

Ultra High-Performance Elastomers Based on trans-Bis(Isocyanatomethyl Cyclohexane)

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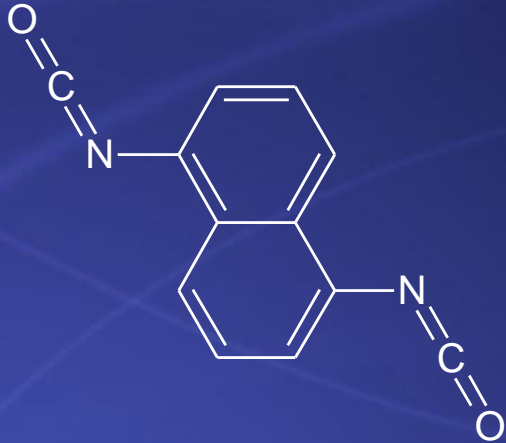
Anderson Development Company
a subsidiary of Mitsui Chemicals



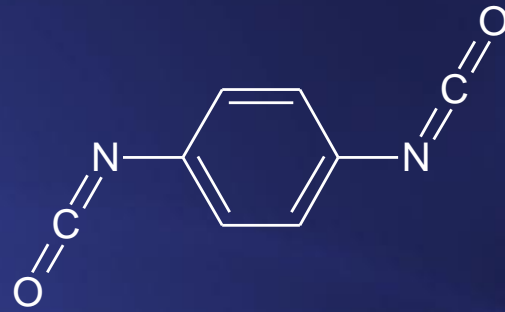
Mitsui Chemical's Concept for a New Diisocyanate



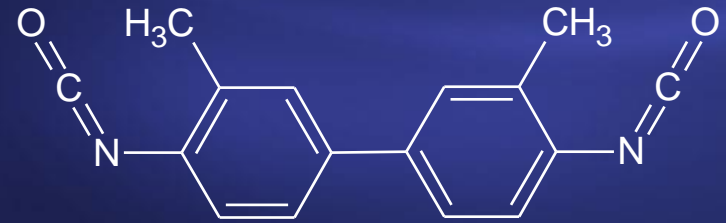
Ultra High-Performance Diisocyanates



1,5-Naphthalene
Diisocyanate
(NDI)

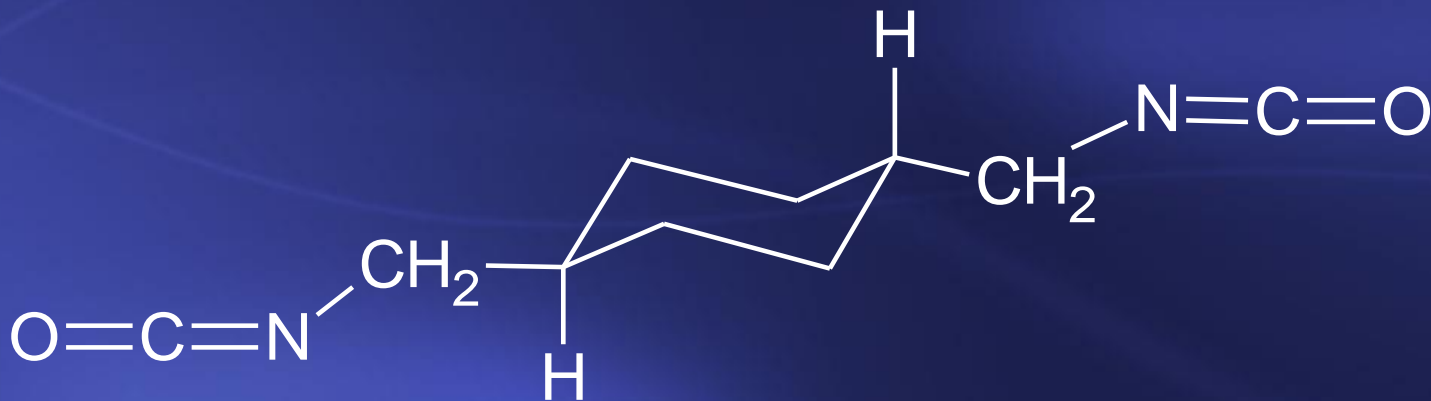


1,4-Phenylene
Diisocyanate
(PPDI)



