THE ROTO-TORSIONAL SPECTRUM OF GLYCOLALDEHYDE

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Glycolaldehyde is the first interstellar monosaccharide, that has been detected in emission toward the Galactic center source Sgr B2(N) . The molecule presents four conformers, three show C_s symmetry (I, II and IV) and one, III, represents a double minimum of C_1 symmetry. Two minima I and IV are cis forms whereas II and III are trans-forms. Cis-I is the most stable geometry that stabilizes by the formation of a hydrogen bond between the OH and the C=O carbonyl group. The relative energies of the remaining minima have been determine to be 1278.2 cm^{-1} (II), 1297.2 cm^{-1} (III) and 1865.2 cm^{-1} (IV) using MP4(SDTQ)/cc-pVQZ. The cis-trans transformation is hindered by a barrier of 1895 cm^{-1} and carries out a significative change of the rotational constants. The roto-torsional energies are obtained by solving the roto-torsional Hamiltonian depending on two coordinates. The potential energy surface is calculated from the MP4/cc-pVQZ energies of a grid of 74 conformations. The rotational constants and the distortion centrifugal constants are obtained in the zero point torsional energies of the cis and the trans forms.