MICROWAVE SPECTROSCOPY OF 2-PENTANONE

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Methyl propyl ketone (MPK) or 2-Pentanone is known to be an alarm pheroromone released by the mandibular glands of the bees. It is a highly volatile compound. This molecule was studied by a combination of quantum chemical calculations and microwave spectroscopy in order to get informations about the lowest energy conformers and their structures.The rotational spectrum of 2-pentanone was measured using the molecular beam Fourier transform microwave spectrometer in Aachen operating between 2 and 26.5 GHz. Ab initio calculations determine 4 conformers but only two of them are observed in our jet-beam conditions.The lowest conformer has a C_1 structure and its spectrum shows internal rotation splittings arising from two methyl groups. The internal splittings of 305 transitions for this conformer were analyzed using the XIAM code [a]. It led to the determination of the values for the barrier heights hindering the internal rotation of two methyl groups of 239 cm^{-1} and 980 cm^{-1} respectively. The next energy conformer has a C_s structure and the analysis of the internal splittings of 134 transitions using the XIAM code and the BELGI code [b] led to the determination of internal rotation barrier height of 186 cm^{-1}. Comparisons of quantum chemistry and experimental results will be discussed.

[a] H. Hartwig, H. Dreizler, Z. Naturforsch. 51a, 923 (1996).

[b] J. T. Hougen, I. Kleiner and M. Godefroid, J. Mol. Spectrosc., 163, 559-586 (1994).