

Technical Data Sheet

XIAMETER™ OFS-6076 Silane

Coupling agent between inorganic and organic materials

Features & Benefits

- Versatile chloroalkyl functionality
- Three hydrolyzable alkoxysilyl groups
- Good wet-out
- Improved adhesion
- Increased dry and wet flexural strength

Composition

• 3-chloropropyltrimethoxysilane supplied as liquid

Applications

XIAMETER™ OFS-6076 Silane is used as a coupling agent. Several articles document its use in improving the adhesion of glass fibers to organic polymers and resins.^{1, 2, 3}

A 3-chloroalkyl-functional silane has been used as an additive in a urethane adhesive formulation.⁴ Its addition to the isocyanate prepolymer caused no adverse effect in the prepolymer viscosity.

High peel strengths were observed for silane - modified urethane - to - aluminum panels, and this adhesion was maintained even after prolonged exposure of the test specimen to elevated temperature and humidity.

The 3-chloropropyltrimethoxysilane is also a good coupling agent for epoxy resins to glass in laminates.² The resin had good wet-out on the treated glass fabric. More important, both flexural strength as well as wet and dry tensile strength were significantly improved over that seen with epoxy- and amine- functional silanes in these evaluations.

XIAMETER OFS-6076 Silane is also an effective coupling agent for treating glass fabric used in polystyrene laminates.^{3, 5} The flexural strength of test laminates was unchanged after two hours in boiling water, and the compressive strength improved slightly over that found under dry conditions.

The wettability and structure of a film of 3-chloropropyltrimethoxysilane deposited on glass, steel and aluminum were also studied.⁶ Measurements indicated that such a film provides a very high critical surface tension compared with other silanes and is similar to polyvinyl chloride in surface polarity.

Typical Properties

Specification Writers: These values are not intended for use in preparing specifications.

Property	Unit	Result
Apperance		Clear, colorless to slightly yellow
Specific Gravity at 25°C (77°F)		1.09
Refractive Index at 25°C (77°F)		1.418
Purity	percent	97
Flash Point, closed cup	°C (°F)	51 (124)
Boiling Point at 760 mm Hg	°C (°F)	196 (385)
Molecular Weight	g/mole	198.5

Description

XIAMETER OFS-6076 Silane is an ambifunctional compound containing chloroalkyl functionality and three hydrolyzable alkoxysilyl groups.

Possessing both organic and inorganic reactivity, the product has a dual nature and can react with organic polymers and also with glass, metal and other inorganic materials. As a coupling agent, it can be used either as an additive to the polymer or as a pretreatment on inorganic surfaces. Many chemical reactions are possible, providing significant improvements in polymer/filler or polymer/substrate interaction.

Chemically, XIAMETER OFS-6076 Silane has the formula:

$$CI(CH2)3Si(OCH3)3.$$

Chemistry

Two types of reactivity must be considered with an organofunctional silane such as XIAMETER OFS-6076 Silane. The reactivity of the chloroalkyl group parallels the reactions of most 1 -chloroalkanes, while the tri-methoxysilyl portion exhibits reactivity typical of any such trialkoxysilane.

Chloroalkyl Reactivity

XIAMETER OFS-6076 Silane is referred to in the following examples as RCI, where "R" is the $(CH_3O)_3Si(CH_2)_3$ – group. For exact reaction conditions, consult the referenced source.

Thiourea⁷

$$S \\ \parallel \\ RCl + H_2NCNH_2 + NH_3 \rightarrow \\ \Delta \\ RSH + (NH_2)_2C = NH_2^+Cl^-$$

Sodium Hydrosulfide8

$$RCl + NaSh \xrightarrow[H,S]{CH,CH} RSH + NaCl$$

Chemistry (Cont.)