o-Tolidine
Diisocyanate
(TODI)

trans-Bis (Isocyanatomethyl Cyclohexane)
trans-1,4-Hydrogenated Xylylene Diisocyanate
Fortimo™ 1,4-H6XDI
trans-1,4-H6XDI



Fortimo™ 1,4-H6XDI Monomer

Characteristics

- Clear water-white liquid
- Equivalent weight – 97.2 gm/equiv.
- 43.2% NCO
- Vapor pressure less than PPDI and TDI
- Vapor pressure higher than NDI, MDI, IPDI and H12MDI

trans-1,4-H6XDI Prepolymers versus PPDI and TODI using 2000 MW Polycaprolactone

		Prepolymer Viscosity (cps) @			
Diisocyanate	% NCO	70°C (158°F)	80°C (176°F)	90°C (194°F)	100°C (212°F)
trans-1,4-H6XDI	7.8	830	570	420	350
PPDI	4.1	2300	1600	1150	950
TODI	6.3	2550	1580	1060	750

Fortimo™ 1,4-H6XDI Prepolymer

Advantages

- Does not sublime like conventional PPDI
- Less reactive with moisture in air
- Less tendency to skin over
- Negligible side reactions to form allophonate crosslinks
- Higher stability at processing temperatures
- Significantly longer shelf life at ambient temperature
- Broader processor base

trans-1,4-H6XDI Prepolymer Processability versus PPDI and TODI

Diisocyanate Prepolymer	Pot Life (minutes)	Demold time (minutes)
trans-1,4-H6XDI	20	>240
PPDI	7	60
TODI	15	90

Prepolymer Temp: 180°F
1,4-Butanediol: Ambient
Mold Temp: 240°F (116°C)
Postcure Conditions: 212°F (100°C) for 16 hours

