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CYTEC

Isocyanic acid, m-phenylenediiso-propylidene, CAS# 2778-42-9

High Production Volume (HPV) Challenge Program

**Test Plan
for**

TMXDI® (META) ALIPHATIC ISOCYANATE

**Isocyanic acid, m-phenylenediiso-propylidene
CAS# 2778-42-9**

Prepared by

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A. INTRODUCTION AND HISTORY

On November 22, 1999, Cytec Industries Inc. (Cytec) voluntarily agreed to participate in the Environmental Protection Agency's (EPA) High Production Volume Chemical Challenge Program. By participating in this program, Cytec agreed to assess the adequacy of existing data, design and submit test plans to fill data gaps where necessary and appropriate, provide test results, and prepare summaries of the data characterizing each chemical.

The sponsored chemical addressed in this test plan is Isocyanic acid, m-phenylenediiso-propylidene (CAS# 2778-42-9) (TMXDI).

This test plan was first submitted to the Environmental Protection Agency and posted on the EPA HPV Chemical Challenge Program website in October 2002. The test plan was revised in April 2003 in response to EPA comments. In October 2003 Cytec provided revised comments to the HPV test plan which were never posted. These comments have been resubmitted for posting to the website. Per agreement with the EPA, the sponsors have conducted studies on stability to water (hydrolysis), developmental toxicity and chromosomal aberration to address initial deficiencies of data for these endpoints. These endpoints have now been addressed satisfactorily, and the study robust summaries have been added to the dossier for this chemical. The test plan has been appropriately revised to reflect the newly generated test data.

B. GENERAL SUBSTANCE INFORMATION**Trade Name: TMXDI® (META) ALIPHATIC ISOCYANATE**

Chemical Name: Isocyanic acid, m-phenylenediiso-propylidene

Inventory Names:

Benzene, 1,3-bis(1-isocyanato-1-methylethyl)-
1,3-Bis(1-isocyanato-1-methylethyl)benzene
1,3-bis(1-isocyanato-1-methylethyl)benzene
1,3-Bis(1-isocyanato-1-methylethyl)benzol
1,3-bis(1-isocianato-1-metiletil)benceno

Other Names:

a,a,a',a'-Tetramethyl-m-phenylenedimethylene diisocyanate
a,a,a',a'-Tetramethyl-m-xylylene diisocyanate
1,3-Bis(a-isocyanatoisopropyl)benzene
Isocyanic acid, a,a,a',a'-tetramethyl-m-xylylene ester
Isocyanic acid, m-phenylenediisopropylidene ester
m-Bis(1-isocyanato-1-methylethyl)benzene
TMXDI
Tetramethyl-m-xylylene diisocyanate

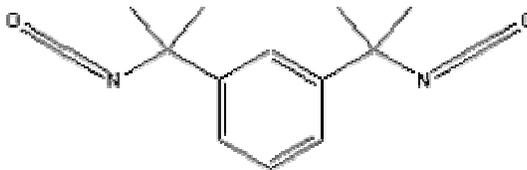
Chemical Abstract Service Registry Number: CAS # 2778-42-9

Common Name: TMXDI

Empirical Formula: C₁₄H₁₆N₂O₂

Molecular Weight: 244.3

Structure:



C. EXPOSURE INFORMATION

1. Use and Exposure Information

Cytec Industries Inc. has produced in excess of 1 million pounds of this material. As such, there are prescribed conditions for its manufacture, processing, distribution, use and disposal. In general, there is low potential for exposure of humans or the environment. In the work place, potential worker exposure is carefully controlled.

2. Manufacture & Processing:

Although diisocyanates are well-known sensitizers, little risk is posed by this chemical. The diisocyanate is manufactured in an essentially closed system with little personnel exposure. Its manufacture is monitored under close technical supervision. Although its vapor pressure is quite low, points of possible exposure are controlled by exhaust systems and, where necessary, carbon filters are used to purify any contaminated air. Protective clothing and respirators are required.

The only worker contact comes from sampling procedures for quality control, and in some instances, during packaging. Exposure would be by skin contact. Inhalation exposure is extremely low due to the use of ventilation and the materials low vapor pressure. Ingestion would not be expected.

In customer applications, this material is used at plants by highly experienced personnel well equipped to handle these materials safely.

