^{29}Si NMR Some Practical Aspects

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1.   Introduction

Silicon is in many respects one of the more important elements in both nature and chemistry. On one hand silicates constitute the main material of the earths crust, and on the other hand organo silicon compounds are often used in element organic chemistry or as building blocks in material science. This is reflected also in literature concerning silicon NMR. For example, one of the fastest growing sections in the last years comprises the application to material sciences and here especially the solid state silicon NMR. Of the naturally occurring isotopes ^{28}Si (92.21%), ^{29}Si (4.70%) and ^{30}Si (3.09%), ^{29}Si only has a spin $^1/_2$ and therefore a magnetic moment. This puts it in the same league together with the other elements of 14 group of the periodic table of the elements such as carbon, tin and lead. All of these elements, with the exception of germanium, have at least one isotope with a spin of $^1/_2$ (Table 1).

Table 1   Group 14 elements, parameter of selected isotopes

	Natural Abundance [%]	Nuclear Spin	Magnetic Moment μ^d	Sensitivity rel.a)	abs.b)	Recept. rel. to ^{13}C
^{13}C	1.108	$^1/_2$	07022	1.59×10^{-2}	1.76×10^{-4}	1
^{29}Si	4.7	$^1/_2$	-0.5548	7.84×10^{-3}	3.69×10^{-4}	2.1
^{73}Ge	7.76	$^9/_2$c)	-0.8768	1.4×10^{-3}	1.08×10^{-4}	0.61
$^{119}Sn^{d)}$	8.58	$^1/_2$	-1.0409	5.18×10^{-3}	4.44×10^{-3}	25.2
^{207}Pb	22.6	$^1/_2$	0.5843	9.16×10^{-3}	2.07×10^{-3}	11.8.

a) at constant field and equal number of nuclei; b) product of relative sensitivity and natural abundance; c) quadrupole moment, -0.18×10^{-28}m; d) isotope used in most tin NMR experiments, for other relevant nuclei see literature [1] and cited reviews.

Table 1 shows that ^{29}Si has a higher share in the isotopic mixture but the absolute value of the magnetic moment is slightly lower than of ^{13}C. This leads to a lower resonance frequency. A complication arises from the fact that spin and magnetic moment are antiparallel leading to a negative sign of the gyromagnetic ratio ?. Concerning these facts silicon NMR had a slow start. After the first report by Lauterbur et al. in 1962 [2] there have been a few papers per year only. However, since the beginning of the 80´s this has changed dramatically. Our own data collection of ^{29}Si chemical shifts now contains about 13.000 data sets for more than 6.500 compounds [3]. A quick search in literature yields around 25.000 compounds with a measured ^{29}Si chemical shift. Because of these huge amounts of material available in silicon NMR, all discussions or reviews must be limited to special and selected research fields.

2.   General aspects

2.1   *Using of standards*

The only magnetic isotope of silicon ^{29}Si has a natural abundance of 4.7%, a spin of $^1/_2$, a magnetic moment of -0.9609 and therefore a receptivity of 3.69×10^{-4} compared to that of ^1H. It can be characterized as a magnetically diluted isotope of medium sensitivity [4]. Similar to ^1H or ^{13}C NMR the referencing is mostly done relatively to tetramethylsilane (Me_4Si, TMS) which has the advantages of having a low boiling point, a relatively short relaxation time and being a chemically relatively inert substance. Therefore, if nescessary, it can be added directly to the sample. However, its resonance is in a shift range where the resonances of many other organosilicon compounds occur and so misinterpretations are possible. Two general strategies are usable to avoid this problem. The first one is the use of secondary standards. Some secondary reference standards as known from literature are collected in Table 2. Unfortuanately, due to their higher reactivity, in contrast to TMS, they are useful only for a limited number of applications.

