عنوان مقاله:

DFT calculations on 2-N-ethylidyneaminiumoxane, 2-N-ethylidyneaminiumthiane, 2-N-ethylidyneaminiumselenane

محل انتشار:

بیستمین کنفرانس شیمی فیزیک ایران (IPCC20) (سال: 1396)

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خلاصه مقاله:

The structural parameters of 2-N-ethylidyneaminiumoxane (1), 2-N-ethylidyneaminiumthiane (2), 2-N-ethylidyneaminiumselenane (3) were calculated by means of the hybrid density functional (B3LYP and M06-2X) theory based methods with the 6-311+G** basis set on all atoms, natural bond orbital (NBO) interpretation and atoms in molecules theory (AIM). Levels of theory used in this work showed that the axial conformations of compounds 1–3 are more stable than their corresponding equatorial forms. The hyper-conjugative anomeric effect (HCAE) is in favor of the axial conformations of compounds 1–3. The axial conformations of compounds 1–3 are harder than their corresponding equatorial conformations but their conformational behaviors could not be interpreted with the Maximum Hardness Principle.

کلمات کلیدی:

DFT-B3LYP, Natural Bond Orbital, 2-N-ethylidyneaminiumoxane

لینک ثابت مقاله در پایگاه سیویلیکا: