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Key indicators

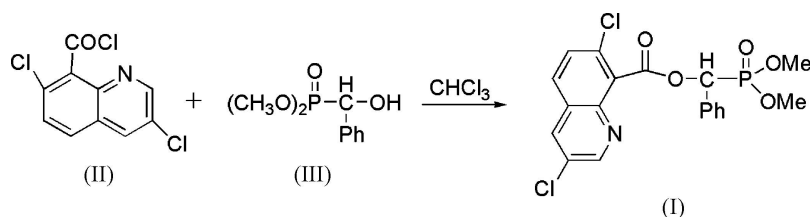
Single-crystal X-ray study
 $T = 292$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.052
 wR factor = 0.131
Data-to-parameter ratio = 15.4For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Dimethyl [(3,7-dichloroquinolin-8-ylcarbonyl-
oxy)(phenyl)methyl]phosphonate

In the title compound, $\text{C}_{19}\text{H}_{16}\text{Cl}_2\text{NO}_5\text{P}$, the P atom is in a distorted tetrahedral configuration, and the carboxylate plane is oriented almost perpendicular to the quinoline ring system. In the crystal structure, molecules are linked by intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds and weak $\pi-\pi$ stacking interactions.

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Comment

Quinoline as a versatile heterocyclic compound has attracted increasing attention because of its high germicidal and pharmacological properties (Adnan *et al.*, 2003). Organic phosphorus compounds play an important role in pesticide science as part of their significant biological properties. The title compound, (I), has been prepared as a part our work on the synthesis of aryl/heterocyclic 1-oxyalkylphosphonic acid derivatives with good biological activities (He *et al.*, 2005), and we report its structure here (Fig. 1 and Table 1).



The bond lengths observed in the quinoline system of (I) do not differ significantly from those in free quinoline (Shetty & Fernando, 1970). The bond angles about atom P1 suggest that it adopts a distorted tetrahedral configuration, as observed previously in a similar compound (Liang & He, 2006). The C10/O1/O2 carboxylate plane is oriented almost perpendicular to the quinoline ring system [dihedral angle $85.6(3)^\circ$].

In the crystal structure, intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen-bonding interactions stabilize the structure (Table 2). In addition, short intermolecular distances between the centroids of the C1-C4/C9/N1 ring ($Cg1$) and the C4-C9 ring ($Cg2$) of an adjacent molecule indicate the existence of $\pi-\pi$ stacking interactions (Janiak, 2000) [$Cg1\cdots Cg2^i = 3.7923(15)$ Å; symmetry code: (i) $1-x, 1-y, 1-z$]. These form inversion-related dimers, which are further stabilized by weak $\text{C}-\text{H}\cdots\text{O}$ intermolecular hydrogen bonds.

Experimental

3,7-Dichloroquinoline-8-carbonyl chloride, (II) (Coutrot, 1986), and *O,O*-dimethyl 1-hydroxy-phenylmethylphosphonate, (III) (Boullet & Foucaud, 1982), were prepared according to literature procedures.

Compound (II) (0.022 mol) in chloroform (10 ml) was added dropwise at 275–277 K to a stirred solution of (III) (0.02 mol) and triethylamine (0.028 mol) in chloroform (25 ml) (He *et al.*, 2005). The mixture was stirred at 283–288 K for 3–5 h, washed with 0.5% hydrochloric acid solution, followed by sodium hydrogen carbonate, dried and evaporated. The residue was purified by chromatography (silica gel with 20% acetone in petroleum ether). Recrystallization from dichloromethane over a period of one week gave colorless block-shaped crystals of (I).

Crystal data

$C_{19}H_{16}Cl_2NO_5P$	$Z = 8$
$M_r = 440.20$	$D_x = 1.460 \text{ Mg m}^{-3}$
Orthorhombic, <i>Pbca</i>	Mo $K\alpha$ radiation
$a = 11.4895 (8) \text{ \AA}$	$\mu = 0.44 \text{ mm}^{-1}$
$b = 15.7158 (11) \text{ \AA}$	$T = 292 (2) \text{ K}$
$c = 22.1792 (16) \text{ \AA}$	Block, colorless
$V = 4004.8 (5) \text{ \AA}^3$	$0.20 \times 0.20 \times 0.20 \text{ mm}$

Data collection

Bruker SMART APEX CCD area-detector diffractometer	3924 independent reflections
φ and ω scans	2968 reflections with $I > 2\sigma(I)$
Absorption correction: none	$R_{\text{int}} = 0.047$
20069 measured reflections	$\theta_{\text{max}} = 26.0^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0582P)^2 + 1.2945P]$
$R[F^2 > 2\sigma(F^2)] = 0.052$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.131$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.06$	$\Delta\rho_{\text{max}} = 0.33 \text{ e \AA}^{-3}$
3924 reflections	$\Delta\rho_{\text{min}} = -0.23 \text{ e \AA}^{-3}$
255 parameters	
H-atom parameters constrained	

Table 1

Selected geometric parameters (\AA , $^\circ$).

