THE MICROWAVE SPECTRUM OF THE MONO DEUTERATED SPECIES OF METHYL FORMATE $HCOOCH_2D$

L. H. COUDERT, *LISA, UMR 7583 CNRS/Universités Paris 12 et 7, 61 Avenue du Général de Gaulle, 94010 Créteil Cedex, France*; L. MARGULÈS, G. WLODARCZAK, and J. DEMAISON, *PhLAM, UMR 8523 CNRS et Université de Lille I, 59655 Villeneuve d'Ascq Cedex, France*.

The normal species of methyl formate ($HCOOCH_3$) is a non-rigid molecule displaying internal rotation of its methyl group. Its microwave spectrum has already been thoroughly studied[a] leading to an accurate value for the height of the barrier to internal rotation: 370.9 cm^{-1}. This corresponds to an A/E tunneling splitting of a few MHz for $v_t = 0$. Much less is known about the mono deuterated species $HCOOCH_2D$ with a partially deuterated methyl group.

In this paper, we present an investigation of the microwave spectrum of $HCOOCH_2D$. This mono deuterated species also undergoes internal rotation of its methyl group, however, due to the deuterium atom, the hindering potential no longer has three fold symmetry. Its still displays three minima, but the minimum corresponding to the C_S-symmetry configuration is roughly 10 cm^{-1} above the two other equivalent minima. The situation is quite similar to the one in the partially deuterated species of methanol CHD_2OH in which[b] for the ground torsional state three states arise: two close lying states of A' and A'' symmetry and an isolated A' symmetry state a few cm^{-1} above.

In the paper the model used to account for the rotation-torsion energy levels will be presented. It makes use of the so called water dimer formalism[c] which turns out to be quite convenient for this high-barrier problem. This model will be used to perform an analysis of the frequencies of the newly measured submillimeterwave transitions in Lille. We hope to obtain an accurate value of the tunneling splitting between the two lowest torsional states and to obtain an estimation of the energy of the isolated A' state.

---

[a] Oesterling, Albert, De Lucia, Sastry, and Herbst, *Astrophys. J.* **521,** 255 (1999); Karakawa, Oka, Odashima, Takagi, and Tsunekawa, *J. Mol. Spec.* **210,** 196 (2001); Ogata, Odashima, Takagi, and Tsunekawa, *J. Mol. Spec.* **225,** 14 (2004); and Carvajal, Willaert, Demaison, and Kleiner, *J. Mol. Spec.* **246,** 158 (2007)

[b] Fu Su and Quade, *J. Chem. Phys.* **90,** 1396 (1989)

[c] Hougen, *J. Mol. Spec.* **114,** 395 (1985) and Coudert and Hougen, *J. Mol. Spec.* **130,** 86 (1988)