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Theoretical Studies of Pyridine-2-carbaldehyde Thiosemicarbazone: A Biological Active Novel Compound

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ABSTRACT

The molecular geometry, net atomic charge and atom electron densities, HOMO-LUMO energy, Hardness-Softness and thermodynamic parameters of the Pyridine-2-carbaldehyde thiosemicarbazone a novel biological active compound, are examined theoretically at the ab-initio HF/STO-3G, HF/3-21G & HF/6-31G levels. The correlation coefficients are reported for bond lengths and bond angles at different levels of calculations. Net atomic charge and atom electron density data reveal the coordination sites in Pyridine-2-carbaldehyde 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 material.

Keywords: Pyridine-2-carbaldehyde thiosemicarbazone, HF/STO-3G, HF/3-21G & HF/6-31G *ab-initio* levels, Correlation Coefficient (CC).
