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N-[2-(Diphenylphosphino)phenyl]-benzamide

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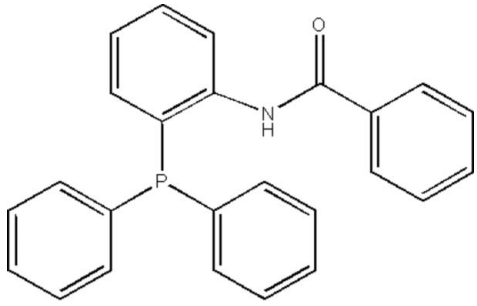
Key indicators: single-crystal X-ray study; T = 153 K; mean σ(C–C) = 0.004 Å; R factor = 0.054; wR factor = 0.152; data-to-parameter ratio = 17.9.

In the molecule of the title compound, $C_{25}H_{20}NOP$, the dihedral angles between pairs of rings are 80.13 (7) and 89.92 (11)°. The arrangement of the rings around P is a propeller structure. The coordination around the P atom is distorted trigonal pyramidal.

Related literature

For related literature, see: Hedden & Roundhill (1982); Soonheum *et al.* (1986); Hedden *et al.* (1986, 1984); Roundhill (1970); Wilson *et al.* (1978). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{25}H_{20}NOP$
M_r = 381.39
Monoclinic, $P2_1/n$
a = 9.936 (5) Å
b = 10.819 (4) Å
c = 19.038 (11) Å
β = 93.49 (2)°
V = 2042.7 (17) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.15 mm^{-1}
T = 153 (2) K
0.16 × 0.12 × 0.10 mm

Data collection

Rigaku Weissenberg IP diffractometer
Absorption correction: multi-scan (*TEXSAN-PC*; Molecular Structure Corporation, 1998)
T_{min} = 0.975, T_{max} = 0.985
18607 measured reflections
4530 independent reflections
2495 reflections with $I > 2\sigma(I)$
R_{int} = 0.067

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.152
S = 1.03
4530 reflections
253 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

P1—C14	1.814 (3)	P1—C13	1.823 (3)
P1—C20	1.820 (2)		
C14—P1—C20	104.20 (11)	C20—P1—C13	101.64 (11)
C14—P1—C13	102.48 (11)	C8—C13—P1	118.60 (17)

Data collection: *TEXSAN-PC* (Molecular Structure Corporation, 1998); cell refinement: *TEXSAN-PC*; data reduction: *TEXSAN-PC*; 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: HK2318).

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supplementary materials

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N-[2-(Diphenylphosphino)phenyl]benzamide

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Comment

The title compound, (I), a new hybrid phosphine amide ligand, has various applications in the fields of synthesis and homogeneous catalysis, and a series of new phosphine amido chelate complexes have been synthesized (Hedden & Roundhill, 1982; Soonheum *et al.*, 1986; Hedden *et al.*, 1986), especially in the reactions of chelate-assisted N—H oxidative addition (Hedden *et al.*, 1984; Roundhill, 1970). The chelate ligands have mixed functionality types in coordination chemistry. We report herein the crystal structure of the title compound, (I).

In the molecule of the title compound, (I), (Fig. 1) the bond lengths and angles (Table 1) are generally within normal ranges (Allen *et al.*, 1987). The coordination around P1 atom is a distorted trigonal pyramid.

Rings 1 (C8–C13), 2 (C14–C19), 3 (C20–C25) and 4 (C1–C6) are, of course, planar and the dihedral angles between them are 1/2 = 88.71 (3)°, 1/3 = 77.92 (3)°, 1/4 = 12.78 (3)°, 2/3 = 88.77 (2)°, 2/4 = 83.93 (2)° and 3/4 = 88.26 (3)°.

In the crystal structure, the molecules are elongated along the *b* axis and stacked along the *a* axis (Fig. 2).

