

Industrial Coatings

Technical Data Sheet

DDI[®] 1410



Product Description	DDI [®] 1410 is a low viscosity, aliphatic diisocyanate liquid that is designed to react with compounds containing active hydrogen to form low molecular weight derivatives or specialty polymers.
Key Features & Benefits	<ul style="list-style-type: none">- Low viscosity at 100% solids- Non-yellowing in outdoor exposure- Low order of toxicity- Flexibility and extensibility- Low water sensitivity- Solubility in a wide range of solvents
Chemical Composition	Diisocyanate

Properties

Product Specifications	Appearance	clear liquid
	NCO	13.6 – 14.4%
	Hydrolyzable chloride	0.05% max
	Gardner color	7 max
Typical Characteristics	Molecular weight	600
	Equivalent weight	300
	Viscosity at 25°C	130 cps
	Density at 25°C	0.924 g/cm ³
	Refractive index	1.479

These typical values should not be interpreted as specifications.

Applications

DDI[®] 1410 is a unique aliphatic diisocyanate designed to react with compounds containing active hydrogen to form low molecular weight derivatives or specialty polymers. It is based on a long chain, dimerized fatty acid backbone containing 36 carbon atoms. This backbone structure provides DDI[®] 1410 an unusual degree of flexibility and water insensitivity along with a low order of toxicity when compared to other aliphatic isocyanates. It is a low viscosity liquid with good solubility in a broad range of polar and non-polar solvents. Because it is an aliphatic diisocyanate, it can be used in applications requiring non-yellowing properties.

DDI[®] 1410 can be used as a chemical building block in a variety of specialized intermediates or polymeric products such as:

- Extensible urea or urethane elastomer products
- Adhesive and sealant applications
- Flexible surface coating formulations
- Paper, leather and textile water-repellent treatments
- Wood stabilization formulations
- Electrical potting applications

Reactivity Data

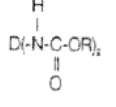
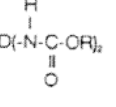
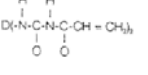
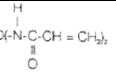
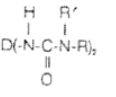
DDI® 1410 is a di-functional and will react with compounds containing two or more active hydrogens to form polymers. This isocyanate is ordinarily used with compounds containing hydroxyl or amine functionality. However, it can also be reacted with amides, carboxylic acids, thiols and ureas.

Polyurethane resins can be formed by reacting DDI® 1410 with polyether, polyester or acrylic polyols that impart unique properties of non-yellowing, excellent flexibility and extensibility, high impact resistance and low water sensitivity. Depending on the core reactant, these polymers may have excellent abrasion, and chemical and solvent resistance. Because the rate of reaction is relatively slow (when compared with lower molecular weight diisocyanates), the use of catalysts such as lead, tin or zinc octoate and/or higher temperatures should be considered. Good results have been obtained using 0.02 – 0.08% zinc (as zinc octoate) based on resin solids. The lower the percentage offers longer pot life but cures more slowly at room temperature.

Hydroxy-terminated polybutadiene diols offer exceptional compatibility and good reactivity with DDI® 1410 and results in polymers with unusually low Shore A hardness properties. These Shore A values are obtained without plasticizers. DDI® 1410 can also be used in combination with other diisocyanates to form co-polyurethane resins with properties varying over a broad range.

Polyurea resins can be formed by the reaction of DDI® 1410 with amine functional resins. This isocyanate-amine reaction takes place at a rapid rate and may require special handling equipment to prevent premature gelation. Special blocked amine materials such as ketimines offer controlled reactivity using a moisture-induced unblocking mechanism. DDI® 1410 can be reacted with a wide variety of polyamines to form elastomer products with a range of tensile strengths, elongations and Shore A hardnesses.

The following table illustrates the reactivity of various functional groups with DDI® 1410 in organic solvent. In each case, a model acrylic monomer is chosen to exemplify a particular functional group.

Reactions of DDI® 1410 with Acrylic Monomers in Organic Solvent					
Type of Functionality	Model Monomer	Catalyst	Product	Structure ¹	Conditions
Hydroxyl	Hydroxyethyl methacrylate	Stannous octoate Lead octoate Bismuth nitrate Dibutyl tin Dilaurate Ferric chloride	Urethane		50% solution in solvent ² at 76°C for 1hr
Methylolamide	Methylol acrylamide	Stannous octoate Bismuth nitrate Ferric chloride	Urethane		50% solution in solvent ² at 76°C for ½ hr
Amide	Acrylamide	None	Acrylure a		50% solution in xylene at 143°C for 1hr
Carboxylic acid	Acrylic acid	Potassium acetate Triethylamine	Amide		50% solution in solvent ² at 78°C for 1hr
Amine	t-Butylaminoethyl methacrylate	None	Urea		50% solution in solvent ² at room temp for 1hr

¹One gram of catalyst used per 300g of DDI® 1410.

