7,12-Dimethylbenz[a]anthracene

Safety Data Sheet

Division of Occupational Health and Safety
National Institutes of Health

WARNING!

This compound is absorbed through the skin and respiratory and intestinal tracts. It is carcinogenic and may irritate tissues and induce sensitivity. Avoid formation and breathing of dusts.

Laboratory operations should be conducted in a fume hood, glove box, or ventilated cabinet.

Avoid skin contact: If exposed, wash with soap and water. Avoid washing with solvents and exposure to UV light.

For eye exposure, irrigate immediately with large amounts of water. For ingestion, induce vomiting. For inhalation, remove victim promptly to clean air. Administer rescue breathing if necessary. Refer to physician.

In case of laboratory spill, wear protective clothing during cleanup. Avoid skin contact or breathing of dust. Use organic solvent (not alcohol) to dissolve compound. Wash down area with soap and water. Check for fluorescence of residues with UV light. Dispose of waste solutions and materials by incineration.

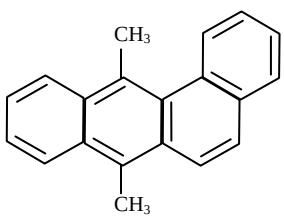
A. Background

7,12-Dimethylbenz[a]anthracene (DMBA) is well established as a highly potent carcinogen. DMBA is not known to be an environmental contaminant. It has no known commercial or industrial use and is employed solely in carcinogenesis research. It is destroyed through photooxidation in the atmosphere and is believed to be degraded slowly by bacteria in the soil.

B. Chemical and Physical Data

1. Chemical Abstract No.: 57-97-6
2. Synonyms: DBA; 9,10-Dimethyl-1,2-benzanthracene; DMBA; Dimethylbenzanethrene; 7,12-DMBA; 1,4-Dimethyl-2,3-benzphenanthrene.
3. Molecular formula, weight and structure:

$C_{20}H_{16}$; 256.36



4. Density: No data.

5. Absorption spectroscopy: UV (Sadtler, 1961; Friedel and Orchin, 1951); UV fluorescence (Sawicki, 1960); IR (Sadtler, 1961; Fuson and Josien, 1956); NMR (Sadtler, 1961; Bartle *et al.*, 1969; Ozubko *et al.*, 1974).
6. Vapor pressure: No quantitative data. Saturated vapor concentration assumed to be in the range of benz[a]anthracene, approximately 3,000 ng/m^3 at 25ºC (Radding *et al.*, 1976).
7. Solubility: Soluble in most organic solvents; slightly soluble in alcohols; very slightly soluble in water.
8. Description, appearance: Colorless plates with greenish-yellow tinge.
9. Melting point: 122-123ºC
10. Stability: Stable in dark at ambient temperature or below. Solutions undergo photooxidation in air and light.
11. Chemical reactivity: Not spontaneously reactive, but enters into numerous types of reactions with organic reagents.
12. Flash point: Does not apply.
13. Autoignition temperature: No data.
14. Flammable limits: Does not apply.

C. Fire, Explosion, and Reactivity Hazard Data

1. DMBA does not require special fire-fighting procedures or equipment. Because of the electrostatic nature of dry DMBA, fire fighters should wear full-face masks.
2. DMBA does not present unusual fire and explosion hazards.
3. DMBA is unstable in the presence of light and is more unstable when UV radiation is present.
4. Incompatibilities: No data.
5. DMBA is not known to produce hazardous decomposition products.
6. DMBA is nonvolatile and does not require nonspark equipment. When handled in flammable solvents such as benzene, the precautions required for such solvents will apply. In powdered form DMBA is electrostatic, and when used in this form, it requires the use of antistatic devices.

D. Operational Procedures

The NIH Guidelines for the Laboratory Use of Chemical Carcinogens describe operational practices to be followed when potentially carcinogenic chemicals are used in NIH laboratories. The Guidelines should be consulted to identify the proper use conditions required and specific controls to be implemented during normal and complex operations or manipulations involving DMBA.

1. Chemical inactivation: No validated method reported.
2. Decontamination: Turn off equipment that could be affected by DMBA or the materials used for cleanup. If more than 1 g has been spilled or if thee is any uncertainty regarding the procedures to be followed for decontamination, call the NIH Fire Department (dial 911) for assistance. Wash surfaces with copious quantities of soap and water. Glassware should be rinsed (in a hood with an organic solvent (not alcohol), followed by soap and water. Animal cages should be washed with soap and water.