Experimental

For the preparation of the title compound, (I), *o*-(Dipheny1phosphino)aniline (2.46 g, 8.9 mmol) and dry pyridine (2.12 g, 26.7 mmol) (Wilson *et al.*, 1978) were dissolved in dry THF (10 ml), under nitrogen atmosphere. Benzoyl chloride (1.25 g, 8.9 mmol) was rapidly added to the stirred solution, the suspension containing pyridine·HCl was stirred for 2 h. The precipitate was filtered and washed with dry THF. Solvent removal left an viscous oil. The oil was washed with water (6× 25 ml), then dissolved in dichloromethane (15 ml) and the solution dried over $MgSO_4$. The filtered solution was reduced in volume to 3 ml, hexane (100 ml) was added, and the cloudy solution was stored at 263 K. The resulting white needles were collected by filtration, lightly washed with hexane (10 ml), and dried *in vacuo* at 298 K (yield; 1.90 g, 56.3%, m.p. 377–379 K).

Refinement

H atoms were positioned geometrically with N—H = 0.86 Å (for NH) and C—H = 0.93 Å for aromatic H atoms, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C,*N*)

Figures

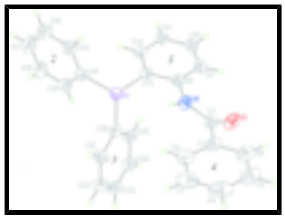

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

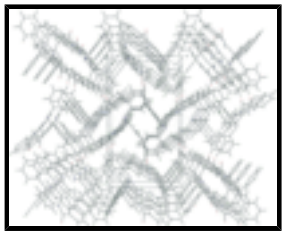

Fig. 2. A packing diagram for (I).

N-[2-(Diphenylphosphino)phenyl]benzamide

Crystal data

$C_{25}H_{20}NOP$	F_{000} = 800
M_r = 381.39	D_x = 1.240 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -p 2yn	Cell parameters from 4530 reflections
a = 9.936 (5) Å	θ = 3.0–27.5º
b = 10.819 (4) Å	μ = 0.15 mm^{-1}
c = 19.038 (11) Å	T = 153 (2) K
β = 93.49 (2)º	Needle, colourless
V = 2042.7 (17) Å^3	0.16 × 0.12 × 0.10 mm
Z = 4	

Data collection

Rigaku Weissenberg IP diffractometer	4530 independent reflections
Radiation source: fine-focus sealed tube	2495 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.067
T = 153(2) K	θ_{max} = 27.5º
scintillation counter scans	θ_{min} = 3.0º
Absorption correction: multi-scan (correct reference required)	h = −12→12
T_{min} = 0.975, T_{max} = 0.985	k = −13→13
18607 measured reflections	l = −24→24

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.054$	H-atom parameters constrained
$wR(F^2) = 0.152$	$w = 1/[\sigma^2(F_o^2) + (0.0651P)^2 + 0.0657P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} < 0.001$
4530 reflections	$\Delta\rho_{max} = 0.44$ e Å^{-3}
253 parameters	$\Delta\rho_{min} = -0.27$ 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 $F^2 > 2$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	0.18732 (6)	0.27331 (6)	0.03471 (3)	0.0569 (2)
N1	0.0906 (2)	0.43689 (17)	−0.08083 (10)	0.0608 (5)
H1A	0.1580	0.4486	−0.0510	0.073*
O1	0.0171 (2)	0.47614 (19)	−0.19282 (10)	0.0928 (6)
C1	0.2309 (3)	0.5556 (2)	−0.15335 (14)	0.0686 (7)
C2	0.3507 (3)	0.5288 (3)	−0.11613 (17)	0.0820 (8)
H2A	0.3546	0.4631	−0.0846	0.098*
C3	0.4651 (3)	0.5985 (3)	−0.1250 (2)	0.1004 (11)
H3A	0.5457	0.5793	−0.0999	0.121*
C4	0.4590 (5)	0.6954 (4)	−0.1709 (3)	0.1107 (13)
H4A	0.5353	0.7433	−0.1765	0.133*
C5	0.3424 (5)	0.7225 (3)	−0.2085 (2)	0.1027 (11)
H5A	0.3399	0.7883	−0.2399	0.123*
C6	0.2267 (3)	0.6534 (3)	−0.20064 (15)	0.0847 (8)
H6A	0.1473	0.6723	−0.2268	0.102*
C7	0.1032 (3)	0.4862 (2)	−0.14497 (14)	0.0647 (6)
C8	−0.0174 (2)	0.36881 (19)	−0.05563 (12)	0.0551 (6)
C9	−0.1477 (3)	0.3825 (2)	−0.08339 (14)	0.0649 (6)

