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# Natural Bonding Orbital and Frontier Molecular Orbital study of 2-Aminoethanethiol

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**Abstract :** 2-Aminoethanethiol is a drug used to treat cystinosis. In the current investigation, the molecular structure of the molecule was modeled using ab initio HF (Hartree-Fock) and DFT (Densiy functional theory) calculations at 6-311+G(d, p) levels. The theoretical vibrational frequencies and parameters like bond lengths and bond angles are calculated and compared with the experimental values. HOMMO-LUMO energies calculated. Stability of the molecule arising from hyperconjugative interactions, charge delocalization have been analyzed using natural bond orbital analysis (NBO). Natural bond orbital (NBO) analysis calculated with DFT/B3LYP/6-311+G(d,p) level shows that charge transfer takes place among the molecule. Besides, molecular electrostatic potential (MESP), HOMO and LUMO analysis, and several other thermodynamic properties were performed at both methods.
**Keywords**:2-Aminoethanethiol**,**HF; DFT; NBO;

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