Table 2   Current and historic reference compounds for silicon NMR

Name	Formula	Common Abbreviation	Chemical shift relative to TMS in ppm
Tetramethylsilane	Me_4Si	TMS	0.0
Tetrakis(trimethylsilyl)methane	$(Me_3Si)_4C$		3.6
Hexamethyldisiloxane	$(Me_3Si)_2O$	M_2	6.53
Octamethylcyclotetrasiloxane	$(Me_2SiO)_4$	D_4	-19.86
Tetramethoxysilane	$(MeO)_4Si$	TMOS	-78.54
Tetraethoxysilane	$(EtO)_4Si$	TEOS	-82.04
Tetrafluorosilane	SiF_4		-113.5
Tetrakis(trimethylsiloxy)silane	$(Me_3SiO)_4Si$	M_4Q	8.62 -104.08
Silicon oil[a]	$(Me_2SiO)_x$		-22.0

a) the use of silicone containing grease for your equipment leads normally also to "impurity" resonances around –22 ppm.

More common, except for precision measurements, is to use no standard compound at all in the sample (tube interchange technique). In such a case the referencing is done relative to a sample containing TMS in the same solvent as it was used in the unknown sample.

Negative values of the silicon chemical shift are to low frequency and high field compared to Me_4Si. Special care must be given by using silicon chemical shift data from earlier reviews and original papers. Some of them employ the magnetic field definition of chemical shifts instead of the currently accepted frequency based one, resulting in a reversed sign for chemical shift data.

2.2   Problems in ^{29}Si NMR, pulse techniques

There are a number of aspects for running into difficulties in measuring silicon NMR. The first of it concerns the fact that silicon containing materials such as glass and ceramics constitute a major part of the construction material of the probe head and probe tube resulting in a broad background signal at approx. -110 ppm. There are three general methods to avoid the problem:

1. In the case of narrow signals, the smallest sweep width possible should be used.
2. Population transfer pulse programs such as DEPT otr INEPT can be used if the silicon atoms are coupling with protons or fluorine for example.
3. If broad lines are measured, you might be able to subtract it from a blanc spectrum obtained under otherwise identical conditions.

One other characteristic feature regarding spectra of organosilicon compounds is usually observed under broad band decoupling of protons. Resonances of silicon atoms containing organic substituents split into many lines by spin-spin couplings with the protons. This is mostly prevented by decoupling experiments. However, the Nuclear Overhauser Effect (NOE) can then lead to zero signals, if the $(^{29}Si,^{1}H)$ dipol-dipol contribution T_1^{DD} to the other longitudinal relaxation paths of the silicon is close to 1.52. The relaxation times depend on the correlation times of a molecule, therefore, the signal intensity of a ^{29}Si spectrum with NOE varies with the temperature. Again there are three ways to turn around the situation:

1. Adding of shiftless relaxation reagents, for example the well-known $Cr(acac)_3$ in a concentration of ~10^{-2} mol/l).
2. Using of inverse gated decoupling. Here proton decoupling is only active during aquisition with long waiting times (3 to 5 times the relaxation time T_1) between scans. The advantage of not polluting the sample is offset by ineffective use of spectrometer time which can be alleviated somewhat by using shorter pulses (40°) and shorter recovery times (20s).
3. Use of population transfer pulse programs such as INEPT or DEPT [5].

A third disadvantage in measuring silicon NMR spectra is related especially with "pure" inorganic compounds containing only ^{29}Si as an, for NMR experiments, useful nucleus. In such cases single pulse experiments are applicable only. Due to the slow relaxation in such compounds, a 30° pulse is used with repetition rates of about 20s.

Solid state silicon-29 NMR differs from these solutions inasmuch as the spatial interactions are not averaged out by particle motion, resulting in broad lines and all the problems are related to that fact. Literature about ^{29}Si solid state NMR is given in reference [6].

3. Chemical shifts

The majority of ^{29}Si NMR shifts are found in a range between +50 and -200 ppm. However, as far as we know the current upfield and downfield "world records" are formed by divalent silicon compounds. The largest upfield shift is measured for the decamethylsilicocene (**1**) with -392 ppm [7]. The highest downfield shift is given for compound **2** with 567 ppm [8].
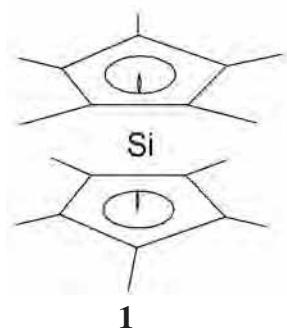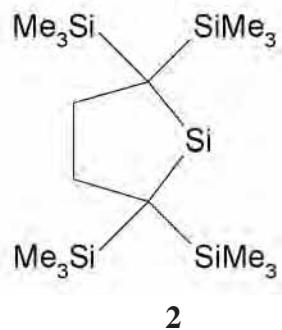
1	**2**
-392 ppm	+567 ppm

