Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

2-[Anilino(diphenylphosphoryl)-methyl]phenol from a three-component Kabachnik–Fields reaction

Ming-Shu Wu,[a]* Qing-Qin Feng,[b] Gao-Nan Li[a] and De-Hui Wan[a]

[a]College of Chemistry and Chemical Engineering, Hainan Normal University, Haikou 571158, People's Republic of China, and [b]College of Chemistry and Chemical Engineering, Anyang Normal University, Anyang, Henan 455000, People's Republic of China
Correspondence e-mail: wumingshu@126.com

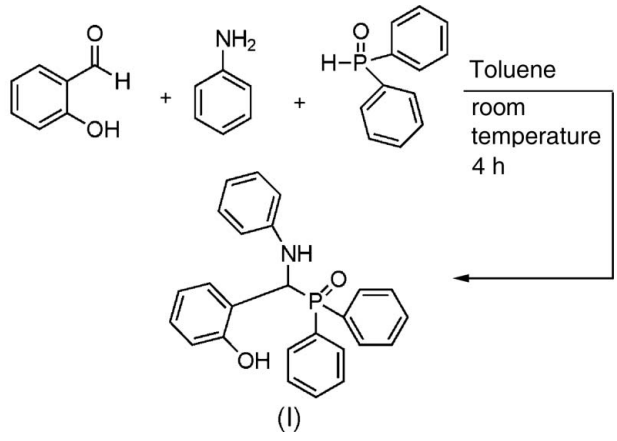
Received 3 July 2013
Accepted 7 August 2013

The title compound, $C_{25}H_{22}NO_2P$, was synthesized in high yield by a three-component Kabachnik–Fields reaction of diphenylphosphine oxide, salicylaldehyde and aniline in dry toluene at room temperature. It precipitates as racemic crystals, in which strong hydrogen bonds between the hydroxy group and the P═O group of a neighbouring molecule form one-dimensional heterochiral chains along the crystallographic *a* axis, with an O···O separation of 2.568 (2) Å. The pseudo-tetrahedral environment of the P atom is distorted, with O—P—C bond angles significantly larger than the C—P—C angles.

Keywords: crystal structure; Kabachnik–Fields reaction; heterochiral chains.

1. Introduction

Chiral phosphorus-containing compounds such as α-aminophosphonic acids and their derivatives have attracted considerable attention due to their promising biological properties (Romanenko & Kukhar, 2006; Haynes *et al.*, 1989, 1991; Shi *et al.*, 2000; Kafarski & Lejczak, 2001). They have found application as antibacterials (Pratt, 1989), antiviral agents (Huang & Chen, 2000) and enzyme inhibitors (Smith *et al.*, 1989; Kafarski & Lejczak, 1991). The absolute configuration of phosphonyl compounds strongly influences their biological properties (Patel *et al.*, 1995). Various methods for the synthesis of α-aminophosphonic acids and α-aminophosphonates have therefore been reported (Moore *et al.*, 2002; Demmer *et al.*, 2011; Bálint *et al.*, 2013; Wu *et al.*, 2013). However, other α-amino phosphorus derivatives, such as α-aminophosphine oxides, have received much less attention for their biological properties due to the lack of direct synthetic access. We report herein a convenient one-pot three-component method using a Kabachnik–Fields reaction for the synthesis of 2-[anilino(diphenylphosphoryl)methyl]phenol, (I), using diphenylphosphine oxide, salicylaldehyde and aniline as starting materials (see Scheme). The notable advantages of this methodology are operational simplicity, mild reaction conditions, higher yields, a reasonable reaction time and ease of isolation of the pure products. In order to confirm further the stereochemistry and structure–activity relationship of α-aminophosphine oxides with potential practical applications, we established the crystal structure of (I).



