

ARON OXETANE

OXT-221 (DOX)

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 an 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

Additionally, 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 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 licences. Please contact us before using oxetanes.

OXT technical report

DOX

OXT-221 (DOX)

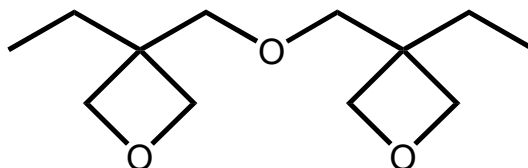
OXT-221 has two oxetanyl functional groups which has polymerization ability. OXT-221 has excellent diluency and cure-promoting effects. OXT-221 has a high degree of cross linking and maintains high elasticity, even above the Tg temperature. Therefore, it is excellent as a chemical resistant coating or heat resistant resin.

Product Name: ARON OXETANE OXT-221 (DOX)

Chemical Name: 3-Ethyl-3- {[(3-ethyloxetane-3-yl)methoxy]methyl} oxetane

Abbreviated Name: DOX (Di Oxetanyl ether)

Chemical Structure:



Purity:	>98%	Molecular Weight:	214.3
Appearance:	clear liquid	Boiling Point:	119°C / 0.67kPa
Freezing Point:	< -20°C	Specific Gravity:	0.999 (25°C)
Viscosity:	12.8 mPa·s (25°C)	Flash Point:	144°C (OPEN CUP)
Skin Irritation:	1.0(P.I.I.)	LD ₅₀ :	300-500mg/kg(oral-rat)
NOEL:	40mg(M), 200mg(F)/kg/day	Ames Test:	negative
CAS No.:	18934-00-4	TSCA Inventory:	included / SNUR
EC No.:	444-140-4(ELINCS)	NDSL Inventory:	included
Main Applications:	Coatings, Inks, Adhesives		
Benefits:	high cross-link, high curing response		

Test Formulation 1 (OXT-221 / Cycloaliphatic Epoxide)

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

Resin Formulation of OXT-221 / Cycloaliphatic Epoxide

		Fomulation No.				
		1	2	3	4	5
Formulation	OXT-221(phr)	0	10	25	50	75
	Cycloaliphatic Epoxide ³⁾ (phr)	100	90	75	50	25
	Cationic Photoinitiator ⁴⁾ (phr)	2	2	2	2	2
	Miscibility	+	+	+	+	+
	Viscosity ⁵⁾ (mPa.s)	360	220	120	51	25
For Thin Coated Film ¹⁾	Pencil Strength	F	H	H	2H	2H
	Adhesion ⁶⁾	100 / 100	100 / 100	100 / 100	100 / 100	100 / 100
	Flexural Test ⁷⁾ 10mm ϕ	-	+	+	+	+
	2mm ϕ	-	-	+	+	+
For Thick Coated Film ²⁾	Acetone Extractability ⁸⁾ (%)	31	23	21	23	16
	Tensile Strength ⁹⁾ (MPa)	5.9	6.4	55	85	86
	Elongation at Break ⁹⁾ (%)	47	30	16	< 3	< 3
	Tensile Modulus ⁹⁾ (MPa)	12	33	600	4,900	5,700
	E''max ¹⁰⁾ (°C)	-5	0	38	51	77
	Tan δ max ¹⁰⁾ (°C)	40	42	63	80	115
	Cross-linking Density ¹⁰⁾ (g/mol)	1.6X10 ⁴	2.4X10 ³	1.2X10 ²	530	83
	Specific Gravity	1.22	1.21	1.18	1.15	1.09
	Shrinking with Curing ¹¹⁾ (%)	4.1	4.5	4.5	5.5	4.6

1) Coated film thickness = about 10 μ m, Substrate:Chroming steel Al plate, Irradiation condition = 120W high press. Mercury lamp / lamp height 10 cm / conveyer speed 10 m / min. 5 pass, 2) Coated film thickness = 200 – 400 μ m, Substrate:PET film, Irradiation condition = 60W high press. Mercury lamp / lamp height 30 cm / 90mW cm², 260sec., 3) 3,4-Epoxycyclohexylmethyl-3',4'-epoxycyclohexyl carboxylate(Dow Chemical UVR-6110), 4) Mixed arylsulfonium hexafluorophosphate salt (Dow Chemical UVI-6990), 5)Rotary Viscometer type E at 25°C, 6) Cross-cut adhesion test, 7) Flexural test, 8) Dipped in acetone for one day and dried. Calculation with loss of weight, 9) Tensile speed = 10mm / min. Chuck interval = 40mm., 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-221 has two oxetanyl functional groups and excellent diluency.
- OXT-221 gives cross-linking density with increasing content.
- OTT-221 has high polymerizability and improves chemical resistance of cured film.

Test Formulation 2 (OXT-221 / 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-221 / Bisphenol-A Epoxide

		Fomulation No.				
		1	2	3	4	5
Formulation	OXT-221(phr)	0	10	25	50	75
	Bisphenol-A Epoxide ³⁾ (phr)	100	90	75	50	25
	Cationic Photoinitiator ⁴⁾ (phr)	2	2	2	2	2
	Miscibility	+	+	+	+	+
	Viscosity ⁵⁾ (mPa.s)	8,900	2,880	790	155	44
For Thin Coated Film ¹⁾	Pencil Strength	H	H	H	2H	2H
	Adhesion ⁶⁾	100 / 100	50 / 100	20 / 100	0 / 100	0 / 100
	Flexural Test ⁷⁾ 10mm ϕ	+	+	+	+	+
	2mm ϕ	+	+	+	+	+
For Thick Coated Film ²⁾	Tensile Strength ⁸⁾ (MPa)	69	43	54	24	22
	Elongation at Break ⁸⁾ (%)	< 3	< 3	< 3	< 3	< 3
	Tensile Modulus ⁸⁾ (MPa)	6,100	7,200	7,000	6,200	3,800
	E''max ⁹⁾ (°C)	76	82	87	90	90
	Tan δ max ⁹⁾ (°C)	97	105	111	107	111
	Shrinking with Curing ⁹⁾ (%)	653	345	234	84	83

1) Coated film thickness = about 10 μ m, Substrate:Chroming steel Al plate, Irradiation condition = 120W high press. Mercury lamp / lamp height 10 cm / conveyer speed 10 m / min. 5 pass, 2) Coated film thickness = 200 – 400 μ m, Substrate:PET film, Irradiation condition = 60W high ppress. Mercury lamp / lamp height 30 cm / 90mW cm², 260sec., 3) Bisphenol-A diglycidylether(Tohto kasei YD-128), 4) Mixed arylsulufoniumu hexafluorophosphate salt (Dow Chemical UVI-6990), 5) Rotary Viscometer type E at 25°C, 6) Cross-cut adhesion test, 7) Flexural test, 8) Tensile speed = 10mm / min. Chuck interval = 40mm., 9) Dynamic modulus measurement: 10 Hz, speed of rising Temp. 4°C / min.

- OXT-221 has two oxetanyl functional groups and excellent diluency.
- OXT-221 gives cross-linking density with increasing content.
- OTT-221 has high polymerizability and improves chemical resistance of cured film.

Solubility of Photo-initiator for OXT-221

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-221 for Solvent

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

Precautions in Handling

OXT-221 is highly reactive and may polymerize by heat, light or contamination with a foreign substance. When handling OXT-221, the following precautions should be taken to avoid accidents.

【Handling】

1. Do not handle OXT-221 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-221.

【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-221, please refer to Material Safety Data Sheet. Feel free to contact the following address for inquiry or request of samples and related documents.

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