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N-Benzylidene-*o*-(diphenylphosphino)-aniline

Aike Li, Jianxin Chen,* Zhongshui Li, Wenjie Zhang and Meiping Zhu

College of Chemistry and Materials Science, Fujian Normal University, Fuzhou, Fujian 350007, People's Republic of China
Correspondence e-mail: jxchen_1964@163.com

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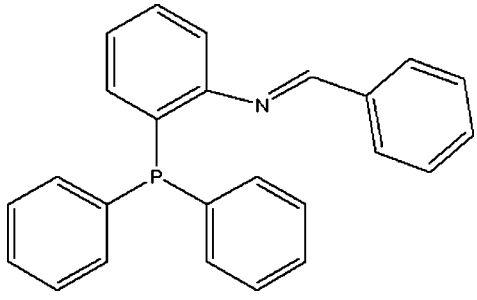
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.047; wR factor = 0.163; data-to-parameter ratio = 18.1.

The title compound, $C_{25}H_{20}NP$, is a Schiff base containing triphenylphosphine. The molecule has a *trans* configuration about the C=N double bond [1.266 (3) Å]. Intermolecular π–π interactions (~3.61 Å) are pronounced in the crystal structure.

Related literature

For related literature, see: Braunstein & Naud (2001); Helmchen & Pfaltz (2000); Li *et al.* (2005); Papathanasiou *et al.* (1997); Reddy *et al.* (2001); Slone *et al.* (1999); Speiser & Braunstein (2004); Wang & Jin (2005); Yang *et al.* (2006).



Experimental

Crystal data

$C_{25}H_{20}NP$
M_r = 366.40
Monoclinic, $P2_1/c$
a = 15.076 (3) Å
b = 6.6127 (13) Å
c = 20.297 (4) Å
β = 98.46 (3)°
V = 2001.5 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.15 mm^{-1}
T = 293 (2) K
0.18 × 0.12 × 0.11 mm

Data collection

Rigaku Weissenberg IP diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.979, T_{max} = 0.984
17296 measured reflections
4416 independent reflections
2664 reflections with $I > 2\sigma(I)$
R_{int} = 0.054

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.163
S = 1.02
4416 reflections
244 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Data collection: *TEXSAN* (Molecular Structure Corporation, 1998); cell refinement: *TEXSAN*; data reduction: *TEXSAN*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXL97*; software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2389).

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supplementary materials

Acta Cryst. (2007). E**63**, o4020 [**doi:10.1107/S1600536807043358**]

N-Benzylidene-*o*-(diphenylphosphino)aniline

A. Li, J. Chen, Z. Li, W. Zhang and M. Zhu

Comment

Schiff base ligands have various applications in the fields of synthesis and catalysis, and exhibit biological activity (Wang *et al.*, 2005; Speiser *et al.*, 2004). At the same time P, N ligands have attracted increasing recent attention because of their bonding versatility with a metal center and the relative ease with which the electronic and steric properties of the donor atoms can be modified (Braunstein *et al.*, 2001; Slone *et al.*, 1999; Helmchen *et al.*, 2000), but few Schiff bases containing phosphorus and nitrogen have been reported (Yang *et al.*, 2006). A Schiff base containing P, N may be expected to be a useful bidentate ligand with new properties, because triphenylphosphine is a well known ligand for coordination compounds. Here we present the title compound (I), a useful Schiff base ligand containing phosphine-imine.

In compound (I), the bond lengths of P1—C1, P1—C13, P1—C1, N1—C25 and N1—C2 are 1.830 (2), 1.831 (2), 1.830 (2), 1.266 (3) and 1.409 (3) Å, respectively. The aromatic ring 1 (C1—C6) is tilted with rings 2 (C7—C12), 3 (C13—C18) and 4 (C19—C24). The dihedral angle of ring 2 and ring 3 is 81.65 (10)°, the dihedral angles of ring 1 with rings 2, 3, 4 are 74.50 (8), 77.73 (7), and 26.61 (15)°, respectively (Fig. 1). The π-π stacking interactions support the crystal packing with distances of about 3.61 Å (Fig. 2).