H9A	−0.1663	0.4346	−0.1216	0.078*
C10	−0.2506 (3)	0.3187 (2)	−0.05418 (15)	0.0699 (7)
H10A	−0.3385	0.3279	−0.0730	0.084*
C11	−0.2251 (3)	0.2416 (2)	0.00228 (14)	0.0679 (7)
H11A	−0.2953	0.2000	0.0222	0.081*
C12	−0.0945 (2)	0.2267 (2)	0.02899 (13)	0.0598 (6)
H12A	−0.0773	0.1740	0.0671	0.072*
C13	0.0125 (2)	0.28804 (19)	0.00078 (12)	0.0526 (5)
C14	0.1732 (2)	0.1743 (2)	0.11078 (12)	0.0578 (6)
C15	0.1525 (3)	0.2295 (3)	0.17442 (14)	0.0797 (8)
H15A	0.1461	0.3151	0.1769	0.096*
C16	0.1410 (4)	0.1604 (4)	0.23404 (16)	0.1054 (11)
H16A	0.1239	0.1989	0.2762	0.127*
C17	0.1549 (4)	0.0342 (4)	0.23152 (19)	0.1050 (11)
H17A	0.1508	−0.0127	0.2723	0.126*
C18	0.1746 (4)	−0.0215 (3)	0.16908 (19)	0.0964 (10)
H18A	0.1815	−0.1072	0.1672	0.116*
C19	0.1845 (3)	0.0459 (2)	0.10894 (14)	0.0733 (7)
H19A	0.1987	0.0061	0.0667	0.088*
C20	0.2567 (2)	0.1730 (2)	−0.03078 (12)	0.0565 (6)
C21	0.3957 (3)	0.1668 (3)	−0.03155 (16)	0.0778 (8)
H21A	0.4488	0.2108	0.0017	0.093*
C22	0.4562 (3)	0.0962 (3)	−0.08090 (18)	0.0908 (9)
H22A	0.5497	0.0920	−0.0803	0.109*
C23	0.3801 (3)	0.0328 (2)	−0.13041 (16)	0.0815 (8)
H23A	0.4213	−0.0140	−0.1640	0.098*
C24	0.2432 (3)	0.0381 (3)	−0.13059 (15)	0.0815 (8)
H24A	0.1911	−0.0056	−0.1644	0.098*
C25	0.1812 (3)	0.1074 (2)	−0.08124 (14)	0.0697 (7)
H25A	0.0876	0.1100	−0.0819	0.084*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P1	0.0542 (4)	0.0626 (4)	0.0536 (4)	0.0002 (3)	0.0002 (3)	−0.0031 (3)
N1	0.0624 (13)	0.0649 (11)	0.0546 (12)	−0.0059 (9)	−0.0010 (10)	0.0008 (9)
O1	0.0976 (16)	0.1228 (16)	0.0570 (12)	−0.0254 (12)	−0.0040 (11)	0.0088 (11)
C1	0.0824 (19)	0.0681 (15)	0.0569 (15)	−0.0070 (13)	0.0170 (14)	−0.0125 (12)
C2	0.075 (2)	0.0842 (18)	0.089 (2)	−0.0015 (15)	0.0167 (17)	−0.0088 (15)
C3	0.075 (2)	0.107 (2)	0.121 (3)	−0.0128 (18)	0.022 (2)	−0.027 (2)
C4	0.108 (3)	0.096 (3)	0.133 (3)	−0.029 (2)	0.048 (3)	−0.032 (2)
C5	0.130 (3)	0.083 (2)	0.099 (3)	−0.028 (2)	0.039 (3)	−0.0034 (18)
C6	0.103 (2)	0.0836 (19)	0.0696 (19)	−0.0125 (16)	0.0173 (17)	−0.0018 (15)
C7	0.0755 (19)	0.0650 (14)	0.0537 (15)	−0.0006 (12)	0.0054 (13)	−0.0064 (11)
C8	0.0566 (14)	0.0553 (12)	0.0533 (14)	0.0012 (10)	0.0030 (11)	−0.0035 (10)
C9	0.0664 (17)	0.0652 (14)	0.0622 (16)	0.0044 (12)	−0.0031 (13)	0.0030 (11)
C10	0.0504 (16)	0.0820 (17)	0.0762 (19)	0.0060 (12)	−0.0039 (13)	−0.0016 (14)
C11	0.0550 (16)	0.0782 (16)	0.0711 (18)	−0.0010 (12)	0.0081 (13)	−0.0022 (13)

