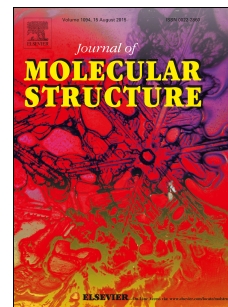


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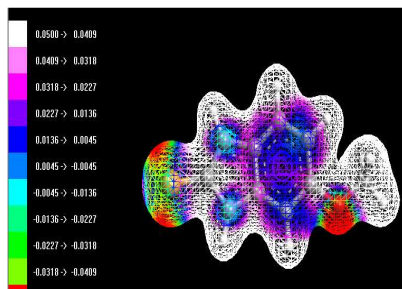
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Graphical abstract

The harmonic vibrational frequencies, infrared intensities, Raman activities, bond lengths, bond angles were calculated for 5-Methoxy-1H-benzo[d]imidazole-2(3H)-thione molecule by DFT method using 6-311++ G(d, p) basis set. The calculated geometrical parameters and frequencies were in good agreement with experimental values. ^1H , ^{13}C NMR, UV-Vis spectral analyses of the title molecule were conducted by experimental and Density Functional Theory (DFT). The HOMO, LUMO energies, Fukui function and NBO analysis were also worked out.



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