# HEXAMINE

## PRODUCT IDENTIFICATION

<table>
<thead>
<tr>
<th>Product Identification</th>
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</thead>
<tbody>
<tr>
<td>CAS NO.</td>
<td>100-97-0</td>
</tr>
<tr>
<td>EINECS NO.</td>
<td>202-905-8</td>
</tr>
<tr>
<td>FORMULA</td>
<td>(CH₂)₆N₄</td>
</tr>
<tr>
<td>MOL WT.</td>
<td>140.19</td>
</tr>
<tr>
<td>H.S. CODE</td>
<td>2933.90</td>
</tr>
<tr>
<td>TOXICITY</td>
<td>Oral, mouse LD₅₀: 569 mg/kg</td>
</tr>
<tr>
<td>SYNONYMS</td>
<td>1,3,5,7-Tetraazaadamantane; Ammonioformaldehyde; Aceto HMT; Aminoform; Ammonform; Cystamin; Cystogen; Esametilentetramina (Italian); Formamine; Formin; Hexaform; Hexamethylenamine; Urotropin; Hexamethyleneamine; Hexamethylenetetraamine; Hexamethylentetramin (German); Hexamethylentetramine; Hexilmethyleneamine; HMT; Methamin; Methenamine; Resotropin; Uritone; Urotropine; Esametilentetramina (Italian); 1,3,5,7-Tetraazatricyclo[3.3.1.1(3,7)]decane;</td>
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</tbody>
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## GENERAL DESCRIPTION

HEXAMETHYLENETETRAMINE (HEXAMINE) is a white crystalline powder with slight amine odor. Specific gravity is 1.27 at 25°C. HEXAMINE is soluble in water, alcohol, and chloroform, but insoluble in ether. Formaldehyde and ammonia yield methenamine, or hexamethylenetetramine, which is used as a urinary antiseptic. Nitration of methenamine gives the explosive cyclonite, or RDX. Formaldehyde and acetaldehyde react with Hexamine in the presence of calcium hydroxide to give pentaerythritol, the tetranitrate of which is the explosive PETN. HEXAMINE is also useful in adhesives, coatings, and sealing compounds. In medicine, it is an antibacterial agent. It is used as a dye fixative and in the preservation of hides. It is used in vulcanizing rubber and as an anti-corrosive agent in steel. It is used in the detection of metals and in the absorption of poisonous gases. It stabilizes lubricating and insulating oils. It is sometimes burned in camping stoves, because it burns without smoke.

## PHYSICAL AND CHEMICAL PROPERTIES

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>PHYSICAL STATE</td>
<td>White crystalline powder with slight amine odor</td>
</tr>
<tr>
<td>MELTING POINT</td>
<td>200°C</td>
</tr>
<tr>
<td>BOILING POINT</td>
<td>280°C (Decomposes)</td>
</tr>
<tr>
<td>SPECIFIC GRAVITY</td>
<td>1.331</td>
</tr>
<tr>
<td>SOLUBILITY IN WATER pH Aqueous solution is alkaline</td>
<td>good</td>
</tr>
<tr>
<td>VAPOR DENSITY</td>
<td>4.9</td>
</tr>
<tr>
<td>AUTOIGNITION</td>
<td>Health: 1 Flammability: 1 Reactivity: 0</td>
</tr>
<tr>
<td>NFPA RATINGS</td>
<td></td>
</tr>
<tr>
<td>REFRACTIVE INDEX</td>
<td></td>
</tr>
<tr>
<td>FLASH POINT</td>
<td>250°C</td>
</tr>
<tr>
<td>STABILITY</td>
<td>Stable under ordinary conditions</td>
</tr>
</tbody>
</table>

## APPLICATIONS

- Vulcanizing agent and rubber blowing agent.
- Explosives (RDX), (HMX), (HMTA), Smokeless pellets.
- Stabilizer for oils and synthetic resin.
- Anti-corrosive agent in steel.
- Absorption of poisonous gases.
- Anti-caking agent for prilled urea.
- Disinfectant.
- Antibacterial agent.

## SALES SPECIFICATION

| Appearance                     | White crystalline powder with slight amine odor |

## CLASSIFICATION

<table>
<thead>
<tr>
<th>DERIVATION</th>
<th>CLASSIFICATION</th>
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## SAFETY DATA SHEET
Amine is a group of basic organic compounds derived from ammonia (NH₃) by replacement of one (primary amines), two (secondary amines), or three (tertiary amines) hydrogen atoms by alkyl, aryl groups or organic radicals. Amines, like ammonia, are weak bases because the unshared electron pair of the nitrogen atom can form a coordinate bond with a proton. Amines react with acids to give salts and with acid anhydrides (or ester) to form amides. They react with halogenoalkanes to form longer chains.

