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# 2-{(2-Chlorophenyl)[(2,4-dichlorophenoxy)acetoxy]methyl}-5,5-dimethyl-1,3,2-dioxaphosphinan-2-one

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In the title compound, $C_{20}H_{20}Cl_3O_6P$, all bond lengths and angles are normal. The P atom is in a distorted tetrahedral configuration. The crystal packing is stabilized by weak intermolecular C—H···O hydrogen bonds and $\pi$–$\pi$ interactions.

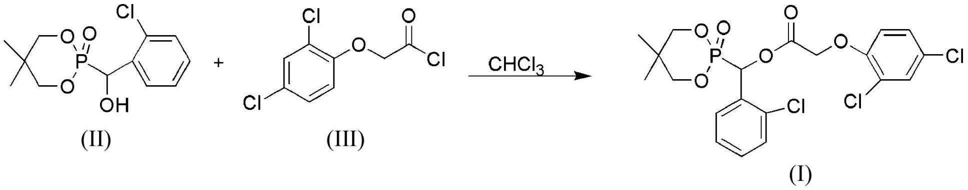
**Key indicators**

Single-crystal X-ray study
*T* = 298 K
Mean $\sigma$(C–C) = 0.004 Å
*R* factor = 0.051
*wR* factor = 0.140
Data-to-parameter ratio = 18.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

## Comment

Some hydroxyphosphonates and their derivatives have shown good biological and pharmaceutical activities (Chen *et al.*, 1995). The title compound, (I), has been prepared as part of our work directed towards the synthesis of oxyalkylphosphonic acid derivatives exhibiting biological activities (He *et al.*, 2005).



Bond distances and angles in (I) are as expected, and the dioxaphosphorinane ring adopts a chair conformation (Fig. 1). The bond angles around atom P1 (Table 1) suggest that its environment adopts a distorted tetrahedral configuration, as observed previously in a similar compound (Zuo & He, 2006). The torsion angles C16—O4—C13—C14, O4—C13—C14—O6 and C14—O6—C15—C20 are −174.38 (18), 163.60 (19) and −0.90 (4)°, respectively.

Weak intermolecular C—H···O hydrogen bonds (Table 2) and $\pi$–$\pi$ interactions [$Cg\cdots Cg^{iv}$ = 3.7939 (18) Å, where *Cg* is the centroid of the C15–C20 ring; symmetry code: (i) $1 - x$, $1 - y$, $1 - z$] stabilize the crystal packing.

## Experimental

2-[Hydroxy(2-chlorophenyl)methyl]-5,5-dimethyl-1,3,2-dioxaphosphinan-2-one, (II) (Sudha *et al.*, 1997), and (2,4-dichlorophenoxy)acetyl chloride, (III) (Klaassens & Schoot, 1956), were prepared according to the 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 (15 ml). The mixture was stirred at 283–288 K for 2–3 h, washed with 0.5% hydrochloric acid solution followed by saturated sodium hydrogen carbonate solution, dried and evaporated. Recrystallization from dichloromethane gave colourless blocks of (I).

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## *Crystal data*

$C_{20}H_{20}Cl_3O_6P$
$M_r = 493.68$
Triclinic, $P\overline{1}$
$a = 8.8627$ (7) Å
$b = 10.4972$ (9) Å
$c = 13.3624$ (11) Å
$\alpha = 79.8340$ (10)°
$\beta = 83.7070$ (10)°
$\gamma = 69.9360$ (10)°
$V = 1147.75$ (16) Å$^3$
$Z = 2$
$D_x = 1.428$ Mg m$^{-3}$
Mo $K\alpha$ radiation
$\mu = 0.50$ mm$^{-1}$
$T = 298$ (2) K
Block, colourless
0.30 × 0.20 × 0.20 mm

## *Data collection*

Bruker SMART APEX CCD area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: none
12883 measured reflections
4976 independent reflections
4228 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.024$
$\theta_{\rm max} = 27.0°$

## *Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.140$
$S = 1.05$
4976 reflections
273 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0677P)^2 + 0.5055P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = 0.001$
$\Delta\rho_{\rm max} = 0.60$ e Å$^{-3}$
$\Delta\rho_{\rm min} = -0.52$ e Å$^{-3}$

**Table 1**
Selected bond angles (°).

| | | | |
|---|---|---|---|
| O3—P1—O2 | 113.75 (10) | O3—P1—C6 | 112.63 (10) |
| O3—P1—O1 | 112.20 (10) | O2—P1—C6 | 105.53 (9) |
| O2—P1—O1 | 106.84 (8) | O1—P1—C6 | 105.26 (9) |

**Table 2**
Hydrogen-bond geometry (Å, °).

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C17—H17···O2$^{\rm i}$ | 0.93 | 2.60 | 3.463 (3) | 155 |
| C20—H20···O3$^{\rm ii}$ | 0.93 | 2.50 | 3.417 (3) | 167 |
| C14—H14*A*···O3$^{\rm ii}$ | 0.97 | 2.43 | 3.311 (3) | 150 |
| C8—H8···O4$^{\rm ii}$ | 0.93 | 2.60 | 3.402 (3) | 145 |
| C5—H5*A*···O5$^{\rm iii}$ | 0.96 | 2.59 | 3.488 (4) | 156 |

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

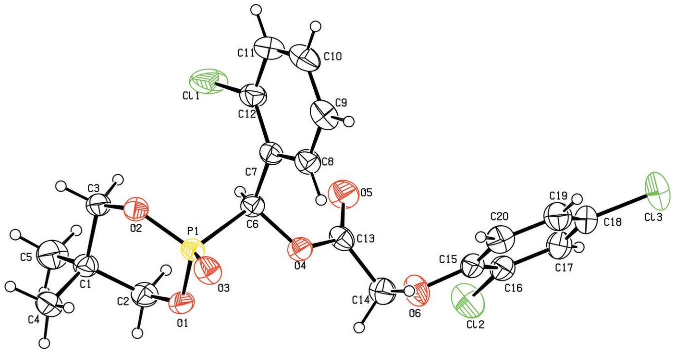

**Figure 1**
The molecular structure of (I), showing the atom-labelling scheme and with 50% probability displacement ellipsoids.

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.93–0.98 Å, and with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(aromatic C, CH, CH$_2$) or 1.5$U_{\rm eq}$(methyl C).

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