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Silane Coupling Agents
Combination of Organic and Inorganic Materials

"Silicon-Etzu Silicone" is a registered trademark of Shin-Etsu Chemical Co., Ltd.

This is an edited version of the product data released on Oct. 2023.

https://www.shinetsusilicone-global.com/guide/

Our diverse array of materials enable users to enhance the quality and functionality of their products, and expand the possibilities for new product development.

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**What are Silane Coupling Agents?**
Silane coupling agents are compounds whose molecules contain functional groups that bond with both organic and inorganic materials. A silane coupling agent acts as a sort of intermediary which bonds organic materials to inorganic materials. It is this characteristic that makes silane coupling agents useful for improving the mechanical strength of composite materials, for improving adhesion, and for resin modification and surface modification.

**Features of Hydrolyzable Silyl Groups**
- **Methoxy type**: Hydrolyzes rapidly. Ethoxy type: Hydrolyzes slowly, and compositions will be highly stable even after addition. This type is more eco-friendly, because the product of hydrolysis is ethanol.
- Dialkoxy type: Good stability after hydrolysis. Condensation products form straight-chain structures.
- Trialkoxy type: High reactivity with high crosslinking density. Strong bonding with inorganic materials.

**Features of Shin-Etsu Silane Coupling Agents**
In addition to general-purpose trimethoxy types, Shin-Etsu offers a wide range of dialkoxy and ethoxy type products. We are also developing products with an emphasis on the following:

1. **High Functionality**
   - Improved adhesion
   - Hydrophobicity
   - Flexibility
   - Compatibility
   - Anti-rust property

2. **Eco-friendly**
   - Reduced VOC
   - Low Volatile Content

3. **Usability**
   - One-component products can be used in place of two-component products
   - Eliminate the step of hydrolysis
   - Excellent storage stability
Our diverse array of materials enable users to enhance the quality and functionality of their products, and expand the possibilities for new product development.

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   - Eliminate the step of hydrolysis
   - Excellent storage stability
4 Types of Silane Coupling Agents Application

**Compound**

- **Model of Unifying Organic Resins and Fillers**
  - Untreated with Silane Coupling Agents
    - The organic resin and filler do not fully combine, so properties do not improve as expected.
  - Treated with Silane Coupling Agents
    - Organic resin and filler bond together, resulting in improved heat resistance, weatherability, moisture resistance, etc.

- **Application Examples**
  - Crosslinked polyethylene (Electrical wire covering)
  - Phenolic resins, grinders, moldings
  - Artificial marble wall materials
  - SBR (tires), rubbers
  - Epoxy Resins (EWC)

**Resulting Properties**
- Heat resistance
- Weatherability
- Water resistance
- Improved durability of resins

**Coating**

- **Model of Improved Adhesion**

- **Application Examples**
  - Adhesives
  - Films
  - Paints & Inks

**Resulting Properties**
- Adhesion
- Water resistance
- Alkali resistance

**Resin Modification**

- **Surface Treatment**

**Filler**

- **Model of Filler Surface Treatment**

- **Application Examples**
  - Inorganic pigments
  - TiC
  - Aluminium hydroxide
  - Titanium oxide
  - Silica

**Resulting Properties**
- Dispersibility
- Hydrophobicity
- Flowability
- High loading

**Inorganic Substrate**

- **Model of Surface Treatment of Inorganic Substrate**

- **Application Examples**
  - Copper foil
  - Steel plate
  - Glass
  - Glass fiber

- **Resulting Properties**
  - Anti-rust property
  - Water resistance
  - Adhesion

- **Model of Interface**
  - Organic functional groups

- **Model of Interface**
  - Organic functional groups
4 Types of Silane Coupling Agents Application

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**Resulting Properties**
- Heat resistance
- Weatherability
- Water resistance
- Improved durability of resins

**Application Examples**
- Crosslinked polyethylene (Electrical wire covering)
- Phenolic resins (grinders, moldings)
- Artificial marble wall materials
- SBR (tires, rubbers)
- Epoxy Resins (EWC)

**Filler**
- **Model of Filler Surface Treatment**
  - Before treatment
  - After treatment
  - Application Examples
    - Inorganic pigments
    - Talc
    - Aluminium hydroxide
    - Titanium oxide
    - Silica

**Surface Treatment**
- Treating a filler material with a silane coupling agent allows the filler and resin to bond together.

**Coating**
- **Model of Improved Adhesion**
  - Application Examples
    - Adhesives
    - Films
    - Paints & Inks
    - Resist
    - Hard coatings

**Resulting Properties**
- Adhesion
- Water resistance
- Alkali resistance

**Inorganic Substrate**
- **Model of Surface Treatment of Inorganic Substrate**
  - Application Examples
    - Copper foil
    - Steel plate
    - Glass
    - Glass fiber

**Resin Modification**
Silane Coupling Agents Usage

Adding into Compound

- Integral blending method
  - In this method, the silane coupling agent is added to the organic materials before the inorganic and organic materials are mixed.

- Application Example of EMC (Epoxy Molding Compound)
  - Epoxide & curing agents
  - Fillers
  - Additives (e.g., wax)
  - Catalysts
  - Pigments

  - Slime couplng agents

  - Mixing
  - Kneading
  - Cooling
  - Grinding
  - Making tablet

  - EMC tablet

Resulting Properties
- Water resistance
- Moisture resistance
- Durability

Adding into Coating

- Adding into Epoxy Paints
  - Improving anticorrosion property

  - Epoxy resin
  - Pigment
  - Filler
  - Solvent

  - Silane (e.g., KMB-403) addition

  - Stirring

Resulting Property
- Anticorrosion property
- Improved adhesion with substrate

- Model of Resin Modification

  - Acrylic resin
  - Improving adhesion

  - Silicone Modified Acrylic Resin (nonvolatile content: about 50 wt%)

Resulting Properties
- Adhesion
- Weatherability
- High cross-linking

Resin Modification

- Surface Treatment with Wet Method
  - Features:
    - Enables even treatment
    - Productivity is low.
    - Silane-containing waste fluid must be disposed of.

- Application Example of Cross-linked Polyethylene
  - Slime Grafted Polyethylene

  - High density polyethylene
  - Peroxide
  - KMB-1003

  - Heating & Mixing

- Slime grafted polyethylene
  - Curing agent masterbatch

  - Mixing
  - Molding

  - Process: 100°C for 3h

  - Cross-linked polyethylene

  - Electrical wire covering

Kneading

Surface Treatment

- Resulting Property
  - Dispersibility
  - Adhesion with Resins

Filler Surface Treatment

- Surface Treatment with Dry Method
  - Features:
    - Productivity is high.
    - Clumping may occur in some cases.

- Preparation Method of Hydrolzed Liquid
  - Use of slime coupling agents when producing acrylic resins (copolymerization)

  - Example: Using a slime coupling agent (KMB-503) to modify acrylic resins via radical copolymerization.

  - Improves adhesion to the substrate and moisture resistance.

- Water Type

  - MMA**-BMA** etc.

  - Total about 50 wt%

  - KMB-503

  - Water

  - Polymerization initiator-surfactant

  - 1-6 wt%

- Solvent Type

  - MMA**-BMA** etc.

  - Total about 50 wt%

  - KMB-503

  - Solvent

  - Polymerization initiator

  - 1-2 wt%

- Solvent

- Reaction

- Silicone Modified Acrylic Emulsion

  - Nonvolatile content: about 50 wt%

- Silicone Modified Acrylic Resin

  - Nonvolatile content: about 50 wt%

- Preparation of hydrolyzed liquid

  - Adjust pH of aqueous solution (alcohol can be used in mix)

  - While stirring, gradually drop in slime coupling agent (0.1-3.0 wt%)

  - Stir until solution is clear (around 30-60 min)

  - Filter with a mesh filter to remove foreign matter if present.

- Treating the substrate

  - Wash the substrate.

  - Treat with the hydrolyzed liquid (brush on, dip, etc.)

  - Dry (at room temp. or by heating)

- Resulting Property

  - Adhesion with Resins

  - Mechanical strength of molding

Primer Treatment

- Glass Cloth Application Example

- Production process of glass fiber

  - Heating

  - Drying

- Production process of glass cloth

  - Hydrolized water solution of slime coupling agent

  - Slime coupling agents was completed.
Silane Coupling Agents Usage

Adding into Compound

- **Integrating blending method**: In this method, the silane coupling agent is added to the organic materials before the inorganic and organic materials are mixed.

  - **Application Example of EMC (Epoxy Molding Compound)**
    - Mixing
    - Kneading
    - Cooling
    - Grinding
    - Making tablet

  - **Slane coupling agents**
    - Epoxy & Curing agents
    - Fillers
    - Additives (i.e. wax)
    - Catalysts
    - Pigments

  - **Resulting Properties**
    - Water resistance
    - Moisture resistance
    - Durability

Adding into Coating

- **Adding into Epoxy Paints** (Improving anticorrosion property)
  - Epoxy resin
  - Pigment
  - Filler
  - Solvent
  - Silane (i.e. KMB-403) adding
  - Stiring
  - Final product

  - **Resulting Property**
    - Anticorrosion property
    - Improved adhesion with substrate

  - **Model of Resin Modification**
    - Acrylic resin
  - Improving adhesion

- **Application Example for Paints**
  - Use of silane coupling agents when producing acrylic resins (copolymerization).
  - Example: Using a silane coupling agent (KMB-503) to modify acrylic resins via radical polymerization.
  - Improves adhesion to the substrate and moisture resistance.

  - **Water Type**
    - MMA®-GMA® Mixed Total about 50 wt%
    - KMB-503
    - Water
    - Polymerization initiator-surfactant: 1-5 wt%

  - **Solvent Type**
    - MMA®-GMA® Mixed Total about 50 wt%
    - KMB-503
    - Solvent
    - Polymerization initiator: 1-2 wt%

  - **Reaction**
    - Silicone Modified Acrylic Emulsion (Non-volatile content : about 50 wt%)

- **Resulting Properties**
  - Adhesion
  - Weatherability
  - High cross-linking

Resin Modification / Surface Treatment

- **Surface Treatment with Wet Method**
  - Features:
    - Enables even treatment
    - Productivity is low.
    - Silane-containing waste fluid must be disposed of.

  - **Preparation Method of Hydrolyzed Liquid**
    - Adjust pH of aqueous solution (alcohol can be used in mix)

  - **While stirring, gradually drop in silane coupling agent (0.1-3.0 wt%)**

  - **Stir until solution is clear (around 30-60 min)**

  - **Filter with a mesh filter to remove foreign matter if present**

  - **Treating the substrate**
    - Wash the substrate.
    - Treat with the hydrolyzed liquid (Brush on, dip, etc.).
    - Dry (at room temp. or by heating)

  - **Resulting Property**
    - Adhesion with Resins (Mechanical strength of molding)

Primer Treatment

- **Glass Cloth Application Example**
  - Preparation process of glass fiber
  - Production process of glass cloth
  - Hydrolyzed water solution of silane coupling agent
  - Production of glass fiber treated with silane coupling agents was completed.

Filler Surface Treatment

- **Surface Treatment with Dry Method**
  - Features:
    - Productivity is high.
    - Clumping may occur in some cases.

