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Triphenylphosphine oxide–succinimide (1/1)

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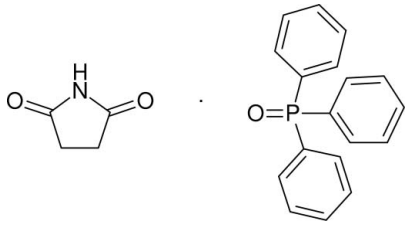
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.044; wR factor = 0.121; data-to-parameter ratio = 18.6.

In the title adduct, $C_{18}H_{15}OP{\cdot}C_4H_5NO_2$, the two components are linked by an N—H···O hydrogen bond. Some weak C—H···O links may help to establish the packing. One of the phenyl rings is disordered over two positions in a 0.551 (15):0.449 (15) ratio.

Related literature

For background, see: Mason (1961); Elding-Pontén (1993). For reference structural data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{18}H_{15}OP{\cdot}C_4H_5NO_2$
M_r = 377.36
Orthorhombic, *Pbca*
a = 8.5825 (4) Å
b = 17.2754 (7) Å
c = 26.6505 (11) Å
V = 3951.4 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.16 mm^{-1}
T = 293 (2) K
0.42 × 0.35 × 0.18 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: none
26415 measured reflections
3887 independent reflections
2454 reflections with $I > 2\sigma(I)$
R_{int} = 0.047

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.121
S = 1.02
3887 reflections
209 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O3	0.86	1.96	2.820 (2)	173
C14—H14···O1^{i}	0.93	2.45	3.368 (3)	170
C18—H18···O1	0.93	2.54	3.256 (3)	135
C22—H22···O1^{ii}	0.93	2.55	3.283 (3)	136

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

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; 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*.

We thank Dhiran Walji for supplying the sample.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2197).

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supplementary materials

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Comment

In the title 1:1 adduct, $C_{18}H_{15}OP{\cdot}C_4H_5NO_2$, (I), the component species interact by an almost linear N—H···O hydrogen bond (Table 1). The five-membered ring of the succinimide (suc) molecule in (I) is close to flat (r.m.s. deviation = 0.006 Å), similar to that in other suc-containing adducts (Elding-Pontén, 1993), whereas in succinimide itself (Mason, 1961), the ring is slightly puckered. One of the phenyl rings in the triphenylphosphine oxide (ppo) molecule in (I) is disordered over two positions, otherwise the geometric parameters for (I) may be regarded as normal (Allen *et al.*, 1987). It is notable that although O1 accepts three of these putative bonds, and O2 none, the C1=O1 and C4=O2 bond lengths are identical.

Some weak C—H···O interactions (Table 1) from ppo to sac help establish the packing in (I). Aromatic π-π stacking interactions in (I) are negligible, as the minimum aromatic ring centroid···centroid separation is greater than 4.1 Å.

Experimental

Triphenylphosphine oxide and succinimide were mixed in a 1:1 ratio in acetonitrile. Colourless blocks of (I) grew as the solvent slowly evaporated.

Refinement

One of the ppo phenyl rings is disordered over two positions in a 0.551 (15):0.449 (15) ratio. The two rings were modelled as regular hexagons with C—C = 1.39Å and U_{iso} values were refined for the C atoms.

The hydrogen atoms were geometrically placed (C—H = 0.93–0.97 Å, N—H = 0.86 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(carrier).

Figures

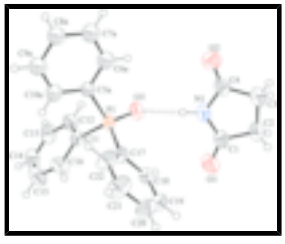


Fig. 1. The molecular structure of (I) showing 50% displacement ellipsoids (arbitrary spheres for the H atoms). Only one orientation of the disordered phenyl ring is shown. The hydrogen bond is indicated by a dashed line.