Many amines are not only bases but also nucleophiles that form a variety of electrophile compounds. They are important intermediates for chemical syntheses due to the basic functionality of the nitrogen atom and electrophilic substitution at nitrogen. Some examples of compounds obtained by reaction of amines are:

- Amides (by reaction with acyl halides or ammonium carboxylate salts)
- N-Alkyl amines (by reaction with halogenoalkanes)
- Isocyanates (by reaction with phosgene)
- Carbamoyl chlorides or Urea derivatives (by reaction with phosgene)
- Alkoxylated amines (by reaction alkylene oxide)
- Quaternary ammonium compounds (by reaction with alkyl halides and dialkyl sulfates)
- N-Alkylcarbamic acids or N,N'- Dialkyl ureas (by reaction with carbon dioxide)
- Urea derivatives (by reaction with isocyanates)
- Schiff bases (by reaction with aldehydes or ketones)
- Aminopropionitriles (by reaction of 1° and 2° amines with acrylonitrile)
- N-Alkylamino acids (by reaction of 1° and 2° amines with monochloroacetic acid or with unsaturated acids)
- Amine oxides (by reaction of 3° amines with hydrogen peroxide)
- Sulfonamide derivatives (by reaction of 1° and 2° amines with benzenesulfonyl chloride)

Low molecular amine names are formed by adding ‘-amine’ as a suffix to the name of the parent compound. In substitutive nomenclature, the prefix ‘amino-’ is placed before the name of the parent compound to denote the functional group in high molecular amines. Synthetic amines are made mostly by reaction of alcohols with ammonia, catalyzed by metals (nickel or copper) or metal oxide at high temperature. Many methods have been devised for the synthesis of the amines; reacting ammonia with an alkyl halide and neutralizing the resulting alkyl ammonium salt with an alkali, e.g., sodium hydroxide. This procedure yields a mixture of primary, secondary, and tertiary amines that is easily separated into its three components by fractional distillation; boiling methyl isocyanate with caustic potash, heating the alkyl iodides with ammonia; reduction of nitriles.
with alcohol and sodium; heating the esters of nitric acid with alcoholic ammonia; reducing on
nitro-paraffins; action of zinc and hydrochloric acid on aldehyde ammonias; reduction of the
phenylhydrazones and oximes of aldehydes and ketones with sodium amalgam in the presence of
alcohol and sodium acetate; action of dilute hydrochloric acid on the isonitriles; heating the
mustard oils with a mineral acid, by the hydrolysis of the alkyl phthalimides. Primary amines contain
the functional group -NH₂ (called amino group) and are converted into secondary and tertiary
amines if heated with alkyl or aryl iodides. Primary amines form various oxidation products violently
with concentrated nitric acid. If the amines are acetylated, they form nitro derivatives with
concentrated nitric acid. Primary amines form diazonium salts with nitrous acid in cold solution in
the presence of excess of mineral acid. Or a diazoamine is obtained in absence of excess of acid.
Other reactions are condensation products with aldehydes; forming anilides; forming alkyl
thioureas; yielding isonitriles with alcoholic potash and chloroform. Tertiary amines combine with
one molecular proportion of an alkyl iodide to form quaternary ammonium salts in which a central
nitrogen atom is joined to four organic radicals and one acid radical. Quaternary ammonium salts
are used as corrosion inhibitor, emulsifying and antiseptic agents. Aliphatic amines which have the
lowest carbon content are water-soluble gases or liquids of low boiling point also readily soluble in
water in case of the next low carbon content. But aliphatic amines which have the high carbon
content are odourless solids of high boiling point and are insoluble in water. They are all bases and
easily form salts with the mineral acids and solid salts with the halogenoalkanes. Amine Salts are
crystalline substances that are readily soluble in water. Many insoluble alkaloids (e.g. quinine and
atropine) are used medicinally in the form of soluble salts. If alkali (sodium hydroxide) is added to
solutions of such salts the free amine is liberated. Short chain alkyl amines are used as raw materials
of solvent, alkyl alkanolamines, and ingredients of rocket fuels. They are used to make other organic
chemicals including rubber vulcanization accelerators, pesticides, quaternary ammonium
compounds, photographic chemicals, corrosion inhibitors, explosives, dyes and pharmaceuticals.

They are used in rayon and nylon industry to improve the tensile strength. Allylamines are used as
intermediates for ion exchange resins, pharmaceuticals, water soluble polymers, herbicide
softeners, rubber chemicals, polymerization initiators and cross-linking agents. Amines are used as
reducing agents for the recovery of precious metals. They are versatile intermediates. They have
active applications in organic synthesis for polymerization catalyst, chain extender in urethane
coatings, agrochemicals, pharmaceuticals, photographic, heat stabilizers, polymerization catalysts,
flame-retardants, blowing agents for plastics, explosives, and colorants. Long chain alkyl amines are
used for the synthesis of organic chemicals and surfactants used as a corrosion inhibitor, detergent,
ore floating agent, fabric softener, anti-static agent, germicide, insecticide, emulsifier, dispersant,
anti-caking agent, lubricant and water treatment agent. Alkyl tertiary Amines are used as fuel
additives and preservatives. They have similar applications with long chain alkyl amines.

Hexamethylenediamine used in the manufacture of nylon-6,6 is prepared by catalytic addition of
hydrogen to nitriles. Aromatic amines also exist, such as phenylamine, which are important for the
production of diazonium salts. They dissociate in water (some very weakly). Aromatic amines are
much weaker bases than the aliphatics. One of the most important aromatic amines is aniline; pale
brown liquid boiling at 184°C, melting at -6°C. Aniline is obtained commercially from chlorobenzene
by heating with ammonia in the presence of copper catalyst or from a product of coal tar
(nitrobenzene) through the reduction reaction. Aniline is the starting material in the dye
manufacturing industry and as in the manufacture of others. Aniline is converted into sulfanilic acid
which is the parent compound of the sulfa drugs. Aniline is also important in the manufacture of
rubber-processing chemicals, antioxidants and varnishes. Amines take part in many kinds of
chemical reactions and offer many applications include in agrochemicals, dyestuffs (the best
known being aniline), pharmaceuticals, and corrosion inhibitors.