

THE ROTO-TORSIONAL SPECTRUM OF GLYCOLALDEHYDE

M.L. SENENT, H.MASSO , *Departamento de Astrofísica Molecular e Infrarroja, Instituto de Estructura de la Materia, C.S.I.C., Madrid 28006, Spain* ; M.VILLA , *Departamento de Química, UAM-I Purísima y Michoacan, s/n , CP 09340, Mexico D.F* ; R. DOMINGUEZ-GOMEZ , *Departamento de Ingeniería Civil, Catedra de Química, E.U.I.T. Obras Publicas, Universidad Politecnica de Madrid.*

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 determined 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 significant 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.