STRUCTURAL PROPERTIES, THEORY FUNCTIONAL CALCULATIONS (DFT), NATURAL BOND ORBITAL AND ENERGIES FOR THE N-(3-CHLORO-1H-INDAZOL-5-YL)-4-METHOXYBENZENESULFONAMIDE

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ABSTRACT

B3LYP/3-21G calculation results indicated that some selected bond length and bond angles values for the C14H12ClN3O3S In this paper, the optimized geometries and frequencies of the stationary point and the minimum-energy paths of new compound with C14H12ClN3O3S chemical formula are calculated by using the DFT methods with 3-21G basis set. The detail group points of compound is C1

Keywords: Methoxybenzenesulfonamide, Electronic structure, DFT Calculations, Vibrational analysis, B3LYP level.