



Crystal structures of 1-(4-chlorophenyl)-2-(diphenylphosphoryl)ethan-1-one and 1-(diphenylphosphoryl)-3,3-dimethylbutan-2-one

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CCDC references: 1058397; 1012828

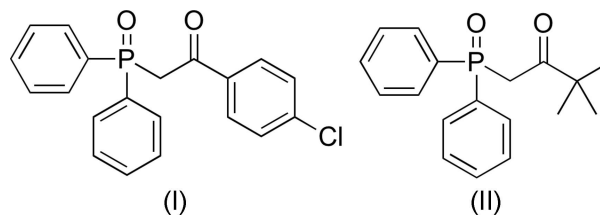
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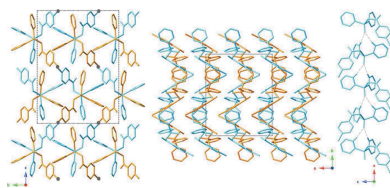
The title compounds, C₂₀H₁₆ClO₂P, (I), and C₁₈H₂₁O₂P, (II), were synthesized *via* an Arbuzov reaction between an α -bromoketone and isopropoxydiphenylphosphane. In the crystals of both compounds, molecules are linked *via* bifurcated C—H...O hydrogen bonds, forming chains propagating along [100] for (I) and along [010] for (II). The chains are linked *via* C—H... π interactions, leading to the formation of sheets lying parallel to (010) for (I) and (001) for (II). The absolute structure of compound (II) was determined by resonant scattering [Fleck parameter = 0.088 (14)].

1. Chemical context

The luminescent properties of lanthanide metals continue to gain attention from researchers interested in the coordination chemistry of *f*-block elements. Direct excitation of lanthanides is difficult due to the parity forbidden *f*–*f* transitions required and relatively low molar absorptivities, but fortunately this excitation can be sensitized with an appropriate organic ligand. The ligand acts as an antenna by harvesting the excitation energy and transferring this energy to the metal emitting state (Weissman, 1942). The resulting emission bands have peak widths less than 10 nm, with a color characteristic of each lanthanide ion. As such, lanthanide metals have found uses in both material and biological applications (de Bettencourt-Dias, 2007; Thibon & Pierre, 2009; Eliseeva & Bünzli, 2010).



Recently, the carbamoylmethylphosphane oxide (CMPO) group has been shown to be an effective ligand for the sensitization of lanthanide luminescence (Sharova *et al.*, 2012; Rosario-Amorin *et al.*, 2013; Sartain *et al.*, 2015). We undertook this work to investigate the role of the aryl carbonyl group on the ability of the CMPO moiety to act as an antenna in this process. Tuning the structure of these organic ligands may be tantamount to potential improvements in the absorption, transfer, and emission of energy by the resultant lanthanide–ligand complex. We report herein on the synthesis and crystal structure of two new CMPO ligands.



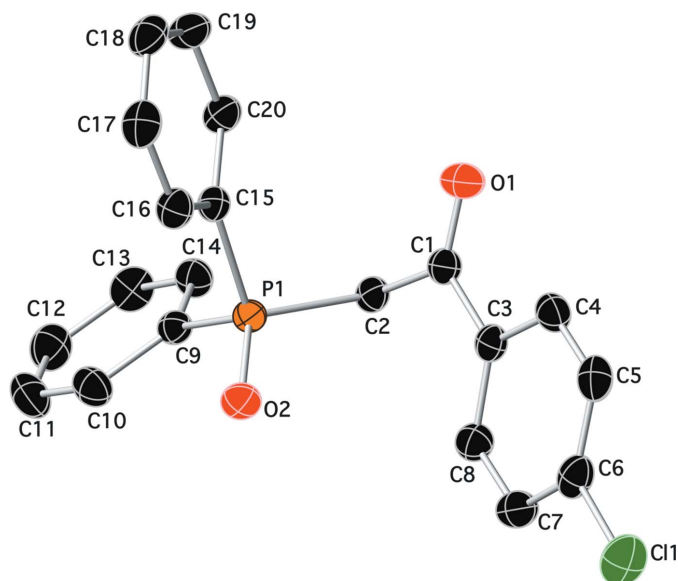


Figure 1
A view of the molecular structure of compound (I), showing the atom labelling. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity.

2. Structural commentary

The molecular structures of compounds (I) and (II) are shown in Figs. 1 and 2, respectively. While compound (I) crystallized in the orthorhombic centrosymmetric space group *Pbca*, compound (II) crystallized in the chiral monoclinic space group *P2*₁. In compound (I), the two phenyl rings (C9–C14

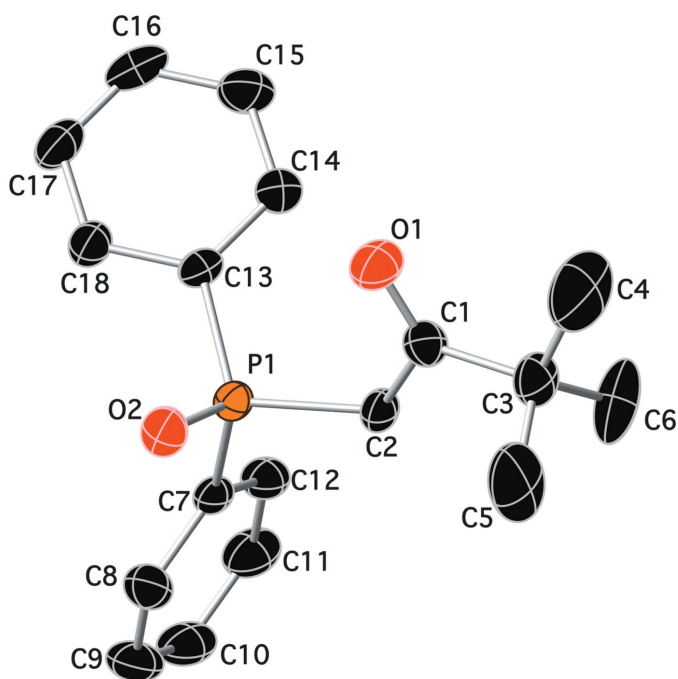


Figure 2
A view of the molecular structure of compound (II), showing the atom labelling. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity.

