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(*R*)-3,3′-Diphenyl-5,6,7,8,5′,6′,7′,8′-octahydro-1,1′-binaphthyl-2,2′-diyl chlorophosphate

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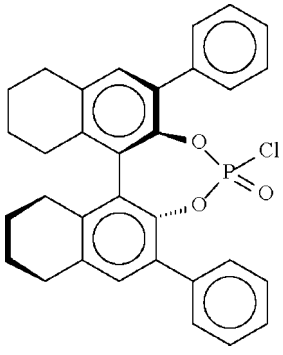
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.036; wR factor = 0.099; data-to-parameter ratio = 16.5.

The two fused ring systems in the 1,1′-bi-2-naphthol derivative title compound, $C_{32}H_{28}ClO_3P$, are twisted by 61.1 (1)° about the linking C—C bond, thus conferring chirality on the molecule. In one of the fused ring systems, the four-atom aliphatic chain is disordered over two sites in a 0.5:0.5 ratio.

Related literature

For a report on the enantioselective catalytic property of the related 3,3′-diphenyl-5,6,7,8,5′,6′,7′,8′-octahydro-[1,1′]-binaphthalenyl-2,2′-phosphate, see Chen *et al.* (2006). For a report on the synthesis of the 3,3′-diphenyl-5,6,7,8,5′,6′,7′,8′-octahydro-[1,1′]-binaphthalenyl-2,2′-diol reactant, see McDougal & Schaus (2003).



Experimental

Crystal data

$C_{32}H_{28}ClO_3P$
M_r = 526.96
Orthorhombic, $P2_12_12_1$
a = 12.6642 (8) Å
b = 13.1613 (8) Å
c = 15.9097 (9) Å
V = 2651.8 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 295 (2) K
0.32 × 0.17 × 0.07 mm

Data collection

Bruker APEX CCD diffractometer
Absorption correction: none
33491 measured reflections
6089 independent reflections
4949 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.099
S = 1.03
6089 reflections
370 parameters
52 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}
Absolute structure: Flack (1983), with 2674 Friedel pairs
Flack parameter: 0.02 (6)

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); 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: HB2462).

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supplementary materials

Acta Cryst. (2007). E**63**, o3359 [**doi:10.1107/S1600536807031479**]

(*R*)-3,3'-Diphenyl-5,6,7,8,5',6',7',8'-octahydro-1,1'-binaphthyl-2,2'-diyl chlorophosphate

Y.-P. Li and S. W. Ng

Comment

3,3'-Diphenyl-5,6,7,8,5',6',7',8'-octahydro-[1,1']-binaphthalenyl-2,2'-phosphate is a highly enantioselective catalyst (Chen *et al.*, 2006) as is starting reactant 3,3'-diphenyl-5,6,7,8,5',6',7',8'-octahydro-[1,1']-binaphthalenyl-2,2'-diol (McDougal & Schaus, 2003). The reaction of the diol with phosphorus oxychloride has yielded the title chlorophosphate, (I), (Fig. 1) which is also expected to exhibit such activity.

Experimental

To a solution of (*R*)-3,3'-diphenyl-5,6,7,8,5',6',7',8'-octahydro-[1,1'] binaphthalenyl-2,2'-diol (2 mmol) in pyridine (5 ml) was added phosphorus oxychloride (4.0 mmol) at room temperature under nitrogen. The mixture was stirred at 343 K for 3 h. The solvent was then removed and the product purified by column chromatography on silica gel. Colorless blocks of (I) were obtained by recrystallization from ethanol.

Refinement

The aliphatic portion of one of the two ten-membered fused rings is disordered over two sites. Its carbon-carbon distances were restrained to within 1.50±0.01 Å, and the U^{ij} values were restrained to nearly isotropic behaviour. As the disorder refined to nearly 50:50, the ratio was fixed as 50:50.

The carbon-bound H-atoms were generated geometrically (C–H 0.93 – 0.97 Å), and were included in the refinement in the riding model approximation, with U(H) set to 1.2U_{eq}(C,*O*).

The configuration in the studied crystal is the *R*-enantiomer.

Figures

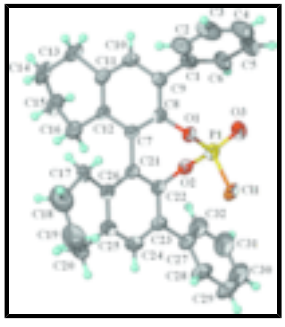


Fig. 1. **Figure 1**. View of the molecular structure of (I) with displacement ellipsoids drawn at the 50% probability level (H atoms as spheres of arbitrary radius). The disorder is not shown.

