

HIGH RESOLUTION FAR-INFRARED FOURIER TRANSFORM SPECTRUM OF THE CD₃OD ISOTOPOMER IN THE GROUND VIBRATIONAL STATE

INDRANATH MUKHOPADHYAY, DAVID S PERRY, *KNIGHT CHEMICAL LABORATORY, UNIVERSITY OF AKRON, AKRON, OH, 44325-3601*; YUN-BO DUAN, *DEPARTMENT OF PHYSICS AND ASTRONOMY, UNIVERSITY OF BRITISH COLUMBIA, VANCOUVER, BC, CANADA V6T 1Z1*; MICHAEL LOCK AND STEFAN KLEE, *PHYSIKALISCH-CHEMISCHES INSTITUT, JUSTUS-LIEBIG-UNIVERSITAET, 35392 GIESSEN, GERMANY*.

High resolution Fourier transform far infrared (FIR) spectra of CD₃OD isotopomer of methanol have been measured in the range 20-350 cm⁻¹ at a resolution of 0.0017 cm⁻¹ using a Bruker spectrometer. The spectra were recorded in various runs at pressure in the range of 0.2 - 0.8 mbar both at room temperature and at -60° C. The spectra show complicated splitting due to strong torsional-rotational interactions in the molecule. Detailed assignments have been achieved mainly for the torsional ground state levels. The assigned transition wavenumbers along with the previously known microwave (MW), and recently measured millimeter-wave (MMW) lines, were fit to an eighth order Hamiltonian with 62 varied parameters [1-4]. The data set consisted of a total of 3211 transitions with 2959 FIR transitions from the ground torsional state with rotational angular momentum K ranging from 0 to 18 and J ranging from 0 to 31, and 237 MW and MMW transitions. The fit converged with a standard deviation of 0.0007 cm⁻¹ for the FIR component of the data and the standard deviation for the MW and MMW transitions was 560 kHz. The standard deviation for the FIR lines is well compared with the estimated experimental accuracy of 0.0002 cm⁻¹ for clean unblended lines.

- [1] Y.B. Duan, H. M. Zhang, and K. Takagi, *J. Chem. Phys.* 104, 3914-3922 (1996).
- [2] Y.B. Duan, L. Wang, I. Mukhopadhyay, and K. Takagi, *J. Chem. Phys.* 110, 927-935 (1999).
- [3] Y.B. Duan, L. Wang, and K. Takagi, *J. Mol. Spectrosc.* 193, 418-433 (1999).
- [4] Li Wang, Y.B. Duan, I. Mukhopadhyay, D.S. Perry and K. Takagi, *Chemical Physics*, 263, 263-270 (2001).