INTERNAL ROTATION OF THE ACETYL METHYL GROUP IN METHYL ALKYL KETONES: THE MICROWAVE SPECTRUM OF OCTAN-2-ONE

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Methyl *n*-alkyl ketones form a class of molecules with interesting internal dynamics in the gas-phase. They contain two methyl groups undergoing internal rotations. To explore the link between structure and barrier heights in ketones, investigations on a series of saturated methyl *n*-alkyl ketones were performed, i.e. pentan-2-one[a] hexan-2-one[b], heptan-2-one[c] and octan-2-one[d]. The molecular jet Fourier-transform microwave spectrum of octan-2-one was recorded between 2.0 and 40.0 GHz, revealing two conformers, one with C_1 and one with C_s symmetry. The barriers to internal rotation of the acetyl methyl group were determined to be 233.340(28) cm^{-1} and 185.3490(81) cm^{-1}, respectively, confirming the link between conformation and barrier height already established for other methyl alkyl ketones. The study combined high level *ab initio* calculations with experimentally dervived rotational and torsional parameters using the XIAM[e] and BELGI-C_1 (or BELGI-C_s)[f] codes. Results from the various fits will be presented. Finally comparisons to molecules in the literature and structural aspects of the conformers generally observed in methyl *n*-alkyl ketones will be reviewed.

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