# VAT YELLOW 4

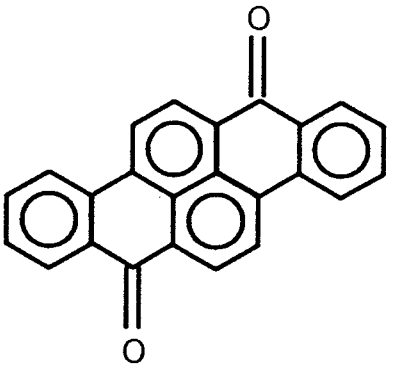
## 1. Chemical and Physical Data

Vat Yellow 4 is produced and used as a mixture of chemicals (see section 1.4). Sections 1.1-1.3 give the chemical and physical characteristics of the principal colour component or of the dye.

### 1.1 Synonyms

*Chem. Abstr. Services Reg. No.*: 128-66-5
(Replaced CAS Reg. Nos 12772-52-0, 39280-74-5 and 115685-46-6)
*Chem. Abstr. Name*: Dibenzo[*b,def*]chrysene-7,14-dione
*IUPAC Systematic Name*: Dibenzo[*b,def*]chrysene-7,14-dione
*Colour Index No.*: 59100
*Synonyms*: CI Vat Yellow 4; dibenzochrysenedione; dibenzo[*a,h*]pyrene-7,14-dione; 3,4:8,9-dibenzopyrene-5,10-dione; dibenzpyrenequinone

### 1.2 Structural and molecular formulae and molecular weight of dibenzo[*b,def*]chrysene-7,14-dione




$C_{24}H_{12}O_2$ Mol. wt: 332.36

### 1.3 Chemical and physical properties of the dye or quinone

(*a*) *Melting-point*: 390°C (Pierce & Katz, 1976) [quinone]; 385°C (Dacre *et al.*, 1979) [dye]

(*b*) *Solubility*: Soluble in nitrobenzene, sulfuric acid, tetrahydronaphthalene and xylene; slightly soluble in acetone, benzene, chloroform, ethanol, pyridine and toluene; insoluble in water (Dacre *et al.*, 1979; Enviro Control, 1981) [dye]

(*c*) *Spectoscopy data*: Ultraviolet, infrared, proton and C-13 nuclear magnetic resonance and mass spectral data have been reported (Pierce & Katz, 1976; Rubin & Buchanan, 1983) [quinone].

## 1.4 Technical products and impurities

*Trade Names*: Ahcovat Printing Golden Yellow GK; Amanthrene Golden Yellow GK; Anthravat Golden Yellow GK; Arlanthrene Golden Yellow GK; Benzadone Gold Yellow GK; Calcoloid Golden Yellow GKWP; Caledon Golden Yellow GK; Caledon Printing Yellow GK; Caledon Yellow GK; Carbanthrene Golden Yellow GK; Cibanone Golden Yellow FGK; Cibanone Golden Yellow GK; Fenanthren Golden Yellow GK; Golden Yellow ZhKh; Helanthrene Yellow GOK; Hostavat Golden Yellow GK; Indanthrene Golden Yellow GK; Indanthren Golden Yellow GK; Indanthren Printing Yellow GOK; Kambanthrene Golden Yellow GK; Leucosol Golden Yellow GK; Mayvat Golden Yellow GK; Mikethrene Gold Yellow GK; Nihonthrene Golden Yellow GK; Novatic Golden Yellow GK; Nyanthrene Golden Yellow GK; Palanthrene Golden Yellow GK; Paradone Golden Yellow GK; Pharmanthrene Golden Yellow GK; Romantrene Golden Yellow FGK; Romantrene Golden Yellow GOK; Sandothrene Golden Yellow GK; Sandothrene Printing Yellow NH; Solanthrene Brilliant Yellow J; Tinon Golden Yellow GK; Tyrian Yellow I-GOK; Vat Golden Yellow ZhKh; Vat Golden Yellow ZhKhD; Yellow GK base

Vat Yellow 4 is available in a commercial grade, with the following specifications: approximately 18% dibenzo[*b*,*def*]chrysene-7,14-dione, 31% sorbitol, 6% dispersant, 3% glycerine and 43% water (National Cancer Institute, 1979). A commercial sample of Vat Yellow 4 analysed in the 1960s was found to contain 0.1% dibenzochrysene (3,4:8,9-dibenzpyrene; Dacre *et al.*, 1979). A US military specification (Anon., 1977) limits the content of dibenzochrysene in Vat Yellow 4 used for smoke screen formulations to a maximum of 0.1%.