The border lines for silicon(IV) compounds are given by the tetraiodosilane (**3**) with a chemical shift of –350 ppm [9] and the central silicon atom of the dihypersilylplumbandiyl (**4**) with +197 ppm [10].

SiI_4 $[(Me_3Si)_3\mathit{Si}]_2Pb$

3 **4**
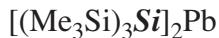
-350 ppm *+197 ppm*

The name hypersilyl is used mainly as abbreviation for the tris(trimethylsilyl)silyl substituent, as supersilyl is used as abbreviation for the tritbutylsilyl group.

Derivatives containing the trimethylsilyl group, $(CH_3)_3Si$-, abbreviated also as TMS, form the largest group of compounds with a known ^{29}Si NMR shift. One reason to introduce one of these groups into a molecule is to obtain a certain substitution pattern in organic chemistry [11]. Another reason is for example the fact to make substances now containing Me_3OSi- or Me_3SiN-groups instead of labile protons in HO- or HN-groups easier to handle. For instance the volatility or the solubility in organic solvents is much better for the derivatized compound. The TMS group is also useful for the characterization of such compounds by NMR methods [20]. The shift of TMS groups ranges from –34.4 ppm for Me_3Si^- K^+ [21] up to 83.6 ppm for $[Me_3Si]^+[B(C_6F_5)_4]^-$ [22]. An overview about typical shift ranges of trimethylsilyl substituted compounds is given in Scheme 1.
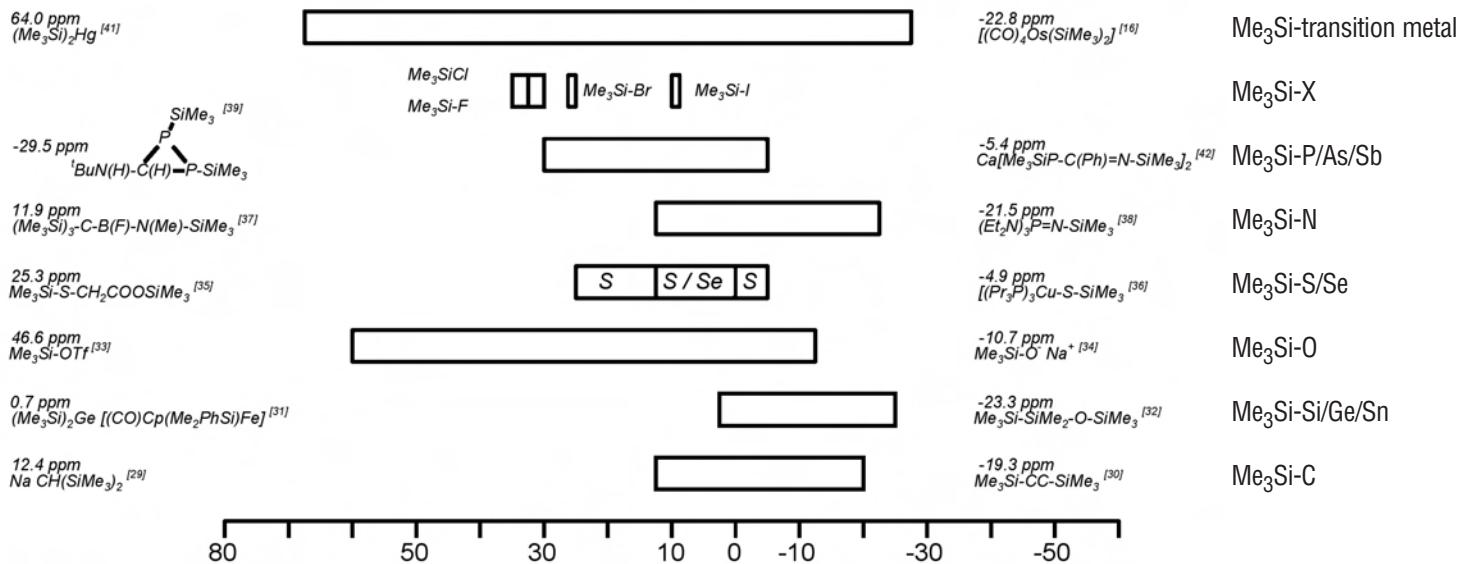
Scheme 1: Typical shift ranges of trimethylsubstituted derivatives.
Selected borderline case examples for each class of compounds are given.

