THE ROTATIONAL-TORSIONAL MICROWAVE SPECTRUM OF MONO DEUTERATED ACETAMIDE

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Acetamide (CH_3CONH_2) is the simplest compound displaying a peptide linkage. It is also a non-rigid molecule displaying a hindered internal rotation of its methyl group characterized by a low barrier.[a] The mono deuterated acetamide molecule (CH_2DCONH_2) displays internal rotation just like the normal species. However, due to the fact that the CH_2D methyl group only has C_s symmetry, its rotation-torsion energy levels are expected to be quite different from those of the normal species. For instance, doubly degenerate E-type levels no longer exist in mono deuterated acetamide.

In this paper the rotation-torsion energy levels of mono deuterated acetamide will be investigated. A four dimensional Hamiltonian in which the overall rotation of the molecule and the large amplitude internal rotation motion are taken into account will be derived. The kinetic energy part of this Hamiltonian will be retrieved from the the generalized inertia tensor, accounting for the fact that the latter, unlike in a molecule with a symmetrical CH_3 group,[b] depends on the angle of internal rotation.[c] The potential energy part of this Hamiltonian will be obtained making reasonable assumptions and using the results of the previous investigations.[a] Using Gaussian Quadrature with weight and notes appropriate for periodic functions, the Hamiltonian matrix will be set up and diagonalized.

Work is still in progress and we hope to predict the frequencies of the rotation-torsion microwave transitions of mono deuterated acetamide with enough accuracy so as to be able to start the assignment of its microwave spectrum.

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[a] Kojima, Yano, Nakagawa, and Tsunekawa, *J. Mol. Spec.* **122,** 408 (1987); Suenram, Golubiatnikov, Leonov, Hougen, Ortigoso, Kleiner, and Fraser, *J. Mol. Spec.* **208,** 188 (2001); Yamaguchi, Hagiwara, Odashima, Takagi, and Tsunekawa, *J. Mol. Spec.* **215,** 144 (2002); and Ilyushin, Alekseev, Dyubko, Kleiner, and Hougen *J. Mol. Spec.* **227,** 115 (2004).

[b] Hougen, Kleiner, and Godefroid, *J. Mol. Spec.* **163,** 559 (1994).

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