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Redetermination of bis(diphenylphosphino)methane at 293 (2) K

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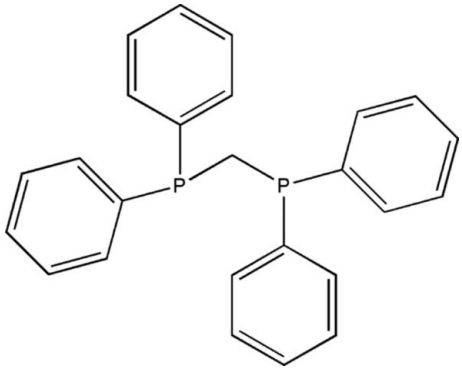
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.049; wR factor = 0.120; data-to-parameter ratio = 21.2.

The structure of the title compound, $C_{25}H_{22}P_2$, at 293 K is isostructural with those determined at 153 K [Di Nicola, Effendy, Fazaroh, Pettinari, Skelton, Somers & White (2005), *Inorg. Chim. Acta*, **358**, 720–734] and 233 K [Schmidbaur, Reber, Schier, Wagner & Muller (1998), *Inorg. Chim. Acta*, **147**, 143–150]. The diphenylphosphine groups are staggered relative to the PCP backbone such that the lone pairs are at an angle of 75.12 (7)° to each other. There are no classical intermolecular interactions.

Related literature

For related literature, see: Allen (2002); de Carvalho *et al.* (1999); Di Nicola *et al.* (2005); Martin & Orpen (1996); Peppe (2004); Powell (1989).



Experimental

Crystal data

$C_{25}H_{22}P_2$
M_r = 384.37
Orthorhombic, *Pbca*
a = 9.8918 (3) Å
b = 10.3368 (4) Å
c = 40.9389 (15) Å
V = 4186.0 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 293 (2) K
0.24 × 0.24 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2006)
T_{min} = 0.840, T_{max} = 1
18346 measured reflections
5171 independent reflections
2927 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.120
S = 1.16
5171 reflections
244 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

*Cg*1 and *Cg*2 are the centroids defined by the atoms C1/C211/C221 and C1/C11/C121, respectively.

P1—C1	1.8463 (19)	P1—C121	1.836 (2)
P2—C1	1.855 (2)	P2—C211	1.841 (2)
P1—C111	1.827 (2)	P2—C221	1.829 (2)
P1—C1—P2	107.63 (10)	C1—P2—C221	103.17 (9)
C1—P1—C111	103.12 (10)	C111—P1—C121	101.98 (9)
C1—P1—C121	101.53 (9)	C211—P2—C221	101.22 (9)
C1—P2—C211	99.94 (9)		
P2—C1—P1—C111	82.33 (11)	P1—C1—P2—C221	−168.57 (10)
P2—C1—P1—C121	−172.30 (10)	P1—C1—P2···*Cg*1	138.70 (12)
P1—C1—P2—C211	87.31 (11)	P2—C1—P1···*Cg*2	135.46 (12)

Data collection: *APEX2*, *BIS* and *COSMO* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT* and *SADABS* (Bruker, 2006); program(s) used to solve structure: *SHELXTL* (Bruker, 2006); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2359).

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supplementary materials

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Redetermination of bis(diphenylphosphino)methane at 293 (2) K

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Comment

Bis(diphenylphosphino)methane, (I), is a ubiquitous ligand in organometallic chemistry, with 1988 compounds reported in the Cambridge Structural Data base (Version 5.28, January, 2007; Allen, 2002). Its crystal structure has been previously determined at 153 K (Di Nicola *et al.*, 2005) and 233 K (Schmidbauer *et al.*, 1998). We present here the structure of the title compound at 293 K, where the precision of the geometric parameters is slightly improved.

The structure of the title compound at 293 K (Fig. 1) is isostructural with those determined at 153 K and 233 K. The bond lengths and angles are as expected (Table 1). Each of the diphenylphosphine moieties adopts a *gauche* conformation relative to the bridging methylene group, with the P atom lone pair pointing in the direction opposite to the methylene H atoms. The resulting configuration forms a nearly planar `W' made up of atoms C121—P1—C1—P2—C222, with two phenyl groups positioned on the plane but only somewhat one coplanar, and two positioned on either side of the plane, as indicated by the P—C—P—C torsion angles (Table 1).

