TORSION-VIBRATION INTERACTIONS IN THE CH_3-ROCKING AND OH-BENDING FUNDAMENTALS OF C-13 METHANOL

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A review is presented of our recent work on the study of the molecular interactions observed in the CH_3-rocking and OH-bending bands of C-13 methanol. The main aim was to find the interaction constants and to estimate the contributions due to the torsional motion. The modelling was done using a Marquardt algorithm and a second order perturbation theory approach.

The frequent Fermi mixing between states of the OH-bending and the first torsionally excited CH_3-rocking modes make it essential to study these bands jointly and not individually [a]. The pattern of torsion-rotation energies for the OH-bending mode is inverted relative to that of the ground state, implying that the usual Hamiltonian used successfully for the ground state cannot describe the excited state energy manifold.

With our new findings, we hope to contribute to better understanding of the torsion-vibration energy structure of the bending modes of methanol.

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[a] A. Predoi, R.M. Lees, G. Mellau, and J.W.C. Johns, 50th Symp. on Mol. Spectrosc., 1995, Paper RA12.