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(*N*-Phenylimino)bis[phosphonic bis(diphenylamide)]

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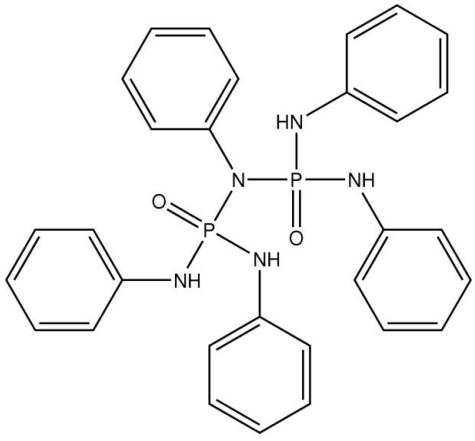
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.003 Å; R factor = 0.039; wR factor = 0.089; data-to-parameter ratio = 15.5.

The title compound, $NC_6H_5[PO(NHC_6H_5)_2]_2$ or $C_{30}H_{29}N_5O_2P_2$, was obtained as a side product during the addition of aniline to an amidoyl chloride, using PCl_5 as chlorinating agent. The title compound was first synthesized by Murray & Woodward [(1989). *Phosphorus Sulfur Silicon*, **41**, 399–403], again as a by-product, but no crystallographic evidence was given. The title compound crystallizes as two crystallographically unique molecules that form layers in the *ab* plane through O···H—N hydrogen-bond interactions, with an O···N minimum distance of 2.769 (2)Å and a maximum distance of 3.117 (2) Å. There is also one intramolecular O···H—N bond present in each of the two molecules, with an average O···N distance of 2.959 (4) Å.

Related literature

Full synthetic details for this compound have been published by Murray & Woodward (1989).



Experimental

Crystal data

$C_{30}H_{29}N_5O_2P_2$
M_r = 553.52
Orthorhombic, *Pbca*
a = 24.5585 (11) Å
b = 18.5726 (8) Å
c = 25.2655 (11) Å
V = 11524.0 (9) Å^3
Z = 16
Cu $K\alpha$ radiation
μ = 1.66 mm^{-1}
T = 150 (2) K
0.25 × 0.15 × 0.03 mm

Data collection

Bruker SMART 6000 diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.758, T_{max} = 0.949
139703 measured reflections
11291 independent reflections
7252 reflections with $I > 2\sigma(I)$
R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.089
S = 1.02
11291 reflections
728 parameters
10 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O11	0.866 (9)	2.386 (14)	3.117 (2)	142.4 (17)
N3—H3A···O11	0.868 (9)	1.911 (10)	2.769 (2)	169.2 (18)
N4—H4A···O12^{i}	0.870 (7)	2.220 (10)	3.032 (2)	155.3 (17)
N4—H4A···O1	0.870 (7)	2.455 (17)	2.959 (2)	117.5 (15)
N12—H12B···O1^{ii}	0.867 (9)	2.221 (11)	3.044 (2)	158.4 (17)
N12—H12B···O12	0.867 (9)	2.471 (18)	2.963 (2)	116.6 (15)
N14—H14B···O2^{iii}	0.872 (7)	2.002 (8)	2.856 (2)	166.0 (18)
N15—H15B···O2^{iii}	0.868 (9)	2.138 (11)	2.962 (2)	158.4 (18)

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *UdMX* (local program).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FI2046).

References

Bruker (1997). *SHELXTL*. Release 5.10. Bruker AXS Inc., Madison, USA.
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supplementary materials

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Comment

The packing along the a-b plane is dominated by hydrogen-bonding interactions. Both crystallographically different molecules show the same interactions. There is one amine which forms an intramolecular hydrogen bond and one intermolecular hydrogen bond; two amines with only one intermolecular interaction, and lastly one that has no intermolecular interactions. Every oxygen atom is implicated in two hydrogen-bonding interactions.

Along the A axis, the intermolecular hydrogen bonds are formed by alternating nitrogen and oxygen atoms, two per molecule. Along the B axis, the interactions zigzag through two nitrogen atoms on one molecule forming an H bond to one oxygen atom on the other molecule. Along the C axis, only weak van der Waals forces can be seen between the aromatic rings, with no π stacking interactions visible.

Experimental

The title compound was formed as a side product from an amidine synthesis, involving excess aniline (reagent grade (99%); purified by distillation prior to use) and PCl_5 (reagent grade (95%)), the latter of which forms $POCl_3$ during the reaction (all reagents are from Sigma-Aldrich). It is believed that $(Ph—NH)_3PO$ is then formed and dimerizes to the title compound once it is treated with aqueous solution of KOH. The title compound was previously published by Murray and Woodward in 1989. The actual crystals were formed by slow evaporation of an ethanolic solution of the title compound.

Refinement

All non-H atoms were refined by full-matrix least-squares with anisotropic displacement parameters. The H atoms bonded to C atoms were generated geometrically (C—H 0.95 Å) and were included in the refinement in the riding model approximation. The H atoms bonded to N atoms were generated geometrically, but their position was left to refine, with a restraint on the N—H distance set to 0.88 Å with a standard deviation of 0.01 Å. Their temperature factors of all H atoms were set to 1.2 times those of the equivalent isotropic temperature factors of the parent site.

Figures

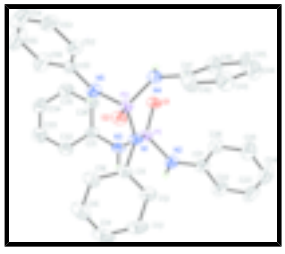


Fig. 1. a *ORTEP* view of the first crystallographically independent molecule of the title compound. Thermal ellipsoids are shown at 50% probability levels, H atoms of C atoms are omitted for clarity.

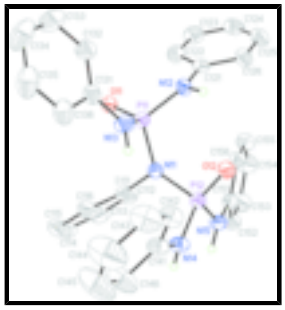


Fig. 2. b *ORTEP* view of the second crystallographically independent molecule of the title compound. Thermal ellipsoids are shown at 50% probability levels, H atoms of C atoms are omitted for clarity.

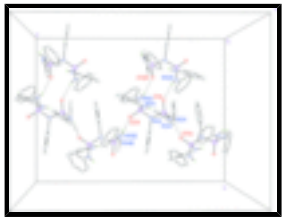


Fig. 3. The packing of the compound, viewed along the *c* axis, showing the intermolecular hydrogen bonding, H atoms of C atoms are omitted for clarity.

