THE ROTATION-TORSION SPECTRUM[a] OF CH_2DOH

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Due to the asymmetry of the CH_2D group, the internal rotation problem in the partially deuterated species of methanol CH_2DOH is a complicated one as, unlike in the normal species CH_3OH, the inertia tensor depends on the angle of internal rotation. The CH_2DOH species also displays a dense far infrared torsional spectrum difficult to assign. Recently 38 torsional subbands of CH_2DOH have been identified,[b] but for most of them there is neither an assignment nor an analysis of their rotational structure.

In this paper an analysis of the rotation-torsion spectrum of CH_2DOH will be presented. The rotational structure of 23 torsional subbands have been assigned. These subbands are $\Delta v_t \geq 1$ perpendicular subbands with a value of v_t' up to 10[b] and values of K' and K'' ranging from 0 to 9. For all subbands, the Q-branch was assigned, for 3 subbands, the R- and P-branches could also be found. The results of the rotational analysis with an expansion in $J(J+1)$ of the new subbands and of already observed ones[c] will be presented. When available, microwave lines within the lower torsional level, recorded in this work or already measured,[d] were added to the data set.

A theoretical approach aimed at calculating the rotation-torsion energy levels has also been developed. It is based on an expansion in terms of rotation-torsion operators with C_s symmetry and accounts for the dependence of the inertia tensor on the angle of internal rotation. This approach will be used to carry out a preliminary global analyses of the wavenumbers and of the frequencies.

[a]This work is supported by the ANR-08-BLAN-0225 contract.

[b]Lauvergnat, Coudert, Klee, and Smirnov, *J. Mol. Spec.* **256** (2009) 204.

[c]Quade, Liu, Mukhopadhyay, and Su, *J. Mol. Spec.* **192** (1998) 378; and Mukhopadhyay, *J. Mol. Struct.* **695-696** (2004) 357.

[d]Liu and Quade, *J. Mol. Spec.* **146** (1991) 252; and Mukhopadhyay *et al., J. Chem. Phys.* **116** (2002) 3710.