The vector defined by the P atom and the centroid of the *ipso*-C atoms of the organic groups bound to the P atom can be used to estimate the vector between the P atom and its lone pair for phosphines (Powell, 1989; Martin & Orpen, 1996). The angle between the vectors P1···centroid(C_{ipso})$_3$ and P2···centroid(C_{ipso})$_3$ is 75.12 (7)°.

There are no intermolecular interactions in the crystal structure of (I). The phenyl groups pack in a herring-bone pattern (Fig. 2).

Experimental

The title compound was obtained unintentionally as colourless blocks by the slow evaporation of tetrahydrofuran from a solution of the white powder precipitated from the reaction of dibromo-bromomethyl-indium(III) (de Carvalho *et al.*, 1999; Peppe, 2004) with bis(diphenylphosphino)methane monoxide in dioxane.

Refinement

All H atoms were located in a difference Fourier map and were placed in idealized positions and refined using a riding model, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for phenyl H atoms and C—H = 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) for methylene H atoms.

Figures

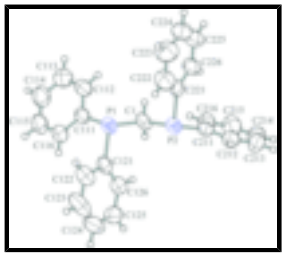

Fig. 1. A view of (I) at 293 K, showing the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

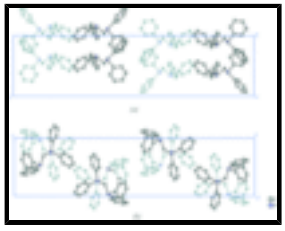

Fig. 2. Views parallel to (a) the a axis and (b) the b axis of the unit cell of (I). Molecules in front are shown with black outlines and those behind are shown with grey outlines; atoms have arbitrary radii.

bis(diphenylphosphino)methane

Crystal data

$C_{25}H_{22}P_2$	$D_x = 1.22$ Mg m^{-3}
$M_r = 384.37$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Orthorhombic, *Pbca*	Cell parameters from 2940 reflections
$a = 9.8918$ (3) Å	$\theta = 2.9$–23.0°
$b = 10.3368$ (4) Å	$\mu = 0.21$ mm^{-1}
$c = 40.9389$ (15) Å	$T = 293$ (2) K
$V = 4186.0$ (3) Å^3	Block, colourless
$Z = 8$	0.24 × 0.24 × 0.18 mm
$F_{000} = 1616$	

Data collection

Bruker SMART CCD area-detector diffractometer	2927 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.041$
$T = 293$(2) K	$\theta_{max} = 28.3^\circ$
φ and ω scans	$\theta_{min} = 2.9^\circ$
Absorption correction: multi-scan (SADABS; Bruker, 2006)	$h = -13 \rightarrow 10$
$T_{min} = 0.840$, $T_{max} = 1$	$k = -13 \rightarrow 13$
18346 measured reflections	$l = -48 \rightarrow 54$
5171 independent reflections	

Refinement

Refinement on F^2	H-atom parameters constrained

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.049$

$wR(F^2) = 0.120$

$S = 1.16$

5171 reflections

244 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

$w = 1/[\sigma^2(F_o^2) + (0.0432P)^2]$

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

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

$\Delta\rho_{max} = 0.30$ e Å^{-3}

$\Delta\rho_{min} = -0.20$ e Å^{-3}

Extinction correction: none

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2$sigma(F^2) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.8024 (2)	0.4568 (2)	0.12237 (5)	0.0592 (5)
H1A	0.7404	0.4616	0.1041	0.071*
H1B	0.8132	0.543	0.1314	0.071*
P1	0.96755 (6)	0.39319 (6)	0.108800 (12)	0.05699 (18)
P2	0.73568 (5)	0.34517 (6)	0.153963 (12)	0.05689 (18)
C111	0.9209 (2)	0.2701 (2)	0.07883 (4)	0.0564 (5)
C112	0.7969 (2)	0.2573 (2)	0.06361 (5)	0.0753 (7)
H112	0.728	0.3154	0.0686	0.09*
C113	0.7734 (3)	0.1599 (3)	0.04116 (6)	0.0982 (9)
H113	0.6888	0.1529	0.0314	0.118*
C114	0.8717 (5)	0.0747 (3)	0.03322 (7)	0.1090 (11)
H114	0.8555	0.0107	0.0177	0.131*
C115	0.9944 (4)	0.0834 (3)	0.04806 (7)	0.1048 (10)
H115	1.0621	0.0243	0.0429	0.126*
C116	1.0189 (3)	0.1797 (2)	0.07069 (6)	0.0801 (7)
H116	1.1031	0.184	0.0807	0.096*
C121	1.02816 (19)	0.5252 (2)	0.08259 (4)	0.0538 (5)
C122	1.0619 (2)	0.5114 (2)	0.04966 (5)	0.0628 (6)
H122	1.0501	0.4318	0.0395	0.075*
C123	1.1129 (2)	0.6149 (3)	0.03200 (5)	0.0766 (7)

