INTENSITY MODELING OF METHANOL IN THE TORSIONAL MANIFOLD

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Methanol is a popular and very important molecule both in astrophysics and atmospheric science, for which reliable line intensities have long been desired by the user communities. Because of the low barrier to the large-amplitude torsional motion, the methanol spectrum is extremely rich and complicated, representing a significant challenge for global modeling. Not until recent years has the torsional manifold of v_t = 0, 1, and 2 levels been successfully globally modeled using a modified version of the BELGI code[a]. The resulting global fit parameters were then used to predict line lists in the THz region, employing both permanent dipole moments[b] and torsional dependence of the dipole moments from ab initio results[c] for the intensity calculations. However, recent direct intensity measurements based on Fourier transform spectra from JPL[d] and THz measurements from the Ohio State University[e] call for improvement of the intensity model. Thus, we have initiated enhanced modeling of the measured intensities in the torsional manifold using an extended set of dipole moment parameters, including permanent (μ_a, μ_b), torsionally dependent ($\mu_{a3n\gamma}$, $\mu_{b3n\gamma}$, $\mu_{c3n\gamma}$), and K and J dependent terms. While we are hopeful that this will improve our intensity predictive power, we also foresee challenges in the modeling for the A torsional species since a substantial body of the measured A doublet transitions exhibit either small asymmetry splittings for low K and high J states or are barely to completely unresolved as K increases. The present status of this work is that the existing database still needs some cleaning up to make it consistent with the new code. We hope to report our early intensity fit results at the conference.

[a] Xu et. al., *J. Mol. Spectrosc.* **251** (2008) p305.
[b] Xu & Lovas, *J. Phys. Chem. Ref. Data* **26** (1997) p17.
[c] Mekhtiev et. al., *J. Mol. Spectrosc.* **194** (1999) p171.
[d] Brauer et. al., *JQSRT* **113** (2012) p128.
[e] DeLucia, private communication.