

Safety Data Sheet

4,4'-Methylene bis- (2-chloroaniline)

Division of Safety
National Institutes
of Health



WARNING!

THIS COMPOUND IS ABSORBED THROUGH THE SKIN AND THE RESPIRATORY AND INTESTINAL TRACTS. IT IS TOXIC, CARCINOGENIC, AND MUTAGENIC. AVOID FORMATION AND BREATHING OF AEROSOLS.

LABORATORY OPERATIONS SHOULD BE CONDUCTED IN A FUME HOOD, GLOVE BOX, OR VENTILATED CABINET.

AVOID SKIN CONTACT: IF EXPOSED, WASH WITH SOAP AND WATER.

FOR EYE EXPOSURE, IRRIGATE IMMEDIATELY WITH LARGE AMOUNTS OF WATER. FOR INGESTION, DRINK WATER, INDUCE VOMITING, OR REFER FOR GASTRIC LAVAGE. 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 AEROSOLS. USE ETHANOL TO DISSOLVE COMPOUND. WASH DOWN AREA WITH SOAP AND WATER. DISPOSE OF WASTE SOLUTIONS AND MATERIALS APPROPRIATELY.

A. Background

4,4'-Methylene bis(2-chloroaniline) (MOCA) is moderately toxic in animals and humans and is carcinogenic in rodents. It is mutagenic in the Ames test. MOCA is used industrially as a curing agent for polyurethane elastomers and in the laboratory as a model compound in the study of carcinogens.

B. Chemical and Physical Data

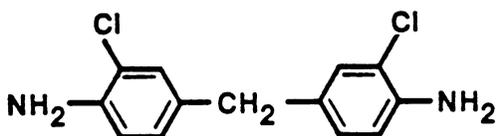
1. Chemical Abstract No.: 101-14-4

issued 8/82

Bis amine	Curene 442
CL-MDA	Di-(4-amino-3-chlorophenyl)methane
Cyanaset	4,4'-Diamino-3,3'-dichlorodiphenylmethane
DACPM	3,3'-Dichloro-4,4'-diaminodiphenylmethane
MBOCA	4,4'-Methylene(bis)-chloroaniline
MOCA	Methylene 4,4'-bis(o-chloroaniline)
Curalin M	4,4'-Methylenebis(2-chlorobenzenamine) (9C)

Molecular
formula:
 $C_{13}H_{12}Cl_2N_2$
weight:
267.17

structure:



Density: 1.39 g/cm³.

Absorption spectroscopy: No data.

Volatility: No data.

Solubility: Insoluble in water; soluble in ethanol, ether, and most organic solvents and lipids (Schmitt and Cagle, 1975)

Description, appearance: Light tan crystals.

Boiling point: No data.

Melting point: 100-105°C.

Stability: Stable under ordinary conditions. Decomposes at temperatures of approximately 200°C.

Chemical reactivity: MOCA exhibits the usual reactivity of primary aromatic amines (salt formation, acylation, alkylation, isocyanide formation, diazotization and tetrazotization oxidation by neutral and basic permanganate) and of aromatic compounds in general (ring substitution).

Flash point: No data.

Autoignition temperature: No data.

Explosive limits in air: No data.

Fire, Explosion, and Reactivity Hazard Data

1. MOCA does not require special fire-fighting procedures or equipment. When exposed to temperatures above 200°C, it undergoes an exothermic and self-sustaining decomposition reaction. In a closed container the pressure buildup can be rapid enough to cause an explosion.
2. No conditions, other than those noted above, contributing to instability are known.
3. No incompatibilities are known.
4. MOCA does not require nonspark equipment. When handled in flammable solvents, the precautions required for such solvents apply.

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 MOCA.

1. Chemical inactivation: No validated method reported.
2. Decontamination: Turn off equipment that could be affected by MOCA or the materials used for cleanup. If more than 1 g has been spilled or if there is any uncertainty regarding procedures to be followed for decontamination, call the NIH Fire Department (dial 116) for assistance. Wipe surfaces with ethanol, then wash with copious quantities of water. Glassware should be rinsed (in a hood) with ethanol, followed by soap and water. Animal cages should be washed with water.
3. Disposal: No waste streams containing MOCA shall be disposed of in sinks or general refuse. Surplus MOCA or chemical waste streams contaminated with MOCA 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 MOCA 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 MOCA 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 MOCA 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 MOCA shall be handled in accordance with the NIH radioactive waste disposal system.