C1–C2	1.402 (4)	C7–C8	1.377 (4)
C4–C9	1.407 (4)	C8–C9	1.407 (3)
C4–C5	1.415 (4)		
O3–P1–O4	116.02 (12)	O3–P1–C11	114.28 (12)
O3–P1–O5	115.63 (11)	O4–P1–C11	101.98 (12)
O4–P1–O5	103.30 (11)	O5–P1–C11	103.86 (12)

Table 2

Hydrogen-bond geometry (\AA , $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C1–H1 \cdots O3 ⁱ	0.93	2.52	3.309 (3)	143
C14–H14 \cdots O3 ⁱⁱ	0.93	2.43	3.302 (4)	157
C3–H3 \cdots O3 ⁱⁱⁱ	0.93	2.65	3.512 (2)	155

Symmetry codes: (i) $x - \frac{1}{2}, -y + \frac{1}{2}, -z + 1$; (ii) $x - \frac{1}{2}, y, -z + \frac{1}{2}$; (iii) $-x + 1, -y + 1, -z + 1$.

All H atoms were refined using a riding model, with C–H = 0.93 \AA and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for aromatic, C–H = 0.98 \AA and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for CH, and C–H = 0.96 \AA and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for CH_3 H atoms.

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve

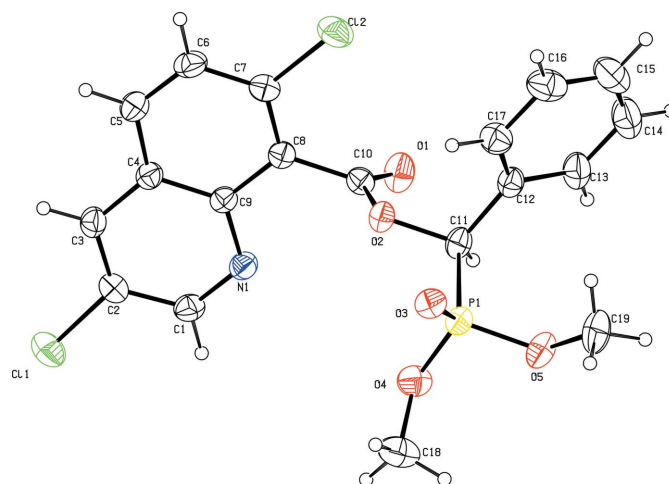


Figure 1
View of (I), showing the atom-labelling scheme, with 50% probability displacement ellipsoids.

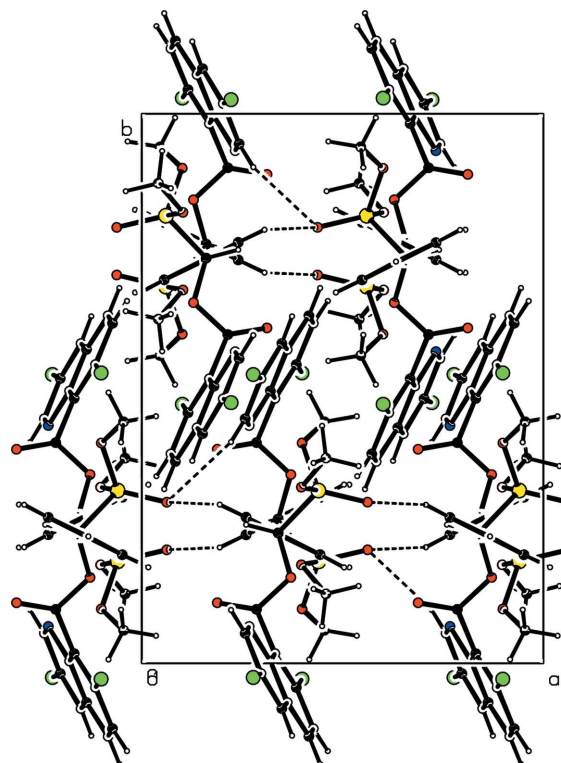


Figure 2

The crystal structure of (I), showing the C–H \cdots O hydrogen bonds (dashed lines).

structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1997); software used to prepare material for publication: SHELXTL.

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