(I)

2. Experimental

2.1. Synthesis and crystallization

A solution of diphenylphosphine oxide (1.01 g, 5 mmol, 1 equivalent) in dry toluene (10 ml) was added to a dry 50 ml flask (equipped with a $CaCl_2$ tube) containing a solution of aniline (1.8 ml, 20 mmol, 4 equivalents) and salicylaldehyde (0.61 g, 5 mmol, 1 equivalent) in dry toluene (20 ml). After stirring for 4 h at room temperature, the reaction was complete; the precipitate was filtered off, washed with cold toluene (10 ml) and then dried under vacuum to afford the pure title product, (I) (yield 1.8 g, 90%), as a colourless solid. Single crystals of (I) suitable for X-ray diffraction were obtained by recrystallization from diethyl ether. Spectroscopic analysis: ^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ 9.82 (*s*, 1H, O*H*), 7.81–6.62 (*m*, 19H, Ar-*H*), 5.46 (*d*, $^2J_{P-H}$ = 8.5 Hz, 1H, C—*H*), 3.73 (*br s*, 1H, N*H*); ^{13}C NMR (100 MHz, $CDCl_3$, 298 K): δ 155.9, 145.8, 132.7, 129.3, 129.7, 129.2, 128.8, 128.6, 128.4, 128.3, 122.4, 120.4, 119.2, 114.4, 56.9 (*d*, $^1J_{P-C}$ = 39.9 Hz); ^{31}P NMR (162 MHz, $CDCl_3$, 298 K): δ 38.4; IR (KBr, ν, cm^{-1}): 3430 (NH), 3228 (OH), 3303 (NH), 3138, 3062, 2969, 2916, 2884, 2827, 1591, 1553, 1485, 1438, 1171 (P═O), 1122, 1096 (P—O), 1070, 1037, 855, 743, 726, 693, 561, 542, 525, 439. Analysis found for $C_{25}H_{22}NO_2P$: C 75.19, H 5.43, N 3.55%; calculated: C 75.18, H 5.55, N 3.51%.

2.2. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. H atoms bound to C or N atoms were positioned geometrically and refined using a

  doi:10.1107/S0108270113022087

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{25}H_{22}NO_2P$
M_r	399.41
Crystal system, space group	Orthorhombic, *Pbca*
Temperature (K)	293
a, *b*, *c* (Å)	12.5489 (4), 16.4560 (5), 20.9643 (6)
V (Å^3)	4329.2 (2)
Z	8
Radiation type	Mo *Kα*
μ (mm^{-1})	0.15
Crystal size (mm)	0.1 × 0.1 × 0.1
Data collection	
Diffractometer	Agilent Xcalibur (Atlas, Gemini ultra) diffractometer
Absorption correction	Multi-scan (*CrysAlis PRO*; Agilent, 2012)
T_{min}, T_{max}	0.774, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14390, 4429, 2951
R_{int}	0.039
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.048, 0.122, 1.02
No. of reflections	4429
No. of parameters	263
No. of restraints	0
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.29, −0.27

Computer programs: *CrysAlis PRO* (Agilent, 2012), *SHELXS97* (Sheldrick, 2008), *SHELXL97* (Sheldrick, 2008) and *OLEX2* (Dolomanov *et al.*, 2009).

riding model, with aryl C—H = 0.93 Å, methine C—H = 0.98 Å and N—H = 0.86 Å, and with U_{iso}(H) = 1.2U_{eq}(C,N). The hydroxy H atom was located from a difference Fourier map and was refined with a combination of riding and rotational motion, with U_{iso}(H) = 1.5U_{eq}(O).