trans-1,4-H6XDI Prepolymer

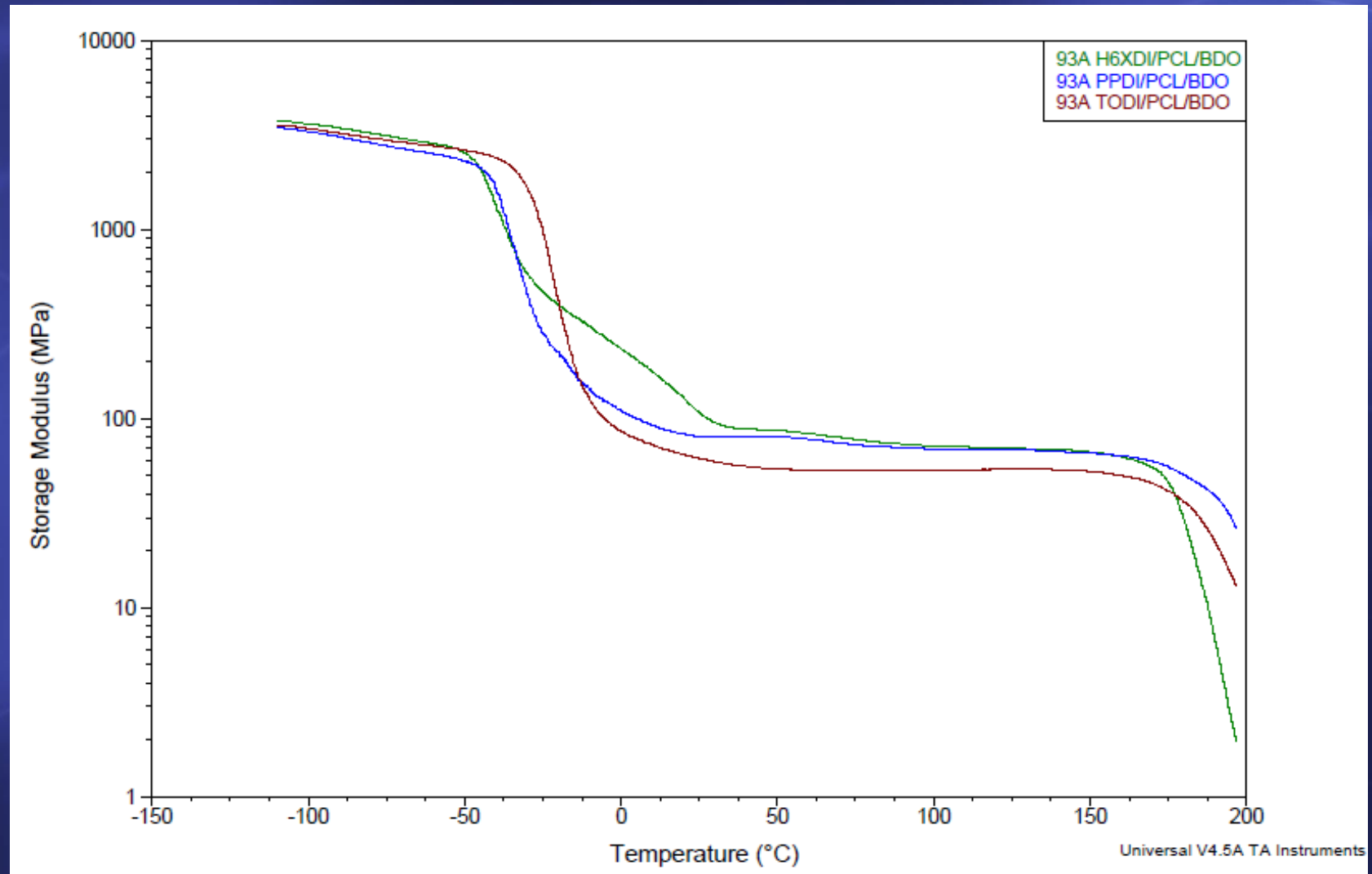
Processability versus PPDI and TODI

Diisocyanate Prepolymer	Catalyst Type	Catalyst Amount (ppm)	Pot Life (minutes)	Demold Time (minutes)
trans-1,4-H6XDI	DBTDL	100	6 to 10	60
		200	3 to 5	40
		300	1.5 to 2.5	20
PPDI	TEDA	200	4 to 6	45
		400	1.5 to 2	30
TODI	TEDA	200	5 to 7	45
		400	2 to 4	30
		800	1.25 to 1.75	15

