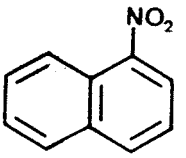
1-NITRONAPHTHALENE

1. Chemical and Physical Data

1.1 Synonyms

Chem. Abstr. Services Reg. No.: 86-57-7
Chem. Abstr. Name: Naphthalene, 1-nitro-
IUPAC Systematic Name: 1-Nitronaphthalene
Synonyms: α-Nitronaphthalene; nitrol

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, recrystallized from ethanol (Weast, 1985)

(*b*) *Boiling-point*: 304°C (Windholz, 1983)

(*c*) *Melting-point*: 61.5°C (Weast, 1985)

(*d*) *Spectroscopy data*: Ultra-violet (National Cancer Institute, 1978), proton and nuclear magnetic resonance (Lucchini & Wells, 1976; Kitching *et al.*, 1977) and mass (Schuetzle & Jensen, 1985) spectral data have been reported.

(*e*) *Relative density*: 1.331 relative to water at 4°C (Buckingham, 1982)

(*f*) *Solubility*: Insoluble in water; soluble in ethanol, diethyl ether, chloroform, carbon disulfide (Windholz, 1983), benzene and pyrene (Weast, 1985)

(*g*) *Flash-point*: 164°C (Sax & Lewis, 1987)

1.4 Technical products and impurities

1-Nitronaphthalene is available for research purposes at 99% purity (Aldrich Chemical Co., 1988). It is also available in a certified purity of 99.61% as a reference material (Belliardo *et al.*, 1988).

2. Production, Use, Occurrence and Analysis

2.1 Production and use

(*a*) *Production*

1-Nitronaphthalene is synthesized by the action of a mixture of nitric and sulfuric acids on finely ground naphthalene (Sax & Lewis, 1987). Reaction of naphthalene with nitric acid and sulfuric acid in dichloromethane (or another suitable inert solvent) was reported to give a 80% yield of 99.2% purity (Kameo & Hirashima, 1986).

There is one producer of this substance in the USA. 1-Nitronaphthalene is reported on the 1985 *Toxic Substances Control Act Chemical Substance Inventory* (US Environmental Protection Agency, 1986).

(*b*) *Use*

The uses of 1-nitronaphthalene include a chemical intermediate in the manufacture of dyes [drugs, perfumes, rubber chemicals, tanning agents and pesticides]; a fluorescence quencher for mineral oils (Sax & Lewis, 1987); a 'debloomer' for petroleum oils (Windholz, 1983); a vapour-phase corrosion inhibitor (Foley & Brown, 1979); a wood preservative; and a fungicide (Kasperczak & Lutomski, 1973; Dominik, 1978). A Chinese patent was issued in which [a compound presumed to be] 1-nitronaphthalene was proposed as a component at 1–2% in sulfur-free, fragrant fireworks powder (Ying *et al.*, 1986).

2.2 Occurrence

(*a*) *Engine exhaust*

1-Nitronaphthalene concentrations of 0.77 mg/kg of particulates were reported in the emissions of a heavy-duty diesel engine run at 100% load and 1200 revolutions/min; at 75% load and 1800 revolutions/min, the same engine produced concentrations of 0.47 mg/kg of particulates (Draper, 1986). Nishioka *et al.* (1982) detected 1-nitronaphthalene in the exhaust emissions of light-duty diesel engines (0.3-0.7 mg/kg), and Liberti *et al.* (1984) found this compound in the gas phase of diesel engine exhaust.

(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). 1-Nitronaphthalene has been detected in formerly available commercial carbon blacks (Fitch *et al.*, 1978; Ramdahl & Urdal, 1982).

1-Nitronaphthalene was detected in urban ambient airborne particulates in St Louis, MO, USA (Ramdahl & Urdal, 1982; Ramdahl *et al.*, 1982), and trace quantities were identified in urban air particulates in Göteborg, Sweden (Brorström-Lundén & Lindskog, 1985). In a laboratory experiment, 1-nitronaphthalene was formed by a gas-phase naphthalene nitration reaction at room temperature and atmospheric pressure with a yield of 18% (Pitts *et al.*, 1985). It was postulated that significant amounts of 1-nitronaphthalene result from the night-time gas-phase reaction of naphthalene with nitrogen pentoxide (Pitts, 1987).

