File No: **NA/5**

Date: 18 February 1991

NATIONAL INDUSTRIAL CHEMICALS NOTIFICATION
AND ASSESSMENT SCHEME

FULL PUBLIC REPORT

# N,N-DIETHYL-6-(DIETHYLAMINO)-9-[2-(METHOXYCARBONYL)PHENYL]- 3H-XANTHENE-3-YLIDENEAMMONIUM TRIFLUOROMETHANE SULFONATE

## (MAGENTA RHODAMINE PIGMENT)

This Assessment has been compiled in accordance with the provisions of the Industrial Chemicals (Notification and Assessment) Act 1989 and Regulations. This legislation is an Act of the Commonwealth of Australia. The National Industrial Chemicals Notification and Assessment Scheme (NICNAS) is administered by Worksafe Australia which also conducts the occupational health & safety assessment. The assessment of environmental hazard is conducted by the Department of the Arts, Sport, the Environment, Territories and Tourism and the assessment of public health is conducted by the Department of Health, Housing and Community Services.

For the purposes of subsection 78(1) of the Act, copies of this full public report may be inspected by the public at the Library, Worksafe Australia, 92-94 Parramatta Road, Camperdown NSW 2050, between the hours of 10.00 a.m. and 12.00 noon and 2.00 p.m. and 4.00 p.m. each week day except on public holidays.

Please find enclosed order form for Full Public Reports.

For Enquiries please contact Ms Karen Bell at:

*Street Address*: 92 Parramatta Rd Camperdown, NSW 2050, AUSTRALIA
*Postal Address:* GPO Box 58, Sydney 2001, AUSTRALIA
*Telephone:* (61) (02) 565-9466 **FAX (61) (02) 565-9465**

Director
Chemicals Notification and Assessment

**Full Public Report**

# N,N-DIETHYL-6-(DIETHYLAMINO)-9-[2-(METHOXYCARBONYL)PHENYL]- 3H-XANTHENE-3-YLIDENEAMMONIUM TRIFLUOROMETHANE SULFONATE

## (MAGENTA RHODAMINE PIGMENT)

## 1. IMPORTER

KODAK (AUSTRALASIA) Pty Ltd, 173 Elizabeth Street, Coburg, Victoria 3058

## 2. IDENTITY OF THE CHEMICAL

**Chemical name:** N,N-Diethyl-6-(diethylamino)-9-[2-(methoxycarbonyl)phenyl]-3H-xanthene-3-ylideneammonium trifluoromethane sulfonate

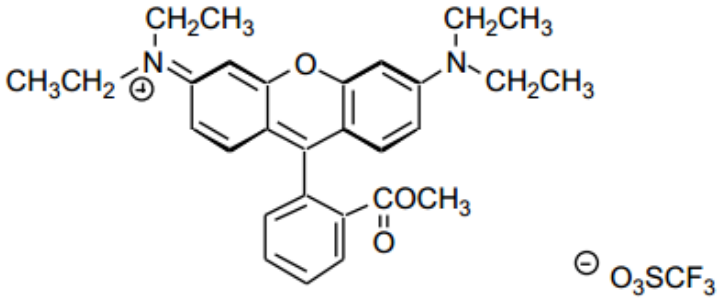
**Chemical Abstract Service (CAS) No.:** 120611-30-5

**Trade name:** Magenta Rhodamine Pigment

**Molecular formula:** $C_{29}H_{33}N_2O_3 \cdot CF_3O_3S$

**Molecular weight:** 606.66

**Structural formula:**




**Spectral Data:** UV-VIS Spectroscopy
Infrared Spectroscopy
NMR

## 3. PHYSICAL AND CHEMICAL PROPERTIES

Magenta Rhodamine Pigment, at room temperature and atmospheric pressure, is a non-volatile, dark purple crystalline solid with no discernible odour. Its physical and chemical properties include:

**Melting point:** 192°C

**Thermal decomposition temperature:** 400°C.

**Pyrolysis products:** On combustion carbon dioxide and toxic fumes such as carbon monoxide, hydrogen fluoride and oxides of nitrogen and sulphur will be produced.

**Water solubility:** < 1gm/L (detection limit)

## 4. METHODS OF DETECTION AND DETERMINATION

Separation: high performance liquid chromatography (HPLC)
Detection: IR, NMR and UV (absorbance band at 555nm) detection.

