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Methyl 2-diphenylphosphoryloxy-2-azabicyclo[2.2.1]hept-5-ene-3-*exo*-carboxylate

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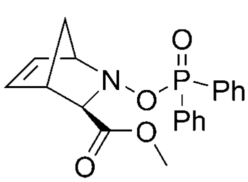
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.035; wR factor = 0.091; data-to-parameter ratio = 15.8.

In the title compound, $C_{20}H_{20}NO_4P$, the dihedral angle between the phenyl rings is 68.52 (7)°. In the crystal structure, the molecules are linked by a weak C—H⋯π(arene) interaction along [010] involving the phenyl CH group and the phenyl rings. There are no further significant intermolecular interactions.

Related literature

For the preparation of the precursor of the title compound, see: Sousa *et al.* (2008). For related literature about this type of bicyclic compound and their relevance see: Vale *et al.* (2006), Alves *et al.* (2006), Yoda *et al.* (1995).



Experimental

Crystal data

$C_{20}H_{20}NO_4P$
M_r = 369.34
Monoclinic, $P2_1/c$
a = 18.4223 (6) Å
b = 8.5522 (3) Å
c = 11.6022 (4) Å
β = 97.1810 (10)°
V = 1813.60 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.18 mm^{-1}
T = 100 (2) K
0.37 × 0.34 × 0.34 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2006)
T_{min} = 0.871, T_{max} = 0.940
14828 measured reflections
3717 independent reflections
3172 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.091
S = 1.05
3717 reflections
236 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C12—H12⋯Cg1^{i}	0.95	2.77	3.566 (2)	142

Symmetry code: (i) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$. Cg1 is the centroid of the C15–C20 ring.

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *WinGX* publication routines (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2188).

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supplementary materials

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Methyl 2-diphenylphosphoryloxy-2-azabicyclo[2.2.1]hept-5-ene-3-*exo*-carboxylate

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Comment

The stucture of the title compound, (I), is shown in Fig. 1. It can be seen the existence of three chiral centers at C2 (*R*), C5 (S) and C6 (*R*). In the crystalline structure, the molecules are linked by a weak C—H···π interaction, Fig. 2 [H12-π^{i} 2.77 Å, C12-H12-π 142°, C12-π 3.566 (2) Å, symmetry code: (i) 1-x,1/2+y, 1/2-z] along [010] directions. There are no further significant intermolecular interactions.

Experimental

The title compound was synthesized from the previously prepared (3*exo*)-2-hydroxy-2-azabicyclo[2.2.1]hept-5-ene-3-carboxylate (Sousa *et al.* 2008). Equimolar amounts of (3*exo*)-2-hydroxy-2-azabicyclo[2.2.1]hept-5-ene-3-carboxylate (0.56 g, 3.3 mmol) and diphenylpfosphinic chloride (0.63 ml, 3.3 mmol), in the presence of 1 eq. of anidrous triethylamine and and a catalytic quantity of DMAP, were let to react overnigth in dichloromethane, at room temperature under argon atmosphere. Water was added and the product was extracted with dichloromethane (3 × 15 ml). The organic layers were dried over sodium sulfate and the solvent was evaporated. The obtained product was purified by flash chromatography (eluent: dichloromethane/diethyl ether 1:1), leading to a light clear yellow oil in 80% yield. Crystals of (I) were made from a slow evaporation of a dichloromethane/hexane solution.

Refinement

All H atoms were found in a difference Fourier map and placed in geometrically idealized and constrained to ride on their parent atoms [C—H = 0.95–1.00 Å and $U_{iso}(H) = 1.2$ or $1.5U_{eq}(C)$].

Figures

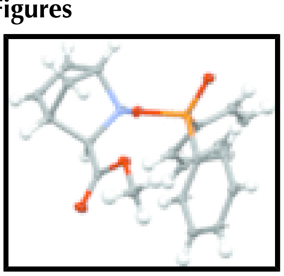


Fig. 1. A view of (I), showing the three chiral carbons C2, C5 and C6 and the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as spheres of arbitary radius.

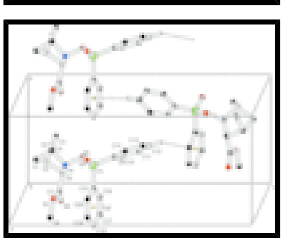


Fig. 2. Part of the crystal structute of (I) viewed along the c axis. Dashed lines show C—H···π (arene) interactions. Only H atoms participating in hydrogen bonding are shown. π is the centroid of the ring defined by atoms C15-C20.

