Available online at **www.joac.info**

ISSN: 2278-1862

Journal of Applicable Chemistry

2013, 2 (1):14-21

(International Peer Reviewed Journal)

Designing of a Novel Biological active compound: AB-Initio Studies of Di-2 Pyridyl KetoneThiosemicarbazone

Hari Singh Barhadiya[1]* and D. Kumar[2]

1. Govt. P.G. Lead (Excellence) College, Tikamgarh, India
2. SMS Govt. Model Science College, Gwalior, India.

Email: haribbb@yahoo.co.in

Received on 06th January and finalized on 16th January 2013

ABSTRACT

The molecular geometry, net atomic charge and atom electron densities, HOMO-LUMO energy, vibrational frequencies and thermodynamic parameters of the Di-2 pyridyl ketone thiosemicarbazone a novel biological active compound, are examined theoretically using ab-initio method at the HF/STO-3G, HF/3-21G and HF/6-31G levels. The correlation coefficients are reported for bond lengths, bond angles and vibrational frequencies at different levels of calculations. Net atomic charge and atom electron density data reveal the coordination sites in Di-2 pyridyl ketone 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: Di-2 pyridyl ketone thiosemicarbazone, HF/STO-3G, HF/3-21G & HF/6-31G a*b-initio* levels, Correlation Coefficient (CC).
