

Molecular Structure and Conformational Preferences of 1-Chloro-1-silacyclohexane, $\text{CH}_2(\text{CH}_2\text{CH}_2)_2\text{SiH-Cl}$, as Studies by Gas-Phase Electron Diffraction and Quantum Chemistry

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Abstract—The molecular structure of axial and equatorial conformer of the 1-chloro-1-silacyclohexane molecule, $\text{CH}_2(\text{CH}_2\text{CH}_2)_2\text{SiH-Cl}$, as well as thermodynamic equilibrium between these species were investigated by means of gas-phase electron diffraction and quantum chemistry on the MP2(full)/AUG-cc-PVTZ level of theory. According to electron diffraction data, the compound exists in the gas-phase as a mixture of conformers possessing the *chair* conformation of the six-membered ring and Cs symmetry and differing in the axial and equatorial position of the Si–Cl bond at 352 K. NBO analysis revealed that axial conformer of 1-chloro-1-silacyclohexane molecule is an example of the stabilization of the form that is unfavorable from the point of view steric effects and effects of conjugations and that stabilization is achieved due to electrostatic interactions.

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