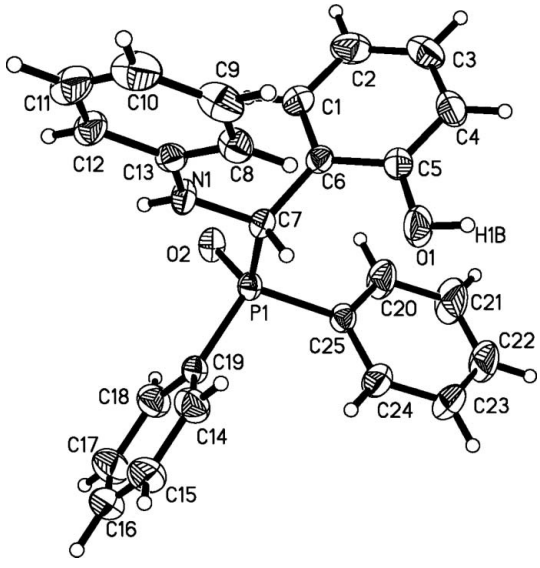


Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

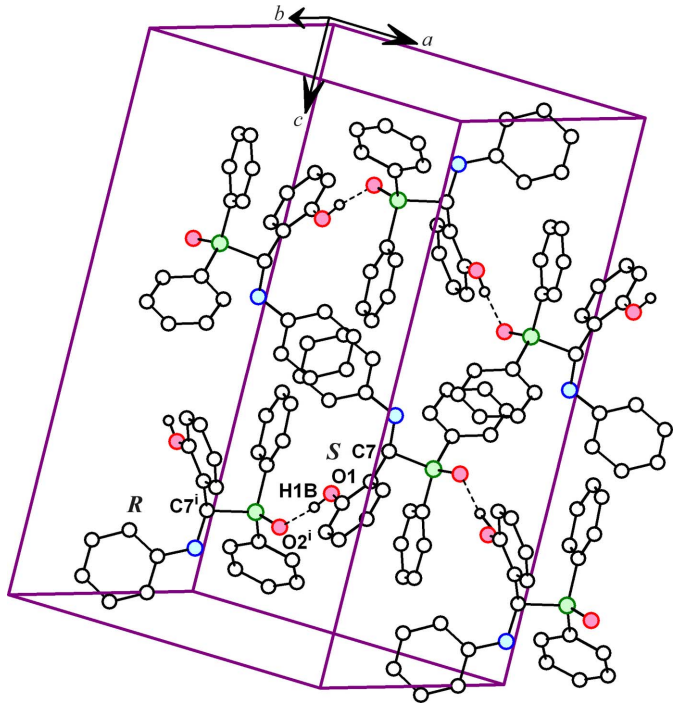


Figure 2
Packing for (I), showing the intermolecular hydrogen-bonding interactions (dashed lines) between atoms H1*B* and O2^i of neighbouring *S* and *R* enantiomers. [Symmetry code: (i) $x - \frac{1}{2}, y, -z + \frac{3}{2}$.]

3. Results and discussion

In compound (I), the formation of P—C bonds between the P atom of diphenylphosphine oxide and the carbonyl C atom of salicylaldehyde generates a stereocentre at atom C7 (Fig. 1). The space group *Pbca* was identified with the help of the program *PLATON* (Spek, 2009). Not surprisingly, (I) forms racemic crystals with one molecule in the asymmetric unit. A displacement ellipsoid plot of the *S* enantiomer is shown in Fig. 1. The O—P—C bond angles are systematically larger than the C—P—C angles (Table 2), indicating a minor distortion in which the phenyl groups are splayed back slightly, away from the phosphoryl function.

An intermolecular O1—H1···O2^i hydrogen bond (details in Table 3, including symmetry code) between the O1—H1 hydroxy group and P-bonded atom O2 links neighbouring

Table 2
Selected bond angles (°).

O2—P1—C7	110.33 (9)	C19—P1—C7	108.59 (9)
O2—P1—C19	110.55 (9)	C25—P1—C7	105.28 (9)
O2—P1—C25	114.61 (9)	C25—P1—C19	107.19 (9)

Table 3
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*B*···O2^i	0.82	1.79	2.5677 (19)	159

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

molecules into heterochiral chains along the crystallographic *a* axis (Fig. 2).

This work was supported by the National Natural Science Foundation of China (grant No. 21162008).

Supplementary data for this paper are available from the IUCr electronic archives (Reference: EG3131). Services for accessing these data are described at the back of the journal.

References

Agilent (2012). *CrysAlis PRO*. Agilent Technologies, Yarnton, Oxfordshire, England.

Bálint, E., Takács, J., Drahos, L. & Juranovic, A. (2013). *Heteroatom Chem.* **24**, 221–225.

Demmer, C. S., Krogsgaard-Larsen, N. & Bunch, L. (2011). *Chem. Rev.* **111**, 7981–8006.

Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.

Haynes, R. K., Loughlin, W. A. & Hambley, T. W. (1991). *J. Org. Chem.* **56**, 5785–5790.

Haynes, R. K., Vonwiller, S. C. & Hambley, T. W. (1989). *J. Org. Chem.* **54**, 5162–5170.

Huang, J. & Chen, R. (2000). *Heteroatom Chem.* **11**, 480–492.

Kafarski, P. & Lejczak, B. (1991). *Phosphorus Sulfur Silicon Relat. Elem.* **63**, 193–215.