One of the first uses of silicon-29 NMR was its application to siloxane polymers. Although it is still possible sometimes to recognize and isolate individual molecules, the main view is to dissect the molecules into building units (see Scheme 2).

End- (M)   Middle- (D)   Trifunctional (T)   Tetrafunctional (Q)
     Groups   Branching Groups
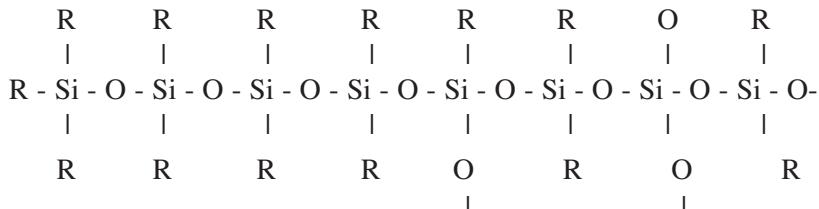
M		**D**		**T**		**(Q)**
R = Me$_3$	7 – 9 ppm	Me$_2$	-17 to –22	Me	-55 to –65	-105 to -115
Me$_2$Cl	~5	Cl$_2$	~ -73	HO	~ -100	
MeCl$_2$	~ -20	Me/H	~ -35	H	~ -85	
Cl$_3$	~ -48	Me/OH	~ -55	Ph	~ -78	
Ph$_3$	~ -10	Ph/OH	~ -70			
		Ph$_2$	-42±3			

Scheme 2: Building units and shift range of selected siloxanes in ppm.

The main difference between the building units is the number of oxygen atoms connected to a silicon atom. Except for the **M** group, the exchange of a R substituent for oxygen leads to an upfield shift. The chemical shifts of the building units are sensitive to neighbor effects in the chain structure revealing the microstructure of polymers. The chemical shifts of all building groups are modified by ring strain if cyclic siloxanes are investigated by ^{29}Si NMR.

Silazenes possess structural similarities to siloxanes and can be rationalized by the analogeous principles, however the range of chemical shifts is smaller. The total region extends from -62 to +18 ppm [12]. The same is true for carbosilanes. Resonances for silicon atoms bonded to 4 carbon atoms are found between -4 and +20 ppm [12]. A new report concerning silthianes has appeared recently [13].

Oligomeric and polymeric silanes are discussed in detail in the literature [14] and some of the appropriate references should looked up there. The ranges of chemical shifts of building components for oligosilanes are collected in Table 3. The skeleton of these compounds is similar to those of alkanes. A number of studies on substituted di- and trisilanes are also discussed in the article mentioned above.

Table 3: Selected chemical shifts of polysilane units in ppm

R	Endgroup $R_3Si\text{-}Si$	Middle group $R_2Si(Si)_2$	Trifunctional group $RSi(Si)_3$	Tetrafunctional group $Si(Si)_4$
Me	-4 ± 5	-28 to –50	-65 to -95	-109 to –165[b)]
Ph	-19 ± 3	-40 to –50	-75 to -85	
Ph/H	-30	-65 ± 5		
Me/H	-35 ± 2	-70 ± 5		
Me$_2$/Cl[a)]	28 ± 2			
^{t}Bu	20 to 30			

a) for BrMe$_2$Si: 21 ppm, IMe$_2$Si: 2 ppm; b) exception Si(SiCl$_3$)$_3$(SiCl$_2$SiCl$_3$): -79.5 ppm