Triphenylphosphine oxide–succinimide (1/1)

Crystal data

$C_{18}H_{15}OP{\cdot}C_4H_5NO_2$	F_{000} = 1584
M_r = 377.36	D_x = 1.269 Mg m^{-3}
Orthorhombic, *Pbca*	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 5293 reflections
a = 8.5825 (4) Å	θ = 2.4–24.8º
b = 17.2754 (7) Å	μ = 0.16 mm^{-1}
c = 26.6505 (11) Å	*T* = 293 (2) K
V = 3951.4 (3) Å^3	Chunk, colourless
Z = 8	0.42 × 0.35 × 0.18 mm

Data collection

Bruker SMART 1000 CCD diffractometer	2454 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.047
Monochromator: graphite	θ_{max} = 26.0º
T = 293(2) K	θ_{min} = 2.4º
ω scans	*h* = −10→10
Absorption correction: none	*k* = −20→21
26415 measured reflections	*l* = −28→32
3887 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.044	H-atom parameters constrained
$wR(F^2)$ = 0.121	$w = 1/[\sigma^2(F_o^2) + (0.0616P)^2 + 0.24P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.02	$(\Delta/\sigma)_{max}$ = 0.001
3887 reflections	$\Delta\rho_{max}$ = 0.32 e Å^{-3}
209 parameters	$\Delta\rho_{min}$ = −0.30 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 $F^2 > 2\text{sigma}(F^2)$ 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}	Occ. (<1)
C1	0.1713 (3)	0.41653 (15)	0.31308 (10)	0.0576 (6)	
C2	0.0888 (4)	0.45266 (16)	0.26964 (12)	0.0853 (9)	
H2A	−0.0221	0.4565	0.2762	0.102*	
H2B	0.1042	0.4223	0.2394	0.102*	
C3	0.1599 (4)	0.53217 (16)	0.26394 (11)	0.0822 (9)	
H3A	0.2056	0.5383	0.2309	0.099*	
H3B	0.0818	0.5721	0.2688	0.099*	
C4	0.2834 (3)	0.53676 (15)	0.30405 (9)	0.0570 (6)	
N1	0.2801 (2)	0.46846 (11)	0.32998 (7)	0.0527 (5)	
H1	0.3412	0.4589	0.3548	0.063*	
O1	0.1478 (2)	0.35331 (11)	0.33060 (8)	0.0800 (6)	
O2	0.3707 (2)	0.59001 (11)	0.31185 (7)	0.0800 (6)	
P1	0.61012 (6)	0.39626 (3)	0.42066 (2)	0.04155 (17)	
O3	0.45860 (17)	0.43822 (9)	0.41661 (5)	0.0551 (4)	
C5A	0.7853 (5)	0.4593 (2)	0.42092 (16)	0.0400 (19)*	0.449 (15)
C6A	0.7718 (6)	0.5331 (2)	0.4007 (2)	0.0610 (18)*	0.449 (15)
H6A	0.6764	0.5500	0.3883	0.073*	0.449 (15)
C7A	0.9008 (8)	0.58172 (19)	0.3991 (3)	0.063 (2)*	0.449 (15)
H7A	0.8917	0.6311	0.3856	0.075*	0.449 (15)
C8A	1.0433 (7)	0.5564 (3)	0.4177 (2)	0.0610 (19)*	0.449 (15)
H8A	1.1296	0.5890	0.4166	0.073*	0.449 (15)
C9A	1.0567 (5)	0.4826 (4)	0.43792 (17)	0.0604 (19)*	0.449 (15)
H9A	1.1521	0.4657	0.4504	0.073*	0.449 (15)
C10A	0.9278 (5)	0.4340 (3)	0.43953 (15)	0.0556 (18)*	0.449 (15)
H10A	0.9368	0.3846	0.4531	0.067*	0.449 (15)
C5B	0.7646 (4)	0.46322 (11)	0.41665 (8)	0.0463 (18)*	0.551 (15)
C6B	0.7367 (6)	0.53136 (14)	0.39039 (13)	0.0577 (15)*	0.551 (15)
H6B	0.6396	0.5402	0.3761	0.069*	0.551 (15)
C7B	0.8542 (7)	0.58627 (15)	0.38555 (17)	0.0728 (17)*	0.551 (15)
H7B	0.8356	0.6319	0.3680	0.087*	0.551 (15)
C8B	0.9994 (7)	0.5730 (2)	0.40696 (16)	0.0628 (16)*	0.551 (15)
H8B	1.0780	0.6098	0.4037	0.075*	0.551 (15)
C9B	1.0273 (5)	0.5049 (3)	0.43322 (14)	0.0627 (15)*	0.551 (15)
H9B	1.1245	0.4960	0.4475	0.075*	0.551 (15)
C10B	0.9098 (3)	0.4500 (2)	0.43806 (10)	0.0510 (14)*	0.551 (15)
H10B	0.9285	0.4044	0.4556	0.061*	0.551 (15)
C11	0.62595 (19)	0.34155 (8)	0.47816 (6)	0.0412 (5)	
C12	0.5739 (2)	0.37552 (10)	0.52185 (6)	0.0600 (6)	