## 5. PURITY OF THE CHEMICAL

Degree of purity (w/w): 95% by HPLC

## 6. INDUSTRIAL USES

The chemical is intended to be used as a magenta colouring agent in a commercial photocopier formulation. It is estimated that less than 50 kg of the pigment will be imported every year for the first five years. The formulated toner will be imported in sealed polyethylene cartridges each containing 350 gm. Magenta Rhodamine Pigment will be a minor (<5%) component in the formulation.

Other ingredients of the formulation, Kodak Coloredge Magenta Toner, are 95-99% 'polyester'* (CAS No. 120611-31-6) and <2% CA-10*.

*Note: full assessment and summary reports for these substances have been published by the Director of Chemicals Notification and Assessment under subsection 38(5) of the Industrial Chemicals (Notification and Assessment) Act 1989

## 7. PUBLIC AND OCCUPATIONAL EXPOSURE

The formulation will be imported and marketed in sealed cartridges ready for use in photocopiers. Only the seal of the cartridges needs to be opened immediately before use. Industrial processes such as manufacture, reformulation, packaging and refilling of

containers will not be carried out in Australia. After use, the formulated product will be fused to paper in a water insoluble polymer matrix.
Therefore, very low public and worker exposure to Magenta Rhodamine pigment and the formulated toner product is expected under normal use conditions.

However, photocopier maintenance workers will have higher exposure to the formulated toner product through skin contact and inhalation during routine maintenance of the machines.

## 8. ENVIRONMENTAL EXPOSURE

### 8.1 Release

As the formulated toner will only be used in photocopying machines, it is expected that only a negligible amount of pigment (as toner waste) would be generated or released to the environment. The chance of accidental spillage should be minimal as the toner is transported and handled in sealed cartridges.

### 8.2 Fate

The quantity of pigment that will need to be incinerated or disposed of in a landfill is expected to be very small. Empty cartridges will be disposed of by contract with a licensed chemical waste disposal agency or returned to the US manufacturer.

Paper to which the polymer is fixed will ultimately be incinerated, disposed of in a landfill, or recycled. When incinerated, the chemical will be degraded to oxides of carbon, sulphur and nitrogen. When disposed in a landfill, it is likely that the pigment will remain encapsulated in the polymer matrix which is not expected to degrade, and therefore is likely to persist.

Waste paper is usually repulped using a number of alkalis, dispersing agents, wetting agents, water emulsifiable organic solvents and bleaching agents. These chemicals enhance fibre separation, ink detachment from the fibres, pulp brightness and whiteness of the paper. After pulping, the contaminants and the ink are separated from the fibres by pumping the stock through various heat washing, screening, cleaning, flotation and dispersion stages (1). As a triflate, the pigment should have a moderate water solubility and may be discharged in the aqueous waste stream from recycling plants. However, any discharges of the pigment during the recycling process will be small as only small amounts of the pigment will be imported (less than 50kg per year).

## 9. EVALUATION OF TOXICOLOGY DATA

### 9.1 Acute Toxicity

TABLE 1. Summary of Acute Toxicity Studies with Magenta Rhodamine Pigment.

| Test | Species | Outcome | Reference |
|---|---|---|---|
| Oral | Rat | $LD_{50}$ = 883 mg/kg (M)<br>= 624 mg/kg (F) | (2) |
| Dermal | Rat | $LD_{50}$ > 2000 mg/kg (M,F) | (3) |
| Skin Irritation | Rabbit | Non-irritant | (4) |
| Eye Irritation | Rabbit | Severe irritant | (5) |
| Skin sensitisation | Guinea Pig | No sensitisation | (6) |

### 9.1. Oral Toxicity

An acute oral toxicity test was carried out in CD(SD)BR rats, using 5 males and 5 females in each group. The animals were administered the following doses of Magenta Rhodamine Pigment, by gavage, using 0.5% guar gum as the vehicle: 312, 625, 1250, 2500 and 5000 mg/kg.