(*R*)-3,3'-Diphenyl-5,6,7,8,5',6',7',8'-octahydro-1,1'-binaphthyl- 2,2'-diyl chlorophosphate

Crystal data

$C_{32}H_{28}ClO_3P$	F_{000} = 1104
M_r = 526.96	D_x = 1.320 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2ac ab	Cell parameters from 7841 reflections
a = 12.6642 (8) Å	θ = 2.2–23.6º
b = 13.1613 (8) Å	μ = 0.24 mm^{-1}
c = 15.9097 (9) Å	T = 295 (2) K
V = 2651.8 (3) Å^3	Block, colorless
Z = 4	0.32 × 0.17 × 0.07 mm

Data collection

Bruker APEX CCD diffractometer	4949 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.032
Monochromator: graphite	θ_{max} = 27.5º
T = 295(2) K	θ_{min} = 2.2º
φ and ω scans	h = −16→16
Absorption correction: None	k = −17→16
33491 measured reflections	l = −20→20
6089 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.037	$w = 1/[\sigma^2(F_o^2) + (0.0547P)^2 + 0.1321P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.099	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.03	$\Delta\rho_{max}$ = 0.16 e Å^{-3}
6089 reflections	$\Delta\rho_{min}$ = −0.23 e Å^{-3}
370 parameters	Extinction correction: none
52 restraints	Absolute structure: Flack (1983), 2674 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.02 (6)
Secondary atom site location: difference Fourier map	

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)

Cl1	0.69670 (4)	0.39625 (5)	0.93762 (4)	0.06273 (16)	
P1	0.82905 (4)	0.40064 (4)	0.87055 (3)	0.04711 (13)	
O1	0.88918 (10)	0.30781 (10)	0.91181 (8)	0.0459 (3)	
O2	0.89086 (10)	0.49825 (10)	0.89966 (8)	0.0464 (3)	
O3	0.81117 (12)	0.39828 (14)	0.78038 (9)	0.0666 (4)	
C1	0.99403 (18)	0.15174 (17)	0.81908 (14)	0.0541 (5)	
C2	1.0106 (2)	0.0517 (2)	0.84163 (17)	0.0743 (7)	
H2	1.0603	0.0361	0.8827	0.089*	
C3	0.9543 (3)	−0.0251 (2)	0.8038 (2)	0.0937 (9)	
H3	0.9651	−0.0921	0.8205	0.112*	
C4	0.8838 (3)	−0.0043 (3)	0.7430 (2)	0.0931 (10)	
H4	0.8458	−0.0568	0.7181	0.112*	
C5	0.8675 (3)	0.0940 (3)	0.71751 (18)	0.0898 (9)	
H5	0.8198	0.1078	0.6746	0.108*	
C6	0.9218 (2)	0.1723 (2)	0.75553 (16)	0.0727 (7)	
H6	0.9100	0.2390	0.7386	0.087*	
C7	1.05299 (14)	0.37665 (14)	0.96221 (11)	0.0398 (4)	
C8	1.00118 (14)	0.30754 (15)	0.91088 (11)	0.0420 (4)	
C9	1.05190 (15)	0.23363 (15)	0.86370 (12)	0.0456 (4)	
C10	1.16196 (16)	0.23720 (16)	0.86518 (13)	0.0497 (5)	
H10	1.1995	0.1878	0.8360	0.060*	
C11	1.21748 (15)	0.31100 (17)	0.90821 (12)	0.0477 (5)	
C12	1.16399 (14)	0.38174 (15)	0.95733 (11)	0.0445 (4)	
C13	1.33695 (16)	0.3147 (2)	0.89788 (15)	0.0648 (6)	
H13A	1.3655	0.2481	0.9108	0.078*	
H13B	1.3531	0.3292	0.8395	0.078*	
C14	1.39153 (16)	0.3922 (2)	0.95210 (17)	0.0703 (7)	
H14A	1.4026	0.3639	1.0077	0.084*	
H14B	1.4602	0.4075	0.9282	0.084*	
C15	1.32899 (18)	0.4890 (2)	0.95974 (18)	0.0704 (7)	
H15A	1.3185	0.5185	0.9045	0.085*	
H15B	1.3677	0.5376	0.9937	0.085*	
C16	1.22350 (17)	0.46740 (19)	0.99976 (16)	0.0612 (6)	
H16A	1.1807	0.5285	0.9978	0.073*	
H16B	1.2344	0.4501	1.0584	0.073*	
C17	1.0695 (7)	0.3533 (7)	1.1426 (6)	0.050 (2)	0.50
H17A	1.0431	0.2891	1.1214	0.059*	0.50
H17B	1.1425	0.3604	1.1251	0.059*	0.50
C18	1.0632 (9)	0.3543 (9)	1.2377 (6)	0.126 (5)	0.50
H18A	1.1287	0.3832	1.2583	0.152*	0.50
H18B	1.0614	0.2841	1.2562	0.152*	0.50
C19	0.9729 (7)	0.4097 (7)	1.2819 (5)	0.092 (2)	0.50
H19A	0.9066	0.3754	1.2707	0.111*	0.50
H19B	0.9846	0.4098	1.3422	0.111*	0.50
C20	0.9683 (8)	0.5169 (7)	1.2499 (5)	0.068 (3)	0.50
H20A	1.0353	0.5512	1.2585	0.081*	0.50
H20B	0.9132	0.5550	1.2782	0.081*	0.50
C17'	1.0817 (8)	0.3751 (8)	1.1556 (6)	0.067 (3)	0.50
H17C	1.1062	0.3204	1.1197	0.081*	0.50