  - **Preparation**
    - Fillers, solvents

  - **Dipping (Lower room temperature)**
    - Slane concentrate or Hydrolyzed solution

  - **Filtering**
    - Liquid waste disposal

  - **Drying 100-150°C**
    - Filtered

  - **Sinter**
    - Typical amounts for treatment Slane: 0.5-1.0 wt% (vs. filler weight)

  - **Resulting Properties**
    - Dispersibility - Adhesion with Resins

  - **Priming process**
    - Slane concentrate or Hydrolyzed solution
**Reaction Mechanism of Silane Coupling Agents**

### Reaction Examples of Organic Functional Groups

<table>
<thead>
<tr>
<th>Functional group</th>
<th>Reacting group</th>
<th>Reaction product</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Epoxy group</strong></td>
<td>H2N-</td>
<td>Epoxide ring-opening reaction</td>
</tr>
<tr>
<td></td>
<td>HO-</td>
<td>Epoxide ring-opening reaction</td>
</tr>
<tr>
<td><strong>Amino group</strong></td>
<td>Cl-</td>
<td>Dehydrochlorination reaction</td>
</tr>
<tr>
<td></td>
<td>C1OC-</td>
<td>Amination reaction</td>
</tr>
<tr>
<td><strong>Isocyanate group</strong></td>
<td>NCO</td>
<td>Ureidation reaction</td>
</tr>
<tr>
<td></td>
<td>H2O-</td>
<td>Urethamation reaction</td>
</tr>
<tr>
<td><strong>Mercapto group</strong></td>
<td>SH</td>
<td>Thioethenation reaction</td>
</tr>
<tr>
<td></td>
<td>HOOC-</td>
<td>Epoxide ring-opening reaction</td>
</tr>
<tr>
<td></td>
<td>HOOC-</td>
<td>Epoxide ring-opening reaction</td>
</tr>
</tbody>
</table>

- **Vinyl group**: Grafting reaction
- **Methylacrylate group**: Copolymerization

### Organic Functional Groups and Compatible Resins

<table>
<thead>
<tr>
<th>Resin</th>
<th>Thermoplastic resins</th>
<th>Thermosetting resins</th>
<th>Elastomer-Rubber</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vinyl</td>
<td>+ + + + + + + + + +</td>
<td>+ + + + + + + + + +</td>
<td>+ + + + + + + + + +</td>
</tr>
<tr>
<td>Epoxy</td>
<td>+ + + + + + + + + +</td>
<td>+ + + + + + + + + +</td>
<td>+ + + + + + + + + +</td>
</tr>
<tr>
<td>Styrene</td>
<td>+ + + + + + + + + +</td>
<td>+ + + + + + + + + +</td>
<td>+ + + + + + + + + +</td>
</tr>
<tr>
<td>Methacryloyl</td>
<td>+ + + + + + + + + +</td>
<td>+ + + + + + + + + +</td>
<td>+ + + + + + + + + +</td>
</tr>
<tr>
<td>Acryloyl</td>
<td>+ + + + + + + + + +</td>
<td>+ + + + + + + + + +</td>
<td>+ + + + + + + + + +</td>
</tr>
<tr>
<td>Amino</td>
<td>+ + + + + + + + + +</td>
<td>+ + + + + + + + + +</td>
<td>+ + + + + + + + + +</td>
</tr>
<tr>
<td>Ureide</td>
<td>+ + + + + + + + + +</td>
<td>+ + + + + + + + + +</td>
<td>+ + + + + + + + + +</td>
</tr>
<tr>
<td>Mercapto</td>
<td>+ + + + + + + + + +</td>
<td>+ + + + + + + + + +</td>
<td>+ + + + + + + + + +</td>
</tr>
<tr>
<td>Isocyanate</td>
<td>+ + + + + + + + + +</td>
<td>+ + + + + + + + + +</td>
<td>+ + + + + + + + + +</td>
</tr>
</tbody>
</table>

*Very effective / Effective
*Not all the functional groups are capable of coupling with the resins in question. This should be taken as a guide.

### Hydrolytic Properties of Alkoxy Groups

Generally speaking, methoxy groups (OCMe3) have higher reactivity than ethoxy groups (OC2H5). In acidic conditions, fewer alkoxy groups will mean a faster reaction, which means that dimethoxy will hydrolyze fastest, followed in order by the trimethoxy, diethoxy and triethoxy types. By contrast, in basic conditions, the order goes from the trimethoxy to the dimethoxy, diethoxy and diethoxy types.

### Types of Inorganic Materials and Reactivity of Silanol

Alkoxy groups hydrolyze to form silanols, which hydrogen-bond to hydroxyls on the surface of inorganic substrates. Typically, Silane coupling agents react more easily with inorganic materials having larger numbers of active hydroxy groups on their surfaces.

<table>
<thead>
<tr>
<th>Numbers of Hydroxyl Group on the Surface</th>
<th>Reactivity</th>
<th>Inorganic material</th>
</tr>
</thead>
<tbody>
<tr>
<td>Large</td>
<td>High</td>
<td>Glass, Silica, Alumina</td>
</tr>
<tr>
<td>Small</td>
<td>Low</td>
<td>Bismuth oxide, Talc, Clay, Micromica, Aluminum Iron, Titanium oxide, Zinc oxide, Iron oxide, Graphite, Carbon black, Calcium carbonate</td>
</tr>
</tbody>
</table>
Reaction Mechanism of Silane Coupling Agents

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<td>Episode ring-opening reaction</td>
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</tr>
<tr>
<td>HO=</td>
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<td></td>
</tr>
<tr>
<td>HODC=</td>
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</tr>
<tr>
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<td>Dehydrochlorination reaction</td>
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</tr>
<tr>
<td>ODC=</td>
<td>Amidation reaction</td>
<td></td>
</tr>
<tr>
<td>OCN=</td>
<td>Episode ring-opening reaction</td>
<td></td>
</tr>
<tr>
<td>HO=</td>
<td>Hydrogen bonding with hydroxyl groups</td>
<td></td>
</tr>
<tr>
<td>HN=</td>
<td>Hydrogen bonding with amino groups</td>
<td></td>
</tr>
<tr>
<td>HO=</td>
<td>Hydrogen bonding with hydroxyl groups</td>
<td></td>
</tr>
<tr>
<td>HOSO=</td>
<td>Salt formed with sulfonic acid</td>
<td></td>
</tr>
<tr>
<td>HODC=</td>
<td>Salt formed with carboxylic acid</td>
<td></td>
</tr>
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</tr>
<tr>
<td>Vinyl</td>
<td>++ +</td>
<td>++ +</td>
<td>++ ++</td>
</tr>
<tr>
<td>Epoxy</td>
<td>++ + ++</td>
<td>++ + ++</td>
<td>++ ++ ++ ++ ++</td>
</tr>
<tr>
<td>Styrene</td>
<td>++ + ++</td>
<td>++ ++ ++ ++ ++ ++ +</td>
<td></td>
</tr>
<tr>
<td>Methacryloyx</td>
<td>++ ++ ++ ++ ++ ++ +</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Acryloyx</td>
<td>++ + ++ ++ ++ ++ ++</td>
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</tr>
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<td>Amino</td>
<td>++ ++ ++ ++ + ++ ++</td>
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<tr>
<td>Isocyanate</td>
<td>++ ++ ++ ++ ++ ++</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*Note: Not all functional groups are capable of coupling with the resins in question. This should be taken as a guide.

### Hydrolytic Properties of Alkoxy Groups

Generally speaking, methoxy groups (OCMe3) have higher reactivity than ethoxy groups (OC2H5). In acidic conditions, fewer alkoxy groups will mean a faster reaction, which means that dimethoxy types will hydrolyze fastest, followed in order by the trimethoxy, diethoxy and triethoxy types. By contrast, in basic conditions, the order goes from the trimethoxy to the dimethoxy, diethoxy and triethoxy types.

### Types of Inorganic Materials and Reactivity of Silanol

Alkoxy groups hydrolyze to form silanols, which hydrogen-bond to hydroxyls on the surface of inorganic substrates. Typically, Silane coupling agents react more easily with inorganic materials having larger numbers of active hydroxyl groups on their surface.

#### Numbers of Hydroxyl Group on the Surface

- Large
- Small

#### Reactivity

- High
- Low

#### Inorganic material

- Glass
- Silica
- Alumina
- Talc
- Clay
- Mica
- Aluminum
- Iron
- Titanium oxide
- Zinc oxide
- Iron oxide
- Graphite
- Carbon black
- Calcium carbonate

---

* Images and diagrams are not translated and are intended for visual representation only.*
### Main Products Lineup

#### Product List

<table>
<thead>
<tr>
<th>Functional group</th>
<th>Product name</th>
<th>Chemical name</th>
<th>Structural formula</th>
<th>Flash point (°C)</th>
<th>Minimum covering area (m²/g)</th>
<th>Solubility parameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vinyl</td>
<td>KBM-1003</td>
<td>Vinyltrimethoxysilane</td>
<td>(CH₃OH)₂Si(CH₃)₂OH</td>
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<td>526</td>
<td>7.49</td>
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<td></td>
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<td>8.59</td>
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<td>335</td>
<td>8.53</td>
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<td>3-Methacryloxypropyl trimethoxysilane</td>
<td>(CH₃)(OCH₃)₂Si(OCH₃)₃</td>
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<td>(CH₃)(OCH₃)₂Si(OCH₃)₃</td>
<td>136</td>
<td>300</td>
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<td>110</td>
<td>378</td>
<td>8.87</td>
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<td>KBM-603</td>
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<td>128</td>
<td>351</td>
<td>9</td>
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<td>3-Aminopropyltrimethoxysilane</td>
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<td>3-Aminopropyltrimethoxysilane</td>
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<td></td>
<td>KBM-9103P</td>
<td>3-Trietoxysilyl(1,3-dimethylbutyl) propylamine</td>
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<td>165</td>
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<td>9.15</td>
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<tr>
<td>Ureide</td>
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<td>9.17</td>
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<td>KBM-803</td>
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<td>(CH₃)(OCH₃)₂Si(OCH₃)₃</td>
<td>107</td>
<td>398</td>
<td>8.49</td>
</tr>
</tbody>
</table>

*About Product Name of Shin-Etsu Silane Coupling Agents*

**KBM-1003** ➔ The last digit indicates the number of hydrolyzable groups.

*There are certain exceptions.

**M** indicates methoxy groups,

**E** indicates ethoxy groups.

**Solubility in water**

The alkoxysilyl groups in a silane coupling agent react with water to form silanol groups. These silanol groups are unstable and over time will undergo condensation. This results in formation of siloxane linkages, and ultimately gelation. Silanol groups are generally unstable in aqueous solutions, but their stability improves if the solution is mildly acidic. Meanwhile, amino silanes are very stable in aqueous solutions, due to interaction of the amino groups. Methods for improving a solution’s shelf-life include adjusting the pH of the liquid, combining it with alcohol, and storing it at room temperature or as below.

**Solubility and Stability at Optimum pH**

<table>
<thead>
<tr>
<th>Product name</th>
<th>Solubility (pH of aqueous solution)</th>
<th>Shelf-life</th>
</tr>
</thead>
<tbody>
<tr>
<td>KBM-1003</td>
<td>+(3.9)</td>
<td>Up to 10 days</td>
</tr>
<tr>
<td>KBE-1003</td>
<td>+(3.9)</td>
<td>Up to 10 days</td>
</tr>
<tr>
<td>KBM-303</td>
<td>+(4.0)</td>
<td>Up to 30 days</td>
</tr>
<tr>
<td>KBE-403</td>
<td>+(5.3)</td>
<td>Up to 30 days</td>
</tr>
<tr>
<td>KBE-402</td>
<td>+(4.0)</td>
<td>Up to 10 days</td>
</tr>
<tr>
<td>KBE-403</td>
<td>+(4.0)</td>
<td>Up to 30 days</td>
</tr>
<tr>
<td>KBM-1403</td>
<td>Insoluble</td>
<td>—</td>
</tr>
<tr>
<td>KBM-502</td>
<td>+(4.0)</td>
<td>Up to 1 day</td>
</tr>
<tr>
<td>KBE-503</td>
<td>+(4.2)</td>
<td>Up to 1 day</td>
</tr>
<tr>
<td>KBE-5103</td>
<td>+(4.2)</td>
<td>Up to 3 days</td>
</tr>
<tr>
<td>KBM-602</td>
<td>+(10.0)</td>
<td>Up to 30 days</td>
</tr>
<tr>
<td>KBE-903</td>
<td>+(10.0)</td>
<td>Up to 30 days</td>
</tr>
<tr>
<td>KBE-903</td>
<td>+(10.0)</td>
<td>Up to 30 days</td>
</tr>
<tr>
<td>KBE-903</td>
<td>+(10.0)</td>
<td>Up to 30 days</td>
</tr>
<tr>
<td>KBM-803</td>
<td>+(4.0)</td>
<td>Up to 1 day</td>
</tr>
</tbody>
</table>

*Solubility

++ = 1% silane-water solution can be prepared without adjusting pH of aqueous solution.

