WH07: INTERNAL ROTATION OF THE ACETYL METHYL GROUP IN METHYL ALKYL KETONES: THE MICROWAVE SPECTRUM OF OCTAN-2-ONE

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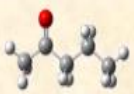
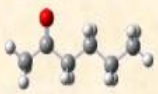
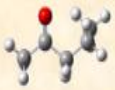
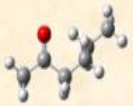
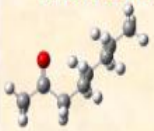
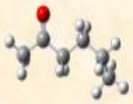
- **Accurate predictions of the barrier height of an acetyl methyl group in ketones are still difficult to make and no conclusive trends could be determined**
- **No previous systematic study of ketones by MW spectroscopy**
- **How does the barrier to internal rotation connect to the molecular structure?**

	Pentan-2-one	Hexan-2-one	Heptan-2-one	Octan-2-one
Status	2 conformers identified[1]	3 conformers identified[2]	2 conformers identified[3]	2 conformers identified[4]
C_s	 188.384 cm^{-1}	 186.920 cm^{-1}	 185.47 cm^{-1}	 185.144 cm^{-1}
C_1	 238.14 cm^{-1}	 233.591 cm^{-1}	 233.38 cm^{-1}	 233.20 cm^{-1}
C_1		 182.248 cm^{-1}		

Quantum Chemical calculations

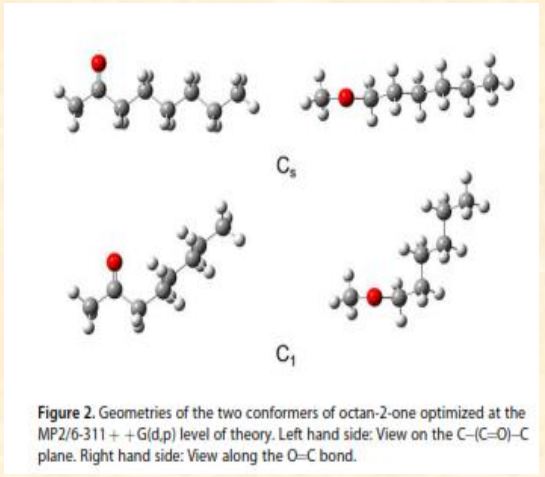


Figure 2. Geometries of the two conformers of octan-2-one optimized at the MP2/6-311++G(d,p) level of theory. Left hand side: View on the C–(C=O)–C plane. Right hand side: View along the O=C bond.

Molecular Jet Fourier Transform Microwave spectroscopy