Experimental

All reagents were of AR grade available commercially and used without further purification. The complex of o-(diphenylphosphino)-*N*-benzaldimine was prepared by simple condensation of o-(diphenylphosphino)-aniline (Reddy *et al.*, 2001} with excess benzaldehyde. o-(Diphenylphosphino)benzenamine was prepared according to the literature (Papathanasiou *et al.*, 1997). To freshly distilled benzaldehyde (16 ml, 0.15 mol) was added o-(diphenylphosphino)-aniline (6 g, 0.02 mol) under nitrogen, and the mixture was stirred at room temperature under nitrogen for 6–7 h. The reaction mixture was poured into cold methanol and kept at low temperature overnight. The desired ligand P, N was crystallized as a white solid. Crystals suitable for X-ray diffraction analysis were obtained by slow evaporation of ethanol solution.

Refinement

H atoms were located geometrically and refined using a riding model with C—H = 0.93 Å, and U_{iso}(H) = 1.2 U_{eq}(C).

Figures

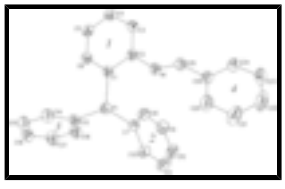


Fig. 1. View of the molecule of (I) showing the atom-labelling scheme. The molecule has a *trans* configuration about the C25═N1 double bond. All H atoms were omitted for clarity.

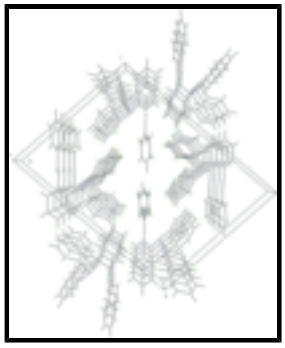


Fig. 2. Packing diagram of (I) showing the π-π stacking along the *b* axis.

N-Benzylidene-*o*-(diphenylphosphino)aniline

Crystal data

$C_{25}H_{20}NP$	F_{000} = 772
M_r = 366.40	D_x = 1.216 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 4416 reflections
a = 15.076 (3) Å	θ = 3.2–27.5º
b = 6.6127 (13) Å	μ = 0.15 mm^{-1}
c = 20.297 (4) Å	T = 293 (2) K
β = 98.46 (3)º	Prism, colourless
V = 2001.5 (7) Å^3	0.18 × 0.12 × 0.11 mm
Z = 4	

Data collection

Rigaku Weissenberg IP diffractometer	4416 independent reflections
Radiation source: fine-focus sealed tube	2664 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.054
T = 293(2) K	θ_{max} = 27.5º
scintillation counter scans	θ_{min} = 3.2º
Absorption correction: ψ scan (North *et al.*, 1968)	h = −19→19
T_{min} = 0.979, T_{max} = 0.984	k = −8→7
17296 measured reflections	l = −26→26

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.047	H-atom parameters constrained
$wR(F^2)$ = 0.163	$w = 1/[\sigma^2(F_o^2) + (0.0897P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