H12	0.5329	0.4253	0.5211	0.072*
C13	0.5825 (3)	0.33567 (18)	0.56671 (10)	0.0728 (8)
H13	0.5467	0.3587	0.5961	0.087*
C14	0.6426 (3)	0.2632 (2)	0.56810 (12)	0.0757 (9)
H14	0.6472	0.2365	0.5984	0.091*
C15	0.6966 (3)	0.22924 (16)	0.52530 (13)	0.0800 (9)
H15	0.7388	0.1797	0.5265	0.096*
C16	0.6886 (3)	0.26835 (14)	0.48007 (10)	0.0628 (7)
H16	0.7255	0.2451	0.4509	0.075*
C17	0.6351 (2)	0.32944 (12)	0.36951 (8)	0.0438 (5)
C18	0.5031 (3)	0.29439 (12)	0.34987 (9)	0.0503 (6)
H18	0.4062	0.3044	0.3641	0.060*
C19	0.5145 (3)	0.24481 (14)	0.30941 (10)	0.0630 (7)
H19	0.4253	0.2216	0.2965	0.076*
C20	0.6566 (4)	0.22971 (16)	0.28827 (10)	0.0754 (8)
H20	0.6636	0.1974	0.2605	0.091*
C21	0.7882 (4)	0.26217 (18)	0.30800 (12)	0.0871 (9)
H21	0.8849	0.2505	0.2942	0.105*
C22	0.7783 (3)	0.31224 (16)	0.34827 (10)	0.0666 (7)
H22	0.8684	0.3346	0.3612	0.080*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0418 (12)	0.0676 (16)	0.0635 (17)	0.0044 (12)	−0.0009 (12)	0.0120 (13)
C2	0.090 (2)	0.0775 (19)	0.089 (2)	0.0031 (17)	−0.0414 (17)	0.0140 (16)
C3	0.102 (2)	0.0731 (18)	0.072 (2)	0.0089 (17)	−0.0285 (17)	0.0176 (15)
C4	0.0675 (16)	0.0589 (15)	0.0445 (14)	0.0091 (13)	0.0034 (12)	0.0048 (12)
N1	0.0472 (11)	0.0651 (12)	0.0458 (11)	0.0052 (10)	−0.0029 (9)	0.0110 (10)
O1	0.0591 (11)	0.0782 (13)	0.1027 (16)	−0.0090 (9)	−0.0085 (10)	0.0330 (12)
O2	0.1052 (15)	0.0678 (12)	0.0669 (13)	−0.0142 (11)	−0.0062 (11)	0.0062 (10)
P1	0.0431 (3)	0.0469 (3)	0.0347 (3)	0.0038 (3)	−0.0016 (3)	0.0005 (2)
O3	0.0542 (9)	0.0655 (10)	0.0457 (10)	0.0169 (8)	−0.0036 (8)	0.0021 (8)
C11	0.0370 (11)	0.0482 (12)	0.0385 (12)	−0.0019 (9)	−0.0011 (9)	0.0019 (9)
C12	0.0745 (17)	0.0624 (15)	0.0432 (14)	0.0115 (13)	−0.0001 (13)	−0.0010 (11)
C13	0.0778 (19)	0.104 (2)	0.0369 (15)	0.0107 (17)	0.0005 (13)	0.0069 (14)
C14	0.0561 (16)	0.107 (2)	0.0641 (19)	−0.0030 (15)	−0.0027 (14)	0.0400 (17)
C15	0.081 (2)	0.0666 (17)	0.093 (2)	0.0156 (15)	0.0052 (18)	0.0334 (17)
C16	0.0696 (17)	0.0570 (14)	0.0617 (16)	0.0137 (13)	0.0104 (14)	0.0102 (12)
C17	0.0444 (12)	0.0509 (12)	0.0360 (12)	0.0001 (10)	0.0000 (10)	−0.0005 (9)
C18	0.0483 (13)	0.0511 (13)	0.0513 (14)	0.0023 (10)	−0.0059 (11)	0.0005 (11)
C19	0.0712 (18)	0.0590 (15)	0.0588 (16)	−0.0061 (13)	−0.0187 (14)	−0.0060 (12)
C20	0.097 (2)	0.0779 (19)	0.0513 (17)	−0.0029 (17)	−0.0004 (16)	−0.0255 (14)
C21	0.0721 (19)	0.118 (2)	0.0712 (19)	−0.0092 (18)	0.0224 (16)	−0.0403 (18)
C22	0.0527 (14)	0.0897 (19)	0.0573 (16)	−0.0121 (14)	0.0087 (13)	−0.0247 (14)

