3. CHEMICAL AND PHYSICAL INFORMATION

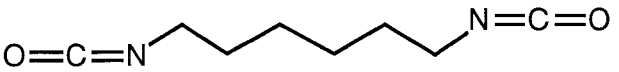
3.1 CHEMICAL IDENTITY

Information regarding the chemical identity of HDI is located in Table 3-1. Most of the HDI manufactured in, or imported into, the United States is converted into HDI prepolymers (polyisocyanates). These prepolymers are biurets and trimers. Information for those prepolymers is shown in Table 3-2.

3.2 PHYSICAL AND CHEMICAL PROPERTIES

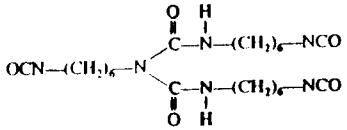
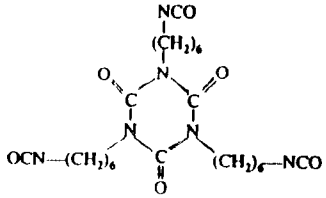
Information regarding the physical and chemical properties of HDI is located in Table 3-3.
HDI is a monomer used in the production of polyurethane foams and other related products, and is found in some industrial paints and spray painting operations. It is a compound which reacts readily with water and alcohols (Von Burg 1993). It has a vapor pressure of 0.05 mm Hg at room temperature, but can be present in aerosol form allowing a potentially higher exposure to individuals. The HDI-BT trimer is often present for similar industrial uses. It would be expected to have a lower vapor pressure; however, the aerosol form can also be present, allowing potentially higher exposure of HDI-BT to individuals.
HDI reacts slowly with water to form carbon dioxide (HSDB 1996). The base-catalyzed reaction of HDI with alcohols should be carried out in inert solvents; the reaction may occur with explosive violence in the absence of solvents (NFPA 1994).

Table 3-1. Chemical Identity of Hexamethylene Diisocyanate

Characteristic	Information	Reference
Chemical name	1,6-Hexamethylene diisocyanate	HSDB 1996
Synonym(s)	1,6-Diisocyanatohexane; HDI; HMDI	HSDB 1996
Registered trade name(s)	TL-78; Desmodur H; Mondur HX	HSDB 1996; Bagon et al. 1984; Dunlap 1976
Chemical formula	$OCN-(CH_2)_6-NCO$	HSDB 1996
Chemical structure		
Identification numbers:		
CAS Registry	822-06-0	Lewis 1993
NIOSH RTECS	MO1740000	HSDB 1996
EPA Hazardous Waste	No data	
OHM/TADS	No data	
DOT/UN/NA/IMCO	UN2281; IMO 6.1	HSDB 1996
HSDB	6134	HSDB 1996
NCI	No data	

CAS = Chemical Abstracts Services; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; HSDB = Hazardous Substance Data Bank; NCI = National Cancer Institute; NIOSH = National Institute for Occupational Safety and Health; OHM/TADS = Oil and Hazardous Materials/Technical Assistance Data System; RTECS = Registry of Toxic Effects of Chemical Substances

Table 3-2. Chemical Identity of Hexamethylene Diisocyanate Prepolymers

Characteristic	HDI biuret	HDI trimer
Chemical name	Hexamethylene diisocyanate biuret	Hexamethyene diisocyanate trimer
Synonym(s)	N,N′,2-tris(6-isocyanatohexyl)-imidodicarbonic diamide; HDI-BT	1,3,5-Tris(6-isocyanatohexyl)-1,3,5-triazine-2,4,6(1H,3H,5H)-trione; HDI isocyanurate
Registered trade name(s)	Desmodur N-75; Desmodur N-100; Desmodur N-3200	Desmodur N-3300; Desmodur N3390
Chemical formula	$C_{23}H_{38}N_6O_5$	$C_{24}H_{36}N_6O_6$
Chemical structure		
Identification numbers:		
CAS registry	4035-89-6	3779-63-3
NIOSH RTECS	NR0195000	None
EPA hazardous waste	None	None
OHM/TADS	None	None
DOT/UN/NA/IMCO shipping	None	None
HSDB	None	None
NCI	None	None

CAS = Chemical Abstracts Service; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; HSDB = Hazardous Substances Data Bank; NCI = National Cancer Institute; NIOSH = National Institute for Occupational Safety and Health; OHM/TADS = Oil and Hazardous Materials/Technical Assistance Data System; RTECS = Registry of Toxic Effects of Chemical Substances

References:

CCOHS 1998
Janko et al. 1992
Maitre et al. 1996
Myer et al. 1993
RTECS 1998

Table 3-3. Physical and Chemical Properties of Hexamethylene Diisocyanate

Property	Information	Reference
Molecular weight	168.22	HSDB 1996
Color	Pale yellow	Von Burg 1993
Physical state	Liquid	Lewis 1993
Melting point	-67 °C	ASTER 1995
Boiling point	255 °C 212.8 °C at 760 mm Hg	ASTER 1995 NIOSH 1978
Density at 25 °C	1.04 g/mL 1.0528 g/mL	HSDB 1996 Weast 1988
Odor	Pungent	Von Burg 1993
Odor threshold:		
Water	Not applicable, reacts with water	HSDB 1996
Air	0.001–0.02 ppm	HSDB 1996
Solubility:		
Fresh water at 20 °C	Poorly soluble; reacts	NIOSH 1978; Von Burg 1993
Salt water at 25 °C	No data	
Organic solvent(s)	Soluble in organic solvents Reacts with alcohols	NIOSH 1978 Von Burg 1993
Partition coefficients:		
Log K_{ow}	3.1956 (estimated)	SRC 1995b
Log K_{oc}	No data	
Vapor pressure at 20 °C	0.014 mbar; 0.05 mm Hg (24 °C)	Morel et al. 1981; NIOSH 1978
Henry's law constant: at 25 °C	4.8×10^{-5} atm-m^3/mole	SRC 1994a
Autoignition temperature	454 °C	Morel et al. 1981
Flashpoint	140 °C; 135 °C (open cup)	NIOSH 1978; Morel et al. 1981
Flammability limits at 25 °C	No data	
Conversion factors (25 °C)	1 µg/m^3 = 0.145 ppb 1 ppb = 6.879 µg/m^3	NIOSH 1978 NIOSH 1978
Explosive limits	1–24%	Von Burg 1993