Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(Dicyclohexylamino)(phenyl)(piperidin-1-yl)phosphine

T. Arun Luiz,[a] Adinarayana Doddi,[a] Babu Varghese[b] and M. N. Sudheendra Rao[a]*

[a]Department of Chemistry, Indian Institute of Technology, Madras, Chennai 600 036, India, and [b]Sophisticated Analytical Instrument Facility, Indian Institute of Technology, Madras, Chennai 600 036, India
Correspondence e-mail: mnsrao@iitm.ac.in

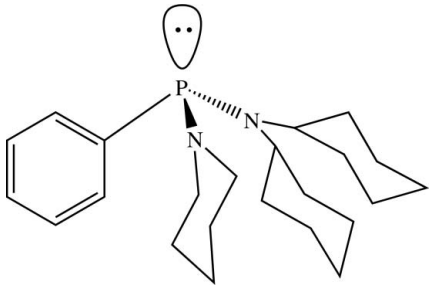
Received 28 June 2007; accepted 1 July 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.007 Å; R factor = 0.060; wR factor = 0.221; data-to-parameter ratio = 16.3.

In the title compound, $C_{23}H_{37}N_2P$, both N atoms have pyramidal geometries, with angle sums of 355.8 and 357.8°. The crystal packing is stabilized by C—H$\cdots\pi$ (H$\cdots\pi$ = 2.797 Å) interactions, leading to centrosymmetric dimers.

Related literature

For related literature, see: Katti *et al.* (1999); Ohta *et al.* (1988).



Experimental

Crystal data

$C_{23}H_{37}N_2P$
M_r = 372.52
Triclinic, $P\overline{1}$
a = 9.5383 (13) Å
b = 10.259 (3) Å
c = 11.413 (10) Å
α = 86.58 (5)°
β = 82.04 (2)°
γ = 81.67 (5)°
V = 1093.4 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.14 mm^{-1}
T = 293 (2) K
0.30 × 0.20 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.959, T_{max} = 0.990
4095 measured reflections
3844 independent reflections
2674 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
3 standard reflections
frequency: 60 min
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.221
S = 1.26
3844 reflections
236 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

Cg is the centroid of the aromatic ring.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C7—H7$A\cdots Cg^{i}$	0.97		2.797 (7)	159

Symmetry code: (i) $-x+2, -y+1, -z$.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

The authors are grateful to the Indian Institute of Technology – Madras, Chennai for financial assistance, and to the Sophisticated Analytical Instruments Facility at IIT Madras for the X-ray data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2466).

References

Altomare, A., Cascarano, G., Giacovazzo, C. & Guagliardi, A. (1993). *J. Appl. Cryst.* **26**, 343–350.
Enraf–Nonius (1989). *CAD-4 Software*. Version 5.0. Enraf–Nonius, Delft, The Netherlands.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.
Katti, K. V., Gali, H., Berning, D. E. & Smith, C. J. (1999). *Acc. Chem. Res.* **32**, 9–17.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Ohta, T., Takaya, H. & Noyori, R. (1988). *Inorg. Chem.* **27**, 566–569.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.

 doi:10.1107/S1600536807032084

supplementary materials

Acta Cryst. (2007). E**63**, o3449 [**doi:10.1107/S1600536807032084**]

(Dicyclohexylamino)(phenyl)(piperidin-1-yl)phosphine

T. A. Luiz, A. Doddi, B. Varghese and M. N. S. Rao

Comment

Phosphines are known to stabilize transition metal centers by σ donation and π-back donation and their complexes have applications in diverse fields (Ohta *et al.*, 1988; Katti *et al.*, 1999). The chemistry of aminophosphines which carry one or more amino substituents on phosphorus is an active area of research as the phosphorus environment can be modified both electronically and sterically by the proper choice of amino substituents. Herein, we report the synthesis and structure of the title compound, (I), (Fig. 1), synthesized by the stepwise aminolysis of dichloro phenyl phosphine.

The structure reveals the pyramidal nature of the phosphorus atom and interestingly near planar geometry at the two nitrogen sites (Σ N1 = 355.8° and Σ N2 = 357.8°). The P—N bonds due to amino substituents are significantly shorter [P1—N1 = 1.701 (4)Å and P1—N2 = 1.702 (4) Å] than the reference P—N single bond distance (1.76–1.78 Å). The six membered piperidino moeity shows a chair conformation as do the two cyclohexane rings.