S = 1.02	$(\Delta/\sigma)_{max}$ = 0.015
4416 reflections	$\Delta\rho_{max}$ = 0.21 e Å^{-3}
244 parameters	$\Delta\rho_{min}$ = −0.21 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}
P1	0.20484 (4)	0.75168 (8)	0.17396 (3)	0.04508 (19)
N1	0.18326 (12)	1.0677 (3)	0.27147 (9)	0.0464 (4)
C2	0.10879 (14)	1.0673 (3)	0.22061 (11)	0.0426 (5)
C1	0.11152 (13)	0.9309 (3)	0.16779 (11)	0.0415 (5)
C7	0.30187 (14)	0.9120 (3)	0.16743 (11)	0.0474 (5)
C6	0.03873 (15)	0.9284 (3)	0.11698 (12)	0.0495 (5)
H6A	0.0399	0.8428	0.0808	0.059*
C13	0.18483 (14)	0.6353 (3)	0.09123 (11)	0.0460 (5)
C3	0.03371 (15)	1.1869 (3)	0.22255 (12)	0.0518 (6)
H3A	0.0318	1.2740	0.2583	0.062*
C14	0.12690 (16)	0.4726 (3)	0.08273 (13)	0.0556 (6)
H14A	0.1007	0.4263	0.1186	0.067*
C4	−0.03791 (15)	1.1780 (4)	0.17219 (13)	0.0563 (6)
H4A	−0.0882	1.2583	0.1739	0.068*
C8	0.29742 (16)	1.1050 (4)	0.14107 (14)	0.0614 (7)
H8A	0.2418	1.1607	0.1250	0.074*
C5	−0.03491 (15)	1.0496 (4)	0.11909 (13)	0.0555 (6)
H5A	−0.0828	1.0449	0.0846	0.067*
C15	0.10727 (18)	0.3773 (4)	0.02167 (14)	0.0637 (7)
H15A	0.0674	0.2691	0.0168	0.076*
C25	0.21333 (15)	1.2371 (3)	0.29366 (12)	0.0506 (5)
H25A	0.1866	1.3548	0.2752	0.061*
C19	0.28912 (15)	1.2531 (4)	0.34766 (12)	0.0541 (6)
C16	0.1455 (2)	0.4401 (4)	−0.03098 (15)	0.0702 (7)
H16A	0.1326	0.3742	−0.0718	0.084*
C12	0.38576 (16)	0.8340 (4)	0.19137 (14)	0.0639 (7)
H12A	0.3907	0.7053	0.2100	0.077*

C18	0.22344 (18)	0.6974 (4)	0.03667 (14)	0.0635 (7)
H18A	0.2634	0.8055	0.0410	0.076*
C17	0.2034 (2)	0.6011 (4)	−0.02407 (15)	0.0754 (8)
H17A	0.2292	0.6455	−0.0604	0.090*
C20	0.34628 (19)	1.0935 (4)	0.36478 (15)	0.0711 (8)
H20A	0.3392	0.9737	0.3406	0.085*
C9	0.3737 (2)	1.2162 (4)	0.13814 (16)	0.0745 (8)
H9A	0.3695	1.3458	0.1202	0.089*
C10	0.45611 (19)	1.1356 (5)	0.16167 (17)	0.0805 (9)
H10A	0.5078	1.2108	0.1598	0.097*
C24	0.30210 (18)	1.4321 (5)	0.38267 (17)	0.0818 (9)
H24A	0.2654	1.5426	0.3700	0.098*
C23	0.3692 (2)	1.4476 (6)	0.4362 (2)	0.1007 (12)
H23A	0.3772	1.5679	0.4601	0.121*
C11	0.46217 (18)	0.9470 (6)	0.18761 (18)	0.0820 (9)
H11A	0.5182	0.8925	0.2031	0.098*
C21	0.4143 (2)	1.1115 (6)	0.41809 (18)	0.0941 (11)
H21A	0.4537	1.0046	0.4295	0.113*
C22	0.4237 (3)	1.2881 (7)	0.45426 (18)	0.1019 (12)
H22A	0.4677	1.2981	0.4914	0.122*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P1	0.0462 (3)	0.0455 (3)	0.0424 (3)	0.0021 (2)	0.0029 (2)	0.0013 (2)
N1	0.0466 (10)	0.0520 (10)	0.0405 (11)	−0.0043 (8)	0.0061 (8)	−0.0059 (8)
C2	0.0417 (10)	0.0456 (11)	0.0410 (12)	−0.0054 (9)	0.0078 (9)	−0.0008 (9)
C1	0.0407 (10)	0.0444 (11)	0.0398 (12)	−0.0050 (9)	0.0072 (9)	0.0006 (9)
C7	0.0437 (11)	0.0524 (12)	0.0447 (13)	0.0046 (10)	0.0024 (10)	−0.0068 (9)
C6	0.0490 (12)	0.0534 (12)	0.0449 (13)	0.0032 (10)	0.0025 (10)	−0.0059 (10)
C13	0.0484 (11)	0.0403 (11)	0.0485 (13)	0.0042 (10)	0.0045 (10)	0.0001 (9)
C3	0.0518 (13)	0.0522 (12)	0.0528 (15)	−0.0025 (11)	0.0122 (11)	−0.0100 (10)
C14	0.0640 (14)	0.0505 (12)	0.0506 (15)	−0.0009 (12)	0.0026 (11)	0.0040 (10)
C4	0.0463 (12)	0.0558 (13)	0.0670 (17)	0.0046 (11)	0.0091 (11)	−0.0031 (12)
C8	0.0484 (13)	0.0574 (14)	0.0785 (19)	0.0012 (11)	0.0092 (12)	0.0069 (13)
C5	0.0428 (11)	0.0609 (14)	0.0593 (16)	0.0015 (11)	−0.0038 (11)	−0.0020 (11)
C15	0.0716 (16)	0.0532 (13)	0.0629 (18)	−0.0105 (12)	−0.0016 (14)	−0.0071 (12)
C25	0.0508 (12)	0.0521 (12)	0.0485 (13)	−0.0039 (10)	0.0061 (10)	−0.0041 (10)
C19	0.0465 (12)	0.0651 (14)	0.0509 (14)	−0.0106 (11)	0.0080 (10)	−0.0114 (11)
C16	0.0850 (18)	0.0693 (16)	0.0551 (17)	−0.0018 (15)	0.0057 (15)	−0.0158 (13)
C12	0.0481 (13)	0.0698 (15)	0.0704 (18)	0.0087 (13)	−0.0032 (12)	0.0001 (14)
C18	0.0727 (16)	0.0622 (15)	0.0589 (17)	−0.0140 (13)	0.0213 (13)	−0.0094 (12)
C17	0.091 (2)	0.0811 (19)	0.0590 (18)	−0.0095 (16)	0.0285 (16)	−0.0103 (14)
C20	0.0694 (16)	0.0737 (17)	0.0652 (19)	−0.0076 (14)	−0.0066 (14)	−0.0064 (14)
C9	0.0690 (17)	0.0669 (16)	0.090 (2)	−0.0141 (14)	0.0198 (16)	0.0011 (15)
C10	0.0553 (16)	0.099 (2)	0.088 (2)	−0.0258 (17)	0.0118 (15)	−0.0127 (18)
C24	0.0542 (15)	0.089 (2)	0.100 (2)	−0.0102 (14)	0.0059 (15)	−0.0431 (18)
C23	0.074 (2)	0.125 (3)	0.100 (3)	−0.026 (2)	0.0045 (19)	−0.063 (2)

