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 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.