The asymmetric molecule and its inversion equivalent at (2 − *x*, 1 − *y*, −*z*) form a C—H···π linked dimer with an H···π separation of 2.797 (7) Å. The packing of these dimers in the lattice is through van der Waals interactions (Fig. 2).

Experimental

To a stirred solution of phenyldichlorophosphine (2.00 g, 11.17 mmol) in toluene-hexane mixture (1:1, 30 ml) at 278 K was added a solution of dicyclohexylamine (4.04 g, 22.32 mmol) in toluene (10 ml) over a period of 30 minutes. After complete addition, the reaction mixture was brought to room temperature, stirred for 12 h and filtered to remove the precipitated amine hydrochloride. The hydrochloride was washed with hexane (5 × 3 ml) and the washings were collected along with filtrate. The filtrate was reacted further with piperidine (1.90 g, 22.35 mmol) in toluene (5 ml) in a similar way for 10 h. The resultant mixture was worked up in the same way as above to remove piperidine hydrochloride formed. The solvent was pumped off completely and the residue was extracted with hexane (4 × 5 ml). On removal of hexane, the title compound was obtained as a colourless powdery solid with a yield of 2.90 g (70%). X-ray quality colourless blocks of (I) were grown from hexane solution at 278 K.

Melting Point: 401 K. 1H NMR (400 MHz, CDCl3): 1.10–1.24 (m, 12H), 1.54–1.68(m,14*H*), 2.60–2.76(m,2*H*), 2.90–3.00(m,4*H*), 7.25–7.29 (m,3*H*) 7.52–7.60(m,2*H*). 13 C NMR (101 MHz, CDCl3): 23.6, 25.8, 27.0, 28.1, 33.7, 45.2, 56.1, 126.8, 128.0, 131.7, 145.1. 31P NMR(161 MHz): 79.2

Refinement

All the hydrogen atoms were located in difference maps, relocated in idealized positions (C—H = 0.93–0.97 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C).

Figures

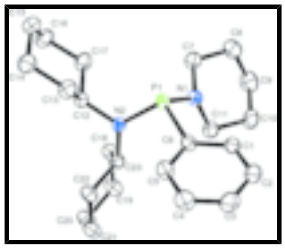


Fig. 1. The molecular structure of (I) showing 30% probability displacement ellipsoids. Hydrogen atoms are omitted for clarity.

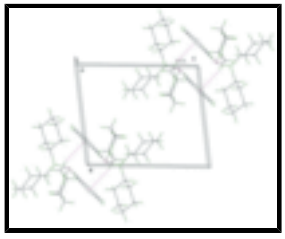


Fig. 2. The packing in (I) showing C—H···π interactions as dashed lines.

(Dicyclohexylamino)(phenyl)(piperdin-1-yl)phosphine

Crystal data

$C_{23}H_{37}N_2P$	$Z = 2$
$M_r = 372.52$	$F_{000} = 408$
Triclinic, $P\overline{1}$	$D_x = 1.131$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.5383$ (13) Å	Cell parameters from 25 reflections
$b = 10.259$ (3) Å	$\theta = 10$–12º
$c = 11.413$ (10) Å	$\mu = 0.14$ mm^{-1}
$\alpha = 86.58$ (5)º	$T = 293$ (2) K
$\beta = 82.04$ (2)º	Block, colourless
$\gamma = 81.67$ (5)º	0.30 × 0.20 × 0.20 mm
$V = 1093.4$ (10) Å^3	

Data collection

Enraf-Nonius CAD-4 diffractometer	$R_{int} = 0.030$
Radiation source: fine-focus sealed tube	$\theta_{max} = 25.0$º
Monochromator: graphite	$\theta_{min} = 2.0$º
$T = 293(2)$ K	$h = 0 \rightarrow 11$
ω–2θ scans	$k = -12 \rightarrow 12$
Absorption correction: ψ scan (North *et al.*, 1968)	$l = -13 \rightarrow 13$
$T_{min} = 0.959$, $T_{max} = 0.990$	3 standard reflections
4095 measured reflections	every 60 min
3844 independent reflections	intensity decay: none
2674 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.060$	$w = 1/[\sigma^2(F_o^2) + (0.077P)^2 + 1.2691P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.221$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.26$	$\Delta\rho_{max} = 0.45$ e Å^{-3}
3844 reflections	$\Delta\rho_{min} = -0.28$ e Å^{-3}
236 parameters	Extinction correction: SHELXL97, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.012 (4)
Secondary atom site location: difference Fourier map	

