TMXDI® (META) aliphatic isocyanate

DESCRIPTION

TMXDI (META) aliphatic isocyanate monomer contains two tertiary aliphatic diisocyanate groups. This functionality provides unique properties as compared to primary and secondary isocyanate containing monomers.

TMXDI[1] monomer is used to prepare solvent-free polyurethane dispersions. These dispersions can be designed to provide adhesion, flexibility, and toughness to light-stable, waterborne adhesives, coatings, and inks.

APPLICATION AREAS

- Solvent-free polyurethane dispersions
- Waterborne automotive OEM basecoat
- Waterborne automotive refinish basecoat
- Waterborne coatings for plastics and wood
- Waterborne primer coat for leather
- Heat activated adhesives
- Laminating adhesives
- Waterborne inks

TYPICAL PROPERTIES

Appearance	Colorless liquid
CAS number	002778-42-9
Molecular Formula	$C_{14}H_{16}N_2O_2$
Molecular Mass	244.3
NCO content (% by weight)	34.4
Boiling Point (°C, 50 mmHg)	150
Flash Point (°C)[2]	153
Specific Gravity at 25°C	1.07

[2] Setaflash Closed Cup

POLYURETHANE DISPERSIONS

The properties of the tertiary isocyanate groups in TMXDI monomer make it more suitable for the preparation of solvent-free polyurethane dispersions than other aliphatic isocyanates. Polyurethane polymers prepared from this tertiary isocyanate have substantially lower and more stable viscosities compared to the same polymers prepared from primary and secondary isocyanate monomers. The steric hindrance also prevents self-condensation of the isocyanate, which stops formation of allophanates, biurets, or isocyanurates. The lack of side reactions and the low reactivity of the tertiary isocyanate with carboxylic acid groups allow prepolymers based on TMXDI monomer to be processed at higher temperatures than is possible with other diisocyanates. Higher processing temperatures, coupled with the lower inherent viscosity of the prepolymers, allow dispersions to be more easily prepared without the use of solvent. As long as the water temperature does not exceed 40°C, the reaction of isocyanate with water is slow enough to be ignored, so chain extension should be done at a 1:1 stoichiometry.

COATINGS APPLICATIONS

Dispersions prepared from TMXDI monomer tend to have lower tensile strength and higher elongation to break than corresponding dispersions prepared from isophorone or hexamethylene diisocyanates. Tensile strength can be increased by the addition of a small amount of trimethylolpropane to the prepolymer formula. The elongation remains high, so tough, flexible coatings are characteristic of dispersions prepared from TMXDI monomer. The properties of dispersions based on TMXDI monomer can be varied from soft, flexible coatings to coatings with hardness approaching that of automotive topcoats. The degree of hardness is achieved by choosing the correct polyester backbone resin and varying the NCO/OH ratio, the number of carboxylic acid groups, and short chain diols. Coalescing solvents or blends with other resins are required for good film formation when hard coatings from these dispersions are desired. Coatings prepared from dispersions based on TMXDI monomer are characterized by having good adhesion to substrates. These dispersions are thermoplastic, so the addition of a crosslinking agent is recommended where solvent resistance is required.

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CYTEC INDUSTRIES INC.
Five Garret Mountain Plaza
West Paterson, NJ 07424-3360
973-357-3100
www.cytec.com

ADHESIVE APPLICATIONS

Dispersions prepared from TMXDI monomer provide lower heat activation temperatures than can be obtained from the same dispersion prepared from either isophorone diisocyanate or hydrogenated methylene diphenylene isocyanate. In addition to lower activation temperature, the activation temperature of applied adhesive remains constant over time. The combination of low heat activation and good adhesion to flexible substrates makes solvent-free dispersions based on TMXDI of interest for applications involving temperature sensitive plastic substrates and flexible films.

INK APPLICATIONS

The adhesion of dispersions prepared from TMXDI monomer to flexible plastic substrates makes them a good choice for binders in the formulation of water-based inks.

BLOCKED PRODUCTS

TMXDI (META) aliphatic isocyanate can be reacted with typical isocyanate blocking agents to allow the formulation of one component thermoset coatings. For a given blocking agent, the tertiary isocyanate group provides a 10-15°C lower deblocking temperature versus primary or secondary isocyanates.

STORAGE

TMXDI (META) aliphatic isocyanate is sensitive to moisture and should be kept in tightly-closed original containers to prevent contamination with moisture and air. If partially filled containers are stored, it is advisable to blanket the liquid surface with dry nitrogen before sealing.

HEALTH AND SAFETY INFORMATION

TMXDI (META) aliphatic isocyanate is harmful if inhaled. The vapor is irritating. The liquid may cause eye irritation and an allergic skin reaction. Where a closed system is not used, good enclosure and local exhaust ventilation should be provided to minimize exposure. For detailed information, see Cytec Industries Inc. Material Safety Data Sheet Number 2344.

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[1] As used herein, all references to TMXDI are understood to be TMXDI® (META) aliphatic isocyanate.

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- **Asia/Pacific** - Cytec Industries Pte. Ltd., Singapore, tel. 65-733-6788, fax. 65-735-7783
- **Europe** - Cytec Netherlands (CRP) B.V., Botlek, the Netherlands, tel. 31-181-295504, fax. 31-181-295401
- **Latin America -** Cytec do Brasil LTDA, Sao Paulo, Brasil tel. 55-11-5505-4588, fax. 55-11-5505-4565
- **United States** - Cytec Industries Inc., West Paterson, NJ, U.S.A., tel. 973-357-3100, fax. 973-357-3065