WEAK INTRAMOLECULAR INTERACTIONS EFFCTS ON THE STRUCTURE AND THE TORSIONAL SPECTRA OF ETHYLENE GLYCOL, AN ASTROPHYSICAL SPECIES

MARIA LUISA SENENT, RAHMA BOUSSESSI, *Inst. Estructura de la Materia, IEM-CSIC, Madrid, Spain*.

A variational procedure of reduced dimensionality based on CCSD(T)-F12 calculations is applied to understand the far infrared spectrum of Ethylene-Glycol. This molecule can be classified in the double molecular symmetry group G8 and displays nine stable conformers, gauche and trans. In the gauche region, the effect of the potential energy surface anisotropy due to the formation of intramolecular hydrogen bonds is relevant. For the primary conformer, the ground vibrational state rotational constants are computed at 6.3 MHz, 7.2 MHz and 3.5 MHz from the experimental parameters.

Ethylene glycol displays very low torsional energy levels whose classification is not straightforward. Given the anisotropy, tunneling splittings are significant and unpredictable. The ground vibrational state splits into 16 sublevels separated approximately 142 cm^{-1}. Transitions corresponding to the three internal rotation modes allow assign previous observed Q branches. Band patterns, calculated between 362.3 cm^{-1} and 375.2 cm^{-1}, between 504 cm^{-1} and 517 cm^{-1} and between 223.3 cm^{-1} and 224.1 cm^{-1}, that correspond to the tunnelling components of the v21 fundamental (ν_{21} = OH-torsional mode), are assigned to the prominent experimental Q branches.