Handbook for the Chemical Analysis of Plastic and Polymer Additives

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Crosslinking Compounds/Accelerators

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CHAPTER 3

Crosslinking Compounds/Accelerators

The chemical crosslinking process has its origins in the Goodyear process by which rubber was transformed from a viscous form into a shape-retaining rubbery material through reaction with sulfur and heat. This 'vulcanizing' process promoted bonding between unsaturated end groups in the natural rubber chains, thus forming 'crosslinks' between chains. With these crosslinks, the rubber molecules were no longer subject to mutual slip, thus a molded object would permanently retain its shape while retaining elastomeric behavior.

Crosslinking is a major commercial process for elastomeric, thermoplastic, and liquid polymeric materials. The approaches for crosslinking reaction imitation vary with the type of polymer, the end application, costs, and technical approach. Many crosslinking processed are thermally initiated. Heat exposure increases oxidation risk, while considerably boosting energy requirements. The rate of crosslinking can be increased by careful technical development of a process and selection of organic compounds that function as cure accelerators. In some cases, the rate of cure may be moderated with chemical retarding agents to control exothermic reactions and physical stability.

Crosslinking of many commercial thermoplastics is conducted with reactive peroxides, including dicumyl peroxide, benzoyl peroxide, and many others, all of which have different activation temperatures. At the crosslinking initiation temperature, the peroxide decomposes and forms free radicals that react with unsaturated end groups on the polymer chains, thus forming chemical crosslinks between chains. For thermoplastic addition, stability of the peroxides is increased for storage and handling by incorporation into master batches that may include waxes, clay, fatty acids, or resins.

A wide range of liquid polymers are crosslinked with reactive peroxides, such as benzoyl peroxide, diacyl peroxide, and various peroxyesters and peroxyketals. These are used to crosslink acrylic resins for a wide range of applications. Since these peroxides are inherently unstable, they are reduced in concentration for safe storage and use by dilution with cyclohexane, diallyl phthalate, or dimethyl phthalate. These diluents must be understood from an analytical perspective for proper role and source identification.

Crosslinking of many thermoplastic polymers can be accomplished by addition of a vinyl silane. In this process, the vinyl silane is mixed into the polymer during extrusion. The heat energy grafts the silane to the polymer chains. The component is then molded or extruded into the desired form. Following this, the crosslinking process is initiated by exposure to moisture and heat. With this process, the processing temperature is reduced. Therefore, the polymer is not oxidized and the vinyl silane is not decomposed into a host of reaction products. Analytically, silane crosslinking initiators can be identified by the vinyl silane signature.

Ionizing radiation is used to crosslink a number of rubber and thermoplastic materials, particularly for applications where precise control of crosslinking density (the proportion of crosslinked to non-crosslinked chains in a given polymer) must be carefully controlled and where chemical purity is a key consideration. Polymers for biomedical applications are typically radiation crosslinked. With this process, an electron beam or gamma radiation source is used to provide ionizing energy. Crosslinking proceeds spontaneously if the polymer contains reactive end groups or if an unsaturated copolymer or unsaturated polymer additive is blended. For rubber compounds, diene
monomers are typically added to provide unsaturated bonds. From an analytical perspective, radiation-crosslinked polymers may contain few chemical signatures that indicate the curing process.

Ultraviolet (UV) crosslinking of polymers is broadly used for many applications where heating is impractical or damaging to the base polymer and where other forms of ionizing radiation may be harmful or excessively costly for the application. UV radiation can be used to decompose a reactant that is blended into a polymer and the free radicals that result will form crosslinks in the polymer. UV curing is used for a wide range of urethanes for cured-in-place coatings, for example. This method is also commonly used for acrylic composite dental restoratives. The crosslinking initiators used for this process must strongly absorb UV radiation and they must be stable and have low volatility in the polymer prior to crosslinking initiation. Benzophenones are a major class of organic compounds used for this process.

