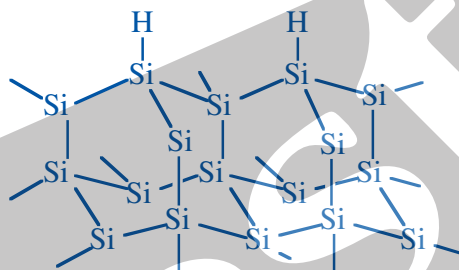


## Volatile Higher Silanes (Perhydridoooligosilanes)

*Volatile Higher Silanes are low temperature, high deposition rate precursors for:*

- Amorphous hydrogenated silicon (a-Si:H) films
- Germanium-doped (Compression-Strained) Silicon
- Carbon-doped (Tensile-Strained) Silicon
- Silicon CVD, ALD, ALE
- Silicon and Silicon-Binary Quantum-Dots by photolytic or laser induction
- Silicon-based Photovoltaics

By appropriate selection of the higher silane precursor and deposition conditions, silicon deposition can be shifted from amorphous hydrogenated silicon toward microcrystalline silicon structures.



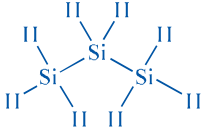
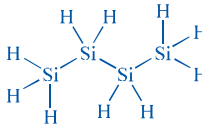
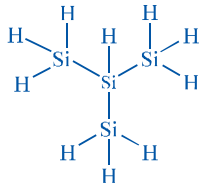
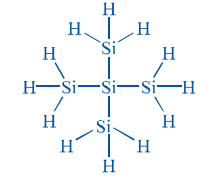
Volatile higher silanes containing three or more silicon atoms and hydrogen are more accurately termed perhydridoooligosilanes. They are volatile pyrophoric liquids with the general formula  $\text{Si}_n\text{H}_{2n+2}$ , which may be depicted as follows:



(where R, R' are H or SiH<sub>3</sub>)

Perhydridoooligosilanes differ from silane and disilane in a number of significant ways. As the number of silicon atoms increases beyond two, electrons are capable of sigma-sigma bond conjugation. The consequences are that the optical absorption of oligosilanes shifts to longer wavelengths with additional silicon atoms. Apart from the obvious advantage oligosilanes possess in CVD by having a greater number of silicon atoms than silane or disilane, the dissociative adsorption of two of the three hydrogen atoms on terminal silicon atoms has a lower energy barrier. This significantly reduces the thermal budget for deposition. While silane and disilane undergo relatively low rates of deposition below 850°C, trisilane and higher linear oligosilanes have demonstrated practical deposition rates as low as 600°C. Branched silanes, such as isotetrasilane and neopentasilane, undergo deposition at lower temperatures than their linear analogs, with practical deposition rates at temperatures as low as 450°C. At atmospheric pressure, isotetrasilane and neopentasilane maintain liquid behavior as high as 100°C, allowing on-substrate photolytic, electron-beam or laser-induced conversion to silicon-rich films.

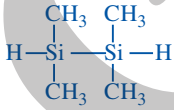
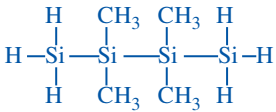
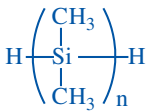
## Volatile Higher Silanes

Name	MW	bp °C/mm (mp)	D <sub>4</sub> <sup>20</sup>	n <sub>D</sub> <sup>20</sup>
SIT8709.6 TRISILANE H <sub>8</sub> Si <sub>3</sub>	92.32	52.9° (-117°)	0.7430	1.4978
 <p>Vapor pressure, 0°: 95.5 mm Bond dissociation energy (Si-Si): 313 kJ/mole Employed in low-temperature CVD of silicon and silicon alloys.<sup>1,2</sup> 1. Akhtar, M. et al. <i>MRS Proc.</i> <b>1986</b>, 70. 2. Todd, M. et al. U.S. Patent 6,821,825, 2004. HYDROLYTIC SENSITIVITY: 10: reacts extremely rapidly with moisture and oxygen - sealed system required [7783-26-8] TSCA-L HMIS: 3-4-3-X</p>				
SIT7880.0 n-TETRASILANE DECAHYDRIDOTETRASILANE H <sub>10</sub> Si <sub>4</sub>	122.42	106° (-85° to -95°)	0.825	
 <p>Contains 10-20% isotetrasilane Vapor pressure, 20°: ~25 mm Employed in low temperature CVD of amorphous silicon.<sup>1</sup> 1. Kanoh, H. et al. <i>Jpn. J. Appl. Phys.</i> <b>1993</b>, 32, 2613. HYDROLYTIC SENSITIVITY: 10: reacts extremely rapidly with moisture and oxygen - sealed system required [7783-29-1] HMIS: 3-4-3-X</p>				
SI16463.4 ISOTETRASILANE (TRISILYL)SILANE H <sub>10</sub> Si <sub>4</sub>	122.42	101° (-99°)	0.793	1.5449
 <p>ΔHvap: 32.5 kJ/mole Precursor for low temp. epitaxy of doped crystalline silicon.<sup>1</sup> Employed in low temperature CVD of amorphous silicon.<sup>2</sup> 1. Francis, T. et al. US Pat. Appl. 20120003819, 2012. 2. Kanoh, H. et al. <i>Jpn. J. Appl. Phys.</i> <b>1993</b>, 32, 2613. HYDROLYTIC SENSITIVITY: 10: reacts extremely rapidly with moisture and oxygen - sealed system required [13597-87-0] TSCA-L HMIS: 3-4-3-X</p>				
SIN6597.07 NEOPENTASILANE H <sub>12</sub> Si <sub>5</sub>	152.52	132-4°		
 <p>Vapor pressure, 25°: 15 mm Vapor pressure, 67°: 50 mm Employed in CVD epitaxy of silicon.<sup>1,2,3</sup> 1. Sturm, J. et al. <i>ECS Transactions</i>, <b>2008</b>, 16, 799. 2. Chung, K. et al. <i>Appl. Phys. Lett.</i> <b>2008</b>, 92, 113506. 3. Singh, K. et al. U.S. Patent 7,645,339, 2010. HYDROLYTIC SENSITIVITY: 10: reacts extremely rapidly with moisture and oxygen - sealed system required [15947-57-6] HMIS: 3-4-3-X</p>				

## Oligomethylsilanes and Polymethylsilanes

Oligomethylsilanes and polymethylsilanes undergo conversion to Carbosilanes at temperatures above 650°.



SIT7541.0 1,1,2,2-TETRAMETHYLDISILANE C <sub>4</sub> H <sub>14</sub> Si <sub>2</sub>	118.32	86-7 (-93)	0.720	1.429
 <p>Flashpoint: -26°C (-15°F) HYDROLYTIC SENSITIVITY: 3: reacts with aqueous base [814-98-2] TSCA HMIS: 2-4-1-X</p>				
SIT7580.0 2,2,3,3-TETRAMETHYLTETRASILANE, 95% C <sub>4</sub> H <sub>18</sub> Si <sub>4</sub>	178.53	125-135		
 <p>Candidate material for nanowires.<sup>1</sup> 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</p>				
PSS-1M01 poly(DIMETHYLSILANE) MW 1000-3000				
 <p>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.<sup>1</sup> 1. Scarlete, M.; et al; US Patent 7,396,563; 2008 (Label Licensed Gelest Product) 2. Yajima, S. et al. <i>J. Mater. Sci.</i> <b>1978</b>, 13, 2569. [30107-43-8] / [28883-63-8] TSCA</p>				