In all the test animals there was a change in the colour of the extremities associated with administration of the chemical. Clinical signs included thymic atrophy, small spleens, and adipose tissue atrophy. From the results, the following oral $LD_{50}$s in rats were determined, males 883mg/kg and females 624mg/kg. (2)

It was also reported that an oral $LD_{50}$ of greater than 5000mg/kg was observed in rats for the formulated product, Kodak Coloredge Magenta Toner, which contained less than 5% of Magenta Rhodamine pigment. (7)

### 9.1.2 Dermal Toxicity:

A limit test was performed on rats. To the clipped backs of 5 female and 5 male CD(SD)BR rats a 2000 mg/kg dose was applied. There were no mortalities and no signs of systemic toxicity. The $LD_{50}$ was >2000 mg/kg and these results indicate that the pigment has a low dermal toxicity in rats. (3)

### 9.1.3 Skin Irritation

A 0.5gm dose of the pigment, moistened with distilled water, was applied to the shaved backs of 3 New Zealand White Rabbits, and

kept in place with an occlusive dressing for 4 hours. No signs of oedema or other irritant responses were noted, but due to colouration of the skin by the pigment evidence of erythema may be masked. However, erythema was not noted at the margins of the stained area where it was reported that staining did not interfere with the detection of irritation. (4)

### 9.1.4 Eye Irritation

In 6 New Zealand White Rabbits 0.1gm of the pigment was placed in the conjunctival sac of one eye of each rabbit (3 washed/3 unwashed). In the unwashed eyes, the pigment caused severe oedema, corneal opacity, and moderate to heavy discharges. In the washed eyes, the pigment caused severe oedema and erythema, moderate to heavy discharges, and necrosis of the nictitating membrane and conjunctivae. Fluorescein staining of the adnexa was observed in all eyes. Fluorescein staining of the cornea was observed in all washed eyes and in 2 of the 3 unwashed eyes. The results indicate that the chemical was a severe eye irritant and that immediate washing was not palliative. (5)

It was also reported that the formulated toner product, Kodak Coloredge Magenta Toner, is only slightly irritating to the eye. (7)

### 9.1.5 Skin Sensitisation

Prior to the induction and sensitisation test, the maximum non-irritant dose was determined in a preliminary irritation study. In this preliminary study 0.5gm of Magenta Rhodamine pigment, moistened with distilled water, was applied under an occlusive wrap to the clipped backs of 3 (HA)BR Hartley guinea pigs. The wraps were removed after six hours and the skin wiped free of excess material. The animals were then examined for signs of erythema and oedema at 24 and 48 hours after the application. No signs of irritation were observed in any of the test animals in this preliminary study.

A Buehler test was carried out in a test group and a control group of 10 (HA)BR Hartley guinea pigs each. In this induction and challenge study, the same dose and application procedures, as for the preliminary study, were used and repeated weekly for three weeks in the 10 test animals. Two weeks after the last induction exposure, a single dose of the pigment was applied to each of the 10 test and 10 control animals using the same application procedures but at different sites on the back of the animals. The animals were examined for signs of erythema and oedema at 24 and 48 hours after the challenge application. No signs of irritation were observed in any animals, however staining by the pigment may have masked any evidence of erythema. These results indicate that Magenta Rhodamine pigment is a non-sensitiser in guinea pigs. (6)

## 9.2 Genotoxicity

Magenta Rhodamine Pigment was assayed for mutagenic activity in the Ames Salmonella/microsome Reverse Mutation Assay using *Salmonella*

*typhimurium* strains TA1535, TA1537, TA1538, TA98, and TA100. The assays were conducted using 3 plates per dose level in the presence and absence of a mammalian metabolic activation system. The doses used were 0.5-100 ug/plate in the absence of microsomes, and 1-300ug/plate in the presence of microsomes. No increase in the number of revertant colonies following exposure to the pigment was noted in any of the strains. The results of these tests indicate that Magenta Rhodamine Pigment, under the conditions of the study, was not genotoxic towards *Salmonella typhimurium*.

### 9.3 Overall Assessment of Toxicology Data

Animal toxicity studies reveal that Magenta Rhodamine Pigment exhibited low acute oral toxicity (Rat $LD_{50}$ 883mg/kg (M), 624 mg/kg (F)) and dermal toxicity (Rat $LD_{50}$ >2000mg/kg). The chemical is likely to be non-irritating to the skin but is a severe eye irritant. It is anticipated that the pigment, if inhaled, will irritate the upper respiratory tract. Magenta Rhodamine Pigment does not cause skin sensitisation.

The pigment was not genotoxic towards *Salmonella typhimurium*.