Rigid polymers such as epoxy and polyurethanes are used in high volume for a wide range of structural, coating, electrical, and other applications. Epoxy formulations vary widely and the chemical signatures of cured resins will vary accordingly. Amine curing agents are the most commonly used for epoxy systems. The selection of the type of amine affects the rate of cure and also impacts the end use of the crosslinked material. Amine-crosslinked epoxies have increased moisture sensitivity compared to those cured with aromatic isocyanates, for example. The amine crosslinking agents include triethylenetetramine, ethylenediamine, diethyltriamine, cycloaliphatic amines, and others. Analytically, these amines might be identified through GC/MS analysis of solvent-extracted or thermally desorbed samples, particularly if unreacted amines remain.

Polyurethanes are also available with a wide range of crosslinking systems, some of which are extremely sensitive to UV exposure. One such curing agent is toluene diisocyanate. Hexamethylene diisocyanate is not subject to UV-induced degradation. As with epoxies, urethanes are highly crosslinked and analytical determination of the ingredients and extractible organics requires careful selection of methodology and knowledge of the polymer systems.

From an analytical perspective, the crosslinking materials and process should be well understood. A reactive peroxide, for example, will generally not be evident in the analysis of a polymer crosslinked with this material. This will be evident when not fully decomposed during a cure process, for example, and the presence of non-reacted peroxide may be a valuable indication of an under-cure condition. Typically, the decomposition products of dicumyl peroxide are what will be found analytically. These include acetic acid, cumyl alcohol, acetophenone, and others. Heating of most thermoplastics to a level that initiates decomposition of the curing agent would also oxidize the base polymer. It is therefore necessary to protect the polymer with an antioxidant. GC/MS analysis of a typical peroxide-crosslinked polyethylene will reveal the peroxide decomposition products, an antioxidant, and no trace of the original peroxide.

Accelerators
The rate of crosslinking of commercial rubber products and a number of other thermosetting plastic compounds can be accelerated by addition of a number of compounds identified as cure accelerators. These are useful for increasing throughput in commercial processes, for locking in transient foam structures, and for controlling recovery in shape-retaining components. These are also useful when a crosslinking agent must be used at the lowest possible temperature to prevent decomposition of the polymer. Accelerators may also enhance tensile properties and improve age resistance of the final product. Cure accelerators are also known as crosslinking synergists.
Crosslinking Compounds/Accelerators

Most accelerators are organic substances that contain either nitrogen or sulfur, or both. Typical accelerators include tetraisobutylthiuram disulfide, n-oxydiethylene thiocarbamyl-N-oxydiethylene sulfonamide, tetrabenzylthiuram disulfide, and others. They can be classed as either primary or secondary accelerators and are often used in combination, depending on the desired final outcome. Crosslinking of many commercial thermoplastics is conducted with reactive peroxides, including dicumyl peroxide, benzoyl peroxide, and many others, all of which have different activation temperatures. At the crosslinking initiation temperature, the peroxide decomposes and forms free radicals that react with the unsaturated end groups on the polymer chains, thus forming chemical crosslinks between chains. For thermoplastic addition, stability of the peroxides is increased for storage and handling by incorporation into master batches that may include waxes, clay, fatty acids, or resins.
Accelerator MBT, MBT/MG

Brand Names & Manufacturers
Captax/Rotax (purified form)  R.T. Vanderbilt Company
Perkacit® MBT  Akzo Nobel Chemicals B.V.
Thiotax  Solutia, Inc.

Physical Properties

Appearance  Off-white to yellow powder
Melting Point  180-182 °C
Solvency (g/100mL 20 °C)  
Water  <0.1  MeOH  U  EtOH  2.0  Acetone  10.0  CH₂Cl₂  U  Hexane  U
Stability  Stable under normal conditions of use.
Boiling Point  260 °C

Application
Used as a vulcanization accelerator for rubber mixes based on natural and synthetic rubbers and in the production of plastics and lacquers.