Methyl 2-diphenylphosphoryloxy-2-azabicyclo[2.2.1]hept-5-ene-3-*exo*- carboxylate

Crystal data

$C_{20}H_{20}NO_4P$	$F_{000} = 776$
$M_r = 369.34$	$D_x = 1.353$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 1953 reflections
$a = 18.4223$ (6) Å	$\theta = 3.1$–25.9º
$b = 8.5522$ (3) Å	$\mu = 0.18$ mm^{-1}
$c = 11.6022$ (4) Å	$T = 100$ (2) K
$\beta = 97.1810$ (10)º	Prism, colourless
$V = 1813.60$ (11) Å^3	0.37 × 0.34 × 0.34 mm
$Z = 4$	

Data collection

Bruker ApexII CCD area-detector diffractometer	3717 independent reflections
Radiation source: sealed tube	3172 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.033$
$T = 100(2)$ K	$\theta_{max} = 26.4$º
phi and ω scans	$\theta_{min} = 2.2$º
Absorption correction: multi-scan (SADABS; Bruker, 2006)	$h = -23 \rightarrow 22$
$T_{min} = 0.871$, $T_{max} = 0.940$	$k = 0 \rightarrow 10$
14828 measured reflections	$l = 0 \rightarrow 14$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.035$	H-atom parameters constrained
$wR(F^2) = 0.091$	$w = 1/[\sigma^2(F_o^2) + (0.0429P)^2 + 0.8843P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} = 0.001$
3717 reflections	$\Delta\rho_{max} = 0.29$ e Å^{-3}
236 parameters	$\Delta\rho_{min} = -0.41$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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.

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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
C1	0.04005 (8)	0.24766 (17)	0.08174 (13)	0.0156 (3)
H1A	−0.005	0.3099	0.0614	0.019*
H1B	0.0318	0.1646	0.1381	0.019*
C2	0.10739 (8)	0.34831 (17)	0.12086 (13)	0.0140 (3)
H2	0.1038	0.4159	0.1902	0.017*
C3	0.11615 (8)	0.43459 (18)	0.00937 (13)	0.0157 (3)
H3	0.1328	0.539	0.003	0.019*
C4	0.09614 (8)	0.33679 (18)	−0.07788 (13)	0.0170 (3)
H4	0.0965	0.358	−0.1582	0.02*
C5	0.07271 (8)	0.18529 (18)	−0.02579 (13)	0.0152 (3)
H5	0.0408	0.1144	−0.0788	0.018*
C6	0.14566 (8)	0.11298 (17)	0.03659 (12)	0.0124 (3)
H6	0.1849	0.1189	−0.0155	0.015*
C7	0.13407 (7)	−0.05517 (17)	0.07081 (12)	0.0126 (3)
C8	0.10791 (9)	−0.23359 (18)	0.21479 (14)	0.0188 (3)
H8A	0.0638	−0.2759	0.1694	0.028*
H8B	0.1021	−0.2364	0.2976	0.028*
H8C	0.1503	−0.2968	0.201	0.028*
C9	0.37374 (8)	0.32042 (17)	0.19955 (13)	0.0135 (3)
C10	0.39313 (8)	0.28107 (18)	0.09030 (13)	0.0156 (3)
H10	0.3592	0.2281	0.0353	0.019*
C11	0.46227 (8)	0.31986 (19)	0.06275 (14)	0.0196 (3)
H11	0.4758	0.2923	−0.011	0.024*
C12	0.51155 (8)	0.3985 (2)	0.14240 (15)	0.0220 (4)
H12	0.559	0.4232	0.1236	0.026*
C13	0.49180 (9)	0.4412 (2)	0.24924 (15)	0.0228 (4)
H13	0.5253	0.4974	0.3029	0.027*
C14	0.42326 (8)	0.40209 (18)	0.27826 (14)	0.0180 (3)
H14	0.41	0.431	0.3519	0.022*
C15	0.29184 (7)	0.05353 (17)	0.27096 (13)	0.0125 (3)
C16	0.31090 (8)	−0.05303 (18)	0.18853 (13)	0.0156 (3)
H16	0.3218	−0.017	0.1151	0.019*
C17	0.31393 (9)	−0.21192 (18)	0.21417 (14)	0.0190 (3)

