عنوان مقاله:

Molecular structure, electronic properties, NBO of Gabapentin with quantum chemical calculations

محل انتشار:

هجدهمین همایش شیمی فیزیک ایران (سال: 1394)

تعداد صفحات اصل مقاله: 4

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خلاصه مقاله:

Gabapentin [1-(amino methyl)cyclohexane acetic acid], a c-amino butyric1acid (GABA) molecule joined to a lipophilic cyclohexane ring, initially introduced in 1994 asan antiepileptic drug (AED), particularly for partial seizures, was soon found to be promisingin treating neuropathic pain associated with postherpetic neuralgia (PHN)[1-2], postpoliomyelitis neuropathy [3], and reflex sympathetic dystrophy [4]. As it is wellknown that amino acids exist as zwitterions as well as in the neutral form depending on theenvironment (solvent, pH, etc.) and that GP is a b,b-disubstituted c amino acid residue, weanalyzed molecular properties of both the zwitterionic and neutral form of GP. In this study,the ground state properties of both zwitterionic and neutral forms of GP have been calculatedemploying a DFT/B3LYP level of theory.

کلمات کلیدی: