APPLICATION OF THE HYBRID PROGRAM FOR FITTING MICROWAVE AND FAR-INFRARED SPECTRA OF METHYLAMINE

ISABELLE KLEINER, *Laboratoire Interuniversitaire des Systèmes Atmosphériques (LISA), CNRS et Universités Paris Est et Paris Diderot, Créteil, France*; JON T. HOUGEN, *Sensor Science Division, National Institute of Standards and Technology, Gaithersburg, MD, USA*.

Last year we presented a new hybrid-model fitting program for methylamine-like molecules, based on an effective Hamiltonian in which the ammonia-like inversion motion is treated using a tunneling formalism, while the internal-rotation motion is treated using an explicit kinetic energy operator and potential energy function. This new hybrid program was successfully applied to 2-methylmalonaldehyde, for which we refit the already published ground state $v_t = 0$ data. This fit[a], which was of almost the same quality as that obtained using an all-tunneling formalism, removed one of the major puzzles in the isotope-dependence of the internal-rotation tunneling parameters found in the all-tunneling fit. This year we are trying to illustrate a second advantage of the new hybrid formalism, which allows one to carry out global fits of data from two or more torsional states in methylamine-like molecules. We are, in fact, trying to simultaneously fit the $v_t = 0$ and $v_t = 1$ microwave and infrared date on methylamine itself. This data is also in the literature, but the all-tunneling Hamiltonians used could only fit each of the two torsional states separately. At the time of writing this abstract, we have preliminary fits of about 1200 methylamine transitions to 25 or 30 torsion-inversion-rotation parameters, but these hybrid-program fits are not yet at the same level as the all-tunneling-program fits in the literature. We hope to report significant further progress on this work in June.

[a] I. Kleiner and J. T. Hougen, J Phys Chem A. 119, 10664-76 (2015)