H17D	1.1425	0.4161	1.1706	0.081*	0.50
C18'	1.0346 (6)	0.3299 (5)	1.2351 (4)	0.0596 (18)	0.50
H18C	0.9663	0.2989	1.2249	0.072*	0.50
H18D	1.0814	0.2808	1.2611	0.072*	0.50
C19'	1.0257 (6)	0.4258 (5)	1.2857 (4)	0.078 (2)	0.50
H19C	1.0103	0.4092	1.3438	0.094*	0.50
H19D	1.0922	0.4623	1.2840	0.094*	0.50
C20'	0.9400 (7)	0.4909 (8)	1.2510 (5)	0.068 (3)	0.50
H20C	0.9433	0.5568	1.2781	0.081*	0.50
H20D	0.8725	0.4606	1.2653	0.081*	0.50
C21	0.99091 (14)	0.44335 (15)	1.01926 (12)	0.0407 (4)	
C22	0.91440 (14)	0.50784 (14)	0.98597 (12)	0.0424 (4)	
C23	0.85660 (15)	0.57704 (15)	1.03315 (14)	0.0490 (5)	
C24	0.87462 (17)	0.57417 (18)	1.11978 (15)	0.0592 (6)	
H24	0.8384	0.6195	1.1541	0.071*	
C25	0.94419 (17)	0.50649 (18)	1.15635 (12)	0.0585 (6)	
C26	1.00400 (15)	0.44054 (16)	1.10670 (12)	0.0484 (5)	
C27	0.77742 (17)	0.64701 (16)	0.99610 (17)	0.0581 (6)	
C28	0.6822 (2)	0.6646 (2)	1.0379 (2)	0.0778 (8)	
H28	0.6687	0.6319	1.0886	0.093*	
C29	0.6082 (2)	0.7297 (3)	1.0048 (3)	0.1066 (12)	
H29	0.5449	0.7405	1.0331	0.128*	
C30	0.6273 (3)	0.7787 (3)	0.9303 (3)	0.1088 (13)	
H30	0.5763	0.8215	0.9076	0.131*	
C31	0.7210 (3)	0.7649 (2)	0.8894 (2)	0.0928 (10)	
H31	0.7350	0.8002	0.8399	0.111*	
C32	0.7958 (2)	0.69762 (18)	0.92191 (18)	0.0714 (7)	
H32	0.8587	0.6869	0.8931	0.086*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0366 (2)	0.0759 (4)	0.0756 (3)	0.0012 (3)	0.0016 (2)	0.0015 (3)
P1	0.0374 (2)	0.0571 (3)	0.0468 (3)	0.0049 (2)	−0.0062 (2)	−0.0003 (2)
O1	0.0359 (6)	0.0487 (8)	0.0532 (8)	0.0021 (6)	−0.0048 (6)	−0.0029 (6)
O2	0.0410 (7)	0.0504 (8)	0.0476 (7)	0.0046 (6)	−0.0005 (5)	0.0040 (6)
O3	0.0625 (9)	0.0863 (11)	0.0510 (8)	0.0101 (9)	−0.0140 (7)	−0.0041 (8)
C1	0.0601 (12)	0.0541 (13)	0.0482 (12)	0.0031 (10)	0.0055 (10)	−0.0119 (10)
C2	0.0904 (19)	0.0542 (15)	0.0783 (18)	0.0092 (13)	−0.0051 (14)	−0.0167 (13)
C3	0.128 (3)	0.0570 (16)	0.096 (2)	0.0008 (18)	0.003 (2)	−0.0223 (15)
C4	0.108 (2)	0.082 (2)	0.089 (2)	−0.0242 (18)	0.0082 (19)	−0.0389 (17)
C5	0.099 (2)	0.097 (2)	0.0735 (17)	−0.0095 (19)	−0.0192 (15)	−0.0266 (17)
C6	0.0865 (18)	0.0690 (16)	0.0626 (15)	−0.0006 (14)	−0.0148 (13)	−0.0146 (12)
C7	0.0365 (8)	0.0427 (10)	0.0403 (9)	0.0039 (7)	−0.0010 (7)	0.0008 (7)
C8	0.0359 (9)	0.0480 (11)	0.0421 (10)	0.0041 (8)	−0.0029 (7)	−0.0002 (8)
C9	0.0485 (10)	0.0461 (11)	0.0423 (10)	0.0068 (8)	−0.0019 (9)	−0.0021 (8)
C10	0.0509 (11)	0.0513 (11)	0.0470 (11)	0.0162 (9)	0.0059 (9)	−0.0005 (9)
C11	0.0387 (9)	0.0582 (12)	0.0463 (10)	0.0090 (9)	0.0007 (8)	0.0103 (9)

