THE TORSIONAL BANDS OF DISILANE

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The most direct determination of hindering potential for ethane-like molecules is through the observation of the torsional spectrum in the ground vibrational state (gs). Unfortunately, these bands are forbidden in the lowest order and are weakly allowed due to intensity borrowing from infrared active bands. While the torsional spectra of ethane and its deuterated isotopomers are relatively well characterized spectroscopically, this is not the case for their silicon analogs. In fact, very few experimental studies of the gs of disilane have been reported in the literature.

We have recorded the torsional spectra of disilane at a resolution of 0.007 cm⁻¹, pressure of 2.9 Kpa and a path length of 172.8 m using the Bruker IFS-120 HR Fourier ransform spectrumeter at the University of Oulu. The spectrum shows five distinct Q branches, one near 130 cm⁻¹ which is a blend of the four components of the torsional fundamental and the remaining four are due to the torsional hot band. A frequency analysis of the torsional bands together with the lower state combination differences from frequencies belonging to the vibrational bands ν_9 and $\nu_9 + \nu_4 - \nu_4$ was made to characterize the torsion-rotation Hamiltonian in the gs. The barrier height and shape were determined to be 404.950(86) and 1.942(68) cm⁻¹, respectively. Twelve other torsion-rotation parameters were required to fit over 800 transitions with the experimental accuracy. Comparison of synthesized and the experimental spectra gives $(\mu_{\parallel} - \mu_{\perp})/\mu_{\perp} \approx -4$ for the torsional dipole moments. This ratio compares well with -3.39 for ethane.