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.