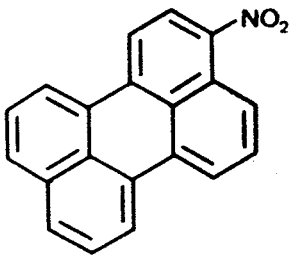
3-NITROPERYLENE

1. Chemical and Physical Data

1.1 Synonyms

Chem. Abstr. Services Reg. No.: 20589-63-3
Chem. Abstr. Name: Perylene, 3-nitro-
IUPAC Systematic Name: 3-Nitroperylene

1.2 Structural and molecular formulae and molecular weight



$C_{20}H_{11}NO_2$ Mol. wt: 297.3

1.3 Chemical and physical properties of the pure substance

(*a*) *Description*: Brick-red crystals from benzene (Buckingham, 1984)

(*b*) *Melting-point*: 210–212°C (Buckingham, 1984)

(*c*) *Spectroscopy data*: Nuclear magnetic resonance and mass spectral data have been reported (Looker, 1972; Eberson & Radner, 1985; Schuetzle & Jensen, 1985).

1.4 Technical products and impurities

No data were available to the Working Group.

2. Production, Use, Occurrence and Analysis

2.1 Production and use

No evidence was found that 3-nitroperylene has been produced in commercial quantities or used for commercial applications.

2.2 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).

3-Nitroperylene was formed when perylene, deposited on high-volume filters, was exposed to simulated atmospheres with 0.5 ppm (1 mg/m^3) nitrogen dioxide and 0.35 ppm (0.9 mg/m^3) gaseous nitric acid, or 0.3–5 ppm (0.6–0.5 mg/m^3) nitrogen dioxide, 0.1 ppm (0.3 mg/m^3) nitric acid, 1.5 ppm (6.6 mg/m^3) nitrogen pentoxide and traces of NO_3 radicals (Pitts *et al.*, 1985). A compound with a mass number of 297 detected in an extract of diesel particulates was characterized tentatively as 3-nitroperylene (Paputa-Peck *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[1]

Skin application

Mouse: In a study of initiating activity, a group of 20 female CD-1 Charles River mice, aged 50–55 days, received ten applications of 0.1 mg 3-nitroperylene (purity, >99%) in 0.1 ml acetone onto shaved back skin every other day for 20 days (total dose, 1.0 mg; El-Bayoumy *et al.*, 1982). A further group received a total dose of 0.05 mg benzo[*a*]pyrene

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

(purity, >99%), and a group of 20 females receiving acetone alone served as vehicle controls. Starting ten days after initiation had been completed, the animals received applications of 2.5 μg 12-*O*-tetradecanoylphorbol 13-acetate in 0.1 ml acetone three times per week for 25 weeks. At the end of this time, skin tumours (mainly squamous-cell papillomas) were observed in 8/20 3-nitroperylene-treated, in 1/20 vehicle controls and in 18/20 benzo[*a*]-pyrene-treated animals. The tumour incidence in the 3-nitroperylene-treated group was significantly greater than that in vehicle controls ($p < 0.01$).

3.2 Other relevant data

(*a*) *Experimental systems*

Absorption, distribution, excretion and metabolism

Incubation of *Salmonella typhimurium* TA98 with [^{3}H]3-nitroperylene in the presence of a rat liver postmitochondrial supernatant gave rise to a number of polar metabolites (Andrews *et al.*, 1983). Similar results were obtained with liver microsomes from Sprague-Dawley rats pretreated with Aroclor 1254 (Anderson *et al.*, 1987).

Toxic effects

No data were available to the Working Group.

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).

3-Nitroperylene induced mutation in *Salmonella typhimurium* TA100 and TA98 in the presence of an exogenous metabolic system from rat liver (Ho *et al.*, 1981; Pitts, 1983; Greibrokk *et al.*, 1984; Löfroth *et al.*, 1984; Anderson *et al.*, 1987).

(*b*) *Humans*

No data were available to the Working Group.

3.3 Epidemiological studies and case reports of carcinogenicity to humans

No data were available to the Working Group.

4. Summary of Data Reported and Evaluation

4.1 Exposure data

No data were available to the Working Group.

4.2 Experimental carcinogenicity data

3-Nitroperylene was tested for carcinogenicity in an initiation-promotion experiment on mouse skin and was active as an initiator.

4.3 Human carcinogenicity data

No data were available to the Working Group.

4.4 Other relevant data

3-Nitroperylene was mutagenic to bacteria in the presence of an exogenous metabolic system.

4.5 Evaluation[1]

There is *inadequate evidence* for the carcinogenicity in experimental animals of 3-nitroperylene.

No data were available from studies in humans on the carcinogenicity of 3-nitroperylene in humans.

Overall evaluation

3-Nitroperylene *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 3-nitroperylene

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
	+																																						

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

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

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