+ = 1% silane-water solution can be prepared if pH of aqueous solution is adjusted.

Insoluble: Silane-water solution cannot be prepared.

*Information on shelf-life should be taken as a guide. Shelf-life will vary depending on usage conditions and intended use.*

---

*Calculated from energy of evaporation and molar volume as determined by the Fedor’s method.*
## Main Products Lineup

### Product List

<table>
<thead>
<tr>
<th>Functional group</th>
<th>Product name</th>
<th>Chemical name</th>
<th>Structural formula</th>
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<th>Minimum covering area m²/g</th>
<th>Solubility parameter</th>
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</thead>
<tbody>
<tr>
<td>Vinyl</td>
<td>KBM-1003</td>
<td>Vinyltrimethoxysilane</td>
<td>(CH₃O)₂Si(CH₃)CH₂</td>
<td>23</td>
<td>526</td>
<td>7.49</td>
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<tr>
<td></td>
<td>KBE-1003</td>
<td>Vinyltrimethoxysilane</td>
<td>(CH₃O)₂Si(CH₃)CH₂</td>
<td>54</td>
<td>410</td>
<td>7.76</td>
</tr>
<tr>
<td>Epoxy</td>
<td>KBM-303</td>
<td>2-(3,4epoxyclohexyl) ethyltrimethoxysilane</td>
<td>(CH₃O)₂Si(CH₃)₃(CH₃)</td>
<td>163</td>
<td>317</td>
<td>8.59</td>
</tr>
<tr>
<td></td>
<td>KBM-402</td>
<td>3-Glycidoxypropyl methyldimethoxysilane</td>
<td>(CH₃O)₂Si(CH₃)OHCH₂CH₂</td>
<td>134</td>
<td>354</td>
<td>8.35</td>
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<tr>
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<td>3-Glycidoxypropyl trimethoxysilane</td>
<td>(CH₃O)₂Si(CH₃)OHCH₂</td>
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<td>330</td>
<td>8.49</td>
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<tr>
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<td>KBE-403</td>
<td>3-Glycidoxypropyl triethoxysilane</td>
<td>(CH₃O)₂Si(CH₃)OHCH₂</td>
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<td>280</td>
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<td>(CH₃O)₂Si(CH₃)OHCH₂</td>
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<td>(CH₃O)₂Si(CH₃)OHCH₂</td>
<td>115</td>
<td>335</td>
<td>8.53</td>
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<td>351</td>
<td>9</td>
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<tr>
<td></td>
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<td>(CH₃O)₂Si(NH₂) CH₂</td>
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<td>435</td>
<td>8.56</td>
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<td>3-TrifluoromethylN-(1,3-dimethylbutylidene) propylamine</td>
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<td>8.41</td>
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<td>165</td>
<td>305</td>
<td>9.15</td>
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<td>(CH₃O)₂Si(CH₃)SH</td>
<td>107</td>
<td>398</td>
<td>8.49</td>
</tr>
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</table>

*flash point °C: calculated from energy of evaporation and molar volume as determined by the Fedor’s method.

$\text{Solubility parameter}$: calculated from energy of evaporation and molar volume as determined by the Fedor’s method.

### About Product Name of Shin-Etsu Silane Coupling Agents

- **KBM-1003** The last digit indicates the number of hydrolyzable groups.
- M indicates methoxy groups.
- E indicates ethoxy groups.

### Solubility in water

The alkoxysil groups in a silane coupling agent react with water to form silanol groups. These silanol groups are unstable and over time will undergo condensation. This results in formation of siloxane linkages, and ultimately gelation. Silanol groups are generally unstable in aqueous solutions, but their stability improves if the solution is mildly acidic. Meanwhile, amino silanes are very stable in aqueous solutions, due to interaction of the amino groups. Methods for improving a solution’s shelf-life include adjusting the pH of the liquid, combining it with alcohol, and storing it at room temperature or as below.

### Solubility and Stability at Optimum pH

<table>
<thead>
<tr>
<th>Product name</th>
<th>Solubility (pH of aqueous solution)</th>
<th>Shelf-life</th>
</tr>
</thead>
<tbody>
<tr>
<td>KBM-1003</td>
<td>+ (3.9)</td>
<td>Up to 10 days</td>
</tr>
<tr>
<td>KBE-1003</td>
<td>+ (3.9)</td>
<td>Up to 10 days</td>
</tr>
<tr>
<td>KBM-303</td>
<td>+ (4.0)</td>
<td>Up to 30 days</td>
</tr>
<tr>
<td>KBE-403</td>
<td>+ (5.3)</td>
<td>Up to 30 days</td>
</tr>
<tr>
<td>KBE-402</td>
<td>+ (4.0)</td>
<td>Up to 10 days</td>
</tr>
<tr>
<td>KBE-403</td>
<td>+ (4.0)</td>
<td>Up to 30 days</td>
</tr>
<tr>
<td>KBM-1403</td>
<td>Incompatible</td>
<td>—</td>
</tr>
<tr>
<td>KBM-502</td>
<td>+ (4.0)</td>
<td>Up to 1 day</td>
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<tr>
<td>KBM-503</td>
<td>+ (4.2)</td>
<td>Up to 1 day</td>
</tr>
<tr>
<td>KBM-5103</td>
<td>+ (4.2)</td>
<td>Up to 3 days</td>
</tr>
<tr>
<td>KBM-602</td>
<td>+ (10.0)</td>
<td>Up to 30 days</td>
</tr>
<tr>
<td>KBE-903</td>
<td>+ (10.0)</td>
<td>Up to 30 days</td>
</tr>
<tr>
<td>KBE-903</td>
<td>+ (10.0)</td>
<td>Up to 10 days</td>
</tr>
<tr>
<td>KBM-803</td>
<td>+ (4.0)</td>
<td>Up to 1 day</td>
</tr>
</tbody>
</table>

*Solubility: 
- + + 1% silane-water solution can be prepared without adjusting pH of aqueous solution.
- + 1% silane-water solution can be prepared if pH of aqueous solution is adjusted.
- Incompatible: Silane-water solution cannot be prepared.

Information on shelf-life should be taken as a guide. Shelf-life will vary depending on usage conditions and intended use.
Development Concept of Shin-Etsu Silane Coupling Agents

Shin-Etsu Chemical is developing a range of new products with many special features. Our offerings include products that not only improve functionality but also allow users to achieve greener product design, and are easier to use by virtue of allowing users to eliminate certain processes.

**Long-chain Spacer Type**
- Improving hydrophobicity and flexibility
- Multi Functional Group Type
  - Low volatility
  - Highly improving adhesion
- VOC Free Type
  - Alcohol released: Reduced by 99% or more
  - Eliminate the step of hydrols.
- Ethoxy Type
  - Product of hydrols is ethanol
  - Hydrolyzes slowly, and compositions will be stable even after addition.

**Multi Functional Group Type → P13**
- Conventional grade (MeO)2Si Spacer Organic functional group
- Long-chain Spacer Type (MeO)2Si Spacer Organic functional group
- Protected Functional Group Type → P16
  - (RO)2Si — Organic functional group
- Dialkoxyl Silane Type → P17
  - Organic functional group
- Ethoxy Type → P17
  - RO — OR

**Polymerizable Type**
- Contains acrylic and styrene groups
- Improved adhesion between inorganic materials and resins

**Liquid Rubber Modified Type**
- Improved compatibility and adhesion with resins
- Improved water resistance

**Anti-rust Properties Imparting Type**
- Improves rust prevention and adhesion to metals

**Protected Functional Group Type → P14**
- One-component products can be used in place of two-component products
- Highly improving adhesion

**Usability**
- Compared to dialkoxyl types: Lower crosslinking density for better shelf life
- Less alcohol is released

**High Functionality**

Highly Functional Products Lineup

**Long-chain Spacer Silane Coupling Agents**

Compared to general-purpose silane coupling agents, these have higher hydrophobicity, which means that fillers treated with them will have greater dispersibility. Another advantage is that the cured material will have improved flexibility.

**Features and Resulting Properties**
- Improving hydrophobicity (lipophilicity)
- Improving compatibility with resins
- Filler high loading
- Improving alkali resistance
- Improving adhesion
- Improving flexibility

**Product List**

<table>
<thead>
<tr>
<th>Organic functional group</th>
<th>Product name</th>
<th>Chemical structure</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vinyl</td>
<td>KBM-1083</td>
<td>(MeO)2Si</td>
</tr>
<tr>
<td>Epoxy</td>
<td>KBM-4803</td>
<td>(MeO)2Si</td>
</tr>
<tr>
<td>Methacryloxy</td>
<td>KBM-5803</td>
<td>(MeO)2Si</td>
</tr>
<tr>
<td>Amino</td>
<td>KBM-6803</td>
<td>(MeO)2Si</td>
</tr>
</tbody>
</table>

**Model of Chemical Structure**

**Measurements of cured materials**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Sample</th>
<th>KBM-4803 treatment</th>
<th>KBM-5803 treatment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Viscosity</td>
<td>Pa·s</td>
<td>120</td>
<td>260</td>
</tr>
</tbody>
</table>

**Epoxy-on-glass adhesion test**

- Roughly 3 times better adhesion than with KBM-4803
- Test method:
  - A 1% aqueous solution is applied to a glass substrate.
  - A cured material (silica resin/methylsilicone): a primer and adhesive strength is tested.
  - Adhesive strength is calculated against a standard of 100% (cured glass).
  - *Model of cure shrinkage:
    - Cured film shrinkage: PET (thickness: 0.2mm) (Not specified value)
    - Wetting: the degree of cure shrinkage

**Dispersibility of treated silicas**

- Long-chain spacer silane coupling agents improve the dispersibility of fillers, and compositions will be more transparent.

Formulation: Silane treated silica 10 wt% / Multifunctional epoxy compounds 90 wt%
Development Concept of Shin-Etsu Silane Coupling Agents

Shin-Etsu Chemical is developing a range of new products with many special features. Our offerings include products that not only improve functionality but allow users to achieve greener product design, and are easier to use by virtue of allowing users to eliminate certain processes.

- **Long-chain Spacer Type**
  - Improving hydrophobicity and flexibility
- **Liquid Rubber Modified Type**
  - Improved adhesion between inorganic materials and resins
- **Multi Functional Group Type**
  - Low volatility
- **VOC Free Type**
  - Alcohol released: Reduced by 99% or more
- **Ethoxy Type**
  - Product of hydrolysis is ethanol
  - Hydrolyzes slowly, and compositions will be stable even after addition.