TMXDI is not sold directly to the consumer market. This material is reacted into the polymers in which they are added, limiting potential exposure in the finished consumer products.

3. Distribution (Transport):

Since diisocyanates are well known sensitizers, distribution of this material is restricted to customers that are highly experienced and well equipped to handle material of this kind. As is well known, plants handling isocyanates routinely use exhaust systems to minimize hazards due to contaminated air, and where required, protective clothing and respirators are used. Our choice of customers is restricted to companies' well respected in the field and having high standards of industrial hygiene.

This material is transported to our customers in drums, totes, or ISO containers by way of truck or ship with little to no risk to the public or the environment.

4. Uses:

TMXDI aliphatic isocyanate is a versatile aliphatic isocyanate finding broad end-use applicability. Application areas include specialty coatings, aqueous dispersions, automotive coatings, wood coatings, inks, sealants, adhesives, thermoplastic urethanes, and lacquers.

This chemical imparts improved physical properties to polyurethane products, affording higher strength and improved adhesion, appearance, and flexibility, resulting in more durable products. Common commercial products that may have been made using TMXDI include, fabric and leather finishes, adhesives, automotive paints, printing inks, sealants, and wood coatings. TMXDI poses little to no risk to the end consumer as there is no exposure to TMXDI.

In addition to these uses, TMXDI is FDA approved for use in food-packaging under specific listings in the Code of Federal Regulations (CFR) Title 21-Food and Drugs Chapter I-Food and Drug Administration, Department of Health and Human Services.

Table 1: 21 CFR Sanctions

21 CFR	Section	Definition
PART 175—Indirect Food Additives: Adhesives and Components of Coatings-- §175.105 (ADHESIVES)	§175.105	Clears meta-tetramethyl xylene diisocyanate for reaction with one or more of the polyols and polyesters listed in §175.105 and dimethylolpropionic acid and triethylamine, N-methyldiethanolamine, 2-dimethylaminoethanol, 2-dimethyl-amino-2-methyl-1-propanol and/or 2-amino-2-methyl-1-propanol in the production of polyurethane resins intended for use as components of adhesive formulations used in food packaging applications. Cytec Industries Petition Oct. 26, 1993, effective March 12, 1996

5. Disposal:

All waste material is drummed and disposed of by approved waste treatment contractors. This material is not regulated as a RCRA hazardous waste

D. SUMMARY TABLE OF AVAILABLE DATA

CAS# 2778-42-9	Study Date	Results	Data Acceptable
Physical/Chemical Characteristics			
Melting Point	1982	-10°C	Yes
Boiling Point	1982/ 2002	292 °C @ 1013 hPa (meas.) 320 °C @ 1013 hPa (est.)	Yes
Vapor Pressure	1986/ 2002	0.0043 hPa (0.0032 mm Hg) @ 25 °C (meas.) 0.00298 mm Hg @ 25 °C (est.)	Yes
Partition Coefficient	2002	Log K _{ow} = 4.74	Yes
Water Solubility	2002/ 2002	Insoluble (reacts with water) 5.833 mg/L @ 25 °C (est.)	Yes
Environmental Fate			
Photodegradation	2002	For reaction with hydroxyl radical, predicted rate constant = 10.1332 x 10 ⁻¹² cm ³ /molecule-sec Predicted half-life = 12.666 hours	Yes
Stability in Water	2003	<i>OECD 111: Hydrolysis as a Function of pH</i> Measured hydrolysis half-lives at 25°C are: pH 4 = 0.4 hours pH 7 = 0.4 hours pH 9 = 0.3 hours Hydrolysis at pH 1.2 and 37°C was too rapid to measure	Yes
Transport between Environmental Compartments: Fugacity Level III Model Default assumption: 1000 kg/hr simultaneously released into air, water, and soil.	2002	Air: 0.779% Water: 18.1% Soil: 62.6% Sediment: 18.5%	Yes
Biodegradation	1988	<i>OECD 301D: Closed Bottle Test</i> Not readily biodegradable by this test procedure	Yes
Ecotoxicity			
Acute Toxicity to Fish	1993	<i>OECD 203: Fish Acute Toxicity Test</i> Lepomis macrochirus: NOEC = >52.19 mg/L 96 hr LC50 = >65.88 mg/L (based on exposure to Water Accommodating Fraction, measured by	Yes