Table 1

Hydrogen-bond geometry (Å, °) for (I).

Cg1 and Cg3 are the centroids of rings C3–C8 and C15–C20, respectively.

<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>
C14–H14...O2 ⁱ	0.95	2.30	3.1899 (19)	156
C20–H20...O2 ⁱ	0.95	2.50	3.4487 (19)	176
C5–H5...Cg3 ⁱⁱ	0.95	3.00	3.8873 (17)	156
C13–H13...Cg1 ⁱ	0.95	2.90	3.5373 (19)	126

Symmetry codes: (i) $x - \frac{1}{2}, y, -z + \frac{3}{2}$; (ii) $-x + 1, -y + 1, -z + 2$.

Table 2

Hydrogen-bond geometry (Å, °) for (II).

Cg1 is the centroid of ring C7–C12.

<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>
C2–H2B...O2 ⁱ	0.99	2.19	3.176 (5)	176
C12–H12...O2 ⁱ	0.95	2.53	3.373 (5)	148
C17–H17...Cg1 ⁱⁱ	0.95	2.80	3.721 (5)	164

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

and C15–C20) are inclined to one another by 75.53 (8)°, and to the chlorobenzene ring (C3–C8) by 47.98 (8) and 62.16 (8)°, respectively. Atom P1 has a distorted tetrahedral geometry with the C–P=O bond angles varying from 112.02 (7) to 114.35 (7)°, while the C–P–C angles vary from 105.04 (7) to 106.60 (7)°. The carbonyl group (C1=O1) and the phosphoryl group (P1=O2) are *anti* to one another, most probably to minimize unfavourable dipole–dipole interactions. In compound (II), the two phenyl rings (C7–C12 and C13–C18) are inclined to one another by 86.4 (2)°. Atom P1 also has a distorted tetrahedral geometry with the C–P=O bond angles varying from 111.47 (16) to 115.06 (16)°, while the C–P–C bond angles vary from 101.84 (15) to 109.21 (16)°. Here the carbonyl group (C1=O1) and the phosphoryl group (P1=O2) are *syn* to one another.

3. Supramolecular features

In the crystal of (I), the phosphoryl groups are aligned with the *a* axis, and as the individual molecules stack in this direction they appear to rotate around the chlorine atom that lies close to the twofold screw axis, creating a pinwheel arrangement of molecules (Fig. 3). The molecules are linked *via* bifurcated C–H...O hydrogen bonds, forming chains propagating along [100]; see Fig. 3 and Table 1. The chains are linked *via* C–H...π interactions (Table 1), forming sheets lying parallel to (010).

Compound (II) packs in a similar arrangement to (I) in the solid state, although subtle differences result in the formation of a chiral crystal from an achiral compound (Fig. 4). For compound (II), the phosphoryl groups are again aligned in one direction (along the *b* axis), but in this case, the P1–C2 bond in the center of the molecule lies about a twofold screw axis and acts as the pivot point for the pinwheel arrangement rather than the terminal chlorine atom as seen in the crystal of

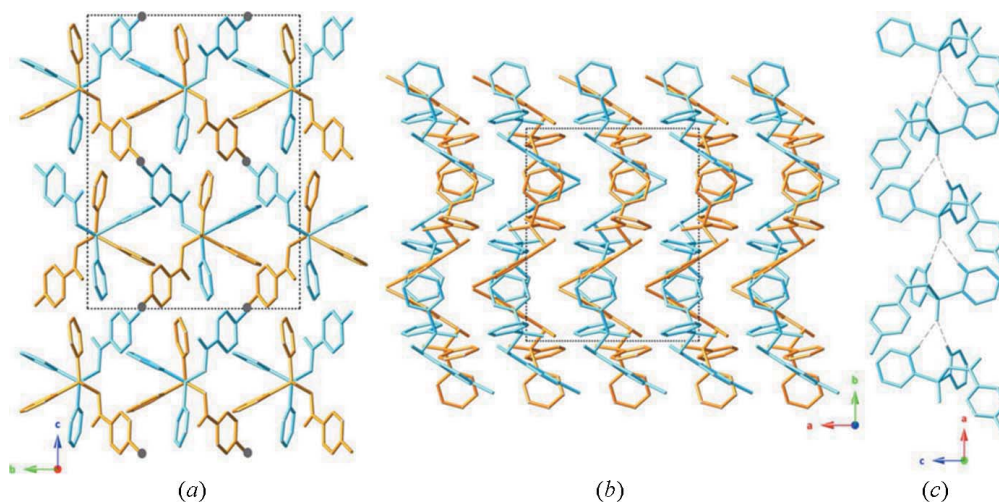


Figure 3

The crystal packing diagram of compound (I) (drawn as blue and orange sticks) viewed along: (a) the *a* axis (the Cl atoms are shown as dark grey dots); (b) the *c* axis; (c) along the *b* axis, with the bifurcated hydrogen bonds shown as dashed lines (see Table 1 for details). H atoms have been omitted for clarity in parts (a) and (b) and only those involved in hydrogen bonding are shown in part (c).

compound (I). The absence of an inversion center or mirror plane results in a chiral twist to the packing within this crystal. Here, molecules are also linked *via* bifurcated C—H...*(O,O)* hydrogen bonds, forming chains propagating along [010] (see Table 2 and Fig. 4) and the chains are linked *via* C—H... π interactions (Table 2), forming sheets parallel to (001).