**High Functionality**
- Polymerizable Type
  - Contains acrylic and styrene groups
  - Improved adhesion between inorganic materials and resins
- **Anti-rust Properties Imparting Type**
  - Improves rust prevention and adhesion to metals
- **Protected Functional Group Type**
  - One-component products can be used in place of two-component products
  - Highly improving adhesion

**Usability**
- **Eco-friendly**
  - Compared to dialkoxy types: Lower crosslinking density for better shelf life
  - Less alcohol is released

**Dialkoxy Silane Type**
- **Model of Chemical Structure**

- **Polymerizable Type**
  - (MeO)₂Si
  - Organic functional group

- **Multi Functional Group Type**
  - Si(OR)₃
  - Organic functional group
  - R = Me, Et

- **VOC Free Type**
  - (RO)₂Si
  - Organic functional group

- **Ethoxy Type**
  - RO – Si – OR

**Highly Functional Products Lineup**

**Long-chain Spacer Silane Coupling Agents**

Compared to general-purpose silane coupling agents, these have higher hydrophobicity, which means that fillers treated with them will have greater dispersibility. Another advantage is that the cured material will have improved flexibility.

- **Features and Resulting Properties**
  - Improving hydrophobicity (lipophilicity)
  - Improving compatibility with resins
  - Filler high loading
  - Improving alkali resistance

- **Model of Chemical Structure**
  - Conventional grade
    - (MeO)₂Si
    - Inorganic part
  - Organic functional group
  - Long-chain Spacer Type
    - (MeO)₂Si
    - Inorganic part
    - Organic functional group
  - Organic part

- **Product List**

<table>
<thead>
<tr>
<th>Organic functional group</th>
<th>Product name</th>
<th>Chemical structure</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vinyl</td>
<td>KBM-1083</td>
<td>(MeO)₂Si</td>
</tr>
<tr>
<td>Epoxy</td>
<td>KBM-4803</td>
<td>(MeO)₂Si</td>
</tr>
<tr>
<td>Methacryloxy</td>
<td>KBM-5803</td>
<td>(MeO)₂Si</td>
</tr>
<tr>
<td>Amino</td>
<td>KBM-6603</td>
<td>(MeO)₂Si</td>
</tr>
</tbody>
</table>

**Measurements of cured materials**

- **Epoxy-on-glass adhesion test**
  - Sample: KBM-4803 (Conventional grade)
  - KBM-4803 (Functional group)
  - KBM-5003 (Conventional grade)
  - KBM-5003 (Functional group)

- **Disperisty of treated silicas**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Sample</th>
<th>KBM-4803 treatment</th>
<th>KBM-403 treatment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Viscosity (Pa-s)</td>
<td>120</td>
<td>260</td>
<td></td>
</tr>
</tbody>
</table>

Long-chain spacer silane coupling agents help hold viscosity down and enable higher filler loadings. Formulation: Silane treated silica 10 wt% / Multifunctional epoxy compounds 90 wt%.

Long-chain spacer silane coupling agents improve the dispersibility of fillers, and compositions will be more transparent.

Formulation: Silane treated silica 10 wt% / Multifunctional acrylic compounds 90 wt%.
Multi Functional Silane Coupling Agents

Compared to monomer types, multifunctional silane coupling agents have lower volatility and a greater number of sites for reaction with resins, so you can expect improved adhesion to the substrate. And because they have film-forming properties, this type of silane coupling agent can also be used as a primer.

**Organic Chain Type : Excellent Compatibility with Resins**

- **Features and Resulting Properties**
  - Low volatile content
  - Can be used in high-temperature conditions. Can be effective even in small amounts.
  - Many reaction sites for resin
  - Improved coupling performance
  - Film forming property
  - Highly functional primers
  - Containing trialkoxysilyl groups
  - Improving adhesion

- **Model of Chemical Structure**

**Product List**

<table>
<thead>
<tr>
<th>Organic functional group</th>
<th>Product name</th>
<th>Alkyl group</th>
<th>Numbers of functional groups*</th>
<th>Viscosity mm^2/s</th>
<th>Resulting functional group reaction rate %</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acrylic</td>
<td>X-12-1048</td>
<td>MeO</td>
<td>1</td>
<td>33</td>
<td>300</td>
</tr>
<tr>
<td>X-12-1050</td>
<td>MeO</td>
<td>5</td>
<td>6,000</td>
<td>1,000</td>
<td>290</td>
</tr>
<tr>
<td>Epoxy</td>
<td>X-12-9815</td>
<td>RO</td>
<td>3</td>
<td>2,000</td>
<td>270</td>
</tr>
<tr>
<td>X-12-9845</td>
<td>RO</td>
<td>2</td>
<td>8</td>
<td>4,000</td>
<td>360</td>
</tr>
<tr>
<td>Mercapto</td>
<td>X-12-1154</td>
<td>MeO</td>
<td>1</td>
<td>1,500</td>
<td>240</td>
</tr>
<tr>
<td>Amino</td>
<td>X-12-9731</td>
<td>RO</td>
<td>1</td>
<td>8.6</td>
<td>600</td>
</tr>
<tr>
<td>X-12-1159N</td>
<td>MeO</td>
<td>2</td>
<td>4</td>
<td>30</td>
<td>360</td>
</tr>
</tbody>
</table>

*15% of alcohol solution
* Number of organic functional groups: each 1 atom

**Epoxy-on-glass Adhesion Test**

Test method:
- A 1% aqueous solution is applied to a glass substrate.
- A cured material (epoxy resin/triethylenetramine) is prepared and adhesive strength is tested.

- *Adhesive strength is calculated against a standard of 100% (untreated glass).

**Non-volatile Content of Silane Coupling Agents**

Multi functional silane coupling agents have lower volatility compared to monomer types.

<table>
<thead>
<tr>
<th>Organic functional group</th>
<th>Product name</th>
<th>Non-volatile content</th>
</tr>
</thead>
<tbody>
<tr>
<td>KBM-5103 (Acryloylamide)</td>
<td>X-12-1048</td>
<td>29</td>
</tr>
<tr>
<td>KBM-503 (Methacryloylamide)</td>
<td>60</td>
<td>0</td>
</tr>
<tr>
<td>X-12-5803 (Methacryloylamide)</td>
<td>98</td>
<td>34</td>
</tr>
<tr>
<td>X-12-1048 (Multi functional acryloylamide)</td>
<td>97</td>
<td>84</td>
</tr>
<tr>
<td>X-12-1050 (Multi functional acryloylamide)</td>
<td>99</td>
<td>87</td>
</tr>
<tr>
<td>X-12-513 (Acryloylamide oligomer)</td>
<td>97</td>
<td>94</td>
</tr>
<tr>
<td>X-4-09296 (Methacryloylamide oligomer)</td>
<td>98</td>
<td>95</td>
</tr>
<tr>
<td>Epoxy</td>
<td>KBM-403 (Epoxy silane)</td>
<td>66</td>
</tr>
<tr>
<td>KBM-4803 (Epoxy silylamine)</td>
<td>98</td>
<td>68</td>
</tr>
<tr>
<td>X-12-9815 (Multi functional epoxy silane)</td>
<td>92</td>
<td>87</td>
</tr>
<tr>
<td>X-12-9845 (Multi functional epoxy silane)</td>
<td>94</td>
<td>90</td>
</tr>
<tr>
<td>SK-516 (Epoxy oligomer)</td>
<td>X-12-1048</td>
<td>85</td>
</tr>
</tbody>
</table>

*Measurements are performed on 2 g of undiluted silane in a 50 cc beaker.

**Polymerizable Type Silane Coupling Agents**

X-12-1290, KBM-1403

- **Resulting Properties**
  - Radical cross-linking is possible due to the inclusion of allyl groups.
  - By adding it to polymerizable resin compositions, it improves the adhesion between inorganic materials such as fillers and resins.
  - Because it contains styrene group, anionic polymerization, cationic polymerization, and radical polymerization are possible.
  - By adding it to polymerizable resin compositions, it improves the adhesion between inorganic materials such as fillers and resins.

- **General Properties**

<table>
<thead>
<tr>
<th>Product name</th>
<th>Chemical name</th>
<th>Refractive index at 25°C</th>
<th>Refractive index at 35°C</th>
<th>Refractive index at 15°C</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vinyl</td>
<td>X-12-1290</td>
<td>1.17</td>
<td>1.483</td>
<td>1.90</td>
</tr>
<tr>
<td>Styrene</td>
<td>KBM-1403</td>
<td>1.06</td>
<td>1.504</td>
<td>1.36</td>
</tr>
</tbody>
</table>

*This product must be stored below 0°C. (Not specified values)

**Liquid Rubber Modified Type Silane Coupling Agents**

**Butadiene Polymer Modified Silane Coupling Agent X-12-12678-ES**

- **Resulting Properties**
  - Improved compatibility and adhesion of various resins
  - Improved water resistance due to high hydrophobicity

**Anti-rust Properties Imparting Type Silane Coupling Agents**

**Silane Coupling Agent with Benztiazazole Groups X-12-1214A**

A silane coupling agent with a benzotrizazole group as an organic functional group, which is effective for rust prevention of metals. By adhering the alkyl group to the inorganic base material, it stays on the surface of the metal base material and exhibits an excellent rust prevention effect over a long period of time.

- **Features**
  - It is effective in preventing rust on metals such as copper, silver, and aluminum.
  - In addition, it can be expected to have the effect of imparting adhesion to metals.

- **Applications**
  - Coating, etc.
  - Copper, silver plating, etc.
  - Metal parts for electrical products, etc.

- **General Properties**

<table>
<thead>
<tr>
<th>Product name</th>
<th>X-12-1214A</th>
</tr>
</thead>
<tbody>
<tr>
<td>Appearance</td>
<td>Pale yellow transparent liquid</td>
</tr>
<tr>
<td>Active ingredient (%)</td>
<td>100</td>
</tr>
<tr>
<td>Viscosity at 25°C (mPa·s)</td>
<td>Not specified</td>
</tr>
</tbody>
</table>

*Not specified values*
Multi Functional Silane Coupling Agents

Compared to monomer types, multi functional silane coupling agents have lower volatility and a greater number of sites for reaction with resins, so you can expect improved adhesion to the substrate. And because they have film-forming properties, this type of silane coupling agent can also be used as a primer.

**Features and Resulting Properties**
- Low volatile content: Can be used in high temperature conditions, can be effective even in small amounts.
- Many reaction sites for resins: Improved coupling performance.
- Film forming property: High fully functional primers.
- Containing trialkoxysilyl groups: Improving adhesion.

**Product List**

<table>
<thead>
<tr>
<th>Organic functional group</th>
<th>Product name</th>
<th>Alkyl group</th>
<th>Numbers of functional groups(a)</th>
<th>Viscosity mm/s</th>
<th>Result functional group reaction time (min)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acrylic</td>
<td>X-12-1048</td>
<td>MeO</td>
<td>1</td>
<td>33</td>
<td>300</td>
</tr>
<tr>
<td></td>
<td>X-12-1050</td>
<td>MeO</td>
<td>5</td>
<td>600</td>
<td>150</td>
</tr>
<tr>
<td>Epoxy</td>
<td>X-12-9815</td>
<td>RO</td>
<td>3</td>
<td>1,000</td>
<td>290</td>
</tr>
<tr>
<td></td>
<td>X-12-9845</td>
<td>RO</td>
<td>3</td>
<td>2,000</td>
<td>270</td>
</tr>
<tr>
<td>Mercapto</td>
<td>X-12-1154</td>
<td>MeO</td>
<td>3</td>
<td>1,500</td>
<td>240</td>
</tr>
<tr>
<td>Amino</td>
<td>X-12-9732</td>
<td>MeO</td>
<td>5</td>
<td>8.6</td>
<td>500</td>
</tr>
<tr>
<td></td>
<td>X-12-1159</td>
<td>MeO</td>
<td>2</td>
<td>4,000</td>
<td>300</td>
</tr>
</tbody>
</table>

(a) 15% of ethanol solution

**Epoxy-on glass Adhesion Test**

Test method:
1. A 1% aqueous solution is applied to a glass substrate.
2. A cured material (epoxy resin/triethylenetetramine) is prepared and adhesive strength is tested.