²Dry tetrahydrofuran

DDI® 1410 reacts with the hydroxyl containing monomers, hydroxyethyl methacrylate and methylol acrylamide, to form urethanes under the conditions shown.

An acryl urea is formed with the unsubstituted amide, acrylamide. Relatively severe conditions are required, although no catalyst is used.

Using the appropriate alkaline catalysts, the diisocyanate reacts with the carboxyl group of acrylic acid. The usual urethane catalysts are not effective for this reaction. The reaction is accompanied by loss of carbon dioxide.

As expected, DDI® 1410 will react readily with amines that contain amino hydrogens, even in the absence of catalyst. t-Butylaminoethyl methacrylate forms the corresponding urea.

When water is present, a competing reaction is the hydrolysis of the isocyanate group forming a polyurea with the concurrent release of carbon dioxide. Most common urethane catalysts accelerate this reaction. DDI® 1410, under certain conditions, however, reacts with some functional groups in preference to water. Two examples are shown below.

Reactions of DDI [®] 1410 Emulsions ³ with Acrylic Monomers					
Type of Functionality	Model Monomer	Catalyst	Product	Structure	Conditions
Hydroxyl	Hydroxyethyl methacrylate	Dibutyl tin Dilaurate	Urethane	$\begin{array}{c} \text{H} \\ \\ \text{D}-(\text{N}-\text{C}-\text{O})_2 \\ \\ \text{O} \end{array}$	Heated at 70 - 75°C for 1hr
Amine	t-Butylaminoethyl methacrylate	None	Urea	$\begin{array}{c} \text{H} \quad \text{R}' \\ \quad \\ \text{D}-(\text{N}-\text{C}-\text{N}-\text{R})_2 \\ \\ \text{O} \end{array}$	Room temp immediate reaction

³35% DDI[®] 1410 emulsion using nonionic emulsifier.

Emulsification Data

DDI[®] 1410, unlike other diisocyanates, exhibits a high degree of hydrolytic stability due to its long chain, hydrophobic backbone. This property permits the preparation of stable water emulsions of DDI[®] 1410 for subsequent use in applications such as emulsion or solution polymerization. Laboratory tests indicate under basic pH conditions, less than 8% of the active isocyanate groups are lost after 24 hours. Under acid or neutral conditions, less than 5% reacts in 24 hours to form the polyurea degradation product. If isocyanate reactivity is desired for periods exceeding 24 – 48 hours and temperatures above 145°C can be tolerated, the 2-butanone oxime adduct of DDI[®] 1410 should be considered. This adduct will unblock in the 145 – 150°C temperature range allowing isocyanate groups to react with other available functional groups.

DDI[®] 1410 can be emulsified in water without auxiliary emulsifiers if extremely high shear agitation is used. However, for a more physically stable emulsion, one of the following three emulsifier compositions would be suitable:

- 25% Polysorbate 20 + 75% Sorbitan laurate
- 60% Polysorbate 80 + 40% Sorbitan mono-oleate
- Nonyl phenol ethoxylate

While the required ration of emulsifier to DDI[®] 1410 will vary depending on the local water source, a recommended starting point would be 7 – 10% emulsifier based on the DDI[®] 1410 solids content. This level is used for simple agitation emulsification, lower levels of emulsifier can be tolerated as mechanical agitation is increased. Emulsifier can be added to the water or the diisocyanate. No special sequence need be followed in emulsification as long as one of the components contains the required emulsifier.

The following 50% solids emulsion has been prepared in our laboratory using efficient agitation equipment:

46 parts water (distilled)
 50 parts DDI[®] 1410
4 parts nonyl phenol ethoxylate
 100 parts

This emulsion can be further diluted with distilled water to achieve lower solids contents.

Solubility Data

DDI[®] 1410 is soluble in a broad range of polar and non-polar solvents. In ratios of 1:10 and 1:1 at room temperature and 0°C, no immiscibility or phase separation was observed in:

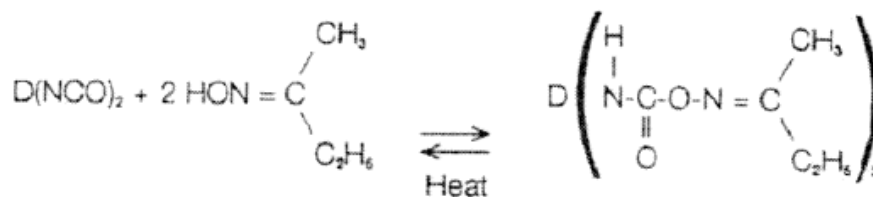
Acetone	Hexane	Tetrachloride
Benzene	Ketone	Toluene
Carbon	Methyl isobutyl	Xylene
Heptane	Mineral spirits	

DDI[®] 1410 will react with hydrogen atoms; therefore, organic solvents such as alcohols should be avoided. It is insoluble in the lower alcohols, such as ethyl and methyl alcohol, although the reaction products are soluble. With ether alcohols, both DDI[®] 1410 and the reaction products are soluble.