4. Database Survey

The Cambridge Structural Database (CSD, Version 5.36, November 2014; Groom & Allen, 2014) contains 11 structures with a β -ketodiphenylphosphoryl moiety. Three of these

structures are related to the title compounds, but have either an alkyl group bonded to the keto function or branching at the α -carbon, *viz.* *E*-(5*SR*,6*SR*)-3,6-dimethyl-5-diphenylphosphinoyl-7-triphenylmethoxyhept-2-en-4-one acetone solvate (SUGWOG; Doyle *et al.*, 1993), anti-(2*S*,4*S*)-2-(*N,N*-dibenzylamino)-4-diphenylphosphinoyl-1-phenylpentan-3-one monohydrate (RIZCEI; O'Brien *et al.*, 1997) and (4*R*,5*R*)-4,5-dihydroxy-1,5-diphenyl-2-(diphenylphosphinoyl)pentan-1-one (FODBUW; Boesen *et al.*, 2005). The last compound (FODBUW) crystallizes in a chiral space group ($P2_12_12_1$), as does compound (II). The phenyl rings of the diphenylphosphinoyl group in each of these three compounds are

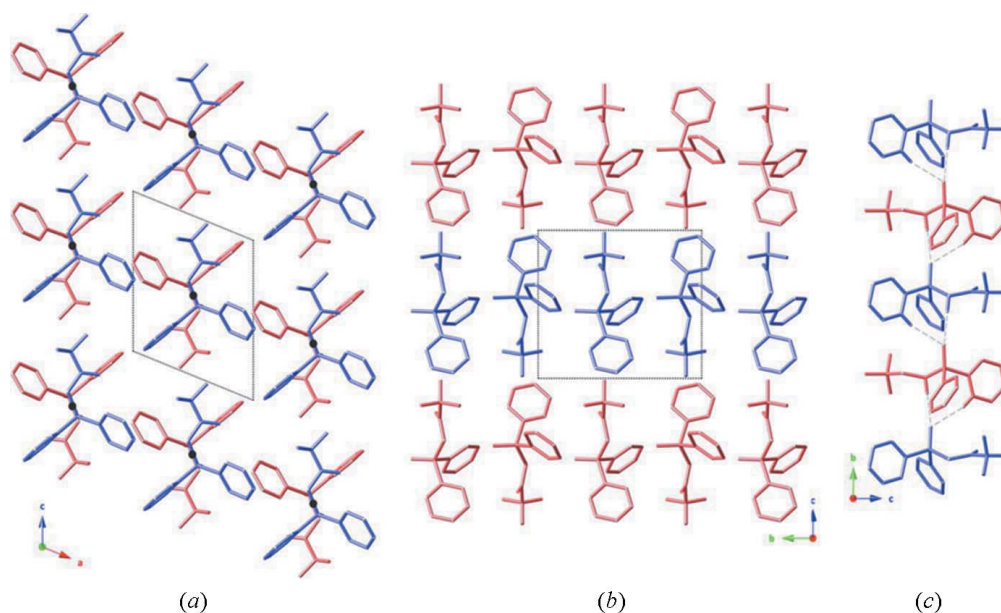


Figure 4

The crystal packing diagram of compound (II) (drawn as purple and pink sticks) viewed along: (a) the *b* axis (the center of the P1—Cl bond that coincides with the twofold screw axis is denoted with a grey dot); (b) the *a* axis; (c) along the *b* axis with the bifurcated hydrogen bonds shown as dashed lines (see Table 2 for details). H atoms have been omitted for clarity in parts (a) and (b) and only those involved in hydrogen bonding are shown in (c).

Table 3
Experimental details.

	(I)	(II)
Crystal data		
Chemical formula	C ₂₀ H ₁₆ ClO ₂ P	C ₁₈ H ₂₁ O ₂ P
<i>M</i> _r	354.75	300.32
Crystal system, space group	Orthorhombic, <i>Pbca</i>	Monoclinic, <i>P2</i> ₁
Temperature (K)	173	173
<i>a</i> , <i>b</i> , <i>c</i> (Å)	11.7380 (2), 14.4453 (3), 19.9515 (3)	8.3416 (2), 10.5161 (2), 10.2790 (2)
α , β , γ (°)	90, 90, 90	90, 112.212 (1), 90
<i>V</i> (Å ³)	3382.95 (10)	834.77 (3)
<i>Z</i>	8	2
Radiation type	Cu <i>K</i> α	Cu <i>K</i> α
μ (mm ⁻¹)	2.97	1.47
Crystal size (mm)	0.36 × 0.17 × 0.13	0.43 × 0.14 × 0.08
Data collection		
Diffractometer	Bruker APEXII CCD	Bruker SMART APEX CCD area detector
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2013)	Multi-scan (<i>SADABS</i> ; Bruker, 2013)
<i>T</i> _{min} , <i>T</i> _{max}	0.599, 0.754	0.631, 0.754
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	17900, 3297, 2880	7043, 3006, 2774
<i>R</i> _{int}	0.033	0.042
(sin θ /λ) _{max} (Å ⁻¹)	0.617	0.617
Refinement		
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.032, 0.089, 1.04	0.042, 0.118, 1.13
No. of reflections	3297	3006
No. of parameters	217	193
No. of restraints	0	1
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
Δρ _{max} , Δρ _{min} (e Å ⁻³)	0.32, -0.39	0.49, -0.38
Absolute structure	—	Flack <i>x</i> determined using 1090 quotients [(<i>I</i> ⁺) - (<i>I</i> ⁻)]/[(<i>I</i> ⁺) + (<i>I</i> ⁻)] (Parsons <i>et al.</i> , 2013)
Absolute structure parameter	—	0.088 (14)

Computer programs: *APEX2*, *SAINT* and *XPRED* (Bruker, 2013), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *CrystalMaker* (Palmer, 2007) and *OLEX2* (Dolomanov *et al.*, 2009; Bourhis *et al.*, 2015).

inclined to one another by *ca* 67.97, 73.25 and 68.24°, respectively, similar to the arrangement in compound (I).

5. Synthesis and crystallization

The title compounds, (I) and (II), were prepared following slightly modified literature procedures (Arnaud-Neu *et al.*, 1996; Schuster *et al.*, 2009) by the Arbuzov reaction of isopropoxydiphenylphosphane (Shintou *et al.*, 2003) with 2-bromo-4'-chloroacetophenone for (I) and 1-bromopinacolone for (II). For both compounds, crystals suitable for X-ray diffraction analysis were grown by slow evaporation of a solution of the compound in CDCl₃.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The hydrogen atoms were placed in calculated positions and refined as riding atoms: C—H = 0.95–0.99 Å with *U*_{iso}(H) = 1.5*U*_{eq}(C) for methyl H atoms and 1.2*U*_{eq}(C) for other H atoms.

