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## Key indicators

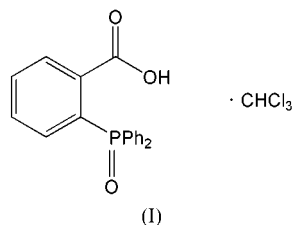
Single-crystal X-ray study  
 $T = 153\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.006\text{ \AA}$   
 $R$  factor = 0.051  
 $wR$  factor = 0.126  
Data-to-parameter ratio = 14.8For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.2-(Diphenylphosphinoyl)benzoic acid  
chloroform solvate

In the solid state, 2-(diphenylphosphinoyl)benzoic acid,  $(\text{C}_6\text{H}_4\text{CO}_2\text{H})\text{P}(\text{O})\text{PPh}_2$ , forms a hydrogen-bonded dimer between the phosphoryl O atom and the O—H group of the benzoic acid moiety, while the O atom of the carbonyl group is involved in an intramolecular contact with the P atom. The molecule exists as the chloroform solvate,  $\text{C}_{19}\text{H}_{15}\text{O}_3\text{P}\cdot\text{CHCl}_3$ .

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## Comment

Commercially available 2-(diphenylphosphino)benzoic acid has been recently used as a building block for the synthesis of more complex ligands (Wroblewski *et al.*, 1984; Correia *et al.*, 2001; Trost *et al.*, 2002; Burger *et al.*, 2003). The phosphine oxide derivative,  $(\text{C}_6\text{H}_4\text{CO}_2\text{H})\text{P}(\text{O})\text{PPh}_2$ , was obtained in moderate yield by addition of hydrogen peroxide to a methanol solution containing 2-(diphenylphosphino)benzoic acid (Chandrasekaran *et al.*, 2001). Unlike Chandrasekaran *et al.*, who obtained crystals of the acid by slow evaporation of a  $\text{CH}_2\text{Cl}_2$ –heptane solution, we obtained crystals of the title solvate, (I), suitable for X-ray analysis, by slow evaporation of a chloroform solution. The presence of chloroform molecules in the crystal generates a completely different mode of packing.



Compound (I) crystallizes with two independent molecules of the acid per asymmetric unit. Fig. 1 shows only one of these independent molecules, and significant bond lengths and angles are given in Table 1. The P atom is in a pseudo-trigonal bipyramidal geometry, the phosphoryl O atom being involved in an intramolecular contact with the O atom of the carbonyl group of the acid function, with  $\text{P1}\cdots\text{O4} = 2.973(3)\text{ \AA}$  and  $\text{P2}\cdots\text{O6} = 2.966(3)\text{ \AA}$ . A similar axial coordination has been observed for  $(\text{C}_6\text{H}_4\text{CO}_2\text{H})\text{P}(\text{O})\text{PPh}_2$  (Chandrasekaran *et al.*, 2001) and the related compounds  $[\text{Et}_2\text{NH}_2][(\text{C}_6\text{H}_4\text{CO}_2)\text{P}(\text{O})\text{PPh}_2]$  (Chandrasekaran *et al.*, 2002) and  $[\text{HN}(\text{CH}_2\text{C}_6\text{H}_2\text{Me}_2\text{OH})_3][(\text{C}_6\text{H}_4\text{CO}_2)\text{P}(\text{O})\text{PPh}_2]$  (Chandrasekaran *et al.*, 2003).

In (I) in the solid state, each independent molecule of the acid exists as a dimer, due to the presence of hydrogen bonds between the phosphoryl O atom and the O—H group of the benzoic acid moiety (Fig. 2 and Table 2). The  $\text{O}\cdots\text{O}$  distances

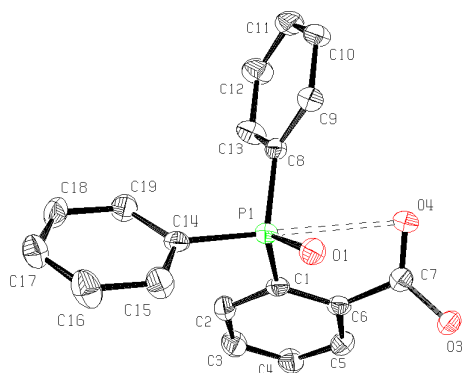


Figure 1

The molecular structure of one independent molecule of 2-(diphenylphosphinoyl)benzoic acid (Farrugia, 1997). H atoms and chloroform molecules have been omitted for clarity. Displacement ellipsoids are drawn at the 50% probability level.