Regulatory Information
FDA approved 1998 for the following materials to be used in contact with food: adhesive preservatives, 21CFR175.105; a rubber accelerator (up to 1.5% of weight of rubber), 21CFR177.2600; in the synthesis of slimicides for use in paper/paperboard, 21CFR178.3010; an adjuvant in the manufacture of foamed plastics, 21CFR178.3010. Listed in 40CFR136.1 and USEPA Method 640: The Determination of Mercaptobenzothiazole in Municipal and Industrial Wastewaters.

Environmental Impact
Does not biodegrade in river water in 8 weeks. Slightly susceptible to indirect photolysis. Medium to low mobility in soil, and marginal to no mobility in sediment. This substance may be hazardous to the environment; special attention should be given to fish. Log Pow value of 2.41 indicates a low potential to bioaccumulate.

Point of Release
Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data
A 2-year NTP study on rats indicates evidence of carcinogenic activity in rats gavaged with 750 mg/kg BW (male) and 375 mg/kg BW (female). No carcinogenic effect on bacteria and yeast cells.
Crosslinking Compounds/Accelerators

Mass Spectrum for Accelerator MBT, MBTMG - PLAS-AC-001

MW = 167.25

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<td>15</td>
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<td>63</td>
<td>15</td>
</tr>
<tr>
<td>123</td>
<td>11</td>
</tr>
</tbody>
</table>
ETU is used as an accelerator in the vulcanization of polychloroprene (Neoprene) and other elastomers; for coated fabrics, for epichlorohydrin, and for chlorosulfonated polyethylene rubbers. It is also an intermediate for antioxidants, insecticides, fungicides, dyes, pharmaceuticals, and synthetic resins.

**Regulatory Information**

FDA: Use of ETU as a food additive is prohibited. EPA (1995): Health Advisory for long-term exposure is 0.4 mg/L. Can be monitored in water by EPA Method 509 - Determination of Ethylene Thiourea (ETU) in Water Using Gas Chromatography with a Nitrogen-Phosphorus Detector. FAO/WHO (1993): ADI: 0.004 mg/kg BW.

**Environmental Impact**

ETU is a trace contaminant and metabolic degradation product of a widely used class of ethylene bisdithiocarbamate fungicides such as Maneb and Zineb. Half-life in H₂O is 7–13 days. Octanol/water partition coefficient as log Pow: ~0.66 (calculated).

**Point of Release**

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

**Toxicological Data**

Ethylene thiourea is toxic and known to produce thyroid neoplasms (thyroid hyperplasia) in rats and liver neoplasms in mice following long-term administration; NIOSH: potential occupational carcinogen; NTP: Suspect carcinogen; OSHA: Possible suspect carcinogen. Acute oral toxicity (LD₅₀): 1832 mg/kg [Rat].
Crosslinking Compounds/Accelerators

Mass Spectrum for Accelerator ETU-22 PM - PLAS-AC-002

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<td>7</td>
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MW=102.16

For Chromatogram See Appendix A - PLAS-AC-002 - page 442
Accelerator BBTS

Chemical Name
N-(1,1-dimethylethyl)-2-benzothiazolesulfenamide

Synonyms
N-(1,1-dimethylethyl)benzothiazolesulfenamide; benzothiazolyl-2-tert-butylsulfenamide; benzothiazyl-2-tert-butylsulfenamide

Brand Names & Manufacturers
Delac® NS
Uniroyal Chemical Co.

Penne® TBBS
Pennwalt Corp.

Perkacit® TBBS
Akzo Nobel Chemicals B

Santocure® NS
Solutia Inc.

Physical Properties
Appearance
Cream to buff powder or pellets

Melting Point
105 °C

Boiling Point
Not available

Stability
Stable under normal conditions of use.

Solubility (g/100mL 20 °C)

<table>
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<tr>
<th>Solvent</th>
<th>Water</th>
<th>MeOH</th>
<th>EtOH</th>
<th>Acetone</th>
<th>CH₂Cl₂</th>
<th>Hexane</th>
</tr>
</thead>
<tbody>
<tr>
<td>Liquid</td>
<td>0.345</td>
<td>U</td>
<td>40-80</td>
<td>40-80</td>
<td>U</td>
<td>U</td>
</tr>
</tbody>
</table>

Application
TBBS is used as a vulcanization accelerator in NR, SBR, BR, and rubber blends. Normally used alone or with small quantities of ultra accelerators in tire compounds or other industrial rubber products.

