TUNNELING EFFECTS AND CONFORMATION DETERMINATION OF THE POLAR FORMS OF 1,3,5-TRISILAPENTANE

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1,3,5-trisilapentane has been synthesized and studied in the microwave region for the first time using CP-FTMW spectroscopy. The lowest calculated energy structure, $C_2$ is essentially non-polar with a calculated dipole of 0.063 D. However, slightly higher in energy at 145 cm$^{-1}$ and 196 cm$^{-1}$ are the calculated energies for the $C_1$ and $C_{2v}$ conformations, respectively. These structures have much larger dipoles calculated at 1.07 D for $C_1$ and 4.88 D for $C_{2v}$. Both of these structures have been confirmed using experiment and the details of such analysis will be discussed.

In addition to the structure determination, 1,3,5-trisilapentane has two terminal -SiH$_3$ groups. The calculated barrier to internal rotation of these groups are calculated to be 327.5 cm$^{-1}$ for $C_{2v}$, and 343.2 cm$^{-1}$ for $C_1$. This barrier is low enough to exhibit internal rotation splitting in the spectra and treatment of these motions in the analysis will be discussed.