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 highest ring-opening polymerizability among various 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-cure 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 System

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

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

Benefits of Oxetane

Additionally, oxetane compounds have the following benefits compared with conventional epoxy compounds.

① Rapid Polymerization → High Molecular Weight, Resilient and Durable Film Properties
② Cure Improvement by formulating with Epoxy Compounds
→ High Manufacturing Efficiency, Low Initiator Content required
③ Not 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 licences. Please contact us before using oxetanes.
**OXT technical report**

**OXT-221 (DOX)**

DOX has two oxetanyl functional groups, with polymerization ability. DOX has excellent diluency and cure promoting effects. DOX 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:** bis[1-Ethyl(3-oxetanyl)]methyl ether

**Abbreviated Name:** DOX (Di Oxetanyl ether)

**Chemical Structure:**

```
  O
 / \
|   |
O---O
```

**Purity:** >98%  
**Molecular Weight:** 214.3

**Appearance:** clear liquid  
**Boiling Temperature:** 119 °C/5 mmHg

**Melting Temperature:** <-20°C  
**Specific Gravity:** 0.999 (25°C)

**Viscosity:** 12.8 mPa·s (25°C)  
**Flash Point:** 144°C (OPEN CUP)

**Primary Irritation Index (PII):** 1.0  
**CAS No.:** 18934-00-4

**Ames Test:** Negative  
**TSCA Inventory:** Now proceeding

**EINECS No.:** Now proceeding(ELINCS)

**Main Applications:** Coatings, Inks, Adhesives

**Benefits:** High cross-link, High cure response
**Test Formulation 1 (DOX/Cycloaliphatic Epoxide)**

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

<table>
<thead>
<tr>
<th>Formation</th>
<th>No.</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>DOX (phr)</td>
<td>0</td>
<td>1.0</td>
<td>2.5</td>
<td>5.0</td>
<td>7.5</td>
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<tr>
<td>Cycloaliphatic Epoxide (phr)</td>
<td>100</td>
<td>9.0</td>
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<td>5.0</td>
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<tr>
<td>Cationic Photoinitiator (phr)</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>2</td>
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<tr>
<td>Miscibility (mPs·s)</td>
<td>360</td>
<td>220</td>
<td>120</td>
<td>51</td>
<td>25</td>
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<tr>
<td>Viscosity (mPs·s)</td>
<td></td>
<td></td>
<td></td>
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</table>

For Thin coated film:

<table>
<thead>
<tr>
<th>Pencil Strength Adhesion (×/×) 100/100</th>
<th>H</th>
<th>H</th>
<th>2H</th>
<th>2H</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flexural Test 10mm φ</td>
<td>×</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Flexural Test 2mm φ</td>
<td>×</td>
<td></td>
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For Thick coated film:

<table>
<thead>
<tr>
<th>Acetone Extractability (%)</th>
<th>31</th>
<th>23</th>
<th>21</th>
<th>23</th>
<th>16</th>
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<tr>
<td>Tensile Strength (MPa)</td>
<td>5.9</td>
<td>6.4</td>
<td>5.4</td>
<td>5.8</td>
<td>6.0</td>
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<tr>
<td>Elongation at Break (%)</td>
<td>4.7</td>
<td>3.0</td>
<td>1.6</td>
<td>&lt;3</td>
<td>&lt;3</td>
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<tr>
<td>Tensile Modulus (MPa)</td>
<td>1.23</td>
<td>3.28</td>
<td>6.00</td>
<td>4.870</td>
<td>5.700</td>
</tr>
<tr>
<td>E′ max (°C)</td>
<td>-5</td>
<td>0</td>
<td>3.8</td>
<td>5.1</td>
<td>7.7</td>
</tr>
<tr>
<td>tan δ max (°C)</td>
<td>4.0</td>
<td>4.2</td>
<td>6.3</td>
<td>8.0</td>
<td>1.15</td>
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<tr>
<td>Cross-linking Density (g/mol)</td>
<td>1.6×10⁴</td>
<td>2.4×10³</td>
<td>1.2×10²</td>
<td>5.30</td>
<td>8.3</td>
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<tr>
<td>Specific Gravity (%)</td>
<td>1.22</td>
<td>1.21</td>
<td>1.18</td>
<td>1.15</td>
<td>1.09</td>
</tr>
<tr>
<td>Shrinking with Curing (%)</td>
<td>4.1</td>
<td>4.5</td>
<td>4.5</td>
<td>5.5</td>
<td>4.6</td>
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</tbody>
</table>