(*N*-Phenylimino)bis[phosphonic bis(diphenylamide)]

Crystal data

$C_{30}H_{29}N_5O_2P_2$	F_{000} = 4640
M_r = 553.52	D_x = 1.276 Mg m^{-3}
Orthorhombic, *Pbca*	Cu *K*α radiation λ = 1.54178 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 9956 reflections
a = 24.5585 (11) Å	θ = 6.9–142.3º
b = 18.5726 (8) Å	μ = 1.66 mm^{-1}
c = 25.2655 (11) Å	*T* = 150 (2) K
V = 11524.0 (9) Å^3	Rectangular, yellow
Z = 16	0.25 × 0.15 × 0.03 mm

Data collection

Bruker SMART 6000 diffractometer	11291 independent reflections
Radiation source: Rotating Anode	7252 reflections with $I > 2\sigma(I)$
Monochromator: Montel 200 optics	R_{int} = 0.046
Detector resolution: 5.5 pixels mm^{-1}	θ_{max} = 72.1º
T = 150(2) K	θ_{min} = 3.5º
ω scans	*h* = −30→30
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*k* = −21→22
T_{min} = 0.758, T_{max} = 0.949	*l* = −30→31
139703 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.039$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.089$	$w = 1/[\sigma^2(F_o^2) + (0.0532P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} = 0.001$
11291 reflections	$\Delta\rho_{max} = 0.39$ e Å^{-3}
728 parameters	$\Delta\rho_{min} = -0.36$ e Å^{-3}
10 restraints	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.000171 (8)

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}
P1	0.65576 (2)	0.48585 (3)	0.754249 (19)	0.02444 (12)
P2	0.53618 (2)	0.50155 (3)	0.73556 (2)	0.02467 (12)
O1	0.65139 (5)	0.56457 (7)	0.75262 (5)	0.0290 (3)
O2	0.48667 (5)	0.45736 (7)	0.74287 (5)	0.0286 (3)
N1	0.59122 (6)	0.45317 (8)	0.75373 (6)	0.0248 (4)
N2	0.68598 (7)	0.44726 (9)	0.80493 (7)	0.0293 (4)
H2A	0.7132 (6)	0.4203 (9)	0.7958 (7)	0.035*
N3	0.69061 (7)	0.44926 (9)	0.70599 (7)	0.0281 (4)
H3A	0.7037 (7)	0.4068 (6)	0.7128 (7)	0.034*
N4	0.53229 (6)	0.57819 (9)	0.76724 (6)	0.0263 (4)
H4A	0.5573 (6)	0.6086 (8)	0.7574 (7)	0.032*
N5	0.54844 (7)	0.52345 (9)	0.67328 (7)	0.0297 (4)
H5A	0.5804 (5)	0.5158 (10)	0.6614 (7)	0.036*
C11	0.58426 (7)	0.37484 (10)	0.75339 (8)	0.0291 (5)
C12	0.58079 (8)	0.33875 (11)	0.80111 (9)	0.0353 (5)
H12A	0.5838	0.3642	0.8336	0.042*
C13	0.57285 (9)	0.26438 (12)	0.80081 (10)	0.0473 (7)
H13A	0.5708	0.2387	0.8333	0.057*
C14	0.56801 (9)	0.22814 (13)	0.75364 (10)	0.0504 (7)

H14A	0.5625	0.1775	0.7537	0.061*
C15	0.57104 (9)	0.26442 (13)	0.70659 (11)	0.0509 (7)
H15A	0.5671	0.2390	0.6742	0.061*
C16	0.57988 (8)	0.33834 (12)	0.70596 (9)	0.0389 (6)
H16A	0.5829	0.3634	0.6733	0.047*
C21	0.67473 (8)	0.45363 (11)	0.85936 (8)	0.0309 (5)
C22	0.70931 (9)	0.41966 (12)	0.89513 (9)	0.0408 (6)
H22A	0.7394	0.3924	0.8827	0.049*
C23	0.69967 (11)	0.42569 (14)	0.94892 (9)	0.0537 (7)
H23A	0.7235	0.4027	0.9732	0.064*
C24	0.65608 (11)	0.46445 (14)	0.96771 (9)	0.0593 (8)
H24A	0.6498	0.4683	1.0047	0.071*
C25	0.62165 (11)	0.49771 (13)	0.93227 (9)	0.0520 (7)
H25A	0.5913	0.5242	0.9450	0.062*
C26	0.63085 (9)	0.49286 (12)	0.87810 (8)	0.0375 (5)
H26A	0.6071	0.5164	0.8540	0.045*
C31	0.68792 (8)	0.46881 (11)	0.65188 (8)	0.0300 (5)
C32	0.68773 (10)	0.41429 (13)	0.61464 (9)	0.0525 (7)
H32A	0.6882	0.3654	0.6256	0.063*
C33	0.68685 (12)	0.43123 (15)	0.56134 (10)	0.0706 (9)
H33A	0.6868	0.3936	0.5358	0.085*
C34	0.68613 (11)	0.50187 (14)	0.54469 (9)	0.0583 (7)
H34A	0.6858	0.5133	0.5080	0.070*
C35	0.68586 (10)	0.55557 (13)	0.58215 (9)	0.0495 (7)
H35A	0.6852	0.6045	0.5712	0.059*
C36	0.68658 (9)	0.53923 (12)	0.63550 (8)	0.0374 (5)
H36A	0.6862	0.5769	0.6609	0.045*
C41	0.51105 (8)	0.58915 (10)	0.81928 (8)	0.0282 (5)
C42	0.46391 (8)	0.55543 (12)	0.83649 (9)	0.0375 (5)
H42A	0.4446	0.5238	0.8136	0.045*
C43	0.44509 (9)	0.56827 (13)	0.88754 (9)	0.0459 (6)
H43A	0.4134	0.5440	0.8996	0.055*
C44	0.47129 (10)	0.61517 (13)	0.92088 (9)	0.0467 (6)
H44A	0.4581	0.6234	0.9557	0.056*
C45	0.51736 (10)	0.65031 (13)	0.90268 (9)	0.0480 (6)
H45A	0.5354	0.6840	0.9249	0.058*
C46	0.53746 (9)	0.63701 (12)	0.85246 (8)	0.0400 (6)
H46A	0.5695	0.6608	0.8407	0.048*
C51	0.51003 (8)	0.54874 (11)	0.63601 (8)	0.0298 (5)
C52	0.45839 (9)	0.57113 (11)	0.65102 (8)	0.0365 (5)
H52A	0.4480	0.5703	0.6872	0.044*
C53	0.42208 (9)	0.59473 (12)	0.61288 (9)	0.0434 (6)
H53A	0.3868	0.6101	0.6234	0.052*
C54	0.43579 (10)	0.59647 (14)	0.56070 (10)	0.0569 (7)
H54A	0.4105	0.6131	0.5350	0.068*
C55	0.48704 (11)	0.57370 (15)	0.54554 (10)	0.0634 (8)
H55A	0.4970	0.5748	0.5092	0.076*
C56	0.52398 (10)	0.54928 (13)	0.58302 (9)	0.0477 (6)
H56A	0.5589	0.5329	0.5722	0.057*