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supporting information

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Crystal structures of 1-(4-chlorophenyl)-2-(diphenylphosphoryl)ethan-1-one and 1-(diphenylphosphoryl)-3,3-dimethylbutan-2-one

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Computing details

For both compounds, data collection: *APEX2* (Bruker, 2013); cell refinement: *APEX2* and *SAINT* (Bruker, 2013); data reduction: *SAINT* and *XPREF* (Bruker, 2013); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *CrystalMaker* (Palmer, 2007); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009; Bourhis *et al.*, 2015).

(I) 1-(4-Chlorophenyl)-2-(diphenylphosphoryl)ethan-1-one

Crystal data

$C_{20}H_{16}ClO_2P$

$M_r = 354.75$

Orthorhombic, *Pbca*

$a = 11.7380$ (2) Å

$b = 14.4453$ (3) Å

$c = 19.9515$ (3) Å

$V = 3382.95$ (10) Å³

$Z = 8$

$F(000) = 1472$

$D_x = 1.393$ Mg m⁻³

Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å

Cell parameters from 9053 reflections

$\theta = 4.4\text{--}72.0^\circ$

$\mu = 2.97$ mm⁻¹

$T = 173$ K

Needle, colourless

$0.36 \times 0.17 \times 0.13$ mm

Data collection

Bruker APEXII CCD

diffractometer

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

(SADABS; Bruker, 2013)

$T_{\min} = 0.599$, $T_{\max} = 0.754$

17900 measured reflections

3297 independent reflections

2880 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.033$

$\theta_{\max} = 72.2^\circ$, $\theta_{\min} = 4.4^\circ$

$h = -14 \rightarrow 14$

$k = -17 \rightarrow 17$

$l = -24 \rightarrow 23$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.032$

$wR(F^2) = 0.089$

$S = 1.04$

3297 reflections

217 parameters

0 restraints

Primary atom site location: structure-invariant

direct methods

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0502P)^2 + 1.0258P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.32$ e Å⁻³

$\Delta\rho_{\min} = -0.39$ e Å⁻³

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C11	0.80844 (4)	0.25495 (3)	0.98830 (2)	0.04355 (14)
P1	0.47545 (3)	0.53879 (3)	0.75031 (2)	0.02092 (11)
O1	0.33462 (10)	0.47690 (9)	0.89963 (6)	0.0366 (3)
O2	0.60062 (9)	0.52376 (8)	0.75506 (6)	0.0292 (3)
C1	0.40409 (13)	0.43971 (11)	0.86325 (8)	0.0257 (3)
C2	0.38970 (12)	0.44712 (10)	0.78795 (7)	0.0243 (3)
H2A	0.3084	0.4587	0.7777	0.029*
H2B	0.4109	0.3873	0.7673	0.029*
C3	0.50328 (13)	0.38850 (10)	0.89190 (7)	0.0252 (3)
C4	0.51562 (14)	0.38806 (11)	0.96164 (8)	0.0293 (3)
H4	0.4594	0.4170	0.9887	0.035*
C5	0.60803 (15)	0.34632 (12)	0.99183 (8)	0.0328 (4)
H5	0.6163	0.3468	1.0392	0.039*
C6	0.68856 (14)	0.30356 (11)	0.95145 (9)	0.0314 (4)
C7	0.67686 (14)	0.30005 (12)	0.88247 (9)	0.0324 (4)
H7	0.7316	0.2685	0.8559	0.039*
C8	0.58415 (14)	0.34315 (11)	0.85264 (8)	0.0289 (3)
H8	0.5758	0.3417	0.8053	0.035*
C9	0.42652 (13)	0.54676 (10)	0.66510 (7)	0.0236 (3)
C10	0.50496 (14)	0.57592 (12)	0.61691 (8)	0.0319 (4)
H10	0.5815	0.5886	0.6293	0.038*
C11	0.47052 (16)	0.58623 (13)	0.55074 (9)	0.0391 (4)
H11	0.5234	0.6071	0.5180	0.047*
C12	0.35988 (17)	0.56633 (13)	0.53235 (8)	0.0384 (4)
H12	0.3372	0.5726	0.4869	0.046*
C13	0.28230 (15)	0.53745 (12)	0.57968 (9)	0.0347 (4)
H13	0.2063	0.5238	0.5667	0.042*
C14	0.31441 (13)	0.52817 (11)	0.64629 (8)	0.0283 (3)
H14	0.2603	0.5092	0.6789	0.034*
C15	0.43163 (12)	0.64440 (10)	0.79158 (7)	0.0230 (3)
C16	0.51476 (14)	0.70315 (11)	0.81674 (8)	0.0290 (3)
H16	0.5927	0.6859	0.8143	0.035*
C17	0.48423 (15)	0.78728 (12)	0.84549 (8)	0.0338 (4)
H17	0.5413	0.8276	0.8624	0.041*
C18	0.37069 (16)	0.81216 (12)	0.84948 (8)	0.0345 (4)
H18	0.3498	0.8701	0.8683	0.041*
C19	0.28765 (15)	0.75256 (12)	0.82598 (9)	0.0345 (4)
H19	0.2097	0.7692	0.8299	0.041*
C20	0.31663 (13)	0.66892 (11)	0.79674 (8)	0.0286 (3)