H123	1.1345	0.6041	0.0101	0.092*
C124	1.1318 (2)	0.7329 (3)	0.04649 (7)	0.0846 (7)
H124	1.1655	0.8021	0.0345	0.102*
C125	1.1002 (3)	0.7479 (3)	0.07903 (7)	0.0867 (8)
H125	1.1129	0.8277	0.0891	0.104*
C126	1.0499 (2)	0.6454 (2)	0.09677 (5)	0.0714 (6)
H126	1.0299	0.6571	0.1188	0.086*
C211	0.8150 (2)	0.4150 (2)	0.19062 (4)	0.0526 (5)
C212	0.9291 (2)	0.3579 (3)	0.20334 (6)	0.0802 (7)
H212	0.9646	0.2849	0.1932	0.096*
C213	0.9921 (3)	0.4073 (3)	0.23097 (7)	0.0996 (9)
H213	1.0698	0.3681	0.2391	0.12*
C214	0.9397 (3)	0.5135 (3)	0.24619 (6)	0.0900 (9)
H214	0.981	0.5455	0.2649	0.108*
C215	0.8273 (3)	0.5730 (3)	0.23410 (6)	0.0865 (8)
H215	0.7923	0.646	0.2443	0.104*
C216	0.7658 (2)	0.5235 (2)	0.20641 (5)	0.0692 (6)
H216	0.6892	0.5644	0.1982	0.083*
C221	0.5605 (2)	0.3984 (2)	0.15895 (4)	0.0568 (5)
C222	0.5074 (2)	0.5138 (2)	0.14730 (5)	0.0695 (6)
H222	0.5635	0.5711	0.1362	0.083*
C223	0.3728 (3)	0.5455 (3)	0.15183 (6)	0.0864 (8)
H223	0.3398	0.6238	0.144	0.104*
C224	0.2882 (3)	0.4627 (4)	0.16777 (7)	0.0928 (9)
H224	0.1976	0.484	0.1705	0.111*
C225	0.3374 (3)	0.3469 (3)	0.17984 (6)	0.0885 (8)
H225	0.2802	0.2903	0.1908	0.106*
C226	0.4733 (2)	0.3153 (2)	0.17545 (5)	0.0693 (6)
H226	0.5061	0.2375	0.1837	0.083*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0728 (14)	0.0612 (14)	0.0436 (10)	0.0072 (11)	0.0088 (9)	−0.0010 (9)
P1	0.0604 (3)	0.0673 (4)	0.0432 (3)	0.0049 (3)	0.0014 (2)	0.0001 (3)
P2	0.0648 (4)	0.0594 (4)	0.0464 (3)	−0.0003 (3)	0.0049 (2)	−0.0015 (3)
C111	0.0624 (13)	0.0606 (14)	0.0462 (11)	0.0033 (11)	0.0105 (10)	0.0032 (9)
C112	0.0679 (15)	0.0940 (19)	0.0641 (14)	−0.0084 (13)	0.0102 (12)	−0.0125 (13)
C113	0.100 (2)	0.122 (3)	0.0720 (17)	−0.0489 (19)	0.0117 (15)	−0.0204 (18)
C114	0.172 (4)	0.084 (2)	0.0704 (19)	−0.038 (2)	0.032 (2)	−0.0190 (15)
C115	0.164 (3)	0.074 (2)	0.0755 (18)	0.027 (2)	0.035 (2)	−0.0087 (15)
C116	0.0928 (18)	0.0824 (19)	0.0652 (14)	0.0204 (15)	0.0094 (12)	−0.0022 (13)
C121	0.0511 (11)	0.0643 (15)	0.0461 (10)	0.0031 (10)	0.0019 (9)	−0.0016 (9)
C122	0.0674 (14)	0.0672 (16)	0.0539 (12)	−0.0025 (11)	0.0084 (10)	−0.0040 (11)
C123	0.0845 (17)	0.088 (2)	0.0571 (13)	−0.0011 (14)	0.0175 (12)	0.0061 (13)
C124	0.0933 (19)	0.0726 (19)	0.0879 (18)	−0.0035 (15)	0.0238 (14)	0.0098 (15)
C125	0.0991 (19)	0.0681 (18)	0.0930 (19)	−0.0101 (15)	0.0133 (15)	−0.0110 (14)
C126	0.0867 (17)	0.0712 (17)	0.0562 (12)	−0.0049 (13)	0.0094 (11)	−0.0086 (12)