1) Coated film thickness = About 10 μm, Substrate: Chroming steel Al plate
   Irradiation condition = 120W high press. mercury lamp / lamp height 10cm / conveyor speed 10m/min. 5 pass
2) Coated film thickness = 200-400 μm, Substrate: PET film
   Irradiation condition = 60W high press. mercury lamp / lamp height 30cm / 90mW/cm², 260sec
3) 3,4-Epoxydicyclohexylmethyl-3,4-Epoxydicyclohexylcarboxylate (DOW UVR 6110, Daicel Chemical Cellosolve 2021p)
4) Triaryl-sulfonium - Hexafluorine salt mixture (DOW UVI-6990, Daicel UC8 Ureacure 1591, Lamberti Esacure1064)
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 = 10mm/min. Chuck interval = 40mm
10) Dynamic modulus measurement: 10Hz, Speed on rising temp.: 4 °C/min
11) Calculation from specific gravity between the cured item and each of the raw materials.

- DOX has two oxetanyl function and excellent diluency.
- DOX gives high cross-linking density with increasing content.
- DOX has high polymerizability and improves chemical resistance of cured film.
Test Formulation 2 (DOX/Bisphenol-A Epoxide)

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

<table>
<thead>
<tr>
<th>Formation</th>
<th>No.</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
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</thead>
<tbody>
<tr>
<td>DOX</td>
<td>(phr)</td>
<td>0</td>
<td>10</td>
<td>25</td>
<td>50</td>
<td>75</td>
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<tr>
<td>Bisphenol-A Epoxide</td>
<td>(phr)</td>
<td>100</td>
<td>90</td>
<td>75</td>
<td>50</td>
<td>25</td>
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<tr>
<td>Cationic Photoinitiator</td>
<td>(phr)</td>
<td>2</td>
<td>2</td>
<td>2</td>
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<td>Miscibility</td>
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<tr>
<td>Viscosity</td>
<td>(mPa·s)</td>
<td>8,900</td>
<td>2,880</td>
<td>790</td>
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<tr>
<td>Pencil Strength</td>
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<td>H</td>
<td>H</td>
<td>2H</td>
<td>2H</td>
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<tr>
<td>Adhesion</td>
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<td>2mm</td>
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<tr>
<td>Tensile Strength</td>
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<td>6.9</td>
<td>4.3</td>
<td>1</td>
<td>5.3</td>
<td>6</td>
</tr>
<tr>
<td>Elongation at Break</td>
<td>(%)</td>
<td>&lt;3</td>
<td>&lt;3</td>
<td>&lt;3</td>
<td>&lt;3</td>
<td>&lt;3</td>
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<tr>
<td>Tensile Modulus</td>
<td>(MPa)</td>
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<td>7.22</td>
<td>6.96</td>
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<tr>
<td>For Thick coated film</td>
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<td></td>
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<tr>
<td>E' max</td>
<td>(°C)</td>
<td>76</td>
<td>82</td>
<td>87</td>
<td>90</td>
<td>90</td>
</tr>
<tr>
<td>tan δ max</td>
<td>(°C)</td>
<td>97</td>
<td>105</td>
<td>111</td>
<td>107</td>
<td>111</td>
</tr>
<tr>
<td>Cross-linking Density</td>
<td>(g/mol)</td>
<td>6.53</td>
<td>3.45</td>
<td>2.34</td>
<td>8.4</td>
<td>8.3</td>
</tr>
</tbody>
</table>

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- DOX has two oxetanyl function and excellent diluency.
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- DOX has high polymerizability and improves chemical resistance of cured film.
Precautions in Handling

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

[Handling]
1. Do not handle DOX 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 DOX.

[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 eye with lots of running water for at least 15 minutes. Get immediate medical attention.
3. If inhaled, remove person 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 packaging.
2. Keep container closed to avoid absorbing moisture.

[Waste Disposal method]
Send to a licensed reclaimor or to a permitted incinerator.

For more detailed information about DOX, 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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1-14-1, Nishi-Shinbashl, Minato-ku, Tokyo, JAPAN
TEL: 03-3597-7332  FAX: 03-3597-7380