The chemistry of silicon containing double bonds was a rapid growing field during the last 15-20 years. For silicon-silicon double bonds, ^{29}Si NMR chemical shifts are reported from ~50 ppm up to ~160 ppm (examples: 49.4 ppm [Mes((Me$_3$Si)$_2$N)Si]$_2$ [25]; 156.2 ppm (^{t}BuMe$_2$Si)$_2$Si=Si(Si^{i}Pr$_2$Me)$_2$ [26]) and for silicon carbon double bonds a range of ~130 ppm is given (13.1 ppm [2,4,6-^{i}Pr$_3$C$_6$H$_2$]$_2$Si=C=C(Ph)^{t}Bu [27]; 144.2 ppm Me$_2$Si=C(SiMe$_3$)Si^{t}Bu$_2$Me [28]). The chemical shifts of silicon having a double bond to a transition metal

strongly depends on the substituents on the transition metal and the metal itself. Chemical shifts are observed in a range of ~ -10 ppm (for example: –9.4 ppm for $[(^tBuO)_2Si=Fe(CO)_4]*THF$ [23]) and nearly 145 ppm (for example: 141.9 ppm for $[(Me_2N-C_{10}H_6)(H)Si=Mn(CO)_2(MeCp)]$ [24]).

The data of a number of other transition metal complexes are collected in some reviews [12, 14, 15, 16]. Due to the large variety for the bonding situations of the silicon a great spread of chemical shifts ranging from 289 ppm [17] up to -150 ppm [18] is observed.

For other compounds, especially for higher coordinated silicon derivatives, general collections of silicon chemical shifts might be consulted [3, 12, 19].

4.   Coupling constants

All magnetic nuclei in a molecule interact and the splitting caused by this gives rise to typical coupling patterns. Two cases can be distinguished:

1. Coupling with 100% isotopes such as ^1H, ^{19}F or ^{31}P gives the well-known splitting patterns in the ^{29}Si spectra. Couplings with quadrupolar nuclei such as the isotopes of chlorine are usually not observed.
2. Coupling with other rare spins such as ^{29}Si, $^{119/117}Sn$ or ^{13}C leads to smaller satellite lines left and right to the main line according to their abundance in the usual ^{29}Si spectra.

The ranges of some silicon-element coupling constants are found in Table 4. The sign of coupling constants over one bond is mostly negative because of the negative magnetogyric ratio of the ^{29}Si. Exceptions are found if the silicon is connected to an element with tightly bonded s-electrons e.g. ^{19}F or ^{31}P.

Table 4   Ranges of selected silicon element coupling constants (without sign)

Si-X coupling (X)	^1J(Si-X) in Hz (largest – smallest)	^2J(Si-X) in Hz (largest – smallest)	^3J(Si-X) in Hz (largest – smallest)
^1H	420 - 75	10 – 3 (SiCH$_3$) 13 – 1 (SiXH)	8 – 1
^{19}F	488 - 108	91 – 17	16 – 2
^{31}P	256 - 16	44 - <1	
^{13}C	113 - 37	18 – 4	
^{29}Si	186 - 23	24 - <1	
^{119}Sn	750 - 120	100 – 35	60 – 12

5   Reviews, Databases of ^{29}Si NMR Data

A large number of review articles deal with selected and special fields of ^{29}Si NMR but, only a limited number of general collections of ^{29}Si NMR chemical shifts or coupling constants exist. An electronic version of a ^{29}Si NMR database is available from the authors of this article [3]. Further information is available via the world wide web (http:\\www.silicium-nmr.de) or directly from the authors. A printed general review and an (incomplete) ^{29}Si NMR data collection will be available within the Landolt-Börnstein series (Springer publishing house) hopefully in 2003/2004.

