

# Safety Data Sheet

# 3-Methyl- cholanthrene

Division of 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

3-Methylcholanthrene (MC) is well established as a highly potent carcinogen. MC 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.

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## Chemical and Physical Data

1. Chemical Abstract No.: 56-49-5

2. Synonyms:

MC 1,2-Dihydro-3-methyl-benz(j)aceanthrylene (9CI)

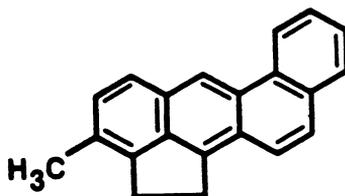
MCA 20-Methylcholanthrene (obsolete)

3-MC

20-MC

3. Molecular  
formula:  
 $C_{21}H_{16}$

structure:



weight:  
286.37

4. Density: 1.28 g/cm<sup>3</sup>.

5. Absorption spectroscopy: UV (Friedel and Orchin, 1951; Sawicki et al., 1960); UV fluorescence (Sawicki et al., 1960); IR (Sadtler, 1961); NMR (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<sup>3</sup> at 25°C (Radding et al., 1976).

7. Solubility: Soluble in most organic solvents; slightly soluble in alcohol; and very slightly soluble in water.

8. Description, appearance: Pale yellow prisms.

9. Boiling point: 280°C at 80 mm Hg.

Melting point: 179°C.

10. Stability: Stable in dark at ambient temperature or below. Solutions undergo photooxidation in air and light.

11. Chemical reactivity: Not spontaneously reactive; 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.

### Fire, Explosion, and Reactivity Hazard Data

1. MC does not require special fire-fighting procedures or equipment. Because of the electrostatic nature of dry MC, fire fighters should wear full-face masks.
2. MC does not present unusual fire and explosion hazards.
3. MC is unstable in presence of light and is more unstable when UV radiation is present.
4. Incompatibilities: No data.
5. MC is not known to produce hazardous decomposition products.
6. MC 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 MC is electrostatic, and when used in this form, it requires the use of antistatic devices.

### 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 MC.

1. Chemical inactivation: No validated method reported.
2. Decontamination: Turn off equipment that could be affected by MC or the materials used for cleanup. If more than 1 g has been spilled or if there is any uncertainty regarding the procedures to be followed for decontamination, call the NIH Fire Department (dial 116) 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 MC shall be disposed of in sinks or general refuse. Surplus MC or chemical waste streams contaminated with MC 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 MC 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 MC 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 MC 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 MC shall be handled in accordance with the NIH radioactive waste disposal system.
4. Storage: Store solid MC and its solutions in dark-colored, tightly closed containers, preferably under refrigeration.

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 adsorption 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 MC is GC-MS. This method allows for accurate identification in the nanogram to picogram 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.

## Biological Data (Animal and Human)

1. Absorption: MC is readily absorbed through the skin and by intravenous and intraperitoneal injection, ingestion, and inhalation.
2. Distribution: MC and/or its derivatives are distributed to, and concentrated in, a variety of tissues, principally the ovaries, fat, adrenals, kidney, and intestine.
3. Metabolism and excretion: MC is metabolized in the mammalian liver by the aryl hydrocarbon hydroxylase system to a variety of epoxides, diols, phenols, and quinones. Hydroxymethyl-cholanthrene, 11,12-epoxy MC, and 11,12-dihydroxy MC have been identified, but other metabolites undoubtedly exist. Some of them are conjugated with glucuronic acid, sulfate, and reduced glutathione and are excreted in the urine and feces via the bile (Goodall et al., 1963).
4. Toxic effects: There are no data on the acute toxicity of MC. As a class, polycyclic aromatic hydrocarbons are regarded as having low acute toxicity in animals and man (Boyland et al., 1965; Heidelberger, 1975). There is no specific target organ but rather a general toxic (and carcinogenic) effect on epithelial and fibroblastic cells.
5. Carcinogenic effects: MC is strongly carcinogenic in experimental animals. Skin application produces various skin tumors and some lung adenocarcinomas. Oral administration to rats and mice results in mammary tumors and leukemias, and subcutaneous injection produces pulmonary tumors and local fibrosarcomas.
6. Mutagenic and teratogenic effects: MC is mutagenic in the Ames test (in the presence of a metabolizing system) and in mice. There is no evidence for teratogenicity.

## Emergency Treatment

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.

## References

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