H2O 0.2591 0.6286 0.7803 0.034*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.0357 (2)	0.0428 (3)	0.0521 (3)	0.00128 (18)	−0.01410 (19)	0.00816 (19)
P1	0.0163 (2)	0.0199 (2)	0.0265 (2)	−0.00157 (13)	−0.00033 (13)	−0.00008 (13)
O1	0.0337 (6)	0.0397 (7)	0.0364 (6)	0.0080 (5)	0.0075 (5)	−0.0014 (5)
O2	0.0181 (5)	0.0310 (6)	0.0386 (6)	−0.0002 (5)	−0.0015 (4)	0.0010 (5)
C1	0.0251 (7)	0.0207 (7)	0.0311 (8)	−0.0041 (6)	0.0033 (6)	−0.0002 (6)
C2	0.0215 (7)	0.0207 (7)	0.0307 (8)	−0.0029 (6)	−0.0001 (6)	0.0011 (6)
C3	0.0264 (7)	0.0203 (7)	0.0289 (7)	−0.0046 (6)	0.0017 (6)	0.0012 (6)
C4	0.0330 (8)	0.0259 (8)	0.0292 (8)	−0.0031 (7)	0.0059 (6)	0.0006 (6)
C5	0.0416 (9)	0.0299 (9)	0.0269 (8)	−0.0052 (7)	−0.0015 (7)	0.0036 (6)
C6	0.0291 (8)	0.0255 (8)	0.0395 (9)	−0.0037 (7)	−0.0057 (7)	0.0052 (7)
C7	0.0303 (8)	0.0305 (9)	0.0365 (9)	0.0029 (7)	0.0014 (7)	−0.0023 (7)
C8	0.0314 (8)	0.0279 (8)	0.0275 (7)	0.0008 (6)	−0.0002 (6)	−0.0012 (6)
C9	0.0231 (7)	0.0207 (7)	0.0269 (7)	−0.0003 (6)	0.0003 (6)	−0.0011 (5)
C10	0.0281 (8)	0.0333 (9)	0.0342 (8)	−0.0055 (7)	0.0053 (7)	−0.0028 (7)
C11	0.0454 (10)	0.0409 (10)	0.0310 (8)	−0.0048 (8)	0.0106 (7)	0.0015 (7)
C12	0.0508 (11)	0.0371 (10)	0.0273 (8)	0.0020 (8)	−0.0037 (7)	0.0012 (7)
C13	0.0328 (9)	0.0356 (10)	0.0357 (9)	−0.0013 (7)	−0.0088 (7)	−0.0015 (7)
C14	0.0241 (8)	0.0299 (8)	0.0308 (8)	−0.0027 (6)	−0.0008 (6)	0.0011 (6)
C15	0.0242 (7)	0.0207 (7)	0.0240 (7)	−0.0016 (6)	0.0001 (6)	0.0007 (5)
C16	0.0277 (8)	0.0277 (8)	0.0315 (8)	−0.0037 (6)	−0.0027 (6)	−0.0001 (6)
C17	0.0440 (9)	0.0269 (9)	0.0307 (8)	−0.0075 (7)	−0.0060 (7)	−0.0030 (6)
C18	0.0511 (10)	0.0234 (8)	0.0291 (8)	0.0056 (7)	−0.0006 (7)	−0.0021 (6)
C19	0.0341 (9)	0.0302 (9)	0.0393 (9)	0.0088 (7)	0.0007 (7)	−0.0002 (7)
C20	0.0258 (7)	0.0256 (8)	0.0345 (8)	0.0008 (6)	−0.0026 (6)	0.0008 (6)

Geometric parameters (\AA , $^\circ$)

C11—C6	1.7360 (16)	C9—C14	1.395 (2)
P1—O2	1.4882 (11)	C10—H10	0.9500
P1—C2	1.8251 (15)	C10—C11	1.389 (2)
P1—C9	1.7982 (15)	C11—H11	0.9500
P1—C15	1.8083 (15)	C11—C12	1.380 (3)
O1—C1	1.2168 (19)	C12—H12	0.9500
C1—C2	1.515 (2)	C12—C13	1.377 (3)
C1—C3	1.493 (2)	C13—H13	0.9500
C2—H2A	0.9900	C13—C14	1.388 (2)
C2—H2B	0.9900	C14—H14	0.9500
C3—C4	1.399 (2)	C15—C16	1.387 (2)
C3—C8	1.394 (2)	C15—C20	1.399 (2)
C4—H4	0.9500	C16—H16	0.9500
C4—C5	1.380 (2)	C16—C17	1.391 (2)
C5—H5	0.9500	C17—H17	0.9500
C5—C6	1.387 (2)	C17—C18	1.383 (3)

C6—C7	1.384 (2)	C18—H18	0.9500
C7—H7	0.9500	C18—C19	1.382 (3)
C7—C8	1.388 (2)	C19—H19	0.9500
C8—H8	0.9500	C19—C20	1.384 (2)
C9—C10	1.396 (2)	C20—H20	0.9500
O2—P1—C2	114.35 (7)	C14—C9—C10	119.68 (14)
O2—P1—C9	112.64 (7)	C9—C10—H10	120.2
O2—P1—C15	112.02 (7)	C11—C10—C9	119.67 (16)
C9—P1—C2	105.04 (7)	C11—C10—H10	120.2
C9—P1—C15	106.60 (7)	C10—C11—H11	119.9
C15—P1—C2	105.54 (7)	C12—C11—C10	120.30 (16)
O1—C1—C2	119.05 (14)	C12—C11—H11	119.9
O1—C1—C3	120.86 (14)	C11—C12—H12	119.9
C3—C1—C2	120.09 (13)	C13—C12—C11	120.22 (16)
P1—C2—H2A	108.9	C13—C12—H12	119.9
P1—C2—H2B	108.9	C12—C13—H13	119.8
C1—C2—P1	113.43 (10)	C12—C13—C14	120.44 (16)
C1—C2—H2A	108.9	C14—C13—H13	119.8
C1—C2—H2B	108.9	C9—C14—H14	120.2
H2A—C2—H2B	107.7	C13—C14—C9	119.69 (15)
C4—C3—C1	117.63 (14)	C13—C14—H14	120.2
C8—C3—C1	123.27 (14)	C16—C15—P1	118.74 (12)
C8—C3—C4	119.09 (15)	C16—C15—C20	119.81 (15)
C3—C4—H4	119.4	C20—C15—P1	121.42 (12)
C5—C4—C3	121.18 (15)	C15—C16—H16	119.9
C5—C4—H4	119.4	C15—C16—C17	120.17 (15)
C4—C5—H5	120.8	C17—C16—H16	119.9
C4—C5—C6	118.47 (15)	C16—C17—H17	120.0
C6—C5—H5	120.8	C18—C17—C16	119.95 (15)
C5—C6—C11	119.11 (13)	C18—C17—H17	120.0
C7—C6—C11	119.12 (13)	C17—C18—H18	120.1
C7—C6—C5	121.75 (15)	C19—C18—C17	119.88 (16)
C6—C7—H7	120.4	C19—C18—H18	120.1
C6—C7—C8	119.20 (15)	C18—C19—H19	119.6
C8—C7—H7	120.4	C18—C19—C20	120.89 (16)
C3—C8—H8	119.9	C20—C19—H19	119.6
C7—C8—C3	120.25 (15)	C15—C20—H20	120.4
C7—C8—H8	119.9	C19—C20—C15	119.27 (15)
C10—C9—P1	117.37 (12)	C19—C20—H20	120.4
C14—C9—P1	122.92 (12)		
C11—C6—C7—C8	−176.61 (13)	C4—C5—C6—C11	177.30 (13)
P1—C9—C10—C11	−177.86 (13)	C4—C5—C6—C7	−1.5 (3)
P1—C9—C14—C13	178.80 (13)	C5—C6—C7—C8	2.2 (3)
P1—C15—C16—C17	176.49 (12)	C6—C7—C8—C3	−0.7 (3)
P1—C15—C20—C19	−176.96 (12)	C8—C3—C4—C5	2.2 (2)
O1—C1—C2—P1	97.28 (15)	C9—P1—C2—C1	−170.57 (11)

