GLOBAL FIT FOR CH_3OD AND THE QUESTION OF INTERPRETATION OF GLOBAL FIT PARAMETERS FOR METHANOL AND ITS ISOTOPOMERS

MATTHEW S. WALSH, *Department of Physics, University of New Brunswick, Fredericton, N.B., Canada E3B 5A3*; LI-HONG XU, *Department of Physical Sciences, University of New Brunswick, Saint John, N.B., Canada E2L 4L5*; R. M. LEES, *Department of Physics, University of New Brunswick, Fredericton, N.B., Canada E3B 5A3*.

This talk presents our current progress on global data analysis for the ground vibrational states of methanol and its isotopomers. Global fits of all observed transitions to within assigned experimental accuracies over a certain quantum number range were reported previously for CH_3OH, $^{13}CH_3OH$, and CD_3OH. The fit for CH_3OD will be discussed in the present talk, and shows again that the one-dimensional torsional model can accurately describe methanol energy levels below and immediately above the torsional barrier (i.e. levels of $\nu_t = 0$ and 1). As we now have analyses for essentially all of the isotopic substitutions with the exception of the oxygen atom (global fitting for $CH_3{}^{18}OH$ will soon commence), we have sets of reliable fundamental molecular parameters obtained for different isotopomers in a logical and consistent way and can start to inter-compare these in order to explore the physical origins and mass dependence of the constants.

We will first report the results for the CH_3OD species of our global fit of reported microwave (MW), millimeter-wave (MMW), and Fourier transform far-infrared (FTFIR) spectroscopic data in the ground and first excited torsional states to experimental accuracy. We will then consider initial approaches to the question of interpreting the physical origins and mass dependence of the molecular parameters. For that, the molecular parameters are grouped into two classes depending on whether they are functionally dependent on the kinetic energy terms or the torsional barrier in the Hamiltonian.