

ARON OXETANE

OXT-121

TOAGOSEI CO., LTD.

What is Oxetane?

Oxetanes, 4-membered cyclic ethers, are new cationic monomers for UV-cure system developed by Toagosei Co.,Ltd. With high basicity and ring strain, oxetane compounds have the highest ring-opening polymerizability among various cyclic ethers including epoxy compounds.

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

Benefits of Cationic System

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

- ①Low Shrinkage → Excellent Adhesion to Substrates, High Gloss
- ②Low Skin Irritation → High Safety and Processibility
- ③No Oxygen Inhibition → Fast Cure even on Thin Film

Benefits of Oxetane

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

- ①Rapid Polymerization → High Molecular Weight and Tough Film Property
- ②Cure Improvement by formulating with Epoxy Compounds
→ High Manufacturing Efficiency, Low Initiator Content needed
- ③Not Mutagenic → High Safety
- ④ No Generation of -OH → Water and Humidity Resistance, 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 licenses. Please contact us before using oxetanes.

OXT-121 (XDO)

XDO is bifunctional oxetane compound having two oxetanyl rings in the molecule. XDO shows excellent cure response in cationic formulations and gives cured film with excellent chemical resistance and electric property.

Product Name: ARON OXETANE OXT-121(XDO)
Chemical Name: 1,4-Bis[(3-ethyl-3-oxetanylmethoxy)methyl]benzene
Abbreviated Name: XDO (Xylilene Oxetane)
Chemical Structure:



n=1	80-85%
n=2	10-15%
n=3	<5%

Purity:	>98%	Appearance:	light yellow liquid or solid
Melting Temperature:	41-44°C	Specific gravity:	1.07 (25°C)
Viscosity:	130-170 mPa·s (25°C)	Flash Point:	220°C
Primary Irritation Index(PII):	2.6	Ames Test:	negative

NOEL=♂ 40mg/kg/day, ♀ 200mg/kg/day

CAS No :	142627-97-2	TSCA Inventory:	not included
EINECS No.:	not included		

Main Application: adhesives, Coatings, resist

Benefits: high cure response, chemical resistance, electronic property

Test Formulation 1 (XDO/Cycloaliphatic Epoxide)

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

Resin Formulation of XDO/Cycloaliphatic Epoxide

	No.	1	2	3	4
Formulation	XDO		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
Formulation characteristics	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	-	+	+	+
Formulation characteristics	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)	4300	9000	11300	12900
	E'' ¹⁰⁾ (°C)	33.7	46.2	50.7	61.1
	tan δ ^{max 10)} (°C)	70.3	85.8	82.4	86.4
	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 1m, Substrate: Chroming steel Al
Irradiation condition = 120W metal halide lamp / lamp height 10cm / conveyer speed 10m/min.
- 2) Coated film thickness = 100 μ m, Substrate: OPP
Irradiation condition = 120W metal halide lamp / lamp height 10cm / conveyer speed 10m/min.
- 3) 3,4-Epoxy cyclohexyl methyl-3,4-
(I.C.C. IIR-6110, Daicel chemical Celloxide 2021P)
- 4) Triallylsulfonium - Hexafluorine salt mixture (UCC UVI-6990, Daicel UCB Uracure)
- 5) Rotary Viscometer type E at 25°C
- 6) Dipped in Acetone for one day and dried. Calculation with loss of
- 7) Cross-cut adhesion
- 8) Flexural test
- 9) Tensile speed = 200m/min. Chuck interval =
- 10) Dynamic modulus measurement: 10Hz, speed of rising 1°C/min.
- 11) Calculation from specific gravity between the cured item and each of the raw

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

Test Formulation 2 (XDO/bisphenol-A Epoxide)

Formulations with conventional bisphenol-A type epoxide were investigated and the cured film properties were estimated.

