PURE ROTATIONAL SPECTRUM OF ENOLIC ACETYLACETONE

WALTHER CAMINATI, *Dipartimento di Chimica "G. Ciamician" dell'Università, Via Selmi 2, I-40126 Bologna, Italy*; JENS-UWE GRABOW, *Lehrgebiet Physikalische Chemie A, Institut für Physikalische Chemie und Elektrochemie, Universtät Hannover, Callinstr. 3-3a, D-30167 Hannover, Germany*.

Acetylacetone (AcAc) comprises two tautomeric forms in dynamic equilibrium; together with malonaldheyde[a] it can be considered a prototype molecule for studying the keto-enolic tautomerization. In addition, both forms are complicated systems from a dynamical point of view. The keto-form contains two equivalent methyl rotors and two low energy skeletal torsion, which can originate several conformational species. As to the dynamics of the enolic form, besides the internal proton transfer, the two methyl groups - difficult to say if they are equivalent or not - are characterized by very low barriers to internal rotation. Finally, other tautomeric forms, involving a butadienic frame, are not ruled out. In spite of considerable efforts dedicated to the elucidation of the keto-enolic equilibrium of AcAc,[b] we think that an important information can be given through a rotationally resolved spectroscopic investigation. We will present here the first step in this direction, consisting in the assignment of the pure rotational spectrum of the enolic species of AcAc.

[a] From W. F. Rowe, R. W. Duerst, and E. B. Wilson, J. Am. Chem. Soc. 1976, 98, 402 to R. Meyer and T.-K. Ha, Mol. Phys. 2003, 101, 3263, and references therein.

[b] R. Srinivasa, J. S. Feenstra, S. T. Park, S. Xu, and A. H. Zewail, J. Am. Chem. Soc., 2004, 126, 2266, and references therein.