

CRYSTAL STRUCTURE OF 4-(4-CHLORO-PHENYL)-5-PHENYL ISOXAZOLE

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The isoxazoles are a group of heterocycles, generated by the insertion of nitrogen atom at 2nd -position of the furan. Isoxazoles are unique in their chemical behaviour like aromatic system particularly at the N-O bond.

The structural studies of isoxazoles and their derivatives have attracted considerable attention with their multifaceted applications as monoamine oxidase inhibitors used in psychotherapy, anti-inflammatory and anti-tumor agents. Some of them are industrial important as semiconductors and corrosion inhibitors in fuels and lubricants. In agriculture applications, herbicidal activity has been identified for some isoxazoles. The X-ray structure determination of some isoxazoles have been undertaken to investigate the effect of the substituents on the conformation of the heterocyclic ring with respective to their orientations.

Crystal data: C₃₀ H₂₀ Cl₂ N₂ O₂, Mr = 511.38. Colourless transparent crystals, triclinic, P- $\bar{1}$, a = 6.554(7), b = 25.966(17), c = 7.472(10) Å, α = 90.07(9), β = 106.17(9) γ = 89.78(7)°, V = 1221(2) Å³, ρ_c = 1.391 Mg/m³, Z = 2, (MoK α) = 0.71073Å, & F(000) = 528. Final R = 0.0554 and Rw = 0.1691 for 2845 with $[I \geq 2 \sigma(I)]$.

Isoxazole ring is planar. At the point of linkage of substituents to the isoxazole ring enlargement in bond lengths, bond angles and torsion of the substituted moieties with respect to isoxazole ring are observed. In the crystal, molecules are packed with van der Waals interactions.

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