PSEUDOROTATION IN TETRAHYDROFURAN: SUPPLEMENTARY DATA FROM THE FREE JET ROTATIONAL SPECTRUM OF THE d_8 SPECIES

WALTHER CAMINATI, ASSIMO MARIS, SONIA MELANDRI, *Dipartimento di Chimica "G. Ciamician" dell'Università, Via Selmi 2, I-40126 Bologna, Italy*; JUAN C. LÓPEZ, JOSÉ L. ALONSO, *Departamento de Química-Física y Química-Inorgánica, Facultad de Ciencias, Universidad de Valladolid, E-47005 Valladolid, Spain*; ROLF MEYER, *Sonnenbergstrasse 18, Zufikon, CH-5621, Switzerland*.

Tetrahydrofuran (THF) is a model molecule for the investigation of the hindered pseudorotation in saturated five-membered rings. Two recent papers, based on millimeter-wave investigations, reported the vibrational spacings among the four lowest pseudorotation states of normal THF, and obtained contrastant results on the potential energy function: four equivalent minima[a], or 2 sets of two equivalent minima[b]. In order to have more information on this problem, we planned to investigate the millimeter wave spectrum of the d_8 species. We obtained a vibrational spacing of *ca* 15 GHz between the two lowest pseudorotation states: a result which is not in agreement with both the above mentioned potential energy functions.

[a] R. Meyer, J. C. López, J. L. Alonso, S. Melandri, W. Caminati, and P. G. Favero, J. Chem. Phys. 1999, 111, 7871.
[b] D. G. Melnik, S. Gopalakrishnan, T. A. Miller, F. C. D. Lucia, J. Chem. Phys. 2003, 118, 3589.