عنوان مقاله:

Conformational Analysis of 2-halo-1,3,2-dioxaphosphinanes: A Density Functional Theory (DFT) Investigation

محل انتشار:

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خلاصه مقاله:

This research aimed at evaluating the stability of the 2-halo-1,3,2-dioxaphosphinanes conformers at the LC-BLYP/aug-cc-pVTZ level of theory. The estimation of the total energy and the dipole moments of the axial and equatorial conformations were first done for the aforementioned molecules. Intermediate states of the transformations of the axial to equatorial conformer were determined. In the basis of the calculations, the axial conformer was found to be more stable than the equatorial conformer in these molecules. Transition states of these transformations were studied, as well. IN addition, the energetic and thermodynamics parameters of these transformations were investigated. Change of the P=O bond distances were illustrated with endo and exo-anomeric effects. The comparison of the P-O bond distances indicated the shorter bonds in the axial conformer compared to the equatorial conformer. These changes attributed to a dominant LP (2)O ® σ* (P-X) negative hyperconjugation interaction between a pair of non-bonded electrons on oxygen and the adjacent P-X bond in axial conformer. The partitioning of the total electronic energy E(tot) into Lewis E(L) and non-Lewis E(NL) parts was performed using the concept of the natural bond orbital (NBO) analysis. Then, the natural coulomb electrostatic (NCE) potential energies, total energies into Lewis components, and total steric exchange energies were estimated. Calculations revealed that axial conformer was more stable than the equatorial conformer in the studied molecules. In addition, the barrier energy values of the transformations of axial®boat®equatorial conformers enhanced with decreasing the electronegativity of halogen.

کلمات کلیدی:

Halo-1, 3, 2-dioxaphosphinanes, anomeric effect, conformers, natural bond orbital analysis-2