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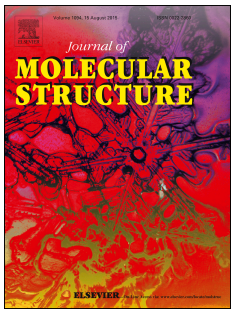

Investigations based on non-covalent interactions in 1-(4-chloromethylbenzoyl)-3-(4, 6-di-substituted pyrimidine-2-yl)thioureas: Synthesis, characterizations and quantum chemical calculations

Yu Zhang, Jie Huang, Lei Qiao, Xing Zhang, Weili Cao, Zimei Ding, Xiaojing Hang, Baofu Qin, Jirong Song

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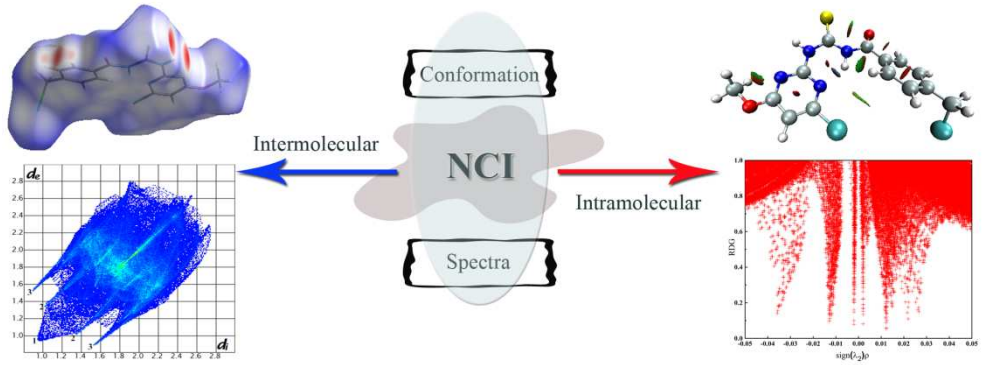
Investigations based on non-covalent interactions in 1-(4-chloromethylbenzoyl)-3-(4, 6-di-substituted pyrimidine-2-yl)thioureas: synthesis, characterization and quantum chemical calculations

Yu Zhang, Jie Huang, Lei Qiao, Xing Zhang, Weili Cao, Zimei Ding, Xiaojing Hang, Baofu Qin, Jirong Song

Two novel 1-(4-chloromethylbenzoyl)-3-(4, 6-di-substituted pyrimidine-2-yl)thiourea derivatives were synthesized and characterized using spectra and single crystal X-ray studies. The non-covalent interactions (NCI) of the two compounds were investigated by reduced density gradient (RDG) function and Hirshfeld surfaces. Wherein, the RDG function was discussed for understanding intramolecular interactions, and the Hirshfeld surfaces was used to investigate intermolecular interactions of pyrimidine thiourea derivatives. Moreover, the spectra and structural conformation analysis were completed, and the results showed that hydrogen bonds are the main influencing factor in molecules.



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