INTERACTION OF THE HYPERFINE COUPLING AND THE INTERNAL ROTATION IN METHYL FORMATE[a]

M. TUDORIE, D. JEGOUSO, G. SEDES, T. R. HUET, *Laboratoire de Physique des Lasers, Atomes et Molécules (PhLAM) UMR 8523 CNRS, Bât. P5, Université des Sciences et Technologies de Lille 1, 59655 Villeneuve d'Ascq Cedex, France*; and L. H. COUDERT, *LISA, CNRS/Universités Paris 12 et 7, 61 Avenue du Général de Gaulle, 94010 Créteil, France*.

Experimental and theoretical analysis of the hyperfine structure of the non-rigid methyl formate ($HCOOCH_3$) molecule will be reported. 25 A-type rotation-torsion lines (nondegenerate levels) and 24 E-type rotation-torsion lines (doubly degenerate levels) were recorded in the 2–20 GHz range using the new Lille FTMW spectrometer, characterized by an instrumental resolution of 0.46 kHz. The high resolution of this spectrometer, limited by the Doppler widths, allowed us to resolve most hyperfine patterns. As in this molecule, the hyperfine coupling is due to four hydrogen atoms ($I = 1/2$), magnetic spin-spin and spin-rotation couplings[b] take place. A theoretical calculation of the hyperfine energy levels was carried out, taking into account these two couplings, and using an effective hyperfine Hamiltonian accounting for the averaging effects due to the large amplitude internal rotation.[c]

In the paper, comparisons between observed and calculated hyperfine patterns will be presented. As the present measurements indicate that hyperfine patterns arising for A-type rotation-torsion lines are systematically wider than those arising for E-type rotation-torsion lines, we hope to confirm this result theoretically.

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[b]Thaddeus, Krisher, and Loubser, *J. Chem. Phys.* **40** (1964) 257

[c]Coudert and Lopez, *J. Mol. Spectrosc.* **239** (2006) 135