Blocked Derivatives

The primary isocyanate group on DDI[®] 1410 can be blocked in typical manner using compounds such as phenols or oximes. A blocked adduct of DDI[®] 1410 may be useful in systems requiring one package stability and where water emulsions of the isocyanate are desired.

The chemical reactions associated with the preparation and activation of an oxime derivate of DDI[®] 1410 are depicted by the equation below:



DDI® 1410 2-Butanone oxime

DDI® 1410 derivative

This derivative is activated by heating to regenerate the isocyanate and make it available for reaction with active hydrogen containing substances such as polyols, polyamines, etc.

To prepare an emulsion of this derivative, a variety of emulsifier systems can be used. One suitable emulsifier system is based on nonyl phenol ethoxylate. A recommended starting level is 5 – 10% based on weight of oxime derivative. The amount of emulsifier required will depend on the concentration of oxime derivative, the local water source, and the method of emulsification.

The preferred emulsification method is to incorporate the emulsifier in the DDI® 1410 derivative and then lend the mixture with water. An effective way to use this derivative in emulsions is first to prepare a 50% emulsion, then dilute to the desired concentration level.

The emulsified DDI® 1410 derivatives are chemically stable at normal temperatures. Any physical separation that occurs can be overcome by simple agitation.

The DDI® 1410 derivative can be activated by heating to an elevated temperature to regenerate the isocyanate. The by-product is 2-butanone oxime. This regeneration depends on temperature and the environment in which the product is heated. When a sample of this material is heated at 150°C for 15 minutes, its infrared spectrum develops a strong isocyanate band with the simultaneous weakening of its urethane band. This shows that unblocking takes place at 150°C making the isocyanate available for reaction. Since this occurs above the boiling point of water, residual water from the emulsion is driven off prior to isocyanate release.

Lower temperatures require correspondingly longer heating times. The presence of functional groups containing active hydrogens may result in a lower activation temperature. For instance, compounds such as polyamides that can aid in the displacement of the blocking agent, might function in this way.

Textile Treatments

DDI® 1410 has shown promising initial results as a water repellent softener for textiles. Because it is less sensitive to water than aromatic diisocyanates, a stable water emulsion can be prepared. Application at 0.125% level imparts a durable softness; after 26 washes a treated cotton cloth was considered similar in softness to a cotton freshly treated with a non-durable cationic softener. Application at 1% concentration provides durable water repellency equal to or better than commercial fatty pyridinium repellents as measured at AATCC tests.

Water-Oil Repellency

DDI® 1410 and its derivatives can serve as efficient and effective synergistic extenders for fluorochemicals used to impart oil/water repellency to textiles. When used with commercially available fluorochemical products, DDI® 1410 greatly improves water repellency properties while extending the oil repellency properties as well. In addition, laboratory and field evaluations have shown DDI® 1410 to enhance wash and dry cleaning durability, not only of fluorochemicals but also auxiliary textile additives such as anti-static finishes.

The following table shows the water-oil repellency properties using Scotchgard⁴ FC 208 emulsion and DDI® 1410. All weight values given represent solids add-on to the fabric. The laboratory evaluation procedure involved preparation of the proper percent solids fluorochemical emulsion taking into account pickup with cotton twill and the amount of water added with the emulsified diisocyanate. DDI® 1410 was prepared as a 50% stock emulsion and added with slow stirring to the prediluted Scotchgard⁴ FC 208 emulsion.

⁴Registered trademark of 3M Company.

Water-Oil Repellancy Data						
Textile Finish Add On	Oil Repellancy (3M Test)		Spray Rating		Hydrostatic Pressure	
	0 Wash	5 Wash	0 Wash	5 Wash	0 Wash	5 Wash
0.50% DDI [®] 1410	0	0	90	70/80	29	19
1.00% DDI [®] 1410	0	0	80	80/90	29	21
0.15% Scotchgard FC 208	50	0	50	50	18	9
0.50% Scotchgard FC 208	90	60	100	80	34	26
0.50% DDI [®] 1410 + 0.15% Scotchgard FC 208	70	60	100	100	31	26
0.50% DDI [®] 1410 + 0.50% Scotchgard FC 208	100	90	100	100	33	25
1.00% DDI [®] 1410 + 0.15% Scotchgard FC 208	80	70	100	90/100	36	24
1.00% DDI [®] 1410 + 0.50% Scotchgard FC 208	110	100	100	100	30	2

Safety

General

The usual safety precautions when handling chemicals must be observed. These include the measures described in Federal, State, and Local health and safety regulations, thorough ventilation of the workplace, good skin care, and wearing of protective goggles.

Material Safety Data Sheet

All safety information is provided in the Material Safety Data Sheet for DDI[®] 1410.

Important

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