P11	0.78654 (2)	0.27729 (3)	0.73290 (2)	0.02464 (12)
P12	0.90624 (2)	0.29401 (3)	0.75486 (2)	0.02492 (12)
O11	0.73709 (5)	0.32157 (7)	0.73999 (5)	0.0295 (3)
O12	0.90202 (5)	0.21522 (7)	0.75375 (5)	0.0298 (3)
N11	0.84200 (6)	0.32634 (8)	0.74910 (6)	0.0243 (4)
N12	0.78249 (6)	0.20195 (8)	0.76629 (6)	0.0251 (4)
H12B	0.8073 (6)	0.1707 (8)	0.7580 (7)	0.030*
N13	0.79872 (7)	0.25319 (9)	0.67107 (6)	0.0309 (4)
H13B	0.8304 (5)	0.2642 (10)	0.6590 (7)	0.037*
N14	0.94452 (7)	0.33005 (9)	0.70872 (7)	0.0283 (4)
H14B	0.9577 (7)	0.3717 (6)	0.7180 (7)	0.034*
N15	0.93244 (7)	0.33257 (9)	0.80766 (6)	0.0286 (4)
H15B	0.9548 (6)	0.3671 (8)	0.7995 (7)	0.034*
C111	0.83487 (7)	0.40416 (11)	0.74594 (8)	0.0271 (5)
C112	0.82790 (8)	0.44297 (11)	0.79193 (9)	0.0344 (5)
H11A	0.8290	0.4193	0.8252	0.041*
C113	0.81929 (9)	0.51689 (12)	0.78940 (10)	0.0464 (6)
H11B	0.8146	0.5438	0.8210	0.056*
C114	0.81759 (9)	0.55119 (12)	0.74101 (11)	0.0497 (7)
H11C	0.8117	0.6017	0.7394	0.060*
C115	0.82449 (9)	0.51218 (12)	0.69487 (10)	0.0471 (6)
H11D	0.8230	0.5358	0.6615	0.057*
C116	0.83359 (8)	0.43834 (11)	0.69735 (9)	0.0362 (5)
H11E	0.8389	0.4115	0.6658	0.043*
C121	0.75911 (8)	0.19211 (10)	0.81755 (7)	0.0264 (5)
C122	0.71505 (8)	0.23221 (11)	0.83540 (8)	0.0342 (5)
H12C	0.6996	0.2687	0.8137	0.041*
C123	0.69384 (9)	0.21837 (13)	0.88524 (8)	0.0413 (6)
H12D	0.6641	0.2464	0.8977	0.050*
C124	0.71469 (9)	0.16517 (12)	0.91707 (8)	0.0400 (6)
H12E	0.6995	0.1564	0.9510	0.048*
C125	0.75813 (9)	0.12454 (11)	0.89901 (8)	0.0381 (6)
H12F	0.7727	0.0872	0.9205	0.046*
C126	0.78043 (8)	0.13834 (11)	0.84969 (8)	0.0325 (5)
H12G	0.8106	0.1108	0.8377	0.039*
C131	0.75926 (8)	0.23638 (10)	0.63213 (8)	0.0303 (5)
C132	0.70794 (9)	0.21190 (11)	0.64540 (8)	0.0377 (5)
H13C	0.6983	0.2051	0.6815	0.045*
C133	0.67069 (10)	0.19726 (13)	0.60574 (10)	0.0501 (7)
H13D	0.6354	0.1804	0.6150	0.060*
C134	0.68368 (11)	0.20655 (14)	0.55348 (10)	0.0573 (8)
H13E	0.6578	0.1960	0.5266	0.069*
C135	0.73497 (11)	0.23142 (13)	0.54034 (9)	0.0516 (7)
H13F	0.7444	0.2380	0.5042	0.062*
C136	0.77265 (10)	0.24683 (12)	0.57930 (8)	0.0396 (6)
H13G	0.8077	0.2645	0.5700	0.048*
C141	0.94267 (8)	0.31258 (12)	0.65441 (8)	0.0340 (5)
C142	0.93114 (9)	0.24394 (12)	0.63629 (8)	0.0395 (6)
H14C	0.9248	0.2061	0.6608	0.047*

C143	0.92889 (10)	0.23030 (14)	0.58253 (9)	0.0566 (7)
H14D	0.9206	0.1831	0.5704	0.068*
C144	0.93847 (13)	0.28417 (17)	0.54632 (10)	0.0787 (10)
H14E	0.9361	0.2747	0.5094	0.094*
C145	0.95154 (13)	0.35178 (16)	0.56418 (10)	0.0830 (11)
H14F	0.9593	0.3889	0.5394	0.100*
C146	0.95355 (11)	0.36668 (14)	0.61791 (9)	0.0575 (8)
H14G	0.9624	0.4138	0.6298	0.069*
C151	0.90887 (8)	0.33299 (11)	0.85851 (8)	0.0286 (5)
C152	0.92385 (9)	0.38581 (12)	0.89471 (8)	0.0379 (5)
H15C	0.9511	0.4200	0.8856	0.045*
C153	0.89929 (10)	0.38867 (13)	0.94370 (9)	0.0485 (6)
H15D	0.9096	0.4251	0.9681	0.058*
C154	0.85972 (9)	0.33911 (13)	0.95780 (9)	0.0459 (6)
H15E	0.8428	0.3414	0.9916	0.055*
C155	0.84527 (9)	0.28639 (12)	0.92205 (8)	0.0370 (5)
H15F	0.8182	0.2521	0.9314	0.044*
C156	0.86962 (8)	0.28287 (11)	0.87282 (7)	0.0294 (5)
H15G	0.8595	0.2460	0.8487	0.035*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P1	0.0215 (3)	0.0230 (3)	0.0288 (3)	−0.0004 (2)	−0.0015 (2)	0.0018 (2)
P2	0.0216 (3)	0.0234 (3)	0.0289 (3)	0.0001 (2)	−0.0015 (2)	0.0010 (2)
O1	0.0247 (8)	0.0224 (7)	0.0399 (9)	−0.0023 (6)	−0.0011 (6)	0.0000 (6)
O2	0.0234 (8)	0.0250 (8)	0.0375 (8)	−0.0015 (6)	−0.0006 (6)	−0.0009 (6)
N1	0.0214 (9)	0.0196 (9)	0.0333 (10)	−0.0009 (7)	−0.0024 (7)	0.0017 (7)
N2	0.0244 (10)	0.0333 (11)	0.0303 (10)	0.0041 (8)	−0.0009 (8)	0.0025 (8)
N3	0.0284 (10)	0.0223 (10)	0.0335 (10)	0.0044 (7)	0.0032 (8)	0.0036 (8)
N4	0.0235 (9)	0.0238 (10)	0.0316 (9)	−0.0035 (7)	0.0019 (7)	0.0019 (8)
N5	0.0240 (10)	0.0350 (10)	0.0301 (10)	0.0035 (8)	0.0009 (8)	0.0031 (8)
C11	0.0193 (11)	0.0226 (11)	0.0454 (13)	0.0000 (8)	−0.0020 (9)	0.0004 (10)
C12	0.0294 (13)	0.0303 (13)	0.0462 (14)	−0.0034 (9)	−0.0085 (10)	0.0064 (10)
C13	0.0335 (14)	0.0321 (14)	0.0763 (19)	−0.0060 (11)	−0.0137 (13)	0.0190 (13)
C14	0.0383 (15)	0.0219 (13)	0.091 (2)	−0.0028 (10)	−0.0063 (14)	0.0001 (13)
C15	0.0436 (15)	0.0357 (15)	0.0735 (19)	−0.0064 (11)	0.0061 (13)	−0.0171 (13)
C16	0.0363 (14)	0.0316 (13)	0.0489 (14)	−0.0031 (10)	0.0037 (11)	−0.0055 (11)
C21	0.0300 (12)	0.0309 (13)	0.0317 (12)	−0.0065 (9)	−0.0040 (9)	0.0052 (9)
C22	0.0413 (14)	0.0396 (14)	0.0416 (14)	−0.0001 (11)	−0.0066 (11)	0.0100 (11)
C23	0.0658 (19)	0.0572 (18)	0.0383 (15)	−0.0027 (14)	−0.0118 (13)	0.0168 (13)
C24	0.083 (2)	0.065 (2)	0.0302 (14)	−0.0045 (16)	0.0029 (14)	0.0099 (13)
C25	0.0602 (18)	0.0575 (18)	0.0384 (14)	0.0019 (14)	0.0087 (12)	0.0023 (13)
C26	0.0388 (14)	0.0409 (14)	0.0326 (12)	0.0001 (11)	−0.0013 (10)	0.0040 (10)
C31	0.0267 (12)	0.0309 (12)	0.0324 (12)	0.0030 (9)	0.0023 (9)	0.0045 (9)
C32	0.087 (2)	0.0325 (15)	0.0375 (14)	0.0138 (13)	0.0048 (13)	0.0008 (11)
C33	0.129 (3)	0.0465 (18)	0.0360 (15)	0.0196 (17)	0.0039 (16)	−0.0059 (13)
C34	0.090 (2)	0.0552 (18)	0.0301 (13)	0.0126 (15)	0.0068 (13)	0.0077 (13)