Regulatory Information
FDA approved 1998 for use as an accelerator in the manufacture of rubber material intended for use in all stages of production, processing, packaging, and transport of food. 21CFR177.2600.

Environmental Impact
TBBS does not ionize at environmental pHs, is not readily biodegradable, but hydrolyzes in less than 1 day at pH 9 or less. The identified hydrolysis products: mercaptobenzothiazole, di(benzothiazoyl)disulfide, t-butylamine, and benzothiazoleare are non-volatile, with a low potential for bioaccumulation, and are not readily biodegradable. Indirect photo-oxidation by hydroxyl radicals is predicted with a half-life estimated at 2.8 hours. Log Pow of 3.9 at room temperature.

Point of Release
Due to the vulcanization process, finished rubber products contain only small amounts of TBBS or synthesis by-products (benzothiazole, 2-mercaptobenzothiazole, and 2-mercaptobenzothiazole disulfide). Release to the environment of these chemicals may occur during the use of rubber products. Fugacity model (Mackay level III) data suggest that it would mostly distribute to soil (if released to the air or soil compartments) and to water (if released to the water compartment).

Toxicological Data
TBBS may be absorbed by the gastro-intestinal route, undergoing hydrolysis in vivo. Studies suggest that the hydrolysis products are toxic primarily to the liver and kidney. It was not found to be mutagenic in bacteria or in vitro mammalian gene mutation assays. It was not genotoxic in an in vivo mouse micronucleus assay. (LD50): >7940 mg/kg dermal [Rabbit]. It did induce chromosomal aberrations in mouse lymphoma cells in vitro with metabolic activation. Carcinogenicity not known.
Crosslinking Compounds/Accelerators

**Mass Spectrum for Accelerator BBTS - PLAS-AC-003**

For Chromatogram See Appendix A - PLAS-AC-003 - page 440
Accelerator CBTS

CAS Number 95-33-0
RTECS Number DL6250000
Abbreviation CBTS

Formula \( \text{C}_{13}\text{H}_{16}\text{N}_{2}\text{S}_{2} \)
Molecular Weight 264.41

Chemical Name
N-(1,3-benzothiazol-2-ylsulfanyl)cyclohexanamine

Synonyms
N-cyclohexyl-2-benzothioazole sulfenamide

Brand Names & Manufacturers
Accelerator CBTS
Akrochem Corporation
Santocure

Physical Properties

<table>
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<tr>
<th>Property</th>
<th>Value</th>
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<tbody>
<tr>
<td>Appearance</td>
<td>White to tan powder</td>
</tr>
<tr>
<td>Melting Point</td>
<td>102 °C</td>
</tr>
<tr>
<td>Boiling Point</td>
<td>Decomposes</td>
</tr>
<tr>
<td>Stability</td>
<td>Stable under normal conditions of use.</td>
</tr>
<tr>
<td>Solubility (g/100mL 20 °C)</td>
<td>Water 0.002 MeOH S</td>
</tr>
</tbody>
</table>

Application, Regulatory & Environmental Information

Delayed action sulfenamide accelerator for natural and synthetic rubbers. It provides better scorch resistance than thiazoles and can be accelerated by thiurams and dithiocarbamates to give shorter cure times. It can also be used as a retarder for ETU-cured polychloroprene and high thiuram cures.

Regulatory Information
Not FDA approved for food contact applications.

Environmental Impact
Not expected to be an environmental hazard.