Geometric parameters (Å, °)

C1—O1	1.205 (3)	C6B—H6B	0.9300

C1—N1	1.371 (3)	C7B—C8B	1.3900
C1—C2	1.494 (3)	C7B—H7B	0.9300
C2—C3	1.511 (4)	C8B—C9B	1.3900
C2—H2A	0.9700	C8B—H8B	0.9300
C2—H2B	0.9700	C9B—C10B	1.3900
C3—C4	1.507 (4)	C9B—H9B	0.9300
C3—H3A	0.9700	C10B—H10B	0.9300
C3—H3B	0.9700	C11—C16	1.375 (3)
C4—O2	1.205 (3)	C11—C12	1.3784
C4—N1	1.368 (3)	C12—C13	1.381 (3)
N1—H1	0.8600	C12—H12	0.9300
P1—O3	1.4928 (15)	C13—C14	1.355 (4)
P1—C5B	1.763 (2)	C13—H13	0.9300
P1—C17	1.799 (2)	C14—C15	1.364 (4)
P1—C11	1.8056 (16)	C14—H14	0.9300
P1—C5A	1.856 (3)	C15—C16	1.384 (4)
C5A—C6A	1.3900	C15—H15	0.9300
C5A—C10A	1.3900	C16—H16	0.9300
C6A—C7A	1.3900	C17—C22	1.386 (3)
C6A—H6A	0.9300	C17—C18	1.387 (3)
C7A—C8A	1.3900	C18—C19	1.380 (3)
C7A—H7A	0.9300	C18—H18	0.9300
C8A—C9A	1.3900	C19—C20	1.369 (4)
C8A—H8A	0.9300	C19—H19	0.9300
C9A—C10A	1.3900	C20—C21	1.366 (4)
C9A—H9A	0.9300	C20—H20	0.9300
C10A—H10A	0.9300	C21—C22	1.381 (3)
C5B—C6B	1.3900	C21—H21	0.9300
C5B—C10B	1.3900	C22—H22	0.9300
C6B—C7B	1.3900		
O1—C1—N1	125.4 (2)	C7B—C6B—C5B	120.0
O1—C1—C2	126.8 (2)	C7B—C6B—H6B	120.0
N1—C1—C2	107.7 (2)	C5B—C6B—H6B	120.0
C1—C2—C3	105.4 (2)	C6B—C7B—C8B	120.0
C1—C2—H2A	110.7	C6B—C7B—H7B	120.0
C3—C2—H2A	110.7	C8B—C7B—H7B	120.0
C1—C2—H2B	110.7	C7B—C8B—C9B	120.0
C3—C2—H2B	110.7	C7B—C8B—H8B	120.0
H2A—C2—H2B	108.8	C9B—C8B—H8B	120.0
C4—C3—C2	105.1 (2)	C10B—C9B—C8B	120.0
C4—C3—H3A	110.7	C10B—C9B—H9B	120.0
C2—C3—H3A	110.7	C8B—C9B—H9B	120.0
C4—C3—H3B	110.7	C9B—C10B—C5B	120.0
C2—C3—H3B	110.7	C9B—C10B—H10B	120.0
H3A—C3—H3B	108.8	C5B—C10B—H10B	120.0
O2—C4—N1	125.7 (2)	C16—C11—C12	119.14 (16)
O2—C4—C3	126.9 (2)	C16—C11—P1	122.84 (15)
N1—C4—C3	107.4 (2)	C12—C11—P1	118.02 (9)
C4—N1—C1	114.4 (2)	C11—C12—C13	120.11 (18)