C35	0.0700 (19)	0.0373 (15)	0.0411 (14)	−0.0001 (13)	0.0034 (13)	0.0105 (12)
C36	0.0467 (15)	0.0295 (13)	0.0359 (13)	−0.0020 (10)	0.0037 (11)	0.0032 (10)
C41	0.0277 (12)	0.0246 (12)	0.0322 (12)	0.0060 (9)	−0.0020 (9)	0.0025 (9)
C42	0.0318 (13)	0.0374 (14)	0.0433 (13)	−0.0028 (10)	0.0049 (10)	−0.0086 (11)
C43	0.0396 (15)	0.0496 (16)	0.0485 (15)	−0.0009 (12)	0.0117 (12)	−0.0034 (12)
C44	0.0524 (17)	0.0537 (17)	0.0340 (13)	0.0093 (13)	0.0050 (12)	−0.0034 (12)
C45	0.0565 (17)	0.0503 (17)	0.0373 (14)	−0.0059 (13)	−0.0046 (12)	−0.0095 (12)
C46	0.0412 (14)	0.0402 (14)	0.0386 (13)	−0.0092 (11)	−0.0026 (11)	−0.0019 (11)
C51	0.0313 (12)	0.0266 (12)	0.0314 (12)	−0.0017 (9)	−0.0056 (9)	0.0025 (9)
C52	0.0392 (14)	0.0335 (13)	0.0366 (13)	0.0045 (10)	−0.0066 (10)	0.0013 (10)
C53	0.0371 (14)	0.0413 (15)	0.0518 (15)	0.0074 (11)	−0.0113 (11)	0.0038 (12)
C54	0.0501 (18)	0.071 (2)	0.0498 (17)	0.0030 (14)	−0.0197 (13)	0.0154 (14)
C55	0.0606 (19)	0.095 (2)	0.0342 (15)	0.0061 (17)	−0.0092 (13)	0.0147 (14)
C56	0.0385 (15)	0.0673 (19)	0.0374 (14)	0.0020 (12)	−0.0021 (11)	0.0071 (12)
P11	0.0224 (3)	0.0238 (3)	0.0277 (3)	−0.0001 (2)	0.0000 (2)	0.0015 (2)
P12	0.0217 (3)	0.0230 (3)	0.0301 (3)	0.0007 (2)	0.0011 (2)	0.0004 (2)
O11	0.0238 (8)	0.0254 (8)	0.0394 (8)	0.0018 (6)	0.0009 (6)	0.0057 (6)
O12	0.0270 (8)	0.0213 (7)	0.0410 (9)	0.0020 (6)	0.0014 (6)	0.0004 (6)
N11	0.0213 (9)	0.0201 (9)	0.0314 (10)	0.0012 (7)	0.0000 (7)	0.0000 (7)
N12	0.0248 (9)	0.0217 (9)	0.0290 (9)	0.0038 (7)	0.0032 (7)	0.0006 (7)
N13	0.0271 (10)	0.0383 (11)	0.0274 (10)	−0.0055 (8)	0.0023 (8)	−0.0006 (8)
N14	0.0276 (10)	0.0250 (10)	0.0324 (10)	−0.0046 (8)	0.0047 (8)	−0.0036 (8)
N15	0.0257 (10)	0.0299 (11)	0.0302 (10)	−0.0057 (7)	0.0006 (8)	0.0010 (8)
C111	0.0178 (11)	0.0247 (11)	0.0390 (13)	0.0007 (8)	0.0000 (9)	0.0008 (9)
C112	0.0284 (12)	0.0296 (13)	0.0451 (14)	0.0045 (9)	−0.0043 (10)	−0.0043 (10)
C113	0.0355 (14)	0.0324 (14)	0.0714 (18)	0.0062 (11)	−0.0059 (12)	−0.0135 (13)
C114	0.0356 (14)	0.0215 (13)	0.092 (2)	0.0035 (10)	0.0057 (14)	0.0059 (14)
C115	0.0384 (14)	0.0342 (15)	0.0688 (18)	0.0025 (11)	0.0093 (12)	0.0188 (13)
C116	0.0313 (13)	0.0305 (13)	0.0469 (14)	0.0011 (10)	0.0091 (10)	0.0069 (10)
C121	0.0250 (11)	0.0243 (12)	0.0299 (11)	−0.0062 (8)	−0.0001 (9)	−0.0011 (9)
C122	0.0289 (12)	0.0387 (14)	0.0351 (12)	0.0017 (10)	0.0043 (10)	0.0049 (10)
C123	0.0316 (13)	0.0504 (16)	0.0419 (14)	−0.0012 (11)	0.0105 (10)	−0.0005 (12)
C124	0.0436 (15)	0.0479 (15)	0.0286 (12)	−0.0145 (12)	0.0060 (10)	0.0022 (11)
C125	0.0513 (16)	0.0321 (14)	0.0310 (12)	−0.0066 (11)	−0.0033 (11)	0.0052 (10)
C126	0.0390 (14)	0.0245 (12)	0.0339 (12)	0.0006 (9)	−0.0013 (10)	0.0002 (9)
C131	0.0358 (13)	0.0241 (12)	0.0310 (12)	0.0029 (9)	−0.0041 (9)	0.0001 (9)
C132	0.0421 (14)	0.0346 (14)	0.0365 (13)	−0.0067 (11)	−0.0038 (11)	−0.0006 (10)
C133	0.0404 (15)	0.0519 (17)	0.0579 (17)	−0.0046 (12)	−0.0089 (13)	−0.0176 (13)
C134	0.0557 (18)	0.0668 (19)	0.0493 (16)	0.0148 (14)	−0.0231 (14)	−0.0260 (14)
C135	0.0667 (19)	0.0588 (18)	0.0292 (13)	0.0174 (14)	−0.0086 (12)	−0.0064 (12)
C136	0.0471 (15)	0.0389 (14)	0.0329 (12)	0.0071 (11)	−0.0009 (11)	−0.0003 (10)
C141	0.0312 (13)	0.0366 (13)	0.0342 (12)	−0.0014 (10)	0.0089 (10)	−0.0030 (10)
C142	0.0450 (15)	0.0375 (14)	0.0359 (13)	−0.0016 (11)	0.0076 (11)	−0.0041 (10)
C143	0.072 (2)	0.0527 (18)	0.0447 (15)	−0.0124 (14)	0.0109 (14)	−0.0123 (13)
C144	0.122 (3)	0.078 (2)	0.0360 (16)	−0.028 (2)	0.0170 (17)	−0.0129 (16)
C145	0.142 (3)	0.068 (2)	0.0389 (16)	−0.031 (2)	0.0199 (18)	0.0012 (15)
C146	0.091 (2)	0.0434 (16)	0.0379 (14)	−0.0185 (14)	0.0134 (14)	−0.0015 (12)
C151	0.0261 (12)	0.0295 (12)	0.0302 (11)	0.0019 (9)	−0.0039 (9)	0.0017 (9)
C152	0.0394 (14)	0.0381 (14)	0.0361 (13)	−0.0116 (10)	−0.0064 (10)	−0.0003 (10)