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 $F^2 > 2$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}
C1	0.7411 (5)	0.4058 (4)	0.0138 (4)	0.0468 (11)
H1	0.7291	0.4971	0.0178	0.056*
C2	0.6625 (5)	0.3492 (5)	−0.0564 (4)	0.0562 (12)
H2	0.5992	0.4025	−0.0998	0.067*
C3	0.6768 (6)	0.2135 (5)	−0.0630 (4)	0.0620 (14)
H3	0.6233	0.1757	−0.1106	0.074*
C4	0.7704 (6)	0.1355 (5)	0.0010 (4)	0.0610 (14)
H4	0.7798	0.0442	−0.0020	0.073*
C5	0.8515 (5)	0.1935 (4)	0.0707 (4)	0.0500 (11)
H5	0.9160	0.1396	0.1127	0.060*
C6	0.8386 (4)	0.3291 (4)	0.0792 (3)	0.0386 (9)
C7	0.9409 (5)	0.6506 (4)	0.2249 (4)	0.0524 (12)
H7A	1.0357	0.6385	0.1801	0.063*
H7B	0.9516	0.6469	0.3083	0.063*
C8	0.8642 (6)	0.7832 (5)	0.1921 (6)	0.0692 (15)
H8A	0.8628	0.7909	0.1071	0.083*