Analysis of a Vat Yellow 4 standard revealed the presence of at least six compounds: dibenzochrysenedione, benzanthrone (a starting material in the manufacture of Vat Yellow 4), three diketones (possibly 3-benzoylbenzanthrone and 1,5-dibenzoylnaphthalene, both of which may be intermediates in the manufacture of Vat Yellow 4) and an unknown (Rubin & Buchanan, 1982).

Analysis of a yellow smoke screen formulation for military use showed the presence of dibenzochrysenedione, benzanthrone, some hydrocarbon impurities (possibly the antidusting agent), anthraquinone and an unspecified diketone. Analysis of a green smoke screen formulation showed the presence of dibenzochrysenedione, 1,4-di-*para*-toluidinoanthraquinone, benzanthrone, some hydrocarbon impurities (possibly the antidusting agent) and several unidentified impurities (Rubin & Buchanan, 1982).

# 2. Production, Use, Occurrence and Analysis

## 2.1 Production and use

(*a*) *Production*

Vat Yellow 4 was reportedly first synthesized by Kränzlein and co-workers in 1922 (Society of Dyers and Colourists, 1971). It has been prepared by the following methods: benzoylation of benzanthrone (the original synthetic route) and ring closure of 3-benzoylbenzanthrone with aluminium chloride and an oxidizing agent; ring closure of 1,5-dibenzoylnaphthalene in the presence of aluminium chlorides; benzoylation of 1-benzoylnaphthalene, followed by ring closure; and direct condensation of naphthalene with benzoyl chloride (see IARC, 1987a) in aluminium chloride at 160°C (Society of Dyers and Colourists, 1971; Savoca, 1974; Dacre *et al.*, 1979).

US production of Vat Yellow 4 was reported to be 161 tonnes in 1972 (US Tariff Commission, 1974). Separate figures were not reported after 1972. Production of all Vat Yellow dyes was approximately 880 tonnes in 1975 and 5 tonnes in 1987 (US International Trade Commission, 1977, 1988).

(*b*) *Use*

Vat Yellow 4 has an anthraquinoid structure. In the dye process, the keto groups are first reduced to hydroxyls to facilitate penetration of the fibre by the dye; the dye is then fixed by oxidation back to the keto form. Vat Yellow 4 is used to dye cellulose fibres, some cellulose synthetics (e.g., cellulose acetate, cellulose polyester), wool, silk and paper (National Cancer Institute, 1979; Enviro Control, 1981).

Vat Yellow 4 has also been used to manufacture Vat Orange 1, another commercial vat dye (Savoca, 1974).

The dye has been used by the US and other armed services to colour smoke screens and as a signalling agent (National Cancer Institute, 1979; Enviro Control, 1981). The dye mixture is approximately 40-50% of the total pyrotechnic composition, which also includes an oxidizer (potassium chlorate), a fuel (sugar), a coolant (sodium bicarbonate) and a binder (diatomaceous earth; see IARC, 1987b). For example, a typical green-coloured smoke contains 44% green dye mix (benzanthrone, Solvent Green 3 and Vat Yellow 4), 28.5% potassium chlorate, 23% sugar, 2.5% sodium bicarbonate and 2.0% diatomaceous earth (Chin & Borer, 1982; Smith & Stewart, 1982).

(*c*) *Regulatory status and guidelines*

No regulatory standard or guideline has been established for Vat Yellow 4.

## 2.2 Occurrence

(*a*) *Natural occurrence*

Vat Yellow 4 is not known to occur as a natural product.

(*b*) *Occupational exposure*

During the 1940s and 1950s, soldiers were exposed to chemical smoke screens that contained Vat Yellow 4, sometimes for several months. No data on exposure levels were available (National Cancer Institute, 1979).

