HIGH RESOLUTION FOURIER TRANSFORM FAR-INFRARED SPECTROSCOPY OF CH_3OD: GLOBAL FIT OF TORSION-ROTATIONAL TRANSITIONS IN THE FIRST THREE TORSIONAL STATES

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The results of a new analysis of the high resolution Fourier transform far infrared (FIR) absorption spectrum of the torsion-rotational band of CH_3OD will be presented. Based on a recently determined set of molecular constants for CH_3OD[a] we have been able to assign 1126 assigned Fourier transform far-infrared (FIR) transitions that involve the second excited torsional levels with $v_t = 2$. A CH_3OD data set that contains 460 microwave (MW), millimeter wave (MMW) transitions and 3474 Fourier transform FIR transitions with $v_t \leq 2$ and $J \leq 21$ has been fit using a reduced torsion-rotational Hamiltonian obtained from the one-large-amplitude internal rotation model. The MW and MMW transitions have been fit with a root-mean-square (rms) deviation of 0.12 MHz while FIR transitions have a rms deviation of 0.00026 cm^{-1} using 61 parameters. These deviations are on the order of the experimental uncertainties, indicating that the MW, MMW and FIR spectral transitions have been fit to the desired accuracy and the reduced torsion-rotational Hamiltonian model is capable of accurately describing CH_3OD energy levels up through the second excited torsional level. The success of the fit demonstrates that the increased general asymmetry in CH_3OD, compared to CH_3OH, can be accounted for adequately by the reduced Hamiltonian model.

[a] Y. B. Duan and A. B. McCoy, *J. Mol. Spectrosc.*, **199**, 302-306 (2000).