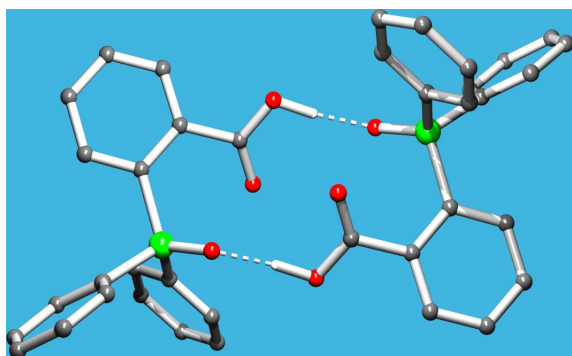


Figure 2

Dimeric structure of (I), showing the intermolecular hydrogen bonds. (Anger *et al.*, 1991)

are 2.578 (3) and 2.566 (4) Å, with the O—H...O angles both 166°. The distances observed between the two P atoms of the dimers are 6.904 (2) and 6.995 (2) Å, respectively. The chloroform molecules in (I) participate in the hydrogen-bonding network (Table 2). The C—H group of one independent molecule of chloroform interacts weakly with the carbonyl O atom of one independent molecule of acid, *i.e.* atom H40 with atom O4<sup>ii</sup> and atom H41 with atom O6<sup>i</sup> (see Table 2).

## Experimental

Compound (I) was prepared according to the literature method of Chandrasekaran *et al.* (2001). Crystals suitable for X-ray analysis were obtained by slow evaporation of a chloroform solution.

### Crystal data

C<sub>19</sub>H<sub>15</sub>O<sub>3</sub>P·CHCl<sub>3</sub>  
*M<sub>r</sub>* = 441.65  
 Triclinic, *P* $\bar{1}$   
*a* = 8.6828 (9) Å  
*b* = 13.3850 (14) Å  
*c* = 17.8678 (18) Å  
 $\alpha$  = 91.572 (12)°  
 $\beta$  = 98.950 (12)°  
 $\gamma$  = 104.045 (12)°  
*V* = 1985.4 (4) Å<sup>3</sup>

*Z* = 4  
*D<sub>x</sub>* = 1.477 Mg m<sup>-3</sup>  
 Mo *K* $\alpha$  radiation  
 Cell parameters from 8000 reflections  
 $\theta$  = 2.0–25.9°  
 $\mu$  = 0.56 mm<sup>-1</sup>  
*T* = 153 (2) K  
 Plate, colourless  
 0.53 × 0.30 × 0.12 mm

### Data collection

Stoe IPDS diffractometer  
 $\varphi$  oscillation scans  
 Absorption correction: multi-scan (Blessing, 1995)  
 $T_{\min} = 0.884$ ,  $T_{\max} = 0.935$   
 15762 measured reflections  
 7227 independent reflections

4039 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.070$   
 $\theta_{\max} = 26.0^\circ$   
 $h = -10 \rightarrow 10$   
 $k = -16 \rightarrow 16$   
 $l = -21 \rightarrow 21$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.051$   
 $wR(F^2) = 0.127$   
 $S = 0.97$   
 1727 reflections  
 487 parameters

H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0524P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.38 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{\min} = -0.40 \text{ e } \text{Å}^{-3}$

Table 1

Selected geometric parameters (Å, °).

C1—P1	1.816 (4)	C27—O6	1.210 (4)
C7—O4	1.218 (4)	C27—O5	1.317 (4)
C7—O3	1.311 (4)	C28—P2	1.801 (4)
C8—P1	1.803 (3)	C34—P2	1.809 (4)
C14—P1	1.806 (4)	O1—P1	1.490 (3)
C21—P2	1.822 (4)	O2—P2	1.493 (3)
O1—P1—C8	114.21 (16)	O2—P2—C28	115.51 (17)
O1—P1—C14	108.38 (16)	O2—P2—C34	108.77 (15)
C8—P1—C14	106.24 (17)	C28—P2—C34	106.35 (18)
O1—P1—C1	113.43 (16)	O2—P2—C21	115.03 (17)
C8—P1—C1	106.94 (16)	C28—P2—C21	105.25 (17)
C14—P1—C1	107.20 (17)	C34—P2—C21	105.13 (16)

Table 2

Hydrogen-bonding geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O5—H5A...O2 <sup>i</sup>	1.06	1.54	2.578 (3)	166
C41—H41...O6 <sup>i</sup>	0.98	2.29	3.255 (5)	170
C40—H40...O4 <sup>ii</sup>	0.98	2.55	3.355 (5)	139
O3—H3A...O1 <sup>iii</sup>	1.03	1.56	2.566 (4)	166

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

The H atoms of the acid functions were located in a difference Fourier map and their positions fixed, while the remaining H atoms were included in calculated positions and treated as riding atoms (C—H = 0.93 Å and  $U_{\text{iso}} = 1.5U_{\text{eq}}$  of the parent atom)

Data collection: *EXPOSE* in *IPDS Software* (Stoe & Cie, 2000); cell refinement: *CELL* in *IPDS Software*; data reduction: *INTEGRATE* in *IPDS Software*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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