	1986	analysis) <i>USEPA 660/3-75-009: Fish Acute Toxicity Test</i> Pimephales promelas NOEC = 0.32 mg/L 96 hr LC50 = 0.67 mg/L (based on material dissolved in acetone)	Yes
Acute Toxicity to Invertebrates	1986	<i>USEPA 660/3-75-009: Daphnia magna Acute Toxicity Test</i> Daphnia magna NOEC = <1.0 mg/L 24-hour LC50 = 6.5 mg/L 48-hr LC50 = 5.2 mg/L (based on material dissolved in acetone)	Yes
Acute Toxicity to Algae	1987	<i>OECD 201: Alga. Growth Inhibition Test</i> Selenastrum capricornutum: NOEC = 0.34 mg/L EbC50 = 2.1 mg/L (based on material dissolved in acetone)	Yes
Mammalian Toxicity			
Acute Toxicity			
Oral	1981	Rat: oral LD50 = 5000 mg/kg	Yes
Dermal	1981	Rabbit: dermal LD50 = >2,000 mg/kg	Yes
Inhalation	1995	Rat: inhalation 4 hr LC50 = 0.27 mg/l	Yes
Eye Irritation	1981	Mild Eye Irritant	Yes
Skin Irritation	1981	Moderate Skin Irritant	Yes
Dermal Sensitization	1981	Skin Sensitizer	Yes
Respiratory Sensitization	1984	No Sensitization Response Elicited	Yes
Repeat Dose Toxicity	1990	(90 day inhalation) rat/mice: NOAEL < 0.4 ppm for both species LOAEL = 0.4 ppm for both species	Yes
	1987	(28 day inhalation) rat: NOAEL = 1.5 mg/m³ LOAEL = 5.0 mg/m³	Yes
	2005	<i>OECD 421: Oral Reproduction/ Developmental Toxicity Screen, Rat</i> NOAEL (systemic) = 150 mg/kg bw LOAEL (systemic) = 250 mg/kg bw	Yes
Genetic Toxicity: Gene Mutations	1983	Salmonella typhimurium: Not mutagenic	Yes
Genetic Toxicity: Chromosomal Aberration	2003	<i>OECD 473 and Method B10 of Commission Directive 2000/32/EC</i> Chinese Hamster Ovary (CHO) Cells: Not clastogenic	Yes
Reproductive Toxicity	2005	<i>OECD 421: Oral Reproduction/</i>	Yes

	1981	<p><i>Developmental Toxicity Screen, Rat</i> NOAEL (systemic) = 150 mg/kg bw NOAEL (reproductive) = 250 mg/kg bw (highest concentration tested)</p> <p>Based on the results of the 90-day repeat dose inhalation study there were no macro or microscopic changes in any of the male or female reproductive organs that could be attributed to exposure to TMXDI. Thus suggestive that at the concentrations tested the material would not be a reproductive toxicant.</p>	Yes
Developmental Toxicity	2005	<p><i>OECD 421: Oral Reproduction/ Developmental Toxicity Screen, Rat</i> NOAEL (systemic) = 150 mg/kg bw NOAEL (developmental) = 250 mg/kg bw (highest concentration tested)</p>	Yes

E. TEST PLAN FOR Isocyanic acid, m-Phenylenediiso-Propylidene, CAS# 2778-42-9

CAS# 13893-53-3	Data Available	Data Acceptable	Testing Required
Study	Y/N	Y/N	Y/N
Physical/Chemical Characteristics			
Melting Point	Y	Y	N
Boiling Point	Y	Y	N
Vapor Pressure	Y	Y	N
Partition Coefficient	Y	Y	N
Water Solubility	Y	Y	N
Environmental Fate			
Photodegradation	Y	Y	N
Hydrolysis	Y	Y	N
Fugacity	Y	Y	N
Biodegradation	Y	Y	N
Ecotoxicity			
Acute Toxicity to Fish	Y	Y	N
Acute Toxicity to Invertebrates	Y	Y	N
Acute Toxicity to Algae	Y	Y	N
Mammalian Toxicity			
Acute Toxicity	Y	Y	N
Repeat Dose Toxicity	Y	Y	N
Genetic Toxicity: Gene Mutations	Y	Y	N
Genetic Toxicity: Chromosomal Aberration	Y	Y	N
Reproductive Toxicity	Y	Y	N
Developmental Toxicity	Y	Y	N