C211	0.0523 (12)	0.0606 (14)	0.0450 (10)	−0.0053 (10)	0.0059 (9)	0.0076 (9)
C212	0.0807 (17)	0.0864 (19)	0.0734 (15)	0.0126 (14)	−0.0096 (13)	−0.0005 (13)
C213	0.0875 (19)	0.123 (3)	0.088 (2)	0.0104 (18)	−0.0303 (16)	0.0082 (19)
C214	0.089 (2)	0.127 (3)	0.0545 (14)	−0.0161 (18)	−0.0143 (13)	−0.0048 (15)
C215	0.0851 (18)	0.109 (2)	0.0659 (15)	−0.0035 (16)	−0.0066 (14)	−0.0264 (14)
C216	0.0660 (14)	0.0867 (18)	0.0550 (12)	0.0042 (12)	−0.0044 (11)	−0.0086 (12)
C221	0.0594 (13)	0.0693 (15)	0.0417 (10)	−0.0097 (11)	−0.0016 (9)	−0.0059 (10)
C222	0.0576 (14)	0.0847 (18)	0.0662 (14)	0.0012 (13)	−0.0001 (10)	0.0054 (12)
C223	0.0724 (17)	0.109 (2)	0.0774 (16)	0.0110 (16)	−0.0011 (13)	0.0039 (15)
C224	0.0590 (16)	0.137 (3)	0.0826 (18)	−0.0002 (18)	−0.0035 (14)	−0.0097 (19)
C225	0.0703 (17)	0.115 (2)	0.0800 (17)	−0.0315 (17)	0.0130 (14)	−0.0094 (17)
C226	0.0729 (15)	0.0776 (18)	0.0574 (13)	−0.0116 (13)	−0.0001 (11)	−0.0066 (11)

Geometric parameters (Å, °)

P1—C1	1.8463 (19)	C124—H124	0.93
P2—C1	1.855 (2)	C125—C126	1.378 (3)
C1—H1A	0.97	C125—H125	0.93
C1—H1B	0.97	C126—H126	0.93
P1—C111	1.827 (2)	C211—C212	1.376 (3)
P1—C121	1.836 (2)	C211—C216	1.383 (3)
P2—C211	1.841 (2)	C212—C213	1.389 (3)
P2—C221	1.829 (2)	C212—H212	0.93
C111—C112	1.382 (3)	C213—C214	1.365 (4)
C111—C116	1.387 (3)	C213—H213	0.93
C112—C113	1.384 (3)	C214—C215	1.364 (3)
C112—H112	0.93	C214—H214	0.93
C113—C114	1.351 (4)	C215—C216	1.384 (3)
C113—H113	0.93	C215—H215	0.93
C114—C115	1.361 (4)	C216—H216	0.93
C114—H114	0.93	C221—C222	1.388 (3)
C115—C116	1.381 (4)	C221—C226	1.392 (3)
C115—H115	0.93	C222—C223	1.384 (3)
C116—H116	0.93	C222—H222	0.93
C121—C126	1.389 (3)	C223—C224	1.364 (4)
C121—C122	1.396 (3)	C223—H223	0.93
C122—C123	1.386 (3)	C224—C225	1.384 (4)
C122—H122	0.93	C224—H224	0.93
C123—C124	1.369 (3)	C225—C226	1.394 (3)
C123—H123	0.93	C225—H225	0.93
C124—C125	1.377 (3)	C226—H226	0.93
P1—C1—P2	107.63 (10)	C126—C125—C124	120.3 (2)
P1—C1—H1A	110.2	C126—C125—H125	119.8
P2—C1—H1A	110.2	C124—C125—H125	119.8
P1—C1—H1B	110.2	C125—C126—C121	121.6 (2)
P2—C1—H1B	110.2	C125—C126—H126	119.2
H1A—C1—H1B	108.5	C121—C126—H126	119.2
C1—P1—C111	103.12 (10)	C212—C211—C216	117.3 (2)
C1—P1—C121	101.53 (9)	C212—C211—P2	119.32 (17)