3. Disposal: No waste streams containing DMBA shall be disposed of in sinks or general refuse. Surplus DMBA or chemical waste streams contaminated with DMBA shall be handled as hazardous chemical waste and disposed of in accordance with the NIH chemical waste disposal system. Nonchemical waste (*e.g.*, animal carcasses and bedding) containing DMBA shall be handled and packaged for incineration in accordance with the NIH medical-pathological waste disposal system. Potentially infectious waste (*e.g.*, tissue cultures) containing DMBA shall be disinfected by heat using a standard autoclave treatment and packaged for incineration, as above. Burnable waste (*e.g.*, absorbent bench top liners) minimally contaminated with DMBA shall be handled as potentially infectious waste and packaged for incineration, as above. Absorbent materials (*e.g.*, associated with spill cleanup) grossly contaminated shall be handled in accordance with the chemical waste disposal system. Radioactive waste containing DMBA shall be handled in accordance with the NIH radioactive waste disposal system.
4. Storage: Store solid DMBA and its solutions in dark-colored, tightly closed containers, preferably under refrigeration.

E. Monitoring and Measurement Procedures Including Direct Field Measurements and Sampling for Subsequent Laboratory Analysis (Jones and Freudenthal, 1978)

1. Sampling: Two methods are recommended: using an absorption sampler in which cooled air is passed through Tenax and using high-volume filtration through fiberglass filter traps.
2. Separation and analysis: Several methods are available and offer various degrees of sensitivity. For separation, TLC, HPLC, and GC are useful. TLC is the least efficient of these three methods. HPLC and GC are highly efficient. The most useful and sensitive method for separation and analysis of DMBA is GC-MS. This method allows for accurate identification in the nanogram to pictogram level; it is still desirable to confirm the identification by other analytical methods. UV spectroscopy is useful but is limited because of possible similarity in spectra with a related compound. Fluorescence spectroscopy gives both excitation and emission spectra and its sensitivity level is in the nanogram range. It is more sensitive than UV by a factor of 10^2 or 10^3 or greater. Other methods are phosphorescence, NMR, and IR spectroscopy.

F. Biological Data (Animal and Human)

1. Absorption: DMBA is readily absorbed through the skin and by intravenous and intraperitoneal injection, ingestion, and inhalation.
2. Distribution: The label (^{3}H or ^{14}C) of orally-administered DMBA in rats appears in lymph and bile shortly after dosing and is then distributed to lipid-containing tissue except the brain.
3. Metabolism and excretion: DMBA is metabolized by oxidative enzymes of mammalian live, mainly to the mono- and dihydroxymethyl derivatives, and further by the aryl hydrocarbon hydroxylase system to a variety of epoxides, diols, phenols, and quinones. The specific metabolic pathway of DMBA to its ultimate carcinogen is not known but a diol-epoxide is suspect (Moschel *et al.*, 1977). In analogy with other polycyclic hydrocarbons, urinary excretion products probably consists of conjugated products of diols and/or epoxides with glucuronic acid, sulfate and reduced glutathione.
4. Toxic effects: Acute LD_{50}s are 340 mg/kg (orally, mouse) and 54 mg/kg (intravenous, rat). There is no specific target organ but rather a general toxic effect in epithelial and fibroblastic cells. High chronic doses produce adrenal necrosis (Boyland *et al.*, 1965; Heidelberger, 1975); the responsible metabolite appears to be the 7-hydroxymethyl derivative (Juchau *et al.*, 1976).

5. Carcinogenic effects: DMBA is highly carcinogenic in experimental animals. Large single and multiple doses produce tumors of the skin, breast, and stomach or leukemias regardless of route of administration. Skin is particularly sensitive to low, topically applied doses.
6. Mutagenic and teratogenic effects: DMBA is a strong mutagen after metabolic activation. Teratogenicity is found in the fetuses of rats injected with DMBA and its 7-hydroxymethyl metabolite during gestation.

G. Emergency

1. Skin and eye exposure: For skin exposure, remove contaminated clothing and wash skin with soap and water. Skin should not be rinsed with organic solvents or scanned with UV light. For eye exposure, irrigate immediately with copious quantities of running water for at least 15 minutes.
2. Ingestion: Drink plenty of water. Induce vomiting.
3. Inhalation: Remove victim promptly to clean air. Administer rescue breathing if necessary.
4. Refer to physician.

H. References

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