Resin Formulation of XDO/bisphenol-A Epoxide

		No.	1	2	3	4
Formulation	XDO			10	25	50
	bisphenol-A Epoxide ³⁾	(phr)	100	90	75	50
	Cationic Photoinitiator ⁴⁾	(phr)	3	3	3	3
	Viscosity ⁵⁾	(mPa.s)	8900	5040	2720	1070
Coating	Pencil Strength		H	H	F	F
	Adhesion ⁶⁾		100/100	100/100	88/100	0/100
	Flexural Test ⁷⁾ 10mm ϕ		-	+	+	+
Physical Properties	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)		64.0	64.0	64.0	64.0
	tan δ max ⁹⁾ (°C)		83.0	77.0	77.2	76.0
	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	

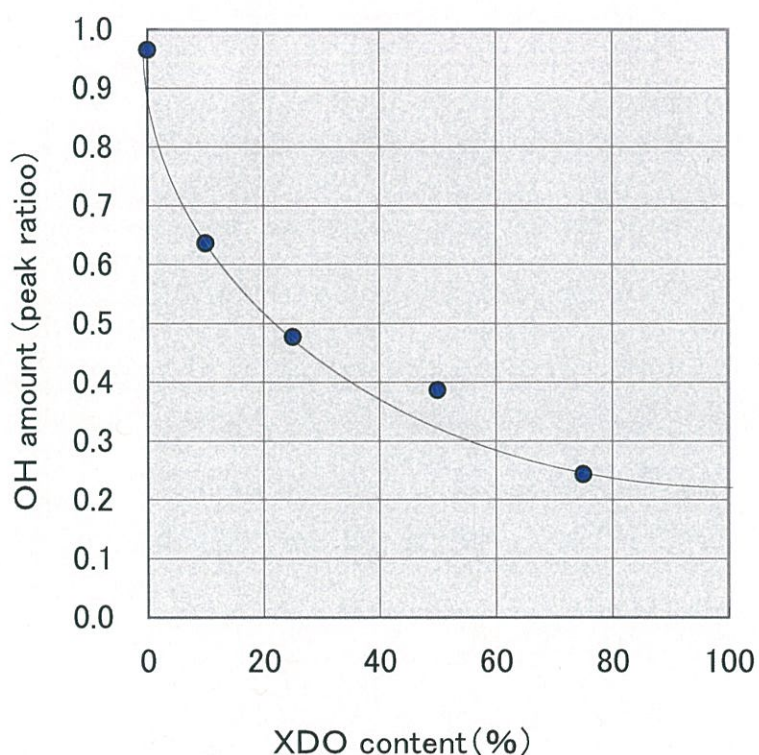
- 1) Coated film thickness = About 100 μ m, Substrate: Chroming steel Al
Irradiation condition = 120W metal halide lamp / lamp height 10cm / conveyer speed 10m/min.
- 2) Coated film thickness = 100 μ m, Substrate: OPP
Irradiation condition = 120W metal halide lamp / lamp height 10cm / conveyer speed 10m/min.
- 3) bisphenol-A diepoxide/epoxy resin Tototasei Y-128
- 4) Triallylsulfonium - Hexafluorine salt mixture (UCC UVI-6990, Daicel UCB Uracure)
- 5) Rotary Viscometer type E at 25°C
- 6) Cross-cut adhesion
- 7) Flexural test
- 8) Tensile speed = 200m/min. Chuck interval = 10mm
- 9) Dynamic modulus measurement: 10Hz, speed of rising 1°C/min.
- 10) Calculation from specific gravity between the cured item and each of the raw materials

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

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 XDO 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% XDO content has only a quarter of OH amount of reference film (cycloaliphatic epoxide 100%).



Formulation : XDO/Cycloaliphatic epoxide

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

Precautions in Handling

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

【Handling】

1. Do not handle XDO near fire or heat sources.
2. Use with adequate ventilation. Avoid breathing vapor.
3. Wear appropriate protective equipment such as protective gloves, goggles, 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 XDO.

【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.
3. Store XDO according to fire-fighting regulations in your country.

【Waste Disposal method】

Send to a licensed reclaimer or to a permitted incinerator.

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

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