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SILICONES & SILICON-CONTAINING POLYMERS

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AMBER GLASS BOTTLES



WHITE PLASTIC BOTTLES



WHITE PLASTIC PAILS		WHITE STEEL PAIL
1 Gallon	5 Gallons	5 Gallons



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Container photos are to show packaging options only – UCT does not sell empty containers.

Note:

Not all products are available in all sizes.

ORGANOSILICON NOMENCLATURE

The nomenclature of organosilanes follows some simple rules. Where feasible, as with the simple systems, they are named as derivatives of silane or disilane, etc.

> SiH₄ H₃SiSiH₃

silane disilane

When the silicon contains two or more different groups attached these are named in alphabetical order when this does not create confusion. For example,

> Me₂SiCl₂ MePhSiCl₂

dichlorodimethylsilane methylphenyldichlorosilane (not dichloromethylphenylsilane, which could be misconstrued as being Cl₂CHPhSiH₂)

Silazanes are named disilazane, trisilazane and so forth depending on the number of silicon atoms in the structure.



Siloxanes are named in a similar fashion to the silazanes.

H ₃ Si–O–SiH ₃	disiloxane
Me ₃ Si–O–SiMe ₃	hexamethyldisiloxane
Me ₃ Si–O–SiMe ₂ –O–SiMe ₂ CH=CH ₂	1-vinylheptamethyltrisiloxane

When the silicon group must be named as a unit, the following general names are used:

H₃Si–	silyl
$H_2Si=$	silylene
H₃SiSiH₂–	disilanyl
H₃SiO–	siloxanyl
Me3Si–	trimethylsilyl
tBuMe₂Si–	tert-butyldimethylsilyl
Me₃SiO–	trimethylsiloxy

The cyclic silanes are named:



Hydroxy derivatives are named as silanols:

H₃SiOH	silanol
$H_2Si(OH)_2$	silane diol
PhSi(OH)₃	phenylsilane triol
Ph₃SiONa	sodium triphenylsilanolate

When the question of whether to use organic or organosilicon nomenclature arises, the tendency is to employ the organic nomenclature.

Me ₃ SiCH ₂ CN	α-trimethylsilylacetonitrile
Me ₃ SiCHCICH ₃	1-trimethylsilyl-1-chloroethane
	or (1-chloroethyl)trimethylsilane
Me ₃ SiCH(OH)CH ₃	1-trimethylsilylethanol
PhCO ₂ SiEt ₃	triethylsilylbenzoate

The General Electric siloxane notation is used as a shorthand notation for the methylsiloxanes and polymethylsiloxanes.

The various groups utilized in this format are:



MM $MD_{10}M$ M_3QDTM_2

Examples are:

Me ₃ Si–O–SiMe ₃	
Me ₃ Si(OSiMe ₂) ₁₀ OSiMe ₃	
(Me ₃ SiO) ₃ Si-O-SiMe ₂ -OSiMe(OMe) ₂	



AN INTRODUCTION TO ORGANOSILICON CHEMISTRY

Organosilicon compounds have been known since 1863 when Friedel and Crafts¹ first reported the synthesis of tetraethylsilane from diethylzinc and silicon tetrachloride. The first systematic studies on organosilanes were carried out by Frederick S. Kipping and his coworkers at the University of Nottingham from 1898 to 1939,² work which the American Chemical Society has memorialized by presenting the biannual Frederick Stanley Kipping award for "distinguished achievement in research and organosilicon chemistry." It was not until the 1940's, however, that organosilicon chemistry bloomed following the success of the silicone polymers. Today on the industrial and commercial side of the ledger, organosilanes are found in applications ranging from solutions to synthetic problems to healthcare products to computer chips. On the research side of the ledger they are being investigated as synthetic reagents and pushed ever further in the quest for knowledge of just what silicon can achieve in terms of their bonding. All of these things make organosilanes interesting subjects, indeed.

Silicon, in the form of polysilicates, accounts for ca. 25 percent of the earth's crust. This compares with carbon, which is less than 1 percent. The three isotopes of silicon along with their nuclear spins are:

²⁸ Si	92.18%	I = 0
²⁹ Si	4.17%	$ = \frac{1}{2}$
³⁰ Si	3.12%	I = 0

The 29Si isotope, with its spin of ½ allows NMR studies on the silicon nucleus to be performed. This has added much to the knowledge of silicon-containing species, especially solids.

Silicon, a second row element of group 14, is frequently compared to carbon. Although this can be "dangerous" in many ways, a direct comparison of their respective physical properties is instructive. A few of these are:

Carbon		Silicon
66 pm	atomic radius	106 pm
77 pm	covalent radius	117 pm
2.5	electronegativity	1.8
	(Pauling)	
259.0 kcal/mol	First Ionization	187.9 kcal/mol
	Potential	

It is also interesting to point out that silicon is more electropositive than hydrogen, their respective Pauling electronegativities being 1.8 and 2.1.

As there are no naturally occurring organosilanes, all organosilanes have their beginning in silicon dioxide. This abundant and extremely thermodynamically stable material can be directly converted to the valuable starting materials, silicon tetrachloride and related species.

$$SiO_2 + C + 2Cl_2 \xrightarrow{1000^\circ} SiCl_4 + 2CO$$

Berzelius had shown as early as 1924 that silicon dioxide could be converted to silicon metal via the fluoride.

$$SiO_2 + 4HF \longrightarrow SiF_4 + 2H_2O$$

 $SiF_4 + 2KF \longrightarrow K_2SiF_6 \longrightarrow 6KF + Si$

More commonly, however, metallic silicon is prepared and then converted to the oxidized forms.



The direct process,³ known as Rochow's reaction, though independently discovered by E. Rochow and R. Muller, allows the direct reaction of organic halides with silicon metal in the presence of electrontransfer catalysts, usually copper. The general reaction is:

RX + Si(Cu)
$$\longrightarrow$$
 RSiX₃ + R₂SiX₂ + R₃SiX + R₄Si + various silicon hydrides and others

The most common usage of this reaction is to form dimethyldichlorosilane under conditions selected to maximize this important precursor to the polydimethylsiloxanes. Useful and important "byproducts" of this process are methyltrichlorosilane and trimethylchlorosilane, which are used to prepare several other organosilanes. Typical results from the reaction of chloromethane with silicon-copper are:

Compound	% Composition	bp °C
Me ₂ SiCl ₂	75	70
MeSiCl ₃	10	66
Me ₃ SiCl	4	58
MeSiHCl ₂	6	41
SiCl ₄ , Me ₄ Si, HSiCl ₃ and	5	
disilanes		

It is also possible to prepare vinyl- and arylsilanes from the direct process. It happens that for the vinylsilanes, the better catalyst is nickel rather than copper and for the arylsilanes it is silver, which is better than iron, which is in turn better than copper.

The reaction of halo-, alkoxy- or even hydridosilanes with organometallic reagents, especially organomagnesium and organolithium reagents provides the silicon-carbon bond. Thus, it is clear why those products directly available from silicon metal as described above are so important to the preparation of the numerous organosilicons that now exist. The scope and limitations of this approach to organosilanes is essentially determined by the ability to prepare the appropriate organometallic reagent.



UCT, Inc. | 2731 Bartram Rd | Bristol, PA 19007 | USA P. 800.541.0559 | 215.781.9255 | F. 215.785.1226 www.unitedchem.com The reaction can be carried out in an "in situ" manner, which serves well for the preparation of organosilanes from organometallic reagents that tend to couple upon formation, such as allyl- or benzyllithium.



The reaction can be performed in an intramolecular sense, an approach that has been very successfully applied to silacyclobutyl systems as well as others.



The addition of the silicon-hydrogen bond to a carbon-carbon multiple bond, termed hydrosilation, is another excellent method of preparing the silicon-carbon bond.⁴ This reaction is not only quite general and clean, but further allows one to maintain the functionality of silicon. The reaction is induced in a variety of ways, including heat, peroxides, light, amines and transitional metal complexes. The free radical reaction pathway, brought about by heat, peroxides or irradiation, proceeds via the R3Si• radical, which then adds to the double bond. This thus explains the anti-Markovnikov addition of Si–H to the double bond.

 $R_{3}SiH + In \bullet \longrightarrow R_{3}Si \bullet + In - H$ $R_{3}Si \bullet + R'CH = CH_{2} \longrightarrow R'CH - CH_{2}SiR_{3}$ $R'CHCH_{2}SiR_{3} + R_{3}SiH \longrightarrow R'CH_{2}CH_{2}SiR_{3} + R_{3}Si \bullet$

Electronegative groups on silicon help the reaction with a general reactivity sequence of Cl3SiH > Cl2MeSiH > Et2SiH2 > Et3SiH. Some examples are:

Ph SiH

$$CH_{3}CH_{2}CH_{2}CH_{2}CH=CH_{2} \xrightarrow{\text{PH}_{3}SiH} CH_{3}CH_{2}CH_{2}CH_{2}CH_{2}CH_{2}CH_{2}SiPh_{3}$$

$$CH_{3}CH_{2}CH_{2}CH=CH_{2} \xrightarrow{\text{Cl}_{3}SiH} CH_{3}CH_{2}CH_{2}CH_{2}CH_{2}CH_{2}SiCl_{3}$$

$$98\%$$

$$CH_{2}=CHCN \xrightarrow{\text{Cl}_{3}SiH} Cl_{3}SiCH_{2}CH_{2}CH_{2}CN$$

$$51\%$$

$$Et_{2}SiH_{2} + CH_{2}=CHSCH=CH_{2} \xrightarrow{\text{CPA}} \xrightarrow{\text{CPA}} Et_{2}Si \xrightarrow{\text{CH}_{3}} CH_{3}$$

The most common catalyst used for hydrosilylations is chloroplatinic acid (CPA or Speier's catalyst). ^{4a} It has the advantages of being effective at very low concentrations (10-5M or even less in certain cases), the avoidance of excessive heat to carry out the reaction and the ability to carry out the reaction in the absence of a solvent. It is also very tolerant of a range of organic functionality, including nitro, cyano, ester, amino, sulfonic esters, borate esters and even phosphine oxides, among others. As with the free radical induced hydrosilylations, the hydrosilylation with CPA occurs regioselectively to place the silicon on the terminal carbon. The reaction does not proceed will with internal olefins, in which cases olefin isomerization is often observed.

$$CH_{3}CH_{2}CH_{2}CH_{2}CH=CH_{2} \xrightarrow{(EtO)_{3}SiH} CH_{3}CH_{2}CH_{2}CH_{2}CH_{2}CH_{2}Si(OET)_{3}$$

$$CH_{2}CH_{3} \xrightarrow{CI_{3}SiH} SiCI_{3}$$

Terminal double bonds react preferentially over internal double bonds as evidenced from the hydrosilylation of the diene below



The reaction can be intramolecular.



The hydrosilylation of alkynes is also possible with the addition being predominantly trans with free-radical catalysis and cis with the CPA. Alkynes are more reactive than olefins.



Carbonyls react with silanes in the presence of Wilkinson's catalyst $(Ph_3P)_3RhCl$ to give reductive-silylation. Triethylsilane is often used for these reactions due to its ease of handling.



UCT, Inc. | 2731 Bartram Rd | Bristol, PA 19007 | USA P. 800.541.0559 | 215.781.9255 | F. 215.785.1226 www.unitedchem.com α , β -Unsaturated ketones react in a 1, 4 manner with R₃SiH, but in a 1, 2 manner with R₂SiH₂ or RSiH₃.



The reductive-silulation of conjugated systems provides another route to the silicon-carbon bond. Some examples are shown below. The reductive-silulation of styrene can lead to silacyclpentanes.



Nucleophilic cleavage of the silicon-carbon bond is possible, though it is in general a difficult process. The reaction is especially facile if the silicon is part of a strained ring or the carbon ligand represents a somewhat stable anion.



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The reaction of certain alkylsilanes with fluoride ion gives rise to the corresponding anion. The reaction is particularly useful when carried out in the presence of our electrophile as the examples below show.





The reaction can be intramolecular as well:



The reaction of acylsilanes with fluoride ion in the presence of a carbonyl provides the product of the acyl anion directly.



A more common reaction is the electrophilic cleavage of organosilanes. Alkylsilanes electrophilically cleave in the presence of Lewis acids.

$$Et_4Si + I_2 \xrightarrow{AII_3} CH_3CH_2I + Et_3SiI \longrightarrow Et_2SiI_2$$

Due in large part to the fact that carbocations β to silicon are stabilized relative to their desilylated counterparts, the electrophilic cleavage of aryl-, vinyl- and allylsilanes are more rapid than others. Examples, together with the proposed intermediates, all of which involve a β -silyl carbocation, are



As can be seen this explains the regioselective replacement of the silyl group in aryl-, vinyl-, and allylsilanes as well as the double bond transposition in the cleavage of the allylsilanes.

Enol silyl ethers undergo a similar reaction pathway to that of the allylsilanes. In this instance the carbocation is not only stabilized by the α -oxygen, but also by the presence of the β -silicon moiety. Enol silyl ethers are, in fact, excellent reagents for cross-aldol reactions and for electrophilic α -substitution of ketones and aldehydes, which complement the nucleophilic substitution via enolate chemistry.



 α -Substituted organosilanes are quite readily cleaved by nucleophiles. The better the leaving group, the easier the cleavage.

 $Me_3SiCH_2CI \longrightarrow CH_3CI + Me_3SiOSiMe_3$

$$Me_3SiCHCl_2 \xrightarrow{KOH} CH_2Cl_2 + (Me_3Si)_2O$$

It has been shown that in the gas phase and under certain conditions in solution a migration of alkyl groups from silicon to an α -carbon occur.

 $\begin{array}{c} \mathsf{Me}_3\mathsf{SiCH}_2\mathsf{CI} \xrightarrow[]{\mathsf{KF/xylene}} \\ 40\mathsf{C}/18\mathsf{-}\mathsf{C-6} \\ \mathsf{CI} \end{array} \xrightarrow{\mathsf{Me}_2\mathsf{SiCH}_2\mathsf{CH}_3} \\ \end{array}$

Thermally an α -elimination can occur giving rise to carbenes as seen from the examples below.



A dyotropic thermal rearrangement occurs with a-substituted organosilanes



 β -Functional organosilanes are particularly vulnerable to nucleophilic attack at silicon with concomitant loss of the β -functionality resulting ultimately in double bond formation.



This approach has been used to generate benzyne.



The benzylsilane below provides a vinylogous version of this same concept, applied here in the construction of the steroid skeleton.



It has been shown that thermally the elimination of β -functional organosilanes is a first order process with strict stereochemical requirements for success. This can be seen from the examples shown below.



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β-Carbonylsilanes thermally rearrange to the thermodynamically more stable enol silyl ethers. This fact has led to a regio- and stereospecific synthesis of the synthetically highly useful enol silyl ethers.



γ-Functional organosilanes undergo elimination to form cyclopropanes.

$$Me_3Si$$
 $Br \xrightarrow{AlBr_3}$ Me_3SiBr

There are a number of applications wherein the organosilyl group is utilized as a large or otherwise special hydrogen atom. This is most commonly found in the protection of alcohols, acids, amines, thiols and the like. It is seen in the presence of enhanced stability in other systems as well. Terminal acetylenes are readily silylated and provide enhanced stability over their protonated precursors. The silyl group can be cleaved with alkali, cyanide ion or fluoride ion.

Diazomethane, well known for its explosive potential, becomes thermally stable when silylated.



UCT, Inc. | 2731 Bartram Rd | Bristol, PA 19007 | USA P. 800.541.0559 | 215.781.9255 | F. 215.785.1226 www.unitedchem.com There exist a number of silvlated reagents that are no more stable than the protonated species, but are in general more easily handled and more selective in their reactivity. Trimethylsilyl iodide has proven to be an excellent Lewis acid for selective cleavage of esters and ethers. These can be isolated as the trimethylsilyl protected species directly or hydrolyzed during workup.



Trimethylsilyltrifluoromethane sulfonate (trimethylsilyl triflate) is proving to be a useful, easily handled and soluble Lewis acid in a number of applications.



Trimethylsilyl nitrile (cyanotrimethylsilane) provides a more easily managed alternative to that of hydrogen cyanide. It adds to aldehydes and ketones to provide the protected cyanohydrins.



The tert-butyldimethylsilyl derivative has been shown to add to epoxides to give protected β-hydroxy isonitriles.



Significant strides have been made in the preparation, development and study of the chemistry of reactive organosilicon species. The organosilyl radical has long been known and studied.

 $R_3SiH + {}^tBuO' \longrightarrow R_3Si' + {}^tBuOH$

The divalent species, dimethylsilylene, is conveniently generated from photolysis of dodecamethylcyclohexasilane. This electrophilic species undergoes a variety of reactions.



Several silacyclopropanes have been prepared and studied, this despite several early failures and predictions that they could not exist due to the large size of the silicon atom. They are, understandably, reactive towards a number of reagents.



Transient disilenes have been prepared and trapped.



X-ray crystal structures have been determined for the sterically hindered, and therefore isolable, disilenes:



Though argued through the years, both correctly and incorrectly, as intermediates in a number of reactions of organosilanes, silenes (Si=C species) of sufficient stability for isolation were prepared only recently. X-ray structures have been performed on the two silenes:



The first good indication of the existence of a silabenzene intermediate was obtained from the reaction:



A retro-ene reaction was successfully employed to prepare 1-silatoluene.



To date only transient species containing the Si=N and Si=O bonds have been reported. The inability to place only three (Si=N) or two (Si=O) sterically demanding groups, and thereby significantly reduce the kinetic instability of such species, makes the preparation of isolable species containing these interesting double bonded silicons a much more challenging endeavor.



Although it had been known for many years that the silenium ion was thermodynamically more stable than the carbenium ion (first ionization potentials are 187.9 and 259 kcal/mol, respectively) and that the silenium ion appeared as principle fragments in the mass spectra of organosilanes, their observation in solution escaped detection. This was correctly attributed to the fact that the organosilanes simply had lower energy alternate reaction pathways available that did not demand the intermediacy of a silenium ion. The first successful preparation of a silenium ion was based on the concept that in order to give stability to such a species it would be necessary to place ligands on the silicon which had filled 3p orbitals (as opposed to 2p orbitals) to successfully donate electrons back to the empty 3p orbital on silicon in the silenium ion. Thus tris(triisopropylmercapto) silane was deprotonated as shown to give the silenium ion:

 $({}^{i}PrS)_{3}SiH + Ph_{3}C^{+}BPh_{4}^{-} \longrightarrow ({}^{i}PrS)_{3}Si^{+}BPh_{4}^{-} + Ph_{3}CH$

This concept has more recently been employed for the preparation of the triphenylsilenium ion:

 $Ph_{3}SiH + Ph_{3}C^{+}CIO_{4}^{-} \longrightarrow Ph_{3}Si^{+}CIO_{4}^{-} + Ph_{3}CH$

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REFERENCES

- 1. Friedel, C.; Crafts, J. M., Ann., 1865, 136, 203
- 2. A summary of this work is to be found in: Kipping, F. S. Proc. Roy. Soc. A, 1937, 159, 139
- 3. Voorhoeve, R. J. H., "Organohalosilanes: Precursors to Silicones,: Elsevier, New York, 1967
- a. Speier, J. L., "Homogeneous Catalysts of Hydrosilyaton by Transition Metals," Advanced Organometal. Chem, **1979**, 17, 407
 - b. Lukevits, E. Y.; Voronkov, M. G., "Organic Insertion Reactions of Group IV Elements," Plenum Publ. New York, 1966
 - c. Cundy, C. S.; Kingston, B. M.; Lappert, M. F. Advan. Organometal. Chem, 1973, 11, 253

ADDITIONAL READING:

- 1. Weber, W. P., "Silicon Reagents for Organic Synthesis," Springer-Verlag, New York, 1983
- 2. Colvin, E., "Silicon in Organic Synthesis," Butterworths, Boston, 1981
- 3. Pawlenko, S., "Organosilicon Chemistry," Walter de Gruyter, New York, 1986.
- Fleming, I., "Organosilicon Chemistry," in Comprehensive Organic Chemistry, 1979, 3, 541. Barton, D. H. R.; Ollis, W. D.; Neville, J. D. Eds. Pergamon Press, Oxford
- Annual surveys for organosilicon chemistry to be found in J. Organometal. Chem. Libr., Elsevier, New York, published since 1976.

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SILANE BLOCKING AGENTS

Silyl groups have long been employed to derivatize and protect various substrates during chemical and synthetic sequences. Initial work involved derivatizing compounds by replacing active hydrogen atoms with silyl groups. These classic silylation reactions have not changed.^{1, 2, 3} The early utilization of silylation was in the area of analysis. The more volatile silyl derivatives of alcohols, carboxylic acids, phenols, amino acids, carbohydrates and amines could be analyzed through their retention times by gas chromatography. Later it was noted that silylation had great synthetic potential. Replacement of active hydrogens with silyl groups afforded products which were more chemically stable and would undergo subsequent chemical reactions at sites other than the silyl blocked one. Hydrolysis would then regenerate the unprotected functionality. A major factor contributing to the wide acceptance of silyl blocking groups is that both blocking and de-blocking reactions are high yield reactions and often quantitative. This has led to the introduction of a wide range of specialty blocking agents which have been designed for specific purposes such as selectivity, degree of reactivity for less reactive substrates, nature of silylation by product for sensitive substrates, and the stability of the blocked substrate toward other reagents.

Some of the more prominent silvlating agents are discussed individually below. The accompanying table is a more comprehensive selection guide.

MONOFUNCTIONAL BLOCKING AGENTS

The Trimethylsilyl Group

The trimethylsilyl moiety is the most common blocking group employed today. It is used to derivatize an astounding number of organic and inorganic materials. The main application has been to block and protect hydroxyl groups in natural compounds.⁷ The trimethylsilyl group may be introduced into a substrate through a variety of reagents, the majority of which are listed below. It is readily removed through acidic or basic hydrolysis.

Trimethylchlorosilane (T2950)

A powerful silvlation reagent, the byproduct of silvlation is hydrochloric acid. It is commonly employed with substrates not affected by strong acidic byproducts such as phenols. It may also be used in conjunction with proton acceptors such as ammonia, triethylamine, pyridine and hexamethyldisilazane in solvents such as toluene, ether, hexane, methylene chloride and dimethylformamde. The use of proton acceptors permits silvlation of acid-sensitive substrates such as amines and amides. It has also been employed to convert ketones and aldehydes to the corresponding silvl enol derivatives. Reaction of T2950 with metal salts of alcohols, carboxylic acids and thiols produces the trimethylsilvl blocked derivatives usually in good yield.

Hexamethyldisilazane (H7300)

The most commonly used reagent for silylation. Reaction with protic species such as alcohols, phenols, carboxylic acids, amino acids, carbohydrates, thiols and amines affords the silylated derivative and ammonia as a byproduct. Reactions are normally carried out by refluxing the substrate with excess H7300 until evolution of ammonia ceases. This material is particularly effective with alcohols and phenols. Addition of acid catalysts such as sulfuric acid (or ammonium sulfate) increases rate and degree of silylation. Trimethylchlorosilane (T2950) when combined with hexamethyldisilazane in an approximate weight ration of two parts H7300 to 1 part T2950 (1:1 molar ratio preferred) will rapidly and efficiently silylate three molar equivalents of substrate. The byproduct is ammonium chloride. Silylations involving H7300 are usually run without solvent.

Trimethylsilylamides

Bis(trimethylsilyl)acetiamide (B2500) and bis(trimethylsilyl)trifluoroacetamide (B2570) are rapid and powerfull trimethylsilylation reagents for alcohols, acids, amines, and thiols. Byproducts of silylation are neutral acetamides and can be employed for materials which are acid or base sensitive. B2570 is preferred when volatile, neutral byproduct (in this case N-(trimethylsilyltrifluoroacetamide)) is desired. It is advantageous when analysis by gas chromatography is employed.⁹ Silylations with B2500 and B2570 are typically conducted in solvents such as dimethylformamide and acetonitrile. The ability of B2500 to block reactive sites is further increased if T2950 is added to the silylation mixture.

Trimethylsilylamines

Trimethylsilylamines such as dimethylaminotrimethylsilane (D5400) block reactive sites of alcohols, amines, amino acids, amides and ureas with liberation of dimethylamine. The reactions are normally run at or near reflux with a slight excess of silylamine. Rate and degree of blocking of reactive sites are increased by the addition of acid catalysts such as ammonium sulfate or trichloroacetic acid.