C12	0.0354 (8)	0.0522 (11)	0.0458 (10)	0.0026 (8)	−0.0010 (7)	0.0024 (8)
C13	0.0395 (10)	0.0830 (17)	0.0720 (15)	0.0167 (11)	0.0080 (10)	0.0097 (13)
C14	0.0356 (10)	0.0850 (17)	0.0901 (17)	0.0012 (12)	−0.0020 (10)	0.0225 (15)
C15	0.0482 (12)	0.0728 (16)	0.0902 (18)	−0.0076 (11)	−0.0053 (12)	0.0125 (13)
C16	0.0432 (11)	0.0640 (14)	0.0763 (14)	−0.0081 (10)	−0.0002 (10)	−0.0099 (12)
C17	0.041 (3)	0.065 (4)	0.043 (4)	0.001 (3)	−0.008 (2)	−0.003 (3)
C18	0.166 (9)	0.137 (8)	0.076 (5)	0.039 (7)	−0.013 (6)	−0.010 (5)
C19	0.108 (5)	0.121 (6)	0.048 (3)	−0.048 (5)	−0.002 (4)	0.003 (3)
C20	0.069 (5)	0.089 (6)	0.045 (3)	−0.006 (4)	0.006 (3)	−0.016 (3)
C17'	0.072 (5)	0.085 (6)	0.045 (4)	0.011 (4)	−0.012 (3)	−0.001 (4)
C18'	0.075 (3)	0.058 (3)	0.046 (3)	−0.021 (3)	−0.015 (3)	0.014 (2)
C19'	0.081 (4)	0.099 (5)	0.053 (3)	−0.017 (4)	−0.010 (3)	−0.012 (3)
C20'	0.071 (5)	0.084 (6)	0.048 (4)	−0.010 (4)	0.005 (3)	−0.016 (3)
C21	0.0337 (8)	0.0426 (10)	0.0459 (10)	−0.0023 (8)	0.0018 (7)	−0.0036 (8)
C22	0.0345 (8)	0.0467 (11)	0.0459 (10)	−0.0032 (8)	0.0018 (7)	−0.0008 (8)
C23	0.0385 (9)	0.0420 (11)	0.0664 (13)	0.0006 (8)	0.0041 (9)	−0.0078 (9)
C24	0.0507 (11)	0.0632 (14)	0.0636 (13)	0.0060 (10)	0.0095 (10)	−0.0188 (11)
C25	0.0500 (11)	0.0778 (16)	0.0477 (12)	0.0016 (11)	0.0022 (9)	−0.0139 (11)
C26	0.0415 (10)	0.0582 (13)	0.0456 (11)	0.0005 (9)	0.0002 (8)	−0.0038 (9)
C27	0.0485 (11)	0.0443 (11)	0.0814 (16)	0.0058 (9)	−0.0034 (11)	−0.0111 (11)
C28	0.0533 (13)	0.0681 (16)	0.112 (2)	0.0156 (12)	0.0060 (14)	−0.0163 (14)
C29	0.0623 (17)	0.091 (2)	0.166 (4)	0.0345 (17)	−0.009 (2)	−0.033 (2)
C30	0.083 (2)	0.069 (2)	0.175 (4)	0.0355 (17)	−0.043 (2)	−0.025 (2)
C31	0.101 (2)	0.0539 (16)	0.123 (3)	0.0139 (15)	−0.030 (2)	0.0059 (16)
C32	0.0642 (14)	0.0524 (14)	0.0977 (19)	0.0071 (12)	−0.0093 (13)	0.0046 (13)

Geometric parameters (Å, °)

