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BAZI BENZOTİYAZOL SCHİFF BAZLARI İÇEREN $C_{12}H_{18}ClN_3OS$ MOLEKÜLÜNÜN GEOMETRİK, ELEKTRONİK VE SPEKTROSKOPİK ÖZELLİKLERİNİN TEORİK OLARAK İNCELENMESİ

THE TEORETICAL İNVESTIGATION OF GEOMETRICAL, ELECTRONIC AND SPECTROSCOPIC PROPERTIES OF SOME SCHIFF BASES $C_{12}H_{18}CLN_3OS$ MOLECULE

Selim KAYA[1*], Salih Mustafa KARABIDAK[1],Uğur ÇEVİK[2]

[1]Gümüşhane Üniversitesi, Mühendislik ve Doğa Bilimleri Fakültesi, Gümüşhane

[2] Karadeniz Teknik üniversitesi, Fen Fakültesi, Trabzon

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ABSTRACT

In this study electronic and Spectroscopic property of some Schiff bases 2-amino-6-(*N*-isopropyl) amidino-2-methylbenzothiazole hydrochloride ($C_{12}H_{18}ClN_3OS$) molecule has been investigated by using Gauss-View and Gaussian 03W, Revision 2004 E01, Gaussian, Inc., Wallingford Ct. package program.

The molecular structures of C12H18ClN3OS molecule at ground state have been found by HF, B3LYP and BLYP methods. The stable states of the molecule have been found by using geometrical optimization and the bond length and bond angles were calculated by using 6-31G, 6-31G^{+}, 6-31G^{++} and 6-31G^{++}(d,p) basic sets. The infrared vibration frequencies and ^{1}H and ^{13}C NMR chemical shift values of these molecules were theoretically calculated. Obtained theoretical values were compared with experimental data.

The most probable full molecular orbital energy states (εHOMO, eV), the least probable empty orbital molecular orbital energy states ((εLUMO, eV) have been investigated using HF and B3LYP and BLYP methods with 6-31G, 6-31/G^{+}, 6-31G^{++} and 6-31G^{++}(d,p) basic sets at 12 different sets at stable state. The hardness (η) and electro negativity (χ) parameters were determined taking into account these energy values.

It was observed that theoretical and experimental values were in a good agreement within the uncertainty limits.

Key Words: $C_{12}H_{18}ClN_3OS$, B3LYP, BLYP, , HF, ^{1}H and ^{13}C, Structure Analysis, Vibration Labeling, IR Spectrums

***Sorumlu Yazar: selimkaya@gumushane.edu.tr**