

عنوان مقاله:

Tautomerism in Phenytoin: A Theoretical Study in Gas Phase

محل انتشار:

بیست و ششمین سمینار شیمی آلی ایران (سال: 1397)

تعداد صفحات اصل مقاله: 1

نویسندگان:

Hesam Sotoodeh - *Department of Chemistry, Computational Quantum Chemistry Laboratory, University of Sistan and Baluchestan, Zahedan, Iran*

Najmeh Mostafavi - *Department of Chemistry, Computational Quantum Chemistry Laboratory, University of Sistan and Baluchestan, Zahedan, Iran*

Ali Ebrahimi - *Department of Chemistry, Computational Quantum Chemistry Laboratory, University of Sistan and Baluchestan, Zahedan, Iran*

خلاصه مقاله:

Phenytoin (Pht) has anticonvulsive, antiepileptic, and antiarrhythmic effects in the human organism (see Fig. 1). Tautomerism can affect the chemical and biological activities of Pht. In the present work, the tautomerism in Pht has been investigated. The geometries of compounds were optimized at the B3LYP/6-31G (d,p) level of theory using the Gaussian 09 program [2]. As can be seen in Table 1, Pht with two H atoms on the N atoms of hydantoin ring is more stable than other tautomers with respect to the relative energy values (ΔE_g). The stability greatly decreases when two H atoms are located on the O atoms, (Pht4). The steric effects seem to be very effective in the stability of tautomers.

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