NEW MEASUREMENTS AND ASSIGNMENTS IN THE $v_t = 0$, 1, 2 TORSIONAL STATES OF CD₃OH AND CH₃OD: FROM MILLIMETER-WAVE TO FIR SPECTRA

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We present^b the results of our new study of the torsion-rotation spectra of the two deuterated isotopologues of methanol: CD_3OH and CH_3OD . The new microwave measurements were carried out from the millimeter wave range (starting at 34 GHz) to the THz range (up to 1.1 THz) using spectrometers in Kharkiv and Köln. The new measurements in the FIR range were carried out in Braunschweig for CD_3OH from 20 to 900 cm⁻¹. In this work we significantly extend the rotational quantum number coverage for both isotopologues (from $J_{up} = 26$ [1] to $J_{up} = 55$ for CD_3OH and from $J_{up} = 21$ [2] to $J_{up} = 40$ for CH_3OD). The analysis is done using the rho axis method and the RAM36 program code. Our preliminary fits show that for both isotopologs the $v_t = 2$ torsional state is significantly affected by intervibrational interactions with non-torsional vibrational modes which propagate down through intertorsional interactions. At the same time, for CD_3OH we were able to get a fit within experimental error for $v_t = 0$, 1 states. For CH_3OD analysis is in progress now. In the talk the details of this new study will be discussed.

[1] A. Predoi-Cross, Li-Hong Xu, M.S. Walsh, R.M. Lees, M. Winnewisser, and H. Lichau J. Mol. Spectrosc. 188, 94–101 (1998). [2] Y.-B. Duan, I. Ozier, S. Tsunekawa, and K. Takagi, J. Mol. Spectrosc. 218 (2003) 95–107.

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