Kafarski, P. & Lejczak, B. (2001). *Curr. Med. Chem.* **1**, 301–312.

Moore, J. D., Sprott, K. T. & Hanson, P. R. (2002). *J. Org. Chem.* **67**, 8123–8129.

Patel, D. V., Rielly-Gauvin, K., Ryono, D. E., Charles, A. F., Rogers, W. L., Smith, S. A., Deforrest, J. M., Oehl, R. S. & Petrillo, E. W. (1995). *J. Med. Chem.* **38**, 4557–4569.

Pratt, R. F. (1989). *Science*, **246**, 917–919.

Romanenko, V. D. & Kukhar, V. P. (2006). *Chem. Rev.* **106**, 3868–3965.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Shi, J.-C., Chao, H.-Y., Fu, W.-F., Peng, S.-M. & Che, C.-M. (2000). *J. Chem. Soc. Dalton Trans.* **18**, 3128–3132.

Smith, M. M., Merlie, J. P. & Lawrence, J. C. (1989). *J. Biol. Chem.* **264**, 12813–12819.

Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

Wu, M.-S., Liu, R.-D. & Wan, D.-H. (2013). *Heteroatom Chem.* **24**, 110–115.

supplementary materials

Acta Cryst. (2013). C**69**, 1070-1072 [doi:10.1107/S0108270113022087]

2-[Anilino(diphenylphosphoryl)methyl]phenol from a three-component Kabachnik–Fields reaction

Ming-Shu Wu, Qing-Qin Feng, Gao-Nan Li and De-Hui Wan

Computing details

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO* (Agilent, 2012); data reduction: *CrysAlis PRO* (Agilent, 2012); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: OLEX2 (Dolomanov *et al.*, 2009); software used to prepare material for publication: OLEX2 (Dolomanov *et al.*, 2009).

2-[Anilino(diphenylphosphoryl)methyl]phenol

Crystal data

$C_{25}H_{22}NO_2P$
$M_r = 399.41$
Orthorhombic, *Pbca*
$a = 12.5489$ (4) Å
$b = 16.4560$ (5) Å
$c = 20.9643$ (6) Å
$V = 4329.2$ (2) Å^3
$Z = 8$
$F(000) = 1680$
$D_x = 1.226$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3813 reflections
$\theta = 2.3$–$29.7°$
$\mu = 0.15$ mm^{-1}
$T = 293$ K
Prism, colourless
0.1 × 0.1 × 0.1 mm

Data collection

Agilent Xcalibur (Atlas, Gemini ultra) diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)
$T_{min} = 0.774$, $T_{max} = 1.000$
14390 measured reflections
4429 independent reflections
2951 reflections with $I > 2\sigma(I)$
$R_{int} = 0.039$
$\theta_{max} = 26.4°$, $\theta_{min} = 2.3°$
$h = -14 \rightarrow 15$
$k = -20 \rightarrow 16$
$l = -26 \rightarrow 25$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.122$
$S = 1.02$
4429 reflections
263 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0503P)^2 + 0.6207P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}

Special details

Experimental. CrysAlisPro, Agilent Technologies, Version 1.171.36.21 (release 14-08-2012 CrysAlis171 .NET) (compiled Sep 14 2012,17:21:16) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