C12	0.0595 (16)	0.0632 (13)	0.0572 (14)	0.0007 (11)	0.0064 (12)	0.0011 (11)
C13	0.0567 (14)	0.0519 (12)	0.0493 (13)	0.0012 (10)	0.0045 (11)	−0.0056 (10)
C14	0.0476 (14)	0.0733 (15)	0.0520 (14)	0.0003 (10)	−0.0015 (10)	0.0001 (11)
C15	0.094 (2)	0.0893 (18)	0.0558 (17)	−0.0006 (15)	0.0018 (15)	−0.0094 (14)
C16	0.118 (3)	0.149 (3)	0.0502 (19)	−0.004 (2)	0.0071 (18)	−0.0022 (19)
C17	0.114 (3)	0.126 (3)	0.074 (2)	−0.008 (2)	−0.002 (2)	0.032 (2)
C18	0.111 (3)	0.088 (2)	0.089 (2)	0.0025 (17)	0.000 (2)	0.0226 (18)
C19	0.082 (2)	0.0716 (16)	0.0657 (17)	0.0064 (13)	0.0006 (14)	0.0077 (13)
C20	0.0562 (15)	0.0604 (13)	0.0529 (14)	0.0010 (10)	0.0032 (11)	0.0030 (10)
C21	0.0542 (17)	0.0925 (18)	0.086 (2)	0.0031 (13)	0.0027 (14)	−0.0219 (16)
C22	0.0651 (19)	0.106 (2)	0.103 (2)	0.0102 (16)	0.0181 (17)	−0.0206 (19)
C23	0.091 (2)	0.0790 (18)	0.077 (2)	0.0086 (15)	0.0274 (17)	−0.0072 (15)
C24	0.091 (2)	0.0877 (18)	0.0656 (18)	−0.0050 (15)	0.0055 (16)	−0.0180 (14)
C25	0.0623 (17)	0.0840 (17)	0.0629 (16)	−0.0032 (13)	0.0050 (13)	−0.0131 (13)

Geometric parameters (Å, °)

P1—C14	1.814 (3)	C11—H11A	0.9300
P1—C20	1.820 (2)	C12—C13	1.389 (3)
P1—C13	1.823 (3)	C12—H12A	0.9300
N1—C7	1.345 (3)	C14—C15	1.378 (3)
N1—C8	1.410 (3)	C14—C19	1.394 (3)
N1—H1A	0.8600	C15—C16	1.370 (4)
O1—C7	1.216 (3)	C15—H15A	0.9300
C1—C2	1.378 (4)	C16—C17	1.374 (5)
C1—C6	1.388 (4)	C16—H16A	0.9300
C1—C7	1.492 (4)	C17—C18	1.357 (5)
C2—C3	1.383 (4)	C17—H17A	0.9300
C2—H2A	0.9300	C18—C19	1.366 (4)
C3—C4	1.364 (5)	C18—H18A	0.9300
C3—H3A	0.9300	C19—H19A	0.9300
C4—C5	1.356 (5)	C20—C25	1.378 (3)
C4—H4A	0.9300	C20—C21	1.384 (4)
C5—C6	1.386 (5)	C21—C22	1.377 (4)
C5—H5A	0.9300	C21—H21A	0.9300
C6—H6A	0.9300	C22—C23	1.358 (4)
C8—C9	1.377 (3)	C22—H22A	0.9300
C8—C13	1.402 (3)	C23—C24	1.361 (4)
C9—C10	1.378 (4)	C23—H23A	0.9300
C9—H9A	0.9300	C24—C25	1.377 (4)
C10—C11	1.372 (4)	C24—H24A	0.9300
C10—H10A	0.9300	C25—H25A	0.9300
C11—C12	1.374 (4)		
C14—P1—C20	104.20 (11)	C13—C12—H12A	119.0
C14—P1—C13	102.48 (11)	C12—C13—C8	117.5 (2)
C20—P1—C13	101.64 (11)	C12—C13—P1	123.83 (18)
C7—N1—C8	129.1 (2)	C8—C13—P1	118.60 (17)
C7—N1—H1A	115.5	C15—C14—C19	118.1 (2)
C8—N1—H1A	115.5	C15—C14—P1	118.0 (2)

