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Conformational Space of Hydroxyacetone Studied by Matrix-Isolation FTIR Spectroscopy and Quantum Chemical Methods[1] A. SHARMA, I. REVA, R. FAUSTO, University of Coimbra, Portugal — The matrix-isolation FTIR spectrum of hydroxyacetone monomers isolated in Ar matrix at 12K was studied. Interpretation of the experiment was aided by MP2 and DFT calculations at the 6-311++G(d,p) level. A 2D potential energy surface, in the space of OCCO and HOCC dihedral angles, revealed 4 non-equivalent minima, Cc, Tt, Tg and Ct. The energy barriers for Tg->Tt and Ct->Cc conversions (0.7 kJ/mol both) were found to be below the zero-point vibrational level associated with the isomerization coordinate of the higher energy form in each pair (Tg and Ct). Then, only Cc and Tt forms have physical meaning. In accord with the relative energy calculated for Tt (>11 kJ/mol), its estimated population in gas phase at 298K is only 1%. Indeed, only Cc form was experimentally detected. Its characterization included the full interpretation of the vibrational spectrum and the calculation of the NMR spectra of the compound in different media.

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