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}
P1	0.68854 (4)	0.10727 (3)	0.67088 (2)	0.03680 (16)
O1	0.43871 (13)	0.17634 (11)	0.75461 (7)	0.0704 (5)
H1B	0.3989	0.1774	0.7856	0.106*
O2	0.79368 (10)	0.14729 (9)	0.66206 (6)	0.0484 (4)
N1	0.59018 (14)	0.21014 (10)	0.59205 (7)	0.0476 (4)
H1	0.6477	0.2017	0.5708	0.057*
C1	0.65930 (19)	0.30369 (13)	0.71138 (11)	0.0559 (6)
H1A	0.7084	0.3083	0.6784	0.067*
C2	0.6630 (2)	0.35799 (15)	0.76194 (13)	0.0732 (7)
H2	0.7144	0.3987	0.7629	0.088*
C3	0.5904 (2)	0.35127 (16)	0.81021 (12)	0.0693 (7)
H3	0.5931	0.3876	0.8442	0.083*
C4	0.5139 (2)	0.29207 (15)	0.80944 (10)	0.0603 (6)
H4	0.4646	0.2885	0.8424	0.072*
C5	0.51038 (17)	0.23744 (13)	0.75920 (9)	0.0466 (5)
C6	0.58356 (16)	0.24296 (11)	0.70957 (9)	0.0392 (5)
C7	0.58122 (15)	0.17948 (12)	0.65686 (8)	0.0384 (5)
H7	0.5136	0.1500	0.6602	0.046*
C8	0.41040 (18)	0.26471 (13)	0.59454 (10)	0.0514 (6)
H8	0.3999	0.2444	0.6355	0.062*
C9	0.3292 (2)	0.30678 (15)	0.56417 (12)	0.0668 (7)
H9	0.2646	0.3146	0.5850	0.080*
C10	0.3430 (3)	0.33700 (16)	0.50364 (14)	0.0758 (8)
H10	0.2881	0.3651	0.4836	0.091*
C11	0.4382 (3)	0.32536 (16)	0.47317 (12)	0.0740 (8)
H11	0.4478	0.3458	0.4322	0.089*
C12	0.5201 (2)	0.28378 (13)	0.50237 (10)	0.0561 (6)
H12	0.5843	0.2763	0.4810	0.067*
C13	0.50706 (18)	0.25279 (11)	0.56411 (9)	0.0433 (5)
C14	0.5774 (2)	−0.00203 (15)	0.59125 (10)	0.0621 (6)
H14	0.5149	0.0253	0.6019	0.075*
C15	0.5736 (3)	−0.06854 (17)	0.55043 (12)	0.0788 (8)
H15	0.5086	−0.0861	0.5342	0.095*
C16	0.6647 (3)	−0.10775 (17)	0.53429 (13)	0.0860 (10)