O1—C1—C3—C4	−2.5 (2)	C9—P1—C15—C16	−117.67 (13)
O1—C1—C3—C8	178.73 (16)	C9—P1—C15—C20	60.42 (14)
O2—P1—C2—C1	65.44 (12)	C9—C10—C11—C12	−1.1 (3)
O2—P1—C9—C10	−25.46 (15)	C10—C9—C14—C13	1.0 (2)
O2—P1—C9—C14	156.68 (13)	C10—C11—C12—C13	1.0 (3)
O2—P1—C15—C16	5.96 (14)	C11—C12—C13—C14	0.1 (3)
O2—P1—C15—C20	−175.96 (12)	C12—C13—C14—C9	−1.1 (3)
C1—C3—C4—C5	−176.70 (15)	C14—C9—C10—C11	0.1 (2)
C1—C3—C8—C7	177.34 (15)	C15—P1—C2—C1	−58.14 (12)
C2—P1—C9—C10	−150.53 (13)	C15—P1—C9—C10	97.79 (13)
C2—P1—C9—C14	31.61 (15)	C15—P1—C9—C14	−80.08 (14)
C2—P1—C15—C16	130.99 (12)	C15—C16—C17—C18	0.5 (2)
C2—P1—C15—C20	−50.92 (14)	C16—C15—C20—C19	1.1 (2)
C2—C1—C3—C4	176.67 (14)	C16—C17—C18—C19	1.2 (3)
C2—C1—C3—C8	−2.1 (2)	C17—C18—C19—C20	−1.7 (3)
C3—C1—C2—P1	−81.86 (15)	C18—C19—C20—C15	0.6 (3)
C3—C4—C5—C6	−0.7 (2)	C20—C15—C16—C17	−1.6 (2)
C4—C3—C8—C7	−1.4 (2)		

Hydrogen-bond geometry (Å, °)

Cg1 and Cg3 are the centroids of rings C3–C8 and C15–C20, respectively.

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C14—H14 \cdots O2 ⁱ	0.95	2.30	3.1899 (19)	156
C20—H20 \cdots O2 ⁱ	0.95	2.50	3.4487 (19)	176
C5—H5 \cdots Cg3 ⁱⁱ	0.95	3.00	3.8873 (17)	156
C13—H13 \cdots Cg1 ⁱ	0.95	2.90	3.5373 (19)	126

Symmetry codes: (i) $x-1/2, y, -z+3/2$; (ii) $-x+1, -y+1, -z+2$.

(II) 1-(Diphenylphosphoryl)-3,3-dimethylbutan-2-one

Crystal data

C₁₈H₂₁O₂P
 $M_r = 300.32$
 Monoclinic, $P2_1$
 $a = 8.3416$ (2) Å
 $b = 10.5161$ (2) Å
 $c = 10.2790$ (2) Å
 $\beta = 112.212$ (1)°
 $V = 834.77$ (3) Å³
 $Z = 2$

$F(000) = 320$
 $D_x = 1.195$ Mg m^{−3}
 Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
 Cell parameters from 5567 reflections
 $\theta = 4.7\text{--}72.0^\circ$
 $\mu = 1.47$ mm^{−1}
 $T = 173$ K
 Needle, colourless
 $0.43 \times 0.14 \times 0.08$ mm

Data collection

Bruker SMART APEX CCD area-detector
 diffractometer
 Radiation source: sealed tube
 Graphite monochromator
 Detector resolution: 8 pixels mm^{−1}
 ω and ϕ scans

Absorption correction: multi-scan
 (SADABS; Bruker, 2013)
 $T_{\min} = 0.631, T_{\max} = 0.754$
 7043 measured reflections
 3006 independent reflections
 2774 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.042$

$\theta_{\max} = 72.0^\circ$, $\theta_{\min} = 4.7^\circ$
 $h = -9 \rightarrow 10$

$k = -12 \rightarrow 12$
 $l = -12 \rightarrow 12$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.042$
 $wR(F^2) = 0.118$
 $S = 1.13$
 3006 reflections
 193 parameters
 1 restraint
 Primary atom site location: structure-invariant
 direct methods