H17	0.3284	−0.2841	0.1591	0.023*
C18	0.29590 (8)	−0.26536 (18)	0.31971 (15)	0.0200 (3)
H18	0.2972	−0.3742	0.3364	0.024*
C19	0.27594 (8)	−0.16006 (19)	0.40103 (14)	0.0185 (3)
H19	0.2629	−0.197	0.4729	0.022*
C20	0.27503 (8)	−0.00078 (18)	0.37771 (13)	0.0149 (3)
H20	0.2629	0.0713	0.4346	0.018*
N1	0.16332 (6)	0.21932 (14)	0.13812 (11)	0.0116 (3)
O1	0.11889 (6)	−0.07336 (12)	0.17981 (9)	0.0166 (2)
O2	0.13582 (6)	−0.16137 (12)	0.00278 (9)	0.0190 (2)
O3	0.23563 (5)	0.28855 (12)	0.12671 (9)	0.0131 (2)
O4	0.27071 (6)	0.34776 (12)	0.34900 (9)	0.0158 (2)
P1	0.288697 (19)	0.26111 (4)	0.24650 (3)	0.01112 (11)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0105 (7)	0.0152 (8)	0.0210 (8)	0.0011 (6)	0.0016 (6)	0.0022 (6)
C2	0.0121 (7)	0.0126 (7)	0.0175 (7)	0.0026 (6)	0.0025 (6)	−0.0004 (6)
C3	0.0118 (7)	0.0132 (7)	0.0218 (8)	0.0026 (6)	0.0016 (6)	0.0041 (6)
C4	0.0154 (7)	0.0179 (8)	0.0172 (7)	0.0029 (6)	0.0000 (6)	0.0060 (6)
C5	0.0130 (7)	0.0149 (8)	0.0167 (7)	−0.0011 (6)	−0.0020 (6)	0.0021 (6)
C6	0.0112 (7)	0.0123 (7)	0.0135 (7)	−0.0005 (6)	0.0008 (5)	0.0000 (6)
C7	0.0081 (6)	0.0149 (7)	0.0145 (7)	0.0003 (6)	−0.0001 (5)	−0.0004 (6)
C8	0.0206 (8)	0.0145 (8)	0.0209 (8)	−0.0045 (6)	0.0010 (6)	0.0058 (6)
C9	0.0106 (7)	0.0116 (7)	0.0180 (7)	0.0001 (6)	0.0005 (6)	0.0035 (6)
C10	0.0133 (7)	0.0161 (8)	0.0169 (7)	−0.0018 (6)	−0.0003 (6)	0.0041 (6)
C11	0.0170 (8)	0.0232 (8)	0.0192 (8)	0.0001 (6)	0.0047 (6)	0.0046 (6)
C12	0.0131 (7)	0.0242 (9)	0.0289 (9)	−0.0026 (6)	0.0031 (6)	0.0075 (7)
C13	0.0152 (8)	0.0235 (9)	0.0283 (9)	−0.0056 (7)	−0.0031 (7)	−0.0009 (7)
C14	0.0157 (7)	0.0174 (8)	0.0205 (8)	−0.0009 (6)	0.0002 (6)	−0.0009 (6)
C15	0.0086 (7)	0.0114 (7)	0.0165 (7)	−0.0001 (5)	−0.0021 (5)	0.0011 (6)
C16	0.0139 (7)	0.0163 (8)	0.0162 (7)	0.0004 (6)	0.0008 (6)	0.0004 (6)
C17	0.0188 (8)	0.0145 (8)	0.0226 (8)	0.0031 (6)	−0.0022 (6)	−0.0060 (6)
C18	0.0166 (8)	0.0120 (8)	0.0296 (9)	−0.0001 (6)	−0.0043 (7)	0.0042 (7)
C19	0.0151 (7)	0.0198 (8)	0.0202 (8)	−0.0022 (6)	0.0002 (6)	0.0068 (6)
C20	0.0121 (7)	0.0154 (8)	0.0169 (7)	−0.0008 (6)	0.0008 (6)	−0.0007 (6)
N1	0.0071 (6)	0.0117 (6)	0.0161 (6)	−0.0022 (5)	0.0017 (5)	−0.0004 (5)
O1	0.0224 (6)	0.0119 (5)	0.0163 (5)	−0.0032 (4)	0.0049 (4)	0.0011 (4)
O2	0.0245 (6)	0.0139 (6)	0.0189 (6)	−0.0012 (4)	0.0038 (5)	−0.0031 (5)
O3	0.0079 (5)	0.0142 (5)	0.0168 (5)	−0.0033 (4)	0.0003 (4)	0.0029 (4)
O4	0.0165 (5)	0.0135 (5)	0.0177 (5)	−0.0003 (4)	0.0030 (4)	−0.0014 (4)
P1	0.00981 (19)	0.01024 (19)	0.0131 (2)	−0.00066 (14)	0.00083 (14)	0.00053 (14)