Point of Release
Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data
LD\(_{50}\) (oral): 5300 mg/kg [Rat]
LD\(_{50}\) (oral): >8000 mg/kg [Mouse]
LD\(_{50}\) (dermal): >7490 mg/kg [Rabbit]
Embryotoxic LD\(_{50}\) (intravenous): 32 mg/kg [Mice, Rodents]
Crosslinking Compounds/Accelerators

Mass Spectrum for Accelerator CBTS - PLAS-AC-007

For Chromatogram See Appendix A - PLAS-AC-007 - page 441
Cure-Rite® IBT

Noveon, Inc.

CAS Number 3064-73-1
RTECS Number N/A
Abbreviation TIBTD

Formula C_{18}H_{36}N_2S_4
Molecular Weight 408.76

Chemical Name
tetraisobutylthiuram disulfide

Synonyms
tetra(isobutyl)thioperoxydicarbamic acid

**Physical Properties**

<table>
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<th>Value</th>
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<tr>
<td>Appearance</td>
<td>Pale yellow to white powder</td>
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<tr>
<td>Melting Point</td>
<td>70-73 °C</td>
</tr>
<tr>
<td>Stability</td>
<td>Stable under normal conditions</td>
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<tr>
<td>Solubility (g/100mL 20 °C)</td>
<td>Water &lt;0.01 MeOH U EtOH U Acetone U CH_2Cl_2 U Hexane U</td>
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</table>

**Application**

Used as an accelerator and vulcanizing agent in rubber (EPDM, SBR, Nitrile, and Natural). Especially useful when the formation of nitrosamines is a concern.

**Regulatory Information**

FDA approved for use with rubber food-contact materials per 21CFR178.2010 and 178.3860.

**Environmental Impact**

Due to its low solubility in water and therefore the non-availability to species, this product is not expected to be toxic to aquatic organisms. Estimated log Kow value of 3.4 indicates a low to moderate potential to bioaccumulate.

**Point of Release**

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

**Toxicological Data**

Not listed as a carcinogen by IARC, NTP, ACGIH, or OSHA.
Crosslinking Compounds/Accelerators

Mass Spectrum for Cure-Rite® IBT - PLAS-AC-004

MW = 408.76

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For Chromatogram See Appendix 4 - PLAS-AC-004 - page 447
### Activator OT Urea

**Akrochem Corporation**

![Chemical Structure](image)

- **Chemical Name**: urea
- **Synonyms**: carbonyl diamide; carbamide; isourea

#### Physical Properties

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<td><strong>Boiling Point</strong></td>
<td>Decomposes 135 °C</td>
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<td><strong>Stability</strong></td>
<td>Decomposes at 135 °C (MP)</td>
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<tr>
<td><strong>Solubility</strong></td>
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<td>Water (g/100mL 20 °C)</td>
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<tr>
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<td>~16</td>
</tr>
<tr>
<td>EtOH</td>
<td>U</td>
</tr>
<tr>
<td>Acetone</td>
<td>U</td>
</tr>
<tr>
<td>CH$_2$Cl$_2$</td>
<td>U</td>
</tr>
<tr>
<td>Hexane</td>
<td>U</td>
</tr>
</tbody>
</table>

#### Application

Urea is used in the manufacture of urea-formaldehyde plastics, adhesives, polymers, synthetic fibers, dyes, etc.

#### Regulatory Information


#### Environmental Impact

Although urea has generally low ecotoxicity to organisms, its well-documented indirect and long-term effects to the ecosystems, e.g., eutrophication, groundwater pollution, soil acidification, and ammonia emissions to air, should be considered. When released to soil, this material will hydrolyze into ammonium in a matter of days to several weeks. This material is not anticipated to bioaccumulate — it has a BCF < 100.

#### Point of Release

Occupational and environmental exposure during production is possible due to accidental process breakdown and disorders in reactor operations, pumping cycles, evaporation, and crystallization processes; in maintenance, loading and unloading operations. Potential occupational exposure occurs via inhalation of aerosols from urea melt and hot saturated solutions, splashed to skin or eyes, or inhalation of dust.

