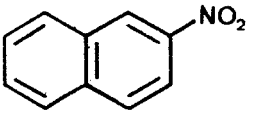
2-NITRONAPHTHALENE

1. Chemical and Physical Data

1.1 Synonyms

Chem. Abstr. Services Reg. No.: 581-89-5
Chem. Abstr. Name: Naphthalene, 2-nitro-
IUPAC Systematic Name: 2-Nitronaphthalene
Synonym: β-Nitronaphthalene

1.2 Structural and molecular formulae and molecular weight



$C_{10}H_7NO_2$ Mol. wt: 173.2

1.3 Chemical and physical properties of the pure substance

(*a*) *Description*: Yellow needles or plates from ethanol (Weast, 1985)

(*b*) *Boiling-point*: 165°C at 15°C (Weast, 1985)

(*c*) *Melting-point*: 79°C (Weast, 1985)

(*d*) *Spectroscopy data*: Proton and nuclear magnetic resonance and mass spectral data have been reported (Lucchini & Wells, 1976; Kitching *et al.*, 1977; Schuetzle & Jensen, 1985).

(*e*) *Solubility*: Soluble in ethanol and diethyl ether (Weast, 1985)

1.4 Technical products and impurities

2-Nitronaphthalene is available for research purposes (Aldrich Chemical Co., 1988). It is also available at a purity of 99.7% as a reference material (Belliardo *et al.*, 1988).

2. Production, Use, Occurrence and Analysis

2.1 Production and use

(*a*) *Production*

2-Nitronaphthalene is a by-product (2–3%) from the commercial preparation of 1-nitronaphthalene by direct nitration of naphthalene (Verschueren, 1983). It can be produced by the Bucherer reaction, starting with 2-naphthalenol (2-naphthol), and by other indirect methods; however, the Bucherer method, which yields 2-naphthylamine (see IARC, 1987), is seldom used (Gaydos, 1981).

(*b*) *Use*

No evidence was found that 2-nitronaphthalene has been used for commercial applications.

2.2 Occurrence

(*a*) *Engine exhaust*

Emissions from a heavy-duty diesel engine contained 2-nitronaphthalene at concentrations of 0.94 mg/kg in particulates when the engine was run at 100% load and 1200 revolutions/min and 0.87 mg/kg in particulates when the same engine was run at 75% load and 1800 revolutions/min (Draper, 1986).

(*b*) *Other occurrence*

Toners for use in photocopy machines have been produced in quantity since the late 1950s and have seen widespread use. 'Long-flow' furnace black was first used in photocopy toners in 1967; its manufacture involved an oxidation whereby some nitration also occurred. Subsequent changes in the production technique reduced the total extractable nitropyrene content from an uncontrolled level of 5–100 mg/kg to below 0.3 mg/kg (Rosenkranz *et al.*, 1980; Sanders, 1981; Butler *et al.*, 1983), and toners produced from this carbon black since 1980 have not been found to contain detectable levels of mutagenicity or, hence, nitropyrenes (Rosenkranz *et al.*, 1980; Butler *et al.*, 1983). One sample of a formerly available commercial carbon black was reported to contain detectable concentrations of unspecified nitronaphthalene (Ramdahl & Urdal, 1982).

2-Nitronaphthalene was detected in urban ambient airborne particulates in St Louis, MO, USA (Ramdahl & Urdal, 1982; Ramdahl *et al.*, 1982). In a laboratory experiment, 2-nitronaphthalene was formed by a gas-phase napthhalene nitration reaction at room temperature and atmospheric pressure with a yield of about 8% (Pitts *et al.*, 1985). It was postulated that significant amounts of 2-nitronaphthalene result from the night-time gas-phase reaction of naphthalene with nitrogen pentoxide (Pitts, 1987). Approximately equal

amounts of 1- and 2-nitronaphthalene were found in day-time samples of ambient air in Torrance, CA, USA. 2-Nitronaphthalene concentrations were 1.1 ng/m^3 of sample during night-time sampling and 2.9 ng/m^3 of sample during day-time sampling (Arey *et al.*, 1987).