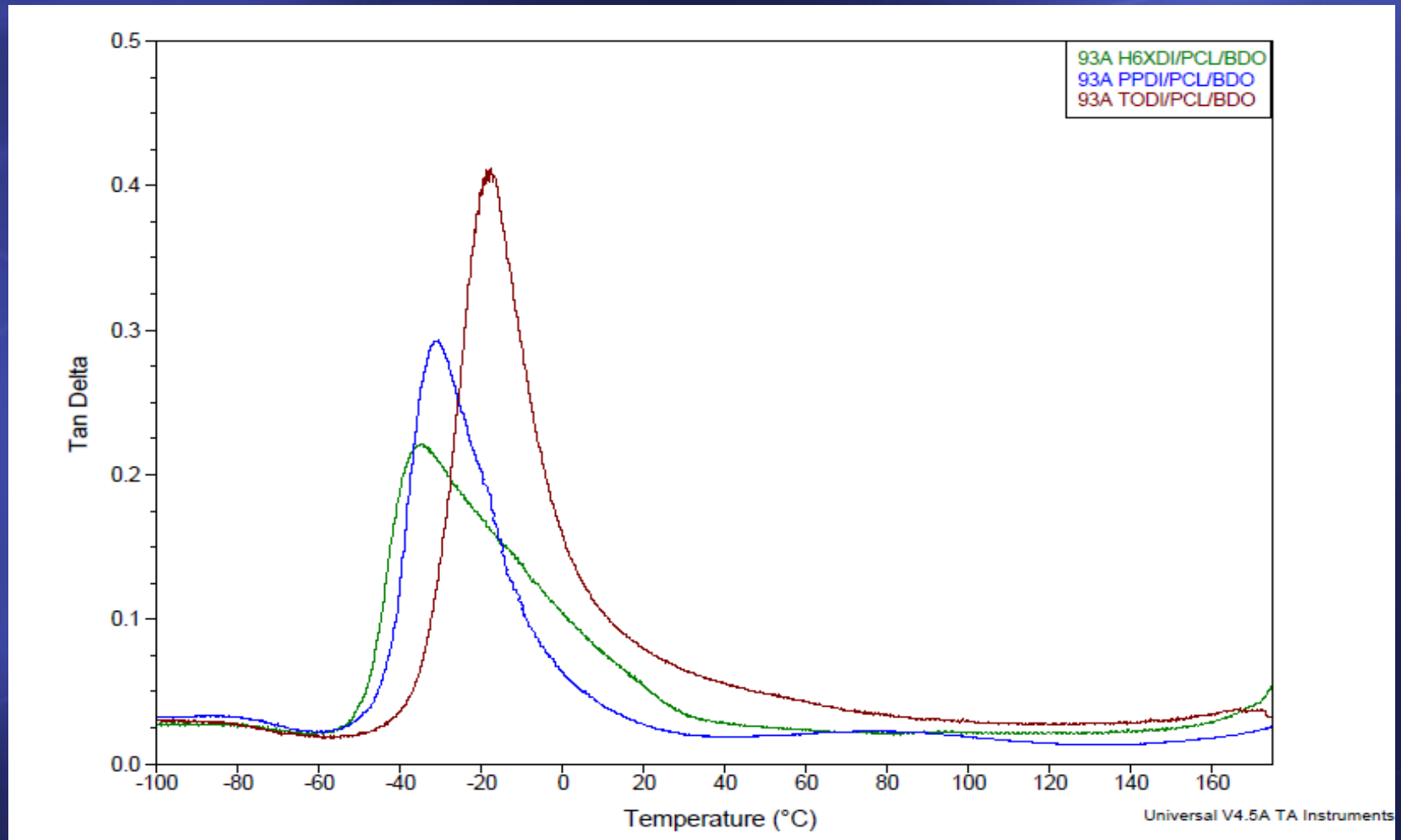
Elastomer Physical/Mechanical Properties: Fortimo™ 1,4-H6XDI versus PPDI and TODI (PCL-2000 Prepolymer; 1,4-BDO Curative)

	trans-1,4-H6XDI	PPDI	TODI
Hardness, Shore	93A	93A	93A
Elongation, %	760	580	650
Tensile Strength, psi (MPa)	7400 (51.0)	6100 (42.1)	5000 (34.4)
Die C Tear, pli (kN/m)	650 (114)	590 (104)	570 (100)
Split Tear, pli (kN/m)	490 (86)	400 (70)	440 (77)
Bashore Rebound, %	68	68	57
Compression Set, % (22 hrs @ 70°C)	28	32	28
Abrasion Resistance, (Volume Loss,mm ³) ASTM D5963	43	32	88