4. Storage: Store in glass ampoules or in screw-capped bottles with Teflon cap liners, preferably under refrigeration.

Monitoring and Measurement Procedures Including Direct Field Measurement and Sampling for Subsequent Laboratory Analysis

1. Sampling: For airborne particles smaller than 0.3 μm , impingers or bubblers filled with a mixture of acetic and hydrochloric acid are used (Linch et al., 1971). For larger particles, a high-volume air sampler with a fiberglass filter trap can be used. For surface sampling, the surface is rubbed with a cloth of undyed 100% polyester wetted with isopropanol. The cloth is then treated with a color reagent (chloranil in chlorobenzene) (Dietrich, 1974). Techniques for sampling metal, painted, and concrete surfaces have been reported (Weeks et al., 1976).
2. Separation and analysis: MOCA can be determined by GC, using a flame ionization detector. This procedure has been applied to urine and air samples (Linch et al., 1971). In the presence of interfering substances, separation by TLC has been used. Colorimetric procedures, based on diazotization and coupling with Chicago acid or N-(1-naphthyl)ethylene diamine (Meddle and Wood, 1970), are convenient but not specific (other primary aromatic amines give interfering colored products and, if present, should be removed by separation procedures).

Biological Effects (Animal and Human)

1. Absorption: MOCA is absorbed by animals and humans through intact skin, by inhalation, and by ingestion.
2. Distribution: In animals receiving MOCA in their diet, it is distributed to the liver, lungs, mammary glands, and skin (Stula et al., 1975).
3. Metabolism and excretion: There are few data. In humans, a monohydroxy derivative has been identified. This plus unchanged MOCA has been identified in the urine of workers engaged in the manufacture of MOCA (Linch et al., 1971).
4. Toxic effects: Data on LD50 in animals are not known. Lethal doses in rats are 2.5 g/kg/week for 88 weeks subcutaneously and 25 mg/kg/week for 89 weeks orally. No specific target organs have been identified; acute MOCA poisoning results in methemoglobinemia and anemia.
5. Carcinogenic effects: Ingestion of MOCA by mice and rats results in malignancies of liver, lung, stomach, kidney, and mammary gland (Russfield et al., 1975; Stula et al., 1975).

6. Mutagenic and teratogenic effects: MOCA is an active mutagen in the Ames test; there are no data concerning its teratogenicity.

Emergency Treatment

1. Skin and eye exposure: For skin exposure, remove contaminated clothing and wash skin with soap and water. For eye exposure, irrigate immediately with copious quantities of running water for at least 15 minutes. Consider ophthalmological consultation.
2. Ingestion: Drink plenty of water. Induce vomiting or refer for gastric lavage.
3. Inhalation: Remove victim promptly to clean air. Administer rescue breathing if necessary.
4. Refer to physician. Oxygen may be necessary during transport. Observe for methemoglobinemia.

References

- Dietrich, W.C. 1974. A rapid field test for MOCA. Prepared for the U.S. Atomic Energy Commission by Oak Ridge Y-12 Plant. Contract No. W-7406-eng-26. UC-4 Y-1943.
- Linch, A.L., G.B. O'Connor, J.R. Barnes, A.S. Killian, Jr., and W.E. Neeld, Jr. 1971. Methylene-bis-ortho-chloroaniline (MOCA): Evaluation of hazards and exposure control. *Am Ind Hyg Assoc J* 32:802-819.
- Meddle, D.W., and R. Wood. 1970. A method for the determination of aromatic isocyanates in air in the presence of primary aromatic amines. *Analyst* 95:402-407.
- Russfield, A.B., F. Homburger, E. Boger, C.G. Van Dongen, E.K. Weisburger, and J.H. Weisburger. 1975. The carcinogenic effect of 4,4-methylene-bis-(2-chloroaniline) in mice and rats. *Toxicol Appl Pharmacol* 31:47-54.
- Schmitt, C.R., and G.W. Cagle. 1975. Sulfamic acid cleaning solution for 4,4-methylene-bis orthochloroaniline (MOCA). *Am Ind Hyg Assoc J* 36:181-186.
- Stula, E.F., H. Sherman, J.A. Zapp, Jr., and J.W. Clayton, Jr. 1975. Experimental neoplasia in rats from oral administration of 3,3'-dichlorobenzidine, 4,4'-methylene-bis(2-chloroaniline) and 4,4'-methylene-bis(2-methylaniline). *Toxicol Appl Pharmacol* 31:159-176.
- Weeks, R.W., B.J. Dean, and S.K. Yasuda. 1976. Detection limits of chemical spot tests toward certain carcinogens on metal, painted and concrete surfaces. *Anal Chem* 48:2227-2233.