Silicones Simplified

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*A Guide to Silane Solutions*

# The Basics of Silane Chemistry

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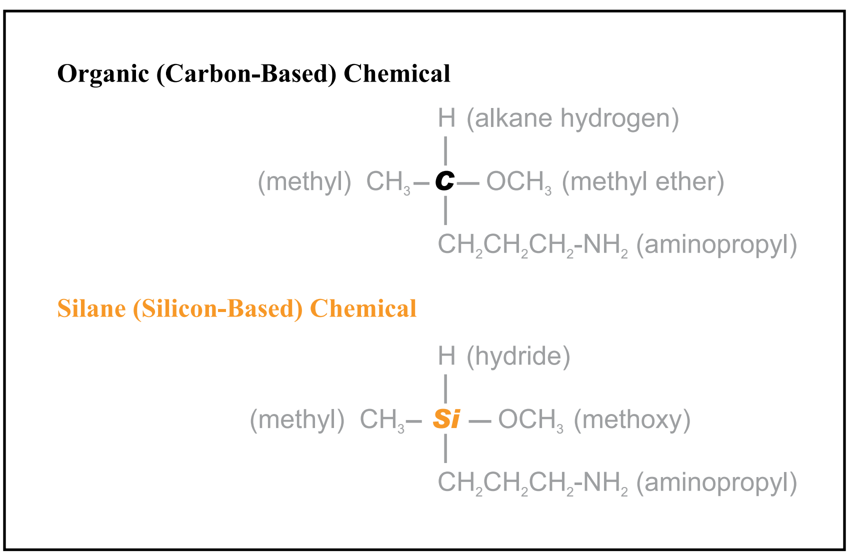
Silicon is in the same family of elements as carbon in the periodic table. In their most stable state, silicon and carbon will both conveniently bond to four other atoms; but silicon-based chemicals exhibit significant physical and chemical differences compared to analogous carbon-based chemicals. Silicon is more electropositive than carbon, does not form stable double bonds, and is capable of very special and useful chemical reactions. Silicon-based chemicals include several types of monomeric and polymeric materials.

**Figure 1. Carbon vs. silicon chemistry.**



Monomeric silicon chemicals are known as silanes. A silane structure and an analogous carbon-based structure are shown in Figure 1. The four substituents have been chosen to demonstrate differences and similarities in physical and chemical properties between silicon- and carbon-based chemicals. A silane that contains at least one carbon-silicon bond ($CH_3$-Si-) structure is known as an organosilane. The carbon-silicon bond is very stable, very non-polar and gives rise to low surface energy, non-polar, hydrophobic effects. Similar effects can be obtained from carbon-based compounds, although these effects are often enhanced with silanes. The silicon hydride (–Si-H) structure is very reactive. It reacts with water to yield reactive silanol (-Si-OH) species and, additionally, will add across carbon-carbon double bonds to form new carbon-silicon-based materials. The methoxy group on the carbon compound gives a stable methyl ether, while its attachment to silicon gives a very reactive and hydrolyzable methoxysilyl structure. The organofunctional group, the aminopropyl substituent, will act chemically the same in the organosilicon compound as it does in the carbon-based compound. The distance of the amine, or other organofunctional group, from silicon will determine whether the silicon atom affects the chemistry of the organofunctional group. If the organic spacer group is a propylene linkage (e.g., $-CH_2CH_2CH_2-$), then the organic reactivity in the organofunctional silane will be similar to organic analogs in carbon chemistry. Certain reactive silanes, particularly vinyl silanes ($-Si-CH=CH_2$) and silicon hydrides (-Si-H), are useful reactive groups in silicon chemistry, even though the reactive group is attached directly to the silicon atom.

Attachment of chlorine, nitrogen, methoxy, ethoxy or acetoxy directly to silicon yields chlorosilanes, silylamines (silazanes), alkoxysilanes and acyloxysilanes, respectively, that are very reactive and exhibit unique inorganic reactivity. Such molecules will react readily with water, even moisture adsorbed on a surface, to form silanols. These silanols then can react with other silanols to form a siloxane bond (-Si-O-Si-), a very stable structure; or in the presence of metal hydroxyl groups on the surface of glass, minerals or metals, silanols will form very stable –Si-O-metal bonds to the surface. This is the key chemistry that allows silanes to function as valuable surface-treating and coupling agents.

Chloro-, alkoxy-, and acetoxy-silanes, and silazanes (-Si-NH-Si) will react readily with an active hydrogen on any organic chemical (e.g., alcohol, carboxylic acid, amine, phenol or thiol) via a proc-ess called silylation.

$$R_3Si\text{-}Cl + R'OH \rightarrow R_3Si\text{-}OR' + HCl$$

Silylation is very useful in organic synthesis to protect functional groups while other chemical manipulations are being performed. The silylated organofunctional group can be converted back to the original functional group once the chemical operation is completed. Silylation is very important in the manufacture of pharmaceutical products.

