

ARON OXETANE

OXT-121 (XDO)

TOAGOSEI CO., LTD.

What's Oxetane ?

ARON OXETANE, 4-membered cyclic ether compounds, are new cationic monomers for UV-curing system developed by TOAGOSEI. With high basicity and ring strain, oxetane compounds show higher ring-opening polymerizability than other cyclic ethers including epoxy compounds.

Although oxetane was recognized as a excellent cationic monomer, few industrial applications had been developed. We paid attention to the potential of oxetane as a new UV-curing monomer and have established industrial manufacturing recently. With its beneficial performances as photo-curable monomer, we believe oxetane helps cationic system broaden its application field.

Benefits of Cationic Curing System

In comparison with conventional radical curing systems, cationic system generally have the following benefits.

- 1. Low Shrinkage → Excellent Adhesion to Substrates and High Gloss
- 2. Low Skin Irritation → High Safety and Easy Handling
- 3. No Oxygen Inhibition → Fast Curing at even Thin Thickness

Benefits of Oxetane

Additionaly, oxetane compounds have the following strong points as photo-cationic monomer, compared with conventional epoxy compounds.

- 1. Rapid Polymerization → High Molecular Weight and Tough Film Property
- 2. Cure Improvement by formulating with Epoxy Compounds
→ High Manufacturing Efficiency, Low Initiator Content Needed
- 3. Not Mutagenic → High Safety
- 4. Few Generation of -OH → Water and Humidity Resistnace, Excellent Electric Properties
- 5. High Stability under High Temperature or Basic Condition → Long Shelf Life

We have been pursuing R&D of Oxetanes for many years and hold wide-ranged patent licences. Please contact us before using oxetanes.

OXT-121 (XDO)

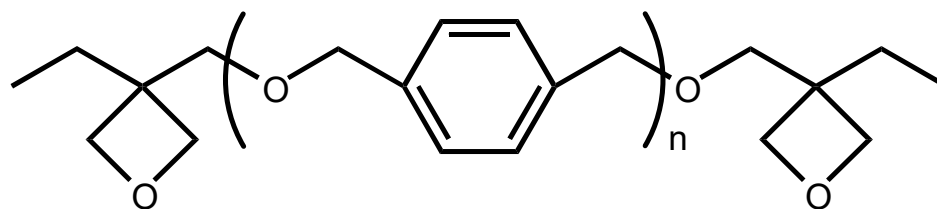
OXT-121 is bifunctional compound having both oxetanyl ring and alcoholic -OH. In cationic systems, appropriate amount of OH function is known to accelerate cure speed by reacting with propagating chain ends (chain transfer). OXT-121 has excellent diluency and cure promoting effects. Films cured with OXT-121 generally show improved thermal and chemical resistance.

Product Name: ARON OXETANE OXT-121(XDO)

Chemical Name: 1,4-Bis{[(3-ethyloxetane-3-yl)methoxy]methyl}benzene

Abbreviated Name: XDO (Xylilene Oxetane)

Chemical Structure:



n=1: 80-90%

n=2: 5-15%

n=3: 0-8%

Purity: >95% Molecular Weight: 334.4(main component)

Appearance: pale yellowish liquid or solid Boiling Point: not available

Freezing Point: 41-44°C Specific Gravity: 1.07 (25°C)

Viscosity: 150-185 mPa·s (25°C) Flash Point: 220°C(OPEN CUP)

Skin Irritation: 2.6(P.I.I.) Ames Test: negative

Chromosomal Aberration Study in Cultured Mammalian Cells: positive

NOEL: ♂: 40mg/kg/day ♀: 250mg/kg/day

CAS No.: 142627-97-2 TSCA Inventory: LVE

EC No.: not included NDSL Inventory: not included

Main Applications: Adhesive, Coatings, Resist

Benefits: high curing response, chemical resistance, electronic property

Test Formulation 1 (OXT-121 / Cycloaliphatic Epoxide)

Formulations with cycloaliphatic epoxide, available as photo-cationic monomer, were investigated and the cured film properties were estimated.