DMA Storage Modulus Curves: trans-1,4-H6XDI versus PPDI and TODI



DMA Tan Delta Curves: trans-1,4-H6XDI versus PPDI and TODI



De mattia Flex Fatigue Tester



<apparatus>

De mattia Flexural tester

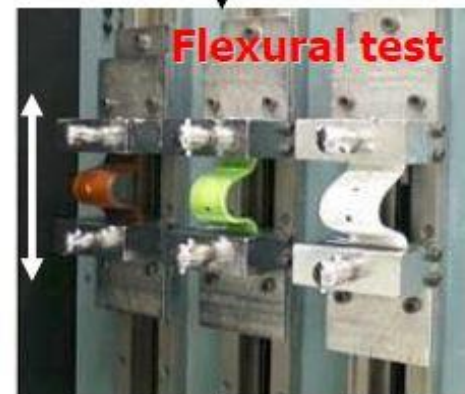
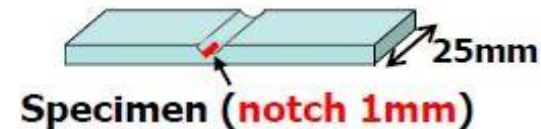
<Test condition>

Tested according to JIS K-7312

Temperature; ambient

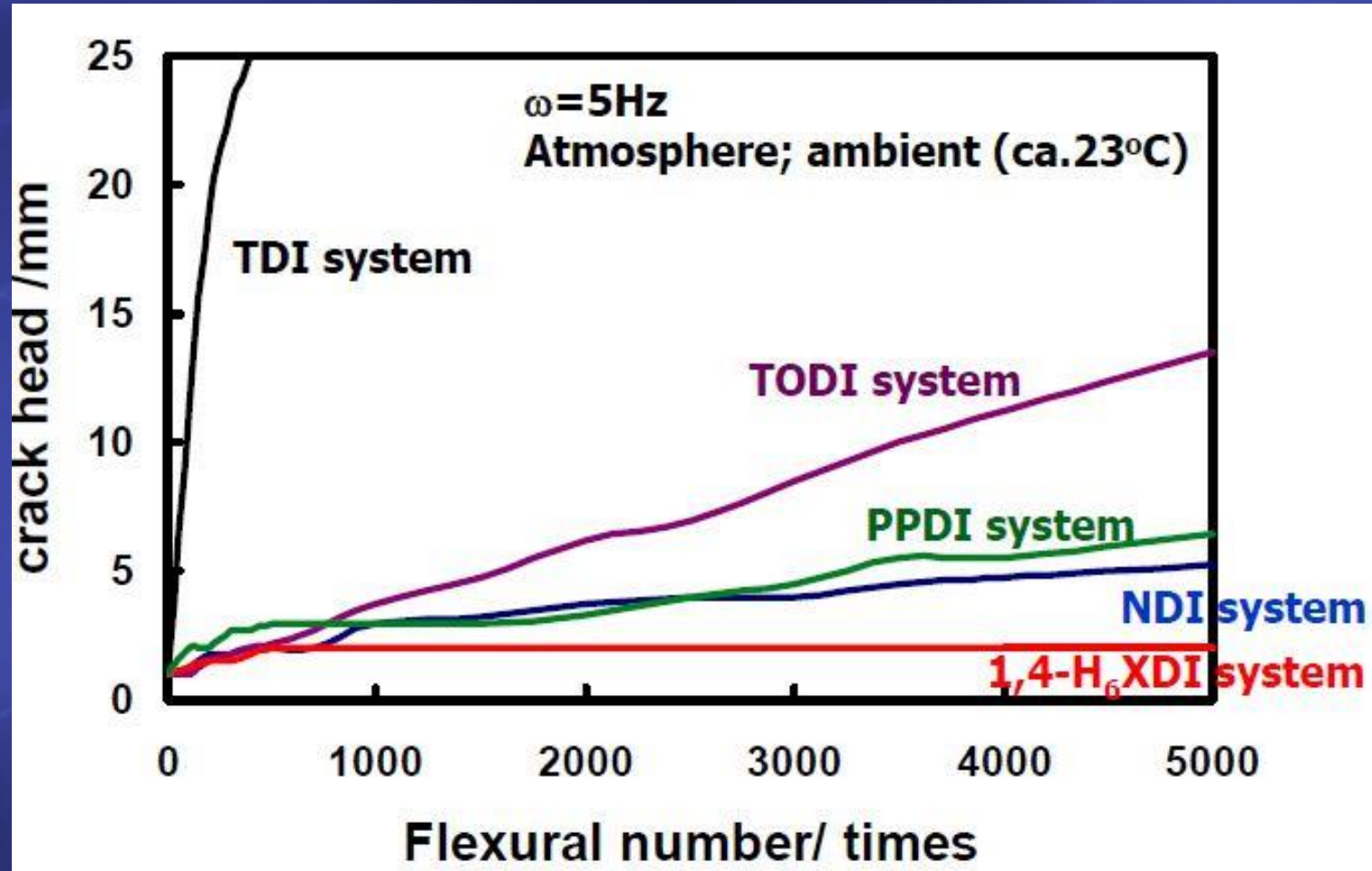