**Non-volatile Content of Silane Coupling Agents**

Multi functional silane coupling agents have lower volatility compared to monomer types.

**Polymerizable Type Silane Coupling Agents**

- **X-12-1290, KBM-1403**
  - **Resulting Properties**
    - Radical cross-linking is possible due to the inclusion of allyl groups.
    - By adding to it polymerizable resin compositions, it improves the adhesion between inorganic materials such as fillers and resins.
  - **General Properties**
    - *This product must be stored below 0°C. (Not specified values)*

**Chemical Structure**

**Liquid Rubber Modified Type Silane Coupling Agents**

- **X-12-12678-ES**
  - **Resulting Properties**
    - Improved compatibility and adhesion of various resins.
    - Improved water resistance due to high hydrophobicity.

**General Properties**

**Butadiene Polymer Modified Silane Coupling Agent X-12-12678-ES**

**Chemical Structure**

**Anti-rust Properties Imparting Type Silane Coupling Agents**

A silane coupling agent with a benzotriazole group as an organic functional group, which is effective for rust prevention of metals. By adhering the alkoy group to the inorganic base material, it stays on the surface of the metal base material and exhibits an excellent rust prevention effect over a long period of time.

**Features**

- It is effective in preventing rust on metals such as copper, silver, and aluminum. In addition, it can be expected to have the effect of imparting adhesion to metals.

**Applications**

- Forging, etc.
- Copper, silver plating, etc.
- Metal parts for electrical products, etc.

**General Properties**

**Copper Plate Treatment**

1. Wash the copper plate with sulfuric acid and water
2. Epoxy silane, benzotriazole, X-12-1214A 1:1 w/w, solution immersed for 5 minutes, dried

<table>
<thead>
<tr>
<th>Product name</th>
<th>X-12-1214A</th>
</tr>
</thead>
<tbody>
<tr>
<td>Appearance</td>
<td>Pale yellow transparent liquid</td>
</tr>
<tr>
<td>Active ingredient</td>
<td>100</td>
</tr>
<tr>
<td>Viscosity at 25°C mm²/s</td>
<td>170</td>
</tr>
</tbody>
</table>

*Measurements are performed on 2 g of undiluted silane in a 50 cc beaker.*
**Protected Functional Group** Silane Coupling Agents

The functional groups of these silane coupling agents are protected. This means they can be added at the same time to systems that would otherwise be too reactive, and this enables use of a one-component product where a two-component product would have been necessary.

**Features**
Can be added to organic materials with which silane coupling agents could not normally be used.

**Product List**

<table>
<thead>
<tr>
<th>Product name</th>
<th>Functional group</th>
</tr>
</thead>
<tbody>
<tr>
<td>X-12-1056ES</td>
<td>Protected mercapto group silane coupling agent</td>
</tr>
<tr>
<td>KBE-9103P</td>
<td>Amino group (amine type)</td>
</tr>
<tr>
<td>X-12-1172ES</td>
<td>Amino group (aldehyde type)</td>
</tr>
<tr>
<td>X-12-967C</td>
<td>Acid anhydride type</td>
</tr>
</tbody>
</table>

**Benefit of Protecting Functional Groups**

**Model for Improving Stability in Resin**

- Conventional grade: Reaction starts immediately after the product is added to the resin.
- Protected functional group type: Reaction is suppressed, and stability is high. (One-component product can be used.)

**Stability after addition to various resins**

- Shell life of KBE-9103P in epoxy resin:
  - Epoxy resin: 50 wt. part
  - Silane coupling agent: 5 wt. part
  - Toluene: 50 wt. part

**Test Result of Viscosity**

<table>
<thead>
<tr>
<th>Product name</th>
<th>Condition</th>
<th>No additive</th>
<th>KBE-9103P</th>
<th>KBE-903</th>
</tr>
</thead>
<tbody>
<tr>
<td>After 3 days</td>
<td>mm/s</td>
<td>4.2</td>
<td>4.4</td>
<td>7.8</td>
</tr>
<tr>
<td>After 14 days</td>
<td>mm/s</td>
<td>4.3</td>
<td>4.7</td>
<td>8.6</td>
</tr>
</tbody>
</table>

**Change in viscosity when mixed with isocyanate compound**

- Isocyanate compound: 95 wt. part
- Silane coupling agent: 5 wt. part

**Application of Urethane Adhesive**

- Tensile Lap-shear Strength Test Result of Urethane Adhesive

**Model of Chemical Structure**

- Protecting organic functional group
- (RO)₂Si
- Organic functional group

**Model for Improving Adhesion**

Functional groups are protected and migrate to surfaces with substrates. Because there is no reaction, the resin does not thicken.

- Many reaction sites contribute to adhesion.

**Features**

- The protective groups are removed by water or moisture, then the reaction begins.

**Resulting Properties**

- Primer
- Surface treatment
- Binder
- Mixing with water paints

**Product List**

<table>
<thead>
<tr>
<th>Product name</th>
<th>Organic functional groups</th>
<th>Active ingredient wt%</th>
<th>Solvent</th>
<th>pH*</th>
</tr>
</thead>
<tbody>
<tr>
<td>KBE-90</td>
<td>Amino -NH₂</td>
<td>30</td>
<td>Water</td>
<td>10-12</td>
</tr>
<tr>
<td>X-12-1355</td>
<td>Amine, vinyl -NH₂ and -CH=CH₂</td>
<td>20</td>
<td>Water</td>
<td>10-12</td>
</tr>
<tr>
<td>X-12-1355M</td>
<td>Amino, methyl -NH₂ and -CH₃</td>
<td>20</td>
<td>Water</td>
<td>10-12</td>
</tr>
<tr>
<td>KBE-64</td>
<td>Ethylenediamine-NH₂</td>
<td>30</td>
<td>Water</td>
<td>10-12</td>
</tr>
<tr>
<td>X-12-954</td>
<td>Ethylenediamine -NH₂</td>
<td>30</td>
<td>Water</td>
<td>10-12</td>
</tr>
<tr>
<td>X-12-1135</td>
<td>Carboxylic acid -COOH</td>
<td>30</td>
<td>Water</td>
<td>1-3</td>
</tr>
<tr>
<td>X-12-1139</td>
<td>Quaternary ammonium -NMe₂⁺</td>
<td>30</td>
<td>Water</td>
<td>8-10</td>
</tr>
<tr>
<td>X-12-1126</td>
<td>Quaternary ammonium -NMe₃⁺</td>
<td>30</td>
<td>Water</td>
<td>8-10</td>
</tr>
</tbody>
</table>

*Stability suffers once pH is outside this zone.

**VOC Free** Silane Coupling Agents

All the alkoxysilyl groups are silanols, which means the amount of methanol or ethanol released is reduced by 99% or more. The alcohol normally released when a conventional silane coupling agent undergoes hydrolysis can be minimized.

- (Ex.) When 100 kg of KBE-903 is hydrolyzed, 62 kg of ethanol is released.

**Features**
- The step of hydrolysis can be eliminated.
- The amount of alcohol released is reduced by 99% or more.
- Nonflammable
- Lower amounts of VOCs released

**Resulting Properties**
- Primer
- Surface treatment
- Binder
- Mixing with water paints

**Model of Chemical Structure**

- Organic functional group
- (EtO)₃Si
- Organic functional group

**Features and Resulting Properties**

- Hydrolysis is slower compared to methoxy types.
- Good shelf life after addition
- Product of hydrolysis is ethanol
- Eco-friendly

*For data on ease of hydrolysis, see graph on PB.
Protected Functional Group Silane Coupling Agents

The functional groups of these silane coupling agents are protected. This means they can be added at the same time to systems that would otherwise be too reactive, and this enables use of a one-component product where a two-component product would have been necessary.

**Features**
Can be added to organic materials with which silane coupling agents could not normally be used.

**Product List**

<table>
<thead>
<tr>
<th>Product name</th>
<th>Functional group</th>
</tr>
</thead>
<tbody>
<tr>
<td>X-12-1056E5</td>
<td>Protected mercapto group silane coupling agent</td>
</tr>
<tr>
<td>KBE-9103P</td>
<td>Protected amino group (ketimine type)</td>
</tr>
<tr>
<td>X-12-1172E5</td>
<td>Protected amino group (alimine type)</td>
</tr>
<tr>
<td>X-12-967C</td>
<td>Acid anhydride type</td>
</tr>
</tbody>
</table>

**Model of Chemical Structure**

[Diagram showing the structure of a protected organic functional group (RO)_2Si, where R represents a protecting group.]

**Benefit of Protecting Functional Groups**

**Model for Improving Stability in Resin**

- Conventional grade: Reaction starts immediately after product is added to resin.
- Protected functional group type: Product does not react after addition to resin and stability is high. (One-component product can be used.)

**Stability after addition to various resins**

- Shell life of KBE-9103P in epoxy resin: Formulation: Epoxy resin --- 50 wt. part; Silane coupling agent --- 5 wt. part; Toluene --- 50 wt. part. Test Result of Viscosity: No additive --- KBE-9103P --- KBE-903
  - Initial: 3.9, 7.6, 6.1
  - Water resistance test at 95°C×10 h: 3.4, 6.4, 5.2

**Change in viscosity when mixed with isocyanate compound**

- Formulation: Isocyanate compound --- 95 wt. part; Silane coupling agent --- 5 wt. part.
  - Application of Urethane Adhesive: Tensile Lap-shear Strength Test Result of Urethane Adhesive: X-12-1056E5, X-12-1172E5, KBE-903

**Model for Improving Adhesion**

- Functional groups are protected and migrate to interface with substrate. Because there is no reaction, the resin does not thicken.
- Many reaction sites contribute to adhesion.

**Model of Chemical Structure**

[Diagram showing the structure of a silane coupling agent with a functional group attached to silicon.]

**Product List**

<table>
<thead>
<tr>
<th>Product name</th>
<th>Organic functional group</th>
<th>Active ingredient wt%</th>
<th>Solvent</th>
<th>pH*</th>
</tr>
</thead>
<tbody>
<tr>
<td>KBE-90</td>
<td>Amine −NH₂</td>
<td>30</td>
<td>Water</td>
<td>10-12</td>
</tr>
<tr>
<td>X-12-1353</td>
<td>Amine, vinyl (−NH₂ and =CH=CH₂)</td>
<td>20</td>
<td>Water</td>
<td>10-12</td>
</tr>
<tr>
<td>X-12-1353M</td>
<td>Amine, methyl (−NH₂ and =CH₃)</td>
<td>20</td>
<td>Water</td>
<td>10-12</td>
</tr>
<tr>
<td>KBE-64</td>
<td>Ethylenediamine (−NH₂=CH₂-NH₂)</td>
<td>30</td>
<td>Water</td>
<td>10-12</td>
</tr>
<tr>
<td>X-12-954</td>
<td>Ethylenediamine (−NH₂=CH₂-NH₂)</td>
<td>30</td>
<td>Water</td>
<td>10-12</td>
</tr>
<tr>
<td>X-12-1135</td>
<td>Carboxylic acid (−COOH)</td>
<td>30</td>
<td>Water</td>
<td>1-3</td>
</tr>
<tr>
<td>X-12-1139</td>
<td>Quaternary ammonium (−NH₃=CH₂-N⁺)</td>
<td>30</td>
<td>Water</td>
<td>8-10</td>
</tr>
<tr>
<td>X-12-1126</td>
<td>Quaternary ammonium (−NH₃=CH₂-N⁺)</td>
<td>30</td>
<td>Water</td>
<td>8-10</td>
</tr>
</tbody>
</table>

*Stability suffers once pH is outside the zone.