2.3 Analysis

See the monograph on 1-nitropyrene.

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

3.1 Carcinogenicity studies in animals[1]

(*a*) *Oral administration*

Monkey: One female rhesus monkey (*Macaca mulatta*) that had been infected with a laboratory strain of *Plasmodium cynomolgi* and cured with chloroquine at least 12 weeks before the beginning of the experiment received a daily dose of 242 mg/kg bw 2-nitronaphthalene ['purified' but purity not given] administered orally in hard gelatin capsules on six days per week for 54 months. The monkey was then killed (terminal weight, 5.7 kg) and necropsied, three papillomas were found in the urinary bladder; no tumour was found in other organs (Conzelman *et al.*, 1970). [The Working Group noted that results were available for only one animal.]

(*b*) *Bladder implantation*

Mouse: Three groups of 41, 76 and 80 mice [strain and age unspecified] received a surgical implant of a cholesterol pellet containing 2-nitronaphthalene [dose and purity unspecified] into the urinary bladder (Bryan *et al.*, 1964). Three groups of 72, 82 and 140 controls received implants of cholesterol only. In a further group of 38 mice, a sham operation was performed which consisted of incising the bladder, momentarily inserting a pellet of pure cholesterol, removing the pellet, closing the bladder and suturing the abdomen. Animals were observed for up to 490 days, and only animals surviving longer than 175 days were evaluated. At the end of the experiment, the incidences of carcinomas and benign tumours of the bladder did not differ significantly between the various groups: 2/41, 2/76 and 7/80 in the treated groups; 4/72, 1/82 and 2/140 in the cholesterol controls and none in the sham-operated animals.

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[1]The Working Group was aware of studies in progress by single subcutaneous injection in mice (IARC, 1988).

3.2 Other relevant data

(a) *Experimental systems*

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

2-Naphthylamine (see IARC, 1987) was detected in the urine of male Sprague-Dawley rats administered single intraperitoneal doses of 100 mg/kg bw 2-nitronaphthalene (Johnson & Cornish, 1978).

After male Wistar rats had been administered 2 mmol[350 mg]/kg bw 2-nitronaphthalene orally, the following metabolites (either free or conjugated) were excreted in the urine over the subsequent 32 h: 2-amino-1-naphthyl sulfate, 2-amino-1-naphthol and *N*-hydroxy-2-naphthylamine. All of these products were detected in the urine of rats treated similarly with 2-naphthylamine (Kadlubar *et al.*, 1981). [The Working Group noted that *N*-hydroxy-2-naphthylamine is tumorigenic to experimental animals. See, for example, Garner *et al.* (1984).] The urine of monkeys given oral doses of 2-nitronaphthalene was found to contain 2-amino-1-naphthyl sulfate and 2-acetamido-6-naphthyl glucuronide (Conzelman *et al.*, 1970).

As reported in an abstract, in male Sprague-Dawley rats treated orally with 0.5 mmol[87 mg]/kg bw 2-nitronaphthalene, covalent binding to haemoglobin was detected, although the level was lower than that found with 2-naphthylamine (Suzuki *et al.*, 1987).

Under anaerobic conditions, liver postmitochondrial supernatants and cytosol from male Fischer rats and female Swiss mice catalysed the stoichiometric conversion of 2-nitronaphthalene to 2-naphthylamine (Poirier & Weisburger, 1974).

Incubation of 2-nitronaphthalene with liver postmitochondrial supernatants from Wistar rats pretreated with sodium phenobarbital, 3-methylcholanthrene or Kanechlor-500 resulted in a time-dependent loss of substrate. The rate of metabolism was faster with homogenates from animals pretreated with 3-methylcholanthrene or Kanechlor-500 than with those from animals given phenobarbital (Ohe, 1985).