Swedish workers were reported to be exposed to Vat Yellow 4 contained in a paste used to polish steel; no data were provided on exposure levels (Järvholm *et al.*, 1982).

(*c*) *Air*

Vat Yellow 4 has been identified in particulate matter from air samples collected in Toronto, Ontario, Canada (Pierce & Katz, 1976).

### 2.3 Analysis

One method for the analysis of polycyclic quinones, including Vat Yellow 4, involves isolation by column and thin-layer chromatography and spectral analysis by ultraviolet, visible and fluorescence spectrophotometry and mass spectrometry (Pierce & Katz, 1976).

Vat Yellow 4 is a component in two coloured smoke mixes — yellow and green. Vat Yellow 4 was separated from the yellow smoke mix by vacuum sublimation, Soxhlet extraction and differential solubility. For the green smoke mix, Vat Yellow 4 was separated by chromatography on a basic alumina column and vacuum sublimation (Rubin & Buchanan, 1982).

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

### 3.1 Carcinogenicity studies in animals

*Oral administration*

*Mouse*: Groups of 50 male and 50 female B6C3F$_1$ mice, six weeks of age, were fed 25 000 or 50 000 (males) and 12 500 and 25 000 (females) mg/kg of diet (ppm) Vat Yellow 4 (commercial formulation containing approximately 18% of the dyestuff dibenzo[*b*,*def*]chrysene-7,14-dione) for 106 weeks. Groups of 20 males and 20 females served as untreated controls. Neither survival nor body weight gain was affected by the treatment. A significant increase ($p = 0.002$, Cochran-Armitage test) in the incidence of lymphomas was observed in male mice (control, 3/20; low-dose, 7/47; high-dose, 22/50). The incidences of hepatic tumours (all considered to be hepatocellular carcinomas) in treated mice were: 3/20 in male controls, 22/47 in low-dose males ($p = 0.012$; Fisher exact test), 21/50 in high-dose males ($p = 0.027$; Fisher exact test), 2/19 in control females, 6/48 in low-dose females and 9/50 in high-dose females. The trend was not significant for either sex (National Cancer Institute, 1979).

*Rat*: Groups of 50 male and 50 female Fischer 344 rats, six weeks of age, were fed 3500 or 7000 mg/kg of diet Vat Yellow 4 (commercial formulation containing approximately 18%

dibenzo[*b*,*def*]chrysene-7,14-dione) for 104 weeks. Groups of 20 males and 20 females served as untreated controls. Mean body weights of the treated rats were lower than those of the corresponding controls; survival was not affected by the treatment. The incidences of tumours were not significantly higher in treated groups than in controls (National Cancer Institute, 1979). [The Working Group noted the small number of control animals used.]

### 3.2 Other relevant biological data

(*a*) *Experimental systems*

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

No data were available to the Working Group.

(ii) *Toxic effects*

No data relevant to an evaluation of carcinogenicity were available to the Working Group.

(iii) *Effects on reproduction and prenatal toxicity*

No data were available to the Working Group.

(iv) *Genetic and related effects* (see Appendix 1)

Vat Yellow was not mutagenic to several strains of *Salmonella typhimurium* in the presence or absence of an exogenous metabolic system from Aroclor 1254-induced rat or Syrian hamster liver (Zeiger *et al.*, 1987).

(*b*) *Humans*

No data were available to the Working Group.

### 3.3 Case reports and epidemiological studies of carcinogenicity to humans

No data were available to the Working Group.

## 4. Summary of Data Reported and Evaluation

### 4.1 Exposure data

Vat Yellow 4 is an anthraquinone-type dyestuff which is used to colour fabrics and paper and in smoke-screen formulations for military use. No data on occupational exposure levels were available.

### 4.2 Experimental carcinogenicity data

Vat Yellow 4 was tested for carcinogenicity by oral administration in one strain of mice and in one strain of rats, producing an increased incidence of lymphomas and hepatocellular tumours in male mice.

### 4.3 Human carcinogenicity data

No data were available to the Working Group.

### 4.4 Other relevant data

In a single study, Vat Yellow 4 was not mutagenic to bacteria in the presence or absence of an exogenous metabolic system.