**VOC Free Silane Coupling Agents**

All the alkoxysilyl groups are silanols, which means the amount of methanol or ethanol released is reduced by 99% or more. The alcohol normally released when a conventional silane coupling agent undergoes hydrolysis can be minimized. (Ex.) When 100 kg of KBE-903 is hydrolyzed, 62 kg of ethanol is released. Users are looking to eliminate VOCs from their operations.

**Features**

- The step of hydrolysis can be eliminated.
- The amount of alcohol released is reduced by 99% or more.
- Nonflammable
- Lower amounts of VOCs released

**Resulting Properties**

- Primer
- Surface treatment
- Binder
- Mixing with water paints

**Model of Chemical Structure**

[Diagram showing the structure of an organic functional group attached to a silane coupling agent with a hydrolysable protective group removed.]

**Product List**

<table>
<thead>
<tr>
<th>Product name</th>
<th>Organic functional group</th>
<th>Aromatic isocyanate</th>
<th>Water resistance test (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>X-12-1056E5</td>
<td>(RO)₂Si</td>
<td>KBE-9103P</td>
<td>222 mPa-s, 139 mPa-s, 174 mPa-s</td>
</tr>
<tr>
<td>X-12-1172E5</td>
<td>(RO)₂Si</td>
<td>KBE-903</td>
<td>223 mPa-s, 176 mPa-s, 380 mPa-s</td>
</tr>
<tr>
<td>(EtO)₃Si</td>
<td>Organic functional group</td>
<td></td>
<td>2,070</td>
</tr>
</tbody>
</table>

**Diaxoxyl Silane Coupling Agents**

**Ethoxy Silane Coupling Agents**

**Features and Resulting Properties**

- Hydrolysis is slower compared to methoxy types.
- Good shelf life after addition
- Product of hydrolysis is ethanol
- Eco-friendly

*For data on ease of hydrolysis, see graph on PB.
Silane

Shin-Etsu’s silane products are a group of organosilicon compounds comprised of alkoxy silanes and silazanes. Silanes have many applications in a wide variety of fields. They are commonly applied to the surface of inorganic substrates to improve water repellency, added to inorganic fillers to improve their dispersibility in organic polymers, and used for surface modification of inorganic materials.

General Properties

<table>
<thead>
<tr>
<th>Type</th>
<th>Product name</th>
<th>Chemical name</th>
<th>Structural formula</th>
<th>Molecular weight (g/mol)</th>
<th>Density (g/cm³)</th>
<th>Refraction index at 20°C</th>
<th>Flash point (°C)</th>
<th>Minimum flammability limit</th>
<th>UN hazard classification</th>
<th>Melting point (°C)</th>
<th>Boiling point (°C)</th>
<th>Minimum flammability limit</th>
<th>CAS No.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methoxy type</td>
<td>KBM-13</td>
<td>Methyltrimethoxysilane</td>
<td>(CH₃O)₃SiH</td>
<td>136.2</td>
<td>0.95</td>
<td>1.399</td>
<td>102</td>
<td>8</td>
<td>573</td>
<td>—</td>
<td>2052</td>
<td>2855</td>
<td>1185-55-3</td>
</tr>
<tr>
<td></td>
<td>KBM-22</td>
<td>Dimethyldimethoxysilane</td>
<td>(CH₃O)₂SiH</td>
<td>120.2</td>
<td>0.86</td>
<td>1.371</td>
<td>82</td>
<td>10</td>
<td>649</td>
<td>—</td>
<td>2052</td>
<td>2112-39-6</td>
<td>121-79-6</td>
</tr>
<tr>
<td></td>
<td>KBM-103</td>
<td>Phenyltrimethoxysilane</td>
<td>(CH₃O)₃SiPh</td>
<td>198.3</td>
<td>1.06</td>
<td>1.473</td>
<td>218</td>
<td>94</td>
<td>393</td>
<td>—</td>
<td>2052</td>
<td>2163-92-1</td>
<td>126-98-6</td>
</tr>
<tr>
<td></td>
<td>KBM-2025S</td>
<td>Octamethyldimethoxysilane</td>
<td>(CH₃O)₄Si</td>
<td>244.4</td>
<td>1.08</td>
<td>1.541</td>
<td>304</td>
<td>145</td>
<td>120</td>
<td>—</td>
<td>2052</td>
<td>843-66-9</td>
<td>26293-26-3</td>
</tr>
<tr>
<td></td>
<td>KBM-3033</td>
<td>n-Propyltrimethoxysilane</td>
<td>(CH₃O)₃SiCH₃</td>
<td>164.3</td>
<td>0.93</td>
<td>1.388</td>
<td>142</td>
<td>36</td>
<td>47</td>
<td>—</td>
<td>2052</td>
<td>1867-25-0</td>
<td>121-59-3</td>
</tr>
<tr>
<td></td>
<td>KBM-3063</td>
<td>Hexamethyldimethoxysilane</td>
<td>(CH₃O)₆SiH</td>
<td>206.4</td>
<td>0.91</td>
<td>1.406</td>
<td>202</td>
<td>81</td>
<td>378</td>
<td>—</td>
<td>2052</td>
<td>3689-19-0</td>
<td>1181-02-8</td>
</tr>
<tr>
<td></td>
<td>KBM-3103C</td>
<td>Decamethyldimethoxysilane</td>
<td>(CH₃O)₁₀SiH</td>
<td>262.5</td>
<td>0.90</td>
<td>1.421</td>
<td>122</td>
<td>122</td>
<td>297</td>
<td>—</td>
<td>2052</td>
<td>5575-48-4</td>
<td>1181-02-8</td>
</tr>
<tr>
<td></td>
<td>KBM-3066</td>
<td>Trifluoropropyltrimethoxysilane</td>
<td>(CH₃O)₃SiCF₃</td>
<td>326.5</td>
<td>1.02</td>
<td>1.420</td>
<td>121</td>
<td>64</td>
<td>379</td>
<td>—</td>
<td>2052</td>
<td>97136-01-1</td>
<td>1181-02-8</td>
</tr>
<tr>
<td>Ethenyl type</td>
<td>KBM-04</td>
<td>Tetraethoxysilane</td>
<td>(C₂H₅O)₄SiH</td>
<td>208.3</td>
<td>0.93</td>
<td>1.381</td>
<td>168</td>
<td>54</td>
<td>375</td>
<td>—</td>
<td>2052</td>
<td>7810-4</td>
<td>1181-02-8</td>
</tr>
<tr>
<td></td>
<td>KBM-13</td>
<td>Triethoxysilane</td>
<td>(C₂H₅O)₃SiH</td>
<td>178.3</td>
<td>0.89</td>
<td>1.383</td>
<td>143</td>
<td>40</td>
<td>437</td>
<td>—</td>
<td>2052</td>
<td>2022-67-6</td>
<td>1181-02-8</td>
</tr>
<tr>
<td></td>
<td>KBM-22</td>
<td>Dimethyldiethoxysilane</td>
<td>(C₂H₅O)₂SiH</td>
<td>148.3</td>
<td>0.83</td>
<td>1.384</td>
<td>114</td>
<td>19</td>
<td>526</td>
<td>—</td>
<td>2052</td>
<td>7826-2</td>
<td>1181-02-8</td>
</tr>
<tr>
<td></td>
<td>KBM-103</td>
<td>Phenyltriethoxysilane</td>
<td>(C₂H₅O)₃SiPh</td>
<td>240.4</td>
<td>0.99</td>
<td>1.459</td>
<td>236</td>
<td>111</td>
<td>324</td>
<td>—</td>
<td>2052</td>
<td>7806-98-9</td>
<td>1181-02-8</td>
</tr>
<tr>
<td></td>
<td>KBM-3033</td>
<td>n-Propyltriethoxysilane</td>
<td>(C₂H₅O)₃SiCH₃</td>
<td>206.4</td>
<td>0.89</td>
<td>1.394</td>
<td>179</td>
<td>77</td>
<td>378</td>
<td>—</td>
<td>2052</td>
<td>20020-09-7</td>
<td>1181-02-8</td>
</tr>
<tr>
<td></td>
<td>KBM-3063</td>
<td>Hexamethyldiethoxysilane</td>
<td>(C₂H₅O)₆SiH</td>
<td>248.4</td>
<td>0.88</td>
<td>1.408</td>
<td>126</td>
<td>98</td>
<td>314</td>
<td>—</td>
<td>2052</td>
<td>8166-375</td>
<td>1181-02-8</td>
</tr>
<tr>
<td></td>
<td>KBM-3083</td>
<td>Octyloxydimethoxysilane</td>
<td>(C₈H₁₇O)₂SiH</td>
<td>276.5</td>
<td>0.88</td>
<td>1.415</td>
<td>126</td>
<td>97</td>
<td>282</td>
<td>—</td>
<td>2052</td>
<td>2943-75-1</td>
<td>1181-02-8</td>
</tr>
<tr>
<td>Silazane</td>
<td>SZ-31</td>
<td>Hexamethyldisilazane</td>
<td>(SiH₃N)₃SiH</td>
<td>161.4</td>
<td>1.77</td>
<td>1.404</td>
<td>126</td>
<td>14</td>
<td>967</td>
<td>—</td>
<td>2052</td>
<td>999-97-3</td>
<td>1181-02-8</td>
</tr>
<tr>
<td></td>
<td>KPM-3504</td>
<td>Silicon with hydrolysable groups</td>
<td>Proprietary</td>
<td>—</td>
<td>0.97</td>
<td>1.405</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>—</td>
</tr>
</tbody>
</table>

*1: Closed cup *2: Open cup at 1 kPa; 7.5 min.

(condensed table values)

Reaction of SZ-31
In this reaction, hydrolysis results in formation of ammonia.

Water repellency (surface properties)

1. Silane repellency on glass substrate

<table>
<thead>
<tr>
<th>Silane</th>
<th>Water contact angle (°)</th>
</tr>
</thead>
<tbody>
<tr>
<td>KBM-13</td>
<td>63</td>
</tr>
<tr>
<td>SZ-31</td>
<td>66</td>
</tr>
<tr>
<td>KBM-3103C</td>
<td>84</td>
</tr>
</tbody>
</table>

2. Surface energy reduction

Silane | γ (mN/m) |
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>KBM-13</td>
<td>20.6</td>
</tr>
<tr>
<td>KBM-13</td>
<td>22.5</td>
</tr>
<tr>
<td>KBM-103</td>
<td>40.0</td>
</tr>
</tbody>
</table>

Condensation reaction properties

Condenosal reaction behavior of methyl and phenyl silanes

- **Trifunctional type**
  In comparing methyltrimethoxysilane (KBM-13) with phenyltrimethoxysilane (KBM-103), it was found that condensation proceeds more slowly for phenyltrimethoxysilane.

  - Me-Si(OH)₃
  - Ph-Si(OH)₃
  - Me-Si(OH)₂
  - Ph-Si(OH)₂
  - Me-Si(OH)
  - Ph-Si(OH)

  Conditions: silane 2%, acetic acid 0.3%, ethanol 50%, water 48%, temp. at 28°C

- **Difunctional type**
  In comparing dimethyldimethoxysilane (KBM-22) with diphenyldimethoxysilane (KBM-2025S), it was found that condensation proceeds more slowly for diphenyldimethoxysilane.

  - Me-Si(OH)₂
  - Me-Si(OH)
  - Ph-Si(OH)₂
  - Ph-Si(OH)

  Conditions: silane 2%, acetic acid 0.3%, ethanol 50%, water 48%, temp. at 28°C

Hydrolysis properties

- **Hydrolysis rates of silanes**
  Hydrolytic properties of different functional groups (room temp.)

- **Silanes of phenyl silane (specified temp.)**
  Hydrolytic properties of long-chain allyl silane (room temp.)
Shin-Etsu’s silane products are a group of organosilicon compounds comprised of alkoxy silanes and silazanes. Silanes have many applications in a wide variety of fields. They are commonly applied to the surface of inorganic substrates to improve water repellency, added to inorganic fillers to improve their dispersibility in organic polymers, and used for surface modification of inorganic materials.

### General Properties

**Type** | **Product name** | **Chemical name** | **Structural formula** | **Physical properties** | **Flash point** | **Flash point (°C)** | **UN hazard classification** | **Kнет No.** | **CAS No.** |
--- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
KBM-13 | Methyltrimethoxysilane | (CH₃)₃Si(OH)₃ | 136.2 0.95 1.369 102 8° 573 | UN1993 | 2.052 | 1185-55-3 |
KBM-22 | Dimethylmethoxysilane | (CH₃)₂Si(OH)₂ | 120.2 0.86 1.371 82 10° 569 | UN1993 | 2.052 | 112-39-6 |
KBM-103 | Phenyltrimethoxysilane | (CH₃)₃Si(OH)₃ | 198.3 1.06 1.473 218 94° 393 | Ict applicable | 3.065 | 2996-92-1 |
KBM-2025S | Dichemethoxysilane | (CH₃)₂SiO(Si(CH₃)₂)₂ | 244.4 1.08 1.541 304 145° 220 | UN1082 | 2.065 | 8443-66-5 |
KBM-3033 | n-Propyltrimethoxysilane | (CH₃)₃Si(OH)₃ | 164.2 0.93 1.388 142 36° 475 | UN1993 | 2.052 | 1067-25-0 |
KBM-3063 | Hexymethyloxysilane | (CH₃)₃Si(CH₂)₂OH | 206.4 0.91 1.406 202 81° 378 | Ict applicable | 3.054 | 3669-19-0 |
KBM-3103C | Dimethyldichlorosilane | (CH₃)₂SiCl₂ | 262.5 0.90 1.421 37° 142° 297 | Ict applicable | 3.054 | 5575-48-4 |
KBM-3066 | 1,6-Bis(trimethoxymethyl)hexane | (CH₃)₂Si(OCH₃)₂ | 326.6 1.02 1.420 31°C 124° 164° 239 | Ict applicable | 2.072 | 87135-01-1 |
KBM-7103 | Trifluoropropyltrimethoxysilane | (CH₃)₂Si(CF₃)₂OH | 218.2 1.14 1.352 144 23° 357 | UN1993 | 2.072 | 429-60-7 |
KBE-04 | Tetraethoxysilane | (CH₂)₄Si(OH)₄ | 208.3 0.93 1.381 168 54° 375 | UN1292 | 2.048 | 78-10-4 |
KBE-13 | Triethoxysilane | (CH₂)₃Si(OH)₃ | 178.3 0.89 1.383 143 40° 437 | UN1993 | 2.052 | 103-52-7 |
KBE-22 | Dicyclohexyl silane | (CH₂)₆Si(OH)₂ | 148.3 0.83 1.384 114 50° 526 | UN2380 | 2.052 | 76-62-8 |
KBE-103 | Phenylmethoxysilane | (CH₃)₃Si(OH)₂ | 240.0 1.69 1.419 236 111° 324 | Ict applicable | 3.065 | 780-69-8 |
KBE-3033 | n-Propylmethoxysilane | (CH₃)₃Si(CH₂)₃CH₂OH | 206.4 0.89 1.394 179 9° 378 | UN1993 | 2.052 | 2030-02-9 |
KBE-3063 | Hexyldimethoxysilane | (CH₃)₂Si(CH₂)₆OH | 248.4 0.88 1.408 37° 9° 314 | Ict applicable | 3.065 | 8166-37-5 |
KBE-3083 | Octyldimethoxysilane | (CH₃)₂Si(CH₂)₈OH | 276.5 0.88 1.415 37°C 126° 282 | Ict applicable | 3.065 | 2943-75-1 |

### Methyltrimethoxysilane (KBM-13)

This reaction, hydrolysis results in formation of ammonia.

```
ON
\[ \text{SiO}_2 + \text{H}_2\text{O} \rightarrow \text{H}_4\text{SiO}_4 + \text{NH}_3 \]
```

### Water repellency (surface properties)

1. **Water repellency (on glass substrate)**
   - **KBM-13**: 63
   - **KBM-3033C**: 84

2. **Surface energy reduction**
   - **Critical surface tension of silane treated surfaces** (γ/cm)
     - **KBM-13**: 20.6
     - **KBM-3033C**: 22.5
     - **KBM-103**: 40.0

---

**Hydrolysis properties**

**Hydrolysis rates of silanes**

<table>
<thead>
<tr>
<th>Silane</th>
<th>Hydrolysis products of long-chain allyl silanes (room temp.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>KBM-13</td>
<td>Diphénylméthoxysilane (KBM-13)</td>
</tr>
<tr>
<td>KBM-1703</td>
<td>Diphénylméthoxysilane (KBM-1703)</td>
</tr>
<tr>
<td>KBM-22</td>
<td>Diphénylméthoxysilane (KBM-22)</td>
</tr>
</tbody>
</table>

**Hydrolysis properties of different functional groups (room temp.)**

**Condensation reaction properties**

**Condensation behavior of methyl and phenyl silanes**

- **Trifunctional type**
  - In comparing methyltrimethoxysilane (KBM-13) with phenyltrimethoxysilane (KBM-103), it was found that condensation proceeds more slowly for phenyltrimethoxysilane.
  - Conditions: silane 2%, acetic acid 0.3%, ethanol 50%, water 48%, temp. at 28°C

- **Difunctional type**
  - In comparing dimethylmethoxysilane (KBM-22) with diphenyldimethoxysilane (KBM-2025S), it was found that condensation proceeds more slowly for diphenyldimethoxysilane.
  - Conditions: silane 2%, acetic acid 0.3%, ethanol 50%, water 48%, temp. at 28°C

---

**Silane**

**Hydrolysis properties**

- **Hydrolysis rates of silanes**
- **Hydrolysis properties of different functional groups (room temp.)**
- **Hydrolysis properties of long-chain allyl silanes (room temp.)**

**Condensation reaction properties**

- **Condensation behavior of methyl and phenyl silanes**
  - **Trifunctional type**
  - **Difunctional type**
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<th>Functional group</th>
<th>Product name</th>
<th>Chemical name</th>
<th>Molecular weight</th>
<th>Specific gravity at 25°C</th>
<th>Refractive index at 25°C</th>
<th>Boiling point °C</th>
<th>Flash point °C</th>
<th>Minimum covering area m²/g</th>
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<th>Packaging</th>
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### Product Features & Packaging Options

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<td>250 &lt;</td>
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### VOC Free Type

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### Product Features & Packaging Options

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#### VOC Free Type

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<tr>
<td>Selecting silane coupling agents</td>
<td>Which to use, methoxyethyl groups or ethoxyethyl groups?</td>
<td>Among the alkoxysilyl groups, methoxyethyl groups hydrolyze faster than ethoxyethyl groups. Please refer to P8 for data on the hydrolyzability of alkoxysilyl groups. Methoxyethyl groups hydrolyze to form methanol, while ethoxyethyl groups hydrolyze to form ethanol. If you are concerned about the release of methanol, you should use ethoxyethyl groups. (KBE Series).</td>
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<tr>
<td></td>
<td>Which to use, trialkoxysilyl groups or dialkoxysilyl groups?</td>
<td>Whereas the hydrolytic condensation of trialkoxysilyl groups leads to three-dimensional crosslinking, hydrolytic condensation of dialkoxysilyl groups leads to two-dimensional crosslinking. This means that dialkoxysilyl groups will be more stable when prepared in an aqueous solution. However, because trialkoxysilyl groups will have a higher crosslinking density with the substrate, adhesion will often be higher.</td>
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<td></td>
<td>How do I select the right organic functional group?</td>
<td>Choosing the optimal organic functional groups will depend on the resin or substrate with which they are used. Please see P9 for a chart of organic functional groups and applicable resins.</td>
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<td></td>
<td>Which resins will show improved adhesion with Silane coupling agents, and which won’t?</td>
<td>For a guide on which types of resins are effective with which resins, see the chart on P9 (Organic functional groups and applicable resins).</td>
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<td>Obtaining samples</td>
<td>How can I obtain samples?</td>
<td>Contact us via the website (<a href="https://www.shinetsu-kemico-global.com/showInquiry.do">https://www.shinetsu-kemico-global.com/showInquiry.do</a>), or talk to a ShinEtsu distributor.</td>
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<td>Preparation method</td>
<td>How do I determine how much silane to use?</td>
<td>The optimal amount can be determined based on the specific surface area of the filler and the minimal coverage area of the silane (Product List on P10-11, Product Characteristics &amp; Package Options on P20-23) (See Note 1). As a rough guide, try using 0.5-2.0 wt % silane vs. the weight of the filler. The user should also be aware that silane coupling agents will be more effective with some types of fillers than others.</td>
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<td>Using silane coupling agents</td>
<td>Treating the filler in advance vs. the integral blend method. Do the results differ?</td>
<td>The typical pretreatment method is to treat the inorganic filler first, then mix it into the organic material. In the integral blend method, the inorganic filler, resin and silane are all added at once, with the pretreatment involved. With the integral blend method, there may be some evaporation of the silane if the materials are heat-treated immediately after mixing. We recommend heating after a suitable curing period. (See Note 2)</td>
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<td>What are some tips regarding treatment methods?</td>
<td>For best results, wash the surface of the inorganic material to remove oils, then treat with a primer.</td>
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<td>What are the drying conditions?</td>
<td>To evaporate the water and initiate the dehydration condensation reaction, we recommend drying at 80-120°C. (See Note 3)</td>
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**Note 1**
- **Treatment amount**
The amount of treatment used for fillers is normally 0.5-2% by weight.
The model equation here can be used as a guide with respect to the amount of silane required to surface-treat fillers to produce a monomolecular film on the filler particles.

- **Weight of filler (g) × Specific surface area of filler (m²/g) = Minimum covering area of the silane (m²/g) Silane treatment amount (g) =**

**Note 2**
- **Effects of aging on organic resin blends**
  - **Application to polyester resin**
When coupling agents are added via the integral blending method and aged at room temperature, the coupling agent migrates to the interface with the inorganic material. The effect is close to that achieved with pretreated glassfiber cloth.

**Note 3**
- **Change in performance caused by dehydration condensation reaction**
  - **Comparison of treatment of polyester laminates**
A comparison was made to evaluate the effect of different drying conditions on effectiveness of treatment. It was found that drying the silane coupling agent for around 5 minutes at 110°C after application achieved the best results.

**Note 4**
- **Vapor pressure curve**
Most silane coupling agents are compounds that have boiling points, and have vapor pressures which are unique to each compound.
The graph below shows the relationship between vapor pressure and temperature for some typical silane coupling agents.