Table 5   Selected ^{29}Si NMR chemical shifts (see reference [5])

Formula	Sum formula	Chemical shift [ppm][a)]	Gelest product code
Et_4Si	$C_8H_{20}Si$	7.1	SIT7115.0
Me_4Si	$C_4H_{12}Si$	0	SIT7555.0
Me_3SiCl	C_3H_9ClSi	30	SIT8510.0/.1
Me_3SiBr	C_3H_9BrSi	26	SIT8430.0
Me_3SiI	C_3H_9ISi	8.7	SIT8564.0
Me_3SiF	C_3H_9FSi	31.0	SIT8525.0
$Me_3SiOSO_2CF_3$	$C_4H_9F_3O_4SSi$	44	SIT8620.0
$Me_3SiC \equiv CH$	$C_5H_{10}Si$	-17.5	SIE4904.0
$Me_3SiC \equiv CSiMe_3$	$C_8H_{18}Si_2$	-19.4	SIB1850.0
Me_2SiCl_2	$C_2H_6Cl_2Si$	32	SID4120.0/.1
$MeSiCl_3$	CH_3Cl_3Si	12	SIM6520.0/.1
Ph_4Si	$C_{24}H_{20}Si$	-14	SIT7755.0
Ph_3SiCl	$C_{18}H_{15}ClSi$	1.5	SIT8645.0
Ph_3SiF	$C_{18}H_{15}FSi$	4.35	SIT8655.0
Ph_2SiCl_2	$C_{12}H_{10}Cl_2Si$	6.2	SID4510.0/.1
Ph_2SiF_2	$C_{12}H_{10}F_2Si$	-30	SID4530.0
$PhSiCl_3$	$C_6H_6Cl_3Si$	-0.8	SIP6810.0
$SiCl_4$	Cl_4Si	-18	SIT7085.0
$SiBr_4$	Br_4Si	-92	SIT7050.0
SiI_4	I_4Si	-350	SIT7123.0
SiF_4	F_4Si	-112	SIT7120.0