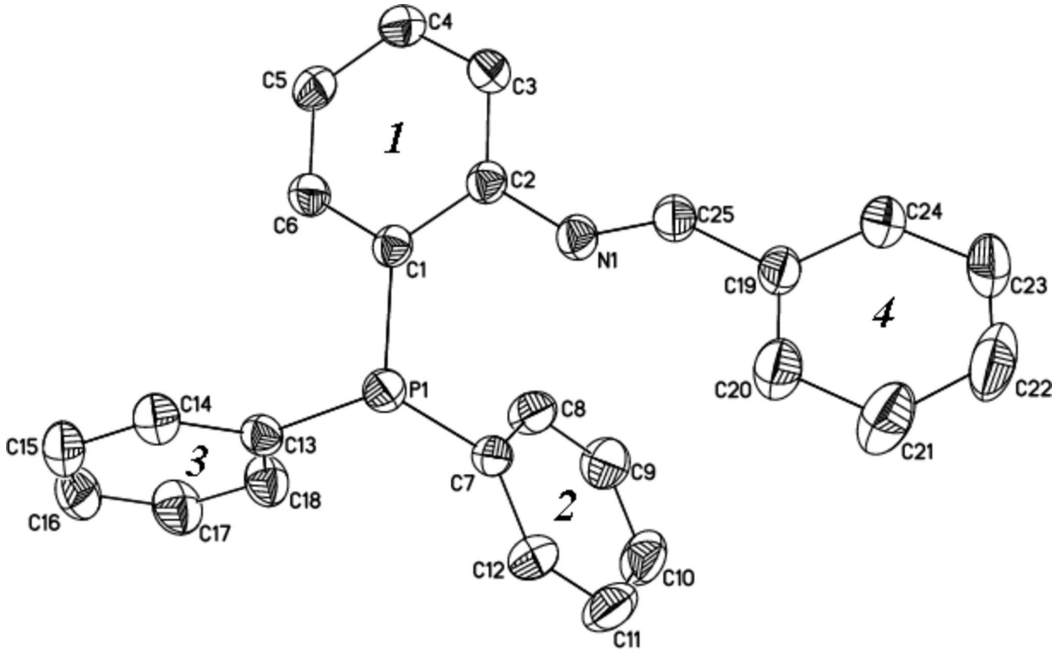
C11	0.0425 (14)	0.109 (2)	0.093 (2)	0.0000 (15)	0.0021 (14)	−0.0030 (19)
C21	0.078 (2)	0.102 (2)	0.091 (3)	−0.0088 (18)	−0.0257 (18)	0.007 (2)
C22	0.084 (2)	0.146 (3)	0.068 (2)	−0.031 (2)	−0.0172 (18)	−0.020 (2)

