UPDATE FOR USERS OF THE METHANOL DATABASE: RECENT IMPROVEMENTS, REMAINING PROBLEMS, AND MORE COMPLICATED REGIONS

LI-HONG XU, *Department of Physics and Centre for Laser, Atomic, and Molecular Sciences, University of New Brunswick, Saint John, NB E2L 4L5, Canada*; J.C. PEARSON, B.J. DROUIN, *Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA USA 91109*; J.T. HOUGEN, *Optical Technology Division, National Institute of Standards and Technology, Gaitherburg, MD 20899-8441*.

Last year, we published a new global fit for normal methanol covering the first three torsional states (v_t = 0, 1 and 2) for J values up to 30[a]. The global fit of approximately 5600 frequency measurements and 19 000 Fourier transform far infrared (FTFIR) wavenumber measurements to 119 parameters reached the estimated experimental measurement accuracy for the FTFIR transitions, and about twice the estimated experimental measurement accuracy for the microwave, submillimeter-wave and terahertz transitions. Due to a number of complications in that data set, we designated the work as a ”living document” and encouraged measurement laboratories represented in the data set to assess carefully how their data were treated, and to partition (if appropriate) their measurements into an optimum set (for which they specify their highest measurement precision) and a less good set (for which they specify a reduced measurement precision). Using the new JPL spectrometer and additional improved measurements, we have recently revisited a large number of transitions. Poor line shapes due either to power saturation or blending were carefully treated with a multi-line peakfinding procedure and assessed with more realistic uncertainties. Assignments were also extended to higher K and J. Several perturbed systems have been identified with complicated networks of interactions. The current data set now contains nearly 9500 frequency measured transitions. While we believe that this represents a substantial improvement on the quantum number coverage of our previous paper[a], we are also aware of continuing problems in our data fitting. Above all, we are facing challenges moving into a more complicated region with networks of interactions coupling different torsional states.

[a] Li-Hong Xu, J. Fisher, R.M. Lees, H.Y. Shi, J.T. Hougen, J.C. Pearson, B.J. Drouin, G.A. Blake, R. Braakman, 2008, J. Mol. Spectrosc., 251, 305-313.