Frequency; 5Hz

Flexural stroke; from 0 to 60 mm



>judged that the durability was good when the crack head was short

De mattia Flex Fatigue Resistance

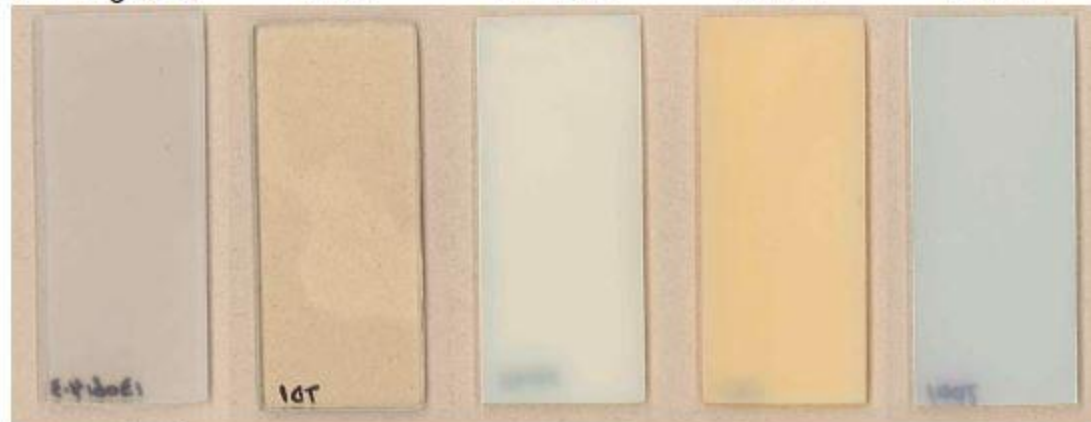


Exposure to UV Light: Yellowing

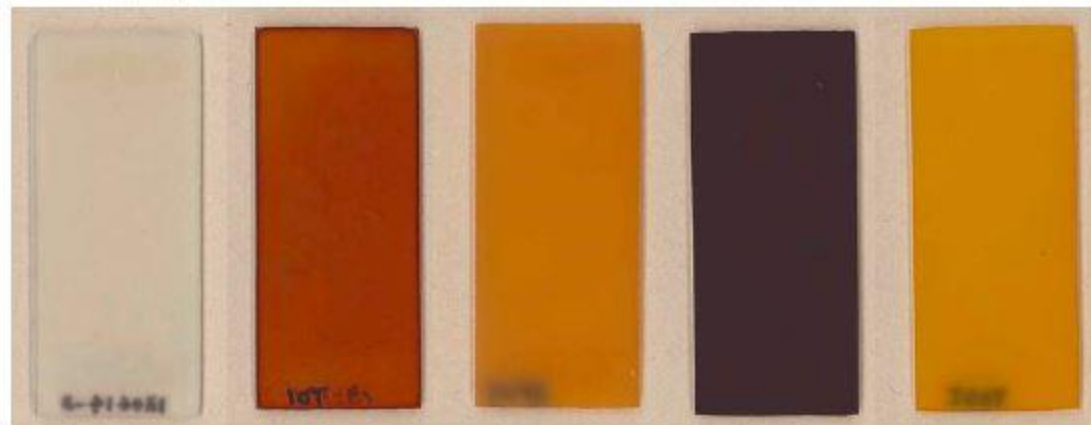
Xe exposure irradiation 100W/m², Black Panel Temperature 89°C, 50%RH
thickness of TSU sheet (specimen) : 2mm (1week)

