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CLS Synchrotron FIR Spectroscopy of High Torsional Levels of CD₃OH: The Tau of Methanol

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Structure from high torsional levels of the CD₃OH isotopologue of methanol has been analyzed in Fourier transform spectra recorded at the Far-Infrared beamline of the Canadian Light Source synchrotron in Saskatoon. Energy term values for *A* and *E* torsional species of the third excited torsional state, $v_t = 3$, are now almost complete up to rotational levels $K = 15$, and thirteen substates have so far been identified for $v_t = 4$. The spectra show interesting close groupings of strong high- v_t sub-bands related by Dennison's torsional symmetry index τ , rather than *A* and *E*, that can be understood in terms of a simple and universal free-rotor "spectral predictor" chart. The energy curves for the $v_t = 3$ and 4 ground-state torsional levels pass through several of the excited vibrational states, and a number of anharmonic and Coriolis interactions have been detected through perturbations to the spectra and appearance of forbidden sub-bands due to strong mixing and intensity borrowing.

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