#### Toxicological Data

No documented toxic effects at low doses. Chronic exposure is carcinogenic and mutagenic: 821 g/kg [Rat] and 394 g/kg [Mouse] for one year results in lymphomas and Hodgkin’s disease. Long-term toxicity: High doses affect cholinergic and bioenergetic processes and modify CNS structure. Acute oral toxicity (LD50): 14.3 g/kg BW [Rat], 11 g/kg [Mouse].

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Crosslinking Compounds/Accelerators

Mass Spectrum for Activator OT Urea - PLAS-AC-005

For Chromatogram See Appendix A - PLAS-AC-005 - page 446

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Accelerator EZ & EZ-SP

Akrochem Corporation

![Chemical Structure](image)

**CAS Number** 14324-55-1  
**RTECS Number** ZH0350000  
**Abbreviation** DEDTZ/ZDEC

**Formula** \( \text{C}_{10}\text{H}_{20}\text{N}_{2}\text{S}_{4} \cdot \text{Zn} \)

**Molecular Weight** 361.93

---

**Chemical Name**
zinc diethyldithiocarbamate

**Synonyms**
- bis(diethylene-dithiocarbamate)zinc
- diethyldithiocarbamic acid, zinc salt
- ethyl zimate

---

**Appearance**
White powder

**Stability**
Stable under normal conditions of use.

**Melting Point** 178-181 °C

**Boiling Point** Not available

**Solubility**
- Water: \(<0.1\) g/100mL 20 °C
- MeOH: U
- EtOH: U
- Acetone: S
- CH₂Cl₂: S
- Hexane: U

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**Application, Regulatory & Environmental Information**

ZDEC is used in the following applications: as a fast primary or secondary vulcanization accelerator in NR, SBR, IIR, EPDM and for natural and synthetic latex; a stabilizer in butyl, butadiene, and urethane rubbers; an antioxidant in rubber-based adhesive systems; a stabilizer in cement; a heat stabilizer for polyethylene.

**Regulatory Information**
FDA approved 1998 for use as an accelerator in the manufacture of rubber material (up to 1.5% of weight of rubber) intended for use in all stages of production, processing, packaging, and transport of food: 21CFR177.2600. Regulated for use under 21CFR175.105 for components of adhesives.

**Environmental Impact**
Ecological impact not determined. Similar compounds show low to moderate biodegradability, but rapid hydrolysis under acidic conditions. Similar compounds are also determined to have low bioaccumulation potential and environmental persistence: 96 hour LC₅₀ 0.23 mg/L [Rainbow Trout], 0.40 mg/L [Bluegill Sunfish], 0.26 mg/L [Fathead Minnow], 48 hour EC₅₀ 0.44 mg/L [Daphnia Magna].

**Point of Release**
Migration of ZDEC into water after 3 days exposure at 20 °C is 0.6 mg/L.

**Toxicological Data**
Not listed as a suspected carcinogen by NTP, IARC, or OSHA. Reactions with nitrosylating agents during vulcanization may yield suspected carcinogens such as nitrosamines. Studies of rats and mice gavaged with ZDEC yield no genotoxic or teratogenic effects. Long-term exposure to large doses may have neurodegenerative effects in addition to altering hydrolytic enzymes in the human brain. Acute oral (LD₅₀): 3530 mg/kg [Rat]. Acute dermal (LD₅₀): >3160 mg/kg [Rabbit].

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Crosslinking Compounds/Accelerators

Mass Spectrum for Accelerator EZ & EZ-SP - PLAS-AC-006

MW=361.93

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For Chromatogram See Appendix A - PLAS-AC-006.D
Handbook for the Chemical Analysis of Plastic and Polymer Additives

N, N'-Diethylthiourea

CAS Number 105-55-5
RTECS Number YS9800000
Abbreviation DETU

Chemical Name
1,3-diethylthiourea

Synonyms
1,3-diethyl-2-thiourea; N,N'-diethylthiocarbamide

Physical Properties

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<td>Boiling Point</td>
<td>169 °C</td>
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<td>Stability</td>
<td>Stable under normal conditions of use.</td>
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<td>U</td>
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<td>Hexane</td>
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Application, Regulatory & Environmental Information

Application
Accelerator for mercaptan-modified chloroprene rubber. Stabilizer for natural, nitrile-butadiene, styrene-butadiene, and chloroprene rubbers. Found in adhesives, animal repellent, cements, condoms, cosmetic applicators, disinfectants, fungicides, gloves, leather shoes, rubber in undergarments, tires and tubes, soaps and shampoo.

