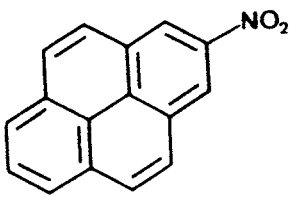
2-NITROPYRENE

1. Chemical and Physical Data

1.1 Synonyms

Chem. Abstr. Services Reg. No.: 789-07-1
Chem. Abstr. Name: Pyrene, 2-nitro-
IUPAC Systematic Name: 2-Nitropyrene

1.2 Structural and molecular formulae and molecular weight



$C_{16}H_9NO_2$ Mol. wt: 247.3

1.3 Chemical and physical properties of the pure substance

(*a*) *Description*: Yellow crystalline solid (Chemsyn Science Laboratories, 1988)

(*b*) *Melting-point*: 197–199°C (Paputa-Peck *et al.*, 1983); 201–202.5°C (Bolton, 1964)

(*c*) *Spectroscopy data*: Nuclear magnetic resonance and ultra-violet spectral data have been reported (Paputa-Peck *et al.*, 1983).

(*d*) *Solubility*: Soluble in toluene and benzene (Chemsyn Science Laboratories, 1988)

1.4 Technical products and impurities

2-Nitropyrene is available for research purposes at ≥95% purity (Chemsyn Science Laboratories, 1988)

2. Production, Use, Occurrence and Analysis

2.1 Production and use

(a) *Production*

2-Nitropyrene can be synthesized by the photoinduced reaction of pyrene with nitrogen dioxide in which monodisperse pyrene on silica particles in nitrogen reacts with nitrogen dioxide in the presence of light (Ramdahl *et al.*, 1986).

No evidence was found that 2-nitropyrene has been produced for other than laboratory use.

(b) *Use*

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

2.2 Occurrence

2-Nitropyrene has been reported to be one of the most abundant nitroarenes in ambient particulate matter (Arey *et al.*, 1987). It was the third most abundant mononitroarene in ambient particles collected in both urban and rural areas of Los Angeles, CA, USA, in winter and in summer (Pitts, 1987). 2-Nitropyrene may result from atmospheric tranformation of pyrene, including the gas-phase reaction of pyrene with nitrogen pentoxide at night and the hydroxyl radical-initiated reaction of pyrene with nitrogen oxides in the day (Arey *et al.*, 1987; Pitts, 1987). 2-Nitropyrene is the only mononitropyrene formed by the hydroxyl radical-initiated reaction (Arey *et al.*, 1986). Atmospheric transformation of pyrene to mononitropyrene, induced in the presence of nitrogen dioxide, is reported to be enhanced in the presence of sulfur dioxide (Tokiwa & Ohnishi, 1986). 2-Nitropyrene was identified in airborne particles in rural Denmark (Nielsen *et al.*, 1984).

A level of 0.17 mg/kg particulate matter was found in an air sample taken in Aurskog, Norway, in winter 1984, and 0.08 mg/kg particulate matter in a sample taken in Claremont, CA, USA, in summer 1985 (Ramdahl *et al.*, 1986). Pitts (1987) reported 0–0.02 mg/kg particulate matter in an air sample taken in Riverside, CA, in summer 1984. A level of 0.04 ng/m^3 was found in a day-time sample of ambient air taken in the winter in Torrance, CA, calculated as the sum of the concentrations on the filter and on three polyurethane foam plugs. A night-time sample contained 0.03 ng/m^3 (Arey *et al.*, 1987).

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).

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

Intraperitoneal injection

Rat: In a study reported as an abstract, female CD rats [initial number unspecified], 30 days of age, received intraperitoneal injections of 67 μmol[16.5 mg]/kg bw 2-nitropyrene [purity unspecified] three times per week for four weeks (Imaida *et al.*, 1985). Surviving rats were killed at 62 weeks. The incidence of mammary tumours [unspecified] was reported to be not significantly different from that in controls (4/29). [The Working Group noted the short periods of treatment and observation and the inadequate reporting of the data.]

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*

No data were available to the Working Group.

(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-Nitropyrene was mutagenic to *Salmonella typhimurium* TA98 and TA100 in the absence of an exogenous metabolic system (Greibrokk *et al.*, 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

2-Nitropyrene has been measured at low concentrations in ambient air.

4.2 Experimental data

No adequate data were available to the Working Group to evaluate the carcinogenicity of 2-nitropyrene in experimental animals.

4.3 Human data

No data were available to the Working Group.

4.4 Other relevant data

2-Nitropyrene was mutagenic to bacteria.

4.5 Evaluation[1]

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

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

Overall evaluation

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

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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-nitropyrene

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

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

5. References

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