Cyanide and Isocyanate Salts^{9,10}

$$\begin{array}{c} \text{DMF} \\ \text{RCl} + \text{NaCN} \rightarrow \text{RCN} + \text{NaCl} \\ \\ \text{RCl} + \text{KNCO} + \text{CH}_3\text{OH} \stackrel{\text{DMF}}{\rightarrow} \\ \\ \text{O} \\ \parallel \\ \text{RNHCCH}_3 \rightarrow \text{RNCO} + \text{CH}_3\text{OH} + \text{KCl} \end{array}$$

Amines and Diamines 11,12

$$\begin{array}{l} RCl + H_2NCH_2CH_2NH_2 \ (\text{in excess}) \longrightarrow \\ RNHCH_2CH_2NH_2 + H_2NCH_2CH_2NH_3 ^+Cl^- \end{array}$$

$$\begin{array}{c} RC1 + NH_{3 \; (in \; excess)} \longrightarrow \\ RNH_{2} + NH_{4}C1 \end{array}$$

The synthesis and chemistry of over fifty 3-aminopropyl silicon compounds have also been described.¹³

Trimethoxysilyl Reactivity

The trimethoxysilyl portion of the molecule undergoes the typical chemistry of alkoxysilanes:

Hydrolysis

The alkoxysilyl group is subject to hydrolysis in water or water/alcohol solutions. Investigations have been conducted to determine the optimum conditions for maximum solubility and the nature of the hydrolysis product in aqueous solutions.⁵

In either case, the initial product of hydrolysis is a silanol; or in the case of XIAMETER OFS-6076 Silane, a silanetriol.

$$Cl(CH_2)_3Si(OCH_3)_3 + 3H_2O \rightarrow$$

 $[Cl(CH_2)_3Si(OH)_3] + 3CH_3OH$

This silanetriol will eventually con-dense to form a resinous material. The ultimate product of condensation is a silsesquioxane:

$$\begin{aligned} \text{[Cl(CH2)3Si(OH)3]} \rightarrow \\ \text{Cl(CH2)3SiO3/2 + 1.5 H2O} \end{aligned}$$

Alcoholysis

Alkoxysilanes will react with alcohols to form an equilibrium mixture of products.

Equilibrium is rapidly established in the presence of acidic or basic catalysts.

Solubility

XIAMETER OFS-6076 Silane is readily soluble in aliphatic and aromatic solvents, chlorinated solvents, ethers, esters and ketones. It is also soluble in alcohols, but exchange of alkoxy groups on silicon should be expected. This is not nearly so important with higher molecular weight secondary and tertiary alcohols as with lower primary alcohols:

≡SiOCH₃ + ROH ← ≡SiOR + CH3OH

XIAMETER OFS-6076 Silane is partially soluble in formamide.

In water, its solubility is a function of pH.5 Dilute aqueous solutions of XIAMETER OFS-6076 Silane in water are made by:

- 1. Acidify water to pH 3.5 to 4.0 with acetic acid.
- 2. Add XIAMETER™ OFS-6076 Silane (less than 3.0 percent) to the acidified water with stirring.
- 3. Stir until the silane is dissolved (may take 15 minutes or longer).

	Approximate Solubility (Parts XIAMETER OFS-6076 Silane to pH 100 parts H2O)	
4	3	
7	<1	
10	<1	

Handling Precautions

PRODUCT SAFETY INFORMATION REQUIRED FOR SAFE USE IS NOT INCLUDED IN THIS DOCUMENT. BEFORE HANDLING, READ PRODUCT AND SAFETY DATA SHEETS AND CONTAINER LABELS FOR SAFE USE, PHYSICAL AND HEALTH HAZARD INFORMATION. THE SAFETY DATA SHEET IS AVAILABLE ON THE DOW WEBSITE AT WWW.CONSUMER.DOW.COM, OR FROM YOUR DOW SALES APPLICATION ENGINEER, OR DISTRIBUTOR, OR BY CALLING DOW CUSTOMER SERVICE.

Usable Life And Storage

When stored in original, unopened containers at or below 32°C (90°F), this product has a usable life of 36 months from date of production.

Limitations

This product is neither tested nor represented as suitable for medical or pharmaceutical uses.

Shipping Limitations

DOT Classification: Combustible.

Health And Environmental Information

To support customers in their product safety needs, Dow has an extensive Product Stewardship organization and a team of product safety and regulatory compliance specialists available in each area.

For further information, please see our website, www.consumer.dow.com or consult your local Dow representative.

References

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