Formula	Sum formula	Chemical shift [ppm][a)]	Gelest product code
H_2SiCl_2	H_2Cl_2Si	-11.3	SID3368.0/.2
$HSiCl_3$	HCl_3Si	-9.4	SIT8155.0
$(CH_2=CH-CH_2)_4Si$	$C_{12}H_{20}Si$	-2	SIT7020.0
$CH_2=CH-CH_2SiMe_2Cl$	$C_5H_{11}ClSi$	27.2	SIA0460.0
$CH_2=CH-CH_2SiMeCl_2$	$C_4H_8Cl_2Si$	26.8	SIA0470.0
$CH_2=CH-CH_2SiCl_3$	$C_3H_5Cl_3Si$	8	SIA0520.0
$CH_2=CHSiCl_3$	$C_2H_3Cl_3Si$	-3	SIV9110.0
$PhCH_2SiCl_3$	$C_7H_7Cl_3Si$	7.2	SIB0970.0
$MeSi(CH_2Cl)Cl_2$	$C_2H_5Cl_3Si$	21.6	SIC2290.0
$Me_2Si(CH_2Cl)_2$	$C_4H_{10}Cl_2Si$	-3.5	SIB1051.0
	$C_8H_{19}ClSi$	35.8	SIT7906.0
$^tBuMe_2SiCl$	$C_6H_{15}ClSi$	33	SIB1935.0
$PhMeSi(H)Cl$	C_7H_9ClSi	1.3	SIP6738.0
$Me_2(H)SiCl$	C_2H_7ClSi	-11.1	SID4070.0
$PhSiH_3$	C_6H_8Si	-60	SIP6750.0
Ph_2SiH_2	$C_{12}H_{12}Si$	-34	SID4559.0
Ph_3SiH	$C_{18}H_{16}Si$	-17 to -22	SIT8665.0
Me_2SiH_2	C_2H_8Si	-37 to -48	SIM6515.0
$MeSiH_3$	CH_6Si	-65	SID4230.0
Me_3SiH	$C_3H_{10}Si$	-17	SIT8570.0
Et_3SiH	$C_6H_{16}Si$	0.2	SIT8330.0
$(EtO)_3SiH$	$C_6H_{16}O_3Si$	-60 to -65	SIT8185.0
$(EtO)_4Si$; TEOS	$C_8H_{20}O_4Si$	-82	SIT7110.0/.1
$(PhO)_4Si$	$C_{24}H_{20}O_4Si$	-101.1	-
$(MeO)_4Si$, TMOS	$C_4H_{12}O_4Si$	-79.5	SIT7510.0/.2
$(MeO)_3SiCl$	$C_3H_9ClO_3Si$	-66.6	-
$(MeO)_2SiCl_2$	$C_2H_6Cl_2O_2Si$	-52.6	-
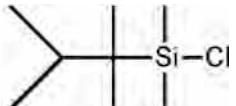
Formula	Sum formula	Chemical shift [ppm][a)]	Gelest product code
MeOSiCl$_3$	CH$_3$Cl$_3$OSi	-36.1	-
EtOSiCl$_3$	C$_2$H$_5$Cl$_3$OSi	-38.3	-
Ph$_2$Si(OH)$_2$	C$_{12}$H$_{12}$O$_2$Si	-33.9	SID4560.0
Ph$_3$SiOH	C$_{18}$H$_{16}$OSi	-12 to -24	SIT8695.0
Et$_3$SiOH	C$_6$H$_{16}$OSi	19.3	SIT8332.0
Me$_3$SiONa	C$_3$H$_9$NaOSi	-4 to -11	SIS6988.0
Me$_3$Si-O-SiMe$_3$	C$_6$H$_{18}$OSi	6	SIH6115.0
Me$_3$Si-O-O-SiMe$_3$	C$_6$H$_{18}$O$_2$Si	27.3	SIB1868.0
Me$_3$Si-S-SiMe$_3$	C$_6$H$_{18}$SSi	13	SIH6116.0
Me$_3$Si-O-Me$_2$Si-O-SiMe$_3$, MDM	C$_8$H$_{24}$O$_2$Si$_3$	6.5 (Me$_3$Si) -22(Me$_2$Si)	SIO6703.0
Me$_3$SiO(Me$_2$SiO)$_3$SiMe$_3$, MD$_3$M	C$_8$H$_{24}$O$_2$Si$_3$	6.8 (Me$_3$Si) -21.9 (2xMe$_2$Si) -22.6 (Me$_2$Si)	SID4626.0
(Me$_3$Si-O)$_4$Si, M$_4$Q	C$_{12}$H$_{36}$O$_4$Si$_5$	8 (Me$_3$Si) -105 (Si)	SIT7298.0
(Me$_3$Si-O)$_3$SiMe, M$_3$T	C$_{10}$H$_{30}$O$_3$Si$_4$	7 (Me$_3$Si) -65 (Si)	SIM6592.0
(-Me$_2$Si-O-)$_3$, D$_3$	C$_6$H$_{18}$O$_3$Si$_3$	-9	SIH6105.0/.1
(-PhMeSi-O-)$_3$	C$_{21}$H$_{24}$O$_3$Si$_3$	-20.8	SIT8705.0
(-Ph$_2$Si-O-)$_3$	C$_{36}$H$_{30}$O$_3$Si$_3$	-33.8	-
(-Me$_2$Si-O-)$_4$, D$_4$	C$_8$H$_{24}$O$_4$Si$_4$	-20	SIO6700.0
(-Me(H)Si-O-)$_4$, D´$_4$	C$_4$H$_{16}$O$_4$Si$_4$	-32.5	SIT7530.0
(-Ph$_2$Si-O-)$_4$	C$_{48}$H$_{40}$O$_4$Si$_4$	-46	SIO6705.0
(-Me$_2$Si-O-)$_x$, silicon oil	Molecular weight 160-423,000	-22	DMS-TXX