H8B	0.9145	0.8518	0.2140	0.083*
C9	0.7113 (6)	0.8013 (5)	0.2553 (6)	0.0747 (16)
H9A	0.7125	0.8043	0.3399	0.090*
H9B	0.6606	0.8842	0.2284	0.090*
C10	0.6344 (5)	0.6883 (5)	0.2300 (5)	0.0613 (13)
H10A	0.6228	0.6920	0.1467	0.074*
H10B	0.5400	0.6971	0.2756	0.074*
C11	0.7183 (5)	0.5556 (4)	0.2620 (4)	0.0505 (11)
H11A	0.7210	0.5480	0.3468	0.061*
H11B	0.6707	0.4848	0.2406	0.061*
C12	1.1441 (4)	0.2548 (4)	0.2894 (4)	0.0402 (10)
H12	1.1418	0.1947	0.3594	0.048*
C13	1.2366 (5)	0.1796 (5)	0.1887 (4)	0.0547 (12)
H13A	1.1958	0.1010	0.1765	0.066*
H13B	1.2364	0.2343	0.1164	0.066*
C14	1.3897 (5)	0.1401 (5)	0.2135 (5)	0.0671 (15)
H14A	1.4460	0.0983	0.1450	0.081*
H14B	1.3914	0.0765	0.2799	0.081*
C15	1.4562 (5)	0.2588 (5)	0.2417 (5)	0.0683 (15)
H15A	1.5519	0.2299	0.2612	0.082*
H15B	1.4633	0.3186	0.1727	0.082*
C16	1.3667 (5)	0.3296 (6)	0.3443 (5)	0.0681 (15)
H16A	1.4087	0.4066	0.3594	0.082*
H16B	1.3661	0.2717	0.4147	0.082*
C17	1.2137 (5)	0.3722 (5)	0.3188 (4)	0.0550 (12)
H17A	1.2137	0.4362	0.2527	0.066*
H17B	1.1579	0.4143	0.3874	0.066*
C18	0.8764 (5)	0.3260 (4)	0.4734 (4)	0.0462 (11)
H18A	0.9635	0.2950	0.5075	0.055*
H18B	0.8723	0.4202	0.4572	0.055*
C19	0.7475 (6)	0.2988 (4)	0.5619 (4)	0.0565 (13)
H19A	0.7503	0.3405	0.6354	0.068*
H19B	0.6604	0.3369	0.5308	0.068*
C20	0.7457 (6)	0.1518 (5)	0.5864 (4)	0.0612 (13)
H20A	0.6587	0.1376	0.6375	0.073*
H20B	0.8262	0.1156	0.6273	0.073*
C21	0.7538 (6)	0.0807 (5)	0.4716 (4)	0.0587 (13)
H21A	0.7618	−0.0135	0.4892	0.070*
H21B	0.6661	0.1075	0.4372	0.070*
C22	0.8789 (5)	0.1097 (4)	0.3831 (4)	0.0490 (11)
H22A	0.8756	0.0676	0.3099	0.059*
H22B	0.9669	0.0724	0.4133	0.059*
C23	0.8798 (4)	0.2572 (4)	0.3575 (3)	0.0373 (9)
H23	0.7894	0.2905	0.3273	0.045*
N1	0.8629 (4)	0.5432 (3)	0.2006 (3)	0.0423 (9)
N2	0.9943 (3)	0.2908 (3)	0.2651 (3)	0.0377 (8)
P1	0.96640 (12)	0.40271 (11)	0.15159 (9)	0.0375 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.054 (3)	0.047 (3)	0.042 (2)	−0.014 (2)	−0.012 (2)	0.0025 (19)
C2	0.061 (3)	0.068 (3)	0.045 (3)	−0.014 (2)	−0.020 (2)	0.003 (2)
C3	0.070 (3)	0.075 (4)	0.049 (3)	−0.020 (3)	−0.021 (3)	−0.009 (3)
C4	0.082 (4)	0.051 (3)	0.056 (3)	−0.012 (3)	−0.019 (3)	−0.014 (2)
C5	0.066 (3)	0.043 (3)	0.043 (3)	−0.005 (2)	−0.014 (2)	−0.006 (2)
C6	0.046 (2)	0.041 (2)	0.029 (2)	−0.0068 (18)	−0.0059 (18)	−0.0007 (17)
C7	0.055 (3)	0.047 (3)	0.058 (3)	−0.005 (2)	−0.015 (2)	−0.010 (2)
C8	0.079 (4)	0.040 (3)	0.090 (4)	−0.007 (3)	−0.016 (3)	−0.008 (3)
C9	0.083 (4)	0.050 (3)	0.085 (4)	0.012 (3)	−0.007 (3)	−0.012 (3)
C10	0.048 (3)	0.060 (3)	0.069 (3)	0.011 (2)	−0.002 (2)	−0.007 (3)
C11	0.049 (3)	0.051 (3)	0.049 (3)	−0.001 (2)	−0.003 (2)	−0.004 (2)
C12	0.040 (2)	0.040 (2)	0.040 (2)	−0.0045 (18)	−0.0079 (18)	0.0011 (18)
C13	0.049 (3)	0.051 (3)	0.062 (3)	0.000 (2)	−0.002 (2)	−0.016 (2)
C14	0.049 (3)	0.060 (3)	0.086 (4)	0.002 (2)	0.003 (3)	−0.003 (3)
C15	0.044 (3)	0.073 (4)	0.087 (4)	−0.011 (3)	−0.009 (3)	0.014 (3)
C16	0.054 (3)	0.081 (4)	0.075 (4)	−0.017 (3)	−0.022 (3)	−0.003 (3)
C17	0.054 (3)	0.054 (3)	0.060 (3)	−0.002 (2)	−0.020 (2)	−0.015 (2)
C18	0.059 (3)	0.042 (2)	0.038 (2)	−0.007 (2)	−0.006 (2)	−0.0044 (19)
C19	0.073 (3)	0.046 (3)	0.045 (3)	−0.004 (2)	0.006 (2)	−0.006 (2)
C20	0.075 (4)	0.056 (3)	0.046 (3)	−0.009 (3)	0.009 (2)	0.006 (2)
C21	0.070 (3)	0.047 (3)	0.061 (3)	−0.016 (2)	−0.007 (3)	0.008 (2)
C22	0.065 (3)	0.040 (2)	0.041 (2)	−0.006 (2)	−0.004 (2)	−0.0018 (19)
C23	0.040 (2)	0.038 (2)	0.033 (2)	−0.0045 (17)	−0.0049 (17)	0.0013 (16)
N1	0.045 (2)	0.0368 (19)	0.046 (2)	−0.0045 (15)	−0.0088 (16)	−0.0062 (15)
N2	0.0373 (19)	0.0408 (19)	0.0348 (18)	−0.0038 (15)	−0.0060 (14)	−0.0002 (14)
P1	0.0418 (6)	0.0381 (6)	0.0326 (6)	−0.0044 (4)	−0.0059 (4)	−0.0023 (4)

Geometric parameters (Å, °)