Hydrogen site location: inferred from
 neighbouring sites
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0722P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.49 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.38 \text{ e } \text{\AA}^{-3}$
 Absolute structure: Flack x determined using
 1090 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
 Absolute structure parameter: 0.088 (14)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
P1	0.46337 (9)	0.13395 (7)	0.54974 (7)	0.0247 (2)
O1	0.2783 (3)	0.1230 (4)	0.2325 (3)	0.0450 (7)
O2	0.4313 (3)	0.2739 (3)	0.5441 (3)	0.0352 (6)
C1	0.4309 (5)	0.1015 (3)	0.2672 (3)	0.0328 (8)
C2	0.5430 (4)	0.0741 (4)	0.4198 (3)	0.0286 (7)
H2A	0.6592	0.1108	0.4399	0.034*
H2B	0.5572	-0.0192	0.4317	0.034*
C3	0.5199 (5)	0.0970 (4)	0.1613 (4)	0.0403 (9)
C4	0.3850 (8)	0.0965 (11)	0.0140 (5)	0.105 (4)
H4A	0.3118	0.0210	0.0006	0.157*
H4B	0.4422	0.0952	-0.0536	0.157*
H4C	0.3133	0.1731	-0.0008	0.157*
C5	0.6294 (11)	0.2154 (7)	0.1830 (7)	0.090 (3)
H5A	0.5596	0.2900	0.1842	0.135*
H5B	0.6712	0.2237	0.1062	0.135*
H5C	0.7284	0.2094	0.2726	0.135*
C6	0.6318 (9)	-0.0220 (7)	0.1848 (6)	0.0713 (17)
H6A	0.7288	-0.0159	0.2757	0.107*
H6B	0.6765	-0.0295	0.1096	0.107*
H6C	0.5619	-0.0970	0.1842	0.107*
C7	0.6358 (4)	0.0881 (4)	0.7129 (3)	0.0280 (7)
C8	0.7278 (5)	0.1814 (4)	0.8067 (4)	0.0400 (9)
H8	0.6982	0.2684	0.7865	0.048*
C9	0.8634 (5)	0.1477 (6)	0.9304 (4)	0.0518 (12)
H9	0.9264	0.2117	0.9946	0.062*

C10	0.9069 (5)	0.0207 (5)	0.9603 (4)	0.0485 (11)
H10	0.9994	−0.0023	1.0449	0.058*
C11	0.8157 (5)	−0.0721 (5)	0.8669 (4)	0.0459 (10)
H11	0.8455	−0.1590	0.8873	0.055*
C12	0.6802 (4)	−0.0389 (4)	0.7431 (4)	0.0341 (8)
H12	0.6178	−0.1031	0.6790	0.041*
C13	0.2784 (4)	0.0408 (4)	0.5431 (3)	0.0270 (6)
C14	0.2209 (5)	−0.0666 (4)	0.4600 (4)	0.0399 (9)
H14	0.2786	−0.0945	0.4012	0.048*
C15	0.0789 (6)	−0.1332 (5)	0.4632 (5)	0.0486 (11)
H15	0.0387	−0.2059	0.4051	0.058*
C16	−0.0046 (5)	−0.0952 (5)	0.5495 (5)	0.0462 (10)
H16	−0.1014	−0.1416	0.5513	0.055*
C17	0.0532 (5)	0.0105 (4)	0.6328 (4)	0.0422 (9)
H17	−0.0035	0.0366	0.6930	0.051*
C18	0.1936 (5)	0.0793 (4)	0.6298 (4)	0.0337 (7)
H18	0.2320	0.1528	0.6870	0.040*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P1	0.0238 (4)	0.0270 (4)	0.0251 (3)	−0.0011 (3)	0.0113 (3)	0.0003 (3)
O1	0.0312 (12)	0.068 (2)	0.0324 (11)	0.0044 (14)	0.0085 (10)	0.0033 (14)
O2	0.0398 (13)	0.0270 (14)	0.0428 (14)	0.0012 (10)	0.0200 (11)	0.0020 (10)
C1	0.0345 (17)	0.037 (2)	0.0268 (15)	−0.0019 (13)	0.0119 (13)	−0.0008 (13)
C2	0.0276 (15)	0.0364 (18)	0.0257 (15)	0.0004 (13)	0.0143 (12)	−0.0003 (13)
C3	0.043 (2)	0.054 (3)	0.0278 (16)	0.0021 (17)	0.0182 (16)	0.0016 (15)
C4	0.068 (3)	0.218 (12)	0.027 (2)	0.022 (5)	0.018 (2)	−0.004 (4)
C5	0.138 (6)	0.084 (5)	0.094 (5)	−0.045 (5)	0.096 (5)	−0.025 (4)
C6	0.092 (4)	0.080 (4)	0.067 (3)	0.029 (3)	0.059 (3)	0.011 (3)
C7	0.0222 (13)	0.0427 (18)	0.0212 (14)	−0.0043 (13)	0.0106 (12)	−0.0009 (12)
C8	0.0411 (19)	0.047 (2)	0.0348 (19)	−0.0138 (17)	0.0173 (16)	−0.0079 (15)
C9	0.0411 (19)	0.079 (3)	0.0333 (17)	−0.027 (2)	0.0120 (15)	−0.016 (2)
C10	0.0291 (17)	0.083 (3)	0.0281 (17)	−0.006 (2)	0.0045 (14)	0.0044 (19)
C11	0.0315 (18)	0.063 (3)	0.038 (2)	0.0070 (18)	0.0082 (16)	0.0108 (19)
C12	0.0267 (16)	0.043 (2)	0.0292 (17)	−0.0013 (14)	0.0066 (14)	0.0005 (14)
C13	0.0200 (13)	0.0328 (16)	0.0276 (15)	0.0006 (12)	0.0083 (12)	0.0047 (13)
C14	0.0336 (18)	0.042 (2)	0.047 (2)	−0.0061 (16)	0.0181 (17)	−0.0107 (16)
C15	0.0392 (19)	0.041 (3)	0.065 (3)	−0.012 (2)	0.019 (2)	−0.0121 (19)
C16	0.0262 (16)	0.052 (2)	0.062 (3)	−0.0053 (18)	0.0184 (18)	0.011 (2)
C17	0.0314 (17)	0.057 (3)	0.044 (2)	0.0000 (17)	0.0216 (16)	0.0036 (18)
C18	0.0292 (16)	0.0431 (19)	0.0306 (16)	0.0007 (15)	0.0133 (14)	−0.0011 (14)

Geometric parameters (Å, °)

P1—O2	1.493 (3)	C7—C12	1.389 (6)
P1—C2	1.814 (3)	C8—H8	0.9500
P1—C7	1.814 (3)	C8—C9	1.391 (6)