C153	0.0618 (17)	0.0493 (16)	0.0342 (13)	−0.0150 (13)	−0.0050 (12)	−0.0093 (11)
C154	0.0575 (17)	0.0507 (17)	0.0294 (13)	−0.0083 (12)	0.0044 (11)	−0.0056 (11)
C155	0.0389 (14)	0.0357 (14)	0.0363 (13)	−0.0035 (10)	0.0041 (10)	−0.0002 (10)
C156	0.0294 (12)	0.0286 (12)	0.0301 (11)	−0.0005 (9)	−0.0013 (9)	−0.0025 (9)

Geometric parameters (Å, °)

P1—O1	1.4665 (13)	P11—O11	1.4775 (13)
P1—N3	1.6374 (17)	P11—N12	1.6368 (16)
P1—N2	1.6444 (17)	P11—N13	1.6522 (17)
P1—N1	1.6973 (16)	P11—N11	1.6888 (16)
P2—O2	1.4787 (13)	P12—O12	1.4672 (13)
P2—N4	1.6359 (17)	P12—N14	1.6404 (17)
P2—N5	1.6530 (17)	P12—N15	1.6451 (17)
P2—N1	1.6866 (15)	P12—N11	1.6944 (15)
N1—C11	1.465 (2)	N11—C111	1.458 (2)
N2—C21	1.408 (2)	N12—C121	1.428 (2)
N2—H2A	0.866 (9)	N12—H12B	0.867 (9)
N3—C31	1.416 (2)	N13—C131	1.416 (2)
N3—H3A	0.868 (9)	N13—H13B	0.860 (9)
N4—C41	1.429 (2)	N14—C141	1.411 (2)
N4—H4A	0.870 (7)	N14—H14B	0.872 (7)
N5—C51	1.413 (2)	N15—C151	1.409 (2)
N5—H5A	0.852 (9)	N15—H15B	0.868 (9)
C11—C16	1.381 (3)	C111—C112	1.378 (3)
C11—C12	1.382 (3)	C111—C116	1.382 (3)
C12—C13	1.395 (3)	C112—C113	1.391 (3)
C12—H12A	0.9500	C112—H11A	0.9500
C13—C14	1.374 (3)	C113—C114	1.379 (3)
C13—H13A	0.9500	C113—H11B	0.9500
C14—C15	1.369 (3)	C114—C115	1.383 (3)
C14—H14A	0.9500	C114—H11C	0.9500
C15—C16	1.390 (3)	C115—C116	1.391 (3)
C15—H15A	0.9500	C115—H11D	0.9500
C16—H16A	0.9500	C116—H11E	0.9500
C21—C26	1.384 (3)	C121—C122	1.389 (3)
C21—C22	1.392 (3)	C121—C126	1.390 (2)
C22—C23	1.384 (3)	C122—C123	1.387 (3)
C22—H22A	0.9500	C122—H12C	0.9500
C23—C24	1.375 (3)	C123—C124	1.373 (3)
C23—H23A	0.9500	C123—H12D	0.9500
C24—C25	1.378 (3)	C124—C125	1.384 (3)
C24—H24A	0.9500	C124—H12E	0.9500
C25—C26	1.390 (3)	C125—C126	1.385 (3)
C25—H25A	0.9500	C125—H12F	0.9500
C26—H26A	0.9500	C126—H12G	0.9500
C31—C36	1.372 (3)	C131—C132	1.381 (3)
C31—C32	1.382 (3)	C131—C136	1.388 (3)
C32—C33	1.383 (3)	C132—C133	1.384 (3)

C32—H32A	0.9500	C132—H13C	0.9500
C33—C34	1.378 (3)	C133—C134	1.369 (3)
C33—H33A	0.9500	C133—H13D	0.9500
C34—C35	1.375 (3)	C134—C135	1.382 (3)
C34—H34A	0.9500	C134—H13E	0.9500
C35—C36	1.382 (3)	C135—C136	1.381 (3)
C35—H35A	0.9500	C135—H13F	0.9500
C36—H36A	0.9500	C136—H13G	0.9500
C41—C46	1.383 (3)	C141—C142	1.384 (3)
C41—C42	1.386 (3)	C141—C146	1.390 (3)
C42—C43	1.391 (3)	C142—C143	1.383 (3)
C42—H42A	0.9500	C142—H14C	0.9500
C43—C44	1.372 (3)	C143—C144	1.376 (3)
C43—H43A	0.9500	C143—H14D	0.9500
C44—C45	1.385 (3)	C144—C145	1.372 (3)
C44—H44A	0.9500	C144—H14E	0.9500
C45—C46	1.384 (3)	C145—C146	1.386 (3)
C45—H45A	0.9500	C145—H14F	0.9500
C46—H46A	0.9500	C146—H14G	0.9500
C51—C56	1.382 (3)	C151—C156	1.388 (3)
C51—C52	1.387 (3)	C151—C152	1.391 (3)
C52—C53	1.384 (3)	C152—C153	1.378 (3)
C52—H52A	0.9500	C152—H15C	0.9500
C53—C54	1.361 (3)	C153—C154	1.385 (3)
C53—H53A	0.9500	C153—H15D	0.9500
C54—C55	1.382 (3)	C154—C155	1.379 (3)
C54—H54A	0.9500	C154—H15E	0.9500
C55—C56	1.388 (3)	C155—C156	1.382 (3)
C55—H55A	0.9500	C155—H15F	0.9500
C56—H56A	0.9500	C156—H15G	0.9500
O1—P1—N3	115.53 (8)	O11—P11—N12	111.31 (8)
O1—P1—N2	119.30 (8)	O11—P11—N13	114.46 (8)
N3—P1—N2	99.38 (9)	N12—P11—N13	105.47 (9)
O1—P1—N1	106.74 (8)	O11—P11—N11	109.46 (8)
N3—P1—N1	109.51 (8)	N12—P11—N11	112.66 (8)
N2—P1—N1	105.77 (8)	N13—P11—N11	103.25 (8)
O2—P2—N4	111.96 (8)	O12—P12—N14	115.70 (8)
O2—P2—N5	113.91 (8)	O12—P12—N15	118.51 (8)
N4—P2—N5	105.21 (9)	N14—P12—N15	100.05 (8)
O2—P2—N1	109.23 (8)	O12—P12—N11	106.62 (8)
N4—P2—N1	112.16 (8)	N14—P12—N11	109.15 (8)
N5—P2—N1	104.13 (8)	N15—P12—N11	106.23 (8)
C11—N1—P2	115.72 (12)	C111—N11—P11	115.12 (12)
C11—N1—P1	117.66 (12)	C111—N11—P12	117.89 (12)
P2—N1—P1	124.05 (9)	P11—N11—P12	125.49 (9)
C21—N2—P1	129.45 (14)	C121—N12—P11	126.94 (13)
C21—N2—H2A	117.5 (13)	C121—N12—H12B	114.6 (12)
P1—N2—H2A	113.1 (13)	P11—N12—H12B	113.9 (13)
C31—N3—P1	126.02 (14)	C131—N13—P11	126.36 (14)