Regulatory Information
Regulated for use under 21 CFR §177.2600 Rubber Articles Intended for Repeated Use in Food Contact.

Environmental Impact
If released to soil, biodegradation of N,N-diethylthiourea may be an important removal process. Because of the estimated low Koc value in soil, N,N-diethylthiourea may rapidly leach in soil. The volatilization of N,N-diethylthiourea from moist soil is not expected to be an important removal process. Neither photolysis nor hydrolysis are expected to be important in water. BCF = 2.

Point of Release
The release of N,N-diethylthiourea in the environment is expected to occur during waste disposal from its production and use.

Toxicological Data
Oral (LD50): = 316 mg/kg [Rat]
Oral (TDLo): = 11 gm/kg/2Y-C [Rat]
Tumorigenic - Carcinogenic by RTECS criteria; Endocrine - thyroid tumors Mutation in mammalian somatic cells (mouse lymphocyte) = 1500 mg/L
Bacteria: Phytobacterium phosphoreum: 761.0 mg/L; 15 minute Microtox test: No data available.

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Mass Spectrum for \(N, N'\)-Diethylthiourea - PLAS-AX-103

Mass Spectrum for \(N, N'\)-Diethylthiourea - PLAS-AX-103

MW = 132.23

For Chromatogram See Appendix A - PLAS-AX-103 - page 444

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1,3-Diphenyl-2-thiourea

**Chemical Name**
1,3-di(phenyl)thiourea

**Synonyms**
N,N'-diphenylthiocarbamide

**Physical Properties**

<table>
<thead>
<tr>
<th>Property</th>
<th>Water</th>
<th>MeOH</th>
<th>EtOH</th>
<th>Acetone</th>
<th>CH₂Cl₂</th>
<th>Hexane</th>
</tr>
</thead>
<tbody>
<tr>
<td>Solubility</td>
<td>&lt;0.01</td>
<td>S</td>
<td>S</td>
<td>S</td>
<td>U</td>
<td>U</td>
</tr>
<tr>
<td>Melting Point</td>
<td>152-155 °C</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Boiling Point</td>
<td>348-350 °C</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Application**
Used as a primary or secondary vulcanization accelerator.

**Regulatory Information**
Regulated for use under the following sections of 21 CFR:
§177.2600 Rubber Articles Intended for Repeated Use in Food Contact
§175.105 Components of Adhesives

**Environmental Impact**

<table>
<thead>
<tr>
<th>Level III Fugacity Model</th>
<th>Mass Amount (%)</th>
<th>Half-Life (h)</th>
<th>Emissions (kg/h)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air</td>
<td>0.0975</td>
<td>3.01</td>
<td>1000</td>
</tr>
<tr>
<td>Water</td>
<td>17</td>
<td>900</td>
<td>1000</td>
</tr>
<tr>
<td>Soil</td>
<td>82.2</td>
<td>1.8e+003</td>
<td>1000</td>
</tr>
<tr>
<td>Sediment</td>
<td>0.626</td>
<td>8.1e+003</td>
<td>0</td>
</tr>
</tbody>
</table>

Persistence Time: 1.17e+003 h

**Point of Release**
Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

**Toxicological Data**

Oral (LD50): 50 mg/kg [Rat]
Intraperitoneal (LD50): 1 gm/kg [Rat]
Intraperitoneal (LD50): 500 mg/kg [Mouse]
Crosslinking Compounds/Accelerators

Mass Spectrum for 1,3-Diphenyl-2-thiourea - PLAS-AC-008

MW=228.31

m/z Abundance

135 100
77 55
51 22
50 12
136 9

For Chromatogram See Appendix A - PLAS-AC-008 - page 449
Dipentamethylenethiuram Tetrasulfide

