THE ROTATION-TORSION SPECTRUM OF DOUBLY DEUTERATED METHANOL CD_2HOH

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Doubly deuterated methanol CD_2HOH is a non-rigid molecule displaying internal rotation of its asymmetrical CD_2H methyl group. Like the isotopic species of methanol with a symmetrical CH_3 or CD_3 group, it displays a strong rotation-torsion Coriolis coupling. Unlike these species, it also displays a dependence of its generalized inertia tensor on the angle of internal rotation. Its complicated rotation-torsion spectrum was investigated in the microwave,[a] submillimeter-wave,[b,c] terahertz,[b] and FIR[b,c] domains. Although more than 3000 transitions have been assigned so far, no global analysis, like the one performed for the similar species CH_2DOH,[d] has been carried out.

In this talk, new assignments in the terahertz and FIR spectra of CD_2HOH will be reported. Parallel and perpendicular transitions, characterized by a higher K-value than in our previous investigation,[b] could be identified up to $J = 35$ for the three lowest lying torsional states. Using the theoretical approach developed for CH_2DOH,[d] a global analysis of the available high-resolution data has been attempted in order to check the new assignments and to retrieve spectroscopic parameters such as those describing the hindering potential and the generalized inertia tensor.[e] So far, this global analysis has been restricted to transitions with $K \geq 4$ as rotation-torsion levels with $K < 4$ are affected by strong rotation-torsion couplings and cannot be properly modeled. Hopefully this issue will be dealt with by the time of the Symposium.

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[a] Liu & Quade, *J. Mol. Spectrosc.* **146** (1991) 252; Su, Liu, & Quade, *J. Mol. Spectrosc.* **149** (1991) 557; Quade, Liu, Mukhopadhyay, & Su, *J. Mol. Spectrosc.* **192** (1998) 378; Su & Quade, *J. Chem. Phys.* **90** (1989) 1396

[b] Ndao, Tchana, Coudert, Motiyenko, Margulès, Barros, Manceron, & Roy, *J. Mol. Spectrosc.* **326** (2015) 136

[c] Mukhopadhyay, *Inf. Phys. Tech.* **75** (2016) 139; *ibid.* **76** (2016) 116

[d] Coudert, Zemouli, Motiyenko, Margulès, & Klee, *J. Chem. Phys.* **140** (2014) 064307

[e] Liu & Quade, *J. Mol. Spectrosc.* **146** (1991) 238; El Hilali, Coudert, Konov, & Klee, *J. Chem. Phys.* **135** (2011) 194309