C2—C1—C6	119.0 (3)	C19—C14—P1	123.95 (19)
C2—C1—C7	123.6 (3)	C16—C15—C14	121.1 (3)
C6—C1—C7	117.5 (3)	C16—C15—H15A	119.5
C1—C2—C3	120.9 (3)	C14—C15—H15A	119.5
C1—C2—H2A	119.6	C15—C16—C17	120.0 (3)
C3—C2—H2A	119.6	C15—C16—H16A	120.0
C4—C3—C2	119.5 (4)	C17—C16—H16A	120.0
C4—C3—H3A	120.3	C18—C17—C16	119.5 (3)
C2—C3—H3A	120.3	C18—C17—H17A	120.3
C5—C4—C3	120.5 (3)	C16—C17—H17A	120.3
C5—C4—H4A	119.8	C17—C18—C19	121.2 (3)
C3—C4—H4A	119.8	C17—C18—H18A	119.4
C4—C5—C6	121.0 (4)	C19—C18—H18A	119.4
C4—C5—H5A	119.5	C18—C19—C14	120.1 (3)
C6—C5—H5A	119.5	C18—C19—H19A	120.0
C5—C6—C1	119.2 (3)	C14—C19—H19A	120.0
C5—C6—H6A	120.4	C25—C20—C21	117.9 (2)
C1—C6—H6A	120.4	C25—C20—P1	124.89 (19)
O1—C7—N1	123.0 (2)	C21—C20—P1	117.12 (19)
O1—C7—C1	122.0 (2)	C22—C21—C20	120.8 (3)
N1—C7—C1	115.0 (2)	C22—C21—H21A	119.6
C9—C8—C13	120.8 (2)	C20—C21—H21A	119.6
C9—C8—N1	122.1 (2)	C23—C22—C21	120.4 (3)
C13—C8—N1	117.1 (2)	C23—C22—H22A	119.8
C8—C9—C10	119.6 (2)	C21—C22—H22A	119.8
C8—C9—H9A	120.2	C22—C23—C24	119.6 (3)
C10—C9—H9A	120.2	C22—C23—H23A	120.2
C11—C10—C9	121.0 (2)	C24—C23—H23A	120.2
C11—C10—H10A	119.5	C23—C24—C25	120.7 (3)
C9—C10—H10A	119.5	C23—C24—H24A	119.7
C10—C11—C12	119.1 (2)	C25—C24—H24A	119.7
C10—C11—H11A	120.4	C24—C25—C20	120.6 (3)
C12—C11—H11A	120.4	C24—C25—H25A	119.7
C11—C12—C13	121.9 (2)	C20—C25—H25A	119.7
C11—C12—H12A	119.0		
C6—C1—C2—C3	0.5 (4)	C20—P1—C13—C12	104.1 (2)
C7—C1—C2—C3	−178.5 (2)	C14—P1—C13—C8	174.36 (17)
C1—C2—C3—C4	0.5 (5)	C20—P1—C13—C8	−78.05 (19)
C2—C3—C4—C5	−1.1 (5)	C20—P1—C14—C15	165.6 (2)
C3—C4—C5—C6	0.7 (6)	C13—P1—C14—C15	−88.8 (2)
C4—C5—C6—C1	0.3 (5)	C20—P1—C14—C19	−13.2 (2)
C2—C1—C6—C5	−0.9 (4)	C13—P1—C14—C19	92.4 (2)
C7—C1—C6—C5	178.2 (3)	C19—C14—C15—C16	−1.0 (4)
C8—N1—C7—O1	−0.8 (4)	P1—C14—C15—C16	−179.9 (2)
C8—N1—C7—C1	178.7 (2)	C14—C15—C16—C17	2.3 (5)
C2—C1—C7—O1	−151.3 (3)	C15—C16—C17—C18	−2.6 (6)
C6—C1—C7—O1	29.7 (4)	C16—C17—C18—C19	1.7 (6)
C2—C1—C7—N1	29.2 (4)	C17—C18—C19—C14	−0.5 (5)
C6—C1—C7—N1	−149.8 (2)	C15—C14—C19—C18	0.2 (4)

