ANALYSIS OF THE MICROWAVE SPECTRUM OF THE THREE-TOP MOLECULE TRIMETHOXYLMETHANE

L. H. COUDERT, *LISA, CNRS/Universités Paris Est et Paris Diderot, 61 Avenue du Général de Gaulle, 94010 Créteil, France*; G. FENG, AND W. CAMINATI, *Dipartimento di Chimica "G. Ciamician," Università di Bologna, Via F. Selmi, 40126 Bologna, Italy*.

Although many investigations about the spectrum of molecules displaying internal rotation of one or two methyl tops have been reported, there are much fewer results about the spectrum of molecules with three methyl tops.

In this paper, we will deal with the microwave spectrum of trimethoxylmethane, $HC(OCH_3)_3$, a molecule displaying three conformers of quite different symmetry which all exhibit internal rotation of their three methyl tops. In a first step, a theoretical approach dedicated to the calculation of the rotation-torsion energy levels of a molecule with three inequivalent tops was developed. The model is based on a DVR approach;[a] it accounts accurately for the rotation-torsion *Coriolis* couplings due to the torsion of each methyl top and leads to matrices which are smaller than those arising with the usual free internal rotation functions. The theoretical approach shows that internal rotation of the three tops leads to 27 tunneling sublevels, including 13 doubly degenerate ones. The statistical weights of the sublevels are 2^4, 2^5, and 2^6.

The microwave spectrum of trimethoxylmethane has been recorded from to 10 to 19 GHz with the molecular beam Fourier transform spectrometer of the University of Bologna. The spectra of the TMM1, TMM2, and TMM3 conformers with C_1, C_3, and C_s symmetry, respectively, have been observed. The theoretical model has been applied to the lowest lying TMM1 conformer since it is the only one with three inequivalent methyl tops. The parameters describing the rotational energy and the rotation-torsion *Coriolis* couplings were obtained from the geometry of the conformer and those corresponding to height of the barriers hindering the internal rotations were retrieved through *ab initio* calculations. Calculated tunneling patterns were compared to experimental ones. As far as the number of tunneling components is concerned, there is a qualitative agreement between experiment and theory. However, the present calculation seems to underestimate the various tunneling splittings and this probably due to the fact that the barrier heights obtained through *ab initio* calculations are too high.

[a] Light and Bačić, *J. Chem. Phys.* **87** (1987) 4008.