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Molecular Structure and HOMO-LUMO Studies of β-N-(3-methoxy phenyl) methylene Thiosemicarbazone Schiff base by *Ab-initio* methods

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ABSTRACT

The molecular geometry, net atomic charge and atom electron densities, HOMO-LUMO energy, ionization energy and thermodynamic parameters of the β-N-(3-methoxy phenyl) methylene thiosemicarbazone, are examined theoretically at the ab-initio HF/STO-3G, HF/3-21G & HF/6-31G levels. The correlation coefficients for bond lengths obtained HF/STO-3G, HF/3-21G and HF/6-31G levels are 0.9391, 0.9927 and 0.8931 respectively. It is evident that HF/3-21G level gives the maximum correlation (CC=0.9927) for bond lengths. In the case of bond angles, correlation coefficients are 0.8460, 0.8472, and 0.7997 for HF/STO-3G, HF3-21G and HF/6-31G methods respectively. It is evident that HF/3-21G method gives most satisfactory correlation (CC=0.8472) for bond angles. Net atomic charge & atom electron density data reveal the coordination sites in β-N-(3-methoxy phenyl) methylene thiosemicarbazone when it undergoes complexation with transition metal ions. Consequently, performance of ab-initio method at different levels of calculations has been tested to find the best auxiliary tool for the designing of a novel biological active compound.

Keywords: β-N-(3-methoxy phenyl) methylene thiosemicarbazone, HF/STO-3G, HF/3-21G and HF/6-31G *ab-initio* levels, Correlation Coefficient (CC) and HOMO-LUMO energy.