Trimethylsilylimidazole (T3600) is a rapid and specific blocking agent for hydroxyl groups. It will silylate alcohols in the presence of amines without silylating the latter. It readily blocks hindered alcohols in steroids and is very effective in the total blocking of sugars. Rate and degree of reaction is enhanced by addition of T2950. Reactions are normally run neat but may be successfully carried out in solvents such as DMF, ether and toluene.

HINDERED MONOFUNCTIONAL BLOCKING GROUPS

Reagents of this type offer increased stability of the derivatized substrate due to steric factors. The larger substituent groups such as t-butyl, phenyl and isopropyl hinder attach at the silicon or silicon-derivatized atom and make the blocked substrate more stable toward hydrolytic, oxidative and reductive procedures which may be encountered in subsequent synthetic sequences.

t-Butyldimethylchlorosilane (B2790)

Because of the steric bulk of the t-butyldimethylsilyl group it is relatively stable against de-blocking in weakly acidic or basic media and mild oxidizing and reducing conditions.⁷ It is unaffected by hydrogenolysis over palladium and lithium aluminum hydride.⁸ Substrates blocked by the t-butyldimethylsilyl group are also stable against Grignard reagents.⁹ The stability of this blocking group has been a major factor in developing syntheses of prostaglandins, and it has found extensive use in terpenoid and carbohydrate chemistry. In addition to the foregoing, B2790 has been utilized in the protection of alcohols, amines, carboxylic acids, phenols and other substrates. Preparation of blocked intermediates is most satisfactorily achieved by reaction of the substrate with B2790 in the presence of a molar excess of imidazole using DMF as solvent. Removal of the t-butyldimethylsilyl group is readily accomplished through hydrolysis using acetic acid, acetic anhydride containing FeCl₃ or with tetrabutylammonium fluoride in THF. ^{10, 11}

t-Butyldiphenylchlorosilane (B2805)

This reagent provides blocked derivatives having even greater stability than can be achieved employing B2790. This blocking agent is utilized where the highest is desired. Hydroxyl derivatives prepared utilizing B2805 are stable to 80% acetic acid (which cleaves t-butyldimethylsilyl derivatives), 50% aqueous trifluoroacetic acid-dioxane, hydrogenation over Pd, Grignard reagents and lithium aluminum hydride. Blocked derivatives are very resistant to hydrolysis and oxidation. Derivatization is efficiently carried out using a molar excess of imidazole in DMF solvent. Hydrolysis is effected with tetrabutylammonium fluoride in THF.

Triisopropylchlorosilane (T2885)

This material has found an application as a blocking group. It has been utilized to prepare blocked derivatives of hydroxy compounds. Derivatization of substrates is accomplished efficiently in DMF containing a slight molar excess of imidazole. Blocked intermediates exhibited acidic hydrolytic stability intermediate between that of a B2790 and B2805 derivatives. Greater stability was obtained with T2885 under basic conditions. With n-butyl alcohol as the substrate, the following half-life stabilities were recorded.¹⁸

Blocking Agent	CAT#	H+	OH.
t-Butyldimethylchlorosilane	B2790	< 1 min	1 h
Triisopropylchlorosilane	T2885	18 min	14 h
t-Butyldiphenylchlorosilane	B2805	244 min	< 14 h

Deblocking is achieved by reaction with tetrabutylammonium fluoride in THF.

CYCLOSILYLATION

Difunctional blocking agents are available to selectively block primary amines, vic-diols or other suitable difunctional sites. This process is termed cyclosilylation. Cyclosilylation typically forms five-, six-, and seven-membered silicon-containing rings which are very stable to hydrolysis, oxidation and reduction. As an example, effective blocking agents for rigid molecules such as steroids, salicyclic, thiosalicyclic or anthranilic acids are dimethyldiacetoxysilane (D5490) and dimethyldimethoxysilane (D5600). ^{13, 14}

A bifunctional blocking agent finding application in nucleoside and glycolipid chemistry is 1,3-dichloro-1,1,3,3tetraisopropyldisiloxane (D4368). This protects the 3'- and 5'-hydroxy groups simultaneously, allowing separate protection of the 2'-position. The 3',5'-diprotected intermediates can be selectively deprotected at the 5'-position with dilute acid.

Protection of primary amines with pka's in the range of 10 – 11 has been successfully carried out through cyclosilylation with 1,1,4,4-tetramethyl-1,4-dichlorosilethylene (T2015) in the presence of triethylamine.¹⁵ Blocked intermediates employing T2015 are typically prepared in yields of greater than 90% and are stable to oxidation, hydrolysis and Grignard reagents.

TRIMETHYLSILYL GROUP, ACIDIC BYPRODUCTS

PRODUCT	APPLICATIONS	REFERENCES
Т2950		
Trimethylchlorosilane	General reagent for most groups	1, 2, 3 ,4
Me ₃ SiCl		

TRIMETHYLSILYL GROUP, BASIC BYPRODUCTS

PRODUCT	APPLICATIONS	REFERENCES
D5400 N,N-Dimethylaminotrimethylsilane Me Me	Employed where removal of the amine from the mixture is desired	
H7300 Hexamethyldisilazane Me ₃ Si Me ₃ Si	One of the most common silylating reagents applicable to alcohols, acids, amines, amides, and thiols. Finds widespread use in pharma-ceutical manufacturing processes.	1, 2, 3
T3600 N-Trimethylsilylimidazole Me ₃ SiN	Protecting agent specific for hydroxyl groups. Reaction with acid chlorides affords acyl-imidazole derivatives.	16

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TRIMETHYLSILYL GROUP, NEUTRAL BYPRODUCTS

PRODUCT	APPLICATIONS	REFERENCES
B2500 Bis(trimethylsilyl)acetamide OSiMe ₃ CH ₃ C=NSiMe ₃	Versatile silylating reagent for amino-acids, amides, phenols, carboxylic acids, ureas, enols, imides, alcohols	5
B2570 Bis(trimethylsilyl)trifluoroacetamide $OSiMe_3$ CF ₃ C—NSiMe ₃	More rapid silylation reagent than B2500. Byproducts are volatile. Suitable for carboxylic acids, alcohols, phenols, amides, and ureas	6

STERICALLY HINDERED BLOCKING AGENTS

PRODUCT	APPLICATIONS	REFERENCES
T2520 Triethylchlorosilane Et Et—Si—Cl I Et	Has been used to protect allylic esters as silylketene acetal. More stable but less volatile derivates than Me ₃ Si–	17
T2885 Triisopropylchlorosilane <i>i</i> -Pr <i>i</i> -Pr Si—Cl <i>i</i> -Pr	For protection of alcohols. Yields derivatives with hydrolytic stability between that of t-butyldimethyl and t-butyldiphenyl derivatives. TIPS derivatives of 1° and 2° alcohols show different reactivity, allowing selective silylation/desilylation of multifunctional compounds. Very useful with nucleosides and nucleotides	12, 18
P0160 Phenyldimethylchlorosilane	Sterically hindered protecting reagent. Derivatives are more stable to acidic and basic conditions than TMS ethers.	

STERICALLY HINDERED BLOCKING AGENTS (CONT.)

PRODUCT	APPLICATIONS	REFERENCES
B2790 t-Butyldimethylchlorosilane	Highly selective protecting reagent for hydroxyl groups based on steric hindrance. Derivative is stable to many	7.8.0.10.11
Me Me ₃ C—Si—Cl Me	reagents allowing other functional group transformations. Finds use in prostaglandin, steroid and nucleoside chemistry	7, 8, 9, 10, 11

DIFUNCTIONAL BLOCKING AGENTS

PRODUCT	APPLICATIONS	REFERENCES
D5490 Dimethyldiacetoxysilane Me OCOCH ₃ Me OCOCH ₃	For derivatizing corticosteroids	13, 14, 19
D5600 Dimethyldiethoxysilane Me_OEt Me_OEt	Protection of vicinal hydroxyl groups	13, 14
D4368 1,3-Dichlorotetraisopropyldisiloxane i-Pr i -Pr Cl—Si—O—Si—Cl i-Pr i -Pr i-Pr	A reagent for the simultaneous protection of the 3'- and 5'-hydroxy groups in nucleosides, allowing selective reaction at the 2'-position. It has also been utilized in the synthesis of glycolipids	20, 21, 22, 23
T2015 1,1,4,4-Tetramethyl-1,4-dichloro- disilethylene $CH_2 - CH_2$ $Me_2Si $ SiMe ₂ Cl Cl	Used to prepare derivatives of primary amines which are stable to strong bases and some oxidizing agents. Has been applied to amino acid synthesis	15

References

- L. Birkofer and A. Ritter, "Newer Methods in Preparative Organic Chemistry," Volv. V. p.211, Academic Press, New Yor, NY 1968.
- 2. A. E. Pierce, "Silylation of Organic Compounds," Pierce Chemical Co., Rockford, III., 1968
- 3. J. F. Klebe, Acc. Chem. Res., 1970 (3) 299.
- 4. E. J. Corey, and B. B. Snider, J. Am. Chem. Soc., 1972 (94) 2549.
- 5. J. F. Klebe, H. Finkbeiner, and D. M. White, J. Am. Chem. Soc., 1966 (88) 3390.
- 6. M. G. Horning, E. A. Boucher, and A. M. Moss, J. Gas. Chromatog., 1967 (5) 297.
- 7. E. J. Corey and A. Ventakeswarlu, J. Am. Chem. Soc., 1972 (94) 6190.
- 8. J. A. Marshall and R. D. Peveler, Synth. Commun., 1963 (3) 167.
- 9. G. D. Prestwich and J. N. Labowitz, J. Org. Chem., 1974 (96) 7103.
- 10. B. Ganem and V. R. Small, J. Org. Chem., 1974 (39) 3728.
- 11. K. K. Ogilvie and D. J. Iwacha, Tetrahedron Lett., 1973 317.
- 12. R. F. Cunico and L. Bedell, J. Org. Chem., **1980** (45) 4797.
- 13. R. W. Kelly, Tetrahedron Lett., 1969 967.
- 14. M. Wieber and M. Schmidt, Chem. Ber., 1963 (96) 1561.
- 15. T. L. Guggenheim, Tetrahedron Lett., 1984 1253.
- 16. S. Torkelson and C. Ainsworth, Synthesis, 1976 722.
- 17. W. C. Still and M. J. Schneider, J. Am. Chem. Soc., 1977 (99) 948.
- 18. K. K. Ogilvie, et al, Tetrahedron Lett., 1974 2861, 2865
- 19. R. W. Kelly, J. Chromatog. 1969 (43) 229.
- 20. W. T. Markiewicz and M. Wienwiorowski, Nucleic Acids Res., 1978 (4) 185.
- 21. M. J. Robins and J. S. Wilson, J. Am. Chem. Soc., 1981 (103) 932.
- 22. K. Pankiewicz, A. Matsuda and K. A. Watanabe, J. Org. Chem., 1982 (47) 485.
- 23. S. A. A. Van Boeckel and J. H. Van Bloom, Chem. Lett., 1981 581.

INFRARED ANALYSIS OF ORGANOSILICON COMPOUNDS: SPECTRA-STRUCTURE CORRELATIONS

The infrared spectrum reveals vibrations of atoms in molecules. The beauty of the spectrum is the close and accessible relationship between infrared bands and molecular structure. Certain groups of atoms have characteristic vibration frequencies which persist in different compounds. These groups, like Si–OCH₃, C=O, Si–CH=CH₂, BF₄, are the very kind of functional groups chemists are interested in. This is why infrared spectroscopy is an indispensable tool for organosilicon research.

The positions of infrared bands characteristic of some organosilicon groups are shown in the following table. Ideally, these correlations should be used for liquids or solutions. Infrared band positions for a crystalline solid often show shifts and splitting when compared with band positions of the sample in the liquid state. However, non-crystalline solids (amorphous polymers, glasses) tend to have infrared spectra that are similar to their solution spectra.

These spectra-structure correlations are the result of work by many investigators. Major contributions have been made by A. Lee Smith and his colleagues at Dow Corning Corporation. In addition to previously-published data, we have included some correlations based on our own experience in the analysis of organosilicon compounds.

There is increasing interest in carbon-containing silicon compounds as precursors of high-performance ceramics. Accordingly, the table gives data on the infrared bands of some silicon-containing ceramics.

This table presents *empirical* correlations between spectra and structure. The table does not show the types of vibrations (stretching, bending, rocking, etc.) that give rise to the infrared bands. Empirical correlations can guide the chemist who is using infrared to follow the course of a reaction, to analyze a commercial product, or to identify an unknown. The correlations become even more useful if the chemist learns the vibrational origins of the bands. The chemist then will be in a better position to anticipate interferences by other groups. Knowledge of the vibrational origins also will help the chemist to understand shifts in a group frequency caused by strain in a bond, coupling of vibrations, or change in the electronegativity of neighboring atoms.

The references list three excellent reviews of spectra-structure correlations for organosilicon compounds. Each review contains some discussion of the molecular vibrations associated with the infrared bands. The reviews also offer a quick way to locate the original literature for many of the correlations.

REFERENCES

D. R. Anderson in "The Analytical Chemistry of Silicones," A. Lee Smith, editor, Wiley-Interscience, New York, 1991, Chapter 10

L. J. Bellamy, "The Infra-red Spectra of Complex Molecules," 3rd ed., Chapman and Hall, London, 1975, Chapter 20

A. Lee Smith, Spectrochim. Acta, 16, 87 (1960).

Group	Frequency in cm-1	Comments
Si–CH ₃ In polysilioxanes	1275–1245, 865–750	
CH ₃ H ₃ C—Si—O—	(M) 1250, 840, 755	
СН ₃ —Si—О— СН ₃	(D) 1260, 860 (weak), 800	The Si–CH ₃ group is easily recognized by a strong, sharp band at about 1260 cm ⁻¹ together with one or more strong bands in the range 865–750 cm ⁻¹ . Some $(CH_3)_3$ Si – compounds show a 1250 cm ⁻¹ band split into two components with the weaker component often appearing as a shoulder on the high-frequency side of the band. Blocks of dimethyl D units show a relatively weak band at 860 cm ⁻¹ . In many copolymers containing dimethyl D units (random or alternating, not block), the 860 cm ⁻¹ band shifts to 845 cm ⁻¹ and becomes stronger
 O H₃C—Si—O— O 	(T) 1270, 780–760	

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Group	Frequency in cm-1	Comments
Si–CH ₂ CH ₃	1250–1220, 1020–1000, 975–945	The 1250–1220 cm ⁻¹ Si–CH ₂ – band is much weaker than the analogous 1260 cm ⁻¹ Si–CH ₃ band.
Si–CH ₂ (CH ₂) _x CH ₃	1220–1170	As the alkyl group becomes longer, the Si–CH2 – band moves to lower frequency: <i>n</i> -propyl, 1220–1200 cm ⁻¹ ; <i>n</i> -butyl, 1200–1190 cm ⁻¹ ; longer chains, 1190–1170 cm ⁻¹ .
Si–CH=CH ₂	1600, 1410, ca. 1010, ca. 960	If other alkenyl groups and aryl groups are absent, C–H bands at 3060 and 3020 cm ⁻¹ help to identify Si–CH=CH ₂ .
Si–CH ₂ –CH=CH ₂	1640–1630, 1190–1140, 990, 930 (appears as shoulder in some compounds), 920– 980.	The isomeric group, Si–CH=CH–CH ₃ , shows a different pattern with a strong band at 970 cm ⁻¹ due to <i>trans</i> –CH=CH–.
Si	1600–1590, 1430, 1130– 1110, 1030, 1000, 760–710, 700–690	
In polysiloxanes:		
CH ₃ -Si-O-	730, 700 intensities approx. equal	The 1430 cm ⁻¹ band is so narrow that its intensity in a recorded spectrum is greatly influenced by the resolution of the spectrometer and the scanning speed. When two phenyl groups are attached to silicon, the strong 1120 cm ⁻¹ band usually is split into a doublet. The 1030 and 1000 cm ⁻¹ bands, normally weak, become much stronger in cylco-trisiloxanes. Specific Si-phenyl compounds often can be identified by the pattern in the range 760–690 cm ⁻¹ where there is a
-si-o-	740, 720, 700 intensities increase as frequency of band decreases	strong band at 700–690 and one to three weak, medium, or strong bands in the region 760–710 cm ⁻¹ .
Si–O–Si	1130–1000	Siloxanes show one or more very strong infrared bands in the region 1130–1000 cm ⁻¹ . Disiloxanes and small-ring cyclosiloxanes show a single Si–O–Si band. As the siloxane chains become longer or branched, the Si–O–Si absorption becomes broader and more complex, showing two or more overlapping bands
R₃SiOSiR₃ Disiloxanes	1080 – 1040	Some unusual shifts in the disiloxane band: $CI_3SiOSiCI_3$, 1115 cm-1 (inductive effect); $(CH_3)_2SiOSi(CH_3)_2CH_2CH_2$, 920 cm-1 (strained ring)

Group	Frequency in cm-1	Comments
[R ₂ SiO] ₃ Cyclic trimers	1080–1010	Cyclic trimers tetramers and pentamers have a single $Si=O=Si$
[R ₂ SiO] ₄₋₅ Cyclic tetramers and pentamers	1090–1075	band. As the ring becomes larger (D_6 , D_7 , etc.), the Si–O–Si band gradually widens and splits
[(CH ₃) ₂ SiO] _x poly(dimethylsiloxane)	1090, 1020	Long chains of dimethyl D units show two very strong, distinct bands of about equal intensity at 1090 and 1020 cm ⁻¹ .
[RSiO _{1.5}] _{8, 10, or 12}	1130–1115	
[RSiO _{1.5}] _x	1160–1000	Polysiloxanes made up of T units, $[RSiO_{1.5}]_x$, often show a broad, structureless absorption covering the entire region 1160–1000 cm ⁻¹ . In other preparations of all T-polymers, there are two distinct bands – one at about 1130 cm ⁻¹ , the other at about 1040 cm ⁻¹
Si–CH ₂ –Si	1080–1040	The disilylmethylene band is strong and sharp. The sharpness helps distinguish it from Si–O–Si bands.
Si–CH ₂ CH ₂ –Si	1180–1120	This is a strong sharp band. Caution: The band does not appear in this range when the disilyl-ethylene group is part of a strained ring.
Si-Si	1135	Compounds containing the <i>p</i> -substituted silphenylene group show a strong, sharp band at 1135 cm ⁻¹
Si–H	2280–2080, 950–800	The Si–H group is readily identified by a strong band in the range 2280–2080 cm ⁻¹ . There usually is no interference from other bands in this part of the spectrum. The exact position of the 2280–2080 band is very sensitive to the electro-negativity of the groups attached to the silicon.
S–H In amorphous silicon	2150–2000	Si–H bands at three or more frequencies in the range 2150–2000 cm-1 have been found in amorphous silicon (a-Si). There still is some uncertainty about the correlations between these band positions and the nature of the other groups on the Si atom.
Si–F	1030–820	SiF_2 and SiF_3 compounds usually show two bands in this range

Group	Frequency in cm-1	Comments
Si–Cl	625–425	$SiCl_2$ and $SiCl_3$ compounds show two or three bands in this range.
Si–OH	3690 (free OH), 3400–3200 (hydrogen-bonded OH), 950 – 810	Isolated Si–OH groups on silica show a sharp band at 3750 cm ⁻¹ [R. S. McDonald, J. Phys. Chem., 62 , 1168 (1958)]. Free silanol groups in organosilicon compounds show a sharp band at about 3690 cm ⁻¹ . Aryl silanols show slightly lower frequencies than alkyl silanols. Two ways to tell the difference between Si–OH and C–OH: The free Si–OH band at 3690 cm ⁻¹ is at a significantly higher frequency than the free C–OH band. Si–OH compounds show absorption, often a single broad band, in the range 950–810 cm ⁻¹ .
Si–O–Metal	1000–900	Silanolates show a strong band in the range 1000–900 cm ⁻¹ . Si–O–Ti compounds show a strong band at ca. 925 cm ⁻¹ .
Si–OR	1110–1000	
Si-OCH ₃	2840 (sharp), 1190, 1100–1080 (strong)	
Si–OCH ₂ CH ₂	1170–1160, 1100 and 1075 (strong doublet), 970–940	SI-alkoxy compounds have one or more strong bands in the 1110–1000 cm ⁻¹ range. If siloxane is present in a sample, the 1110–1000 cm ⁻¹ band is apt to be masked by strong Si–O–Si
Si–OCH ₂ CH ₂ CH ₃	1155 (weak), 1100 and 1085 (strong doublet), 1020	absorption. In such cases, the alkoxy group often can be identified by using other bands.
Si – OCH(CH ₃) ₂	1385 and 1370 (sharp, well- defined doublet), 1175, 1140– 1110, 1055–1030 (strongest band in set), 890	
Si—O—	1240, 975	The phenoxy group attached to silicon has strong bands at about 1240 and 975 cm ⁻¹ .
	1770–1725, 1370, 1260–1195, 1050–1000, 970–925	Two of these bands are sensitive to the number of acetoxy groups attached to a silicon atom. The correlations are not perfect, but here are the tendencies: In the interval 1770–1725 cm ⁻¹ , as the number of acetoxy groups increases, the band shifts to higher frequency. In the interval 1260–1195 cm ⁻¹ , as the number of acetoxy groups increases, the band shifts to lower frequency.
Si–NH ₂	3500–3390 (NH ₂ , doublet in this interval), 1550–1540, 3390	
H Si—N—Si	(NH, single band), 1200– 1150, 950–920	Tris(trimethylsilyl)amine (also called nonamethyl-trisilazane, "NMTS") has a strong Si–N–Si band at 915 cm ⁻¹ .

Group	Frequency in cm-1	Comments
Si–N ₃	2180–2120	Compounds containing the azide group attached to silicon have a strong N=N=N band in the interval 2180–2120 cm ⁻¹ . See W. R. Peterson, Reviews on Silicon, Germanium, Tin and Lead compounds, 1 , 193 (1974).
Si–N=C=O	2280	Trimethylsilylisocyanate has a very strong N=C=O band at 2280 cm ⁻¹ . This band position is close to the high-frequency end of the range $2275 - 2250$ cm ⁻¹ for N=C=O attached to carbon.
Si–CH ₂ CH ₂ CF ₃	1210, 1130, 1070, 1020, 900	The 1210 cm ⁻¹ band is the strongest one of the set.
Si–CH ₂ Cl	1395, 1180	
Si-Cl	1580, 1485, 1380, 1090, 1015, 810	These are strong, narrow bands.
(RO ₃)Si–(CH ₂) ₃ X		
Where X is		Silanes having this general formula, where X is a reactive group
–Cl	1310, 910, 860	are used as coupling agents. For some of the silanes, the infrared
–C≡N	2245 (C≡N), 1190–1175	spectrum is dominated by bands of the $(RO)_3SI-$ part of the structure, and bands due to the reactive group are not obvious. In such cases,
-NH ₂	3370 and 3290 (NH ₂ , weak doublet), 1595 (broad, weak)	it often is a good idea to hydrolyze the trialkoxysilanes to the resin, $[O_{1.5}SiCH_2CH_2CH_2X]_n$, and to record the infrared spectrum of the resin. This eliminates the many bands due to Si–OR and replaces
–SH	2560 (S–H, weak)	them with one or two broad Si-O-Si bands. When 3-amino-propyl compounds are hydrolyzed in the air, the NH, group reacts with
О СН ₃ —О-С-С-С-С-С-С-С-С-С-С-С-С-С-С-С-С-С-С-С	1720 (C=O), 1640 (C=C)	carbon dioxide and water, and one gets a resin containing –NH ₃ ⁺ ¹ HCO ₃ [see S. R. Culler, H. Ishida, and J. K. Koenig, Appl. Spectrosc., 38, 1 (1984)]. This salt structure is characterized by the following bands: 3400–2000 (several broad bands) 1640 (shoulder) 1575
	3045 (C-H of three member- ed ring, weak), 1250	(strong), 1480 cm ⁻¹ (strong).
Q R₃Si—C—C—	1725–1660	In compounds having a carbonyl group β to silicon, the C=O frequency is 10–20 cm ⁻¹ lower than that of the carbon analog. This is attributed to the inductive effect of the R ₃ SiC– group. [see G. L. Larson, D. Hernandez, I. Montes de Lopez-Cepero and L. E. Torres, J. Org. Chem., 50, 5260 (1985) and references therein for examples of these kinds of molecules]

Group	Frequency in cm-1	Comments
Si=C (silenes)	ca. 1000	$(CH_3)HSi=CH_2$, stable at 35°K in argon matrix, has a strong band at 989 cm ⁻¹ due to Si=C stretch (see C. A. Arrington et al., J. Am. Chem. Soc. 106 , 525 (1984); and G. Raabe et al., J. Am. Chem. Soc. 108 , 671 (1986). Solid silenes of the type $[(CH_3)_3Si]_2Si=C[OSi(CH_3)_3]R$, where R is the bulky group, are stable at room temperature in the absence of air. These silenes show a strong band at 1135–1130 cm-1 probably due to the Si–O–C stretch in the Si–O–C=Si group (see A. G. Brook et al., J. Am. Chem. Soc. 104 , 5667 (1982).
CERAMICS: Silicon carbide	ca. 800	Silicon carbide occurs in a bewildering number of crystal modifications. It also occurs as amorphous material (a-SiC). We do not have detailed spectra-structure correlations for these forms. We expect that the different forms will have small differences in their infrared spectra, but that all forms of SiC will show strong absorption at or near 800 cm ⁻¹ .
		Amorphous $Si_{3}N_{4}$ has a strong absorption band at ca. 840 cm ⁻¹ .
Silicon nitride	ca. 840	All forms of SiO_2 show a strong band at $1110 - 1080$ cm ⁻¹ . In addition to this strong band, there are other bands that help to identify the kind of SiO.:
Silicon dioxide	ca. 1100	α -quartz (a crystal form of SiO ₂) – 1170 (sharp band on the slope of the strong 1080 band), 800 and 780 (well-defined, sharp doublet), and 695 cm ⁻¹ . <i>Crystobalite</i> (another crystal form) – 1200 (a narrow shoulder or "step"), 795, and 620 cm ⁻¹ . <i>Amorphous silica</i> (includes silica gel, silica glass, "fused quartz", precipitated silica and fumed silica) – ca. 1220 (a very broad shoulder) and 810 – 800 cm ⁻¹ . The 810 – 800 cm ⁻¹ absorption of amorphous silica is broader and weaker than the 800 cm ⁻¹ region bands of a-quartz and cristobalite.