Cl1—P1	1.9878 (7)	C17—H17B	0.9700
P1—O3	1.4526 (15)	C18—C19	1.528 (8)
P1—O2	1.5741 (14)	C18—H18A	0.9700
P1—O1	1.5822 (14)	C18—H18B	0.9700
O1—C8	1.418 (2)	C19—C20	1.501 (8)
O2—C22	1.411 (2)	C19—H19A	0.9700
C1—C2	1.381 (3)	C19—H19B	0.9700
C1—C6	1.390 (3)	C20—C25	1.525 (7)
C1—C9	1.484 (3)	C20—H20A	0.9700
C2—C3	1.376 (4)	C20—H20B	0.9700
C2—H2	0.9300	C17'—C18'	1.520 (8)
C3—C4	1.346 (5)	C17'—C26	1.522 (8)
C3—H3	0.9300	C17'—H17C	0.9700
C4—C5	1.371 (5)	C17'—H17D	0.9700
C4—H4	0.9300	C18'—C19'	1.502 (7)
C5—C6	1.379 (4)	C18'—H18C	0.9700
C5—H5	0.9300	C18'—H18D	0.9700
C6—H6	0.9300	C19'—C20'	1.489 (8)
C7—C8	1.387 (3)	C19'—H19C	0.9700
C7—C12	1.410 (2)	C19'—H19D	0.9700
C7—C21	1.487 (2)	C20'—C25	1.521 (7)

