CONFORMATIONAL STUDY OF BUTANE WITH THE MULTIPLE MINIMA HYPERSURFACES METHOD.

Lic. Cercis Morera Boado, Lic. Susana González Santana, Dra. Rachel Crespo Otero, Dr. Luis A. Montero Cabrera.
Laboratorio de Química Computacional y Teórica, Facultad de Química, Universidad de la Habana, La Habana, Cuba. cercis@fq.uh.cu.

The multiple Minima Hypersurfaces aproximation (MMH) allows, as one of its applications the study of the molecular environment. This procedure combines quantum mechanical methods for the calculations of energy with statistical thermodynamics to obtain thermodynamic quantities related to the molecular association process. In this work the methodology has been modified to obtain a better exploration of the multiple minima hypersurfaces. Therefore internal rotations have been taken into account. The partition function used until now in the calculation of thermodynamic properties only has the electronic contribution of each randomly generated configuration. The new modification consists in a complete description of the partition function, which is taking into account the translational and roto-vibrational states of the molecules. In the present work a conformational study of the central C-C dihedral angle of butane molecule using this methodology has been done. Optimization and frequency calculations at the HF/3-21G level were performed over 500 conformations randomly created. Finally and after similarity analysis were performed to all created structures, four final conformers were obtained: the eclipsed conformations i.e. the syn (s) and s^+ (120^0)), the anti or fully staggered conformer (a) and the gauche (g^+). Thermodynamical properties were obtained for each conformer following this methodology.