Comparative Investigation of Reactivity, Stability, Structural and Thermodynamic Parameters of Heterocyclic Carboxylic Acids and Their Benzofused Derivatives: A DFT Foresight

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ABSTRACT

Currently, the use of computational chemistry is an effective tool in the development of perceptions regarding the reactivity and stability of organic-inorganic compounds. It has been greatly strengthened by the development of Density Functional Theory (DFT). The present study deals with the computational study of biologically efficacious heterocyclic carboxylic acids, thiophene-2-carboxylic acid (T2CA) and furan-2-carboxylic acid (F2CA) along with their benzofused derivatives benzothiophene-2-carboxylic acid (BT2CA) and benzofuran-2-carboxylic acid (BF2CA). DFT/B3LYP (6-31G*) functional was employed to calculate various reactivity descriptors, thermodynamic properties, structural parameters, Mulliken charge distribution at various atomic sites and optimized molecular structures of the studied heterocyclic carboxylic acids. This study will give an insight into the effect of structural variations on stability, reactivity, structural attributes and Mulliken atomic charge distribution in the heterocycles.

Keywords: DFT; thiophene-2-carboxylic acid; furan-2-carboxylic acid; benzofused derivatives.

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