

Theoretical Study of the Structural, Electronic Properties and GIAO ^1H -NMR, ^{13}C NMR and the Effect of Substitutes on the Succinimide

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الخلاصة

تم في هذه الورقة دراسة نظرية لخصائص وخصائص تزكيتية والاتقونية للسكينيميد المعموش (I, II, III). بـ 3DHF/B3LYP وـ 3DHF/G(3d,3p)، وـ 3DHF/B3LYP+G(3d,3p). تم حساب الطاقة الجلوبالية لجزيئات (I, II, III) على مستوى نظرية DFT/B3LYP، وـ 3DHF/B3LYP+G(3d,3p)، وـ 3DHF/G(3d,3p). تم تحديد الطاقة الجلوبالية لجزيئات (I, II, III) على مستوى نظرية DFT/B3LYP، وـ 3DHF/B3LYP+G(3d,3p)، وـ 3DHF/G(3d,3p). تم حساب الطاقة الجلوبالية لجزيئات (I, II, III) على مستوى نظرية DFT/B3LYP، وـ 3DHF/B3LYP+G(3d,3p)، وـ 3DHF/G(3d,3p). تم حساب الطاقة الجلوبالية لجزيئات (I, II, III) على مستوى نظرية DFT/B3LYP، وـ 3DHF/B3LYP+G(3d,3p)، وـ 3DHF/G(3d,3p). تم حساب الطاقة الجلوبالية لجزيئات (I, II, III) على مستوى نظرية DFT/B3LYP، وـ 3DHF/B3LYP+G(3d,3p)، وـ 3DHF/G(3d,3p).

Abstract

The calculations of Substituted Succinimide (I, II, III) were carried out by using quantum chemical calculations. The optimized structures of the Compounds(I, II, III) were obtained by the Density functional theory DFT/B3LYP level of theory using the basis set 6-311++G(3d,3p). The study shown, the optimized structures of compounds (I, II, III) have the global minimum energy. Also the dipole moment of compound (II) found to have high values compared with the Compounds (I, III). Global descriptors such as the MO energies of HOMO, LUMO levels, ΔE , electron affinity(A),ionization potential(I), hardness(η), electronegativity(X), electrophilicity(α) were determined and used to identify the differences in the stability and reactivity of compounds. In general calculated values lead to the conclusion that the stability of the compounds are I>II>III . On the other hand theoretical calculations for ^1H -NMR and ^{13}C NMR for compound (I) were carried out and compare with experimental data for compound (I) and predicate the ^1H -NMR and ^{13}C -NMR, Charge Density Distribution for compounds (II, III). As well as the calculations show the effect of substitution on the ring leads to change of the bond length and angles.

Key Words: Substituted Succinimide, ^1H NMR and ^{13}C NMR spectra, DFT/B3LYP(6-311++G(3d,3p)).

Introduction

Succinimide its derivatives are biologically and industrially useful compounds. Pharmaceutically they are used as analgesics, nephrotoxic, anticonvulsant, antiepileptic, fungicidal, ionic inhibitors of human leukocyte, etc. They are also used in industries as antifoaming agent, and biodegradable polymer, lubricating oil, lubricating tackifiers, emulsion explosives and also corrosion inhibitors. Some new succinimide and sulfonated derivatives were confirmed to have analgesic activity through abdominal constriction tests in mice. It has been reported that sulfonated derivatives of succinimide are more effective than aspirin and paracetamol. Consideration of these factors lead to undertake the detailed spectral investigation of succinimide [1-6]. Theoretical foundation for modern chemistry was laid more than 70 years ago at this time it becomes possible, in principle, to use this for