<table>
<thead>
<tr>
<th>Category</th>
<th>Question</th>
<th>Answer</th>
</tr>
</thead>
<tbody>
<tr>
<td>Using silane coupling agents</td>
<td>Can materials be treated with silane coupling agents via vapor deposition?</td>
<td>Yes. See Note 4 for the vapor pressure curves of some commonly used products.</td>
</tr>
<tr>
<td></td>
<td>I’m going to polymerize the silane to make a coating agent. Do different silanes have different degrees of heat resistance?</td>
<td>See Note 5 for heat loss data for the hydrolysis products of some commonly used products.</td>
</tr>
<tr>
<td></td>
<td>Which types of silane coupling agents will be stable when prepared as an aqueous solution?</td>
<td>Ammonosilanes are the most stable, and epoxysilanes (KBM-403) are also stable. (See Note 6)</td>
</tr>
<tr>
<td>Evaluating performance</td>
<td>How can I check the silane treatment?</td>
<td>A simple means of evaluating hydrophobicity-tREATED fillers is the methanol wettabiJity test (See Note 7). For more detailed analysis, 2951 NMR is also effective.</td>
</tr>
<tr>
<td>Storage</td>
<td>How should hydrolyzed treatment liquids be stored?</td>
<td>The storage method may differ depending on the type and number of alkoxysilyl groups, and the type, concentration and pH of the organic functional groups. (See Note 8). Also, adding alcohol will improve shelf life and wetting of inorganic materials.</td>
</tr>
<tr>
<td>Disposal</td>
<td>How can I dispose of leftover liquids and old samples?</td>
<td>Be sure to follow the instructions on the Safety Data Sheet. ShinEtsu does not take back leftover liquids or old samples for disposal.</td>
</tr>
<tr>
<td>Other</td>
<td>What are some precautions for cleaning equipment after use?</td>
<td>Clean filters, tanks and lines immediately after use. These can typically be cleaned with solvents or alkaline cleaners. (See Note 9)</td>
</tr>
<tr>
<td></td>
<td>What are the laws and regulations concerning export to foreign countries?</td>
<td>There are restrictions on countries that can be exported to and on applications and quantities. These are subject to change. Also, containers may differ, so check with a sales representative for details.</td>
</tr>
</tbody>
</table>
Here are some of the questions we frequently get from customers. Check here first to see if your own question has been answered.

**Q & A**

<table>
<thead>
<tr>
<th>Category</th>
<th>Question</th>
<th>Answer</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Selecting silane coupling agents</strong></td>
<td>Which to use, methoxysilyl groups or ethoxysilyl groups?</td>
<td>Among the alkoxysilyl groups, methoxysilyl groups hydrolyze faster than ethoxysilyl groups. Please refer to P8 for data on the hydrolysability of alkoxysilyl groups. Methoxysilyl groups hydrolyze to form methanol, while ethoxysilyl groups hydrolyze to form ethanol. If you are concerned about the release of methanol, you should use ethoxysilyl groups. (KBE Series).</td>
</tr>
<tr>
<td></td>
<td>Which to use, trialkoxysilyl groups or diethoxysilyl groups?</td>
<td>Whereas the hydrolytic condensation of trialkoxysilyl groups leads to three-dimensional crosslinking, hydrolytic condensation of diethoxysilyl groups leads to two-dimensional crosslinking. This means that diethoxysilyl groups will be more stable when prepared in an aqueous solution. However, because trialkoxysilyl groups will have a higher crosslinking density with the substrate, adhesion will often be higher.</td>
</tr>
<tr>
<td></td>
<td>How do I select the right organic functional group?</td>
<td>Choosing the optimal organic functional groups will depend on the resin or substrate with which they are used. Please see P9 for a chart of organic functional groups and applicable resins.</td>
</tr>
<tr>
<td></td>
<td>Which resins will show improved adhesion with Silane coupling agents, and which won’t?</td>
<td>For a guide on which types of silanes are effective with which resins, see the chart on P9 (Organic functional groups and applicable resins).</td>
</tr>
</tbody>
</table>

| **Obtaining samples** | How can I obtain samples? | Contact us via the form on our website (https://www.shinetsu-silicone-global.com/showInquiry.do) or talk to a ShinEtsu distributor. |

| **Preparation method** | How do I determine how much silane to use? | The optimal amount can be determined based on the specific surface area of the filler and the minimum coverage area of the silane (Product List on P10-11, Product Characteristics & Packaging Options on P20-23). (See Note 1). As a rough guide, try using 0.5-2.0% vs. silane vs. the weight of the filler. The user should also be aware that silane coupling agents will be more effective with some types of fillers than with others. |
| | Treating the filler in advance vs. the integral blend method. Does the results differ? | The typical pretreatment method is to treat the inorganic filler first, then mix it into the organic material. In the integral blend method, the inorganic filler, resin and silane are all added together, with a pretreatment involved. With the integral blend method, there may be some evaporation of the silane if the materials are heat-treated immediately after mixing. We recommend heating after a suitable curing period. (See Note 2). |

| **Using silane coupling agents** | What are some tips regarding treatment methods? | For best results, wash the surface of the inorganic material to remove oils, then treat with a primer. |
| | What are the drying conditions? | To evaporate the water and initiate the dehydration condensation reaction, we recommend drying at 80-120°C. (See Note 3). |

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**Note 1**

- **Treatment amount**
  - The amount of treatment used for fillers is normally 0.5-2.0% by weight.
  - The model equation here can be used as a guide with respect to the amount of silane required to surface-treat fillers to produce a monomolecular film on the filler particles.

- **Silane treatment amount (g)**
  - Weight of filler (g) × Specific surface area of filler (m²/g) Minimun covering area of the silane (m²/g)

**Note 2**

- **Effects of aging on organic resin blends**
  - **Application to polyester resin**
  - When coupling agents are added via the integral blending method and aged at room temperature, the coupling agent migrates to the interface with the inorganic material. The effect is close to that achieved with pretreated glass fiber cloth.

**Note 3**

- **Change in performance caused by dehydration condensation reaction**
  - **Comparison of treatment of polyester laminates**
  - The graph below shows the relationship between vapor pressure and temperature for some typical silane coupling agents. Most silane coupling agents are compounds that have boiling points, and have vapor pressures which are unique to each compound. The graph below shows the relationship between vapor pressure and temperature for some typical silane coupling agents.

- **Vapor pressure curve**
  - Most silane coupling agents are compounds that have boiling points, and have vapor pressures which are unique to each compound. The graph below shows the relationship between vapor pressure and temperature for some typical silane coupling agents.
Handling Precautions

- **Product quality, storage and handling**
  1. Store in a cool, dark place (out of direct sunlight in a place cooler than room temperature where there is no risk of condensation) and avoid exposure to humidity.
  2. Products containing silanes that polymerize with heat (KBM-1403, KBM-5103, X-12-1048, X-12-1050) should be kept refrigerated (0-5°C).
  3. Shin-Etsu guarantees the quality of its silane coupling agents when in a sealed, unopened state. When exposed to water or moisture, silane coupling agents undergo hydrolysis and degrade, and in the process will release substances which include methanol and hydrogen chloride. Do not leave product containers open, and always close tightly after use to prevent water and moisture from entering the container. Ideally, when closing containers, the air in the container should be replaced with dry nitrogen. After opening, products should be used up as quickly as possible, since products stored in bottles may become degraded through exposure to the alkali content of the glass.
  4. Isocyanate silane and protected functional group silanes cannot be used as part of pretreatment methods that involve adding them to water to induce hydrolysis. Isocyanate silanes will release carbon dioxide gas and deteriorate, while protected functional group silanes will lose their protective groups and deteriorate.

- **Safety & hygiene**
  1. Ensure there is proper ventilation when using these products. Avoid breathing of vapors from products or their hydrolysis products, and avoid bodily contact.
  2. Wear rubber gloves, safety glasses and other protective gear to prevent contact with the skin and mucous membranes. In case of contact, wash immediately and thoroughly with running water.
  3. In case of eye contact, immediately flush eyes with plenty of running water, and consult a physician if necessary.
  4. If products get on clothing, wash off with running water.
  5. Be sure to wash hands thoroughly after handling products and before eating, drinking or smoking.
  6. In case of spills, wash with plenty of water or soak up the spilled liquid using rags or sand and dispose of it by incineration.
  8. Please read the Safety Data Sheets (SDS) before use. SDS can be obtained from our Sales Department.

- **Additional information**
  1. If you need a special high purity product for use in electronics materials manufacturing or other applications, please discuss your needs with a Shin-Etsu sales representative.
  2. Contact the Shin-Etsu Sales Department to discuss issues concerning the export of these products.
Q & A

Note 5
◆ Heating loss of silane hydrolsates
  Measured in a heated state.

Note 6
◆ Condensation behavior of amino silane in aqueous solution
  An amino silane (KBM-903) was found to be very stable in aqueous solutions.

Note 7
◆ Checking the results of hydrophobic treatment
  1. Weigh out 0.5 g of the sample into a 500 mL round-bottomed flask.
  2. Add 50 mL of ion-exchange softened water to it and agitate with a magnetic stirrer.
  3. While continuing agitation, drip in methanol using a burette.
     When all of the sample is in suspension in the softened water, note the amount of methanol that has been dripped in.
  4. Determine hydrophobicity using the following equation.

  Hydrophobicity =
  Methanol drip amount (mL) × 100
  Methanol drip amount (mL) + ion-exchange softened water amount (mL)

Note 8
◆ Stability of epoxy silane-water solutions and pH
  
Note 9
◆ Cleaning silane from reactors, containers, pipes, etc.
  These methods are good for cleaning, but keep in mind that results will vary depending on the type of silane (hydrophilic, hydrophobic), the material being cleaned (glass, metal, plastic), whether the silane has simply adhered to or has reacted onto the surface, and how much has built up. Use proper caution when handling solvents and alcohols.

  1. Cleaning with solvents
     This method involves cleaning the silane by placing equipment in an organic solvent (alcohol, aromatic solvent, etc.). Agitation and heating will yield better cleaning results. With some physical effort, such as scrubbing with a brush, the results will be even better. Clean the inside of pipes by flushing them with large amounts of solvent.

  2. Cleaning with alcohols
     If the silane has reacted to the surface or has built up in significant amounts, cleaning with a solvent will not be sufficient. If so, the silane can be removed by placing equipment in an alkaline water solution (e.g., 50% potassium hydroxide-water solution). Again, agitation and heating will yield better cleaning results. When cleaning stainless steel, the solution can be heated to around 80°C without problems. However, glass-lined equipment will be damaged at this temperature, so such equipment should not be soaked for more than a few hours at temperatures not higher than around 50°C. After cleaning, be sure to remove the alkaline component by washing thoroughly with water or alcohol.

Note 10
◆ Handling Precautions
 ◆ Product quality, storage and handling
  1. Store in a cool, dark place (out of direct sunlight) in a place cooler than room temperature where there is no risk of condensation and avoid exposure to humidity.

  Products containing silanes that polymerize with heat (KBM-1043, KBM-5103, X-12-1048, X-12-1050) should be kept refrigerated (0-5°C).

  2. Shin-Etsu guarantees the quality of its silane coupling agents when in a sealed, unopened state. When exposed to water or moisture, silane coupling agents undergo hydrolysis and degrade, and in the process will release substances which include methanol and hydrogen chloride. Do not leave product containers open, and always close tightly after use to prevent water and moisture from entering the container. Ideally, when closing containers, the air in the container should be replaced with dry nitrogen.

     After opening, products should be used up as quickly as possible, since products stored in bottles may become degraded through exposure to the alkali content of the glass.

  3. Isocyanate silane and protected functional group silanes cannot be used as part of pretreatment methods that involve adding them to water to induce hydrolysis. Isocyanate silanes will release carbon dioxide gas and deteriorate, while protected functional group silanes will lose their protective groups and deteriorate.

 ◆ Safety & hygiene
  1. Ensure there is proper ventilation when using these products. Avoid breathing of vapors from products or their hydrolysis products, and avoid bodily contact.

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  2. Contact the Shin-Etsu Sales Department to discuss issues concerning the export of these products.
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Users are solely responsible for making preliminary tests to determine the suitability of products for their intended use. Statements concerning possible or suggested uses made herein may not be relied upon, or be construed, as a guaranty of no patent infringement.

For detailed information regarding safety, please refer to the Safety Data Sheet (SDS).

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Users must never use the silicone products described herein for the purpose of implantation into the human body and/or injection into humans.

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