Geometric parameters (Å, °)

C1—C2	1.531 (2)	C10—C11	1.392 (2)
C1—C5	1.546 (2)	C10—H10	0.95
C1—H1A	0.99	C11—C12	1.386 (2)

C1—H1B	0.99	C11—H11	0.95
C2—N1	1.5057 (18)	C12—C13	1.384 (2)
C2—C3	1.515 (2)	C12—H12	0.95
C2—H2	1	C13—C14	1.388 (2)
C3—C4	1.329 (2)	C13—H13	0.95
C3—H3	0.95	C14—H14	0.95
C4—C5	1.515 (2)	C15—C20	1.393 (2)
C4—H4	0.95	C15—C16	1.397 (2)
C5—C6	1.571 (2)	C15—P1	1.7976 (15)
C5—H5	1	C16—C17	1.391 (2)
C6—N1	1.4915 (18)	C16—H16	0.95
C6—C7	1.514 (2)	C17—C18	1.386 (2)
C6—H6	1	C17—H17	0.95
C7—O2	1.2064 (18)	C18—C19	1.387 (2)
C7—O1	1.3379 (17)	C18—H18	0.95
C8—O1	1.4505 (18)	C19—C20	1.389 (2)
C8—H8A	0.98	C19—H19	0.95
C8—H8B	0.98	C20—H20	0.95
C8—H8C	0.98	N1—O3	1.4786 (15)
C9—C14	1.395 (2)	O3—P1	1.6133 (10)
C9—C10	1.400 (2)	O4—P1	1.4737 (11)
C9—P1	1.7950 (15)		

C2—C1—C5	92.89 (11)	C11—C10—H10	120.2
C2—C1—H1A	113.1	C9—C10—H10	120.2
C5—C1—H1A	113.1	C12—C11—C10	120.30 (15)
C2—C1—H1B	113.1	C12—C11—H11	119.8
C5—C1—H1B	113.1	C10—C11—H11	119.8
H1A—C1—H1B	110.5	C13—C12—C11	120.11 (14)
N1—C2—C3	109.04 (11)	C13—C12—H12	119.9
N1—C2—C1	98.23 (11)	C11—C12—H12	119.9
C3—C2—C1	100.92 (12)	C12—C13—C14	120.20 (15)
N1—C2—H2	115.5	C12—C13—H13	119.9
C3—C2—H2	115.5	C14—C13—H13	119.9
C1—C2—H2	115.5	C13—C14—C9	120.14 (15)
C4—C3—C2	107.14 (13)	C13—C14—H14	119.9
C4—C3—H3	126.4	C9—C14—H14	119.9
C2—C3—H3	126.4	C20—C15—C16	119.59 (14)
C3—C4—C5	107.46 (13)	C20—C15—P1	117.59 (11)
C3—C4—H4	126.3	C16—C15—P1	122.82 (11)
C5—C4—H4	126.3	C17—C16—C15	119.85 (14)
C4—C5—C1	100.71 (12)	C17—C16—H16	120.1
C4—C5—C6	104.50 (12)	C15—C16—H16	120.1
C1—C5—C6	99.25 (11)	C18—C17—C16	120.24 (15)
C4—C5—H5	116.6	C18—C17—H17	119.9
C1—C5—H5	116.6	C16—C17—H17	119.9
C6—C5—H5	116.6	C17—C18—C19	120.02 (14)
N1—C6—C7	113.33 (11)	C17—C18—H18	120
N1—C6—C5	102.32 (11)	C19—C18—H18	120
C7—C6—C5	110.74 (12)	C18—C19—C20	120.14 (15)

N1—C6—H6	110.1	C18—C19—H19	119.9
C7—C6—H6	110.1	C20—C19—H19	119.9
C5—C6—H6	110.1	C19—C20—C15	120.11 (14)
O2—C7—O1	123.83 (14)	C19—C20—H20	119.9
O2—C7—C6	121.82 (13)	C15—C20—H20	119.9
O1—C7—C6	114.29 (12)	O3—N1—C6	106.47 (10)
O1—C8—H8A	109.5	O3—N1—C2	107.69 (10)
O1—C8—H8B	109.5	C6—N1—C2	105.28 (11)
H8A—C8—H8B	109.5	C7—O1—C8	115.30 (12)
O1—C8—H8C	109.5	N1—O3—P1	108.68 (8)
H8A—C8—H8C	109.5	O4—P1—O3	116.67 (6)
H8B—C8—H8C	109.5	O4—P1—C9	113.30 (7)
C14—C9—C10	119.54 (13)	O3—P1—C9	98.94 (6)
C14—C9—P1	117.84 (12)	O4—P1—C15	112.04 (7)
C10—C9—P1	122.54 (11)	O3—P1—C15	106.49 (6)
C11—C10—C9	119.67 (14)	C9—P1—C15	108.35 (7)