C4—N1—H1	122.8	C11—C12—H12	119.9
C1—N1—H1	122.8	C13—C12—H12	119.9
O3—P1—C5B	109.39 (12)	C14—C13—C12	120.3 (3)
O3—P1—C17	111.15 (9)	C14—C13—H13	119.9
C5B—P1—C17	106.59 (9)	C12—C13—H13	119.9
O3—P1—C11	112.40 (8)	C13—C14—C15	120.3 (3)
C5B—P1—C11	109.78 (10)	C13—C14—H14	119.9
C17—P1—C11	107.35 (9)	C15—C14—H14	119.9
O3—P1—C5A	114.90 (16)	C14—C15—C16	120.1 (3)
C5B—P1—C5A	6.38 (15)	C14—C15—H15	119.9
C17—P1—C5A	106.42 (14)	C16—C15—H15	119.9
C11—P1—C5A	104.05 (15)	C11—C16—C15	120.1 (2)
C6A—C5A—C10A	120.0	C11—C16—H16	120.0
C6A—C5A—P1	118.0 (2)	C15—C16—H16	120.0
C10A—C5A—P1	122.0 (2)	C22—C17—C18	118.5 (2)
C7A—C6A—C5A	120.0	C22—C17—P1	123.57 (17)
C7A—C6A—H6A	120.0	C18—C17—P1	117.95 (16)
C5A—C6A—H6A	120.0	C19—C18—C17	120.5 (2)
C8A—C7A—C6A	120.0	C19—C18—H18	119.7
C8A—C7A—H7A	120.0	C17—C18—H18	119.7
C6A—C7A—H7A	120.0	C20—C19—C18	120.2 (2)
C7A—C8A—C9A	120.0	C20—C19—H19	119.9
C7A—C8A—H8A	120.0	C18—C19—H19	119.9
C9A—C8A—H8A	120.0	C21—C20—C19	120.0 (2)
C8A—C9A—C10A	120.0	C21—C20—H20	120.0
C8A—C9A—H9A	120.0	C19—C20—H20	120.0
C10A—C9A—H9A	120.0	C20—C21—C22	120.4 (3)
C9A—C10A—C5A	120.0	C20—C21—H21	119.8
C9A—C10A—H10A	120.0	C22—C21—H21	119.8
C5A—C10A—H10A	120.0	C21—C22—C17	120.4 (2)
C6B—C5B—C10B	120.0	C21—C22—H22	119.8
C6B—C5B—P1	117.20 (7)	C17—C22—H22	119.8
C10B—C5B—P1	122.80 (7)		
O1—C1—C2—C3	178.8 (3)	C7B—C8B—C9B—C10B	0.0
N1—C1—C2—C3	−1.1 (3)	C8B—C9B—C10B—C5B	0.0
C1—C2—C3—C4	1.3 (3)	C6B—C5B—C10B—C9B	0.0
C2—C3—C4—O2	178.1 (3)	P1—C5B—C10B—C9B	179.49 (9)
C2—C3—C4—N1	−1.1 (3)	O3—P1—C11—C16	138.65 (18)
O2—C4—N1—C1	−178.8 (2)	C5B—P1—C11—C16	−99.36 (19)
C3—C4—N1—C1	0.4 (3)	C17—P1—C11—C16	16.13 (19)
O1—C1—N1—C4	−179.4 (2)	C5A—P1—C11—C16	−96.4 (2)
C2—C1—N1—C4	0.5 (3)	O3—P1—C11—C12	−41.93 (13)
O3—P1—C5A—C6A	−21.7 (3)	C5B—P1—C11—C12	80.06 (14)
C5B—P1—C5A—C6A	9.3 (14)	C17—P1—C11—C12	−164.45 (12)
C17—P1—C5A—C6A	101.7 (3)	C5A—P1—C11—C12	83.00 (15)
C11—P1—C5A—C6A	−145.0 (2)	C16—C11—C12—C13	−1.1 (3)
O3—P1—C5A—C10A	159.7 (2)	P1—C11—C12—C13	179.48 (19)
C5B—P1—C5A—C10A	−169.2 (16)	C11—C12—C13—C14	0.3 (3)
C17—P1—C5A—C10A	−76.8 (3)	C12—C13—C14—C15	0.6 (4)