C1—C2	1.374 (6)	C13—H13A	0.9700
C1—C6	1.397 (6)	C13—H13B	0.9700
C1—H1	0.9300	C14—C15	1.521 (7)
C2—C3	1.384 (7)	C14—H14A	0.9700
C2—H2	0.9300	C14—H14B	0.9700
C3—C4	1.369 (7)	C15—C16	1.507 (8)
C3—H3	0.9300	C15—H15A	0.9700
C4—C5	1.395 (6)	C15—H15B	0.9700
C4—H4	0.9300	C16—C17	1.524 (7)
C5—C6	1.387 (6)	C16—H16A	0.9700
C5—H5	0.9300	C16—H16B	0.9700
C6—P1	1.832 (4)	C17—H17A	0.9700
C7—N1	1.474 (6)	C17—H17B	0.9700
C7—C8	1.501 (7)	C18—C19	1.527 (6)
C7—H7A	0.9700	C18—C23	1.529 (6)
C7—H7B	0.9700	C18—H18A	0.9700

C8—C9	1.526 (8)	C18—H18B	0.9700
C8—H8A	0.9700	C19—C20	1.519 (6)
C8—H8B	0.9700	C19—H19A	0.9700
C9—C10	1.520 (8)	C19—H19B	0.9700
C9—H9A	0.9700	C20—C21	1.524 (7)
C9—H9B	0.9700	C20—H20A	0.9700
C10—C11	1.527 (6)	C20—H20B	0.9700
C10—H10A	0.9700	C21—C22	1.505 (6)
C10—H10B	0.9700	C21—H21A	0.9700
C11—N1	1.450 (6)	C21—H21B	0.9700
C11—H11A	0.9700	C22—C23	1.525 (6)
C11—H11B	0.9700	C22—H22A	0.9700
C12—N2	1.483 (5)	C22—H22B	0.9700
C12—C13	1.523 (6)	C23—N2	1.473 (5)
C12—C17	1.532 (6)	C23—H23	0.9800
C12—H12	0.9800	N1—P1	1.701 (4)
C13—C14	1.519 (7)	N2—P1	1.702 (4)
C2—C1—C6	121.4 (4)	H14A—C14—H14B	108.0
C2—C1—H1	119.3	C16—C15—C14	110.4 (4)
C6—C1—H1	119.3	C16—C15—H15A	109.6
C1—C2—C3	120.6 (5)	C14—C15—H15A	109.6
C1—C2—H2	119.7	C16—C15—H15B	109.6
C3—C2—H2	119.7	C14—C15—H15B	109.6
C4—C3—C2	119.5 (5)	H15A—C15—H15B	108.1
C4—C3—H3	120.3	C15—C16—C17	111.2 (4)
C2—C3—H3	120.3	C15—C16—H16A	109.4
C3—C4—C5	119.7 (5)	C17—C16—H16A	109.4
C3—C4—H4	120.1	C15—C16—H16B	109.4
C5—C4—H4	120.1	C17—C16—H16B	109.4
C6—C5—C4	121.9 (4)	H16A—C16—H16B	108.0
C6—C5—H5	119.1	C16—C17—C12	111.6 (4)
C4—C5—H5	119.1	C16—C17—H17A	109.3
C5—C6—C1	116.9 (4)	C12—C17—H17A	109.3
C5—C6—P1	120.5 (3)	C16—C17—H17B	109.3
C1—C6—P1	121.7 (3)	C12—C17—H17B	109.3
N1—C7—C8	111.5 (4)	H17A—C17—H17B	108.0
N1—C7—H7A	109.3	C19—C18—C23	111.2 (4)
C8—C7—H7A	109.3	C19—C18—H18A	109.4
N1—C7—H7B	109.3	C23—C18—H18A	109.4
C8—C7—H7B	109.3	C19—C18—H18B	109.4
H7A—C7—H7B	108.0	C23—C18—H18B	109.4
C7—C8—C9	110.5 (5)	H18A—C18—H18B	108.0
C7—C8—H8A	109.6	C20—C19—C18	111.4 (4)
C9—C8—H8A	109.6	C20—C19—H19A	109.3
C7—C8—H8B	109.6	C18—C19—H19A	109.3
C9—C8—H8B	109.6	C20—C19—H19B	109.3
H8A—C8—H8B	108.1	C18—C19—H19B	109.3
C10—C9—C8	110.3 (4)	H19A—C19—H19B	108.0
C10—C9—H9A	109.6	C19—C20—C21	111.0 (4)