1-Nitronaphthalene was found at 3.5 mg/kg particulate matter in a hexane/benzene fraction and at 3.1 mg/kg particulate matter in a polycyclic aromatic hydrocarbon fraction of suburban/industrial ambient air in north-west Philadelphia, PA, USA. It was not found in polar I and II fractions (Wise *et al.*, 1985). A level of 2.3 ng/m^3 was found in a night-time sample of ambient air in Torrance, CA, USA, calculated as the sum of the concentrations on the filter and three polyurethane foam plugs. A day-time sample contained 3.0 ng/m^3 in approximately equal amounts of 1- and 2-nitronaphthalene; however, this was considered to be a lower limit, since the adsorption capacity of the three polyurethane foam plugs was exceeded (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]

Oral administration

Mouse: Two groups of 50 male and 50 female B6C3F1 mice, approximately six weeks old, were fed a basal diet containing 0.06% or 0.12% 1-nitronaphthalene ([purity and impurities unspecified] melting-point, 50–53°C) for 78 weeks and observed for a further 18–20 weeks (National Cancer Institute, 1978). Two untreated groups of 50 males and 50 females served as controls. Statistical analyses were based on animals that survived at least 52 weeks; more than 80% of the mice survived to 80 weeks. At the end of the experiment, tumours were observed in the respiratory, digestive and endocrine systems in both treated and control animals; the incidences did not differ significantly among the four groups. [The Working Group noted that the dose administered was not the maximal tolerated dose.]

Rat: Two groups of 50 male and 50 female Fischer 344 rats, approximately six weeks old, were fed a basal diet containing 0.05% then 0.06% or 0.18% 1-nitronaphthalene ([purity and impurities unspecified] melting-point, 50–53°C) for 78 weeks and observed for a further 29–31 weeks (National Cancer Institute, 1978). Two untreated groups of 25 females and 25 males and 50 males and 50 females served as controls for the high- and low-dose groups, respectively. Statistical analyses were based on animals that survived at least 52 weeks; more than 80% of the rats survived to 80 weeks. At the end of the experiment, tumours were observed in the respiratory, digestive and endocrine systems in both treated and control animals; the incidences did not differ significantly among the four groups. [The Working Group noted that the dose administered was not the maximal tolerated dose and that it was changed during treatment of the low-dose group.]

3.2 Other relevant data

(*a*) *Experimental systems*

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

1-Naphthylamine (see IARC, 1987) was detected in the urine of male Sprague-Dawley rats administered single intraperitoneal doses of 100 mg/kg bw 1-nitronaphthalene (Johnson & Cornish, 1978).

Incubation of 1-nitronaphthalene under anaerobic conditions with a postmitochondrial supernatant from the livers of male Fischer rats resulted in the stoichiometric formation of 1-naphthylamine (Poirier & Weisburger, 1974). Under aerobic conditions, a rat liver

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

metabolic system converted 1-nitronaphthalene into dihydrodiol and phenol metabolites (El-Bayoumy & Hecht, 1982).

Under anaerobic conditions, rabbit liver microsomes catalysed the reduction of 1-nitronaphthalene to *N*-hydroxy-1-naphthylamine and 1-naphthylamine (Sternson, 1975; Tatsumi *et al.*, 1986). [The Working Group noted that *N*-hydroxy-1-naphthylamine is carcinogenic to experimental animals. See, for example, Garner *et al.* (1984).]

