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Synthesis and vibrational study of 2-amino, 3-chloro 1,4-naphthoquinone by DFT

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Abstract : 2-amino,3-chloro 1,4-naphthoquinone was synthesized. The Vibrational wave numbers of this compound have been calculated using Gaussian 09 software code, employing Density Functional Theory. The IR data is compared with experimental values. The predicted infrared intensities and Raman activities are reported. The calculated frequencies are in good agreement with the experimental values. The calculated geometrical parameters are also given. The study is extended to calculate the HOMO-LUMO energy gap, Ionization potential (I), Electron affinity (A), Global hardness (η), chemical potential (μ) and global electrophilicity (ω). The calculated HOMO-LUMO energies show the charge transfer occurs in the molecule. Optimized geometrical parameters of the title compound are in agreement with similar reported structures.

Keywords : 2-amino,3-chloro 1,4-naphthoquinone, IR, DFT, Energy gap.

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