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TECHNIQUES FOR SILYLATION

Silylation is the replacement of an active hydrogen of a protic material with a substituted silicon atom. There are two general categories of silylation. Well-defined molecular species can be modified with silyl groups for the purpose of producing blocked intermediates or producing volatile derivatives for analysis by gas chromatography. Macromolecular structures may be modified with functional silane groups to impart specific surface properties to the macromolecule, e.g. wettability, surface energy, partition parameters, orientation, covalent reactivity, and surface potential. The purpose of this presentation is to provide examples of silylation techniques.

SILYLATION OF MOLECULAR SPECIES FOR DERIVATIZATION OR BLOCKED INTERMEDIATES

The most widely used silvlation agents employ the trimethylsilvl group Me₃Si–, The hydrodimethyl-silvl group Me₂HSi– may be used for increased volatility but is less stable and more susceptible to hydrolysis. Increased hydrolytic stability is available with bulkier silvl groups such as phenyldimethylsilvl, t-butyldimethylsilvl and triisopropyl groups. Sensitivity to electron capture techniques may be introduced with chlorodimethylsilvl, or pentafluorophenyldimethylsilvl groups. For industrial scale synthesis, difunctional dimethylsilvl groups offer economic incentive in protecting two molecules simultaneously. Di-functional materials are also employed for silvlation of vicinal hydroxyl groups.

Silvation reagents are selected by a number of factors: specificity, donor strength, byproducts and cost. The most widely used are the trimethylsilyl reagents:



A number of other trimethylsilyl donor reagents are available, but their utility is not as generally recognized. The range of donor reagents for other silyl groups is generally more limited, but analogous to trimethylsilyl reagents.

Difunctional blocking agents include the following materials.

With the exception of basic proton acceptors, solvents used for silylation reactions must be aprotic. If used in analysis or microchemical reactions, they should be dried before use. In most cases allowing the solvent to stand over 3A molecular sieves is adequate. Typical solvents are dimethylformamide, hexane, acetonitrile, tetrahydrofuran, and toluene. When basic proton acceptor solvents are desired, pyridine and triethylamine are preferred.
<u>CHLOROSILANES/BASE</u> – Silylation of most protic compounds can be effected by dissolving the compound in an appropriate solvent with a 20% molar excess of base. Preferred bases are triethylamine, pyridine, and tributylamine. If the reaction is to be run with t-butyldimethylchlorosilane (B2790) instead of trimethylchlorosilane, imidazole is the preferred base. Trimethylchlorosilane is then added at a moderate rate, again in 20% molar excess. In most instances exotherm is minimal, but care should be take with initial reactions to observe heating during addition. Most reactions are completed at room temperature, but a two hour reflux may be necessary. Amides and enol ethers may be silylated by this method, but the base is employed as the solvent in a minimum of 4 - 5 times mole ratio followed by a 6 - 8 hour reflux. While a good general technique, disadvantages of this method are the corrosive chlorosilane and filtration required, and possible difficulties in purification.

HEXAMETHYLDISILAZANE (HMDS) – HMDS may be used directly with alcohols, phenols, amines and carboxylic acids. It is added to the compound to be derivatized as a 0.6 molar equivalent and utilized neat or with an appropriate solvent. The reaction proceeds at room temperature with most primary and secondary alcohols. Other compounds may require refluxing for up to 8 hours. Completion can be judged by halt of ammonia evolution. Silylation of less reactive groups may be facilitated by the addition of a few drops of H_2SO_4 , 2 – 3% ammonium sulfate or better, 10% trimethylchlorosilane.

<u>SILYLAMINES</u> – Silylamines are used for silylation of alcohols, amines, amino acids, amides and ureas. Dimethylaminotrimethylsilane is particularly useful for aminoacid hydrochlorides, converting them directly to silylated amino acids with dimethylamine hydrochloride byproduct. Trimethylsilylimidazole is extremely active in silylation of carbohydrate hydroxyl groups. TMSI reactivity can be considered analogous to the amides. The general procedure for the silylamines yield volatile byproducts, imidazole is precipitated in TMSI reactions.

<u>SILYLAMIDES</u> – Silylamides are the most powerful silylation reagents employed in derivatization for analysis. They include BSA, BSU, and TDPU. BSA is an excellent solvent and may be used neat for many reactions. In general, a slight molar excess of the silylamide is dissolved in 3 - 4 fold volume of solvent. Reactions are generally complete in 5 minutes at $65 - 70^{\circ}$ C. Most reactions will proceed in 20 - 30 minutes at room temperature. Progress can usually be followed by dissolution of the material to be derivatized followed by precipitation of free amide. Potentiation of the silylamides with 10% trimethylchlorosilanes results in systems strong enough to convert ketones to silyl ethers.

SILANE COUPLING AGENT CHEMISTRY

The general formula of an organosilane shows two classes of functionality.

R_nSiX_(4-n)

The X functional group is involved in the reaction with the inorganic substrate. The bond between X and the silicon atom in coupling agents is replaced by a bond between the inorganic substrate and the silicon atom. X is a hydrolyzable group, typically, alkoxy, acyloxy, amine, or chlorine. The most common alkoxy groups are methoxy and ethoxy, which give methanol and ethanol as byproducts during coupling reactions. Since chlorosilanes generate hydrogen chloride as a byproduct during coupling reactions, they are generally utilized less than alkoxysilanes.

R is a nonhydrolyzable organic radical that possesses a functionality which enables the coupling agent to bond with organic resins and polymers. Most of the widely used organosilanes have one organic substituent.

In most cases the silane is subjected to hydrolysis prior to the surface treatment. Following hydrolysis, a reactive silanol group is formed, which can condense with other silanol groups, for example, those on the surface of siliceous fillers, to form siloxane linkages. Stable condensation products are also formed with other oxides such as those of aluminum, zirconium, tin, titanium, and nickel. Less stable bonds are formed with oxides of boron, iron, and carbon. Alkali metal oxides and carbonates do not form stable bonds with Si – O –.

Water for hydrolysis may come from several sources. It may be added, it may be present on the substrate surface or it may come from the atmosphere. Water for hydrolysis may also be generated in situ by dissolving chlorosilanes in excess alcohol. Reaction with alcohol produces alkoxysilanes and HCl, which can react with additional alcohol to form an alkyl halide and water.

Reaction of these silanes involves four steps. Initially, hydrolysis of the three labile X groups attached to silicon occurs.



Condensation to oligomers follows.



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The oligomers then hydrogen bond with OH groups of the substrate.



Finally during drying or curing, a covalent linkage is formed with the substrate with concomitant loss of water. At the interface, there is usually only one bond from each silicon of the organosilane to the substrate surface. The two remaining silanol groups are present either bonded to other coupling agent silicon atoms or in free form.



The number of reactive sites on a surface area and the type of silane deposition sought, i.e. monolayer, multilayer or bulk, are all factors which can be used in calculating the amount of silane necessary to silylate a surface. In order to provide monolayer coverage, the concentration of reactive sites (silanols) should be determined. Most siliceous substrates have 4 – 12 silanols per m μ^2 . Thus, one mole of evenly distributed silane should cover an average of 7500 m². The oligimerization of silanes with multiple groups thwarts the capability of computing stoichiometries, but order of magnitude computations are successful. Silanes with one hydrolyzable group can be utilized to produce surfaces with monolayers of consistent stoichiometry. These materials are more expensive and produce surfaces with less hydrolytic stability. The number of silanols on a surface is varied by thermal history. In one example, a siliceous surface having 5.3 silanols per mu² had only 2.6 after exposure to 400°C and less than one after exposure to 850°C. Higher concentrations of silanol groups may be produced by treating material with warm hydrochloric acid. Silanol anions may be produced by treating the surfaces with alkaline detergent or, more radically, by treatment with methanolic potassium hydroxide. Optimum deposition of silanes with more than one hydrolyzable group is often defined as the as the amount necessary to produce a surface of uniform energy. A value defined as the wetting surface (ws) describes the area in m² one gram of silane deposited from solution will cover. In combination with data on the surface area of a siliceous substrate in m^2/g the amount of silane required for deposition may be calculated. Most composite, adhesive, and coating formulations do not follow any stoichiometry, but simply define optimal concentration by operation success. For most fillers, a treatment level of 0.02 – 1.00% by weight is used.

Selecting a Silane Coupling Agent

Selection of the appropriate coupling agent is accomplished by empirical evaluation of silanes within predicted categories. Exact prediction of the best silane is extremely difficult. Increased bond strength by utilization of silanes is a result of a complex set of factors – wet out, surface energy, boundary layer absorbtion, polar adsorption, acid-base interaction, interpenetrating network formation and covalent reaction. Strategies for optimization must take into account the materials on both sides of the interface and their susceptibilities to the various coupling factors. Generally speaking the initial approach is to select a single coupling agent and assume a direct bond between the two materials. The most common application for silane coupling agents is to bond an inorganic substrate to a polymer.

Inorganic-Si-R-Organic

The number of hydrolyzable X groups on the silane is another important parameter in controlling bond characteristics. The traditional silane coupling agents contain three hydrolyzable groups. They have maximum hydrolytic stability but tend to by hydroscopic. At the opposite end are the silanes with one hydrolyzable group. These yield the most hydrophobic interfaces but have the least long term hydrolytic stability. Silanes with two hydrolyzable groups form less rigid interfaces than silanes with three hydrolyzable groups. They are often used as coupling agents for elastomers and low modulus thermoplastics. Polymeric silanes with recurrent trialkoxy or dialk-oxysilanes offer better film-forming and primer capabilities. For enhanced hydrolytic stability or economic benefit, non-functional silanes such as short chain alkyltrialkoxysilanes or phenyltrialkoxysilanes can be combined in ratios up to 3:1 with functional silanes.

In more difficult bonding situations, mixed silanes or silane network polymers may be employed. These include inorganic to inorganic or organic to organic. In these cases, reaction of the silanes with themselves is critical.

Inorganic-O-Si-R-R-Si-O-Inorganic

Organic-O-Si-R-R-Si-O-Organic

An example of mixed silane application is the use of mixtures of epoxy and amine functional silanes to bond glass plates together. A more general use is bonding organic to organic. Primers, prepared by pre-hydrolyzing silanes to resins in order to form bulk layers on metal substrates, are examples of the application of silanes as network polymers.

Thermal Stability

Most silanes have moderate thermal stability, making them suitable for plastics that process below 350°C or have continuous temperature exposures below 150°C. Silanes with an aromatic nucleus have higher thermal stability. A relative ranking where Z is the functional groups is as follows:

Class	Example	Thermal Limit
ZCH ₂ CH ₂ SiX ₃	N/A	< 150°C
ZCH ₂ CH ₂ CH ₂ SiX ₃	A0700	390°C
ZCH ₂ AromaticCH ₂ CH ₂ SiX ₃	T2902	495°C
Aromatic SiX ₃	P0320	550°C

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Table 1 - Thermosets					
Name	Class	UCT Product			
dially/abthalata	amine	A0698	A0700	A0750	
dialiyiphinalate	styryl	S1590			
	amine	A0700	A0750	T2910	
	ероху	G6720	E6250		
ероху	chloroalkyl	C3300			
	mercapto	M8450	M8500		
	chloromethylaromatic	T2902			
imide	amino	A0698	A0700	A0750	
	armite	T2910			
	amine	A0700	A0750	T2910	
melamine	ероху	G6720	E6250		
	alkanolamine	B2408			
paralene	chloromethylaromatic	T2902			
	amine	A0700	A0750	T2910	
phenolic	chloroalkyl	C3300			
	ероху	G6720	E6250		
	silazane	H7300	D6208		
photoresist, negative	vinyl	D6208	V4900		
	aromatic	P0320			
	silazane	H7300			
photoresist, positive	aromatic	P0320			
	phosphine	D6110			
	amine	A0700	A0750	T2910	
polycostor	methacrylate	M8550			
polyester	styryl	S1590			
	vinyl	V4917	V4910		
	amine	A0700	A0750	T2910	
urothana	alkanolamine	B2408			
	ероху	G6710	G6720	E6250	
	isocyanate	17840			
Table	e 2 - Thermoplastics				
cellulosics	amine	A0700	A0750	T2910	
	isocyanate	17840			
polyacetal	thiouronium	S1590			
polyacrylate	methacrylate	M8550			
	ureido	T2507			
	amina	A0700	A0750	T2910	
polyamide (nylon)	armie	A0742	PS076		
	ureido	T2507			
nolvamide-imide	chloromethylaromatic	T2902			
	amine	A0700	A0750	A0800	
	amine	A0698	A0750		
	isocyanate	17840			

Table 2 - Thermoplastics (cont.)					
polycarbonate	amine	A0700	A0750	T2910	
polyetherketone	amine	A0698	A0750	A0800	
ethylene-vinyl acetate copolymer	ureido	T2507			
	amine	A0700	A0742	A0750	
polyethylene	vinyl	V4910	V4917		
	styryl	S1590			
nalyphanylana ayida	amine	A0700	A0750	T2910	
polyphenylene oxide	aromatic	P0320			
	amina	A0698	A0700	A0750	
nalyphanylana gylfida	annine	T2910			
polyphenylene suilide	mercapto	M8450	M8500	B2494	
	chloromethylaromatic	T2902			
	aromatic	P0320	P0330		
polypropylerie	styryl	S1590			
	aromatic	P0320	P0330		
polystyrene	ероху	G6720	E6250		
	vinyl	V4910	V4917		
polysulfone	amine	A0700	A0750	T2910	
polyvinyl butyral	amine	A0700	A0742	A0750	
	amine	A0700	A0750	T2910	
polyvinyi chloride	alkanolamine	B2408			
	Table 3 - Sealants	_			
	acrylic	A0380	M8550		
acrylic	styryl	S1590			
	ероху	G6710	G6720	E6250	
	mercapto	B2494	M8500	M8450	
polysulfides	amino	A0699	A0700	A0742	
	annine	A0750	T2910		
	Table 4 - Rubbers				
butyl	epoxide	G6710	G6720	E6250	
neoprene	mercapto	M8450	M8500		
isoprene	mercapto	M8450	M8500		
fluorocarbon	amine	A0698			
Indorocarbon	styryl	S1590			
	amino	A0699	A0700	A0742	
epichlorohydrin		A0750			
	mercapto	M8450	M8500		
silicone	amine	A0700	A0750		
	allyl	A0567			
Table 5 - Water S	Soluble and Hydrophilic p	olymers			
	epoxy	G6710	G6720		
Cellulosic	isocvanate	17840			

Table 5 - Water Soluble and Hydrophilic polymers (cont.)				
	amine	A0800	PS076	
heparin	ероху	G6710	G6720	
	isocyanate	17840		
polyethylene oxide	isocyanate	17840		
polybydroxyetbylmetbacrylate	ероху	G6710	G6720	
polytryuloxyettryimethaciylate	isocyanate	17840		
polysaccharida	ероху	G6710	G6720	
polysacchande	isocyanate	17840		
polywinyl alcohol	ероху	G6710	G6720	
	isocyanate	17840		
siliceous	all listed in Table 1	A0700		
aluminum, zirconium, tin and titanium metals	all listed in Table 1, but the epoxies, acrylates and quats preferred	S1590	M8540	
connor iron	polyamine	T2910	PS076	
copper, non	phosphine	D6110		
add procious motals	phosphine	D6110		
	mercapto	B2494	M8500	
silicon	vinyl	D6208		

APPLYING A SILANE COUPLING AGENT

Deposition from aqueous alcohol solutions is the most facile method for preparing silylated surfaces. A 95% ethanol – 5% water solution is adjusted to pH 4.5 – 5.5 with acetic acid. Silane is added with stirring to yield a 2% final concentration. Five minutes should be allowed for hydrolysis and silanol formation. Large objects, e.g. glass plates, are dipped into the solution, agitated gently, and removed after 1 – 2 minutes. They are rinsed free of excess materials by dipping briefly in ethanol. Particles, e.g. fillers and supports, are silylated by stirring them in solution for 2 – 3 minutes and then decanting the solution. The particles are usually rinsed twice briefly with ethanol. Cure of the silane layer is for 5 – 10 minutes at 110°C or for 24 hours at room temperature (<60% relative humidity).

For aminofunctional silanes such as A0700 and A0750 this procedure is modified by omitting the additional acetic acid. The procedure is not acceptable for chlorosilanes as bulk polymerization often occurs. Silane concentration of 2% is a starting point. It usually results in deposition of trialkoxysilanes as 3 - 8 molecular layers. Monoalkoxysilanes are always deposited in monolayers or incomplete monolayers. Caution must be exercised if oven curing. Exhausted, explosion-proof ovens should always be used.

Deposition from aqueous solutions is employed for most commercial fiberglass systems. The alkoxysilane is dissolved at 0.5 - 2.0% concentration in water. For less soluble silanes, 0.1% of a non-ionic surfactant is added prior to the silane and an emulsion rather than a solution is prepared. If the silane does not contain an amine group, the solution is adjusted to pH 5.5 with acetic acid. The solution is either sprayed onto the substrate or employed as a dip bath. Cure is at 110 - 120°C for 20 - 30 minutes.

Stability of aqueous silane solutions varies from hours for the simple alkyl silanes to weeks for the aminosilanes. Poor solubility parameters limit the use of long chain alkyl and aromatic silanes by this method. Distilled water is not necessary, but water containing fluoride ions must be avoided.

Bulk deposition onto powders, e.g. filler treatment, is usually accomplished by a spray-on method. It assumes that the total amount of silane necessary is known and that sufficient adsorbed moisture is present on the filler to cause hydrolysis of the silane. The silane is prepared as a 25% solution in alcohol. The powder is placed in a high intensity solid mixer, e.g. twin cone mixer with intensifier. The solution is pumped into the agitated powder as a fine spray. In general, this operation is completed within 20 minutes. Dynamic drying methods are most effective. If the filler is dried in trays, care must be taken to avoid wicking or skinning of the top layer of treated material by adjusting heat and air flow.

Integral blend methods are used in composite formulations. In this method the silane is used as a simple additive. Composites can be prepared by the addition of alkoxysilanes or silazanes to dry-blends of polymer and filler prior to compounding. Generally 0.2 - 1.0 weight percent of silane (on the total mix) is dispersed by spraying the silane in an alcohol carrier onto a pre-blend. The addition of the silane to non-dispersed filler is not desirable in this technique since it can lead to agglomeration. The mix is dry-blended briefly and then melt compounded. Vacuum devolatization of byproducts of silane reaction during melt compounding is necessary to achieve optimum properties. Properties are sometimes enhanced by adding 0.5 - 1.0% of tetrabutyl titanate or benzyldimethylamine to the silane prior to dispersal. Amino-functional silanes are available in concentrate form for dry-blending with nylons and polyesters. Concentrates eliminate any need for solvent dispersion and devolatization and reduce variability due to relative humidity and shelf-aging.

Deposition as a primer is employed where a bulk phase is required as a transition between a substrate and a final coating. The silane is dissolved at 50% concentration in alcohol. One to three molar equivalents of water are added. The mixture is allowed to equilibrate for 15 - 20 minutes and then diluted to 10% concentration with a higher boiling polar solvent. Materials to be coated with the primer are dipped or sprayed and then cured at $110 - 120^{\circ}$ C for 30 - 45 minutes.

Chlorosilanes such as V4900 may be deposited from alcohol solution. Anhydrous alcohols, particularly ethanol or isopropanol are preferred. The chlorosilane is added to the alcohol to yield a 2 - 5% solution. The chlorosilane reacts with the alcohol producing an alkoxysilane and HCl. Progress of the reaction is observed by halt of HCl evolution. Mild warming of the solution ($30 - 40^{\circ}$ C) promotes completion of the reaction. Part of the HCl reacts with the alcohol to produce small quantities of alkyl halide and water. The water causes formation of silanols from alkoxy silanes. The silanols condense with those on the substrate. Treated substrates are cured for 5 - 10 minutes at 110° C or allowed to stand 24 hours at room temperature.

Chlorosilanes and silylamines may also be employed to treat substrates under aprotic conditions. Toluene, tetrahydrofuran or hydrocarbon solutions are prepared containing 5% silane. The mixture is refluxed for 12 – 24 hours with the substrate to be treated. It is washed with the solvent. The solvent is then removed by air or explosion-proof oven drying. No further cure is necessary. This reaction involves a direct nucleophilic displacement of the silane chlorines by the surface silanol. If monolayer deposition is desired, substrates should be pre-dried at 150°C for 4 hours. Bulk deposition results if adsorbed water is present on the substrate. This method is cumbersome for large scale preparations and rigorous controls must be established to ensure reproducible results. More reproducible coverage is obtained with monochlorosilanes.

Silazanes such as H7300 and D6208 may be used as treatments in concentrated form or as 10 - 20% solutions in aprotic solvents. In some applications, parts are exposed for 5 - 10 minutes by dipping or in microelectronics by spin-on techniques. Optimum reactivity is at $30 - 50^{\circ}$ C. An alternate method of treatment is to expose parts to 50° C vapor for 2 - 6 hours. Ammonia is the byproduct of silazane reaction and areas should be ventilated.