C31—N3—H3A	116.2 (13)	C131—N13—H13B	115.2 (13)
P1—N3—H3A	115.0 (13)	P11—N13—H13B	115.7 (13)
C41—N4—P2	126.54 (13)	C141—N14—P12	125.38 (14)
C41—N4—H4A	115.3 (12)	C141—N14—H14B	118.6 (13)
P2—N4—H4A	112.6 (13)	P12—N14—H14B	112.6 (13)
C51—N5—P2	126.47 (14)	C151—N15—P12	125.52 (14)
C51—N5—H5A	115.9 (14)	C151—N15—H15B	118.2 (13)
P2—N5—H5A	117.5 (13)	P12—N15—H15B	112.0 (13)
C16—C11—C12	120.9 (2)	C112—C111—C116	120.4 (2)
C16—C11—N1	120.11 (18)	C112—C111—N11	119.16 (18)
C12—C11—N1	118.93 (18)	C116—C111—N11	120.45 (18)
C11—C12—C13	118.9 (2)	C111—C112—C113	119.8 (2)
C11—C12—H12A	120.5	C111—C112—H11A	120.1
C13—C12—H12A	120.5	C113—C112—H11A	120.1
C14—C13—C12	120.1 (2)	C114—C113—C112	120.1 (2)
C14—C13—H13A	119.9	C114—C113—H11B	120.0
C12—C13—H13A	119.9	C112—C113—H11B	120.0
C15—C14—C13	120.5 (2)	C113—C114—C115	120.1 (2)
C15—C14—H14A	119.7	C113—C114—H11C	120.0
C13—C14—H14A	119.7	C115—C114—H11C	120.0
C14—C15—C16	120.3 (2)	C114—C115—C116	119.9 (2)
C14—C15—H15A	119.8	C114—C115—H11D	120.1
C16—C15—H15A	119.8	C116—C115—H11D	120.1
C11—C16—C15	119.2 (2)	C111—C116—C115	119.8 (2)
C11—C16—H16A	120.4	C111—C116—H11E	120.1
C15—C16—H16A	120.4	C115—C116—H11E	120.1
C26—C21—C22	119.5 (2)	C122—C121—C126	119.29 (19)
C26—C21—N2	122.08 (19)	C122—C121—N12	122.61 (18)
C22—C21—N2	118.5 (2)	C126—C121—N12	118.06 (18)
C23—C22—C21	119.8 (2)	C123—C122—C121	119.2 (2)
C23—C22—H22A	120.1	C123—C122—H12C	120.4
C21—C22—H22A	120.1	C121—C122—H12C	120.4
C24—C23—C22	121.0 (2)	C124—C123—C122	121.7 (2)
C24—C23—H23A	119.5	C124—C123—H12D	119.2
C22—C23—H23A	119.5	C122—C123—H12D	119.2
C23—C24—C25	119.2 (2)	C123—C124—C125	119.1 (2)
C23—C24—H24A	120.4	C123—C124—H12E	120.4
C25—C24—H24A	120.4	C125—C124—H12E	120.4
C24—C25—C26	120.7 (2)	C124—C125—C126	120.0 (2)
C24—C25—H25A	119.6	C124—C125—H12F	120.0
C26—C25—H25A	119.6	C126—C125—H12F	120.0
C21—C26—C25	119.8 (2)	C125—C126—C121	120.7 (2)
C21—C26—H26A	120.1	C125—C126—H12G	119.7
C25—C26—H26A	120.1	C121—C126—H12G	119.7
C36—C31—C32	119.5 (2)	C132—C131—C136	119.7 (2)
C36—C31—N3	122.46 (19)	C132—C131—N13	121.90 (19)
C32—C31—N3	118.01 (19)	C136—C131—N13	118.37 (19)
C31—C32—C33	119.8 (2)	C131—C132—C133	119.5 (2)
C31—C32—H32A	120.1	C131—C132—H13C	120.3

C33—C32—H32A	120.1	C133—C132—H13C	120.3
C34—C33—C32	120.9 (2)	C134—C133—C132	121.3 (2)
C34—C33—H33A	119.5	C134—C133—H13D	119.4
C32—C33—H33A	119.5	C132—C133—H13D	119.4
C35—C34—C33	118.7 (2)	C133—C134—C135	119.1 (2)
C35—C34—H34A	120.6	C133—C134—H13E	120.5
C33—C34—H34A	120.6	C135—C134—H13E	120.5
C34—C35—C36	120.8 (2)	C136—C135—C134	120.6 (2)
C34—C35—H35A	119.6	C136—C135—H13F	119.7
C36—C35—H35A	119.6	C134—C135—H13F	119.7
C31—C36—C35	120.3 (2)	C135—C136—C131	119.8 (2)
C31—C36—H36A	119.9	C135—C136—H13G	120.1
C35—C36—H36A	119.9	C131—C136—H13G	120.1
C46—C41—C42	119.5 (2)	C142—C141—C146	119.1 (2)
C46—C41—N4	118.55 (19)	C142—C141—N14	122.70 (19)
C42—C41—N4	121.95 (18)	C146—C141—N14	118.2 (2)
C41—C42—C43	119.4 (2)	C143—C142—C141	120.1 (2)
C41—C42—H42A	120.3	C143—C142—H14C	119.9
C43—C42—H42A	120.3	C141—C142—H14C	119.9
C44—C43—C42	121.5 (2)	C144—C143—C142	120.9 (2)
C44—C43—H43A	119.3	C144—C143—H14D	119.6
C42—C43—H43A	119.3	C142—C143—H14D	119.6
C43—C44—C45	118.6 (2)	C145—C144—C143	119.1 (3)
C43—C44—H44A	120.7	C145—C144—H14E	120.4
C45—C44—H44A	120.7	C143—C144—H14E	120.4
C46—C45—C44	120.8 (2)	C144—C145—C146	120.9 (3)
C46—C45—H45A	119.6	C144—C145—H14F	119.6
C44—C45—H45A	119.6	C146—C145—H14F	119.6
C41—C46—C45	120.2 (2)	C145—C146—C141	119.9 (2)
C41—C46—H46A	119.9	C145—C146—H14G	120.0
C45—C46—H46A	119.9	C141—C146—H14G	120.0
C56—C51—C52	119.3 (2)	C156—C151—C152	119.05 (19)
C56—C51—N5	118.84 (19)	C156—C151—N15	121.27 (18)
C52—C51—N5	121.86 (19)	C152—C151—N15	119.66 (19)
C53—C52—C51	119.6 (2)	C153—C152—C151	120.1 (2)
C53—C52—H52A	120.2	C153—C152—H15C	119.9
C51—C52—H52A	120.2	C151—C152—H15C	119.9
C54—C53—C52	121.5 (2)	C152—C153—C154	120.8 (2)
C54—C53—H53A	119.3	C152—C153—H15D	119.6
C52—C53—H53A	119.3	C154—C153—H15D	119.6
C53—C54—C55	119.1 (2)	C155—C154—C153	119.0 (2)
C53—C54—H54A	120.4	C155—C154—H15E	120.5
C55—C54—H54A	120.4	C153—C154—H15E	120.5
C54—C55—C56	120.4 (2)	C154—C155—C156	120.8 (2)
C54—C55—H55A	119.8	C154—C155—H15F	119.6
C56—C55—H55A	119.8	C156—C155—H15F	119.6
C51—C56—C55	120.1 (2)	C155—C156—C151	120.22 (19)
C51—C56—H56A	120.0	C155—C156—H15G	119.9
C55—C56—H56A	120.0	C151—C156—H15G	119.9