Formula	Sum formula	Chemical shift [ppm][a)]	Gelest product code
T8-silsesquioxane			
R=vinyl	$C_{16}H_{24}O_{12}Si_8$	-79.4	SIO6706.0
$Me_2(H)Si$	$C_{16}H_{56}O_{20}Si_{16}$	0.5 $Me_2Si(H)$	SIO6696.5
H	$H_8O_{12}Si_8$	-84.5	
$Me_2(H)Si$-O-$Si(H)Me_2$	$C_4H_{14}OSi_2$	-5	SIT7546.0
$Me_2(Cl)Si$-O-$Si(Cl)Me_2$	$C_4H_{12}Cl_2OSi_2$	9.6	SID3372.0
$Me_2(Cl)Si$-O-Me_2Si-$Si(Cl)Me_2$	$C_6H_{18}Cl_2O_2Si_3$	-18.3 (Me_3Si) 2.3 (SiCl)	SID3360.0
Cl_3Si-O-$SiCl_3$	Cl_6OSi_2	-46	SIH5910.0
$(MeO)_3Si$-$Si(OMe)_3$	$C_6H_{18}O_6Si_2$	-52.5	SIH6101.0
R = vinyl	$C_8H_{15}NO_3Si$	-80	SIV9097.0
Me	$C_7H_{15}NO_3Si$	-63	SIM6518.0
$(Me_2N)_4Si$	$C_8H_{24}N_4Si$	-28.1	SIT7276.0
$(Me_2N)_3SiMe$	$C_7H_{21}N_3Si$	-17	SIT8712.0
$(Et_2N)_2SiMe_2$	$C_6H_{18}N_2Si$	-1.8	SIB1095.0
Me_2N-$SiMe_3$	$C_5H_{15}NSi$	-6	SID3605.0
$(Me_3Si)_2NH$; HMDZ, HMDS	$C_6H_{19}NSi_2$	2.2	SIH6110.0
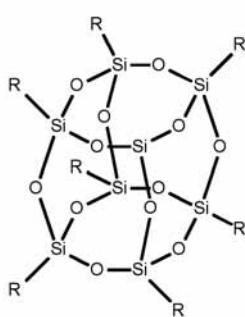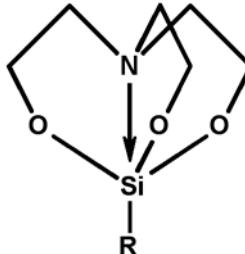
Formula	Sum formula	Chemical shift [ppm][a)]	Gelest product code
$(Me_3Si)_3N$	$C_9H_{27}NSi_3$	2.4	SIN6595.0
$(-Me_2Si-NH-)_3$	$C_6H_{21}N_3Si_3$	-4	SIT6102.0
$(-Me_2Si-NH-)_4$	$C_8H_{28}N_4Si_4$	-8.2	SIO6698.0
$(Me_3Si-O)_3B$	$C_9H_{27}BO_3Si_3$	12.3	SIT8718.0
$(Me_3Si-O)_3P=O$	$C_9H_{27}O_4PSi_3$	20	SIT8723.0
$(Me_3Si)_3P$	$C_9H_{27}PSi_3$	0.2	-
$Me_3Si-SiMe_3$	$C_6H_{18}Si_2$	-19.5	SIH6109.0
$PhMe_2Si-SiMe_2Ph$	$C_{16}H_{22}Si_2$	-21.8	SID4584.0
$Ph_2MeSi-SiMePh_2$	$C_{26}H_{26}Si_2$	-22	SID4238.0
$Ph_3Si-SiPh_3$	$C_{36}H_{30}Si_2$	-26.5	SIH6155.0
$ClMe_2Si-SiMe_2Cl$	$C_4H_{12}Cl_2Si_2$	17	SID3370.0
$Cl_2MeSi-SiMe_2Cl$	$C_3H_9Cl_3Si_2$	15.4 (SiCl) 25 (SiCl$_2$)	-
$Cl_2MeSi-SiMeCl_2$	$C_2H_6Cl_4Si_2$	18	-
$Cl_3Si-SiCl_3$	Cl_6Si_2	-6.2	SIH5905.0
$(-Me_2Si-)_6$	$C_{12}H_{36}Si_6$	-41.6	SID4623.0
$(Me_3Si)_3SiMe$	$C_{10}H_{30}Si_4$	-12.5 (Me$_3$Si) -87.9 (SiMe)	-
$(Me_3Si)_4Si$	$C_{12}H_{36}Si_5$	-9.8 (Me$_3$Si) -135.5 (Si)	SIT7308.0
$n-Bu_3Sn-SiMe_3$	$C_{15}H_{36}SiSn$	-8	SNT8585

a) chemical shifts without decimal point are due to different values with deviations of ±2 ppm.

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