Poster Presentation

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Crystal structure of 1-(3-chlorophenyl)-3-(5-chlorothiophen-2-yl)-5-phenyl-4,5-dihydro-1H-pyrazole

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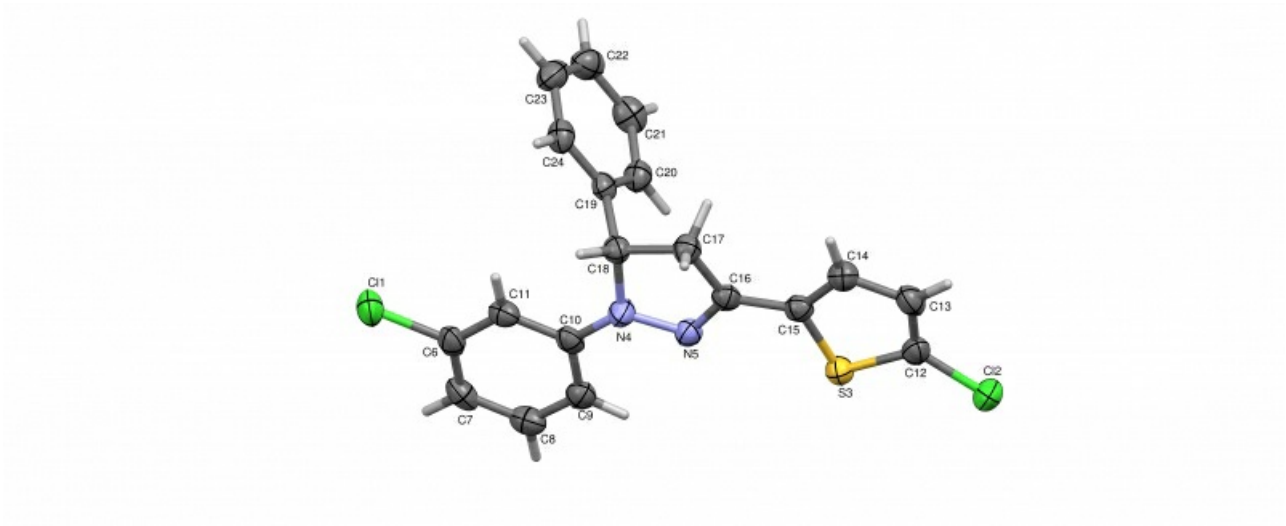
The five membered heterocyclic compounds pyrazolines were found as the core structure in a large variety of organic compounds. Pyrazoles have been the recent target of numerous methodologies, due to their prevalence as scaffolds in synthesis of bioactive pharmaceutical and agrochemicals. Development of novel and accessible procedure for the transformation of a simple molecule in to bioactive pyrazole and its derivative is a worthwhile contribution in organic synthesis. In view of this, we synthesized pyrozole derivative, 1-(3-chlorophenyl)-3-(5-chlorothiophen-2-yl)-5-phenyl-4,5-dihydro-1H-pyrazole. The title compound is characterized by ^{1}H-NMR, FT-IR, TGA, UV-Visible Spectra and finally the structure was confirmed by X-ray diffraction studies. The title compound is crystallized in the monoclinic crystal system with the space group P21/c with unit cell parameters are a = 18.560(3) Å, b = 5.563(9) Å, c = 17.194(3) Å, β = 108.557(4)°, V = 1683.0(5)Å^3 and Z = 4. The crystal structure exhibits C – H . . .π and C – Cl…..π interactions.

[1]. Ajay Kumar, K. Govindaraju, M. (2015) Int. J. ChemTech Res. 8(1), 313-322.
[2]. Spek, A. L. PLATON, (1990) Acta. Crystallogr.A46, C34-C34.
[3]. Prabhuswamy, M. Lokanath, N. K. (2016) Chem. Dat. Coll. 3, 26-35.



Keywords: Spectral characterization, X - ray diffraction, π - interactions.