

Highly correlated ab initio calculations of non-rigid molecules: Ethylene Glycol

R. Boussessi^{a,b}, M.L.Senent^a and N.Jäidane^b

^a Departamento De Química y Física Teóricas, Instituto de Estructura de la Materia, C.S.I.C., Serrano 121, Madrid 28006, Spain.

^b Laboratoire de Spectroscopie Atomique, Moléculaire et Applications-LSAMA, LR01ES09, Faculté des sciences de Tunis, Université de Tunis El Manar, 2092, Tunis, Tunisie.

Ethylene glycol (EG) represents a relevant organic molecule for astrochemical and atmosphere studies in gas phase. The most abundant isotopomer of ethylene glycol was detected in the interstellar medium [1]. Given its astrophysical importance, this discovery has been followed with great interest and a large number of ab initio studies have been carried out. Our main interest concerns internal rotation. Ethylene glycol is a non-rigid molecule since their ground state potential energy surface contains various minima. This molecule can exist in one of 27 conformers, and out of these 9 are unique. Very anharmonic torsional modes intertransform these minima which are separated by potential energy barriers. Tunneling effect splits their vibrational states.

We present highly correlated ab initio calculations performed to help the assignments of spectra measured at very low temperatures. Using level CCSD(T) of theory, we determine the structures of the conformers, the energy barriers and the torsional potential energy surfaces. To obtain spectroscopic parameters for 24 modes neglected in the 3D-model, a full-dimensional analysis has been performed for all the conformers. Anharmonic spectroscopic properties were determined using second order Möller-Plesset theory (MP2). Our theoretical results are in good agreement with experimental microwave spectroscopy [2].

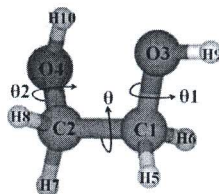


FIG. 1: The most stable geometry of ethylene glycol and the independent variables θ , θ_1 and θ_2 .

[1] J. M. Hollis, F. J. Lovas, P. R. Jewell, and L. H. Coudert, *Astrophys.J.* 571, L59 (2002).

[2] D. Christen, L. H. Coudert, J. A. Larsson, D. Cremer, *J. Mol.Spectrosc.*, 205, 185-196 (2001).