H16	0.6619	−0.1523	0.5071	0.103*
C17	0.7601 (3)	−0.08252 (17)	0.55751 (14)	0.0857 (9)
H17	0.8221	−0.1096	0.5458	0.103*
C18	0.7655 (2)	−0.01646 (14)	0.59873 (11)	0.0640 (7)
H18	0.8310	0.0006	0.6145	0.077*
C19	0.67364 (17)	0.02364 (12)	0.61607 (9)	0.0428 (5)
C20	0.7151 (2)	0.10357 (17)	0.80119 (10)	0.0719 (8)
H20	0.7624	0.1463	0.7948	0.086*
C21	0.6948 (3)	0.0757 (2)	0.86265 (12)	0.0975 (11)
H21	0.7280	0.1003	0.8973	0.117*
C22	0.6265 (3)	0.0125 (2)	0.87217 (12)	0.0874 (9)
H22	0.6143	−0.0067	0.9133	0.105*
C23	0.5764 (2)	−0.02250 (17)	0.82197 (13)	0.0783 (8)
H23	0.5290	−0.0651	0.8287	0.094*
C24	0.5956 (2)	0.00505 (14)	0.76081 (10)	0.0609 (6)
H24	0.5609	−0.0193	0.7266	0.073*
C25	0.66542 (16)	0.06800 (12)	0.74989 (9)	0.0426 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P1	0.0374 (3)	0.0433 (3)	0.0297 (3)	−0.0013 (2)	−0.0015 (2)	0.0009 (2)
O1	0.0646 (11)	0.0858 (12)	0.0609 (10)	−0.0245 (10)	0.0271 (8)	−0.0124 (9)
O2	0.0378 (8)	0.0683 (9)	0.0391 (7)	−0.0077 (7)	−0.0011 (6)	−0.0007 (7)
N1	0.0492 (11)	0.0603 (11)	0.0333 (8)	0.0079 (9)	0.0064 (8)	0.0097 (8)
C1	0.0629 (15)	0.0474 (13)	0.0574 (14)	−0.0102 (12)	0.0067 (12)	0.0012 (11)
C2	0.0790 (19)	0.0521 (15)	0.089 (2)	−0.0140 (14)	−0.0039 (16)	−0.0097 (14)
C3	0.084 (2)	0.0586 (16)	0.0657 (16)	0.0075 (15)	−0.0063 (15)	−0.0203 (13)
C4	0.0673 (16)	0.0659 (16)	0.0479 (12)	0.0117 (14)	0.0073 (12)	−0.0074 (11)
C5	0.0465 (12)	0.0501 (12)	0.0430 (11)	0.0012 (11)	0.0035 (10)	0.0010 (10)
C6	0.0421 (12)	0.0384 (11)	0.0370 (10)	0.0008 (9)	0.0000 (9)	0.0045 (9)
C7	0.0390 (11)	0.0429 (11)	0.0332 (10)	−0.0034 (9)	0.0006 (8)	0.0051 (8)
C8	0.0570 (14)	0.0535 (13)	0.0436 (12)	0.0074 (11)	−0.0110 (11)	−0.0036 (10)
C9	0.0662 (17)	0.0640 (16)	0.0702 (16)	0.0141 (13)	−0.0229 (13)	−0.0157 (13)
C10	0.093 (2)	0.0604 (17)	0.0743 (18)	0.0103 (15)	−0.0419 (17)	−0.0013 (14)
C11	0.108 (2)	0.0609 (16)	0.0527 (14)	−0.0108 (16)	−0.0350 (16)	0.0141 (12)
C12	0.0759 (16)	0.0524 (13)	0.0400 (11)	−0.0113 (12)	−0.0120 (11)	0.0062 (10)
C13	0.0567 (14)	0.0371 (11)	0.0362 (10)	−0.0034 (10)	−0.0102 (10)	−0.0019 (9)
C14	0.0703 (17)	0.0622 (15)	0.0539 (13)	−0.0032 (13)	−0.0079 (13)	−0.0116 (12)
C15	0.109 (2)	0.0678 (17)	0.0595 (16)	−0.0205 (18)	−0.0115 (16)	−0.0111 (14)
C16	0.148 (3)	0.0524 (16)	0.0574 (16)	−0.006 (2)	0.0084 (19)	−0.0091 (13)
C17	0.116 (3)	0.0599 (17)	0.081 (2)	0.0229 (18)	0.0206 (19)	−0.0111 (15)
C18	0.0740 (18)	0.0570 (15)	0.0609 (14)	0.0125 (14)	0.0016 (13)	−0.0042 (12)
C19	0.0567 (14)	0.0400 (11)	0.0318 (10)	0.0011 (10)	−0.0007 (10)	0.0016 (9)
C20	0.0852 (19)	0.0932 (19)	0.0372 (12)	−0.0216 (16)	−0.0057 (12)	0.0073 (13)
C21	0.129 (3)	0.128 (3)	0.0357 (14)	−0.021 (2)	−0.0097 (15)	0.0118 (16)
C22	0.125 (3)	0.092 (2)	0.0450 (15)	0.011 (2)	0.0147 (17)	0.0264 (15)
C23	0.100 (2)	0.0636 (17)	0.0714 (18)	−0.0068 (16)	0.0200 (17)	0.0246 (14)
C24	0.0745 (17)	0.0593 (15)	0.0491 (13)	−0.0074 (13)	0.0037 (12)	0.0112 (11)
C25	0.0475 (12)	0.0456 (11)	0.0347 (10)	0.0048 (10)	−0.0008 (9)	0.0043 (9)

Geometric parameters (Å, º)