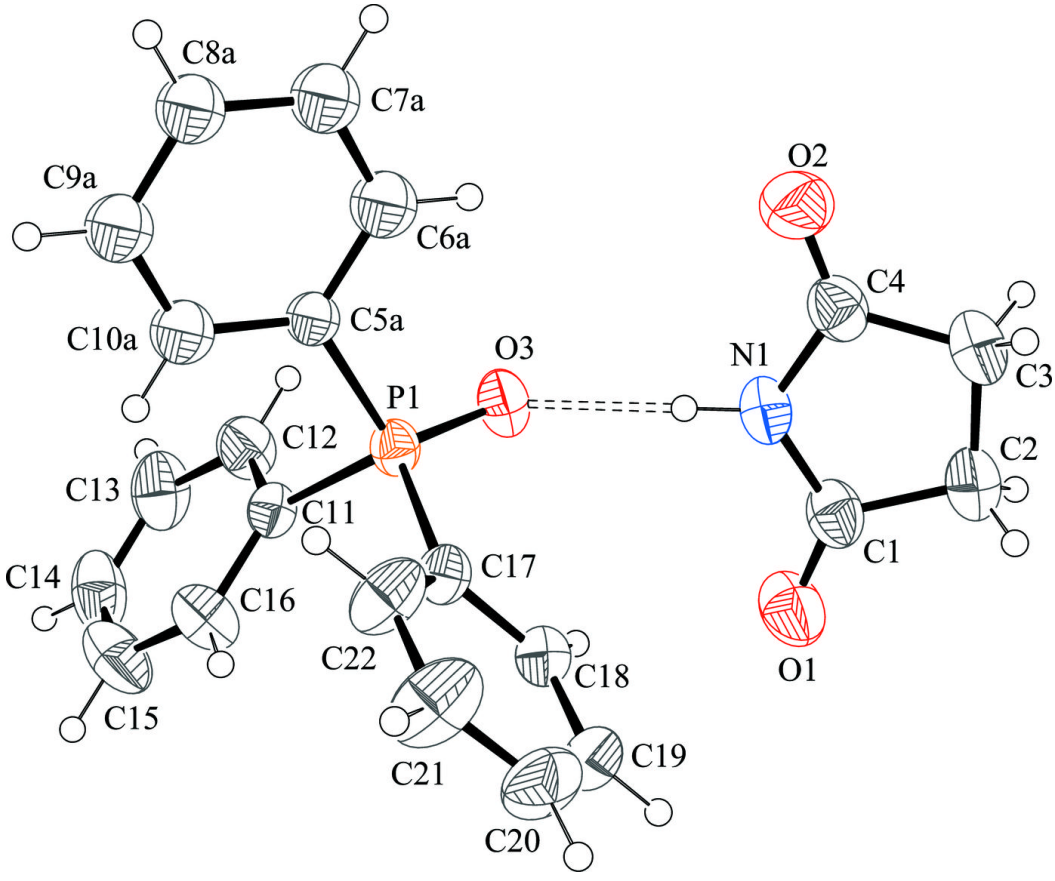
C11—P1—C5A—C10A	36.4 (3)	C13—C14—C15—C16	−0.7 (4)
C10A—C5A—C6A—C7A	0.0	C12—C11—C16—C15	1.0 (3)
P1—C5A—C6A—C7A	−178.6 (3)	P1—C11—C16—C15	−179.6 (2)
C5A—C6A—C7A—C8A	0.0	C14—C15—C16—C11	−0.1 (4)
C6A—C7A—C8A—C9A	0.0	O3—P1—C17—C22	146.5 (2)
C7A—C8A—C9A—C10A	0.0	C5B—P1—C17—C22	27.4 (2)
C8A—C9A—C10A—C5A	0.0	C11—P1—C17—C22	−90.2 (2)
C6A—C5A—C10A—C9A	0.0	C5A—P1—C17—C22	20.7 (3)
P1—C5A—C10A—C9A	178.5 (3)	O3—P1—C17—C18	−32.4 (2)
O3—P1—C5B—C6B	−26.77 (10)	C5B—P1—C17—C18	−151.50 (19)
C17—P1—C5B—C6B	93.50 (11)	C11—P1—C17—C18	90.92 (18)
C11—P1—C5B—C6B	−150.54 (9)	C5A—P1—C17—C18	−158.1 (2)
C5A—P1—C5B—C6B	−177.1 (14)	C22—C17—C18—C19	−1.3 (3)
O3—P1—C5B—C10B	153.73 (14)	P1—C17—C18—C19	177.61 (18)
C17—P1—C5B—C10B	−86.01 (16)	C17—C18—C19—C20	0.0 (4)
C11—P1—C5B—C10B	29.96 (18)	C18—C19—C20—C21	1.7 (4)
C5A—P1—C5B—C10B	3.4 (14)	C19—C20—C21—C22	−2.1 (5)
C10B—C5B—C6B—C7B	0.0	C20—C21—C22—C17	0.8 (5)
P1—C5B—C6B—C7B	−179.52 (9)	C18—C17—C22—C21	0.9 (4)
C5B—C6B—C7B—C8B	0.0	P1—C17—C22—C21	−177.9 (2)
C6B—C7B—C8B—C9B	0.0		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O3	0.86	1.96	2.820 (2)	173
C14—H14···O1^{i}	0.93	2.45	3.368 (3)	170
C18—H18···O1	0.93	2.54	3.256 (3)	135
C22—H22···O1^{ii}	0.93	2.55	3.283 (3)	136

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

Fig. 1


C8a
C7a
C9a
C6a
C10a
C5a
O3
P1
N1
O2
C4
C3
C12
C13
C11
C2
C1
C14
C16
C17
C22
C18
O1
C15
C21
C19
C20