Lung and liver microsomes from male Swiss-Webster mice metabolized 1-nitronaphthalene to products that bound microsomal macromolecules. The binding was NADPH- and oxygen-dependent and was inhibited by carbon monoxide, nitrogen and SKF-525A. Little binding was detected with kidney microsomes. Pretreatment of the mice with β-naphthoflavone enhanced the binding to lung microsomal macromolecules; phenobarbital pretreatment increased the binding to liver microcomes. Incubations were also conducted with lung slices and isolated lung cells. Autoradiographs of the lung slices showed that most of the binding occurred in the epithelial cells of the bronchioles and smaller airways. With the isolated lung cells, there was preferential binding of 1-nitronaphthalene to cell populations enriched in Clara cells. β-Naphthoflavone pretreatment increased the binding of 1-nitronaphthalene in both the lung slices and isolated lung cells (Rasmussen, 1986).

(ii) *Toxic effects*

A single intraperitoneal injection of 1-nitronaphthalene (25–200 mg/kg bw) to male Sprague-Dawley rats resulted in respiratory distress, which generally developed within 24 h (ED_{50}, 60 mg/kg bw). At necropsy at 24 h, there was diffuse, irregular red mottling on the pleural surface of the lungs and necrosis of nonciliated bronchiolar epithelial cells (Clara cells). Hepatotoxicity was also observed after intraperitoneal injection of 100 mg/kg bw, increasing in severity over 72 h after injection (Johnson *et al.*, 1984).

No toxic effect was observed in mice administered 1-nitronaphthalene for 78 weeks at doses up to 0.12% or in rats at doses up to 0.18% in the diet (National Cancer Institute, 1978).

(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).

1-Nitronaphthalene (100 μg/disc) preferentially inhibited the growth of DNA repair-deficient *Bacillus subtilis* (Tokiwa *et al.*, 1987) and induced DNA damage in *Salmonella typhimurium* (lowest effective dose, 19 μg/ml; Nakamura *et al.*, 1987).

1-Nitronaphthalene was mutagenic to *S. typhimurium*, TA1535, TA1538, TA98 and TA100 (Scribner *et al.*, 1979; El-Bayoumy *et al.*, 1981; Matsuda, 1981; McCoy *et al.*, 1981; Tokiwa *et al.*, 1981; Löfroth *et al.*, 1984; Vance & Levin, 1984; Dunkel *et al.*, 1985; Mortelmans *et al.*, 1986). It was not mutagenic to TA97 or TA1537 (McCoy *et al.*, 1981;

Dunkel *et al.*, 1985; Rosenkranz *et al.*, 1985; Mortelmans *et al.*, 1986) or to *Escherichia coli* WP2 *uvr*A (Dunkel *et al.*, 1985).

This compound did not induce sex-linked recessive lethal mutation in *Drosophila melanogaster* when administered orally or by injection (Valencia *et al.*, 1985).

1-Nitronaphthalene has been reported [data not given] to induce chromosomal aberrations but not sister chromatid exchange [in Chinese hamster CHO cells] (Shelby & Stasiewicz, 1984).

(*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

1-Nitronaphthalene is used as an intermediate in chemical synthesis. It has been detected in some carbon blacks and in particulate exhaust of diesel engines and has been found at low concentrations in ambient air.

4.2 Experimental data

1-Nitronaphthalene was tested for carcinogenicity in mice and rats by oral administration. No carcinogenic effect was observed, but the dose used did not induce toxic effects.

4.3 Human data

No data were available to the Working Group.

4.4 Other relevant data

N-Hydroxy-1-naphthylamine (which has been shown to induce tumours in experimental animals) has been detected as a metabolite of 1-nitronaphthalene *in vitro*. A single intraperitoneal injection of 1-nitronaphthalene to rats caused hepatotoxicity and necrosis of Clara cells of the lung. 1-Nitronaphthalene induced DNA damage and mutation in bacteria but was not mutagenic to *Drosophila melanogaster*.

Summary table of genetic and related effects of 1-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]																													

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 negative, but only one valid study was available to the Working Group

4.5 Evaluation[1]

There is *inadequate evidence* for the carcinogenicity in experimental animals of 1-nitronaphthalene.

No data were available from studies in humans on the carcinogenicity of 1-nitronaphthalene.

Overall evaluation

1-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.

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