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Theorical Studies on the Structural Properties of 2,3-Bis(Furan-2-Yl)Pyrazino[2,3-F][1,10]Phenanthroline Derivaties

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Abstract : This paper reports on the geometrical parameters optimized of the stationary point for the 2,3-Bis(furan-2-yl)pyrazino[2,3-f][1,10]phenanthroline. The calculations are performed using density functional theory (DFT) method at the B3LYP/LanL2DZ level. We determined bond lengths and bond angles values for the compound and calculate the amount of bond hybridization according to the natural bond orbital theory (NBO) too. The energy of frontier orbital (HOMO and LUMO) are computed. In addition, calculated data are accurately compared with the experimental result. This comparison show that the our theoretical data are in reasonable agreement with the experimental values.

Keywords : 2,3-Bis(furan-2-yl)pyrazino[2,3-f][1,10]phenanthroline, density functional theory, theorical calculations, LanL2DZ level, B3LYP level
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