

# Molecular Structure and UV Absorption Spectra of OH and NH<sub>2</sub> Derivatives of Dodecamethylcyclohexasilane: A Combined Experimental and Computational Study

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*Dedicated to Professor Hubert Schmidbaur on the occasion of his 75<sup>th</sup> birthday*

The monofunctionalized cyclohexasilanes XSi<sub>6</sub>Me<sub>11</sub> [X = -OH (**2**); -NH<sub>2</sub> (**3**)] are easily accessible from XSi<sub>6</sub>Me<sub>11</sub> and H<sub>2</sub>O/Et<sub>3</sub>N or NH<sub>3</sub>, respectively. The crystal structure of **2** as determined by single crystal X-ray crystallography exhibits the cyclohexasilane ring in chair conformation with the OH group in an unusual equatorial position due to intermolecular hydrogen bonding. Full geometry optimization (B3LYP/6-31+G\*) of the gas-phase structures of **2** and **3** affords six minima on the potential energy surface for *chair*, *twist* and *boat* conformers with the heterosubstituents either in axial or equatorial positions all being very close in energy. According to time-dependent DFT B3LYP/TZVP calculations contributions of several conformers to the observed solution UV absorption spectra of dodecamethylcyclohexasilane (**1**), **2** and **3** need to be considered in order to achieve satisfactory agreement of calculated and experimental data.

*Key words:* Cyclopolysilanes, Aminosilanes, Silanols, UV Absorption Spectra, Molecular Structure