

## C~6~0SiH~2的结构和电子光谱的量子化学研究

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**摘要** 用INDO系列方法研究了C~6~0SiH~2的两种结构: 一是SiH~2加在两个六元环之间的键上形成C~2~v构型; 另一是SiH~2加在一个五元环和一个六元环之间的键上形成C~s构型。从总能量和LUMO-HOMO能级差看, C~6~0SiH~2的稳定结构应是C~2~v构型, 其中桥C(15)-C(30)的键长为0.1508nm, 键序为0.9369, 说明不开环, 形成类环丙烷结构。文中计算了两种构型的电子吸收光谱和NMR谱, 此类计算是基于对C~6~0SiH~2的等电子体C~6~0O和C~6~0CH~2的研究之上, 且后两者的研究结果与实验相一致。

**关键词** [量子化学](#) [构型](#) [微分重叠忽略近似](#) [碳13核磁共振](#) [电子光谱](#) [富勒烯](#) [其它基金](#) [C~6~0SiH~2](#)

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## Quantum chemical studies on the structures and electronic spectra of C~6~0SiH~2

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**Abstract** The INDO series of methods are used to study two kinds of structures of C~6~0SiH~2: one is C~2~v isomer with a bridging SiH~2 across the bond between two fused six-membered rings in C~6~0, and the other is C~s isomer with a bridging SiH~2 across the bond between a five- and a six-membered rings in C~6~0. From the view of total energy and LUMO- HOMO energy gap, the most stable structure of C~6~0SiH~2 is C~2~v geometry in which bridging C(15)-C(30) bond length and bond order are 0.1508nm and 0.9369, thus forming a cyclopropane-like structure. The electronic spectra and NMR spectra of both isomers have been calculated based on the similar studies about the isoelectronic molecules C~6~0O and C~6~0CH~2, the electronic spectra of which are in good agreement with the experimental results.

**Key words** [QUANTUM CHEMISTRY](#) [CONFIGURATION](#) [INTERMEDIATE NEGLECT OF DIFFERENTIAL OVERLAP APPROXIMATION \(INDO\)](#) [CARBON-13 NMR SPECTROMETRY](#) [ELECTRONIC SPECTROSCOPY](#) [FULLERENES](#)

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