عنوان مقاله:

(Investigation of Thermodynamic Properties and Hardness by DFT Calculations of S۲X۲ isomers (X: F, Cl, Br

محل انتشار:

نشریه متدهای شیمیایی, دوره 6, شماره 1 (سال: 1401)

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نویسنده:

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خلاصه مقاله:

Studying S۲X۲ compounds is of great importance due to their biochemical, atmospheric chemistry properties and protein structure, and because of the importance of this combination, it has received attention in the review. The compounds of disulfide S۲X۲ [X: F (۱), Cl (۲), Br (۳)] and their isomers were studied with long-range-corrected functional (LC-ωPBE, LC-BLYP) with basis set Aug/pVmZ (m: ۳). The analysis performed for the two forms of product (C۲) and reactant (CS) showed that conformation C۲ is a more stable thermodynamic parameter due to greater HOMO-LUMO gap and chemical hardness higher. The difference between Gibbs free energy (ΔG) and enthalpy (ΔH), and corrected electronic energy (ΔE۰) for compounds ۱ to ۳ was increasing. The global hardness (η) and electronegativity (χ), ionization energy (I), electron affinity energy (A), and electrophilicity index (ω) were investigated .in these compounds. There was a direct relationship between the difference in global hardness and Gibbs free energy

کلمات کلیدی:

Thermodynamic properties, Hardness, index electrophilicity, long-range corrected