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Vibrational Spectra, DFT Calculations, and the Unusual Structure and Vibrations of 1,3-Disilacylobutane[1] 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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