FT-MW AND PERMUTATION-INVERSION GROUP THEORETICAL INVESTIGATIONS OF THE MICROWAVE SPECTRUM OF $(CH_3)_3SnCl$

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The rotational spectrum of the C_{3v}-symmetric trimethyl-tin-chloride $(CH_3)_3SnCl$, a molecule with three methyl tops connected to a tin atom, has been studied using a pulsed supersonic jet COBRA Fourier-transform microwave spectrometer. The spectrum exhibits rather dense line patterns, which arise from the internal rotation of the three methyl tops, the quadrupole coupling interaction of the chlorine atom, and the large number of isotopic combinations of tin and chlorine.

To support a spectroscopic analysis we are exploring the high barrier group-theoretical tunneling-rotational formalism appropriate for the PI group G_{162}. We will discuss different tunneling pathways and compare the resulting splitting patterns for rotational levels with the FT-MW results. Stark-effect measurements can be used to distinguish between levels of the six different species of G_{162}, since the I_1, I_2, I_3 and E_2 levels will exhibit first-order Stark-splittings, while the A_1 and I_4 levels will have only a second-order Stark-effect. We suspect that levels of A_1 and A_2 species in G_{162} can be fitted to a rigid rotor Hamiltonian. At the time of writing the abstract, a theoretical proof that a rigid rotor fit is indeed possible for these G_{162} species is in progress.

We have also recorded the spectrum of $(CH_3)_2SiH - Sn(CH_3)_3$, a molecule with a Si-Sn atom backbone and three inequivalent internal rotor locations containing a total of five methyl tops. Our G_{162} results will be extended to the G_{486} group appropriate for this molecule.