Crystal and Molecular Structure of 2-(2-chlorophenoxy)-3,4-dihydro-3-(3'-chloro 4'-flurophenyl)-2H-[1,3,2] benzoxazaphosphorin 2-oxide

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Orgnophosphorus compounds are widespread in nature and they have unique multifaceted applications as insecticides, anticancer agents and lubricating oil additives and polymer stabilizers. The title compound has both antimicrobial and pesticidal activity, which promoted us to undertake crystal structure determination to know the influence of the substituents on the conformation of the heterocyclic ring. In the title compound C19 H13 Cl2F N O3 P, the six-membered phosphorinring exhibits a sofa conformation with phosphoryl O atom occupying an equatorial and chlorophenoxy group in an axial position. The P=O distance is 1.446(2) and the average length of the three P --- O bonds is 1.574(2). The chlorophenoxy ring is oriented at an angle of 36.2(1)degrees; to the heterocyclic phosphorin ring. Crystals obtained from 2-propanal by slow evaporation are monoclinic, space group P2 1n with cell parameters a=6.731(2), b=18.652(3) and c=15.045(3); beta=101.9(3) degrees, V=1847.7(7)3. The structure was solved by direct methods and refined by full matrix least squares using SHELXL-97 to final values of R = 0.0598 and Rw = 0.1642.