The Gas-phase Structure of the Hexasilsesquioxane $Si_6O_9(OSiMe_3)_6$

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Dedicated to Professor Hubert Schmidbaur on the occasion of his 75th birthday

The equilibrium molecular structure of the hexasilsesquioxane, $Si_6O_9(OSiMe_3)_6$, has been determined in the gas phase by electron diffraction. With OSi-containing substituents on the cage silicon atoms, this molecule closely resembles the moiety that if reproduced in a periodic manner would yield a zeolite-type structure. Semi-empirical molecular-dynamics (SE-MD) calculations were used to give amplitudes of vibration, vibrational distance corrections (differences between interatomic distances in the equilibrium structure and the vibrationally averaged distances that are given directly by the diffraction data) and anharmonic constants. A number of different SE-MD methods were tested, and their results are compared. The inclusion of *d*-type orbitals in the SE-MD method is crucial for obtaining accurate vibrational quantities for $Si_6O_9(OSiMe_3)_6$, with the PM6 and MNDO/D methods both giving acceptable values.

Key words: Silsesquioxane, Gas Electron Diffraction, Molecular Dynamics