Vibrational Spectra, DFT Calculations, and the Unusual Structure and Vibrations of 1,3-Disilacyclobutane

MOHAMED Z.M. RISHARD, RICHARD M. IRWIN, JAAN LAANE, Department of Chemistry, Texas A&M University, College Station, TX 77843-3255 — The infrared and Raman spectra of 1,3-disilacyclobutane and its 1,1,3,3-d$_4$ isotopomer have been reexamined and partially reassigned based on DFT and ab initio calculations. These calculations are in excellent agreement with the observed spectra in both frequency and intensity. They also demonstrate that this molecule has CH$_2$ wagging and twisting vibrations with frequencies below 1000 cm$^{-1}$, about 200 cm$^{-1}$ lower than expected. These unprecedented low values can be explained by the decreased slope in the potential energy curves for these vibrations as the sideways motions of the CH$_2$ groups result in attractive forces between the positively-charged hydrogens on the carbon atoms and the negatively charged hydrogens on the silicon atoms. The theoretical calculations also confirm the previous conclusions that the individual molecules in the vapor have C$_{2v}$ symmetry while in the solid the molecules become planar with D$_{2h}$ symmetry.

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