### 4.5 Evaluation[1]

There is *limited evidence* for the carcinogenicity of Vat Yellow 4 in experimental animals.

No data were available from studies in humans on the carcinogenicity of Vat Yellow 4.

**Overall evaluation**

Vat Yellow 4 is *not classifiable as to its carcinogenicity to humans (Group 3)*.

## 5. References

Anon. (1977) *Military Specification, Dye, Vat Yellow 14 (MIL-D-0050029D (MA))*, Fort Detrick, Frederick, MD, US Army Medical Research and Development Command

Chin, A. & Borer, L. (1982) Investigations of the effluents produced during the functioning of Navy colored smoke devices. *Proc. Int. Pyrotech. Semin., 8*, 129-148

Dacre, J.C., Burrows, W.D., Wade, C.W.R., Hegyeli, A.F., Miller, T.A. & Cogley, D.R., eds (1979) *Problem Definition Studies on Potential Environmental Pollutants. V. Physical, Chemical, Toxicological, and Biological Properties of Seven Chemicals used in Pyrotechnic Compositions (Technical Report 7704; US NTIS AD-A090631)*, Fort Detrick, Frederick, MD, US Army Medical Research and Development Command, pp. 66-73

Enviro Control (1981) *Anthraquinone Dye Toxicological Profiles (CSPC-Mono-82-2; US NTIS PB83-166033)*, Rockville, MD

IARC (1987a) *IARC Monographs on the Evaluation of Carcinogenic Risks to Humans*, Suppl. 7, *Overall Evaluations of Carcinogenicity: An Updating of* IARC Monographs *Volumes 1 to 42*, Lyon, pp. 126-127

IARC (1987b) *IARC Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans*, Vol. 42, *Silica and Some Silicates*, Lyon, pp. 39-143

[1]For description of the italicized terms and criteria for making the evaluation, see Preamble, pp. 25-29.

## Summary table of genetic and related effects of Vat Yellow 4

| **Nonmammalian systems** | | | | | | | | | | | | | **Mammalian systems** | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
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| Proka-ryotes | | 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 symbol indicates the consensus of the Working Group with regard to the results for each endpoint:*

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

Järvholm, B., Thiringer, G. & Axelson, O. (1982) Cancer morbidity among polishers. *Br. J. ind. Med., 39*, 196-197

National Cancer Institute (1979) *Bioassay of C.I. Vat Yellow 4 for Possible Carcinogenicity (CAS No. 128-66-5) (Technical Report No. 134; DHEW Publ. No. (NIH) 79-1389)*, Bethesda, MD, US Department of Health, Education, and Welfare

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Rubin, I.B. & Buchanan, M.V. (1982) The preparative scale separation and the identification of constituents of anthraquinone-derived dye mixtures. Part 2. Benzanthrone, dibenzochrysenedione, and 1,4-di-*p*-toluidino-anthraquinone. *Anal. chim. Acta, 135*, 121-128

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Smith, M.D. & Stewart, F.M. (1982) Environmentally acceptable smoke munitions. *Proc. int. Pyrotech. Semin., 8*, 623-635

Society of Dyers and Colourists (1971) *Colour Index*, 3rd ed., Vol 4, Bradford, Yorkshire, p. 4524

US International Trade Commission (1977) *Synthetic Organic Chemicals, US Production and Sales, 1975 (USITC Publication 804)*, Washington DC, US Government Printing Office, p. 53

US International Trade Commission (1988) *Synthetic Organic Chemicals, US Production and Sales, 1987 (USITC Publication 2118)*, Washington DC, US Government Printing Office, p. 4-5

US Tariff Commission (1974) *Synthetic Organic Chemicals, US Production and Sales, 1972 (TC Publication 681)*, Washington DC, US Government Printing Office, p. 64

Zeiger, E., Anderson, B., Haworth, S., Lawlor, T., Mortelmans, K. & Speck, K. (1987) *Salmonella* mutagenicity tests. III. Results from the testing of 255 chemicals. *Environ. Mutagenesis, 9 (Suppl. 9)*, 1-110