0.00	Weill-Thevenet *et al.* (1981)
SA9, *Salmonella typhimurium* TA98, reverse mutation (spot test)	–	–	350	Florin *et al.* (1980)
SA9, *Salmonella typhimurium* TA98, reverse mutation	–	–	0.00	Weill-Thevenet *et al.* (1981)
SA9, *Salmonella typhimurium* TA98, reverse mutation	–	–	385	US National Toxicology Program (1989)
SAS, *Salmonella typhimurium* TA98NR, reverse mutation	–	–	0.00	Weill-Thevenet *et al.* (1981)
G5T, Gene mutation, mouse lymphoma L5178Y cells, *tk* locus *in vitro*	+	0	100	McGregor *et al.* (1988)
SIC, Sister chromatid exchange, Chinese hamster ovary (CHO) cells *in vitro*	+	+	37	US National Toxicology Program (1989)
CIC, Chromosomal aberrations, Chinese hamster ovary (CHO) cells *in vitro*	+	+	280	US National Toxicology Program (1989)

[a] +, considered to be positive; –, considered to be negative; 0, not tested

[b] LED, lowest effective dose; HID, highest ineffective dose; in-vitro tests, mg/ml; in-vivo tests, mg/kg bw; 0.00, dose not given

5. Summary and Evaluation

5.1 Exposure data

Benzofuran is produced by isolation from coal-tar oils, which are obtained as by-products of coking coal. Its major use is in the production of coumarone–indene resins. Human exposure can occur during coke production, coal gasification, the production of coumarone–indene resins or the combustion of coal and from tobacco smoke.

5.2 Human carcinogenicity data

No data were available to the Working Group.

5.3 Animal carcinogenicity data

Benzofuran was tested for carcinogenicity by oral administration in one study in mice and in one study in rats. In mice, benzofuran increased the incidence of hepatocellular adenomas in animals of each sex and of hepatoblastomas and forestomach papillomas and carcinomas in males; the incidence of alveolar–bronchiolar adenomas was increased in both males and females. Female rats had an increased incidence of renal-cell adenocarcinomas, which occur rarely in animals of this sex.

5.4 Other relevant data

No data were available on the toxicokinetics of benzofuran. Repeated administration of benzofuran to rats and mice caused renal toxicity; rats also developed slight hepatic toxicity.

Induction of gene mutation, sister chromatid exchange and chromosomal aberrations was seen in cultured rodent cells treated with benzofuran in single studies. Benzofuran was not mutagenic to bacteria.

5.5 Evaluation[1]

There is *inadequate evidence* in humans for the carcinogenicity of benzofuran.

There is *sufficient evidence* in experimental animals for the carcinogenicity of benzofuran.

Overall evaluation

Benzofuran *is possibly carcinogenic to humans (Group 2B).*

[1] For definition of the italicized terms, see Preamble, pp. 22–26.

6. References

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