(ii) *Toxic effects*

A single intraperitoneal injection of 2-nitronaphthalene (100 mg/kg bw) to male Sprague-Dawley rats did not cause respiratory distress or lung or liver toxicity, in contrast to observations made with 1-nitronaphthalene (see monograph on 1-nitronaphthalene; Johnson *et al.*, 1984).

(iii) *Genetic and related effects*

The genetic and related effects of nitroarenes and of their metabolites have been reviewed (Rosenkranz & Mermelstein, 1983; Beland *et al.*, 1985; Rosenkranz & Mermelstein, 1985; Tokiwa & Ohnishi, 1986).

2-Nitronaphthalene preferentially inhibited the growth of DNA repair-deficient *Escherichia coli* (Rosenkranz & Poirier, 1979; DeFlora *et al.*, 1984) and *Bacillus subtilis* (at 100 μg/disc; Tokiwa *et al.*, 1987) and induced DNA damage in *Salmonella typhimurium* (lowest effective dose, 6 μg/ml; Nakamura *et al.*, 1987).

2-Nitronaphthalene was mutagenic to *S. typhimurium* strains TA1535, TA1537, TA1538, TA98 and TA100 (McCann *et al.*, 1975; Wang *et al.*, 1978; De Flora, 1979; Rosenkranz & Poirier, 1979; Scribner *et al.*, 1979; Simmon, 1979a; Wang *et al.*, 1980; De Flora, 1981; El-Bayoumy *et al.*, 1981; Ho *et al.*, 1981; Löfroth, 1981; McCoy *et al.*, 1981; De Flora *et al.*, 1984; Morotomi & Watanabe, 1984) but not to strain TA97 (Rosenkranz *et al.*, 1985).

This compound induced recombination in the yeast, *Saccharomyces cerevisiae* D3 (Simmon, 1979b).

In a host-mediated assay in mice, 2-nitronaphthalene (at 125–1300 mg/kg) induced mutation in *S. typhimurium* TA1530 and TA1538 but not recombination in *S. cerevisiae* D3 (Simmon *et al.*, 1979).

2-Nitronaphthalene did not induce unscheduled DNA synthesis in cultured rat or mouse hepatocytes (Mori *et al.*, 1987) but did induce morphological transformation of Syrian hamster embryo cells (Pienta, 1980).

(*b*) *Humans*

No data were available to the Working Group.

3.3 Epidemiological studies and case reports of carcinogenicity in humans

No data were available to the Working Group.

4. Summary of Data Reported and Evaluation

4.1 Exposure data

2-Nitronaphthalene has been detected in particulate emissions from diesel engines. It has also been found at low concentrations in ambient air.

4.2 Experimental data

2-Nitronaphthalene was tested for carcinogenicity by prolonged oral administration in one monkey, producing papillomas in the urinary bladder. Implantation of cholesterol pellets containing 2-nitronaphthalene into the bladder of mice did not increase the incidence of urinary bladder tumours.

4.3 Human data

No data were available to the Working Group.

4.4 Other relevant data

N-Hydroxy-2-naphthylamine (which has been shown to induce tumours in experimental animals) and 2-naphthylamine (which is causally associated with cancer in humans) have been detected as metabolites of 2-nitronaphthalene in the urine of rats.

2-Nitronaphthalene induced morphological transformation in cultured animal cells but did not induce DNA damage in cultured rodent hepatocytes. It induced DNA damage and mutation in bacteria and recombination in yeast.

4.5 Evaluation[1]

There is *inadequate evidence* for the carcinogenicity in experimental animals of 2-nitronaphthalene.

No data were available from studies in humans on the carcinogenicity of 2-nitronaphthalene.

Overall evaluation

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

5. References

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[1]For definitions of the italicized terms, see Preamble, pp. 25–28.

Summary table of genetic and related effects of 2-nitronaphthalene

Nonmammalian systems													Mammalian systems																									
Prokaryotes		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 table, the following symbols indicate the consensus of the Working Group with regard to the results for each endpoint:

\+ considered to be positive for the specific endpoint and level of biological complexity

+[1] considered to be positive, but only one valid study was available to the Working Group

− considered to be negative

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