Volatile Carbosilanes

Volatile carbosilanes are the preeminent precursors for:

- Silicon Carbide films and buffer layers
- Carbon-doped (Tensile-Strained) Silicon
- ALD promoted patterning and seed layers
- SiCO:H films for low-k, barrier layers and etch-stop
- Silicon Carbonitride utilized in passivation of silicon-based photovoltaics

By appropriate selection of the carbosilane precursor and deposition conditions the silicon carbide framework can be shifted toward substituted silicon and diamond-like structures.

Carbosilanes are compounds in which the elements of silicon and carbon alternate in a molecular framework or polymeric backbone in an approximate ratio of 1:1 according to the following general structure:

$$H\left[\left(\begin{array}{c}H\\ |\\ Si\\ |\\ R\end{array}\right)_{1-2}\left(\begin{array}{c}H\\ |\\ C\\ |\\ R'\end{array}\right)_{1-2}\right]H$$

Carbosilane Compounds

Name	MW	bp °C/mm (mp)	D_4^{20}	n_D^{20}
SIM6515.0 METHYLSILANE CH_6Si *1MS*	46.14	-57 (-157)	0.628 [-58]	

CAUTION: CAN FORM EXPLOSIVE MIXTURES WITH AIR

ΔHcomb: -624 kcal/mole
ΔHform: -7 kcal/mole
ΔHvap: 4.6 kcal/mole
Vapor pressure, -80°: 241 mm
Vapor pressure, 21°: 14 atm (210 psia)

Flashpoint: <-40°C (<-40°F)
Autoignition temperature: 130°C
Critical temperature: 79.3°
Dipole moment: 0.73 debye

$$CH_3-\overset{\displaystyle H}{\underset{\displaystyle H}{Si}}-H$$

Plasma polymerization yields dry process photoresist.[1]
Intermediate for poly(methylsilane) precursor to silicon carbide.[2]
Deposits SiC on Si and Ge at 400 - 500°C.[3]
Source for hydrogenated amorphous silicon carbide films.[4]

1. Dabbagh, G. et al. *J. Photopolym. Sci. Tech.* **1998,** *11*, 651.
2. Fhang, Z. et al. *J. Am. Ceram. Soc.* **1991,** *74*, 670.
3. Takatsuka, T. et al. *Appl. Surf. Sci.* **2000,** *162*, 156.
4. Lee, M. et al. in "*Chemical Aspects of Electronic Ceramics Processing*" Arkles, B. ed., MRS Proc. **1998**, *495*, 153.

HYDROLYTIC SENSITIVITY: 9: reacts extremely rapidly with atmospheric moisture - may be pyrophoric - glove box or sealed system required

[992-94-9] TSCA EC 213-598-5 HMIS: 3-4-3-X

Name	MW	bp °C/mm (mp)	D_4^{20}	n_D^{20}
SID4230.0 DIMETHYLSILANE C_2H_8Si	60.17	-20 (-150)	0.68 [-20]	

ΔHcomb: -624 kcal/mole
ΔHform: -23 kcal/mole
ΔHvap: 5.5 kcal/mole

Flashpoint: <-40°C (<-40°F)
Vapor pressure, -80: 30 mm
Dipole moment: 0.75 debye

$$CH_3-\overset{\displaystyle H}{\underset{\displaystyle H}{Si}}-CH_3$$

Generates cubic silicon carbide by plasma CVD.[1]
Epitaxial growth of cubic silicon carbide carried out by triode plasma CVD.[2]

1. Hashim, A. et al. *Semiconductor Electronics, IEE Int'l. Conf. Proc.* **2006**, 646.
2. Yasuiet, K. et al. *Appl. Surf. Sci.* **2000**, *159*, 556.

HYDROLYTIC SENSITIVITY: 3: reacts with aqueous base

[1111-74-6] TSCA EC 214-184-7 HMIS: 3-4-1-X

Name	MW	bp °C/mm (mp)	D_4^{20}	n_D^{20}
SID4595.0 1,3-DISILAPROPANE *DISILMETHYLENE* CH_8Si_2	76.24	14.7	0.697 [4]	1.4115 [4]

$$H-\overset{\displaystyle H}{\underset{\displaystyle H}{Si}}-CH_2-\overset{\displaystyle H}{\underset{\displaystyle H}{Si}}-H$$

CAUTION: PYROPHORIC, FORMS EXPLOSIVE MIXTURES WITH AIR
AIR TRANSPORT FORBIDDEN

HYDROLYTIC SENSITIVITY: 9: reacts extremely rapidly with atmospheric moisture - may be pyrophoric - glove box or sealed system required

[1759-88-2] HMIS: 4-4-2-X

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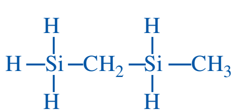
Name	MW	bp °C/mm (mp)	D_4^{20}	n_D^{20}



