A SIMULTANEOUS FIT OF v_t = 0 AND 1 TORSION-WAGGING-ROTATIONAL LEVELS OF METHYLAMINE USING A HYBRID (TUNNELING AND NON-TUNNELING) HAMILTONIAN FORMALISM

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This work is in memory of Dr. Jon Hougen deceased on January 28th 2019 who dedicated his life to spectroscopy and worked on the present project very actively untill the end of December 2018. We will show the latest results obtained with Jon on the fit of more than 15000 rotational-torsional-wagging transitions in the MW and FIR of v_t = 0,1 of CH_3NH_2. We used the recently written hybrid program to fit rotational levels in molecules with one CH_3 internal-rotation large-amplitude motion, one NH_2 inversion large-amplitude motion, and symmetry described by the G_{12} PI group[a]. We will first present an overview of our present best least-squares fit. The data set contains slightly less than 2500 MW and 12754 FIR transitions, which are fit to a weighted standard deviation of 1.13 using 74 parameters. Most of the FIR transitions are taken from recent measurements of the v_t = 1-0 band centered near 265 cm^{-1}[b], but a number of lines were re-assigned or remeasured. The ground torsional state (taken mostly from Motyienko et al[c]) fit within measurement uncertainty but 75 older MW measurements in the v_t = 1 showed large observed-calculated residuals and were presently discarded from the fit. We believe that our fit, as well as the predictive abilities of the program, are now sufficiently good that we can begin a new measurement campaigns of v_t = 1 MW data and v_t = 2, 3 IR data. This new project will be discussed in the talk[d].

[a] J. T. Hougen and I. Kleiner, J. Phys. Chem. A, 2015, 119, 10664

[b] I. Gulaczyk, M. Kreglewski, V.-M. Horneman, J. Mol. Spectrosc. 2017,342, 25

[c] R.A. Motiyenko, V.V. Ilyushin, B.J. Drouin, S. Yu, L. Margulès, Astron.and Astrophys. 2014, 563, A1

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