Appendix

Calculations of necessary silane to obtain minimum uniform multilayer coverage can be obtained knowing the values of the wetting surface of silane (ws) and the surface area of filler

Amount of silane (g) = (amount of filler) x (surface area of filler)

wetting surface (ws)

Relative surface area of common fillers m²/g

E-Glass	0.1 – 0.12
Silica, ground	1 – 2
Kaolin	7
Clay	7
Talc	7
Si, diatomaceous	1 – 3.5
Calcium silicate	2.6
Silica, fumed	150 - 250

UCT SPECIALTIES SILANES



ABBREVIATIONS

CAS#	Chemical Abstract Service Registry Number
MW	Molecular Weight
BP	Boiling Point
SG	Specific Gravity
RI	Refractive Index
LCLO	Lethal Concentration Low
LD100	Lethal Dose 100%
LD50	Median Lethal Dose
LDLO	Lethal Dose Low
TSCA	Listed on the Toxic Substances Control Act inventory
R&D Only	Appoved for research & development only
	(not listed on TSCA)



A0300 2-ACETOXYETHYLTRICHLOROSILANE



CAS# 18204-80-3	MW 221.54	C ₄ H ₇ Cl ₃ O ₂ Si	TSCA
Flash Pt. 82°C	BP 143°C/70 mm	SG @ 20°C 1.272	
97% Purity	RI @ 20°C 1.4427		

C₇H₁₂Cl₂O₂Si

SG @ 20°C 1.15

TSCA

R&D ONLY

A0394

3-ACRYLOXYPROPYLMETHYLDICHLOROSILANE



CAS# 71550-63-5 Flash Pt. >110°C 97% Purity - Isomers RI @ 25°C 1.4585

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MW 227.15

BP 73°C/0.1 mm

A0396

3-ACRYLOXYPROPYLTRICHLOROSILANE



CAS# 385 Flash Pt. 97% Purity

595-89-0	MW 247.58	$C_6H_9CI_3O_2Si$
34°C	BP 63°C/0.4 mm	SG @ 20°C 1
ty	RI @ 20°C 1.4631	

.26





CAS# 4369-14-6	MW 234.32	$C_9H_{18}O_5Si$	TSCA
Flash Pt. 123°C	BP 95-100°C/3 mm	SG @ 20°C 1.00	
92% Purity			

ADAMANTYLETHYLTRICHLOROSILANE A0400

CAS# 37843-11-1	MW 297.73	$C_{12}H_{19}CI_3Si$	TSCA
Flash Pt. 155°C	BP 135°C/3 mm	SG @ 20°C 1.2204	
80% Purity	RI @ 20°C 1.5135	Melting Pt. 36°C	
	CAS# 37843-11-1 Flash Pt. 155°C 80% Purity	CAS# 37843-11-1MW 297.73Flash Pt. 155°CBP 135°C/3 mm80% PurityRI @ 20°C 1.5135	CAS# 37843-11-1 MW 297.73 C12H19Cl3Si Flash Pt. 155°C BP 135°C/3 mm SG @ 20°C 1.2204 80% Purity RI @ 20°C 1.5135 Melting Pt. 36°C



A0555 ALLYLMETH		E			
$ \begin{array}{c} CI \\ H_2C = CH - CH_2 - \overset{I}{Si} - CH_3 \\ CI \\ \end{array} $	CAS# 1873-92-3 Flash Pt. 27°C 95% Purity	MW 155.10 BP 119-120°C RI @ 20°C 1.4419	C₄H ₈ Cl₂Si SG @ 20°C 1.076	TSCA	
A0560 ALLYLTRICH	LOROSILANE				
CI	CAS# 107-37-9	MW 175.52	C₃H₅Cl₃Si	TSCA	
H ₂ C=CH-CH ₂ -Si-Cl	Flash Pt. 18°C	BP 117-118°C	SG @ 20°C 1.201		
	95% Purity	RI @ 20°C 1.446			
	TOXICITY: ivn mus, L	D50: 56 mg/kg			
A0564 ALLYLTRIETI	HOXYSILANE				
CH ₃ CH ₂	CAS# 2550-04-1	MW 204.34	$C_9H_{20}O_3Si$	TSCA	
H ₂ C=CH-CH ₂ -Si-O-CH ₂ -CH ₃	Flash Pt. 70°C	BP 176°C	SG @ 25°C 0.903		
O CH ₂	97% Purity	RI @ 25°C 1.406			
ĊH ₃					
A0567 ALLYLTRIME	THOXYSILANE				
CH ₃ O	CAS# 2551-83-9	MW 162.26	$C_6H_{14}O_3Si$	TSCA	
$H_2C = CH - CH_2 - Si - O - CH_3$	Flash Pt. 46°C	BP 146-148°C	SG @ 25°C 0.963		
	97% Purity	RI @ 25°C 1.4036			
A0570 ALLYLTRIME	THYLSILANE				

'		IIILSILANL			
	CH ₂	CAS# 762-72-1	MW 114.26	C ₆ H ₁₄ Si	TSCA
	H ₂ C=CH-CH ₂ Si-CH ₃	Flash Pt. 7°C	BP 85-86°C/0.4 mm	SG @ 20°C 0.719	
	CH ₃	97% Purity	RI @ 25°C 1.4074		

A0695	4-AMINOBUT	YLDIMETHYLMETH	IOXYSILANE		
	CH₂	CAS# 3663-43-2	MW 161.32	C ₇ H ₁₉ NOSi	TSCA
H ₂ N-(C	$H_2)_4$ $ Si$ $-OCH_3$	Flash Pt. 85°C	BP 85°C/17 mm	SG @ 20°C 0.85	
	CH ₃	95% Purity	RI @ 20°C 1.4325		







A0750 **3-AMINOPROPYLTRIETHOXYSILANE**

СН ₃ СН ₂	CAS# 919-30-2	MW 221.37	C ₉ H ₂₃ NO ₃ Si	TSCA
Н₂N−(CH₂) <u>3−</u> Şi—O−CH <u>2</u> −CH ₃	Flash Pt. 96°C	BP 122-123°C/30 mi	n SG @ 20°C 0.951	
O C H ₂	97% Purity	RI @ 20°C 1.4225		
CH ₃	TOXICITY - orl rat, LD50: 1780 mg/kg			

A0800

3-AMINOPROPYLTRIMETHOXYSILANE

CH3
Ó I
$H_2N-(CH_2)_{\overline{3}}-Si-O-CH_3$
O I
ĊH ₃

CAS# 13822-56-5 Flash Pt. 104°C 97% Purity

BP 80°C/8 mm RI @ 25°C 1.420

MW 179.29

ŀ	40805 3-AMINOPROPYLTRIS(TRIMETHYLSILOXY)SILANE					
	OSi(CH ₂)2	CAS# 25357-81-7	MW 353.76	$C_{12}H_{35}NO_3Si_4$	TSCA
	H ₂ N—(CH ₂) ₃ —Si—OSi	(CH ₃) ₃	Flash Pt. >93°C	BP 152°C/47 mm	SG @ 25°C 0.891	
	ÖSi(CH ₃)3	97% Purity	RI @ 25°C 1.5135		

B1597 BENZYLDIMETHYLSILANE



Flash Pt. 65°C 97% Purity

CAS# 1631-70-5

MW 150.30	C ₉ H ₁₄ Si
BP 70°C/15 mm	SG @ 20°C 0.949
RI @ 20°C 1.5040	

 $C_6H_{17}NO_3Si$

SG @ 25°C 1.01

TSCA

TSCA

B1710 1,3-BIS(3-AMINOPROPYL)-1,1,3,3-TETRAMETHYLDISILOXANE

$H_2N-(CH_2)_3$	CH ₃ - Si— O- CH ₃	СН ₃ –Si— (СН ₂) ₃ — NH ₂ СН ₃	2

CAS# 2469-55-8	MW 248.52	$C_{10}H_{28}N_2OSi_2$	TSCA
Flash Pt. 91°C	BP 132-139°C/11 mm	SG @ 25°C 0.897	
97% Purity	RI @ 25°C 1.4480		

B1724 1,3-BIS(3-CARBOXYPROPYL)TETRAMETHYLDISILOXANE CAS# 3353-68-2 MW 306.51 $C_{12}H_{26}O_5Si_2$ TSCA CH_3 CH_o -Śi—(CH₂)3—C-OH но-с (CH) -0сн_з ĊНз 97% Purity Melting Pt. 47-49°C

51







•			
CAS# 52217-53-5	MW 381.10	$C_8H_{16}CI_6Si_2$	R&D ONL
Flash Pt. 120°C	BP 140°C/1 mm	SG @ 20°C 1.282	
97% Purity	RI @ 20°C 1.4757		

B2491.5

1,2-BIS(TRIETHOXYSILYL)ETHANE



CAS# 16068-37-4	MW 354.59	$C_{14}H_{34}O_6Si_2$	TSCA
Flash Pt. 107°C	BP 96°C/0.3 mm	SG @ 20°C 0.957	
97% Purity	RI @ 20°C 1.4052		



B2494

BIS[3-(TRIETHOXYSILYL)PROPYL]TETRASULFIDE



CAS# 40372-72-3 $C_{18}H_{42}O_6S_4Si_2$ MW 538.94 Flash Pt. 91°C **BP** 250°C SG @ 20°C 1.074 22% Sulfur TOXICITY: orl rat, LD50: 17,500 mg/kg

B2495.6

1,4-BIS(TRIMETHOXYSILYLETHYL)BENZENE



CAS# 58298-01-4 **MW** 374.58 $C_{16}H_{30}O_6Si_2$ BP 148-150°C/0.1 mm SG @ 20°C 1.08 Flash Pt. 193°C 97% Purity - Isomers RI @ 20°C 1.4734

B2495.7 1,6-BIS(TRIMETHOXYSILYL)HEXANE



MW 326.54 $C_{12}H_{30}O_6Si_2$ **BP** 161°C/2 mm 97% Purity

BIS(TRIMETHYLSILOXY)METHYLSILANE



CAS# 1873-88-7	MW 222.51
Flash Pt. 22°C	BP 141-142°C
95% Purity	RI @ 20°C 1.3815

B2500

B2497

BIS(TRIMETHYLSILYL)ACETAMIDE



CAS# 10416-59-8 MW 203.43 C₈H₂₁NOSi₂ **TSCA** Flash Pt. 42°C **BP** 71-73°C/35 mm SG @ 20°C 0.832 92% Purity - Isomers RI @ 20°C 1.418 TOXICITY: ipr mus, LDLO: 500 mg/kg

C7H22O2Si3

SG @ 20°C 0.814

BIS(TRIMETHYLSILYL)TRIFLUOROACETAMIDE B2570



CAS# 25561-30-2 **MW** 257.40 $C_8H_{18}F_3NOSi_2$ Flash Pt. 23°C **BP** 45-50°C/15 mm SG @ 20°C 0.97 97% Purity - Isomers RI @ 25°C 1.381



53

TSCA

R&D ONLY

R&D ONLY

TSCA

TSCA



B2614.4 BROMOPHENYLTRIMETHOXYSILANE



CAS# 17043-05-9 **MW** 277.19 C₉H₁₃BrO₃Si **R&D ONLY** Flash Pt. 105°C SG @ 20°C 1.631 **BP** 136°C/13.5 mm 97% Purity - Isomers RI @ 20°C 1.5388

B2785 n-BUTYLDIMETHYLCHLOROSILANE



CAS# 1000-50-6	MW 150.72
Flash Pt. 39°C	BP 138°C
97% Purity	RI @ 20°C 1

BP 138°C	
RI @ 20°C 1.4205	

TSCA

SG @ 20°C 0.875

C₆H₁₅CISi





CAS# 69739-34-0 Flash Pt. 35°C 90% Purity

MW 264.33 BP 65°C/10 mm RI @ 20°C 1.385

 $C_7H_{15}F_3O_3SSi$ **R&D ONLY** SG @ 20°C 1.151

tert-BUTYLDIPHENYLCHLOROSILANE



CAS# 58479-61-1	MW 274.84	C ₁₆ H ₁₉ CISi	R&D ONLY
Flash Pt. >112°C	BP 90°C/0.015 mm	SG @ 20°C 1.074	
97% Purity	RI @ 20°C 1.568		

tert-BUTYLDIPHENYLMETHOXYSILANE



CAS# 76358-47-9	MW 270.45	C ₁₇ H ₂₂ OSi	R&D ONLY
Flash Pt. >43°C			
97% Purity		Melting Pt. 49-51°C	

B2805

B2806



B2850 n-BUTYLTRICHLOROSILANE



CAS# 7521-80-4	MW 191.56	C₄H ₉ Cl₃Si	TSCA
Flash Pt7°C	BP 142-143°C	SG @ 20°C 1.161	
97% Purity	RI @ 20°C 1.436		

C14H29CIO2Si

C2895

C3005

(10-CARBOMETHOXYDECYL)DIMETHYLCHLOROSILANE



Flash Pt. 105°C
95% Purity

CAS# 53749-38-5

RI @ 20°C 1.4483

BP 133°C/0.3 mm

MW 292.92

C	2905 2-(CARBOMET	HOXY)ETHYLTRICH	ILOROSILANE		
	0 0	CAS# 18147-81-4	MW 221.54	$C_4H_7CI_3O_2Si$	TSCA
	$H_3C = O = C = (CH_2)_2 = Si = CI$	Flash Pt. 43°C	BP 90-92°C/25 mm	SG @ 20°C 1.325	
	CI	95% Purity - Isomers	RI @ 20°C 1.448		

2-CHLOROETHYLMETHYLDICHLOROSILANE



CAS# 7787-85-1	MV
Flash Pt. 32°C	BP
97% Purity	RI

5-1 MW 177.53 C BP 157°C RI @ 20°C 1.4399 C₃H₇Cl₃Si **TSCA SG** @ 20°C 1.261

 C3270
 CHLOROMETHYLDIMETHYLCHLOROSILANE

 $C_{1} = CH_{3}$ CAS# 1719-57-9 MW 143.09
 $C_{3}H_{8}Cl_{2}Si$ TSCA

 $CI = CH_{2} = Si = CI$ GH_{3} CAS# 1719-57-9 MW 143.09
 $C_{3}H_{8}Cl_{2}Si$ TSCA

 $Flash Pt. 21^{\circ}C$ BP 115-116^{\circ}C
 SG @ 20^{\circ}C 1.087
 97% Purity
 RI @ 20^{\circ}C 1.436



R&D ONLY







C3360 2-(4-CHLOROSULFONYLPHENYL)ETHYLTRIMETHOXYSILANE



C3445

3-CYANOPROPYLDIMETHYLCHLOROSILANE



 CAS# 18156-15-5
 MW 161.71
 C₆H₁₂CINSi

 Flash Pt. 108°C
 BP 108-109°C/15 mm
 SG @ 20°C 0.993

 97% Purity - Isomers
 RI @ 20°C 1.446

C3447 3-CYANOPROPYLDIMETHYLMETHOXYSILANE $\begin{bmatrix} CH_3 \\ -Si-O-CH_3 \\ -H_3 \end{bmatrix}$ CAS# 143203-47-8 MW 157.29 C₇H₁₅NOSi R&D ONLY $N = C - (CH_2)_3 - Si-O-CH_3 \\ -Si-O-CH_3 \\ -Si-O-CH_3 \end{bmatrix}$ Flash Pt. 74°C 97% Purity - Isomers 97% Purity - Isomers

MW 182.18

BP 79-82°C/1 mm

C3450 3-CYANOPROPYLMETHYLDICHLOROSILANE



CAS#	119	90-16-5
Flack	D4	0000

Flash Pt. 92°C

97% Purity - Isomers RI @ 25°C 1.455

TOXICITY: orl rat, LD50: 2,830 mg/kg

C3555 3-CYANOPROPYLTRICHLOROSILANE



 CAS# 1071-27-8
 MW 231.37
 C4H6Cl3NSi
 TSCA

 Flash Pt. 75°C
 BP 93-94°C/8 mm
 SG @ 20°C 1.280

 97% Purity
 RI @ 20°C 1.465
 SCA

C₅H₉Cl₂NSi

SG @ 20°C 1.22

CYCLOHEXYLTRICHLOROSILANE



C3660

CAS# 98-12-4 MW 217.60 C ₆ H ₁₁ Cl ₃ Si	ISCA
Flash Pt. 94°C BP 90-91°C/10 mm SG @ 20°C 1.222	
97% Purity RI @ 20°C 1.4774	

TSCA

TSCA







 CAS# 13829-21-5
 MW 275.72
 C10H21Cl3Si
 TSCA

 Flash Pt. >10°C
 BP 133-137°C/5 mm
 SG @ 20°C 1.0640
 SCA

 96% Purity - Isome
 RI @ 20°C 1.4528
 SCA
 SCA

D4280

1,5-DICHLOROHEXAMETHYLTRISILOXANE



CAS# 3582-71-6	MW 277.37	$C_6H_{18}CI_2O_2Si_3$	TSCA
Flash Pt. 76°C	BP 184°C	SG @ 20°C 1.018	
95% Purity	RI @ 20°C 1.4071	Melting Pt53°C	



D4320 1,7-DICHLOROOCTAMETHYLTETRASILOXANE

CI—s	CH ₃ 8i—O− CH ₃	CH ₃ -Si—O- CH ₃	CH ₃ 	CH₃ -Si—CI -CH₃

CAS# 2474-02-4 MW 351.52 Flash Pt. 98°C BP 222°C 90% Purity RI @ 20°C 1.403

90% **Purity**

D4368

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1,3-DICHLOROTETRAISOPROPYLDISILOXANE



CAS# 69304-37-6	
Flash Pt. 45°C	
96% Purity	

BP 120°C/15 mm **RI** @ 20°C 1.4543

MW 315.43

C₁₂H₂₈Cl₂OSi **R&D ONLY** SG @ 20°C 1.001

TSCA

C₈H₂₄Cl₂O₃Si₄

SG @ 20°C 1.011

Melting Pt. -62°C

04370 1,3-DICHLORO	DTETRAMETHYLDI	SILOXANE		
ÇH ₃ ÇH ₃	CAS# 2401-73-2	MW 203.22	$C_4H_{12}CI_2OSi_2$	TSCA
CI—Și—O—Și—CI	Flash Pt. 15°C	BP 138°C	SG @ 20°C 1.039	
ĊH ₃ ĊH ₃	97% Purity	RI @ 20°C 1.4054	Melting Pt37°C	

D4477 (N,N-DIETHYL-3-AMINOPROPYL)TRIMETHOXYSILANE



CAS# 41051-80-3 Flash Pt. 100°C 95% Purity

3 MW 235.40 C₁₀H₂₅NO₃Si TSCA BP 120°C/20 mm

D4850 DIISOPROPYL	CHLOROSILANE			
н.с. Н. сн.	CAS# 2227-29-4	MW 150.72	C ₆ H ₁₅ CISi	R&D ONLY
$\begin{array}{ c c } H_{3} & J_{3} \\ H_{-} C_{-} Si_{-} C_{-} H \end{array}$	Flash Pt. <37.7°C	BP 137°C	SG @ 20°C 0.872	
H ₃ C CI CH ₃	95% Purity	RI @ 20°C 1.4278		
D4895 DIISOPROPYL	ETHOXYSILANE			

H_3C H CH_3 H-C-Si-C-H	CAS# 90633-16-2	MW 160.33	$C_8H_{20}OSi$	TSCA
H ₃ C O CH ₃ 	96% Purity			







D5600 DIMETHYLDIE	THOXYSILANE			
СН	CAS# 78-62-6	MW 148.28	$C_6H_{16}O_2Si$	TSCA
$H_3C-H_2C-O-Si-O-CH_2-CH_3$	Flash Pt. 11°C	BP 114-115°C	SG @ 20°C 0.865	
ĊН ₃	97% Purity	RI @ 20°C 1.3805	Melting Pt87°C	
	TOXICITY: orl rat, LDL	O: 1,000 mg/kg		
D5605 DIMETHYLDIM	IETHOXYSILANE			
CH ₃	CAS# 1112-39-6	MW 120.22	$C_4H_{12}O_2Si$	TSCA
	Flash Pt8°C	BP 82°C	SG @ 20°C 0.865	
CH ₃	97% Purity	RI @ 20°C 1.3708		
D5635 DIMETHYLETH	IOXYSILANE			
CH ₃	CAS# 14857-34-2	MW 104.22	C ₄ H ₁₂ OSi	TSCA
H-Si-O-CH ₂ CH ₃	Flash Pt. 23°C	BP 54-55°C/15 mm	SG @ 20°C 0.757	
	95% Purity	RI @ 20°C 1.3683		
	TOXICITY: orl rat, LD5	0: 5,000 mg/kg		
D5636 DIMETHYL-n-C	OCTADECYLCHLOR	OSILANE		
CH ₃	CAS# 18643-08-8	MW 347.10	C20H43CISi	TSCA
H ₃ C-(CH ₂) ₁₇ -Si-Cl	Flash Pt. 10°C	BP 159°C/0.1 mm	20 10	
CH ₃	97% Purity - Isomers		Melting Pt. 27°C	
	-		-	
D5830 1,3-DI-n-OCTY	LTETRAMETHYLDIS	ILAZANE		
	CAS# 69519-51-3	MW 357.77	$C_{20}H_{47}NSi_2$	R&D ONLY
$H_3C^-(CH_2)_7^-Si^-N^-Si^-(CH_2)_7^-CH_3$	Flash Pt. >110°C	BP 160-165°C/1 mm	SG @ 20°C 0.826	
СН ₃ Н СН ₃	95% Purity - Isomers	RI @ 20°C 1.4500		
D5950 DIPHENYLDIC	HLOROSILANE			
CL	CAS# 80-10-4	MW 253.20	$C_{12}H_{10}CI_2Si$	TSCA



CAS# 80-10-4	MW 253.20	$C_{12}H_{10}CI_2Si$	TSCA	
Flash Pt. 157°C	BP 309-310°C	SG @ 20°C 1.222		
97% Purity	RI @ 20°C 1.582			
TOXICITY: ipr mus LD50: 383 mg/kg				







D6220 n-DODECYLTRICHLOROSILANE



CAS# 4484-72-4	MW 303.77	$C_{12}H_{25}CI_3Si$	TSCA
Flash Pt. 165°C	BP 155°C/10 mm	SG @ 20°C 1.30	
95% Purity - Isomers	RI @ 20°C 1.4581		

D6221 n-DODECYLTRIETHOXYSILANE



CAS# 18536-91-9	MW 332.60	$C_{18}H_{40}O_3Si$
Flash Pt. >110°C	BP 152-153°C/3 mm	SG @ 20°C 0.89
97% Purity - Isomers	RI @ 20°C 1.472	

E	E6250 2-(3,4-EPOXY	CYCLOHEXYL)ETH	IYLTRIMETHOX	YSILANE
	CH3	CAS# 3388-04-3	MW 246.38	$C_{11}H_{22}O_4Si$
		Flash Pt. 146°C	BP 310°C	SG @ 20°C 1.070



CAS# 3388-04-3	MW 246.38	$C_{11}H_{22}O_4$
Flash Pt. 146°C	BP 310°C	SG @ 2
97% Purity	RI @ 20°C 1.449	
TOXICITY: orl rat, LD50	0: 12,300 mg/kg	

E6350

ETHYLTRICHLOROSILANE

H ₃ C-CH ₂ -SI-CI CI	
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CAS# 115-21-9 Flash Pt. 27°C 92% Purity

MW 163.51	$C_2H_5CI_3Si$	TSCA
BP 100-101°C	SG @ 20°C 1.237	
RI @ 20°C1.426	Melting Pt106°C	

E6380	ETHYLTRIETH	OXYSILANE			
	СН ₃ Г СН ₂	CAS# 78-07-9	MW 192.33	$C_8H_{20}O_3Si$	TSCA
H ₃ C-CH ₂	0 −Si − O−CH <u>2−</u> CH ₃	Flash Pt. 40°C	BP 158-159°C	SG @ 20°C 0.896	
		97% Purity	RI @ 20°C 1.3955	Melting Pt78°C	
	CH ₃	TOXICITY: orl rat, LD5	i0: 13,720 mg/kg		

G6720

3-GLYCIDOXYPROPYLTRIMETHOXYSILANE



CAS# 2530-83-8	MW 236.34	$C_9H_{20}O_5Si$		
Flash Pt. 57°C	BP 120°C/2 mm	SG @ 20°C 1.070		
97% Purity	RI @ 20°C 1.428			
TOXICITY: orl rat, LD50: 8,400 mg/kg				

63

TSCA

TSCA

TSCA





H7280 HEXAMETHYLDISILANE

CH ₃ CH ₃	CAS# 1450-14-2	MW 146.38	$C_8H_{18}Si_2$	TSCA
H ₃ C—Si—Si—CH ₃	Flash Pt10°C	BP 112-113°C	SG @ 20°C 0.729	
CH ₃ CH ₃	96% Purity	RI @ 20°C 1.4214		



