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Synthesis, single crystal X-ray, Hirshfeld surface analysis and characterization of novel 4-(2,4-dichlorophenyl)-*N*-(2,6-dichlorophenyl)-1,3-thiazol-2-amine

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Abstract:

In the present study, the spectroscopic characterization of a novel thiazole scaffold was studied. The formation of title compound 4-(2,4-dichlorophenyl)-*N*-(2,6-dichlorophenyl)-1,3-thiazol-2-amine(**6**) was evidenced through the changes in FTIR, ¹H-NMR, LCMS Data. The X-ray diffraction studies revealed that compound (**6**) crystallized in monoclinic crystal system with $P2_1/c$ Space group with $Z=4$. The percentage of intermolecular contacts contributing to the Hirshfeld surface in thiazole crystal was resolved by Hirshfeld surface analyses with 2D fingerprint plots.

Key words: 1, 3-thiazole, crystal structure, Hirshfeld surfaces, 2,6-dichloroaminophenyl.

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1. Introduction:

Thiazole is a stable heterocyclic compound and has Bird IA value of 79. It possesses both electron donating and an electron accepting groups (C=N). Diverse modification of the thiazole ring at various positions led to synthesis of variety of novel compounds with wide spectrum of pharmacological activities such as antibacterial[1], antifungal[2]. anti-inflammatory [3], antihypertensive,

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