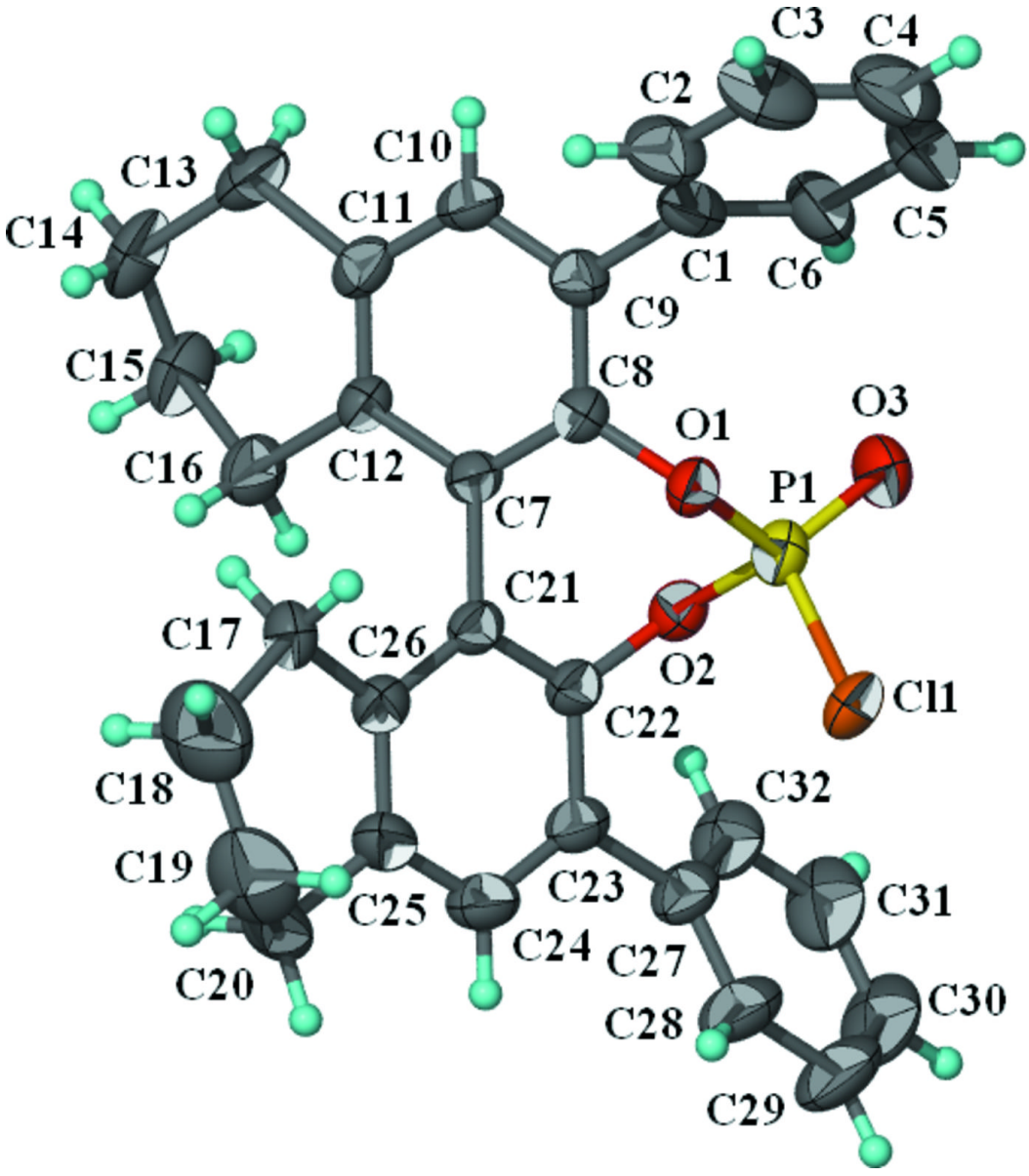
C8—C9	1.386 (3)	C20'—H20C	0.9700
C9—C10	1.395 (3)	C20'—H20D	0.9700
C10—C11	1.381 (3)	C21—C22	1.393 (3)
C10—H10	0.9300	C21—C26	1.401 (3)
C11—C12	1.391 (3)	C22—C23	1.389 (3)
C11—C13	1.523 (3)	C23—C24	1.398 (3)
C12—C16	1.515 (3)	C23—C27	1.484 (3)
C13—C14	1.505 (4)	C24—C25	1.381 (3)
C13—H13A	0.9700	C24—H24	0.9300
C13—H13B	0.9700	C25—C26	1.397 (3)
C14—C15	1.505 (3)	C27—C32	1.375 (4)
C14—H14A	0.9700	C27—C28	1.396 (3)
C14—H14B	0.9700	C28—C29	1.375 (4)
C15—C16	1.507 (3)	C28—H28	0.9300
C15—H15A	0.9700	C29—C30	1.371 (5)
C15—H15B	0.9700	C29—H29	0.9300
C16—H16A	0.9700	C30—C31	1.367 (5)
C16—H16B	0.9700	C30—H30	0.9300
C17—C18	1.514 (8)	C31—C32	1.396 (4)
C17—C26	1.528 (7)	C31—H31	0.9300
C17—H17A	0.9700	C32—H32	0.9300
O3—P1—O2	112.68 (9)	C19—C18—H18B	107.3
O3—P1—O1	117.92 (9)	H18A—C18—H18B	106.9
O2—P1—O1	105.59 (7)	C20—C19—C18	108.7 (8)
O3—P1—Cl1	113.46 (7)	C20—C19—H19A	110.0
O2—P1—Cl1	106.56 (6)	C18—C19—H19A	110.0
O1—P1—Cl1	99.24 (6)	C20—C19—H19B	110.0
C8—O1—P1	118.61 (13)	C18—C19—H19B	110.0
C22—O2—P1	117.68 (12)	H19A—C19—H19B	108.3
C2—C1—C6	118.3 (2)	C19—C20—C25	104.8 (6)
C2—C1—C9	119.5 (2)	C19—C20—H20A	110.8
C6—C1—C9	122.1 (2)	C25—C20—H20A	110.8
C3—C2—C1	120.5 (3)	C19—C20—H20B	110.8
C3—C2—H2	119.7	C25—C20—H20B	110.8
C1—C2—H2	119.7	H20A—C20—H20B	108.9
C4—C3—C2	120.6 (3)	C18'—C17'—C26	113.1 (7)
C4—C3—H3	119.7	C18'—C17'—H17C	109.0
C2—C3—H3	119.7	C26—C17'—H17C	109.0
C3—C4—C5	120.3 (3)	C18'—C17'—H17D	109.0
C3—C4—H4	119.8	C26—C17'—H17D	109.0
C5—C4—H4	119.8	H17C—C17'—H17D	107.8
C4—C5—C6	120.1 (3)	C19'—C18'—C17'	98.4 (7)
C4—C5—H5	120.0	C19'—C18'—H18C	112.1
C6—C5—H5	120.0	C17'—C18'—H18C	112.1
C5—C6—C1	120.1 (3)	C19'—C18'—H18D	112.1
C5—C6—H6	120.0	C17'—C18'—H18D	112.1
C1—C6—H6	120.0	H18C—C18'—H18D	109.7
C8—C7—C12	118.06 (17)	C20'—C19'—C18'	109.8 (7)
C8—C7—C21	119.75 (15)	C20'—C19'—H19C	109.7

