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# TMI<sup>®</sup> (META)

## Unsaturated Aliphatic Isocyanate



## About allnex



## Table of Contents

TMI <sup>®</sup> (META) Unsaturated Aliphatic Isocyanate
Uses of TMI
Modified Polymers Containing TMI
Improved Performance of Modified Latex Films Co
Reactivity Ratios of TMI
Improved Tensile Properties of a Modified Latex C
Blocked Isocyanates
Deblock Temperatures of Tertiary Aliphatic Isocya
Physical Attributes of Blocked Isocyanates
Cure Temperatures of Blocked TMI Self-Crosslinki

## Facts & Figures

- Global company with over €2.1 billion in sales
- Broad Technology portfolio: liquid coating resins, energy curable resins, powder coating resins, crosslinkers and additives, composites and construction materials
  Approximately 4000 employees
  Customers in more than 100 countries

#### • 33 manufacturing facilities

- 23 research and technology centers
- 5 joint ventures
- Extensive range of solutions for key coating segments: automotive, industrial, packaging coating and inks, protective, industrial plastics and specialty architectural

With manufacturing, R&D and technical facilities located throughout Europe, North America, Asia Pacific and Latin America, allnex offers global and reliable supply of resins and additives combined with local, responsive customer support.

	1
	4
	5
ntaining TMI	5
6	ŝ
ontaining TMI6	ŝ
	7
nates	7
	3
ng Copolymers	3

### TMI<sup>®1</sup> (META) Unsaturated Aliphatic Isocyanate



α,α -Dimethyl meta-Isopropenyl Benzyl Isocyanate

#### **Physical Properties**

Chemical Abstract Registry No.	2094–99–7
Molecular Weight	201.3
NCO (Isocyanate group) Content, % By Weight	20.9
Appearance	Clear, Colorless Liquid
Boiling Point, 1 atm	270°C
Density, g/mL. 25°C	1.0
Viscosity, cp, 27°C	3.0
Vapor Pressure, Torr, 100°C	2

### Uses of TMI

#### **Polymer Modification**

Use NCO to attach desired functionality and polymerize.

Copolymerize TMI monomer with a variety of other monomers to create a polymer with free isocyanate groups available for crosslinking.

#### Coatings

Blocked version in acrylic copolymer for 1K acid etch resistant topcoat.

Unblocked version in acrylic copolymer for ambient cure paint.

#### **Plastics Modification**

Grafting to PP and TPO for improved surface properties.

## Modified Polymers Containing TMI®

#### Two Approaches

React –NCO group and then polymerize to incorporate specic functional groups.



- deblock and cure
- rheology modiers
- polymerizable surfactants
- wet adhesion modifers

Copolymerize TMI monomer into latex and moisture cure for selfcrosslinked lms for improved strength and scrub resistance.

 $\rightarrow$  NCO +H<sub>2</sub>O OCN  $\rightarrow$   $\rightarrow$  NHCONH  $\rightarrow$  +CO<sub>2</sub>

## Improved Performance of Modified Latex Films Containing TMI

### **Critical Parameters**

Polymerization conditions <sup>1</sup>	<ul> <li>polymerize &lt;40°C to prevent hydrolysis</li> <li>increasing the concentration of TMI monomer can reduce polymerization rate</li> <li>2-5 wt% recommended</li> </ul>		
Location of TMI in latex	<ul> <li>location a ects both Im properties and storage stability</li> <li>optimum location needs to be determinined for particular application</li> </ul>		
Catalyst choice	<ul> <li>catalyst affects film performance</li> <li>incorporation of 2-5 wt% of (meth) acrylic acid recommended for speed of cure; will reduce NCO stability in latex</li> </ul>		

<sup>1</sup> Data obtained from sponsored research program at the Emulsion Polymers Institute, Lehigh University



## Reactivity Ratios of TMI®

Bulk Polymerization at 70°C1 TMI as M1			Bulk Polymerization at 110°C2 TMI as M1	
$M_2$	r <sub>1</sub>	r <sub>2</sub>	M <sub>2</sub>	r <sub>1</sub>
Styrene	0.16	0.84	Styrene	0.72
MMA	0.03	0.43	MMA	0.62
BA	0.38	0.08	BA	0.53

## Improved Tensile Properties of a Modified Latex Containing TMI



Improved tensile property poly (MMA/ BA/TMI/MAA) (40/55/3/2) compared to poly (MMA/BA) (45/55) control. Cast lms dried at room temperature for 10 days prior to testing.

Tensile property of poly (MMA/BA/TMI/ MAA) latex stored at room temperature

for one year compared to that of the fresh latex; TMI = 3%, MAA = 2%.

10 days.

Cast films dried at room temperature for

 $r_2$ 

0.80

0.31 0.13

## Improved Tensile Properties of one-year-old Modified Latex Containing TMI



<sup>1</sup> Lehigh data calculated using Kelen Tudos Method, J. Marcomol. Sci, Chem A9 (1), 1 (1975) <sup>2</sup> TMI (META) Unsaturated Aliphatic Isocyanate Technical Data Sheet, Allnex

## Blocked Isocyanates

Products Based on TMxdI<sup>®</sup> and TMI<sup>®</sup> in Powder Coatings Products deblock at lower temperature vs. HDI and IPDI

### TMI in Solvent Borne Coatings

Acid etch resistant OEM topcoat system based on TMI is reported in patent literature

## Deblock Temperatures of Tertiary Aliphatic Isocyanates

Blocking Group	NCO Onset, Deblock Temperature °C
3,5-Dimethylpyrazole	55 - 65
2,6-Dimethyl-4-Heptanone Oxime	60 - 75
Methyl Ethyl Ketoxime	65 - 80
2-Heptanone Oxime	70 - 80
1,2,4-Triazole	80 - 90
ε-Caprolactam	95 - 105
Nonylphenol	145 - 165
t-Butanol	150 - 185
Propylene Glycol	> 180
Isopropanol	190 - 210
Methanol	200 - 220
n-Butanol	200 - 230
n-Hexanol	215 - 230
n-Pentanol	215 - 235

## Physical Attributes of Blocked Isocyanates

Allnex's Isocyanate	Blocking Material	Physical State	Melting Point °C
	МЕКО	Liquid	-
	3,5-Dimethylpyrazole	Liquid	-
	n-butanol	Solid	~ 27
TMI®	Methanol	Solid	~ 37
	t-butanol	Solid	~ 60
	ε–Caprolactam	Solid	~ 70
	Nonylphenol	Solid	~ 80
	МЕКО	Resinous	-
TMXDI®	n-butanol	Solid	~ 68
	ε–Caprolactam	Solid	~ 117
	1,2,4-Triazole	Solid	~ 117
	Acetone Oxime	Solid	~ 125
	Methanol	Solid	~ 130

## Cure Temperatures of Blocked TMI Self-Crosslinking Copolymers

Blocking Agent	Temperature <sup>1</sup> , °C
Methyl ethyl ketoxime	120
N-Hydroxysuccimide	130
ε–Caprolactam	135



NOLES		

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