Resin Formulation of OXT-121 / Cycloaliphatic Epoxide

		Fomulation No.			
		1	2	3	4
Formulation	OXT-121(phr)		10	25	50
	Cycloaliphatic Epoxide ³⁾ (phr)	100	90	75	50
	Cationic Photoinitiator ⁴⁾ (phr)	3	3	3	3
	Viscosity ⁵⁾ (mPa.s)	362	334	310	270
For Thin Coated Film ¹⁾	Acetone Extractability ⁶⁾ (%)	14.4	6.7	4.9	7.9
	Pencil Strength	3H-4H	3H	3H	2H
	Adhesion ⁷⁾	100 / 100	100 / 100	97 / 100	77 / 100
	Flexural Test ⁸⁾ 10mm ϕ	-	+	+	+
	2mm ϕ	-	-	+	+
For Thick Coated Film ²⁾	Acetone Extractability ⁶⁾ (%)	30.0	22.4	16.4	7.9
	Tensile Strength ⁹⁾ (kg/cm ²)	43	331	226	297
	Elongation at Break ⁹⁾ (%)	1.0	3.7	2.0	2.3
	Tensile Modulus ⁹⁾ (kg/cm ²)	4,300	9,000	11,300	12,900
	E''max ¹⁰⁾ (°C)	34	46	51	61
	Tan δ max ¹⁰⁾ (°C)	70	86	82	86
	Cross-linking Density ¹⁰⁾ (mol/m ³)	9.2 X 10 ⁴	1.4 X 10 ⁵	2.2 X 10 ⁵	3.6 X 10 ⁵
	Specific Gravity	1.23	1.22	1.20	1.17
	Shrinking with Curing ¹¹⁾ (%)	4.8	4.7	4.5	4.5

1) Coated film thickness = about 10 μ m, Substrate:Chroming steel Al plate, Irradiation condition = 120W metal halide lamp / lamp height 10 cm / conveyer speed 10 m / min., 2) Coated film thickness = 100 μ m, Substrate:OPP film, Irradiation condition = 120W metal halide lamp / lamp height 10 cm / conveyer speed 10 m / min., 3) 3,4-Epoxycyclohexylmethyl-3',4'-epoxycyclohexyl carboxylate(Dow Chemical UVR-6110), 4) Mixed arylsulfonium hexafluorophosphate salts(Dow Chemical UVI-6990), 5) Rotary Viscometer type E at 25°C, 6) Dipped in acetone for one day and dried. Calculation with loss of weight., 7) Cross-cut adhesion test, 8) Flexural test, 9) Tensile speed = 200mm / min. Chuck interval = 100mm., 10) Dynamic modulus measurement: 10 Hz, speed of rising Temp. 4°C / min., 11) Calculation from specific gravity between the cured item and each of the raw materials.

- OXT-121 gives cured film with excellent flexibility and processibility.
- OXT-121 improves cure response and the cured film has excellent chemical resistance.
- OXT-121 gives tough film with high tensile strength.

Test Formulation 2 (OXT-121 / Bisphenol-A Epoxide)

Formulations with bisphenol-A type epoxide, most commonly used as thermosetting resin, were investigated and the cured film properties were estimated.

Resin Formulation of OXT-121 / Bisphenol-A Epoxide

		Formulation No.			
		1	2	3	4
Formulation	OXT-121(phr)		10	25	50
	Bisphenol-A Epoxide ³⁾ (phr)	100	90	75	50
	Cationic Photoinitiator ⁴⁾ (phr)	3	3	3	3
	Viscosity ⁵⁾ (mPa.s)	8,900	5,040	2720	1070
For Thin Coated Film ¹⁾	Pencil Strength	H	H	F	F
	Adhesion ⁶⁾	100 / 100	100 / 100	88 / 100	0 / 100
	Flexural Test ⁷⁾ 10mm ϕ	-	+	+	+
	2mm ϕ	-	-	-	+
For Thick Coated Film ²⁾	Tensile Strength ⁸⁾ (kg/cm ²)	358	324	341	461
	Elongation at Break ⁸⁾ (%)	2.0	2.0	2.0	3.0
	Tensile Modulus ⁸⁾ (kg/cm ²)	17,900	16,200	17,000	15,400
	E''max ⁹⁾ (°C)	64	64	64	64
	Tan δ max ⁹⁾ (°C)	83	77	77	76
	Cross-linking Density ⁹⁾ (mol/m ³)	2.3 X 10 ⁵	2.8 X 10 ⁵	3.1 X 10 ⁵	3.9 X 10 ⁵
	Specific Gravity	1.21	1.19	1.18	1.16
	Shrinking with Curing ¹⁰⁾ (%)	3.1	2.8	3.1	3.4

1) Coated film thickness = about 10 μ m, Substrate:Chroming steel Al plate, Irradiation condition = 120W metal halide lamp / lamp height 10 cm / conveyer speed 10 m / min., 2) Coated film thickness = 100 μ m, Substrate:OPP film, Irradiation condition = 120W metal halide lamp / lamp height 10 cm / conveyer speed 10 m / min., 3) Bisphenol-A diglycidylether(Tohto kasei YD-128), 4) Mixed arylsulfonium hexafluorophosphate salts(Dow Chemical UVI-6990), 5) Rotary Viscometer type E at 25°C, 6) Cross-cut adhesion test, 7) Flexural test, 8) Tensile speed = 200mm / min. Chuck interval = 100mm., 9) Dynamic modulus measurement: 10 Hz, speed of rising Temp. 4°C / min., 10) Calculation from specific gravity between the cured item and each of the raw materials.

- By using OXT-121, it is possible to establish practical cationic formulation including glycidyl ether type epoxide, which has usually poor cationic polymerizability.
- OXT-121 gives cured film with excellent chemical resistance and processibility.