P1—C13	1.807 (3)	C9—H9	0.9500
O1—C1	1.207 (5)	C9—C10	1.387 (8)
C1—C2	1.520 (5)	C10—H10	0.9500
C1—C3	1.533 (5)	C10—C11	1.378 (7)
C2—H2A	0.9900	C11—H11	0.9500
C2—H2B	0.9900	C11—C12	1.390 (5)
C3—C4	1.507 (6)	C12—H12	0.9500
C3—C5	1.509 (7)	C13—C14	1.388 (6)
C3—C6	1.525 (7)	C13—C18	1.391 (5)
C4—H4A	0.9800	C14—H14	0.9500
C4—H4B	0.9800	C14—C15	1.387 (6)
C4—H4C	0.9800	C15—H15	0.9500
C5—H5A	0.9800	C15—C16	1.378 (7)
C5—H5B	0.9800	C16—H16	0.9500
C5—H5C	0.9800	C16—C17	1.375 (7)
C6—H6A	0.9800	C17—H17	0.9500
C6—H6B	0.9800	C17—C18	1.387 (5)
C6—H6C	0.9800	C18—H18	0.9500
C7—C8	1.387 (5)		
O2—P1—C2	115.06 (16)	H6B—C6—H6C	109.5
O2—P1—C7	111.47 (16)	C8—C7—P1	119.5 (3)
O2—P1—C13	113.25 (15)	C8—C7—C12	119.6 (3)
C7—P1—C2	101.84 (15)	C12—C7—P1	120.9 (3)
C13—P1—C2	109.21 (16)	C7—C8—H8	120.0
C13—P1—C7	104.98 (16)	C7—C8—C9	120.0 (4)
O1—C1—C2	120.6 (3)	C9—C8—H8	120.0
O1—C1—C3	122.4 (3)	C8—C9—H9	119.9
C2—C1—C3	117.0 (3)	C10—C9—C8	120.1 (4)
P1—C2—H2A	108.3	C10—C9—H9	119.9
P1—C2—H2B	108.3	C9—C10—H10	120.1
C1—C2—P1	116.1 (2)	C11—C10—C9	119.9 (4)
C1—C2—H2A	108.3	C11—C10—H10	120.1
C1—C2—H2B	108.3	C10—C11—H11	119.9
H2A—C2—H2B	107.4	C10—C11—C12	120.2 (4)
C4—C3—C1	109.6 (4)	C12—C11—H11	119.9
C4—C3—C5	109.4 (6)	C7—C12—C11	120.1 (4)
C4—C3—C6	109.7 (5)	C7—C12—H12	119.9
C5—C3—C1	107.3 (3)	C11—C12—H12	119.9
C5—C3—C6	110.7 (5)	C14—C13—P1	123.8 (3)
C6—C3—C1	110.1 (4)	C14—C13—C18	119.4 (3)
C3—C4—H4A	109.5	C18—C13—P1	116.8 (3)
C3—C4—H4B	109.5	C13—C14—H14	120.1
C3—C4—H4C	109.5	C15—C14—C13	119.7 (4)
H4A—C4—H4B	109.5	C15—C14—H14	120.1
H4A—C4—H4C	109.5	C14—C15—H15	119.6
H4B—C4—H4C	109.5	C16—C15—C14	120.8 (4)
C3—C5—H5A	109.5	C16—C15—H15	119.6

C3—C5—H5B	109.5	C15—C16—H16	120.3
C3—C5—H5C	109.5	C17—C16—C15	119.5 (4)
H5A—C5—H5B	109.5	C17—C16—H16	120.3
H5A—C5—H5C	109.5	C16—C17—H17	119.7
H5B—C5—H5C	109.5	C16—C17—C18	120.6 (4)
C3—C6—H6A	109.5	C18—C17—H17	119.7
C3—C6—H6B	109.5	C13—C18—H18	120.0
C3—C6—H6C	109.5	C17—C18—C13	120.0 (4)
H6A—C6—H6B	109.5	C17—C18—H18	120.0
H6A—C6—H6C	109.5		
P1—C7—C8—C9	−178.3 (3)	C3—C1—C2—P1	158.4 (3)
P1—C7—C12—C11	178.3 (3)	C7—P1—C2—C1	−177.5 (3)
P1—C13—C14—C15	179.1 (3)	C7—P1—C13—C14	−102.8 (3)
P1—C13—C18—C17	−178.4 (3)	C7—P1—C13—C18	75.6 (3)
O1—C1—C2—P1	−23.1 (5)	C7—C8—C9—C10	0.0 (6)
O1—C1—C3—C4	−11.3 (7)	C8—C7—C12—C11	0.3 (5)
O1—C1—C3—C5	107.4 (6)	C8—C9—C10—C11	0.1 (6)
O1—C1—C3—C6	−132.0 (5)	C9—C10—C11—C12	−0.1 (6)
O2—P1—C2—C1	−56.8 (3)	C10—C11—C12—C7	−0.1 (6)
O2—P1—C7—C8	−5.5 (3)	C12—C7—C8—C9	−0.2 (5)
O2—P1—C7—C12	176.4 (3)	C13—P1—C2—C1	71.8 (3)
O2—P1—C13—C14	135.4 (3)	C13—P1—C7—C8	−128.5 (3)
O2—P1—C13—C18	−46.2 (3)	C13—P1—C7—C12	53.5 (3)
C2—P1—C7—C8	117.7 (3)	C13—C14—C15—C16	−1.0 (7)
C2—P1—C7—C12	−60.4 (3)	C14—C13—C18—C17	0.0 (6)
C2—P1—C13—C14	5.8 (4)	C14—C15—C16—C17	0.3 (7)
C2—P1—C13—C18	−175.8 (3)	C15—C16—C17—C18	0.5 (7)
C2—C1—C3—C4	167.2 (5)	C16—C17—C18—C13	−0.7 (6)
C2—C1—C3—C5	−74.1 (5)	C18—C13—C14—C15	0.8 (6)
C2—C1—C3—C6	46.5 (5)		

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

Cg1 is the centroid of ring C7–C12.

$D\cdots H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C2—H2B \cdots O2 ⁱ	0.99	2.19	3.176 (5)	176
C12—H12 \cdots O2 ⁱ	0.95	2.53	3.373 (5)	148
C17—H17 \cdots Cg1 ⁱⁱ	0.95	2.80	3.721 (5)	164

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