**Chemical Name**

**Synonyms**
1,1’-(tetraethydcarbonothioyl)-bis-piperidine

**Brand Names & Manufacturers**

Westco DPTT
Tetrone A

**Physical Properties**

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Melting Point</td>
<td>115 °C</td>
</tr>
<tr>
<td>Boiling Point</td>
<td>510 °C</td>
</tr>
<tr>
<td>Solubility (g/100mL 20 °C)</td>
<td>Water &lt;0.01, MeOH U, EtOH U, Acetone S, CH₂Cl₂ U, Hexane U</td>
</tr>
<tr>
<td>Appearance</td>
<td>Light yellow to gray powder</td>
</tr>
<tr>
<td>Stability</td>
<td>Stable under normal conditions of use.</td>
</tr>
</tbody>
</table>

**Application**

This compound is used as primary or secondary accelerator or sulfur donor for both natural rubber and synthetic.

**Regulatory Information**

Regulated for use in articles in contact with food as specified under FDA §175.105, §175.300, §177.1210 (indirect food contact).

**Environmental Impact**

Contains no hazardous air pollutants or ozone depleting substances. It is also not listed under the US Clean Water Act Priority Pollutant List.

**Point of Release**

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

**Toxicological Data**

Oral (LD₅₀): > 2000 mg/kg [Rat]
Crosslinking Compounds/Accelerators

Mass Spectrum for Dipentamethylenethiuram Tetrasulfide - PLAS-AC-009

For Chromatogram See Appendix A - PLAS-AC-009 - page 450

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1,3-Di-o-tolylguanidine

Chemical Name
1,2-bis(2-methylphenyl)guanidine

Synonyms
Di-o-tolylguanidine

Brand Names & Manufacturers

| Accelerator | Timeliall |
| DOTG        | Western Reserve Chemical |
| Sovchem® DOTG | Sovereign Chemical Company |
| VANAX® DOTG | RT Vanderbilt |

Physical Properties

| Appearance       | White powder       |
| Melting Point    | 175 - 178 ºC       |
| Boiling Point    | N/A                |
| Stability        | Stable under normal conditions of use. |
| Solubility (g/100mL 20 ºC) |
| Water <0.01 | MeOH S | EtOH S | Acetone S | CH₂Cl₂ U | Hexane U |
| Application, Regulatory & Environmental Information

Seldom used alone, commonly used with thiazoles, thiurams, dithiocarbamates, and sulfenamides to promote its activity as an accelerant. Mainly used in processing thick rubber products, tread rubber, breaker rubber, and rubber roll cover.

Regulatory Information
Regulated for use under the following sections of 21 CFR:
§177.2600 Rubber Articles Intended for Repeated Use in Food Contact
§175.105 Components of Adhesives
§178.3120 Animal Glue

Environmental Impact
Contains no hazardous air pollutants or ozone-depleting substances. It is also not listed under the US Clean Water Act Priority Pollutant List.

Point of Release
Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data
LD50 Oral - Mammal - 120 mg/kg
LD50 Oral Rat 56 mg/kg

CAS Number 97-39-2
RTECS Number MF1400000
Abbreviation DOTG

Formula C₁₅H₁₇N₃
Molecular Weight 239.32
**Mass Spectrum for 1,3-Di-o-tolylguanidine - PLAS-AC-010**

MW = 239.32

<table>
<thead>
<tr>
<th>m/z</th>
<th>Abundance</th>
</tr>
</thead>
<tbody>
<tr>
<td>107</td>
<td>100</td>
</tr>
<tr>
<td>106</td>
<td>42</td>
</tr>
<tr>
<td>239</td>
<td>31</td>
</tr>
<tr>
<td>91</td>
<td>20</td>
</tr>
<tr>
<td>224</td>
<td>14</td>
</tr>
</tbody>
</table>

For Chromatogram See Appendix A - PLAS-AC-010.0