P1—O2	1.4862 (14)	C11—H11	0.9300
P1—C7	1.820 (2)	C12—C11	1.378 (3)
P1—C19	1.803 (2)	C12—H12	0.9300
P1—C25	1.8015 (19)	C13—C8	1.384 (3)
O1—H1B	0.8200	C13—C12	1.401 (3)
N1—H1	0.8600	C14—H14	0.9300
N1—C13	1.387 (3)	C14—C15	1.390 (3)
C1—H1A	0.9300	C15—H15	0.9300
C1—C2	1.387 (3)	C16—C15	1.356 (4)
C2—H2	0.9300	C16—H16	0.9300
C2—C3	1.366 (4)	C16—C17	1.357 (4)
C3—H3	0.9300	C17—H17	0.9300
C4—C3	1.368 (3)	C18—C17	1.390 (3)
C4—H4	0.9300	C18—H18	0.9300
C5—O1	1.352 (2)	C19—C14	1.382 (3)
C5—C4	1.385 (3)	C19—C18	1.377 (3)
C6—C1	1.380 (3)	C20—H20	0.9300
C6—C5	1.391 (3)	C20—C21	1.391 (3)
C7—N1	1.454 (2)	C21—H21	0.9300
C7—C6	1.521 (3)	C22—C21	1.363 (4)
C7—H7	0.9800	C22—H22	0.9300
C8—H8	0.9300	C23—C22	1.355 (4)
C8—C9	1.387 (3)	C23—H23	0.9300
C9—H9	0.9300	C24—C23	1.381 (3)
C9—C10	1.374 (4)	C24—H24	0.9300
C10—H10	0.9300	C25—C20	1.374 (3)
C11—C10	1.368 (4)	C25—C24	1.376 (3)
O2—P1—C7	110.33 (9)	C10—C11—C12	120.9 (2)
O2—P1—C19	110.55 (9)	C12—C11—H11	119.6
O2—P1—C25	114.61 (9)	C11—C12—H12	119.9
C19—P1—C7	108.59 (9)	C11—C12—C13	120.3 (2)
C25—P1—C7	105.28 (9)	C13—C12—H12	119.9
C25—P1—C19	107.19 (9)	N1—C13—C12	119.1 (2)
C5—O1—H1B	109.5	C8—C13—N1	122.41 (17)
C7—N1—H1	119.6	C8—C13—C12	118.4 (2)
C13—N1—H1	119.6	C15—C14—H14	119.9
C13—N1—C7	120.81 (16)	C19—C14—H14	119.9
C2—C1—H1A	119.6	C19—C14—C15	120.2 (3)
C6—C1—H1A	119.6	C14—C15—H15	120.0
C6—C1—C2	120.7 (2)	C16—C15—C14	120.0 (3)
C1—C2—H2	120.3	C16—C15—H15	120.0
C3—C2—C1	119.5 (2)	C15—C16—H16	119.7
C3—C2—H2	120.3	C15—C16—C17	120.6 (3)
C2—C3—H3	119.4	C17—C16—H16	119.7
C2—C3—C4	121.1 (2)	C16—C17—H17	119.8
C4—C3—H3	119.4	C16—C17—C18	120.3 (3)
C3—C4—H4	120.2	C18—C17—H17	119.8

C3—C4—C5	119.6 (2)	C17—C18—H18	120.1
C5—C4—H4	120.2	C19—C18—C17	119.9 (3)
O1—C5—C4	123.9 (2)	C19—C18—H18	120.1
O1—C5—C6	115.74 (18)	C14—C19—P1	124.35 (17)
C4—C5—C6	120.4 (2)	C18—C19—P1	116.58 (17)
C1—C6—C5	118.79 (19)	C18—C19—C14	119.1 (2)
C1—C6—C7	122.05 (18)	C21—C20—H20	119.9
C5—C6—C7	119.09 (18)	C25—C20—H20	119.9
P1—C7—H7	107.8	C25—C20—C21	120.1 (3)
N1—C7—P1	108.69 (13)	C20—C21—H21	119.9
N1—C7—C6	116.05 (16)	C22—C21—C20	120.2 (3)
N1—C7—H7	107.8	C22—C21—H21	119.9
C6—C7—P1	108.47 (13)	C21—C22—H22	119.9
C6—C7—H7	107.8	C23—C22—C21	120.2 (2)
C9—C8—H8	119.9	C23—C22—H22	119.9
C13—C8—H8	119.9	C22—C23—H23	120.0
C13—C8—C9	120.2 (2)	C22—C23—C24	120.0 (3)
C8—C9—H9	119.6	C24—C23—H23	120.0
C10—C9—C8	120.8 (3)	C23—C24—H24	119.6
C10—C9—H9	119.6	C25—C24—C23	120.8 (2)
C9—C10—H10	120.3	C25—C24—H24	119.6
C11—C10—C9	119.4 (2)	C20—C25—P1	119.59 (17)
C11—C10—H10	120.3	C20—C25—C24	118.65 (19)
C10—C11—H11	119.6	C24—C25—P1	121.71 (16)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*B*···O2^{i}	0.82	1.79	2.5677 (19)	159

Symmetry code: (i) *x*−1/2, *y*, −*z*+3/2.