H73	00 HEXAMETHYL	DISILAZANE			
	H ₃ C CH ₃ H ₃ C-Si	CAS# 999-97-3	MW 161.39	C ₈ H ₁₉ NSi ₂	TSCA
	H ₃ C—Si	Flash Pt. 12°C	BP 126-127°C	SG @ 20°C 0.774	
	H₃C CH₃	98% Purity	RI @ 20°C 1.4080		
LI72		TOXICITY: ipr mus, LD	LO: 650 mg/kg		
			MW 161 20		TOCA
	H ₃ C—Si	CAS# 999-97-3	NIV 101.39		ISCA
	Ň—H	Flash Pt. 12°C	BP 126-127°C	SG @ 25°C 0.774	
	$H_{3}C$ CH_{3}	99% Purity	RI @ 20°C 1.4080		
		TOXICITY: ipr mus, LD	LO: 650 mg/kg		
H73 ⁻	10 HEXAMETHYL	DISILOXANE			
	CH ₃ CH ₃	CAS# 107-46-0	MW 162.38	$C_6H_{18}OSi_2$	TSCA
H ₃	$C - Si - O - Si - CH_3$	Flash Pt1°C	BP 99-100°C	SG @ 20°C 0.764	
	CH_3 CH_3	97% Purity	RI @ 20°C 1.3774	Melting Pt67°C	
	0 0	TOXICITY: orl gpg, LDI	_O: 32,500 mg/kg		
H732	29.8 5-HEXENYLTR	IMETHOXYSILANE			
	CH3	CAS# 58751-56-7	MW 204.35		R&D ONLY
	H O │ H₂C=C−(CH₂)₄─Şi−O−CH₃	Flash Pt . 68.5°C	BP 193°C	SG @ 20°C 0.9	
	0	97% Purity - Isomers	BI @ 20°C 1 419		
	CH ₃	Si /o i unty isomers	N @ 20 0 1.413		
H73	31 n-HEXYLMETH	HYLDICHLOROSILAN	NE		
	CH₂	CAS# 14799-94-1	MW 199.19	C ₇ H ₁₆ Cl ₂ Si	TSCA
	H₂C−(CH₂)₌−Si−−Cl	Flash Pt. 85°C	BP 204-206°C	SG @ 20°C 0.993	
	° (2/3 ∣ CH₂	97% Purity - Isomers	RI @ 20°C 1.4390		
	5				
H73	32 n-HEXYLTRIC	HLOROSILANE			
		CAS# 928-65-4	MW 219 61	CallaClaSi	TSCA
.		Elach Dt 0500	BD 101 102°C		IUUA
	$I_3C^-(CH_2)_{\overline{5}}^-Si^-Cl$			JU @ 20 C1.10/	
	CI	97% Purity - Isomers	RI @ 20°C 1.3473		





CH₃



	CAS# 18395-30-7	MW 178.30	$C_7H_{18}O_3Si$	TSCA
CH ₃	Flash Pt. 42°C	BP 154-157°C	SG @ 20°C 0.933	
	95% Purity - Isomers	RI @ 20°C 1.3960		

17840 3-ISOCYANATOPROPYLTRIETHOXYSILANE



M8450

3-MERCAPTOPROPYLMETHYLDIMETHOXYSILANE



CAS# 31001-77-1	MW 180.34	$C_8H_{16}O_2SSi$
Flash Pt. 93°C	BP 96°C/30 mm	SG @ 20°C 1.00
95% Purity - Isomers	RI @ 20°C 1.4502	

R&D ONLY



M8500 **3-MERCAPTOPROPYLTRIMETHOXYSILANE**

	CH ₃
	Ó I
HS-(CH ₂) ₃ -	-Si-O-CH ₃
	CH ₃

CAS# 4420-74-0

Flash Pt. 88°C 97% **Puritv**

BP 93°C/40 mm RI @ 20°C 1.4440 C₆H₁₆O₃SSi

 $C_{10}H_{20}O_5Si$

SG @ 20°C 1.045

SG @ 20°C 1.04

TSCA

R&D ONLY

TSCA

MW 196.34

M8543

3-METHACRYLOXYPROPYLDIMETHYLETHOXYSILANE



CAS# 13731-98-1	MW 230.38	$C_{11}H_{22}O_3Si$
Flash Pt. 87°C	BP 75-76°C/0.4 mm	SG @ 20°C 0.926
95% Purity - Isomers	RI @ 20°C 1.4371	

Ν	18545 3-METHACRYI	OXYPROPYLMETH	YLDICHLOROSIL	ANE	
		CAS# 18301-56-9	MW 241.19	$C_8H_{14}CI_2O_2Si$	TSCA
	$\begin{array}{c} O & CI \\ H_{2}C - C - C - O - (CH_{2})_{2} - Si - CH_{2} \end{array}$	Flash Pt. 92°C	BP 75°C/2 mm	SG @ 20°C 1.108	
	CH ₂ CI	97% Purity - Isomers	RI @ 20°C 1.4552		

MW 248.35

BP 78-81°C/1 mm

M8550

3-METHACRYLOXYPROPYLTRIMETHOXYSILANE



CAS#	2530-85-0

Flash Pt. 92°C

97% Purity - Isomers RI @ 25°C 1.429

TOXICITY: orl rat, LD50: 3,000 mg/kg

N-METHYL-N-(t-BUTYLDIMETHYLSILYL)-TRIFLUOROACETAMIDE M8637.1 CAS# 77377-52-7 **MW** 241.33 $C_9H_{18}F_3NOSi$



R&D ONLY Flash Pt. 52°C **BP** 168-170°C SG @ 20°C 1.121 97% Purity RI @ 20°C 1.4018

METHYLDICHLOROSILANE M8750



CAS# 75-54-7	MW 115.03	CH ₄ Cl ₂ Si	TSCA
Flash Pt32°C	BP 41-42°C	SG @ 20°C1.105	
97% Purity	RI @ 20°C 1.422	Melting Pt93°C	
TOXICITY: inh rat, LCL ipr rat, LD50	O: 300 ppm/4H): 150 mg/kg		





O CH ₃ O	CAS# 4253-34-3	MW 220.25	$C_7H_{12}O_6Si$	TSCA
H ₃ C-C-O-Si-O-C-CH ₃ O	Flash Pt. 85°C	BP 87-88°C/3 mm	SG @ 20°C 1.175	
C=O CHo	95% Purity	RI @ 20°C 1.4083	Melting Pt. 40°C	





UCT, Inc. | 2731 Bartram Rd | Bristol, PA 19007 | USA P. 800.541.0559 | 215.781.9255 | F. 215.785.1226 www.unitedchem.com SG @ 20°C 0.89

Flash Pt. 11°C

50% in Methanol

CĪ CH₃

 $H_3C^{-}(CH_2)_{17} - \dot{N}_{-}^{+}(CH_2)_{3}^{-}$

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Si-O-CH3







 CAS# 1000-05-1
 MW 282.63
 C

 Flash Pt. 78°C
 BP 169-170°C
 S

 95% Purity
 RI @ 20°C 1.3875

C₈H₂₆O₃Si₄ **TSCA SG** @ 20°C 0.863

O9816 OCTAMETHYLTRISILOXANE

	CAS# 107-51-7	MW 236.53	$C_8H_{24}O_2Si_3$	TSCA
$H_3C - Si - O - Si - O - Si - CH_3$ $H_3C - Si - O - Si - CH_3$	Flash Pt. 29°C	BP 152-153°C	SG @ 20°C 0.820	
	97% Purity	RI @ 20°C 1.3848	Melting Pt86°C	



O9817.1 OCTAPHENYLCYCLOTETRASILOXANE



CAS# 546-56-5	MW 793.18	$C_{48}H_{40}O_4Si_4$	TSCA
Flash Pt. 392°C	BP 332°C/1 mm	SG @ 22°C 1.185	
N/A Purity		Melting Pt. 200°C	

09817.2 7-OCT-1-ENYLDIMETHYLCHLOROSILANE



CAS# 17196-12-2	MW 204.81	$C_{10}H_{12}CISi$
Flash Pt. 95°C	BP 98°C/11 mm	SG @ 20°C 0.80
96% Purity - Isomers	RI @ 20°C 1.4455	

O9818 7-OCT-1-ENYLTRICHLOROSILANE



CAS# 52217-52-4	MW 245.65	$C_8H_{15}CI_3Si$	TSCA
Flash Pt. 63°C	BP 223-224°C	SG @ 20°C 1.07	
97% Purity - Isomers	RI @ 20°C 1.4578		

O9818.3 7-OCT-1-ENYLTRIMETHOXYSILANE



 CAS# 52217-57-9
 MW 232.39

 Flash Pt. 95°C
 BP 48-49°C/0.1 mm

97% Purity - Isomers



09830 n-OCTYLTRICHLOROSILANE



CAS# 5283-66-9	MW 206.83	C ₈ H ₁₇ Cl ₃ Si	R&D ONLY
Flash Pt. 97°C	BP 224-226°C	SG @ 20°C 1.074	
97% Purity - Isomers	RI @ 20°C 1.447		

 $C_{11}H_{24}O_3Si$

TSCA

TSCA





09840 n-OCTYLTRIMETHOXYSILANE



CAS# 3069-40-7	MW 234.41	$C_{11}H_{26}O_3Si$	R&D ONLY
Flash Pt. 68°C	BP 191-192°C	SG @ 20°C 0.907	
95% Purity - Isomers	RI @ 20°C 1.417		

TSCA



PHENETHYLTRICHLOROSILANE



CAS# 940-41-0	MW 239.60	$C_8H_9CI_3Si$
Flash Pt. 91°C	BP 93-96°C/3 mm	SG @ 20°C 1.240
97% Purity - Isomers	RI @ 20°C 1.5185	
TOXICITY: orl rat, LD50: 2,830 mg/kg		

P0113

P0110



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PHENETHYLTRIMETHOXYSILANE

PHENYLDIMETHYLCHLOROSILANE

CAS# 49539-88-0	MW 226.35	$C_{11}H_{18}O_3Si$	TSCA
Flash Pt. 109°C	BP 95-96°C/2 mm	SG @ 20°C 1.037	
97% Purity - Isomers	RI @ 20°C 1.4753		

P0160

CH₃ Si-Cl CH₃

CAS# 768-33-2	MW 170.71	C ₈ H ₁₁ CISi	TSCA
Flash Pt. 61°C	BP 192-193°C	SG @ 20°C 1.032	
97% Purity	RI @ 25°C 1.5082		

P0172 PHENYLMETHYLVINYLCHLOROSILANE



CAS# 17306-05-7	MW 182.72	C ₉ H ₁₁ CISi	TSCA
Flash Pt. 72°C	BP 79-80°C/3-4 mm	SG @ 20°C 1.034	
97% Purity	RI @ 20°C 1.5197		




97% Purity - Isomers **RI** @ 25°C 1.429

CI





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RI @ 20°C 1.395

SG @ 20°C 0.91



T1750 TETRA-n-BUTOXYSILANESILANE

CH ₃ (CH ₂) ₃ O	CAS# 4766-57-8	MW 320.54	$C_{16}H_{36}O_4Si$	TSCA
H ₃ C(CH ₂) ₃ -O-SiO(CH ₂) ₃ -CH ₃	Flash Pt. 110°C	BP 115°C/3 mm	SG @ 20°C 0.899	
(CH ₂) ₃ CH ₃	97% Purity	RI @ 25°C 1.4126		

T1800 TETRACHLOROSILANE



CAS# 10026-04-7	MW 169.90	Cl₄Si
Flash Pt. 58°C	BP 57°C	SG @ 20°C 1.481
97% Purity	RI @ 25°C 1.4153	Melting Pt70°C

T1803 n-TETRADECY	LDIMETHYL(3-TRI	METHOXYSILYI	LPROPYL)AMMONIU	M CHLORIDE
ÇH₃	CAS# 41591-87-1	MW 440.18	$C_{22}H_{50}CINO_3Si$	TSCA
$CI CH_3 O' H_3C-(CH_2)_{13} - + I O' - (CH_2)_3 - SI O - CH_3$	Flash Pt. 11°C			
ĊH ₃ Ó ĊH ₃	50% in Methanol			

T1806 1,1,3,3-TETRAETHOXY-1,3-DIMETHYLDISILOXANE

	CH ₃ CH ₂ O	СН ₃ СН ₂ О
H ₃ C-	-Si-O- O CH ₂ CH ₃	–Si—CH ₃ O CH ₂ CH ₃

CAS# 8001-60-0 Flash Pt. 58°C 97% Purity

TETRAETHOXYSILANE

MW 282.48	
BP 205°C	
RI @ 20°C 1.3912	2

C₁₀H₂₆O₅Si₂ SG @ 20°C 0.953

T1807



CAS# 78-10-4	MW 208.33	$C_8H_{20}O_4Si$	TSCA
Flash Pt. 46°C	BP 169°C	SG @ 20°C 1.934	
97% Purity	RI @ 20°C 1.3838	Melting Pt85°C	
TOXICITY: orl rat, LD50: 6,270 mg/kg			

T1808 TETRAETHOXYSILANE



-			
CAS# 78-10-4	MW 208.33	$C_8H_{20}O_4Si$	TSCA
Flash Pt. 46°C	BP 169°C	SG @ 20°C 1.934	
99% Purity	RI @ 20°C 1.3838	Melting Pt85°C	
TOXICITY: orl rat, LD50: 6,270 mg/kg			

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R&D ONLY

TSCA





	CH3	CH3
H-	\$i-O-	-Śi — H
	ĊH ₃	с́Н3

CAS# 30110-74-8	
Flash Pt12°C	
97% Purity	

MW 134.33	C ₄ H ₁₄ OS
BP 70-71°C RI @ 20°C 1.3669	SG @ 2

Si₂ 20°C 0.757



T2090 TETRAPROPOXYSILANE

с ¬	CAS# 682-01-9	MW 264.44	$C_{12}H_{28}CI_4Si$	TSCA
Si-O-CH ₂ -CH ₂ -CH ₃ 4	Flash Pt. 156°C	BP 1224-225°C	SG @ 20°C 0.916	
	98% Purity	RI @ 20°C 1.401		

T2160

T2450

1,3,5,7-TETRAVINYLTETRAMETHYLCYCLOTETRASILOXANE



CAS# 27342-69-4	MW 344.66
Flash Pt. 112°C	BP 110°C/10
97% Purity	RI @ 20°C 1.

MW 344.66	$C_{12}H_{24}O_4Si_4$
BP 110°C/10 mm	SG @ 20°C 0.998
RI @ 20°C 1.4342	Melting Pt42°C

T2190 TRIACONTYLTRICHLOROSILANE



CAS# 70851-48-8	MW 556.26	$C_{30}H_{61}CI_3Si$	TSCA
Flash Pt. >200°C			
80% Purity			

TRICHLOROSILANE



CAS# 10025-78-2	MW 135.45	Cl₃HSi
Flash Pt13°C	BP 31.9°C	SG @ 20°C 1.342
97% Purity	RI @ 20°C 1.402	Melting Pt128°C

T2455 1-TRICHLOROSILYL-2-(p,m-CHLOROMETHYLPHENYL)ETHANE



CAS# 58274-32-1	MW 288.08	$C_9H_{10}O_4Si$	R&D ONL
Flash Pt. >93°C	BP 111-112°C/1.5 mm	SG @ 20°C 1.32	
97% Purity			

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TSCA

TSCA

TSCA



T2490 (TRIDECAFLU	ORO-1,1,2,2-TETRA	HYDROOCTYL)-1	-DIMETHYLCHLORC	SILANE
CH ₃	CAS# 102488-47-1	MW 440.70	C ₁₀ H ₁₀ CIF ₁₃ Si	R&D ONLY
$F_{3}C - (CF_{2})_{5} - (CH_{2})_{2} - Si - CI$	Flash Pt. 52°C	BP 189-191°C	SG @ 20°C 1.473	
CH ₃	97% Purity	RI @ 20°C 1.3453		
T2491 (TRIDECAFLU	ORO-1,1,2,2-TETRA	HYDROOCTYL)-1	-METHYLDICHLORO	SILANE
CI	CAS# 73609-36-3	MW 461.12	$C_9H_7Cl_2F_{13}Si$	R&D ONLY
$F_3C - (CF_2)_5 - (CH_2)_2 - Si - CH_3$	Flash Pt. 51°C	BP 189-190°C		
Ċı	97% Purity			
T2492 (TRIDECAFLU	ORO-1,1,2,2-TETRA	HYDROOCTYL)-1	-TRICHLOROSILANE	
CI	CAS# 78560-45-9	MW 481.54	C ₈ H ₄ CI ₃ F ₁₃ Si	TSCA
F_3C —(CF ₂) ₅ —(CH ₂) ₂ —Si—Cl	Flash Pt. >200°C	BP 189-190°C	SG @ 20°C 1.30	
ĊI	97% Purity	RI @ 20°C 1.351	Melting Pt13°C	
T2494 (TRIDECAFLU	ORO-1,1,2,2-TETRA	HYDROOCTYL)-1	-TRIETHOXYSILANE	1
$CH_3\\ H_2\\ CH_2$	CAS# 51851-37-7	MW 510.36	$C_{14}H_{19}F_{13}O_3Si$	TSCA
$F_{3}C$ —(CF ₂) ₅ —(CH ₂) ₂ — $\stackrel{O}{I}_{I}$ —O—CH ₂ –CH ₃	Flash Pt. 84°C	BP 86°C/1.5 mm	SG @ 20°C 1.351	
О СН ₂	97% Purity	RI @ 20°C 1.3436		
T2507 N-(TRIETHOX)	SILYLPROPYL)UR	EA		
СН ₃ СН ₂	CAS# 23779-32-0	MW 266.64	$C_{10}H_{24}N_2O_4Si$	TSCA
0 0 H ₂ N-C-N-(CH ₂) ₃ -Si-O-CH ₂ -CH ₃	Flash Pt. 10°C		SG @ 20°C 1.91	
Ч Ó СН ₂	97% Purity	RI @ 20°C 1.386		
CH ₃				
T2520 TRIETHYLCHL	OROSILANE			
CH ₃	CAS# 994-30-9	MW 150 72	CoHaclisi	TSCA



T2523 TRIETHYLSILANE



CAS# 617-86-7	MW 116.28	C ₆ H₁8Si	TSCA
Flash Pt3°C	BP 107-108°C	SG @ 20°C 0.731	
97% Purity	RI @ 20°C 1.4123	Melting Pt157°C	

C₃H₄CI

SG @ 20°C 1.395

T2845

(3,3,3-TRIFLUOROPROPYL)TRICHLOROSILANE



CAS# 592-09-6	MW 231.50
Flash Pt. 15°C	BP 113-114°C
97% Purity - Isomers	RI @ 20°C 1.385

T2847 (3,3,3-TRIFL	JOROPROPYL)TRIME	THOXYSILANE		
CH ₃	CAS# 429-60-7	MW 218.25	$C_6H_{13}O_3F_3Si$	TSCA
F = O $F = C - (CH_2)_2 - Si = O - CH_3$	Flash Pt. 37°C	BP 144°C	SG @ 20°C 1.3546	
F O CHa	97% Purity - Isomers	RI @ 20°C 1.137		
3				

T2885

TRIISOPROPYLCHLOROSILANE

H ₃ C CH ₃	CAS# 13154-24-0	MW 192.80	C ₉ H ₂₁ CISi	TSCA
H ₃ C, C⊓ HC−Şi−Cl	Flash Pt. 62°C	BP 80°C/10 mm	SG @ 20°C 0.903	
H ₃ C CH H ₃ C CH ₃	97% Purity	RI @ 25°C 1.4515		

T2895	TRIMETHOXY	SILANE			
	CH ₃	CAS# 2487-90-3	MW 122.20	$C_3H_{10}O_3Si$	R&D ONLY
	О Н ₃ С—О—Şi—Н	Flash Pt9°C	BP 86-87°C	SG @ 20°C 0.860	
	о Сн _з	97% Purity	RI @ 20°C 1.3687	Melting Pt114°C	

_						
	2902 1	-TRIMETHOX	(YSILYL-2(p,m-CHL	OROMETHYL)PHE	NYLETHANE	
	CI	CH ₃	CAS# 68128-25-6	MW 274.82	$C_{12}H_{19}CIO_3Si$	TSCA
	CH ₂	О I H ₂) ₂ —Şi—О—СН ₃	Flash Pt. 130°C	BP 115°C/1.5 mm	SG @ 20°C 1.12	
		о Сн _а	97% Purity			

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R&D ONLY







T2992 TRIMETHYLMETHOXYSILANE

CH ₃	CAS# 1825-61-2	MW 104.44	C ₄ H ₁₂ OSi	TSCA
$CH_3 = Si = OCH_3$	Flash Pt11°C	BP 57-58°C	SG @ 0.756 g/mL	
CH ₃	96% Purity	RI @ 20°C 1.3678		

T3060

2-(TRIMETHYLSILOXY)ETHYLMETHACRYLATE



CAS# 17407-09-9
Flash Pt. 42°C
96% Purity

)	BP 65°C/0.9 mm	SG @ 20°C 0.995
	RI @ 20°C 1.4300	

MW 202.32

T3100 p-

p-TRIMETHYLSILOXYNITROBENZENE



CAS# 114-66-0	MW 221.29	C ₉ H ₁₃ NO ₃ Si	TSCA
Flash Pt. 105°C	BP 104°C/1 mm	SG @ 25°C 1.099	
97% Purity	RI @ 20°C 1.5293		

T3254

O-TRIMETHYLSILYLACETATE

$\begin{vmatrix} O & CH_3 \\ H_3C - C - O - Si - CH \\ CH_3 \end{vmatrix}$	I ₃
--	----------------

CAS# 2754-27-0 Flash Pt. 4°C 97% Purity

MW 132.23	$C_5H_{12}O_2Si$	TSCA
BP 103-104°C	SG @ 20°C 0.891	
RI @ 20°C 1.3890	Melting Pt32°C	

 $C_9H_{18}O_3Si$

 T3258
 TRIMETHYLSILYLACETYLENE

 GH_3 GH_3
 H_3C GH_3
 GH_3 GH_3

T3259.5 N-TRIMETHYLSILYLALLYLAMINE

H CH₃	CAS# 10519-97-8	MW 129.28	C ₆ H ₁₅ NSi	R&D ONLY
$H_2C = CH - CH_2 - N - Si - CH_3$	Flash Pt. 10°C	BP 110-112°C		
ĊH ₃	94% Purity	RI @ 25°C 1.4127		

TSCA







V4790 VINYLMETHYLDIETHOXYSILANE

CH ₃ CH ₂	CAS# 5507-44-8	MW 160.29	$C_7H_{16}O_2Si$	TSCA
Ó H₂C=CH−Şi−CH₃	Flash Pt. 16°C	BP 133-134°C	SG @ 20°C 0.858	
о Н СН ₂ СН ₃	97% Purity	RI @ 20°C 1.4000		

V4910 VINYLTRIETHOXYSILANE



CAS# 78-08-0	MW 190.31	$C_9H_{18}O_3Si$	
Flash Pt. 45°C	BP 160-161°C	SG @ 20°C 0.903	
97% Purity - Isomers	RI @ 20°C 1.396		
TOXICITY: orl rat, LD50: 22,500 mg/kg			

VINYLTRIMETHOXYSILANE V4917



	CAS# 2768-02-7	MW 148.23	$C_5H_{12}O_3Si$	TSCA
H ₃	Flash Pt. 23°C	BP 123°C	SG @ 20°C 0.970	
-	97% Purity	RI @ 20°C 1.3930		

V4930

VINYLTRIPHENOXYSILANE



Flash Pt15°C
97% Purity

CAS# 18666-65-4	MW 334-45	$C_{20}H_{18}O_3Si$
Flash Pt15°C	BP 210°C/7 mm	SG @ 25°C 1.130
97% Purity	RI @ 25°C 1.562	

 $C_{14}H_{25}K_{3}O_{9}Si$

N-[(3-TRIMETHOXYSILYL)PROPYL]ETHYLENEDIAMINE TRIACETIC ACID, T2913.1 **TRIPOTASSIUM SALT**

MW 482.73



50% in Water

CAS# N/A

TSCA

TSCA

R&D ONLY

UCT SPECIALTIES Silicone Fluids



USING THIS SECTION

The format of this presentation does not allow full descriptions of many of the polymer materials listed. The following guidelines may be helpful in understanding our chemistry: Polymer viscosities can vary \pm 10% although normally they are controlled within much closer tolerances. Homopolymer fluids are more closely controlled. The fluids are usually polymerized to data sheet viscosity. Occasionally the fluids have been blended within decades to adjust viscosity. Molecular weights reported are not determinations, but correlations to viscosity. Unless otherwise noted, fluids are usually trimethylsiloxy terminated.

Composition of copolymers listed in the tables is indicated by mole percent in parentheses immediately preceding each comonomer.

