GLOBAL MODELLING OF THE FIRST THREE TORSIONAL STATES OF METHANOL (v_t = 0, 1, 2, J_{max} = 30): CH_3OH AND $CH_3^{18}OH$

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Methanol is an important interstellar molecule that was first discovered in space in 1970. Because of the torsional motion, the methanol spectrum is extremely rich and complicated, representing a significant challenge for global modeling. Previous successful modeling efforts from the UNB group included the first two torsional states (v_t = 0 and 1) up to J_{max} = 20 for CH_3OH, CD_3OH, CD_3OD and $^{13}CH_3OH$. With new telescopes and space missions, there are increased demands for methanol data, in order to help astronomers remove interstellar methanol "grass" and thus uncover new molecular species in the interstellar medium.

We have quite recently managed to model the $CH_3^{18}OH$ Fourier-Transform far-infrared data and literature microwave and millimeter-wave measurements to their respective experimental uncertainties for the first three torsional states (v_t = 0, 1 and 2). The fitted data set includes about 500 microwave and millimeter-wave lines and 16762 Fourier-transform transitions covering the quantum number ranges J_{max} = 30, K_{max} = 15 and v_{tmax} = 2. With incorporation of about 80 adjustable parameters, the global fit achieved convergence with an overall weighted standard deviation of 1.12, essentially to within the assigned measurement uncertainties of ±50 kHz for almost all of the microwave and millimeter-wave lines and ±6 MHz (0.0002cm^{-1}) to ±15 MHz (0.0005cm^{-1}) for the Fourier transform far-infrared measurements.

The challenges to model the $CH_3^{16}OH$ data set are several times larger than those for the ^{18}O species, because we have several thousand newly measured THz transitions from the new JPL spectrometer. After carefully scrutinizing measurement uncertainties and assignments, there are good indications that a similar quality fit may be achieveable for $CH_3^{16}OH$ as was achieved for the ^{18}O species. We hope that information will be available for presentation in June on results from global fits of the normal species up to v_t = 2 and J_{max} = 30.