C12—C7—C21	122.19 (16)	C18'—C19'—H19C	109.7
C9—C8—C7	124.03 (16)	C20'—C19'—H19D	109.7
C9—C8—O1	118.08 (17)	C18'—C19'—H19D	109.7
C7—C8—O1	117.72 (16)	H19C—C19'—H19D	108.2
C8—C9—C10	115.48 (18)	C19'—C20'—C25	114.8 (7)
C8—C9—C1	122.66 (17)	C19'—C20'—H20C	108.6
C10—C9—C1	121.74 (18)	C25—C20'—H20C	108.6
C11—C10—C9	122.75 (18)	C19'—C20'—H20D	108.6
C11—C10—H10	118.6	C25—C20'—H20D	108.6
C9—C10—H10	118.6	H20C—C20'—H20D	107.5
C10—C11—C12	120.08 (17)	C22—C21—C26	118.42 (17)
C10—C11—C13	118.4 (2)	C22—C21—C7	119.69 (16)
C12—C11—C13	121.5 (2)	C26—C21—C7	121.84 (17)
C11—C12—C7	118.99 (18)	C23—C22—C21	124.11 (18)
C11—C12—C16	120.40 (17)	C23—C22—O2	118.26 (17)
C7—C12—C16	120.46 (17)	C21—C22—O2	117.55 (16)
C14—C13—C11	114.6 (2)	C22—C23—C24	115.42 (19)
C14—C13—H13A	108.6	C22—C23—C27	123.27 (19)
C11—C13—H13A	108.6	C24—C23—C27	121.26 (19)
C14—C13—H13B	108.6	C25—C24—C23	122.48 (19)
C11—C13—H13B	108.6	C25—C24—H24	118.8
H13A—C13—H13B	107.6	C23—C24—H24	118.8
C15—C14—C13	112.25 (19)	C24—C25—C26	120.55 (19)
C15—C14—H14A	109.2	C24—C25—C20'	118.8 (4)
C13—C14—H14A	109.2	C26—C25—C20'	119.7 (4)
C15—C14—H14B	109.2	C24—C25—C20	118.7 (4)
C13—C14—H14B	109.2	C26—C25—C20	119.9 (5)
H14A—C14—H14B	107.9	C25—C26—C21	118.74 (18)
C14—C15—C16	109.9 (2)	C25—C26—C17'	114.4 (4)
C14—C15—H15A	109.7	C21—C26—C17'	126.8 (4)
C16—C15—H15A	109.7	C25—C26—C17	123.4 (4)
C14—C15—H15B	109.7	C21—C26—C17	117.1 (4)
C16—C15—H15B	109.7	C32—C27—C28	118.3 (2)
H15A—C15—H15B	108.2	C32—C27—C23	121.8 (2)
C15—C16—C12	113.2 (2)	C28—C27—C23	119.8 (2)
C15—C16—H16A	108.9	C29—C28—C27	120.7 (3)
C12—C16—H16A	108.9	C29—C28—H28	119.7
C15—C16—H16B	108.9	C27—C28—H28	119.7
C12—C16—H16B	108.9	C28—C29—C30	120.3 (3)
H16A—C16—H16B	107.8	C28—C29—H29	119.9
C18—C17—C26	109.8 (7)	C30—C29—H29	119.9
C18—C17—H17A	109.7	C31—C30—C29	120.2 (3)
C26—C17—H17A	109.7	C31—C30—H30	119.9
C18—C17—H17B	109.7	C29—C30—H30	119.9
C26—C17—H17B	109.7	C30—C31—C32	119.8 (3)
H17A—C17—H17B	108.2	C30—C31—H31	120.1
C17—C18—C19	120.3 (9)	C32—C31—H31	120.1
C17—C18—H18A	107.3	C27—C32—C31	120.7 (3)
C19—C18—H18A	107.3	C27—C32—H32	119.6