Abbreviations

- bp Boiling Point in °C
- cSt Centistoke
- D.C. Dielectric Constant
- F.P. Flash Point in °C
- mp Melting Point in °C
- M.W. Molecular Weight
- R.I. Refractive Index at 25°C for polymers and 20°C for monomers
- P.P. Pour Point in °C
- S.G. Specific Gravity at 25°C
- S.T. Surface Tension in dynes/cm
- Tc Thermal Conductivity at 25°C g.cal/sec/cm2/°C/1 cm thickness x 10-4
- Te Coefficient of Thermal Expansion cc/cc/°C x 10-4
- Tg Glass Transition Temperature, °C
- Visc. Viscosity in centistokes at 25°C
- V.T.C. Viscosity-Temperature Coefficient [1-(visc @ 100°C/visc @ 38°C)]

INTRODUCTION

Silicone fluids have truly amazing versatility and new uses are continually being developed. We hope the wide range of products presented in this section encourages researchers to build better polymers and uncover novel applications.

The name "silicone" denotes a polymer

where n is between 0-3 and m is 2 or larger. The term "silicone" arose from very old work in which investigators erroneously assumed that oxygen was bound to silicon by a double bond similar to that in ketones.

The simplest silicones are polydimethylsiloxanes. Polydimethylsiloxanes exhibit the basic structure of silicones.

 $\begin{array}{c} CH_{3} \\ H_{3}C \xrightarrow{I}{} Si \xrightarrow{I}{} O \xrightarrow{I}{} Si \xrightarrow{I}{} O \xrightarrow{I}{} Si \xrightarrow{I}{} O \xrightarrow{I}{} Si \xrightarrow{I}{} CH_{3} \\ CH_{3} \\ CH_{3} \\ CH_{3} \\ \end{array} \xrightarrow{I}{} D \xrightarrow{I}{} D \xrightarrow{I}{} O \xrightarrow{I$

The repeating unit of the polymer (Me_2SiO), the dimethyl siloxane unit, is referred to as a D unit. The termination unit (Me_3SiO), the trimethylsiloxy group, is referred to as an M unit. The structure drawn above may be described as MDnM. The silicones do not have to be linear. They can contain branch points, $MeSiO_3$ and SiO_4 , referred to as T and Q groups, respectively. The branch points introduce rigidity in the structure. This relatively simple chemistry at low molecular weights leads to fluids, and at high molecular weights leads to gums which may be crosslinked to form elastomeric products.

The methyl group in silicone may be substituted by a variety of other groups including, most commonly, phenyl, vinyl and hydrogen. When the substituents of the silicon are not methyl, a superscript is added to the unit. DPh indicates a phenylmethyl siloxane unit. MVi indicates a vinyldimethylsiloxane unit. M' indicates a dimethyl hydrogen siloxane unit. In some naming systems the apostrophe is not specific for hydrogen but indicates any non-methyl unit. The substitution, branching and molecular weight of the polymers dictate uses.

Low molecular weight siloxanes are most widely used as monomers and terminators in the polymerization of higher molecular weight silicones. Two general methods of polymerization are employed. Gums and non-silanol terminated fluids are produced by base-catalyzed (anionic) polymerization. Under typical conditions potassium, sodium or tetramethylammonium silanolate catalysts are introduced into a mixture of monomers and endcappers. The mixtures are equilibrated by heating under moderate conditions (60-150°C). Polydimethylsiloxanes may be prepared from hexamethylcyclotrisiloxane, octamethylcyclotetrasiloxane or decamethylcyclopentasiloxane monomers with an endcapper like hexamethyldisiloxane or the less volatile decamethyltetrasiloxane. Cyclic siloxanes can also be polymerized with mineral acid catalysts. This method is used primarily for low molecular weight silanol terminated, or hydride functional siloxanes.

The relative reactivity towards acids is: $D_3 > MM > MDM > MD_2M > D_4$ The relative reactivity towards bases is: $D_3 > D_4 > MD_2M > MDM > MM$ Many important end-use applications that do not involve further polymerization have been developed for the lower molecular weight siloxanes. The cyclic siloxanes provide a unique hydrophobic treatment for reactive siliceous fillers. This includes such applications as treatment of precipitated silicas for use as reinforcing fillers and roofing granules to improve the weatherability of shingles. The high volatility of the cyclic siloxanes has led to the introduction of specially purified cosmetic grades as carriers in idry feelî deodorants. Diphenylmethylsiloxy endcapped fluids are used in diffusion pump applications. These fluids are useful in vacuums as low as 10⁻¹⁰ torr. (see section on diffusion pump fluid).

UCT now offers a wide variety of substituted polymers. The vinyl (p. 95), hydride (p. 98), and silanol (p. 100), fluids are widely used in silicone RTV systems. These polymers, together with the catalysts (p. 106) and crosslinkers (p. 101), that are also offered, provide the raw materials for RTV systems. Some two part RTV user-ready system are offered (p. 118).

Organically substituted fluids are readily available in a number of varying forms. Polymers and copolymers containing amino, methacryl, mercapto, and other functionalities are available. In addition, UCT research staff is constantly endeavoring to produce new and novel polymers to meet the needs of new applications.

POLYDIMETHYLSILOXANE FLUIDS, TRIMETHYLSILOXY TERMINATED

Silicone fluids have unique properties because they are not products of petroleum or organic chemistry. They were the first, and are still the only, major class of polymers that are products of inorganic chemistry. Silicone fluids consist of a broad range of different materials with the following characteristics:

- Wide Service Temperature Range
- Low Viscosity Change vs. Temperature
- Thermal Stability
- Low Flammability
- Shear Stability
- Dielectric Stability
- High Compressibility
- Low Surface Tension
- Low Toxicity

These features have facilitated the adoption of silicones as dielectric, hydraulic, heat transfer, power transmission and damping fluids. They have found applications when incorporated as additives in plastics and rubbers as process and release aids, into coatings for flow and level control and into process streams as antifoams. Other unique properties have led to their introduction in acoustical applications as ultrasonic sensor and sonar buoys. Light refractive and index matching properties have allowed the use of silicones in fiberoptic and optoelectronics. This proliferation of applications has engendered many improvements and refinements of silicone fluids.

Conventional fluids are the well-known general purpose silicones described in chemical notation as polydimethylsiloxanes. They are commercially produced in viscosities ranging from 0.65 to 2,500,000 cSt.

Conventional silicone fluids are composed of polymer chains with unique flexibility. Polydimethylsiloxane has virtually no energy barrier for rotation. This results in one of the lowest glass-transition temperatures of any polymer. The liquid surface tension of polydimethylsiloxane is lower than the critical surface tension of wetting (24 dynes/cm). This causes polymers to spread over their own adsorbed films. An important consequence of the low intermolecular forces in polysiloxanes is the highest permeability coefficients of any polymer for oxygen and nitrogen.

The fluids are thermally stable indefinitely at 150°C in air. Fluids with viscosities of 50 cSt or greater have negligible vapor pressure.

At viscosities greater than 1,000 cSt correlating to molecular weights greater than 30,000, polymer chain entanglement occurs, resulting in leveling of physical property change vs. viscosity. Refractive index, surface tension, density, and viscosity-temperature coefficients are strikingly flat.

Low viscosity fluids (0.65 – 20 cSt) offer maximum compressibility, lowest temperature service and heat transfer properties. They are soluble in a greater variety of solvents than higher viscosity fluids including petroleum oils. Their dispersibility and surface active properties make them excellent antifoams and leveling and flow control aids in coating applications. Low temperature applications include heat exchangers, bath and thermostats. They are used as dielectric media in rectifiers and electronic modules. The combined temperature and electronic characteristics make these polydimethylsiloxanes suited for cooling in magnetrons and other electric power transduction applications. Ultrasonic applications are based on low viscosity fluids due to their low acoustical velocities.

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Low viscosity fluids are utilized in many precision applications. Apart from the obvious mechanical advantages of the low viscosity, they offer higher purity levels and more discrete vapor pressure control than higher viscosity fluids. The different types are described below.

Intermediate viscosity fluids (50 – 1000 cSt) have a remarkable diversity of uses, from brake fluids to electronics to hand creams. They make excellent, safe, low-volatility heat transfer media, mold releases for rubber, plastic and glass parts, lubrication for most non-metal to metal contact, and toners for photocopiers.

They are found in hydraulic systems, inertial guidance systems, delicate timing and photographic devices, and as dielectric fluids in electronic components, such as capacitors and transformers.

These fluids are suitable for polish and other high-gloss water-repellent coatings, antifoams, grease and oil formulations (when mixed with thickeners, such as silica and bentonite). High performance greases can be produced by compounding the silicone fluid with extreme pressure additives, such as polytetrafluoroethylene or molybdenum disulfide.

High viscosity fluids (5,000 – 2,500,000 cSt) are employed as internal lubricants and process aids for thermoplastics and die casting. They are used as band-ply lubricants in the rubber industry, damping fluids for meters, and liquid springs in shock absorbers and load cell applications. The paint industry employs 100,000 cSt Fluid additives to create "hammer" finishes. Fluids with viscosities of 1,000,000 cSt or greater serve as impact modifiers for thermoplastic resins and as mold release agents.

Other fluids

Silahydrocarbons are thermally stable fluids which possess superior metal lubrication and wear characteristics when compared to conventional silicones. Four ball wear scar at 40 kg load (75°C) is 0.9 mm, the best value reported for any unmodified silicone fluid. Their discrete branched structure gives them low volatility characteristics when compared to equivalent viscosity organic oils. They also have lower viscosity-temperature coefficients. They exhibit liquid behavior between -60 and 205°C. They do not affect finishing and painting operations.

The tetraalkoxysilanes possess excellent thermal stability and a broad temperature range of liquid behavior that widens as length and branching is introduced in the substituents. The alkosysilanes maintain fluidity at extremely low temperatures. A variety of heat exchange applications include solar panels utilize tetrabutoxysilane (T1750), and tetrakis(2- ethylbutoxy)silane (T1920). The alkoxysilanes are also excellent dielectric fluids and have been employed in airborne radar where lubricity at low temperature conditions is required.

Oligomeric siloxanes are low molecular weight versions of conventional silicones. They are available in high purity and are used in applications in which their low toxicity, inertness and low solubility parameters are desirable. They have been used as cleaning, polishing and damping media. The lowest viscosity member of the series – hexamethyldisiloxane (H7310) and octamethyltrisiloxane (O9816) have compressibilities at 20,000 psi of 11.9% respectively.

PROPERTIES OF CONVENTIAL SILICONE FLUIDS

The properties of specific viscosity grades of polydimethylsiloxanes are given on the following pages. Other properties which do not vary significantly with viscosity are listed below for 5 to 2,500,000 cSt fluids.

Electrical				
	Dielectric strength		350 – 400 V/mil	
	Dielectric constant 10 ² - 10 ⁶ Hz,	20°	2.44 – 2.76	
	Dissipation factor		0.0001	
	Volume resistivity		1 x 10 ¹⁵ ohm-cm at 2	0°C
Thermal				
	Specific heat		0.37 cal/g/°C	
	Heat of formation		-2.41 Kcal/g	
	Heat of combustion (>50 cSt)		6.13 Kcal/g	
	Glass transition temperature		-128°C	
	Gel time, 150°C		indefinite	
	Gel time for intermediate		200 hours	
	viscosity fluids, 200°C			
	Gel time for high viscosity fluids 200°C	i	100 hours	
	Autoignition temperature		greater than 460°C	
Mechanical				
	Coefficient of adiabatic comprese Volume reduction of 100 cSt flu	ssibility id	1.0x10- ¹⁰ cm- ² /dyne	
	at 1,000 psi		0.70 - 0.75%	
	at 10,000 psi		5.50 - 5.90%	
	at 20,000 psi		9.00 - 9.20%	
	at 40,000 psi		13.30 – 13.80%	
Acoustical				
	Velocity of sound, m/s			
	Fluid viscosity (cSt)	<u>30°C</u>	<u>50.7°C</u>	
	0.65	873	795	
	2.0	931	863	
	20	975	918	
	100	985	930	
	1000	987	933	

Solubility of fluids

Methylene chloride, chlorofluorocarbons, ethyl ether, xylene and methylethyl ketone are typical solvents for dimethylsiloxanes. Low viscosity polymers are also soluble in acetone, ethanol, dioxane and dihexyladipate. They are insoluble in methanol, cyclohexanol and ethylene glycol. The solubility parameter for 100 cSt fluid is 7.4.

Reactivity

While they exhibit low reactivity under many conditions, certain environments are destructive to silicone fluids. Hydrogen fluoride, for example, attacks the silicone-oxygen bond to produce dimethylsilyl fluorides and water. Strong bases, such as methanolic potassium hydroxide, destroy silicone fluids and create resinous by-products.

Thermal degradation at elevated temperatures causes rearrangement of the siliconeoxygen bonds to produce volatile by-products. Free-radical reaction of the methyl groups to form cross-linked materials by oxidation with peroxy compounds increases fluid viscosity and causes the fluid to gel.



VISCOSITY DATA FOR CONVENTIONAL SILICONE FLUIDS SUPPLEMENTARY TABLES

By careful selection polydimethylsiloxane can be used to effect precise viscosity control. Low viscosity fluids are Newtonian in behavior. High viscosity fluids exhibit non-Newtonian viscosity at high shear rates as shown in the following chart.



VISCOSITY VS. SHEAR RATE

VISCOSITY CONVERSION CHART

Centistokes	Poise	SSU	Zahn #1	Zahn #2	Zahn #3	Zahn #4	Zahn #5	Ford #3	Ford #4	Krebs	SAE	Example
1	0.01	31										Water
10	0.10	60	30	16				9	5			
20	0.20	100	37	18				12	10			
40	0.40	210	52	22				25	18			
60	0.60	320	68	27				33	25	33	10	
80	0.80	430	81	34				41	31	37		
100	1.0	530		41	12	10		50	34	40	20	Olive oil
200	2.0	1000		82	23	17	10	90	58	52		
300	3.0	1475			34	24	15	130	74	60	30	
400	4.0	1950			46	30	20	170	112	64	40	Glycerine
500	5.0	2480			58	38	25	218	143	68	90	
1000	10.0	600				69	49	390	264	85		Castor oil
2000	20.0	9400						800	540	103		
3000	30.0	14500						1230	833	121		
4000	40.0	18500						1570	1060	133		
5000	50.0	23500							1350			
6000	60.0	28000							1605			
7000	70.0	32500							1870			
8000	80.0	37000							2120			
9000	90.0	41000							2360			
10000	100	46500							2670			
15000	150	69400										
20000	200	92500										
30000	300	138600										
40000	400	185000										
50000	500	231000										
60000	600	277500										
70000	700	323500										
80000	800	370000										
90000	900	415500										
100000	1000	462000										
125000	1250	578000										
150000	1500	694000										
175000	1750	810000										
200000	2000	925000										

BLENDED SILICONE FLUIDS

Any standard viscosity grade of polydimethylsiloxane can be blended together with another viscosity of the same fluid to produce an intermediate viscosity. The blend chart listed provides a means for determining the proper blend ratio.

The chart should be used as follows:

Decide upon the viscosity grades to be blended. For high accuracy, measure the actual viscosity of the blending fluids. Locate the lower viscosity on the left hand scale. Locate the higher viscosity on the right hand scale. Connect these two points with a straight line

Locate the point where the line indicating the desired blend viscosity intersects the constructed line. From this point, follow down to the horizontal scale to read the percent of the higher viscosity fluid to use in the blend.

This method is reasonably accurate in predicting blend viscosity when the two fluids differ in viscosity by no more than one magnitude (one power of ten). When fluids covering a wider range are blended, the chart will only approximate the finished viscosity. To achieve a viscosity of 800 cSt as shown in the example 68% of 1000 cSt and 32% of 500 cSt fluids are blended.

The following equation can be used in place of the chart to calculate blending ratios:

A log α + B log β $Log \lambda =$ 100

- λ = target viscosity
- α = viscosity of one of the blending silicones

 β = viscosity of other blending silicone

A = percentage of silicone α

B = percentage of silicone β



				c	ONVE	NTIO	NAL SILIO	CONE FLU	JIDS			
					Поср		Vienneity	Coefficient of		Thermal		Dialantria
Catalog #	Viscosity (cSt)	Molecular Weight	Specific Gravity	Refractive Index	Point (°C)	Pour (°C)	Viscosity Temperature Coefficient	Expansion (x 10 ⁻⁴ /°C)	Surface Tension	Conductivity (cal/cm*sec x 10 ⁴ °C)	Dielectric Constant	Dielectric Strength (Volts/mil)
			Pol	ydimethyls	iloxane	s, Trim	ethylsiloxy Te	erminated - C	AS# [63148	-62-9]		
PS034	0.65	162	0.761	1.3750	Ļ	- 68	0.32	13.4	15.9	2.4	2.20	300
PS035	1.0	237	0.818	1.3825	38	- 85	0.37	13.4	17.4	2.4	2.30	350
PS038	5.0	770	0.918	1.3970	135	- 65	0.54	11.2	19.7	2.8	2.60	375
PS039	10	1,250	0.935	1.3990	163	- 65	0.56	10.8	20.1	3.2	2.68	375
PS039.5	20	2,000	0.950	1.4000	232	- 65	0.59	10.7	20.6	3.4	2.72	375
PS040	50	3,780	0.960	1.4015	285	- 65	0.59	10.6	20.8	3.6	2.75	400
PS041	100	5,970	0.966	1.4025	315	- 65	0.60	9.3	20.9	3.7	2.75	400
PS041.2	200	9,430	0.968	1.4030	315	- 60	0.60	9.3	21.0	3.7	2.75	400
PS041.5	350	13,650	0.970	1.4031	315	- 60	0.60	9.3	21.1	3.8	2.75	400
PS042	500	17,250	0.971	1.4033	315	- 55	0.60	9.3	21.1	3.8	2.75	400
PS043	1,000	28,000	0.971	1.4034	315	- 50	0.61	9.3	21.2	3.8	2.75	400
PS044	5,000	49,350	0.973	1.4035	315	- 48	0.61	9.3	21.3	3.8	2.75	400
PS045	10,000	62,700	0.974	1.4035	315	- 48	0.61	9.3	21.5	3.8	2.75	400
PS046	12,500	67,700	0.974	1.4035	315	- 46	0.61	9.3	21.5	3.8	2.75	400
PS047	30,000	91,700	0.976	1.4035	315	- 43	0.61	9.3	21.5	3.8	2.75	400
PS047.5	60,000	116,500	0.976	1.4035	315	- 42	0.61	9.2	21.5	3.8	2.75	400
PS048	100,000	139,000	0.977	1.4035	321	- 41	0.61	9.2	21.5	3.8	2.75	400
PS048.5	350,000	204,000	0.977	1.4035	321	- 41	0.61	9.2	21.5	3.8	2.75	400
PS049	600,000	260,000	0.978	1.4035	321	- 41	0.61	9.2	21.6	3.8	2.75	400
PS049.5	1,000,000	308,000	0.978	1.4035	321	- 39	0.62	9.2	21.6	3.8	2.75	400
PS050	2,500,000	423,000	0.978	1.4035	321	- 38	0.62	9.2	21.6	3.8	2.75	400
						I						

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VINYL POLYMERS AND COPOLYMERS

Vinyl Terminated Siloxanes

Vinyl terminated siloxanes are usually employed in addition cure systems. The addition reaction of polyfunctional silicon hydride to unsaturated groups in polysiloxane chains is achieving increasing importance as a cure method for silicone elastomers. The bond forming chemistry is the hydrosilation reaction which proceeds according to the following equation:

Si—H + CH₂=CHSi $\xrightarrow{}$ SiCH₂CH₂Si

Typical hybrid crosslinkers are methylhydro-dimethylsiloxane copolymers with 20 – 60% methyl hydrogen. In special instances hydride terminated siloxanes are utilized for chain extension. Vinyl terminated polydimethylsiloxanes with viscosities greater than 100 cSt contain less than 1% volatile material. Specialty vinyl terminated materials include phenylmethylvinyl and divinylmethyl materials. Vinyl terminated siloxanes with internal vinyl are used in gel formulations for both dielectrics and orthopedic pads.

Elastomers produced by this method have demonstrated increased toughness, tensile strength and dimensional stability. Both terminal and internal vinyl groups may be cured by this method, although the former usually leads to greater toughness. The most widely used catalyst systems are solutions or complexes of platinum in alcohols, ethers, divinylsiloxanes and cyclic vinylsiloxanes. Moderators of cure rate include cyclic vinyl siloxanes (PS925). In two-part forumations, the A component usually contains 5 – 10 ppm platinum and vinyl-containing siloxane. The part B component usually contains a hydride functional siloxane and a vinylsiloxane. Single component addition cure systems contain fugitive inhibitors of the platinum, usually conjugated polar materials. Enhanced tear strength is achieved by the use of vinyl resin reinforced vinyldimethyl terminated polydimethylsiloxanes. Other mechanical properties are improved and unlike reinforced systems, optical clarity is maintained.

Polydimethylsiloxane	, vinyldimethyl terminated -	- CAS# 68083-19-2	(TSCA)
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	CH ₃	CH ₃	CH ₃
H ₂ C=CH-	−Śi—O−	-Śi-O-	-Śi-CH=CH ₂
	ĊН ₃	_ĊH ₃	n ĊH ₃

Cat#	Visc (cSt)	Mol. Wt.	Wt% vinyl	SG	Comments
PS441	100	6000	0.8 – 1.2	0.97	
PS441.2	200	9400		0.97	Base polymer or blend
PS442	500	17,200		0.97	of liquid RTV systems
PS443	1000	28,000	0.18 – 0.26	0.97	
PS444	5000	49,000		0.97	
PS445	10,000	62,000		0.97	High strength RTV systems
PS447.6	6 65,000	117,000	0.04 - 0.06	0.97	
PS448	100,000	139,000		0.97	
PS448.5	165,000	155,000		0.97	
PS449	600,000	260,000		0.98	High consistency RTV systems

Vinyl Functional Copolymers

Vinylmethylsiloxane copolymers are mostly used in activated cure systems which involve free radical coupling and addition reactions between the vinyl and methyl groups. Peroxide catalysts are normally employed at 140 – 160°C, followed by a post-cure 25 – 30°C higher to remove volatile peroxide decomposition products and stabilize silicone properties. The most widely used peroxides include benzoylperoxide (often as a 50% concentrate in silicone), dicumylperoxide (often 40% on calcium carbonate), di-t-butylperoxide and bis(dichlorobenzoyl)-peroxide. The last peroxide is particularly recommended for aromatic containing siloxanes. While vinylsiloxane chemistry is well-known for gum rubber stocks, the use of lower viscosity materials for gels in electronics and medical devices is growing. Typical applications include orthopedic pads and dielectric encapsulants. Cure chemistry in these cases is not limited to peroxides but includes the addition cure systems already described under vinyl-terminated siloxanes. Vinylfunctional siloxanes are also employed in copolymerization with vinyl monomers and as surfactants for organosols. They also form reactive internal lubricants for vulcanizeable rubber formulations. These polymers can also be utilized in solvent or emulsion copolymerization, or grafting with a number of different olefins (styrene, vinyl chloride, and various alkylenes). They are used to increase glass transition temperature in unsaturated polyesters.

UCT Specialties also offers a line of vinyl terminated silicone fluids containing phenyl functionality. The products are valuable ingredients in addition cure RTV systems where higher refractive index is required. The products are of particular interest to optical and fiberoptical applications. Phenyl functionality also provides greater temperature serviceability. Polymerization continues through the terminal vinyl groups.





Cat#	Visc (cSt)	Wt% vinyl	SG	Comments
PS422	250	1.0	0.97	Peroxide or Platinum cure
PS424	1000	7.5	0.97	
PS426	1000	1.0	0.97	

Vinylmethyl, dimethylsiloxane copolymer, vinyldimethyl terminated - CAS# 68083-18-1 (TSCA)



Cat#	Visc (cSt)	Wt% vinyl	SG	Comments
PS493	1000	0.4	0.97	

Vinyl Q-resin dispersion – CAS# 68584-83-8 (TSCA)



Cat#	Visc (cSt)	Wt% vinyl	SG	Comments
PS496	5000	1.02		High strength RTV systems

VINYL TERMINATED FLUIDS

Diphenyldimethyl copolymer, vinyl terminated - CAS# 68951-96-2 (TSCA)



Cat#	Visc	MW	Mole % Dimethyl	Mole % Diphenyl	RI
PS765	10,000	49,000	95.0	5.0	1.432
PS782	500	9,300	84.0	16.0	1.465
PS783	1,000	18,900	84.0	16.0	1.465
PS786	30,000	N/A	84.0	16.0	1.465
PS793	1,500	12,500	76.5	23.5	1.493

Cyclic vinylmethylsiloxanes - CAS# 68082-23-5



Cat#	Visc (cSt)	Wt% vinyl	SG	Comments
PS925	3 - 7	13.5 – 40.5	0.98	

ORGANO-HYDROSILOXANE POLYMERS AND COPOLYMERS

Polymethylhydrosiloxanes have a unique reactivity among the silicones. They undergo three basic classes of reactions. They can react with silanol terminated polymers and hydroxyl active materials in the presence of tin octoate, zinc octoate and a variety of other metal salt catalysts to form bonds with the evolution of hydrogen.

