TWO-TOP TORSIONAL ASSIGNMENTS IN THE $A^1A_u(S_1) - X^1A_g(S_0)$ TRANSITION OF BIACETYL $CH_3C(=O)C(=O)CH_3$

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The laser-induced fluorescence excitation spectrum of the biacetyl $A^1A_u(S_1) - X^1A_g(S_0)$ transition in the region from 22 182 to 28 000 cm^{-1}shows a complicated absorption line spectrum, which is believed to arise from a long progression in the torsional vibrations of the two equivalent methyl tops in this molecule. In this talk we discuss three topics: (i) a numerical calculation of these energy levels using a kinetic and potential energy formalism and preliminary constants from the literature,[a] (ii) a qualitative description of the calculated energy level pattern using local mode ideas applied to the two equivalent methyl rotors as well as G_{36} permutation-inversion group symmetry species, and (iii) a comparison of the calculated energy levels with the low-resolution spectrum taken in the region from 0 to 500 cm^{-1}above the A-X band origin at IAMS in Taipei. The levels with one quantum of torsional excitation are best described by a normal mode formulation, but levels with more than one quantum of torsional excitation are better described by a local mode formulation. Good agreement with the low resolution spectrum is obtained, but full confirmation of the interpretation will require high resolution studies of some additional bands.

[a] M. L. Senent, D. C. Moule, Y. G. Smeyers, A. Toro-Labbé, and F. J. Peqalver, J. Mol. Spectrosc. **164**, 66-78 (1994).