SID4592.0
1,3-DISILABUTANE — 90.27 — 44-5 — 0.80 — 1.436 [25]
1-METHYLDISILMETHYLENE
$C_2H_{10}Si_2$
Precursor for low temperature CVD of silicon carbide MEMS.[1,2]
1. Stoldt, C. et al. *Sens.Actuators, A* **2002**, *97-8*, 410.
2. Stoldt, C. et al. *Appl. Phys. Lett.* **2001**, 347.
HYDROLYTIC SENSITIVITY: 3: reacts with aqueous base
[6787-86-6] HMIS: 3-4-2-X

SID4593.0
1,4-DISILABUTANE — 90.27 — 45-6 (-15) — 0.697 — 1.4141
1,2-ETHANEDIYLBIS(SILANE) — Flashpoint: -31°C (-24°F)
$C_2H_{10}Si_2$ — Autoignition temperature: 152°C
CAUTION: VAPORS HAVE BEEN REPORTED TO SPONTANEOUSLY IGNITE
Bonds to oxide-free titanium, gold and silicon substrates.[1]
Forms 0.2-1.7% carbon doped silicon films.[2]
1. Arkles, B. et al. *J. Adhes. Sci. Technol.* **2012**, *26*, 41.
2. Okada, L. et al. *Surf. Sci.* **1998**, *418*, 353.
HYDROLYTIC SENSITIVITY: 9: reacts extremely rapidly with atmospheric moisture - may be pyrophoric - glove box or sealed system required
[4364-07-2] HMIS: 2-4-2-X

SIT8709.3
1,3,5-TRISILACYCLOHEXANE — 132.38 — 135 (-10) — 0.9001 — 1.5059
CYCLOTRISILMETHYLENE
$C_3H_{12}Si_3$
Single source precursor for beta-SiC by LPCVD at 800-1,000°.[1]
1. Lienhard, M. et al. in "*Chemical Aspects of Electronic Ceramics Processing*" Arkles, B. ed., MRS Proc. **1998**, *495*, 139.
HYDROLYTIC SENSITIVITY: 3: reacts with aqueous base
[291-27-0] HMIS: 3-4-1-X

SIT8709.8
1,3,5-TRISILAPENTANE — 120.37 — 100 — 0.7628 — 1.4491
BIS(SILYLMETHYL)SILANE — Flashpoint: -16°C (3°F)
$C_2H_{12}Si_3$
Employed in ALD of SiC films
Employed in PECVD of silicon carbide and silicon carbonitride "seed" layers.[1]
1. Weidman, T. et al. US Patent Appl. 2012/0122302 A1, 2012.
HYDROLYTIC SENSITIVITY: 7: reacts slowly with moisture/water
[5637-99-0] TSCA-L HMIS: 3-4-2-X

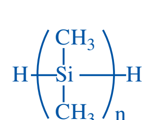
SIT8715.9
TRIS(SILYLMETHYL)SILANE — 164.48 — 61-2 / 30 — 0.806 — 1.4669 [25]
$C_3H_{16}Si_4$ — Flashpoint: 35°C (95°F)
Employed in PECVD of silicon carbide and silicon carbonitride "seed" layers
HYDROLYTIC SENSITIVITY: 7: reacts slowly with moisture/water
[1385027-19-9] HMIS: 3-3-2-X

Oligosilanes and Polysilanes

Oligosilanes and polysilanes undergo conversion to Carbosilanes at temperatures above 650°.

SIT7541.0
1,1,2,2-TETRAMETHYLDISILANE — 118.32 — 86-7 (-93) — 0.720 — 1.429
$C_4H_{14}Si_2$ — Flashpoint: -26°C (-15°F)
HYDROLYTIC SENSITIVITY: 3: reacts with aqueous base
[814-98-2] TSCA HMIS: 2-4-1-X

SIT7580.0
2,2,3,3-TETRAMETHYLTETRASILANE, 95% — 178.53 — 125-135
$C_4H_{18}Si_4$
Candidate material for nanowires.[1]
1. Arkles, B. et al. U.S. Patent Appl. 20120076840, 2012.
HYDROLYTIC SENSITIVITY: 7: reacts slowly with moisture/water
[1364487-19-3] HMIS: 2-4-1-X



PSS-1M01
poly(DIMETHYLSILANE) MW 1000-3000
DP: 25-50 Flashpoint: 103° Tm: 250-270° (substantial degradation before mp)
Solid state source for volatile siliconcarbonitride (SiCN) precursors utilized in passivation of silicon-based photovoltaics
Employed in CVD of silicon carbonitride films.[1]
1. Scarlete, M.; et al; US Patent 7,396,563; 2008 (Label Licensed Gelest Product)
2. Yajima, S. et al. *J. Mater. Sci.* **1978**, *13*, 2569.
[30107-43-8] / [28883-63-8] TSCA

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