Si - H + HOR
$$\longrightarrow$$
 SiOR + H₂

This reaction is used to formulate silicone elastomers with a wide variety of physical and performance properties as well as to impart water repellency to glass, leather, paper and fabric surfaces. It can also impart free flowing characteristics to powders and granular materials. Application is generally from dilute (0.5 - 2.0%) solutions in hydrocarbons or chlorinated solvents. The coating may be cured at 110 - 150°C. Accelerators include dibutyltindilaurate and zinc, iron or tin octoates. In addition to the formal chemistry described above crosslinking due to oxidation also participates in the cure of these systems.

Polymethylhydrosiloxane will hydrosilylate olefins in the presence of precious metal catalysts.

$$Si - H + CH_2 = CHR \longrightarrow SiCH_2CH_2R$$

The widest application of hydrosilylation chemistry is in addition cure RTV and LTV systems. The most widely used polymethylhydrosiloxanes for these applications are the dimethyl copolymers which have more readily controlled reactivity that the homopolymers and result in tougher polymers with a lower crosslink density. Although the reaction with vinyl functional silicones does take place in 1:1 stoichiometry, the ratio of hydride to vinyl in commercial products is typically 2:1 and may be as high as 6:1.

Polymethylhydrosiloxanes behave as mild selective reducing agents. They have been used directly or coupled with a tin hydride or platinum catalyst. While performing many of the same reactions as Dibal-H or sodium borohydride, no hydrolysis is required to destroy the excess material prior to work-up. Reduction of aldehydes and ketones including selective steroid positions has been accomplished with polymethylhydrosiloxane in the presence of a catalytic amount of tributyltin oxide or (dibutylacetoxytin) oxide. Reduction of olefins, nitroaromatics and acid chlorides has been completed in the presence of Pd/C. Reactions can be run in the presence of air, moisture and in solvents such as hexane, methylene chloride and dioxane.

Polymethylhydro fluids exhibit the highest compressibility of silicone fluids – 9.32% at 20000 psi – and the lowest viscosity temperature coefficient – 0.50.

The hydride terminated polymers are usually employed in addition cure elastomers or in metal salt catalyzed reactions with silanol containing materials. The former is discussed in the section entitled Vinyl Fluids. The reaction with silanols is written as follows.

Si - H + HO - Si
$$\longrightarrow$$
 Si - O - Si + H₂

The catalysis for the reaction include ferric, tin and zinc chlorides, acetates and octoates, and platinum complexes.

Polymethylhydrosiloxane, trimethylsilyl terminated - CAS# 63148-57-2 (TSCA)



			Mole %			
Cat#	Visc (cSt)	Mol. Wt	Methyl hydro	SG	RI	Flash Pt
PS118	2 - 5	400	100	0.91	1.382	50°C
PS120	30	2270	100	0.99	1.396	121°C

Methylhydro, dimethylsiloxane copolymer, trimethylsilyl terminated - CAS# 68037-59-2 (TSCA)

	CH ₃	CH ₃		H		CH_3	
H ₃ C-	–Śi—O—	–Śi—O−		-Śi—C	>+	-Śi—	-CH ₃
	ĊH3	_с́н _з	m	ĊH ₃	n	ĊН ₃	

			Mole %			
Cat#	Visc (cSt)	Mol. Wt	Methyl hydro	SG	RI	Flash Pt
PS122.5	10 - 15	900 - 1000	50 - 55	0.99	1.394	70°C
PS123	25 - 30	2000 - 2100	26.5 - 37.5	0.99	1.399	125°C
PS123.5	25 – 35	2000 - 2500	10 – 20	0.99	1.400	>94°C
PS123.8	5000 - 10000	10,000	0.5 – 1.0	0.97	1.404	300°C
PS124.5	250 – 275	13,000	3 – 6	0.97	1.404	>66°C

Polydimethylsiloxane, hydride terminated - CAS# 70900-21-9 (TSCA)

			Wt %			
Cat#	Visc (cSt)	Mol. Wt	Methyl hydro	SG	RI	Flash Pt
PS537	2 - 3	400	0.5	0.905	1.395	>65.5°C
PS542	500	17,500	0.01	0.971	1.403	>93°C
PS543	1000	28,000	0.007	0.971	1.403	>93°C
PS545	10,000	62,000	0.003	0.974	1.403	>93°C

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SILANOL TERMINATED AND RELATED POLYDIMETHYLSILOXANES

In contrast to trimethylsiloxy terminated polydimethylsiloxanes, silanol terminated polydimethylsiloxanes are reactive materials which are almost never used in fluid applications. The terminal silanol (Si–OH) group renders the materials susceptible to condensation under acid or mild base conditions. They are intermediates for most RTV (room temperature vulcanizable) silicone formulations. The silanol terminated siloxanes are generally produced by kinetically controlled hydrolysis of chlorosilanes. Other methods involve hydrolyzeable endcappers such as acetate or stopping equilibrium reactions with low molecular weight silanol terminated silicones.

RTV systems are formulated from silanol terminated polymers with a molecular weight of 26,000 to 200,000. They may be cross-linked with small quantities of multifunctional silanes which condense with the silanol groups. Some model reactions are listed below. The first three are most widely used in moisture activated single component RTVs. Enoxy and alkoxy cure systems have neutral non-complexing byproducts.

ACETOXY	′ ── Si──OH + AcOSi	────> ── Si−O−─Si── + AcOH
		O
ENOXY	— Si—OH + $CH_2 = C(CH_3)OSi$ —	\longrightarrow Si-O-Si + CH ₃ CCH ₃
OXIME	-Si-OH + R ₂ C=N-OSi-	\longrightarrow Si-0-Si- + R ₂ C=NOH
ALKOXY	— Si—OH + CH ₃ OSi—	CATALYST SI-O-SI- + CH ₃ OH
AMINE	— Si–OH + $(CH_3)_2NSi$ —	\longrightarrow Si-O-Si- + (CH ₃) ₂ NH

The cross-linking reactions of the alkoxy type are often catalyzed by titanates and carboxylic acid salts of zinc, iron and tin.

Incorporating SiH containing siloxanes in formulations results in foamed structures. The foam systems are usually two components which are compounded separately and mixed shortly before use.

Low molecular weight silanol terminated polydimethylsiloxanes are employed as filler treatments and structure control additives in silicone rubber compounding.

Intermediate viscosity, 1000 – 10,000 cst, silanol terminated fluids can be applied to textiles as durable fabric softeners. High viscosity silanol terminated polydimethylsiloxanes are used as base gums in compounding elastomers and rubbers. They also form the matrix component in tackifiers and pressure sensitive adhesives.

SILANOL TERMINATED FLUIDS

Polydimethylsiloxane, silanol terminated - CAS# 70131-67-8 (TSCA)

		HO—:	$\begin{array}{c c} CH_3 & CH_3 \\ Si & O & Si & O \\ CH_3 & CH_3 \\ CH_3 & CH_3 \\ CH_3 & CH_3 \end{array}$	CH ₃ -Si—OH CH ₃	
Cat#	Visc (cSt)	Mol. Wt	Wt % OH	SG	Uses
PS340	15 – 35	400 – 700	4.0 - 6.0	0.95	Structure control additive
PS340.5	45 – 85	1500 – 2000	0.9 – 1.2	0.97	Moderator for RTV foams
PS341	100	4200	0.8 - 0.9	0.97	
PS342.5	750	18,000	0.2	0.97	
PS343	1000	26,000	0.1	0.98	One & two part RTVs
PS343.5	2000	36,000	0.09	0.98	
PS343.8	3500	43,600	0.08	0.98	
PS344.5	8000	58,000	0.06	0.98	
PS345.5	18,000	77,000	0.04	0.98	
PS347.5	50,000	110,000	0.03	0.98	
PS349.5	1,000,000	310,000	0.01	0.98	Silicone pressure sensitive Adhesives, silicone curable Solvent dispersions

(82 - 86%) Dimethyl (14 - 18%) diphenylsiloxane copolymer, silanol terminated - CAS# 63148-59-4 (TSCA)



Cat#	Visc	SG	MW	RI
PS084	55	1.05	950	1.473

OTHER MOISTURE CURE PREPOLYMERS

Acetoxy terminated polydimethylsiloxanes provide a controlled method for production of high strength single component RTVs. They are usually used in conjunction with polyalkoxysilanes. The methyldiacetoxy terminated polydimethylsiloxanes are unfilled bases for RTVs and can be cured directly. The monoacetoxy terminated polydimethylsiloxanes react with a variety of hydroxylic materials leading to their use in specialty silicone block copolymers such as urethanes and polycarbonates.

Chlorine terminated and dimethylamine terminated polydimethylsiloxanes are usually employed in ordered chain extension polymer synthesis. They also provide a method for forming bound silicone layers on siliceous and polyhydroxylic surfaces



			Functionality	
Cat#	Visc (cSt)	Mol. Wt	wt %	SG
PS375	2 – 5	425 – 600	13 – 16	1.00

AMINO FUNCTIONAL POLYMERS

Aminopropyl-terminated siloxanes are used to form a variety of block copolymers including polyamides, polyurethanes and polycarbonates. A typical reaction is below:



The silicone is employed to produce silicone modified epoxy resins. It also has improved adhesion to both painted and unpainted metal surfaces allowing use in corrosion resistant coatings and polishes.

Amino functional silicones are reactive additives to both epoxy and urethane formulations.

Aminoalkyl functional T-structure polymers demonstrate the same range of chemical reactivity as the aminopropyl terminated siloxanes (reactivity with epoxides, isocyanates, carboxylic acids, etc.). The branched polymers are more likely to find application as formulative additives rather than as prepolymers. Typical applications include detergent polishes, leather finishes, and an internal mold release for nylon.

Polydimethylsiloxane, aminopropyldimethyl terminated – CAS# 106214-84-0 (TSCA)

Cat#	Visc (cSt)	Amine Number	SG	Mol. Wt
PS510	50	0.38 – 0.90 meq/g	0.98	2500
PS512	1000	0.060 – 0.120 meg/g	0.98	23,000
PS513	2000	0.070 – 0.150 meq/g	0.98	27,000

Amino functional T-Structure - CAS# 71750-80-6 (TSCA)



Cat#	Visc (cSt)	Amine Number	SG
PS401	80 - 130	0.25 – 0.75 meq/g	0.98

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MISCELLANEOUS FUNCTIONALITIES

Mercapto functional siloxanes strongly adsorb onto fibers and painted surfaces. As components in car polish, they are effective rust preventatives. They act as internal mold release agents for rubber and semi-permanent lubricants for automotive weather stripping. Mercapto polymers are valuable additives into cosmetic and hair care products. They also will undergo radical initiated (including UV) addition to unsaturated resins.

Carboxypropylsilicones are employed in polyester and polyamide copolymers. The esterification reaction is probably the most important because it allows reaction is probably the most important because it allows reaction with cellulosic materials

$$\begin{array}{c} \mathsf{CH}_{3} & \mathsf{OH} \\ -\mathsf{Si} - \mathsf{R} - \mathsf{OCH}_{2}\mathsf{CH}_{2}\mathsf{OH} + \mathsf{CH}_{2}\mathsf{CHR} \longrightarrow \begin{array}{c} \mathsf{CH}_{3} & \mathsf{OH} \\ -\mathsf{Si} - \mathsf{R} - \mathsf{OCH}_{2}\mathsf{CH}_{2}\mathsf{OCH}_{2}\mathsf{CHR} \\ -\mathsf{H}_{3} & \mathsf{CH}_{3} \end{array}$$

Such materials can be used in copolymerization with polyols and as a durable softening agent for textiles.

Carboxylic acid functional fluids, when reacted with inorganic bases or amines, perform as anti-static surfactants and lubricants. They are excellent rheology and wetting modifiers for polyesters. They also serve as dispersing agents for metal powders.

Carbinol terminated siloxanes contain primary hydroxyl groups which may be reacted into such systems as polyurethanes, epoxies, polyesters, and phenolics. A typical reaction is shown below:

The material is used as a reactive additive for urethane leather finishes, and as a reactive internal lubricant for polyester fiber melts processing.

Epoxy functional siloxanes are used predominantly in self-crosslinking acrylic latexes. They are also used to treat textiles to increase wrinkle recovery, reduce needle damage and improve water repellency.

Mercapto functional, Polydimethylsiloxane Copolymers – CAS#102783-03-9 (TSCA)



Cat#	Visc (cSt)	Mole % Comonomer	SG
PS848	50	2.0	0.954
PS849	200	2.0	0.973
PS850	100 – 200	5 – 10	0.978

Mercaptomethyl homopolymer – CAS# N/A (R&D Only)



Cat#	Visc (cSt)	Mole % Comonomer	SG
PS927	75 – 150	100	1.06



Cat#	Visc (cSt)	Mole % Comonomer	SG
PS922	100 - 400	45 – 55	1500 – 2000

Carbinol terminated polydimethylsiloxane - (R&D Only)

$$HO - (CH_{2}CH_{2}O)_{n} - R - CH_{2} - Si_{n} - O + Si$$

Cat#	CAS#	Termination	Visc (cSt)	SG	Mol. Wt.
PS555	68037-63-8	Carbinol	300 – 350	1.03	2200 – 2600
PS556	68037-63-8	Carbinol	250 - 330	1.06	1000 – 1500
PS563	158465-59-9	Carboxypropyl	800 – 1200	0.98	28,000

CATALYSTS

UCT Specialties, LLC provides a variety of catalyst concentrates predispersed as solution in appropriate siloxanes. These materials allow uniform compounding in gum or other vulcanizeable compositions.

Zinc and tin octoates are the usual catalysts used independently or together in RTV formulations.

Divinylsiloxane/platinum catalysts are utilized in addition cure systems. Neutralized divinylsiloxane complexes in xylene are generally "hotter" catalysts. Cyclic vinylsiloxane solutions give moderated cures. Relative reactivity rates are PC072 which is greater than PC075 which in turn is greater than PC085.

Zinc and Tin octoate salts					
Cat#	Conc.	Туре	Matrix	Cure Type	
PC040	50%	Zinc octoate	Polydimethylsiloxane Hydrocarbon blend	Si-Hydride/Si-Hydroxide	
PC050	50%	Tin octoate	Polydimethylsiloxane	Si-Hydride/Si-Hydroxide	
PC055	25%	Si-Hydride/Si-Hydroxide			
		CAS#6847	Platinum /8-92-2 and 68585-32-0		
Cat#	Conc.	Туре	Matrix	Cure Type	
PC072	2%	Platinum divinyl complex	Xylene	Si-Hydride/Si-Vinyl	
PC074	2%	Platinum divinyl complex (optically clear)	Xylene	Si-Hydride/Si-Vinyl	
PC075	2%	Platinum divinyl complex	Vinyl terminated	Si-Hydride/Si-Vinyl	
			polydimethylsiloxane		
PC075.3	3%	Platinum divinyl complex	Vinyl terminated	Si-Hydride/Si-Vinyl	
			Polydimethylsiloxane		
PC075.7	10%	Platinum divinyl complex	Vinyl terminated	Si-Hydride/Si-Vinyl	
			Polydimethylsiloxane		
PC076	1%	Platinum divinyl complex	Vinyl terminated	Si-Hydride/Si-Vinyl	
			Polydimethylsiloxane		
PC085	2%	Platinum cyclovinyl complex	Cyclic vinylmethylsiloxanes	Si-Hydride/Si-Vinyl	
PC085.3	3%	Platinum cyclovinyl complex	Cyclic vinylmethylsiloxanes	Si-Hydride/Si-Vinyl	
PC088.3	2%	Platinum octanol complex	Octanol/octanal	Si-Hydride/Si-Vinyl	

Nitrogen/Amine

Cat# PC090 **Type** Tetramethylammonium siloxanolate **Cure Type** Siloxy equilibrium

Inhibitors

Cat#	CAS#	Name	Structure
D6210	2627-95-4	1,3-Divinyltetramethyldisiloxane	$\begin{array}{ccc} CH_3 & CH_3 \\ H_2C=\!CH-\!$
T2160	27342-69-4	1,3,5,7-TetravinyItetramethylcyclotetrasiloxane	$\begin{array}{c} CH_2\\ CH\\ H_3C-Si-O, CH_3\\ O\\ Si-CH=CH_2\\ H_2C=HC-Si\\ CH_3O-Si-CH_3\\ CH\\ CH_2\\ CH_2\\ \end{array}$

Crosslinkers and Chain Extenders

Used in One Part RTV Systems

Cat#	CAS#	Name	Structure
B2300	2537-10-1	Bis(dimethylamino)methylvinylsilane	$H_2C = HC$ Si[NCH ₃) ₂] ₂ H_3C
M8980	4253-34-3	Methyltriacetoxysilane	O [∥] H ₃ C─Si(OCCH ₃) ₃
M9050	2031-67-6	Methyltriethoxysilane	H_3C —Si(OCH ₂ CH ₃) ₃

Used in Two Part RTV Systems

Cat#	CAS#	Name	Structure
D5600	78-62-6	Dimethyldiethoxysilane	$(CH_3)_2Si(OCH_2CH_3)_2$
T1807	78-10-4	Tetraethoxysilane(TEOS)	Si(OCH ₂ CH ₃) ₄
T2090	682-01-9	Tetra-n-propoxysilane	Si(OCH ₂ CH ₂ CH ₃) ₄

Used in Two Part Non-Corrosive RTV Systems

Cat#	CAS#	Name	Structure
T2030	30110-74-8	1,1,3,3-Tetramethyldisiloxane	$\begin{array}{c} CH_3 & CH_3 \\ H -\!$

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SILICONE GUMS

Silicone gums are high molecular weight linear polydiorganosilixanes that can be converted from a highly viscous plastic state into a predominantly elastic state by cross-linking. They are base stocks for most traditional silicone rubbers. The principal method of producing rubbers is cure at elevated temperatures with peroxides. Elevated temperature cure gums usually have molecular weights ranging from 500,000 to 900,000. Introduction of low percentages of vinyl groups reduces vulcanization temperature and imparts greater elasticity and lower compression set to rubbers. Peroxide cure gums may be trimethylsiloxy or vinyldimethylsiloxy terminated. Most gum stocks have methylvinylsiloxane chain components. The peroxides most commonly used are benzoyl peroxide and bis(dichlorobenzoyl)peroxide. Other peroxides are restricted to more specific systems. Ducumyl peroxide, for example, can be used only for vinyl containing polymers. Generally, peroxide loading is 0.2 to 1.0% and cure is at 125°C - 155°C.

	SILICONE GUMS			
3	Cat#	Description	Normal Cure System Used	
	PS255	Poly(dimethylsiloxane)-(0.1-0.3% Methylvinylsiloxane) copolymer, gum	Peroxide	
AROMATIC (PHENYL) CONTAINING SILOXANES

The most commonly used high temperature silicone fluids are the phenyl containing siloxanes. The phenyl group is usually incorporated in two ways. It may be introduced as a phenylmethylsiloxane or diphenylsiloxane. As phenyl groups replace methyl groups in a polysiloxane, several changes occur. Lubricity, oxidation resistance, thermal stability and shear resistance are enhanced. For polymethylphenyl siloxane the service temperature is -55 to 290°C. The gel times of several fluids are as follows:

<u>Cat#</u>	Description	Gel Time at 230°C in air
N/A	Mineral Oil (coking time)	4 hours
PS043	Polydimethylsiloxane	25 hours
PS160	Polymethylphenysiloxane	700 hours

In a closed oxygen-free system, the polymethylphenylsiloxanes are stable for thousands of hours at 230°C. The materials are used in heating baths. They are also base oils for high temperature lubrication.

The phenyl group also introduces rigidity in the silicone chain. When substitution exceeds 75 mole percent, the polymers are solid. Diphenylhomopolymers demonstrate liquid crystal behavior between 250°C and 500°C. Refractive index also increases with phenyl concentrations. At 15 - 20 mole percent phenyl concentrations, the refractive index matches that of amorphous silica and transparent compounds may be prepared.

At low phenyl concentrations, these fluids are dielectric coolants. They also function in place of standard dimethyl fluids where extended service temperature is necessary. One special class of phenyl fluids are the dimer, trimer and tetramer fluids. Because the introduction of a moderate concentration of phenyl groups also improves lubricity, members of the family have found utilization as lubricants for instruments and timing devices. High phenyl content fluids are also used as heat transfer media and chromatographic stationary phases. The polymethylphenyl-siloxanes exhibit good radiation resistance by remaining serviceable up to 200 megarads exposure.

The compressibility of phenyl containing siloxanes is reduced in comparison to dimethyl fluids. Polymethylphenylsiloxane has a compressibility of 5.5% at 20,000 psi.

TRIMETHYLSILOXY TERMINATED FLUIDS

Polymethylphenylsiloxane – CAS# 9005-12-3 (TSCA)



Cat#	Visc	MW	SG	RI	PP	TG
PS160	500	2600	1.11	1.533	-20°C	-86°C

(45 – 55%) Methylphenyl (45 – 55%) diphenylsiloxane copolymer – CAS# N/A (R&D Only)



Cat#	Visc	SG	RI	PP
PS162	200,000 - 500,000	1.15	1.582	-20°C

POLYMETHYLALKYLSILOXANES

Silicones can be modified to impart organic characteristics to their inorganic structure, which makes them more compatible with organic materials, such as petroleum oils and synthetic resins.

Replacement of a methyl group with longer chain aliphatic moieties produces silicones with properties that more closely resemble hydrocarbons. When compared to polydimethyl-siloxanes, methylalkylsiloxanes have greatly improved lubrication characteristics and greater compatibility with organic materials. The fluids have higher viscosity-temperature coefficients, lower compressibility and decreased oxidation stability. This last characteristic has been substantially overcome by compounding the fluids with stabilizers such as BHT and DSTDP or copolymerizing them with aromatic siloxanes as internal stabilizers.

Lubrication properties are optimized when the alkyl unit is at least eight carbons long. Polymethyloctylsiloxane is useful as a lubricant for soft metals such as aluminum, zinc and copper. It is also useful as a rubber and plastic lubricant especially when mated against steel and aluminum. Polymethyloctylsiloxane is employed in aluminum machining operations.

With increasing length of the alkyl substituent, the melting point increases. Conversely, as the pour point of the alkyl modified siloxanes increase, the resemblance and compativility with hydrocarbon oils increases. Polymethyltetradecylsiloxane has a high degree of hydrocarbon compatibility and maintains liquid behavior at room temperature. Polymethyloctadecylsiloxane is a creamy solid with a melt point just above room temperature. It is compatible with paraffin wax. It is used as a component in thread and fiber lubricant formulations and as a process aid in melt spinning. Methylalkylsiloxanes reduce surface tension of many non-aqueous solvents allowing them to act as wetting and leveling agents in coating and ink formations.

