ANALYSIS OF THE ROTATION-TORSION SPECTRUM OF CH_2DOH WITHIN THE e_0, e_1, AND o_1 TORSIONAL LEVELS

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Since the first assignments of Quade and *coworkers,*[a] a more satisfactory understanding of the spectrum of CH_2DOH has now been achieved. Thanks to a multidimensional potential energy surface[b] and to a new theoretical approach accounting for the internal rotation of a partially deuterated methyl group,[c] 76 torsional subbands could be identified in the microwave and FIR domains. 8356 rotation and rotation-torsion transitions were also assigned for the three lowest lying torsional levels, e_0, e_1, and o_1, in the microwave and terahertz domains[d] and were analyzed with empirical models.

In this paper, a new approach aimed at accounting for the rotation-torsion energy levels of CH_2DOH will be presented. It is based on the exact expression of the generalized 4×4 inertia tensor of the molecule[e] and accounts for the C_s symmetry of the partially deuterated methyl group, for the dependence of the rotational constants on the angle of internal rotation, and for the rotation-torsion *Coriolis* coupling. This approach will be used to analyze high-resolution data involving the three lowest lying torsional levels, up to $k = 11$. In addition to the microwave data reported recently,[d] new transitions recorded in the terahertz domain at JPL will be analyzed. The results of the analysis will be presented in the paper and the parameters determined in the analysis will be discussed.

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[a] Quade and Suenram, *J. Chem. Phys.* **73** (1980) 1127; *and* Su and Quade, *J. Mol. Spec.* **134** (1989) 290.
[b] Lauvergnat, Coudert, Klee, and Smirnov, *J. Mol. Spec.* **256** (2009) 204.
[c] El Hilali, Coudert, Konov, and Klee, *J. Chem. Phys.* **135** (2011) 194309.
[d] Pearson, Yu, and Drouin, *J. Mol. Spec.* **280** (2012) 119.
[e] Quade and Lin, *J. Chem. Phys.* **38** (1963) 540.