C5—C1—C2—N1	−60.85 (12)	C18—C19—C20—C15	2.1 (2)
C5—C1—C2—C3	50.47 (12)	C16—C15—C20—C19	−1.2 (2)
N1—C2—C3—C4	68.17 (15)	P1—C15—C20—C19	179.43 (11)
C1—C2—C3—C4	−34.58 (15)	C7—C6—N1—O3	120.70 (12)
C2—C3—C4—C5	0.88 (16)	C5—C6—N1—O3	−120.03 (11)
C3—C4—C5—C1	32.73 (15)	C7—C6—N1—C2	−125.14 (12)
C3—C4—C5—C6	−69.86 (15)	C5—C6—N1—C2	−5.87 (13)
C2—C1—C5—C4	−49.87 (12)	C3—C2—N1—O3	51.25 (14)
C2—C1—C5—C6	56.93 (12)	C1—C2—N1—O3	155.87 (10)
C4—C5—C6—N1	71.20 (13)	C3—C2—N1—C6	−62.06 (14)
C1—C5—C6—N1	−32.48 (13)	C1—C2—N1—C6	42.56 (13)
C4—C5—C6—C7	−167.72 (12)	O2—C7—O1—C8	3.0 (2)
C1—C5—C6—C7	88.59 (13)	C6—C7—O1—C8	−179.72 (12)
N1—C6—C7—O2	−162.95 (13)	C6—N1—O3—P1	−127.24 (9)
C5—C6—C7—O2	82.74 (17)	C2—N1—O3—P1	120.25 (10)
N1—C6—C7—O1	19.76 (17)	N1—O3—P1—O4	−68.47 (10)
C5—C6—C7—O1	−94.56 (14)	N1—O3—P1—C9	169.71 (9)
C14—C9—C10—C11	1.8 (2)	N1—O3—P1—C15	57.44 (9)
P1—C9—C10—C11	−174.85 (12)	C14—C9—P1—O4	18.47 (14)
C9—C10—C11—C12	−0.7 (2)	C10—C9—P1—O4	−164.79 (12)
C10—C11—C12—C13	−1.0 (2)	C14—C9—P1—O3	142.70 (12)
C11—C12—C13—C14	1.6 (3)	C10—C9—P1—O3	−40.56 (14)
C12—C13—C14—C9	−0.4 (2)	C14—C9—P1—C15	−106.51 (13)
C10—C9—C14—C13	−1.3 (2)	C10—C9—P1—C15	70.23 (14)
P1—C9—C14—C13	175.54 (12)	C20—C15—P1—O4	2.24 (13)
C20—C15—C16—C17	−0.9 (2)	C16—C15—P1—O4	−177.14 (11)
P1—C15—C16—C17	178.48 (11)	C20—C15—P1—O3	−126.43 (11)
C15—C16—C17—C18	2.0 (2)	C16—C15—P1—O3	54.19 (13)
C16—C17—C18—C19	−1.1 (2)	C20—C15—P1—C9	127.97 (11)
C17—C18—C19—C20	−1.0 (2)	C16—C15—P1—C9	−51.41 (14)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12···Cg1^{i}	0.95	2.77	3.566 (2)	142

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+1/2.