Geometric parameters (Å, °)

P1—C7	1.827 (2)	C25—C19	1.466 (3)
P1—C13	1.831 (2)	C25—H25A	0.9300
P1—C1	1.830 (2)	C19—C20	1.375 (4)
N1—C25	1.266 (3)	C19—C24	1.379 (3)
N1—C2	1.409 (3)	C16—C17	1.370 (4)
C2—C3	1.386 (3)	C16—H16A	0.9300
C2—C1	1.406 (3)	C12—C11	1.384 (4)
C1—C6	1.391 (3)	C12—H12A	0.9300
C7—C8	1.382 (3)	C18—C17	1.381 (4)
C7—C12	1.386 (3)	C18—H18A	0.9300
C6—C5	1.375 (3)	C17—H17A	0.9300
C6—H6A	0.9300	C20—C21	1.382 (4)
C13—C14	1.381 (3)	C20—H20A	0.9300
C13—C18	1.387 (3)	C9—C10	1.371 (4)
C3—C4	1.374 (3)	C9—H9A	0.9300
C3—H3A	0.9300	C10—C11	1.352 (4)
C14—C15	1.383 (3)	C10—H10A	0.9300
C14—H14A	0.9300	C24—C23	1.375 (4)
C4—C5	1.378 (3)	C24—H24A	0.9300
C4—H4A	0.9300	C23—C22	1.353 (5)
C8—C9	1.374 (4)	C23—H23A	0.9300
C8—H8A	0.9300	C11—H11A	0.9300
C5—H5A	0.9300	C21—C22	1.376 (5)
C15—C16	1.352 (4)	C21—H21A	0.9300
C15—H15A	0.9300	C22—H22A	0.9300
C7—P1—C13	101.71 (10)	C20—C19—C24	119.5 (3)
C7—P1—C1	103.59 (10)	C20—C19—C25	121.6 (2)
C13—P1—C1	100.85 (10)	C24—C19—C25	118.9 (2)
C25—N1—C2	117.86 (19)	C15—C16—C17	119.8 (3)
C3—C2—N1	123.0 (2)	C15—C16—H16A	120.1
C3—C2—C1	120.2 (2)	C17—C16—H16A	120.1
N1—C2—C1	116.76 (18)	C11—C12—C7	120.3 (3)
C6—C1—C2	117.67 (19)	C11—C12—H12A	119.9
C6—C1—P1	123.90 (16)	C7—C12—H12A	119.9
C2—C1—P1	118.15 (16)	C17—C18—C13	120.9 (2)
C8—C7—C12	118.0 (2)	C17—C18—H18A	119.6
C8—C7—P1	124.76 (17)	C13—C18—H18A	119.6
C12—C7—P1	117.25 (18)	C16—C17—C18	120.1 (3)
C5—C6—C1	121.5 (2)	C16—C17—H17A	119.9
C5—C6—H6A	119.3	C18—C17—H17A	119.9
C1—C6—H6A	119.3	C19—C20—C21	119.8 (3)
C14—C13—C18	117.6 (2)	C19—C20—H20A	120.1
C14—C13—P1	117.25 (18)	C21—C20—H20A	120.1

