VIBRATION-TORSION-ROTATION INTERACTIONS IN METHYL MERCAPTAN CH_3SH: v_t=3,4 TORSIONAL, C–S STRETCHING, AND CSH BENDING VIBRATIONAL STATES.

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We present[a] the results of a joint analysis of the MIR, FIR, and microwave spectra of the ν_8 vibrational state (C-S stretch) near 710 cm^{-1}, the ν_7 vibrational state (CSH bend) near 802 cm^{-1}, and torsional stack of levels up to fourth excited torsinal state of methyl mercaptan CH_3SH. The analysis employs a new program which was recently developed for fitting several isolated small-amplitude fundamentals embedded in a pure torsional bath in molecules like methyl mercaptan, in which the frame has C_s symmetry and the methyl top has C_{3v} symmetry. This is the first attempt to perform an analysis of two small amplitude vibrations interacting with torsional bath of states and each other in a molecule with torsional large amplitude motion with this new program. The analysis gave us an opportunity to assign for the first time the pure rotational (microwave) transitions of the ν_7 vibrational state (CSH bend). In our analysis we used data available in the literature [1,2,3] as well as the results of the new measurements from Kharkiv, Köln, and Braunschweig. In the talk the details of this new study will be discussed.

[1] L.-H. Xu, R. M. Lees, G. T. Crabbe, et al., J. Chem. Phys. 137, 104313 (2012).

[2] R.M. Lees, Li-Hong Xu, B.E. Billinghurst, J. Mol. Spectrosc. 352, 30-38 (2016).

[3] R.M. Lees, Li-Hong Xu, B.E. Billinghurst, J. Mol. Spectrosc. 319, 45-56 (2018).

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