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## FIR Spectroscopy at the Canadian Light Source: High Torsional Levels of CD<sub>3</sub>OH and their Coupling to the Methyl Rocking Modes

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High-resolution Fourier transform far-infrared spectra of the CD<sub>3</sub>OH isotopologue of methanol, a well-known interstellar molecule, have been recorded at the Far-Infrared beamline of the Canadian Light Source synchrotron in Saskatoon, supplementing earlier Bomem FTIR spectra from the National Research Council in Ottawa at lower frequency. The primary motivation was to extend our mapping of high torsion-rotation levels of the ground vibrational state in order to explore more systematically the previously identified coupling with the in-plane CD<sub>3</sub>-rocking vibrational mode centred around 859 cm<sup>-1</sup>. The coupling involves principally the third excited torsional state, and  $\nu_t = 3$  sub-state assignments are now complete for all three torsional species up to rotational levels  $K = 9$  plus a further number up to  $K = 16$  with some torsional components still missing. Unexpectedly, we found that sub-bands involving the  $\nu_t = 3$  levels of torsional index  $\tau = 1$  at low  $K$  and  $\tau = 3$  at high  $K$  are significantly shifted from their predicted positions by up to 2.2 cm<sup>-1</sup>, accounting for earlier difficulty in locating these sub-bands in the spectrum. The pattern of the shifts indicates a perturbing state lying at approximately 895 cm<sup>-1</sup>, which must be the out-of-plane CD<sub>3</sub> rock. The gas-phase spectrum of this “dark state” has not yet been identified; hence new insights into its location and the interactions with the torsional modes are of interest. Another unexpected observation in the spectrum was a band with a relatively strong Q branch at around 775 cm<sup>-1</sup>. This cannot be a fundamental of CD<sub>3</sub>OH, yet its structure is clearly methanol-like. From earlier literature results, we can identify it as the OD-bending band of the fully deuterated CD<sub>3</sub>OD species. This has not previously been reported at high resolution so represents an extra bonus, albeit a significant complication in the spectrum, that we hope to be able to analyze in detail.

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