O2—P2—N1—C11	21.87 (16)	O11—P11—N11—C111	−23.10 (15)
N4—P2—N1—C11	146.60 (13)	N12—P11—N11—C111	−147.51 (13)
N5—P2—N1—C11	−100.16 (14)	N13—P11—N11—C111	99.21 (14)
O2—P2—N1—P1	−176.79 (9)	O11—P11—N11—P12	171.23 (10)
N4—P2—N1—P1	−52.06 (13)	N12—P11—N11—P12	46.82 (13)
N5—P2—N1—P1	61.18 (12)	N13—P11—N11—P12	−66.47 (12)
O1—P1—N1—C11	178.04 (13)	O12—P12—N11—C111	−176.42 (13)
N3—P1—N1—C11	52.30 (16)	N14—P12—N11—C111	−50.77 (15)
N2—P1—N1—C11	−53.94 (16)	N15—P12—N11—C111	56.30 (15)
O1—P1—N1—P2	17.03 (13)	O12—P12—N11—P11	−11.10 (13)
N3—P1—N1—P2	−108.70 (11)	N14—P12—N11—P11	114.55 (11)
N2—P1—N1—P2	145.06 (11)	N15—P12—N11—P11	−138.39 (11)
O1—P1—N2—C21	55.5 (2)	O11—P11—N12—C121	−37.91 (18)
N3—P1—N2—C21	−178.12 (18)	N13—P11—N12—C121	−162.60 (16)
N1—P1—N2—C21	−64.6 (2)	N11—P11—N12—C121	85.48 (17)
O1—P1—N3—C31	−42.3 (2)	O11—P11—N13—C131	−34.9 (2)
N2—P1—N3—C31	−171.27 (17)	N12—P11—N13—C131	87.78 (18)
N1—P1—N3—C31	78.20 (18)	N11—P11—N13—C131	−153.80 (16)
O2—P2—N4—C41	41.43 (18)	O12—P12—N14—C141	47.0 (2)
N5—P2—N4—C41	165.65 (16)	N15—P12—N14—C141	175.52 (17)
N1—P2—N4—C41	−81.78 (17)	N11—P12—N14—C141	−73.25 (18)
O2—P2—N5—C51	44.7 (2)	O12—P12—N15—C151	−66.66 (19)
N4—P2—N5—C51	−78.24 (18)	N14—P12—N15—C151	166.65 (17)
N1—P2—N5—C51	163.63 (16)	N11—P12—N15—C151	53.16 (18)
P2—N1—C11—C16	70.9 (2)	P11—N11—C111—C112	103.13 (18)
P1—N1—C11—C16	−91.6 (2)	P12—N11—C111—C112	−90.05 (19)
P2—N1—C11—C12	−107.44 (17)	P11—N11—C111—C116	−75.1 (2)
P1—N1—C11—C12	89.97 (19)	P12—N11—C111—C116	91.74 (19)
C16—C11—C12—C13	0.1 (3)	C116—C111—C112—C113	0.3 (3)
N1—C11—C12—C13	178.48 (18)	N11—C111—C112—C113	−177.92 (18)
C11—C12—C13—C14	−0.7 (3)	C111—C112—C113—C114	0.2 (3)
C12—C13—C14—C15	0.2 (4)	C112—C113—C114—C115	−0.1 (3)
C13—C14—C15—C16	1.0 (4)	C113—C114—C115—C116	−0.5 (3)
C12—C11—C16—C15	1.0 (3)	C112—C111—C116—C115	−0.9 (3)
N1—C11—C16—C15	−177.35 (18)	N11—C111—C116—C115	177.32 (18)
C14—C15—C16—C11	−1.5 (3)	C114—C115—C116—C111	1.0 (3)
P1—N2—C21—C26	4.7 (3)	P11—N12—C121—C122	32.5 (3)
P1—N2—C21—C22	−174.80 (16)	P11—N12—C121—C126	−149.86 (15)
C26—C21—C22—C23	−0.3 (3)	C126—C121—C122—C123	0.9 (3)
N2—C21—C22—C23	179.2 (2)	N12—C121—C122—C123	178.54 (18)
C21—C22—C23—C24	0.4 (4)	C121—C122—C123—C124	−1.1 (3)
C22—C23—C24—C25	0.0 (4)	C122—C123—C124—C125	0.3 (3)
C23—C24—C25—C26	−0.5 (4)	C123—C124—C125—C126	0.8 (3)
C22—C21—C26—C25	−0.2 (3)	C124—C125—C126—C121	−0.9 (3)
N2—C21—C26—C25	−179.7 (2)	C122—C121—C126—C125	0.1 (3)
C24—C25—C26—C21	0.7 (4)	N12—C121—C126—C125	−177.63 (18)
P1—N3—C31—C36	43.0 (3)	P11—N13—C131—C132	−25.2 (3)
P1—N3—C31—C32	−138.28 (19)	P11—N13—C131—C136	153.17 (16)
C36—C31—C32—C33	0.8 (4)	C136—C131—C132—C133	0.7 (3)