C1—P2—C211	99.94 (9)	C216—C211—P2	123.34 (16)
C1—P2—C221	103.17 (9)	C211—C212—C213	121.3 (2)
C111—P1—C121	101.98 (9)	C211—C212—H212	119.4
C211—P2—C221	101.22 (9)	C213—C212—H212	119.4
C112—C111—C116	116.6 (2)	C214—C213—C212	119.8 (3)
C112—C111—P1	126.39 (17)	C214—C213—H213	120.1
C116—C111—P1	117.01 (17)	C212—C213—H213	120.1
C111—C112—C113	121.2 (2)	C215—C214—C213	120.4 (2)
C111—C112—H112	119.4	C215—C214—H214	119.8
C113—C112—H112	119.4	C213—C214—H214	119.8
C114—C113—C112	120.9 (3)	C214—C215—C216	119.2 (3)
C114—C113—H113	119.6	C214—C215—H215	120.4
C112—C113—H113	119.6	C216—C215—H215	120.4
C113—C114—C115	119.5 (3)	C211—C216—C215	121.9 (2)
C113—C114—H114	120.3	C211—C216—H216	119.1
C115—C114—H114	120.3	C215—C216—H216	119.1
C114—C115—C116	120.2 (3)	C222—C221—C226	117.6 (2)
C114—C115—H115	119.9	C222—C221—P2	125.34 (16)
C116—C115—H115	119.9	C226—C221—P2	117.10 (18)
C115—C116—C111	121.6 (3)	C223—C222—C221	121.4 (2)
C115—C116—H116	119.2	C223—C222—H222	119.3
C111—C116—H116	119.2	C221—C222—H222	119.3
C126—C121—C122	117.2 (2)	C224—C223—C222	120.4 (3)
C126—C121—P1	118.13 (15)	C224—C223—H223	119.8
C122—C121—P1	124.51 (17)	C222—C223—H223	119.8
C123—C122—C121	120.8 (2)	C223—C224—C225	119.9 (2)
C123—C122—H122	119.6	C223—C224—H224	120.1
C121—C122—H122	119.6	C225—C224—H224	120.1
C124—C123—C122	120.8 (2)	C224—C225—C226	119.7 (2)
C124—C123—H123	119.6	C224—C225—H225	120.1
C122—C123—H123	119.6	C226—C225—H225	120.1
C123—C124—C125	119.2 (2)	C221—C226—C225	121.0 (2)
C123—C124—H124	120.4	C221—C226—H226	119.5
C125—C124—H124	120.4	C225—C226—H226	119.5
P2—C1—P1—C111	82.33 (11)	C124—C125—C126—C121	−0.6 (4)
P2—C1—P1—C121	−172.30 (10)	C122—C121—C126—C125	1.2 (3)
P1—C1—P2—C211	87.31 (11)	P1—C121—C126—C125	177.45 (19)
P1—C1—P2—C221	−168.57 (10)	C221—P2—C211—C212	153.94 (18)
P1—C1—P2—Cg1	138.70 (12)	C1—P2—C211—C212	−100.36 (18)
P2—C1—P1—Cg2	135.46 (12)	C221—P2—C211—C216	−26.07 (19)
C121—P1—C111—C112	−88.10 (19)	C1—P2—C211—C216	79.64 (18)
C1—P1—C111—C112	16.9 (2)	C216—C211—C212—C213	0.1 (3)
C121—P1—C111—C116	92.48 (17)	P2—C211—C212—C213	−179.9 (2)
C1—P1—C111—C116	−162.49 (16)	C211—C212—C213—C214	0.8 (4)
C116—C111—C112—C113	−0.7 (3)	C212—C213—C214—C215	−1.2 (4)
P1—C111—C112—C113	179.87 (18)	C213—C214—C215—C216	0.8 (4)
C111—C112—C113—C114	−0.6 (4)	C212—C211—C216—C215	−0.5 (3)
C112—C113—C114—C115	1.4 (4)	P2—C211—C216—C215	179.48 (18)
C113—C114—C115—C116	−0.9 (4)	C214—C215—C216—C211	0.1 (4)

