MICROWAVE SPECTRUM OF 1-ADAMANTANOL $C_{10}H_{15}-OH$

OLIVIER PIRALI, MARIE-ALINE MARTIN-DRUMEL, L. H. COUDERT, *Institut des Sciences Moléculaires d'Orsay, Université Paris-Sud, Orsay, France*; MANUEL GOUBET, *Laboratoire PhLAM, Université de Lille 1, Villeneuve de Ascq, France*; SÉBASTIEN GRUET, MELANIE SCHNELL, *CoCoMol, Max-Planck-Institut für Struktur und Dynamik der Materie, Hamburg, Germany*.

1-Adamantanol is a heavy non-rigid molecule consisting of 1-adamantyl and hydroxyl groups. Internal rotation about the 1-adamantyl 3-fold axis of symmetry was evidenced some time ago[a] leading to an estimated value of the A-E splitting of 10 cm^{-1}. The microwave spectrum of 1-adamantanol was recorded later[b] in the 8 to 40 GHz region. Even though individual rotational lines could not be assigned, a value of 410 cm^{-1} was obtained for V_3 the height of the barrier hindering the internal rotation.

A cold molecular beam and a room temperature submillimeter wave spectra of 1-adamantanol were recorded in the 2–12 and 140–220 GHz ranges, respectively. 1404 parallel a-type transitions have been assigned in both spectra. A line frequency analysis of this new data set and of the perpendicular b-type clusters previously observed[b] was carried out using an IAM approach.[c]

In the paper, the new data and the results of the analysis will be presented. As 1-adamantanol is a nearly symmetric top molecule with an asymmetry parameter[b] κ close to -0.99, asymmetry splittings could not be resolved in the new spectra and $B - C$ was set to zero. Owing to the fact that the moment of inertia of 1-adamantyl about the axis of internal rotation is 400 times larger than that of the OH group about the same axis, ρ the parameter describing the rotational dependence of the torsional splitting is 0.9975. The implication for the energy level diagram of a value so close to 1 for this parameter will be discussed. Work is still in progress and it is hoped that it will be possible to identify torsional subbands in the crowded submillimeter wave spectrum recorded at room temperature.

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[a] Craven, *Spectrochim. Acta, 29A* (1973) 679

[b] Corbelli, Degli Esposti, Favero, and Lister, *J. Chem. Soc. Trans. 2,* **83** (1987) 2225

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