Chemical Name

Bis(3-triethoxysilylpropyl)tetrasulfide

Chemical Structure

Background

Heretofore, carbon black has been used as a reinforcing filler for rubber because carbon black provides higher reinforcement and more excellent abrasion resistance than other fillers. Recently, because of social requirements to save energy and to save resources, particularly to cut down fuel consumption of automobiles, a decrease in the heat buildup of rubber compositions is also required.

For decreasing the heat buildup of rubber compositions by using carbon black, use of a small amount of carbon black or carbon black having a large particle size is considered. It is, however, well known that, in both methods, decreasing heat buildup is in a contradictory relation with improving reinforcement and abrasion resistance of a rubber composition.

On the other hand, silica is known as a filler which provides decreased heat buildup of a rubber composition. However, silica particles tend to cohere together due to hydrogen bonding of silanol groups which are functional groups on the surfaces of the silica particles. For improving the dispersion of silica particles into rubber, the mixing time must be increased. When dispersion of silica particles into rubber is insufficient, a problem arises in that processability in processes such as extrusion and the like deteriorates due to the increase in the Mooney viscosity.

Moreover, the surfaces of the silica particles are acidic. Therefore, there are problems in that basic substances used as vulcanization accelerators are absorbed such that vulcanization is not carried out sufficiently, and a sufficient modulus of elasticity is not obtained.
In order to solve these problems, we developed various types of silane coupling agents. For example, SiSiB® PC2000 and SiSiB® PC2200. In the following article we would like to inform you about the silane coupling agent SiSiB® PC2000, SiSiB® PC2200 and its other commercial forms SiSiB® PC2000B and SiSiB® PC2000S.

**Introduction**

SiSiB® PC2000 is a bifunctional polysulfidic organosilane for the rubber industry defined chemically as Bis(3-triethoxysilylpropyl)tetrarsulfide. It is used to improve the reinforcing capability of fillers with silanol group on their surface (e.g., silicas, silicates, clay, etc.), and also as an integral part of curing systems to improve crosslinking network properties.

### Typical Physical Properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>CAS No.</td>
<td>40372-72-3</td>
</tr>
<tr>
<td>EINECS No.</td>
<td>254-896-5</td>
</tr>
<tr>
<td>Empirical Formula</td>
<td>C_{18}H_{42}O_{6}S_{4}Si_{2}</td>
</tr>
<tr>
<td>Molecular Weight</td>
<td>539</td>
</tr>
<tr>
<td>Color and Appearance</td>
<td>Yellowish liquid</td>
</tr>
<tr>
<td>Density (16/24°C) (g/cm³)</td>
<td>1.1 +/- 0.02</td>
</tr>
<tr>
<td>Secondary Components</td>
<td>Propyltriethoxysilane</td>
</tr>
<tr>
<td>Boiling Point at 1013 mbar(°C)</td>
<td>Decomposition above 250</td>
</tr>
<tr>
<td>Pour Point (°C)</td>
<td>App. –80</td>
</tr>
<tr>
<td>Flash Point (°C)</td>
<td>&gt;100</td>
</tr>
<tr>
<td>Volatiles Components(%)</td>
<td>&lt;= 4.0</td>
</tr>
<tr>
<td>Average Chain Length(%)</td>
<td>3.75 +/- 0.15</td>
</tr>
<tr>
<td>Total Sulfur (standard value)(%)</td>
<td>22.7 +/- 0.8</td>
</tr>
</tbody>
</table>

**Solubility:**

Soluble in Primary alcohols, ketones, benzene, toluene, dimethylformamidine, chlorinated hydrocarbons, cetonitrile, dimethylsulfoxide; Insoluble in Water;

**Effects**

When used in rubber compounds, it produces these effects:
Coupling agent for non-black pigments.
Cure equilibrium for reversion resistance.
Curing agent for good heat aging.

**Coupling Agent** - With as little as 0.5 to 1.0 phr with clay fillers and 1.0 to 4.0 phr for silica pigments, SiSiB® PC2000 couples the non-black pigment and elastomers resulting in increases in modulus and increase in abrasion resistance.

**Cure Equilibrium** - SiSiB® PC2000 has four sulfur atoms positioned in the center.

At cure temperatures, these participate with sulfur in producing polysulfidic crosslinks. The SiSiB® PC2000 replaces crosslinks broken during cure, resulting in reversion resistant, and with proper compounding, reversion free compounds. This is known as equilibrium cure. The dynamic flex characteristics, E.G., heat generation and crack growth, are dramatically improved.

**Curing Agent** - Removing all sulfur from the compound for NR, SBR, NBR and replacing it with SiSiB® PC2000 and certain thiuram accelerators, produces compounds with excellent heat aging characteristics in addition to the coupling effects.

SiSiB® PC2000 is a silane coupling agent that has crosslinking and accelerator activity in rubber compounds.

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**Suggest Dosage**

Suggested dosage per 100 parts of filler:
- For silica-------------------3~13 parts
- For clay and talc---------0.5~1.0 parts

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**Application Area**

Footwear
- Abrasion resistance
- Cutting and chunking resistance
- Flex life improvement

Rolls
- Abrasion resistance
- Aging resistance
- Processing
- Set reduction (better load bearing)
- Reduced water swell
- Lower hysteresis

Mechanical Molded Goods
- Increased modulus
- Better heat aging
- Compression set reduction
- Dynamic property improvement
- Reduced swell to polar liquids
- Filler substitution (non-black for black)

Hose
- Improved abrasion on cover
- Better heat aging
- Increased modulus
- Lower compression set
- Improved adhesion to reinforcing elements

Solid Tires
- Improved abrasion
- Lower hysteresis
- Higher modulus
- Improved processing
- Possibly better adhesion

Tires
- Treads for abrasion, hot tear
- Carcass for adhesion and/or filler substitution
- Breaker (belt) stocks for adhesion

Belts
- Increased abrasion
- Improved reversion resistance
- Reduced cost with clay substitution for black
- Improved cord adhesion
- Increased flex life and modulus

V Belts
- Increased modulus
- Improved abrasion
- Longer flex life
- Improved adhesion to reinforcing elements
SiSiB® PC2000 SILANE

Packing and Storage

SiSiB® PC2000 is supplied in net weight 200Kg steel drum or 1000Kg IBC tote.

In the unopened original container SiSiB® PC2000 has a shelf life of five years in a dry and cool place.

Notes

All information in the leaflet is based on our present knowledge and experience. We reserve the right to make any changes according to technological progress or further developments. Performance of the product described herein should be verified by testing.

We specifically disclaim any other express or implied warranty of fitness for a particular purpose or merchantability. We disclaim liability for any incidental or consequential damages.

Please send all technical questions concerning quality and product safety to: silanes@SiSiB.com.