C114—C115—C116—C111	−0.4 (4)	C211—P2—C221—C222	89.39 (18)
C112—C111—C116—C115	1.2 (3)	C1—P2—C221—C222	−13.7 (2)
P1—C111—C116—C115	−179.32 (18)	C211—P2—C221—C226	−91.44 (16)
C111—P1—C121—C126	168.52 (16)	C1—P2—C221—C226	165.43 (15)
C1—P1—C121—C126	62.25 (18)	C226—C221—C222—C223	0.0 (3)
C111—P1—C121—C122	−15.51 (19)	P2—C221—C222—C223	179.12 (17)
C1—P1—C121—C122	−121.78 (17)	C221—C222—C223—C224	−0.6 (4)
C126—C121—C122—C123	−1.0 (3)	C222—C223—C224—C225	0.8 (4)
P1—C121—C122—C123	−177.01 (17)	C223—C224—C225—C226	−0.4 (4)
C121—C122—C123—C124	0.3 (3)	C222—C221—C226—C225	0.5 (3)
C122—C123—C124—C125	0.3 (4)	P2—C221—C226—C225	−178.78 (16)
C123—C124—C125—C126	−0.2 (4)	C224—C225—C226—C221	−0.3 (3)

Fig. 1

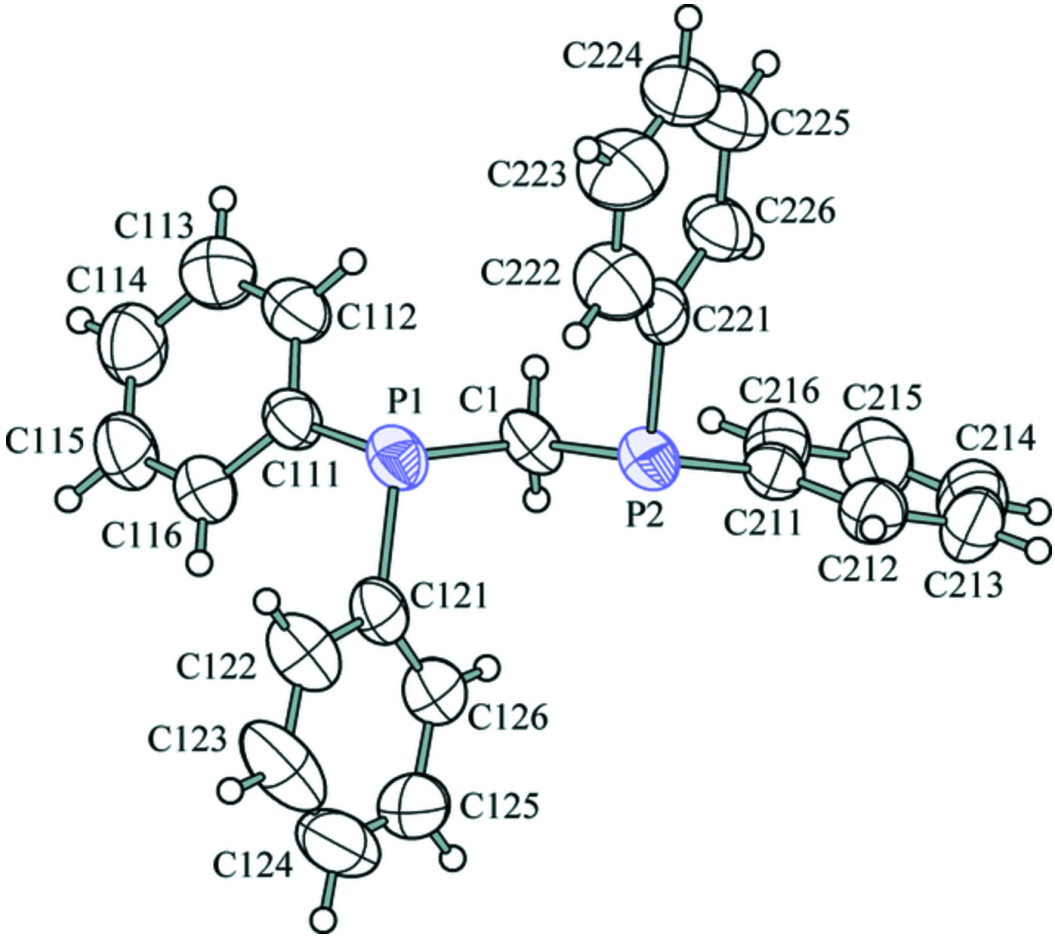
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Fig. 2