Fig. 1

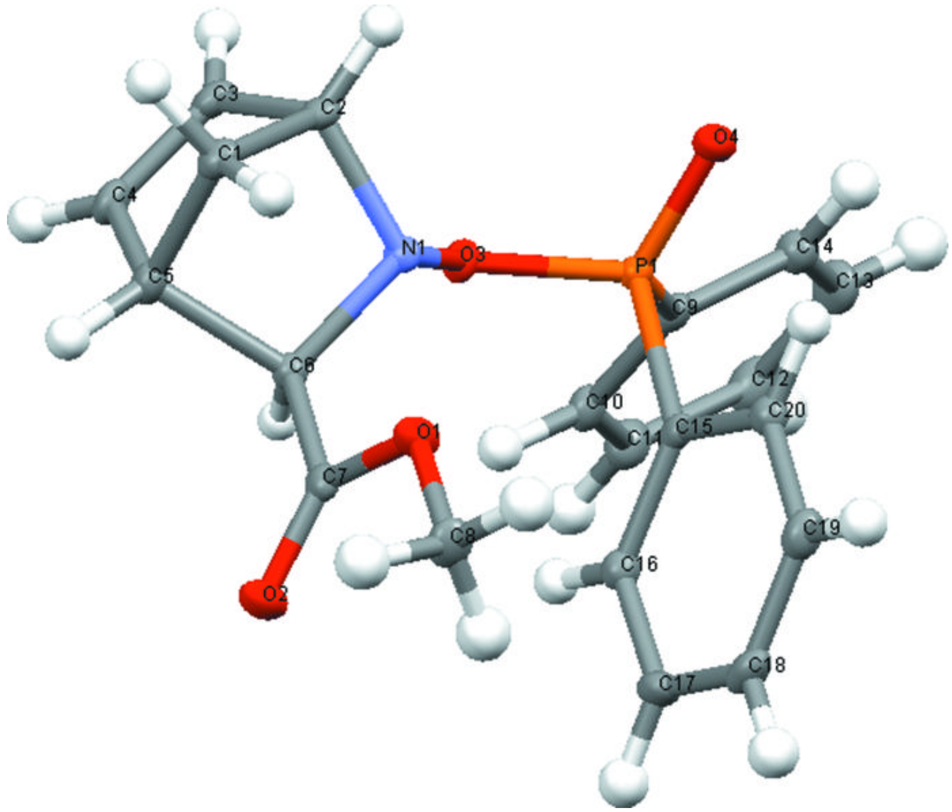
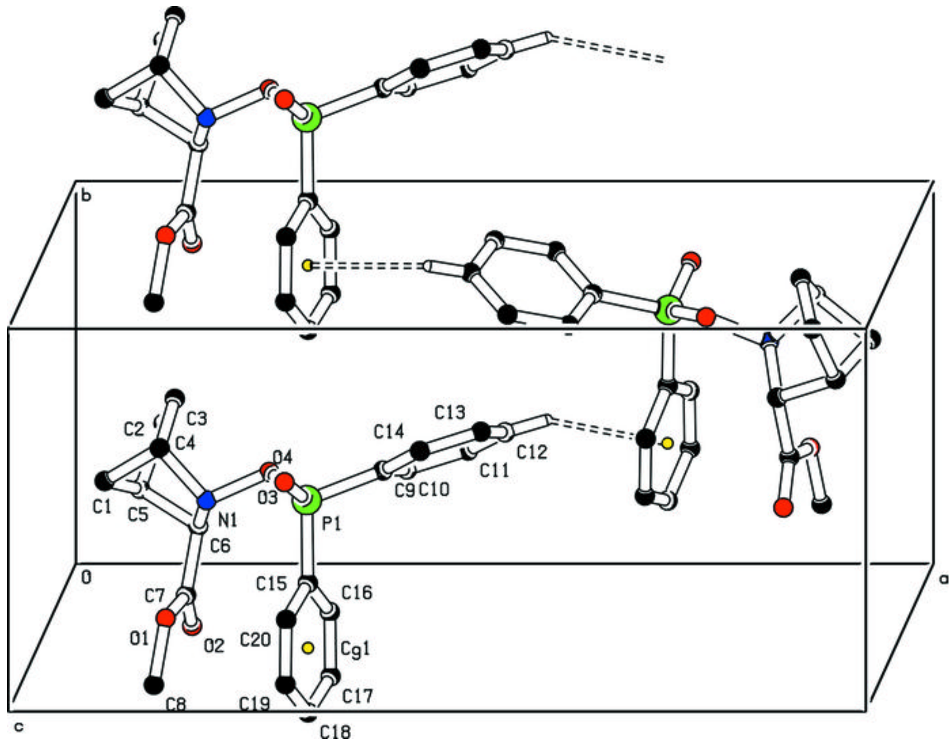

C3
C2
C1
O4
C4
N1
O3
P1
C14
C5
C13
C9
C6
C12
C10
C20
O1
C11
C15
C7
C8
C19
C16
O2
C18
C17

Fig. 2


b
0
a
c
C1
C2
C3
C4
C5
C6
C7
C8
C9
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C11
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C14
C15
C16
C17
C18
C19
C20
Cg1
N1
O1
O2
O3
O4
P1