THE COMPLETE, TEMPERATURE RESOLVED EXPERIMENTAL SPECTRUM OF METHANOL BETWEEN 560 AND 654 GHZ

SARAH M. FORTMAN, CHRISTOPHER F. NEESE, and FRANK C. DE LUCIA, *Department of Physics, The Ohio State University, 191 W. Woodruff Ave., Columbus, OH 43210*.

The complete spectrum of methanol (CH_3OH) in the 560.4–654.0 GHz spectral region has been characterized over a range of astrophysically significant temperatures, 248–397 K. Analysis of experimental spectra recorded with absolute intensity calibration over a slow temperature ramp provides a means for the simulation of the spectrum as a function of temperature without a complete quantum mechanical (QM) model.[a] These results include contributions from $v_t = 3$ and other higher states that are difficult to model via QM techniques. They also contain contributions from the ^{13}C isotopologue in natural abundance. These results are used to both provide catalogs in the usual line frequency, linestrength, and lower state energy format and in a frequency point-by-point format that is particularly well suited for the characterization of blended lines.

In contrast to our earlier work on the semi-rigid species ethyl cyanide and vinyl cyanide, significant intensity difference between these experimental values and those calculated by QM methods were found for some of the lines. Analysis of these differences points to the difficulty of the calculation of dipole matrix elements in the context of the internal rotation of the methanol molecule. We will compare our experimental intensities with the most recent QM model,[b] as well as an earlier QM model that includes the variation of the dipole moment function with the torsional angle.[c]

[a] S. M. Fortman, I. R. Medvedev, C. F. Neese, and F. C. De Lucia, *Astrophys. J.* **737**, 20/1-6 (2011).
[b] L.-H. Xu, *et al. J. Mol. Spectrosc.* **251**, 305-313 (2008).
[c] M. A. Mekhtiev, P. D. Godfrey, and J. T. Hougen, *J. Mol. Spectrosc.* **194**, 171-178 (1999).