FIRST ASSIGNMENT OF SEVERAL TORSIONAL BANDS OF CH_2DOH

M. SMIRNOV, L. H. COUDERT, *LISA, CNRS/Universités Paris 12 et 7, 61 Avenue du Général de Gaulle, 94010 Créteil, France*; S. BLASCO, D. LAUVERGNAT, *Laboratoire de Chimie Physique, Unité mixte du C.N.R.S. et de l'Université Paris-Sud, Bât. 490, Université Paris-Sud, 91405 Orsay Cedex, France*; and S. KLEE, *Physikalisch-Chemisches Institut, Justus-Liebig-Universität Gießen, 35392 Gießen, Germany*.

Although the torsional spectrum of the isotopic species of methanol with a symmetrical CH_3 or CD_3 methyl group has been studied in great details, almost no investigations have been carried out on partially deuterated species of methanol, like CH_2DOH or CD_2HOH, with an asymmetrical CH_2D or CD_2H methyl group. This stems from the fact that these partially deuterated species of methanol require a complicated theoretical treatment[a] in order to compute their rotation-torsion energy levels and that they display a dense far infrared torsional spectrum[b] difficult to assign.

With a view toward understanding this spectrum, a theoretical calculation of the rotation-torsion energy levels of CH_2DOH has been undertaken aided by *ab initio* calculations. This approach accounts for the complicated torsion-rotation interaction displayed by this molecule and for the fact that, due to the low symmetry of the CH_2D methyl group, the inertia tensor is strongly dependent on the torsional angle of rotation. In the theoretical approach, this angle is treated as an active coordinate[c] and matrix elements of the kinetic energy part of the Hamiltonian, involving the inertia tensor, are calculated using Gaussian quadrature.[d] Rotation-torsion energy levels are obtained using a potential energy function retrieved through *ab initio* calculations.

In the paper, a calculated rotation-torsion spectrum will be presented and compared to the experimental one, recorded in Gießen. It will be shown that this allows us to assign about 50 torsional bands.

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[a] Quade and Lin, *J. Chem. Phys.* **38,** 540 (1963).

[b] Mukhopadhyay, Perry, Butler, Herbst, and De Lucia, 57th International Symposium on Molecular Spectroscopy, paper **RH06** (2002) and Mukhopadhyay, Perry, Lock, and Klee, 57th International Symposium on Molecular Spectroscopy, paper **RH07** (2002).

[c] Lauvergnat and Nauts, *J. Chem. Phys.* **116,** 8560 (2002).

[d] Light and Bačić, *J. Chem. Phys.* **87,** 408 (1987).