## Typical Silane Applications

**Coupling Agent:** Organofunctional alkoxysilanes are used to couple organic polymers to inorganic materials. Typical of this application are reinforcements, such as fiberglass and mineral fillers, incorporated into plastics and rubbers. They are used with both thermoset and thermoplastic systems. Mineral fillers, such as silica, talc, mica, wollastonite, clay and others, are either pretreated with silane or treated *in situ* during the compounding process. By applying an organofunctional silane to the hydrophilic, non-organoreactive filler, the surfaces are converted to reactive and organophilic. Fiberglass applications include auto bodies, boats, shower stalls, printed circuit boards, satellite dishes, plastic pipes and vessels, and many others. Mineral-filled systems include reinforced polypropylene, silica-filled molding compounds, silicon-carbide grinding wheels, aggregate-filled polymer concrete, sand-filled foundry resins and clay-filled EPDM wire and cable. Also included are clay- and silica-filled rubber for automobile tires, shoe soles, mechanical goods and many other applications.

**Adhesion Promoter:** Silane coupling agents are effective adhesion promoters when used as integral additives or primers for paints, inks, coatings, adhesives and sealants. As integral additives, they must migrate to the interface between the adhered product and the substrate to be effective. As a primer, the silane coupling agent is applied to the inorganic substrate before the product to be adhered is applied. In this case, the silane is in the optimum position (in the interphase region), where it can be most effective as an adhesion promoter. By using the right silane coupling agent, a poorly adhering paint, ink, coating, adhesive or sealant can be converted to a material that often will maintain adhesion even if subjected to severe environmental conditions.

**Hydrophobing and Dispersing Agent:** Alkoxysilanes with hydrophobic organic groups attached to silicon will impart that same hydrophobic character to a hydrophilic inorganic surface. They are used as durable hydrophobing agents in construction, bridge and deck applications. They are also used to hydrophobe inorganic powders to make them free-flowing and dispersible in organic polymers and liquids.

**Crosslinking Agent:** Organofunctional alkoxysilanes can react with organic polymers to attach the trialkoxysilyl group onto the polymer backbone. The silane is then available to react with moisture to crosslink the silane into a stable, three-dimensional siloxane structure. Such a mechanism can be used to crosslink plastics, especially polyethylene, and other organic resins, such as acrylics and urethanes, to impart durability, water resistance and heat resistance to paints, coatings and adhesives.

**Moisture Scavenger:** The three alkoxy groups on silanes will hydrolyze in the presence of moisture to convert water molecules to alcohol molecules. Organotrialkoxysilanes are often used in sealants and other moisture-sensitive formulations as water scavengers.

**Polypropylene Catalyst "Donor":** Organoalkoxysilanes are added to Ziegler-Natta catalyzed polymerization of propylene to control the stereochemistry of the resultant polypropylene. The donors are usually mono- or di-organo silanes with corresponding tri- or di-alkoxy substitution on silicon. By using specific organosilanes, the tacticity (and hence the properties) of the polypropylene is controlled.

**Silicate Stabilizer:** A siliconate derivative of a phosphonate-functional trialkoxysilane functions as a silicate stabilizer to prevent agglomeration and precipitation of silicates during use. The predominant application is in engine coolant formulations to stabilize the silicate corrosion inhibitors.

## Benefits of Silanes

Below is a listing of some industries that can utilize XIAMETER® brand silanes and the corresponding benefits.

| Industries | Benefit(s) |
|---|---|
| **Fiberglass and Composites** | Improved:<br>• Mechanical strength of the composites<br>• Electrical properties<br>• Resistance to moisture attack at the interface<br>• Wet-out of the glass fiber<br>• Fiber strand integrity, protection and handling<br>• Resistance to hot solder during fabrication<br>• Performance in cycling tests from hot to cold extremes |
| **Mineral and Filler Treatment** | Improved:<br>• Adhesion between the mineral and the polymer<br>• Wet-out of the mineral by the polymer<br>• Dispersion of the mineral in the polymer<br>• Electrical properties<br>• Mechanical properties<br>Reduced viscosity of the filler/polymer mix |
| **Paints, Inks and Coatings** | Improved:<br>• Abrasion resistance<br>• Adhesion<br>• Flow<br>• Crosslinking to improve thermal stability and durability<br>• Pigment and filler dispersion<br>• UV resistance<br>• Water and chemical resistance |
| **Plastics and Rubber** | • Coupling and dispersing agents for fillers in rubber and plastics formulations<br>• Polymerization modifiers in the synthesis of polypropylene<br>• Crosslinking agents for polyethylene homopolymers and copolymers<br>• Inorganic filler in place of carbon black in the reinforcement of rubber |
| **Adhesives and Sealants** | Improved:<br>• Initial adhesion<br>• Adhesive bond with longer life<br>• Temperature resistance<br>• Chemical resistance |
| **Water Repellents and Surface Protection** | Improved:<br>• Water repellency<br>• Long-term durability<br>• UV stability<br>• Depth of penetration<br>• Water vapor permeability<br>• Dilution capability and stability<br>• Appearance |

## Product Information

A complete list of XIAMETER® brand silanes is available at xiameter.com.

In addition, Dow Corning Corporation also offers a wide variety of *Dow Corning*® brand specialty silicone material and service options as well as other silicon-based materials available to help you keep your innovative edge in the marketplace. Visit dowcorning.com to learn more about the many additional silicone and silicon-based options available to you from Dow Corning.



Printed in USA AGP9791 Form No. 95-718-01