## 10. ENVIRONMENTAL ASSESSMENT

### 10.1 Assessment of Environmental Exposure

The main source of environmental exposure to Magenta Rhodamine pigment would occur through the treatment and disposal of waste paper, particularly recycling. During the recycling process, some of the pigment may be discharged in the aqueous waste from recycling plants. However, only small amounts are to be used annually, and it is therefore unlikely that toxic concentrations would result, even before dilution of any discharges by the receiving water.

### 10.2 Assessment of Environmental Hazard

Animal studies show that Magenta Rhodamine pigment has low acute toxicity, except that it is a severe eye irritant. Some aquatic toxic effects may be expected as the pigment is a quaternary ammonium salt. However, as the environmental exposure to Magenta Rhodamine pigment is expected to be low, the environmental hazard would also be low.

## 11. ASSESSMENT OF PUBLIC AND OCCUPATIONAL HEALTH AND SAFETY EFFECTS

Under normal use conditions public and worker exposure to Magenta Rhodamine Pigment and the formulated toner product is likely to be minimal. Results of animal studies indicate that the pigment, and the formulated product, have low acute toxicities, and therefore exposure to the toner (which contains Magenta Rhodamine Pigment only as a minor component) should not pose a significant acute health and safety hazard to the public and workers.

## 12. RECOMMENDATIONS FOR THE CONTROL OF PUBLIC AND WORKER EXPOSURE

To minimise workers exposure to the Magenta Rhodamine pigment and the formulated toner product, in general the following guidelines and precautions should be observed:

. as a good work practice, photocopiers should be located in a well ventilated area to control the accumulation of any dusts, gases or fumes;

. a copy of the Material Safety Data Sheet of the formulated product should be made available to all personnel who may have exposure to the toner product; and

. photocopier maintenance workers who frequently come into direct contact with the toner powder should:

  - wear appropriate gloves (for example cotton or impervious gloves);

  - avoid the generation of a dust cloud; and

  - observe good personal hygiene practices at work.

Note: Guidance on the health hazards and the appropriate control measures are available in Worksafe Australia *Guide on Office Copying Machines*(8).

## 13. REQUIREMENTS FOR SECONDARY NOTIFICATION

Under the Industrial Chemicals (Notification and Assessment) Act 1989 (the Act), secondary notification of Magenta Rhodamine Pigment shall be required by Kodak (Australasia) Pty Ltd if any of the circumstances stipulated under subsection 64(2) of the Act arise. No other specific conditions are prescribed.

## 14. REFERENCES

(1) Forestry Canada, Industry/Trade and Technology Directorate and Environment Canada, Final Report, *Waste Paper Study (to end of 1989)*, p 56-57.

(2) Acute Oral Toxicity of N,N-diethyl-6-(diethylamino)-9-[2-(methoxycarbonyl)phenyl]-3H-xanthene-3-ylideneammonium trifluoromethane sulfonate, Data on File, Eastman Kodak, USA, Report TX-88-54, 1988.

(3) Acute Dermal Toxicity of N,N-diethyl-6-(diethylamino)-9-[2-(methoxycarbonyl)phenyl]-3H-xanthene-3-ylideneammonium trifluoromethane sulfonate, Data on File, Eastman Kodak, USA, Report TX-88-55, 1988.

(4) Acute Skin Irritation of N,N-diethyl-6-(diethylamino)-9-[2-(methoxycarbonyl)phenyl]-3H-xanthene-3-ylideneammonium

trifluoromethane sulfonate, Data on File, Eastman Kodak, USA, Report TX-88-57, 1988.

(5) Acute Eye Irritation of N,N-diethyl-6-(diethylamino)-9-[2-(methoxycarbonyl)phenyl]-3H-xanthene-3-ylideneammonium trifluoromethane sulfonate, Data on File, Eastman Kodak, USA, Report TX-88-56, 1988.

(6) Skin Sensitization study of N,N-diethyl-6-(diethylamino)-9-[2-(methoxycarbonyl)phenyl]-3H-xanthene-3-ylideneammonium trifluoromethane sulfonate, Data on File, Eastman Kodak, USA, Report TX-89-45, 1989.

(7) National Industrial Chemicals Notification and Assessment Scheme, *'Polymer of pentanedioic acid, dimethyl ester; 1,4-benzenedicarboxylic acid, dimethyl ester; 1,2-propanediol and 1,2,3-propanetriol'*, Full Public Report No. NA/7, 1991.

(8) National Occupational Health and Safety Commission, *Office Copying Machines*, AGPS, Canberra, December, 1989.