C18—C13—P1	125.15 (18)	C10—C9—C8	119.9 (3)
C4—C3—C2	120.7 (2)	C10—C9—H9A	120.0
C4—C3—H3A	119.7	C8—C9—H9A	120.0
C2—C3—H3A	119.7	C11—C10—C9	120.0 (3)
C15—C14—C13	121.0 (2)	C11—C10—H10A	120.0
C15—C14—H14A	119.5	C9—C10—H10A	120.0
C13—C14—H14A	119.5	C19—C24—C23	120.2 (3)
C5—C4—C3	119.7 (2)	C19—C24—H24A	119.9
C5—C4—H4A	120.2	C23—C24—H24A	119.9
C3—C4—H4A	120.2	C22—C23—C24	120.2 (3)
C9—C8—C7	121.2 (2)	C22—C23—H23A	119.9
C9—C8—H8A	119.4	C24—C23—H23A	119.9
C7—C8—H8A	119.4	C10—C11—C12	120.7 (3)
C4—C5—C6	120.2 (2)	C10—C11—H11A	119.7
C4—C5—H5A	119.9	C12—C11—H11A	119.7
C6—C5—H5A	119.9	C22—C21—C20	119.8 (3)
C16—C15—C14	120.6 (2)	C22—C21—H21A	120.1
C16—C15—H15A	119.7	C20—C21—H21A	120.1
C14—C15—H15A	119.7	C23—C22—C21	120.4 (3)
N1—C25—C19	121.9 (2)	C23—C22—H22A	119.8
N1—C25—H25A	119.0	C21—C22—H22A	119.8
C19—C25—H25A	119.0		
C25—N1—C2—C3	−45.7 (3)	P1—C7—C8—C9	179.8 (2)
C25—N1—C2—C1	137.2 (2)	C3—C4—C5—C6	1.1 (4)
C3—C2—C1—C6	3.0 (3)	C1—C6—C5—C4	0.2 (4)
N1—C2—C1—C6	−179.87 (19)	C13—C14—C15—C16	0.9 (4)
C3—C2—C1—P1	−171.27 (16)	C2—N1—C25—C19	178.46 (19)
N1—C2—C1—P1	5.9 (2)	N1—C25—C19—C20	17.8 (4)
C7—P1—C1—C6	117.68 (19)	N1—C25—C19—C24	−161.1 (3)
C13—P1—C1—C6	12.7 (2)	C14—C15—C16—C17	−0.8 (4)
C7—P1—C1—C2	−68.48 (18)	C8—C7—C12—C11	−1.0 (4)
C13—P1—C1—C2	−173.49 (16)	P1—C7—C12—C11	179.6 (2)
C13—P1—C7—C8	84.7 (2)	C14—C13—C18—C17	0.9 (4)
C1—P1—C7—C8	−19.7 (2)	P1—C13—C18—C17	−179.3 (2)
C13—P1—C7—C12	−96.0 (2)	C15—C16—C17—C18	0.8 (5)
C1—P1—C7—C12	159.66 (19)	C13—C18—C17—C16	−0.8 (4)
C2—C1—C6—C5	−2.2 (3)	C24—C19—C20—C21	2.0 (4)
P1—C1—C6—C5	171.66 (18)	C25—C19—C20—C21	−176.9 (3)
C7—P1—C13—C14	167.16 (17)	C7—C8—C9—C10	0.0 (5)
C1—P1—C13—C14	−86.34 (18)	C8—C9—C10—C11	0.1 (5)
C7—P1—C13—C18	−12.6 (2)	C20—C19—C24—C23	−2.9 (5)
C1—P1—C13—C18	93.9 (2)	C25—C19—C24—C23	176.0 (3)
N1—C2—C3—C4	−178.8 (2)	C19—C24—C23—C22	0.9 (6)
C1—C2—C3—C4	−1.8 (3)	C9—C10—C11—C12	−0.7 (5)
C18—C13—C14—C15	−0.9 (4)	C7—C12—C11—C10	1.1 (5)
P1—C13—C14—C15	179.26 (19)	C19—C20—C21—C22	0.9 (5)
C2—C3—C4—C5	−0.3 (4)	C24—C23—C22—C21	2.1 (6)
C12—C7—C8—C9	0.5 (4)	C20—C21—C22—C23	−3.0 (6)

Fig. 1


C4
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C8
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C18
C16
C17
C12
C10
C11

Fig. 2