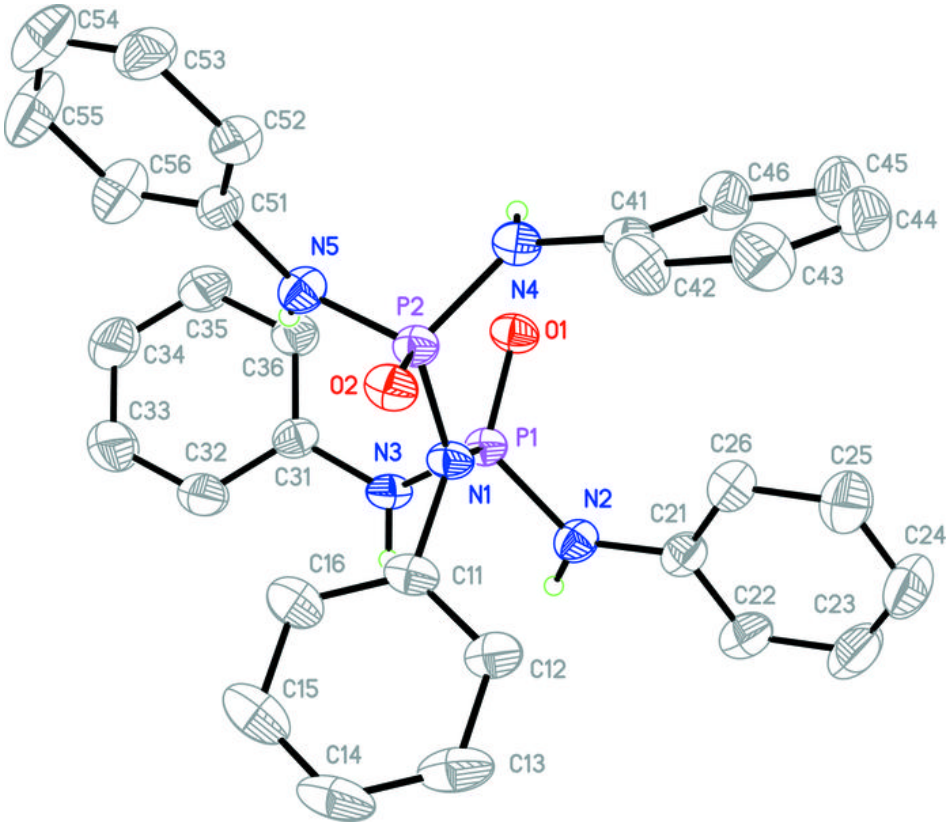
N3—C31—C32—C33	−178.0 (2)	N13—C131—C132—C133	179.1 (2)
C31—C32—C33—C34	0.0 (4)	C131—C132—C133—C134	0.0 (4)
C32—C33—C34—C35	−0.5 (5)	C132—C133—C134—C135	−0.4 (4)
C33—C34—C35—C36	0.3 (4)	C133—C134—C135—C136	−0.1 (4)
C32—C31—C36—C35	−0.9 (3)	C134—C135—C136—C131	0.9 (3)
N3—C31—C36—C35	177.75 (19)	C132—C131—C136—C135	−1.2 (3)
C34—C35—C36—C31	0.4 (4)	N13—C131—C136—C135	−179.58 (19)
P2—N4—C41—C46	140.39 (17)	P12—N14—C141—C142	−33.7 (3)
P2—N4—C41—C42	−42.1 (3)	P12—N14—C141—C146	147.07 (19)
C46—C41—C42—C43	−2.3 (3)	C146—C141—C142—C143	−2.0 (3)
N4—C41—C42—C43	−179.86 (19)	N14—C141—C142—C143	178.8 (2)
C41—C42—C43—C44	1.8 (3)	C141—C142—C143—C144	0.6 (4)
C42—C43—C44—C45	0.2 (4)	C142—C143—C144—C145	1.4 (5)
C43—C44—C45—C46	−1.7 (4)	C143—C144—C145—C146	−1.9 (5)
C42—C41—C46—C45	0.9 (3)	C144—C145—C146—C141	0.5 (5)
N4—C41—C46—C45	178.47 (19)	C142—C141—C146—C145	1.5 (4)
C44—C45—C46—C41	1.2 (4)	N14—C141—C146—C145	−179.3 (2)
P2—N5—C51—C56	−165.66 (17)	P12—N15—C151—C156	19.9 (3)
P2—N5—C51—C52	12.6 (3)	P12—N15—C151—C152	−158.11 (16)
C56—C51—C52—C53	−1.1 (3)	C156—C151—C152—C153	−1.0 (3)
N5—C51—C52—C53	−179.32 (19)	N15—C151—C152—C153	177.1 (2)
C51—C52—C53—C54	0.1 (3)	C151—C152—C153—C154	0.3 (4)
C52—C53—C54—C55	0.4 (4)	C152—C153—C154—C155	0.2 (4)
C53—C54—C55—C56	0.1 (4)	C153—C154—C155—C156	−0.2 (3)
C52—C51—C56—C55	1.6 (3)	C154—C155—C156—C151	−0.5 (3)
N5—C51—C56—C55	179.9 (2)	C152—C151—C156—C155	1.0 (3)
C54—C55—C56—C51	−1.1 (4)	N15—C151—C156—C155	−176.99 (18)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2A···O11	0.866 (9)	2.386 (14)	3.117 (2)	142.4 (17)
N3—H3A···O11	0.868 (9)	1.911 (10)	2.769 (2)	169.2 (18)
N4—H4A···O12^{i}	0.870 (7)	2.220 (10)	3.032 (2)	155.3 (17)
N4—H4A···O1	0.870 (7)	2.455 (17)	2.959 (2)	117.5 (15)
N5—H5A···.	0.852 (9)	.	.	.
N12—H12B···O1^{ii}	0.867 (9)	2.221 (11)	3.044 (2)	158.4 (17)
N12—H12B···O12	0.867 (9)	2.471 (18)	2.963 (2)	116.6 (15)
N13—H13B···.	0.860 (9)	.	.	.
N14—H14B···O2^{iii}	0.872 (7)	2.002 (8)	2.856 (2)	166.0 (18)
N15—H15B···O2^{iii}	0.868 (9)	2.138 (11)	2.962 (2)	158.4 (18)

Symmetry codes: (i) −*x*+3/2, *y*+1/2, *z*; (ii) −*x*+3/2, *y*−1/2, *z*; (iii) *x*+1/2, *y*, −*z*+3/2.

Fig. 1


C54
C53
C55
C52
C56
C51
N5
C41
C46
C45
C44
C42
C43
N4
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C35
C34
C36
O1
O2
C33
C32
C31
N3
P1
N1
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C25
C21
C24
C16
C11
C22
C23
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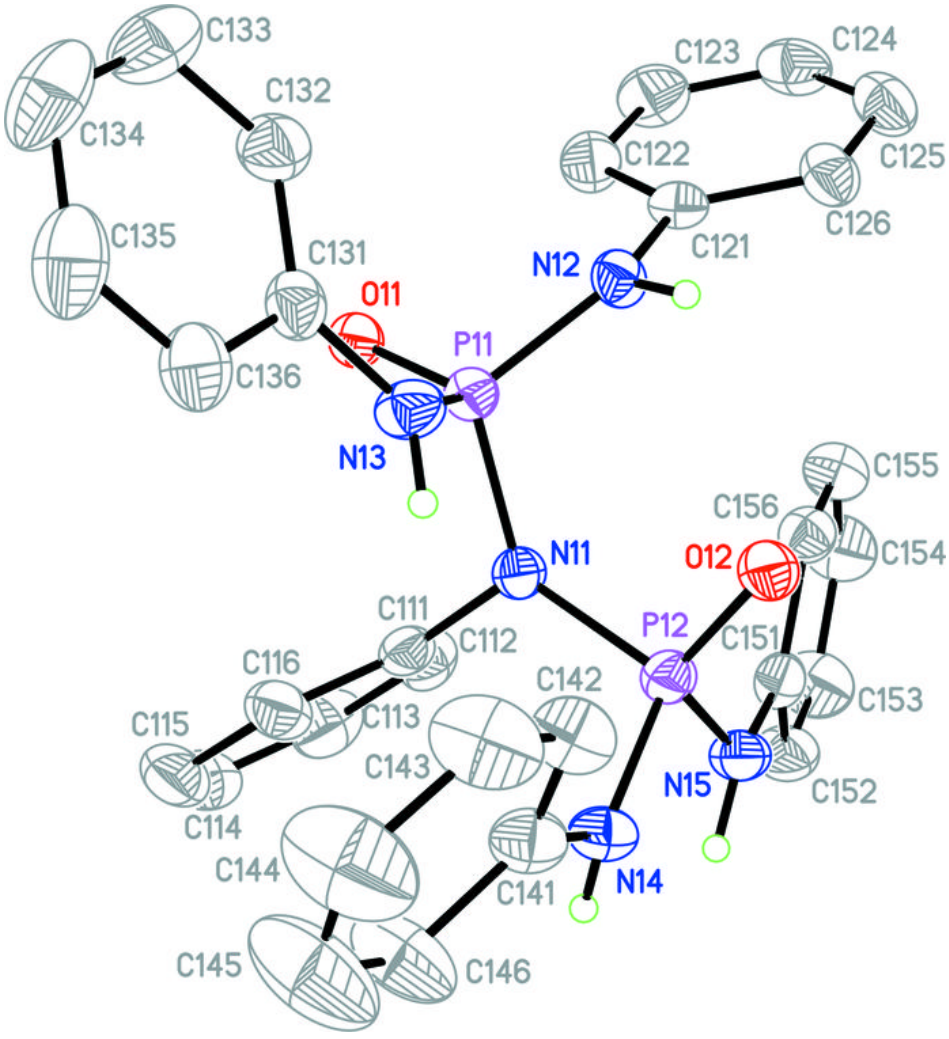
C15
C14
C13

Fig. 2


C133
C132
C134
C135
C131
C136
O11
P11
N13
N12
C123
C124
C122
C125
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C121
C155
C156
C154
O12
N11
C111
C112
P12
C151
C153
C116
C142
C115
C113
C143
N15
C152
C114
C144
C141
N14
C145
C146

Fig. 3