MILLIMETER WAVE SPECTRUM OF CD_3OD FOR ASTRONOMICAL APPLICATION AND GLOBAL ANALYSIS TO EXPERIMENTAL PRECISION

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In order to assist the astronomers in searching for methanol D isotopomers in interstellar regions, we have performed systematic and precision millimeter wave measurements of CD_3OD in the frequency range from 62 to 226 GHz. Currently, more than 400 millimeter-wave (MMW) transitions have been newly measured with a typical measurement accuracy mostly 20–50 kHz. Our new measurements significantly extend previously published work where a combined analysis of FTFIR and MW lines was performed[a]. Our new measurements cover J_{max} = 20 and K_{max} = 7; many internally closed loops permitted to check the assignments and the experimental uncertainties. A global fit of previously reported[a,b] (14 MW lines from Ref. a and 22 MW lines from Ref. b) as well as our newly measured MMW spectroscopic data of CD_3OD has been completed to experimental accuracy in the quantum number ranges of ν_t = 0 and 1 (the ground and first excited torsional states below and straddling the torsional barrier) and J_{max} = 20.
The current global fit for CD_3OD will be included as part of our overall program of global analyses of data in the ground vibrational state for methanol and its isotopomers. This program is intended to obtain reliable molecular parameters in a consistent way for meaningful inter-comparison and to explore the physical origins and mass dependences of the constants.

[a] I. Mukhopadhyay, K. V. L. N. Sastry, and M. Winnewisser, Spectrochimica Acta **A54**, 1375-1379 (1998)
[b] R.M. Lees, J. Chem. Phys. **56**, 5887-5890 (1972)