Solubility of Photo-initiator for OXT-121

Sulfonium Salts

Photo-initiator	Solubility
UVI-6992 ¹⁾	>10wt%
SP-150 ²⁾	>10wt%
SP-152 ²⁾	>10wt%

1)Dow Chemical

2)ADEKA

Iodoniumu Salts

Photo-initiator	Solubility
Irgacure 250 ¹⁾	>10wt%
Rhodosil 2074 ²⁾	>10wt%
WPI-113 ³⁾	>10wt%

1)Ciba Speciality Chemicals

2)Rhodia

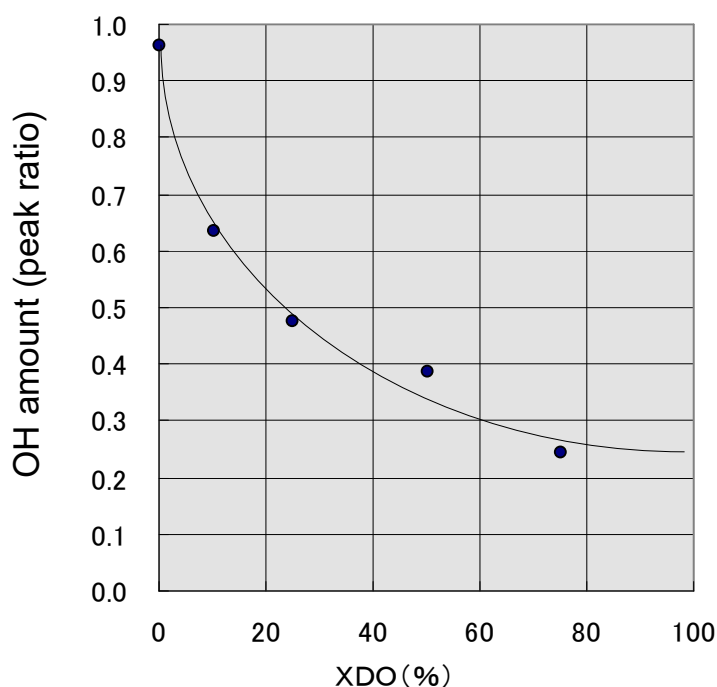
3)Wako Pure Chemical Industries

Solubility of OXT-121 for Solvent

Solvent	Solubility	Solvent	Solubility
Acetone	> 50wt%	Methoxy Propylacetate	> 50wt%
2-Propanol	> 50wt%		
Toluene	> 50wt%	Cyclohexane	> 50wt%

Amount of OH function in Cured Film

As many OH functions are generated in general cationic polymerization, the cured film tends to have poor moisture resistance and insufficient electronic properties. Using OXT-121 decreases OH generation in cationic polymerization, as a result, excellent cured film can be produced. The following graph is the results of the measurement of OH content of cured film by IR spectrum. As seen in this graph, cured film with 80% OXT-121 content has only a quarter of OH amount of reference film (cycloaliphatic epoxide 100%).



Formulation : OXT-121 / Cycloaliphatic epoxide

Irradiation Condition : 120W metal halide lamp, 10m / min. x 2 pass, thickness 10 μ m

Precautions in Handling

Primary Irritation Index (P. I. I.) of OXT-121 is 2.6 which means moderate irritant to skin. Therefore, skin contact of OXT-121 may cause a rash or chemical burn. OXT-121 has highly reactive and may polymerize by heat, light and contamination with a foreign substance. In handling OXT-121, the following precautions should be taken to avoid accidents.

【Handling】

1. Do not handle OXT-121 near fire or heat sources.
2. Use with adequate ventilation. Avoid breathing vapor.
3. Wear appropriate protective equipment such as protective glove, goggle and safety glasses. Avoid direct contact with eyes, skin, mucous membranes and clothing.
4. In case of spilling, wipe up with towel and dispose by incineration or absorb on inert mineral filler and collect in a closed container.
5. Wash hands sufficiently after handling OXT-121.

【First Aid Measures】

1. In case of skin contact, immediately wash with lots of soap and water. Remove contaminated clothing and shoes. Get immediate medical attention if irritates persists after washing.
2. In case of eye contact, immediately flush eyes with lots of running water for at least 15 minutes. Get immediate medical attention.
3. If inhaled, remove to fresh air. If not breathing, give artificial respiration and get medical attention immediately.
4. If swallowed, get immediate medical attention. Do not give anything to an unconscious or convulsing person.

【Storage】

1. Store in a cool dark place in original package.
2. Keep container closed to avoid absorbing moisture.

【Waste Disposal method】

1. Send to a licensed reclaimer or to a permitted incinerator.

For more detailed information about OXT-121, please refer to Safety Data Sheet. Feel free to contact the following address for inquiry or request of samples and related documents.

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