C7—N1—C8—C9	−26.4 (4)	P1—C14—C19—C18	179.0 (2)
C7—N1—C8—C13	155.3 (2)	C14—P1—C20—C25	93.4 (2)
C13—C8—C9—C10	1.7 (4)	C13—P1—C20—C25	−12.9 (2)
N1—C8—C9—C10	−176.4 (2)	C14—P1—C20—C21	−89.6 (2)
C8—C9—C10—C11	0.1 (4)	C13—P1—C20—C21	164.2 (2)
C9—C10—C11—C12	−1.2 (4)	C25—C20—C21—C22	−0.6 (4)
C10—C11—C12—C13	0.4 (4)	P1—C20—C21—C22	−177.8 (2)
C11—C12—C13—C8	1.3 (3)	C20—C21—C22—C23	0.9 (5)
C11—C12—C13—P1	179.21 (19)	C21—C22—C23—C24	−0.7 (5)
C9—C8—C13—C12	−2.4 (3)	C22—C23—C24—C25	0.2 (5)
N1—C8—C13—C12	175.86 (19)	C23—C24—C25—C20	0.1 (4)
C9—C8—C13—P1	179.58 (18)	C21—C20—C25—C24	0.1 (4)
N1—C8—C13—P1	−2.1 (3)	P1—C20—C25—C24	177.1 (2)
C14—P1—C13—C12	−3.5 (2)		

Fig. 1

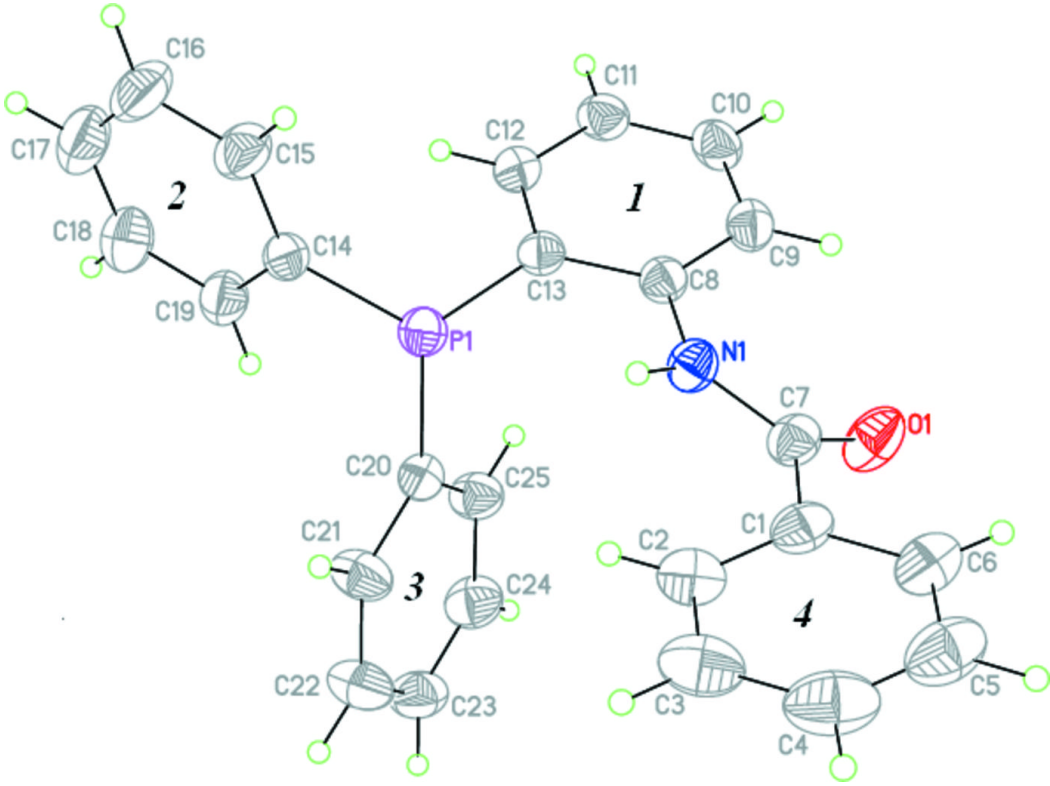
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Fig. 2