1,4-H₆XDI TDI PPDI NDI TODI

Appearance
Before testing



Appearance
After testing



trans-1,4-H6XDI Elastomers: Effect of Stoichiometry

Stoichiometry (OH/NCO)	0.91	0.95	0.98
Hardness, Shore	93A	93A	93A
Elongation, %	770	760	750
Tensile Strength, psi (MPa)	7600 (52.4)	7400 (51.0)	6500 (44.8)
Die C Tear, pli (kN/m)	640 (112)	650 (114)	650 (114)
Split Tear, pli (kN/m)	460 (80.7)	490 (86)	520 (91.2)
Bashore Rebound, %	66	68	68
Compression Set, % (22 hrs @ 70°C)	27	28	38

trans-H6XDI/PCL-2000/1,4-BDO Elastomers: Hardness Variation

Hardness, Shore	93A	86A	77A	60A
Elongation, %	760	720	750	630
Tensile Strength, psi (MPa)	7400 (51.0)	5400 (37.2)	4900 (33.7)	3200 (22.0)
Die C Tear, pli (kN/m)	650 (114)	540 (95)	450 (79)	240 (42)
Split Tear, pli (kN/m)	490 (86)	400 (70)	270 (47)	110 (19)
Bashore Rebound, %	68	69	71	80

trans-H6XDI/PTMEG-2000/1,4-BDO

Elastomers: Hardness Variation

Hardness, Shore	95A	85A	80A	72A
Elongation, %	650	760	650	650
Tensile Strength, psi (MPa)	5900 (40.7)	4800 (33.1)	3900 (26.9)	3800 (26.2)
Die C Tear, pli (kN/m)	620 (109)	420 (74)	360 (63)	240 (42)
Split Tear, pli (kN/m)	360 (63)	90 (16)	75 (13)	45 (8)
Bashore Rebound, %	55	72	74	77

Fortimo™ 1,4-H6XDI versus MDI and TDI Elastomer Systems

	H6XDI /PTMEG 1,4-BDO	MDI /PTMEG 1,4-BDO	TDI-80/PTMEG MBOCA
Hardness, Shore	85A	85A	85A
Elongation, %	760	460	580
Tensile Strength, psi (mPa)	4800 (33.1)	3000 (20.7)	5300 (36.6)
Die C Tear, pli (kN/m)	420 (74)	440 (77)	340 (60)
Split Tear, pli (kN/m)	90 (16)	75 (13)	60 (11)
Bashore Rebound, %	72	68	64

Conclusions (1)

- Prepolymers based on trans-1,4-H6XDI opens ultra high-performance elastomers to a broader processor base:
 - Superior stability at processing temperature.
 - Longer shelf life at ambient temperature.

Conclusions (2)

- Elastomers based on Fortimo™ 1,4-H6XDI exhibit ultra high-performance properties.
 - Stress/Strain properties, tear strength, Bashore rebound and abrasion resistance are superior or comparable to PPDI elastomers.
 - trans-1,4-H6XDI elastomers have superior flex fatigue resistance in comparison to PPDI and NDI.
- Fortimo™ 1,4-H6XDI elastomers being aliphatic have excellent light stability (non yellowing).

Acknowledgements

- Mitsui Chemicals
 - Satoshi Yamasaki
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Questions?