Polymethyloctadecylsiloxane - CAS# 68607-75-0 (TSCA)

$$\begin{array}{c} \mathsf{CH}_{3} \\ \mathsf{H}_{3}\mathsf{C} - \overset{\mathsf{CH}_{3}}{\underset{\mathsf{CH}_{3}}{\overset{\mathsf{I}}{\underset{\mathsf{H}_{3}}}} \mathsf{O} - \overset{\mathsf{CH}_{3}}{\underset{\mathsf{CH}_{3}}{\overset{\mathsf{I}}{\underset{\mathsf{CH}_{3}}}} \mathsf{O} - \overset{\mathsf{CH}_{3}}{\underset{\mathsf{CH}_{3}}{\overset{\mathsf{I}}{\underset{\mathsf{CH}_{3}}}} \mathsf{CH}_{3} \\ \end{array} \\ \begin{array}{c} \mathsf{CH}_{3} \\ \mathsf{CH}_{3} \\ \mathsf{CH}_{3} \\ \mathsf{CH}_{3} \\ \mathsf{CH}_{3} \\ \mathsf{CH}_{3} \end{array}$$

Cat#	Visc	MW	SG	RI	PP	TG
PS130	250 – 300	11,000	0.89	1.443	50°C	39.5°C

(70%) Dimethyl (30%) methyloctadecyl Siloxane Copolymer - CAS# 67762-83-8 (TSCA)

			CH3	
	CH3	CH3	(CH ₂) ₁₇	CH3
H ₃ C-	-Śi—O—	-Śi—O-	ŚiO-	−Śi−−CH ₃
	ĊH ₃	_с́н ₃	ĊH_3	ⁿ ĊH ₃

Cat#	Visc	SG	RI
PS130.5	250 – 350	0.892 1.	.44

Polymethyltetradecylsiloxane - CAS# 76684-67-8 (TSCA)



Cat#	Visc	SG	MW	RI
PS134	1500 – 3000	0.89	9,400	1.455

Polymethylhexadecylsiloxane - CAS# N/A (For R&D Only)



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Cat#	Visc	MW	SG	RI	PP
PS135	200	10,000	0.88	1.451	35°C

Polymethyloctylsiloxane - CAS# 68440-90-4 (TSCA)

		CH3	
	CH3	(CH ₂) ₇	CH3
H ₃ C-	Śi—O—	-Si-O-	—Śi—CH ₃
	ĊH ₃	ĊH ₃	CH ₃

Cat#	Visc	MW	SG	RI	PP	TG
PS140	600 - 1000	6,200	0.91	1.445	-50°C	30.4°C

HYDROPHILLIC SILICONES

Hydrophillic silicones are non-reactive fluids that have been modified to give them slight to complete solubility in water. The chemical description is polyalkylene oxide modified polydimethylsiloxanes.

Polydimethylsiloxanes prepared as copolymers with alkene oxides are widely used as surfactants. By altering the amounts of alkene oxide (hydrophile) and dimethylsiloxane (lipophile) the desired surfactant properties may be balanced. The higher the alkene oxide content the higher the hydrophilicity. Materials with ethylene oxide contents 75% and higher, are freely soluble in water, as well as other commonly used organic solvents such as methanol, iso-propanol, acetone, xylene, and methylene chloride. PS071 is a low molecular weight water-soluble fluid that is used in lithographic and photographic plates to facilitate wetting and spread of developers. It is also used as an anti-fogging treatment for glass and plastic optical surfaces. PS073 is used as an anti-foam in water-based coatings. PS072 is a water-insoluble copolymer employed as a lubricant for fibers and plastics. It also imparts anti-tack and mar resistant quality coatings. PS071, PS072 and PS073 all have excellent long term hydrolytic stability. PS071 and PS072 provide slip in flexographic and gravure inks. PS073.5 reduces the static charge generation of fiber substrates and has been incorporated into rolling oil formulations for metal drawing and stamping. The coefficient of thermal expansion is 8 x 10⁻⁴/°C.

$$(OCH_{2}CH_{2})_{x} - OCH_{3}$$

$$(OCH_{2}CH_{2})_{x} - OCH_{3}$$

$$(OCH_{2})_{x} - OCH_{3}$$

$$(OCH_{3})_{x} - OCH_{3}$$

$$(OCH$$

H

xane ethylen	e oxide block copolymer – CAS	# 27306-78-1 (TSC/	A)		
Visc	Non Siloxane Wt%	RI	MW	SG	ST
20	75	1.4116	600	1.007	23.6
xane(60% pro	opylene oxide-40% ethylene oxid	de) block copolym	er – CAS# 67762-8	85-0 (TSCA)	
Visc	Non Siloxane Wt%	RI	MW	SG	ST
1800	65 - 70	1.4456	20,000	1.023	22
xane(25%)etl	nylene oxide block copolymer –	CAS# 68938-54-5 ((TSCA)		
Visc	Non Siloxane Wt%	RI	MW	SG	ST
130	25	1.4539	4,000	1.066	27
xane(80%)etl	nylene oxide block copolymer –	CAS# 117272-76-1	(TSCA)		
Visc	Non Siloxane Wt%	RI	MW	SG	ST
45	80	1.4521	1,000	1.035	26
	xane ethylen Visc 20 xane(60% pro Visc 1800 xane(25%)eth Visc 130 xane(80%)eth Visc 45	xane ethylene oxide block copolymer – CASViscNon Siloxane Wt%2075xane(60% propylene oxide-40% ethylene oxideViscNon Siloxane Wt%180065 - 70xane(25%)ethylene oxide block copolymer – ViscNon Siloxane Wt%13025xane(80%)ethylene oxide block copolymer – ViscNon Siloxane Wt%4580	xane ethylene oxide block copolymer – CAS# 27306-78-1 (TSC/ ViscViscNon Siloxane Wt%RI20751.4116xane(60% propylene oxide-40% ethylene oxide) block copolymeViscViscNon Siloxane Wt%RI180065 - 701.4456xane(25%)ethylene oxide block copolymer – CAS# 68938-54-5 (ViscNon Siloxane Wt%RI130251.4539xane(80%)ethylene oxide block copolymer – CAS# 117272-76-1 ViscNon Siloxane Wt%RI45801.4521	xane ethylene oxide block copolymer – CAS# 27306-78-1 (TSCA)ViscNon Siloxane Wt%RIMW20751.4116600xane(60% propylene oxide-40% ethylene oxide) block copolymer – CAS# 67762-8ViscNon Siloxane Wt%RIMW180065 - 701.445620,000xane(25%)ethylene oxide block copolymer – CAS# 68938-54-5 (TSCA)ViscNon Siloxane Wt%RIMW130251.45394,000xane(80%)ethylene oxide block copolymer – CAS# 117272-76-1 (TSCA)ViscNon Siloxane Wt%RIMW45801.45211,000	Visc Non Siloxane Wt% RI MW SG 20 75 1.4116 600 1.007 xane(60% propylene oxide-40% ethylene oxide) block copolymer - CAS# 67762-85-0 (TSCA) MW SG Visc Non Siloxane Wt% RI MW SG 1800 65 - 70 1.4456 20,000 1.023 xane(25%)ethylene oxide block copolymer - CAS# 68938-54-5 (TSCA) WW SG Visc Non Siloxane Wt% RI MW SG 130 25 1.4539 4,000 1.066 xane(80%)ethylene oxide block copolymer - CAS# 117272-76-1 (TSCA) Yisc Non Siloxane Wt% RI MW SG 45 80 1.4521 1,000 1.035

POLYMERIC COUPLING AGENTS

Polymeric silanes are preferred in film-forming and primer applications. Multiple bonding opportunities with both inorganic substrates and polymer matricies make these materials desirable in many adhesive bonding formulations. Polymeric coupling agents introduce new considerations when used as additives in composite systems. In general, hydrophilic polymeric silanes are more effective on hydrated substrates such as aluminum trihydrate, a wetting phenomenon, but care must be taken to maintain reactivity with the organic substrate. It has been demonstrated that when polymeric silanes are used in composites, dialkoxy versions generally give higher mechanical properties than trialkoxy-silanes. Vinyl and unsaturated polymeric silanes can be grafted to polyolefins with peroxides. Those with alkoxy groups can be subsequently crosslinked with moisture. The technology is important in enhancing wet electricals and use-temperature ranges for the wire and cable industry. Alkoxy-silane modified polymers are used to transfer the properties of a polymer to inorganic material by displacing alkoxy groups on the silicon. The materials have uses as permanently bonded stationary phases for chromatography and exchange columns. Other polymers with non-reactive silane pendant groups have been used for permeable membranes and as barriers.

(N-Trimethoxysilylpropyl)polyethyleneimine, 50% in Isopropanol – CAS# 75132-84-2 (TSCA)



(N-Dimethoxymethylsilylpropyl)polyethyleneimine, 50% in Isopropanol – CAS# NA (For R&D Only)

$H_3C = O = Si = O = CH_3$	$H_3C = O = Si = O = CH_3$
CH ₃	CH ₃

Cat#	Visc	SG
PS076.5	125 - 175	0.92

(N-Triethoxysilylpropyl) O-polyethylene oxide urethane – CAS# NA (For R&D Only)

$$\begin{array}{ccc} & & & OCH_2CH_3 & & O\\ H_3C-CH_2-O-Si-CH_2-CH_2-CH_2-CH_2-O-(CH_2CHO)_n-H\\ & & OCH_2CH_3 \end{array}$$

Cat#	Visc	SG
PS077	25 – 60	0.93

Vinylmethoxysiloxane oligomer – CAS# NA (For R&D Only)



Cat#	Visc	SG
PS078.9	8 – 11	1.10

T-RESINS AND LADDER POLYMERS

T-resins are highly cross-linked materials with the empirical formula $RSiO_{1.5}$. They are names from the organic group and the one and a half (sesqui) stoichiometry of oxygen. Thus $C_6H_5SiO_{1.5}$ is called polyphenylsilsequioxane. In generally, the resins have an unordered structure. Lower molecular weight, soluble resins (particularly phenyl) are believed to contain substantial ladder structure.

T-resins form the basis of a wide range of coating materials that can be used directly or in combination with other materials. They have been used as planarization layers and reactive ion etch layers in microelectronics. They are employed as binders in high performance mineral filled molding compounds and refractories. Chloromethyl aromatic resins can be crosslinked by ultraviolet radiation. Another applications is silicone carbide fiber production via carbothermal reduction to SiC and CO at 400-600°C.

PR6155	Polymethylsilsesquioxane – CAS# 68554-70-1 (TSCA)
PR6163	Polyphenylpropylsilsesquioxane, 4 OH groups average, 30% Propyl
	CAS# 68037-90-1 (TSCA)

POLYALKOXYSILOXANES-POLYSILICATES

Polyalkoxysilanes are often operationally viewed as liquid sources of silicon dioxide. The hydrolysis reaction, which yields polymers of silicic acid which can be dehydrated to silicon dioxide, is of considerable importance. The stoichiometry of hydrolysis for simple linear polydiethoxysilane is

$$[Si(OC_2H_5)_2O] + H_2O \xrightarrow[Acid or Base]{} SiO_2 + 2CH_2H_5OH$$

Silicon dioxide never forms directly during hydrolysis. Intermediate ethoxy derivatives of silicic acid and polysilicates form as hydrolysis progresses. The polysilicates grow in molecular weight and chain length until most or all of the ethoxy groups are removed and a nonlinear network of Si–O–Si remains. The polyalkoxysiloxanes themselves contain cyclic and linear structures containing 3 – 6 silicon atoms. The viscosity of solutions increases until gelation or precipitation. Partially hydrolyzed materials of this type often contain more than enough silanols (SiOH) to displace most of the remaining ethoxy groups in an acid- or base-catalyzed condensation.

The hydrolysis reaction is catalyzed by acid or base. For binder preparation, dilute hydrochloric, nitric or acetic acids are preferred, since these facilitate formation of stable silanol condensation products. When more complete condensation or gelation is preferred, a wider range of catalysts, including moderately basic ones, is employed. These materials, which are often called hardeners or accelerators, include aqueous or anhydrous ammonia, ammonium carbonate, triethanolamine, calcium hydroxide, magnesium oxide, dicyclohexylamine, alcoholic ammonium acetate and tributylin oxide. For glass formation, hard bases such as sodium methoxide, sodium hydroxide or lithium methoxide are added. The stoichometry of hard base is calculated to give the desired glass decomposition, e.g. 20% Na₂O: 80% SiO₂.

Polydiethoxysilane with 40% SiO₂ content (PS9120) is the most widely used of this class of compounds finding wide use as a binder in investment casting and in zinc rich paints. Polydiethoxysiloxanes with higher SiO₂ content are sometimes preferred in coating formulations since they give less alcohol byproducts and dry faster. Polydimethoxysiloxane is preferred in many sol-gel or law heat glass applications since it has a high SiO₂ content and the methanol byproduct contributes to reduced stress-cracking.

Polydiethoxysiloxane - CAS# 68412-37-3 (TSCA)



Cat#	Visc (cSt)	% SiO ₂ Content	SG
PS9120	4 - 5	40 ⁻ - 42	1.05 – 1.06

Polydimethoxysiloxane - CAS# 25498-02-6 (TSCA)



Cat#	Visc (cSt)	% SiO, Content	SG
PS9130	6 - 9	55 - 60	1.10 – 1.12

PROTOTYPE AND MODEL MAKING SILICONE

HOW MODELING SILICONES WORK

Most of the silicones are supplied as two part kits with "A" and "B" parts, containing at least three components.

- 1. Base
- 2. Crosslinker
- 3. Catalyst

The base and crosslinker combine with each other to form the cured product, but they need a catalyst. In most formulatons the catalyst is premixed with the base, so many kits have only two parts. They are referred to as vinyl-addition silicones.

Other materials can be added by the craftsman to modify the basic properties of the silicones. These include fillers, softening agents, pigments, dyes, additional catalyst or cure retarders. The modifiers are added to the base. After mixing these components, the crosslinker is added. All of UCT Specialties' kits are in ready-to-use form with responses and strengths most widely desired. Only the experienced modelist should consider blending materials other than pigments and dyes, such as softening agents and fillers.

HOW TO USE UCT SPECIALTIES SILICONES

Mixing

It is important to obtain a homogeneous mix of the silicones and to avoid entrapment of air. Mixing can be accomplished with a spoon or mixing stick. If air is entrapped as bubbles, cured rubber will contain weak areas and detail will be lost. In most systems, vacuum de-airing is desirable. Some systems will de-air on standing for 5 to 20 minutes, particularly if the mix container is tapped sharply or placed on a vibrating surface. Bubbles on mold surfaces can be reduced by brushing a layer of catalyzed mix over the surface before pouring.

Work Life

All silicone systems are designed to have a work life of 30 to 90 minutes. The work life can be extended by adding a cure retarder to the initial mix. The section on accelerators and retarders provides details on work life modification. The work life can be shortened by adding additional catalyst or warming the mix.

Curing

Most UCT Specialties silicones will cure at room temperature in 24 hours. The cure can be accelerated by heating the silicones. At a temperature of 110°C (240°F) most will cure within two hours.

Materials to Avoid

The "A" Part, "B" Part and catalyzed mix of A/B can be cure-inhibited by certain contaminants. Avoid contamination with amines, sulfur, chloride or tin containing compounds. These materials are found in epoxy, natural rubber, PVC and moisture silicones respectively.

Shelf Age

The shelf life of these materials is six months. Containers of these products should be kept tightly sealed to avoid contamination by moisture or dirt. Recommended storage temperature is 25°C.

PEM10

Clear Liquid Silicone Elastomer

PEM10 silicone elastomer is supplied as a two part kit comprised of liquid base and curing agent. When the base and the curing agent are thoroughly mixed in a 10:1 weight ratio, the liquid mixture will cure in thick or thin sections to a flexible, transparent elastomer ideally suited for electrical/electronic potting and encapsulating applications.

Properties

Base viscosity	5500 cP
Specific Gravity	1.05
Mixed viscosity	3900 cP
Pot life at 25°C	2 hours
Cure time at 25°C	24 hours

Cured Properties

Appearance	Transparent
Hardness	40 Shore A
Tensile Strength MPa	6.20
Elongation	100%
Tear Strength die B	2.6 kN/m
Brittle Point	- 65°C
Refractive Index	1.430

Processing/Mixing

PEM10 liquid rubber base and crosslinking agent are blended in the ratio of 1 part of the "B" crosslinker to 10 parts of the "A" base, by weight. Thorough mixing is required for uniform cure. For best curing results, glassware, tinned cans as well as glass or metal stirring implements should be used. Mix with a smooth action that will minimize the introduction of excess air. Any entrapped air should be removed before the rubber is poured by using at least 1 - 10 mm vacuum. Apply vacuum slowly to avoid overflow of the container. The container should not be more than half full.

Work Life

The work life of the mixed material depends on the temperature. At room temperature, work life is approximately one hour. The work life of the mixed material may be greatly increased by refrigeration. At a temperature of 0°C, a pot life of 10 days can be expected. During refrigerated storage, care should be taken to avoid moisture contacting the material.

Varying Crosslinking Agent Concentration

Variation of the crosslinking agent concentration has little effect upon the set-up time of the rubber. Lowering the crosslinker concentration will result in softer, weaker material; increasing the concentration will results in overhardening and will tend to degrade physical and thermal properties.

PEG060

Silicone Gels

Silicone gels are solids with fluid characteristics. They maintain good cohesion, high instantaneous deformation and good resilience. The materials are clear with a range of firmness that varies from slow flowing to free standing. These temporarily deformable materials have found application in soft tissue prosthesis and shock absorption. These two part silicone gel systems may be characterized as viscoelastic substances of which only a small portion is crosslinked by an addition cure mechanism. Variation of ratio of base components gives a wide range of firmness.

Processing

PEG060 is a 2 part addition cure system which is comprised of an "A" part and a "B" part which, as supplied, are mixed in a 10 to 1 ratio. After thoroughly mixing 10 parts "A" to 1 part "B," allow the mix to de-air. Cure at $115 - 120^{\circ}$ C for 30 - 60 minutes or at room temperature for 48 hours. If penetration of the cured gel is either too soft or too firm, for the given application, the "A" part to "B" part ratio can be changed.

Too firm – Low penetration – change "A" to "B" ratio to 11:1, 12:1, 13:1, etc.

Too soft – High penetration – change "A" to "B" ratio to 9:1, 8:1, 7:1, etc.

MODIFIERS

Accelerators

In order to shorten cure time or "freshen" two-part silicone systems described, it is often desirable to add additional catalyst. The catalyst is a dilute solution of platinum. One to two drops per 100 g of silicone elastomer is typically used. PC072 is an extremely fast catalyst. It shortens work and cure time. PC075 is room temperature active, but not as fast as PC072.

PC072 Platinum Divinyltetramethyldisiloxane complex, 2% platinum in xylenePC075 Platinum Divinyltetramethyldisiloxane complex, 2% platinum in vinyl terminated polydimethylsiloxane

Inhibitors

In order to extend work-life, PS925 methylvinylsiloxanes are added at a level of 2 - 4 drops per 100 grams. This inhibits the platinum. After the addition of inhibitor, the systems must be cured at elevated temperature ($120 - 150^{\circ}$ C).

PS925 Cyclic vinylmethyl, dimethyl siloxanes

Softening Agents & Thinners

Softening agents include reactive and non-reactive silicone flexiblizers. Non-reactive fluids can be used universally but in proportions greater than 5%, they tend to bleed.

PS040	Polydimethylsiloxane, trimethylsiloxy terminated (50 cS) non-reactive
PS445	Polydimethylsiloxane, vinyl terminated (10,000 cS) for vinyl addition silicones
PS343.8	Polydimethylsiloxane, silanol terminated (3,500 cS) for one-part and tin catalyzed silicones

Fillers

The preferred filler for silicones is hexamethyldisilazane treated silica. The material is very fine and hydrophobic. In order to thicken silicones, the silica should be mixed thoroughly into the base.

SS0216 Silica, hexamethyldisilazane treated

UCT SPECIALTIES GLASSCLAD COATINGS



GLASSCLAD COATINGS

PS200 - GLASSCLAD 18

Glassclad Imparts the Following Properties to Treated Surfaces

- Non-adherent, non-oily surfaces
- Greater scratch resistance
- Easier cleaning, improved appearance
- Reduces the number of surface polar sites

Uses

Applications where PS200 (Glassclad 18) has been used successfully include:

- Laboratory Glassware Improves drainage, reduces breakage
- Porcelain Ware Provides a glide surface and reduces adhesion to other porcelain ware.
- Optical Fibers Provides lubricity and reduces breakage during fabrication and in operational flexing
- **Clinical Analysis** Treatment of analytical equipment extends clotting time of blood, reduces hemolysis, and reduces protein adsorption. PS200 (Glassclad 18) is <u>not</u> for food or drug use.
- Fluorescent Light Bulbs Increases scratch resistance, reducing breakage, increases surface reactivity

Description

PS200 (Glassclad 18) is a monomeric octadecylsilane derivative in a solution of t-butanol and diacetone alcohol that reacts with water to form a silanol-rich prepolymer and an alcohol. The silanol-rich prepolymer is able to condense with available hydroxy groups of glass or other siliceous materials to form a chemically bound alkylsilicone.

Typical Properties of PS200 (Glassclad 18)

% Active	20%
Color, Gardner scale	< 5
Flashpoint	10°C
Specific gravity (25°C)	0.88
Solidification Point	-30°C

Properties of Treated Surfaces

Values reported are for glass slides dipped in 1% solutions of PS200 (Glassclad 18) and cured at 100°C.

Untreated

Treated

Surface Resistivity

Blood Protein Adsorption

1 x 10¹² ohms

1.2 x 10¹³ ohms

Critical Surface Tension

Untreated	$\gamma_c = 78 \text{ dynes/cm}$
Treated (hydrophobic)	γ_{c} = 31 dynes/cm

Coefficient of Friction, static

Untreated	0.9 - 1.0	(glass slide c	on glass slide) comparative
Treated	0.2 - 0.3	100 hour adsorption values for	
		human blood	I on borosilicate glass
		surfaces.	-
		Untreated	0.13 mg/mm ²
		Treated	0.01-0.02 mg/mm ²

These results are not meant to suggest "in vivo" application of PS200 (Glassclad 18). PS200 (Glassclad 18) should be used only in treatment of diagnostic apparatus for clinical analysis in outside the human body applications.

PS220 - GLASSCLAD HT

PS220 is a high temperature modified phenylsiloxane resin which has a continuous use temperature exceeding 350°C. It is used both as a thin film coating and for the production of laminated structures. It has a tensile strength of 3,500 psi and a hardness of 120R (Rockwell). Parts are dipped or sprayed with undiluted resin and cured 20 to 30 minutes at 240°C.

PS225 - GLASSCLAD EG

PS225 is a thermally stable resin which forms a moderately flexible film with excellent adhesion and low chloride content. It provides an oxidation and mechanical barrier for resistors and circuit boards. Part application is by spraying or dipping. Cure is 20 minutes at 220°C.

PS233 - GLASSCLAD RC

PS233 is a methylsilicone resin which forms a coating with high temperature (250°C) serviceability. Its high dielectric strength, thermal resistance and mechanical strength make it ideal as an electrical component and circuit board coating. PS233 reacts covalently with glass and siliceous surfaces to form a permanent bond. It has excellent abrasion resistant properties and can be applied to materials as a protective coating. It is typically applied by dipping or brushing followed by air dry and final cure at 150°C for one hour.

PS234 - GLASSCLAD CR

PS234 is an 80% hard resin in toluene, which is designed to impart an improvement to heat service life and to improve weather stability to an organic surface. PS234 dries in air and can be cured by using a zinc octoate catalyst (PC040) for two hours at 250°C.

PS235 - GLASSCLAD TF

PS235 is employed as a source of thick film (0.2 - 0.4 micron) coatings of silicon dioxide. PS235 is a polymeric precursor of silicon dioxide. Silica formation begins at $110 - 120^{\circ}$ C and is complete by 220°C. The polymer converts to approximately 36% SiO₂. Applications for PS235 include dielectric layers, abrasion resistant coatings and translucent films. PS235 can be applied without solvent or in chlorinated hydrocarbon and ester vehicles. Specific gravity is 1.13. It is 100% solids.

PS252 - GLASSCLAD FF

Applications

PS252 is a source of filler-free silicone rubber in a tough bulk film form. It exhibits high bond strength to a wide range of substrates including other silicones, silica, metals and solvent compatible plastics and fibers. In biomedical equipment, PS252 coatings reduce physiological interaction including protein adsorption and clot initiation. In optical devices, it provides a clear mechanical barrier that seals and gaskets without scratching or initiating notch failure.

Description

PS252 is a moisture-activated silicone RTV dispersed in a solution of tetrahydrofuran and dioxane. In the presence of atmospheric moisture, the coasting undergoes a condensation of silicone prepolymers to a high molecular weight rubber. The system is designed for wet out and adhesion to polar substrates.

Cured Properties

Tensile Strength > 100 psi Elongation > 150% Durometer, Shore A > 8 Tear Strength > 5 pli

Uncured Properties

Percent Solids 48 - 52%Viscosity 350 - 400 cstks Skin over time 30 - 45 minutes Cure time (0.25 mm) 6 - 8 hours

Application Methods

PS252 is applied by dipping or brushing. Solvent is allowed to evaporate, cure is at room temperature.

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