C8—C9—H9A	109.6	C19—C20—H20A	109.4
C10—C9—H9B	109.6	C21—C20—H20A	109.4
C8—C9—H9B	109.6	C19—C20—H20B	109.4
H9A—C9—H9B	108.1	C21—C20—H20B	109.4
C9—C10—C11	110.8 (4)	H20A—C20—H20B	108.0
C9—C10—H10A	109.5	C22—C21—C20	112.3 (4)
C11—C10—H10A	109.5	C22—C21—H21A	109.2
C9—C10—H10B	109.5	C20—C21—H21A	109.2
C11—C10—H10B	109.5	C22—C21—H21B	109.2
H10A—C10—H10B	108.1	C20—C21—H21B	109.2
N1—C11—C10	110.7 (4)	H21A—C21—H21B	107.9
N1—C11—H11A	109.5	C21—C22—C23	112.3 (4)
C10—C11—H11A	109.5	C21—C22—H22A	109.1
N1—C11—H11B	109.5	C23—C22—H22A	109.1
C10—C11—H11B	109.5	C21—C22—H22B	109.1
H11A—C11—H11B	108.1	C23—C22—H22B	109.1
N2—C12—C13	111.9 (3)	H22A—C22—H22B	107.9
N2—C12—C17	113.7 (3)	N2—C23—C22	114.5 (3)
C13—C12—C17	110.3 (4)	N2—C23—C18	113.2 (3)
N2—C12—H12	106.8	C22—C23—C18	109.6 (3)
C13—C12—H12	106.8	N2—C23—H23	106.3
C17—C12—H12	106.8	C22—C23—H23	106.3
C14—C13—C12	112.3 (4)	C18—C23—H23	106.3
C14—C13—H13A	109.1	C11—N1—C7	112.9 (4)
C12—C13—H13A	109.1	C11—N1—P1	127.2 (3)
C14—C13—H13B	109.1	C7—N1—P1	115.7 (3)
C12—C13—H13B	109.1	C23—N2—C12	117.7 (3)
H13A—C13—H13B	107.9	C23—N2—P1	123.5 (3)
C13—C14—C15	111.5 (4)	C12—N2—P1	116.6 (3)
C13—C14—H14A	109.3	N1—P1—N2	111.38 (18)
C15—C14—H14A	109.3	N1—P1—C6	100.57 (19)
C13—C14—H14B	109.3	N2—P1—C6	101.20 (18)
C15—C14—H14B	109.3		
C6—C1—C2—C3	0.8 (7)	C19—C18—C23—N2	174.5 (3)
C1—C2—C3—C4	−0.1 (8)	C19—C18—C23—C22	−56.3 (5)
C2—C3—C4—C5	−0.9 (8)	C10—C11—N1—C7	56.9 (5)
C3—C4—C5—C6	1.2 (8)	C10—C11—N1—P1	−147.5 (3)
C4—C5—C6—C1	−0.5 (7)	C8—C7—N1—C11	−57.5 (5)
C4—C5—C6—P1	−170.0 (4)	C8—C7—N1—P1	143.8 (4)
C2—C1—C6—C5	−0.5 (7)	C22—C23—N2—C12	−64.7 (5)
C2—C1—C6—P1	168.9 (4)	C18—C23—N2—C12	62.0 (4)
N1—C7—C8—C9	55.4 (6)	C22—C23—N2—P1	132.7 (3)
C7—C8—C9—C10	−54.6 (6)	C18—C23—N2—P1	−100.6 (4)
C8—C9—C10—C11	54.6 (6)	C13—C12—N2—C23	129.2 (4)
C9—C10—C11—N1	−55.6 (5)	C17—C12—N2—C23	−105.0 (4)
N2—C12—C13—C14	−179.0 (4)	C13—C12—N2—P1	−67.0 (4)
C17—C12—C13—C14	53.3 (5)	C17—C12—N2—P1	58.9 (4)
C12—C13—C14—C15	−55.0 (6)	C11—N1—P1—N2	−60.1 (4)
C13—C14—C15—C16	56.2 (6)	C7—N1—P1—N2	95.0 (3)

