عنوان مقاله:

Study of Solvent Effect on the Thermodynamic Properties of 2-Halo tetrahydro-pyran and Analogs Containing F, Cl, Br Atoms Using NBO Analysis and Ab Initio

محل انتشار:

بیست و یکمین کنفرانس شیمی فیزیک انجمن شیمی ایران (سال: 1397)

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خلاصه مقاله:

In this study, the correlation between thermodynamic properties and Anomeric effects usinghybrid density functional theory and natural bond orbital analysis were examined. Earlier, Nori-Shargh et al. studied the effects of stereo-electronics on the structural properties of 5-methyl-5-aza-1,3-di-thiocyclohexane and its similar molecules containing three N, P, O atoms [1]. Also,Mousavi et al. studied the effects of exo-anomic and endo-anomic, electrostatic interactions andspatial suppression on the conformational behavior of 2-halo-1,3-dioxan (dithiane and diSelenan)compounds [2].Polarization effects that result from changes in the electron distribution can be obtained fromtransmission electron correlation effects have Anomeric. Furthermore, the correlation betweenthe stability of the central formulation of a saturated heterocyclic six member has electronegativehalogen atoms substituted on carbon 2 in the tropical formations in solvents with differentdielectric constant was examine. Anomeric effects depend on the nature and extent ofsubstitution decreases with increasing dielectric constant environment. Confirmation ofAnomeric with transmission electron orbitals of the linked and non-linked anti-graft emptyorbitals using the link changes have been approved. The structure of some of 2- Halo TetraHydropyran derivatives was evaluated by theory, By measuring the difference in Gibbs freeenergy (G), Anomeric effect (AE) and dipole moment, axial 2-Halo tetrahydropyran formstability than more equatrial form, and also by changing the halogen of fluorine to chlorine tobromine, stability is increase.

کلمات کلیدی:

Halvttrahydrvpyran, Density Functional, B3LYP/6-311+G**, Structural Parameters,Thermodynamic Parameters-2