THE TORSIONAL SPECTRUM OF MONO-DEUTERATED METHANOL CH_2DOH

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Contrary to the isotopic specie of methanol with a symmetrical CH_3 or CD_3 methyl group, in the mono-deuterated species CH_2DOH the hindering potential no longer displays 3-fold symmetry and all moments of inertia depend on the angle of internal rotation.[a] For this reason, this mono-deuterated species displays a fairly dense torsional spectrum difficult to compute and to assign.
In this paper an analysis of the torsional spectrum of mono-deuterated methanol is presented. More than 40 torsional subbands have been assigned in the 20 to 800 cm^{-1} region. The body of data available for CH_2DOH consists of these newly assigned subbands and of the already available ones.[b] The observed torsional subbands are characterized by $K \leq 10$ and $v_t \leq 10$. For 23 subbands, the rotational structure could be analyzed and this provides us with a mean to check their torsional assignment. The positions of the subband centers were analyzed with a theoretical approach accounting for the dependence of the inertia tensor on the angle of internal rotation. This allowed us to reproduce 58 experimental wavenumbers with an RMS value of 0.12 cm^{-1}. The spectroscopic parameters corresponding to the hindering potential and to the inertia tensor were also retrieved.

[a]Quade and Lin,*J. Chem. Phys.* **38** (1963) 54.
[b]Lauvergnat, Coudert, Klee, and Smirnov, *J. Mol. Spec.* **239** (2009) 204.