C14—C15—C16—C17	−57.2 (6)	C11—N1—P1—C6	46.5 (4)
C15—C16—C17—C12	56.8 (6)	C7—N1—P1—C6	−158.4 (3)
N2—C12—C17—C16	179.4 (4)	C23—N2—P1—N1	46.2 (3)
C13—C12—C17—C16	−54.0 (5)	C12—N2—P1—N1	−116.6 (3)
C23—C18—C19—C20	56.7 (5)	C23—N2—P1—C6	−59.9 (3)
C18—C19—C20—C21	−54.3 (6)	C12—N2—P1—C6	137.2 (3)
C19—C20—C21—C22	53.4 (6)	C5—C6—P1—N1	−152.2 (3)
C20—C21—C22—C23	−54.8 (6)	C1—C6—P1—N1	38.8 (4)
C21—C22—C23—N2	−175.9 (4)	C5—C6—P1—N2	−37.7 (4)
C21—C22—C23—C18	55.6 (5)	C1—C6—P1—N2	153.3 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7A···Cg^{i}	0.97	?	2.797 (7)	159

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

Fig. 1

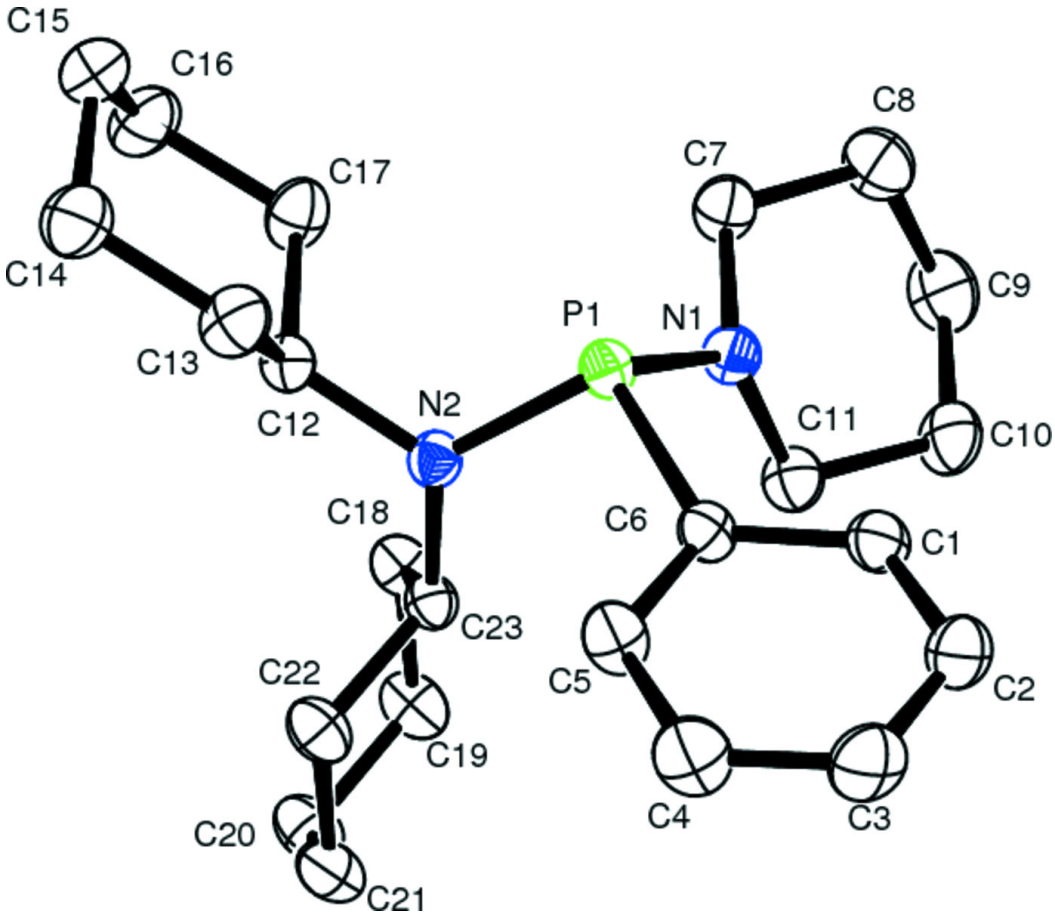

C15
C16
C17
C14
C13
C12
N2
P1
N1
C7
C8
C9
C10
C11
C18
C6
C1
C23
C22
C5
C2
C19
C20
C4
C3
C21

Fig. 2