C17—C18—H18B	107.3	C31—C32—H32	119.6
O3—P1—O1—C8	84.18 (16)	C12—C7—C21—C26	−61.5 (3)
O2—P1—O1—C8	−42.76 (15)	C26—C21—C22—C23	6.4 (3)
Cl1—P1—O1—C8	−152.95 (12)	C7—C21—C22—C23	−176.17 (17)
O3—P1—O2—C22	−178.91 (13)	C26—C21—C22—O2	−170.31 (17)
O1—P1—O2—C22	−48.85 (13)	C7—C21—C22—O2	7.1 (2)
Cl1—P1—O2—C22	56.04 (13)	P1—O2—C22—C23	−105.79 (17)
C6—C1—C2—C3	−2.1 (4)	P1—O2—C22—C21	71.10 (18)
C9—C1—C2—C3	177.0 (2)	C21—C22—C23—C24	−4.2 (3)
C1—C2—C3—C4	1.5 (5)	O2—C22—C23—C24	172.50 (17)
C2—C3—C4—C5	0.3 (5)	C21—C22—C23—C27	178.32 (19)
C3—C4—C5—C6	−1.5 (5)	O2—C22—C23—C27	−5.0 (3)
C4—C5—C6—C1	0.8 (5)	C22—C23—C24—C25	−0.7 (3)
C2—C1—C6—C5	1.0 (4)	C27—C23—C24—C25	176.9 (2)
C9—C1—C6—C5	−178.1 (2)	C23—C24—C25—C26	3.2 (3)
C12—C7—C8—C9	9.3 (3)	C23—C24—C25—C20'	−165.5 (5)
C21—C7—C8—C9	−171.49 (18)	C23—C24—C25—C20	173.0 (4)
C12—C7—C8—O1	−175.67 (17)	C19'—C20'—C25—C24	−173.4 (5)
C21—C7—C8—O1	3.6 (3)	C19'—C20'—C25—C26	17.8 (9)
P1—O1—C8—C9	−113.98 (17)	C19'—C20'—C25—C20	−78 (2)
P1—O1—C8—C7	70.7 (2)	C19—C20—C25—C24	140.2 (6)
C7—C8—C9—C10	−5.0 (3)	C19—C20—C25—C26	−49.9 (8)
O1—C8—C9—C10	179.97 (17)	C19—C20—C25—C20'	45 (2)
C7—C8—C9—C1	171.05 (19)	C24—C25—C26—C21	−0.9 (3)
O1—C8—C9—C1	−4.0 (3)	C20'—C25—C26—C21	167.7 (4)
C2—C1—C9—C8	−117.0 (3)	C20—C25—C26—C21	−170.7 (4)
C6—C1—C9—C8	62.0 (3)	C24—C25—C26—C17'	176.5 (5)
C2—C1—C9—C10	58.8 (3)	C20'—C25—C26—C17'	−14.9 (7)
C6—C1—C9—C10	−122.2 (3)	C20—C25—C26—C17'	6.7 (7)
C8—C9—C10—C11	−2.1 (3)	C24—C25—C26—C17	−170.4 (5)
C1—C9—C10—C11	−178.14 (18)	C20'—C25—C26—C17	−1.8 (7)
C9—C10—C11—C12	4.5 (3)	C20—C25—C26—C17	19.9 (7)
C9—C10—C11—C13	−173.4 (2)	C22—C21—C26—C25	−3.6 (3)
C10—C11—C12—C7	0.0 (3)	C7—C21—C26—C25	179.01 (18)
C13—C11—C12—C7	177.81 (19)	C22—C21—C26—C17'	179.4 (6)
C10—C11—C12—C16	−175.7 (2)	C7—C21—C26—C17'	2.0 (6)
C13—C11—C12—C16	2.2 (3)	C22—C21—C26—C17	166.5 (5)
C8—C7—C12—C11	−6.5 (3)	C7—C21—C26—C17	−10.9 (5)
C21—C7—C12—C11	174.34 (17)	C18'—C17'—C26—C25	44.0 (9)
C8—C7—C12—C16	169.16 (19)	C18'—C17'—C26—C21	−138.8 (5)
C21—C7—C12—C16	−10.0 (3)	C18'—C17'—C26—C17	−87 (3)
C10—C11—C13—C14	−175.55 (19)	C18—C17—C26—C25	−2.9 (10)
C12—C11—C13—C14	6.6 (3)	C18—C17—C26—C21	−172.5 (6)
C11—C13—C14—C15	−38.1 (3)	C18—C17—C26—C17'	53 (3)
C13—C14—C15—C16	61.0 (3)	C22—C23—C27—C32	−42.4 (3)
C14—C15—C16—C12	−51.5 (3)	C24—C23—C27—C32	140.2 (2)
C11—C12—C16—C15	20.8 (3)	C22—C23—C27—C28	139.1 (2)
C7—C12—C16—C15	−154.8 (2)	C24—C23—C27—C28	−38.3 (3)
C26—C17—C18—C19	20.1 (14)	C32—C27—C28—C29	1.0 (4)

C17—C18—C19—C20	−53.2 (13)	C23—C27—C28—C29	179.6 (3)
C18—C19—C20—C25	62.4 (9)	C27—C28—C29—C30	−0.3 (5)
C26—C17'—C18'—C19'	−70.3 (8)	C28—C29—C30—C31	−1.4 (5)
C17'—C18'—C19'—C20'	71.4 (8)	C29—C30—C31—C32	2.4 (5)
C18'—C19'—C20'—C25	−48.8 (10)	C28—C27—C32—C31	0.0 (4)
C8—C7—C21—C22	−58.1 (2)	C23—C27—C32—C31	−178.5 (2)
C12—C7—C21—C22	121.1 (2)	C30—C31—C32—C27	−1.8 (4)
C8—C7—C21—C26	119.3 (2)		

Fig. 1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