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5-[(*tert*-Butyl)(pyridin-2-yl)phosphanyl]-2-(di-*tert*-butylphosphanyl)-1-phenylpyrrole

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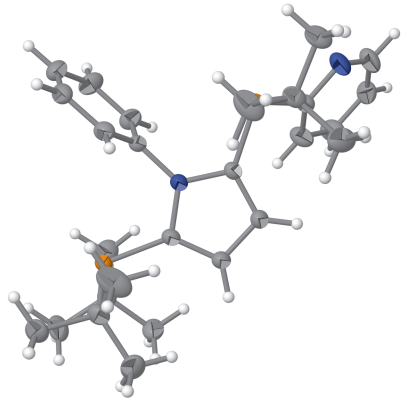
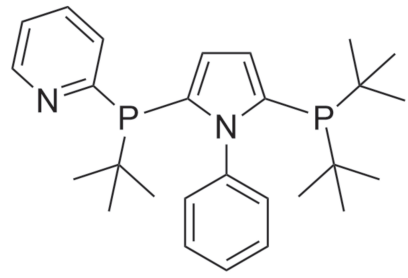
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{27}H_{38}N_2P_2$ is an asymmetric P,P,N ligand consisting of *tert*-butyl(2-pyridyl)phosphino and di-*tert*-butylphosphino groups bridged by a 1-*N*-phenylpyrrole core. The dihedral angle between the pyrrole and phenyl rings is 75.85 (6)°. In the extended structure, inversion dimers linked by pairwise C—H···π interactions are observed.

3D view



Chemical scheme



Structure description

Bidentate ligands are indispensable in homogeneous transition-metal-catalyzed reactions. By modifying the groups attached to the phosphorus atoms, by altering their electronic properties and steric hindrance, it is possible not only to change the bite angle but also to influence both the activity and the selectivity for different kinds of transformations (Clegg *et al.*, 1999; Berens *et al.*, 1996). As well as the substituents, the backbones of the ligands also have a significant influence on the outcome of the transformations; consequently, modifying them can lead to an acceleration or deceleration of the process (Kamer *et al.*, 2001; Fehrmann *et al.*, 2026).

The title compound, $C_{27}H_{38}N_2P_2$, which crystallizes in space group $P\overline{1}$ with one molecule in the asymmetric unit (Fig. 1) is an asymmetric P,P,N ligand and consists of a *tert*-butyl(2-pyridyl)phosphino (atom P1) and a di-*tert*-butylphosphino (P2) group bridged by a 1-*N*-phenylpyrrole core. The dihedral angles between the central C1–C4/N1 pyrrole moiety and the pendant C5–C9/N2 pyridyl and C22–C27 phenyl rings are 63.75 (6) and 75.85 (6)°, respectively, while the dihedral angle between the pyridyl and phenyl rings is 85.69 (6)°.

In the extended structure (Fig. 2), pairwise C—H···π interactions between C25—H25 of the phenyl ring and the π system of the pyridyl ring of an adjacent molecule are observed [C25···Cg^i = 3.6284 (13) Å, H25···Cg^i = 2.73 Å, C25—H25···Cg^i = 159°, Cg^i is the centroid of atoms C5–C9/N2, symmetry code (i) $1-x, -y, 1-z$].

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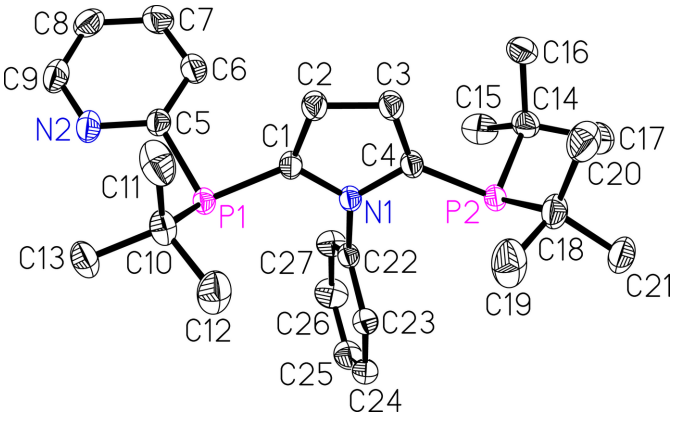

Figure 1
The molecular structure of the title compound with atom labelling and displacement ellipsoids drawn at the 50% probability level.

Synthesis and crystallization

The title compound was obtained by stirring 2-(di-*tert*-butylphosphino)-1-phenyl-1*H*-pyrrole (3.9 mmol, 1.12 g) in diethyl ether (20 ml) for 24 h at room temperature in the presence of *N*,*N*,*N*′,*N*′-tetramethylethylenediamine (3.9 mmol, 0.45 g, 0.6 mL) and *n*-butyllithium (1.6 *M* in hexanes, 2.5 ml). 2-(*tert*-butylchlorophosphanyl)pyridine (3.9 mmol, 0.783 g, 0.71 ml) was added and stirred for additional four h at room temperature before adding degassed water (3 × 10 ml) and extracting the organic phase. The removal of the solvent *in vacuo* afforded the ligand as a white powder. The title compound was crystallized from warm methanol solution (10 ml) as colourless crystals (87% yield, 1.53 g).

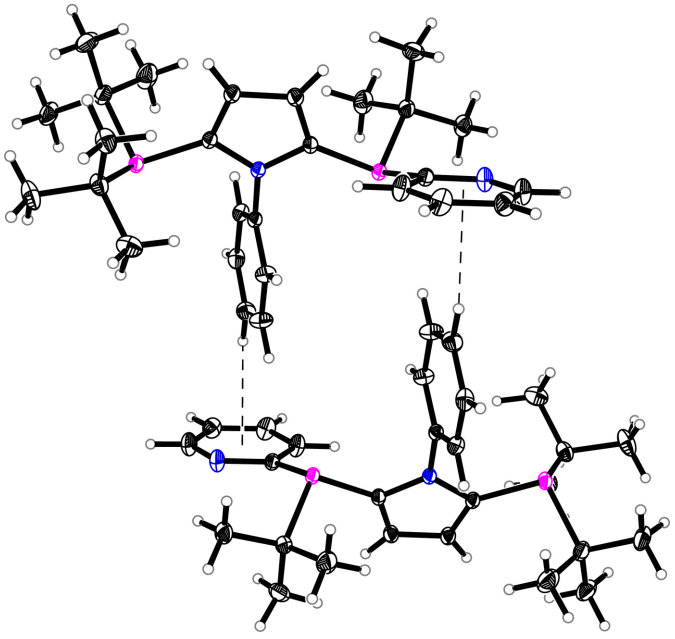

Figure 2
The dimeric structure of the title compound formed by pairwise C—H···π interactions. Displacement ellipsoids are drawn at the 30% probability level.

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{27}H_{38}N_2P_2$
M_r	452.53
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	150
a, b, c (Å)	7.5484 (2), 13.1146 (3), 14.3570 (3)
α, β, γ (°)	71.552 (2), 79.486 (2), 86.193 (2)
V (Å^3)	1325.53 (6)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.18
Crystal size (mm)	0.31 × 0.26 × 0.16
Data collection	
Diffractometer	Stoe IPDS II
Absorption correction	Multi-scan (*LANA*; Stoe & Cie, 2025)
T_{min}, T_{max}	0.95, 0.97
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	21892, 7053, 6547
R_{int}	0.025
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.682
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.037, 0.105, 1.05
No. of reflections	7053
No. of parameters	289
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.42, −0.26

Computer programs: *X-AREA* (Stoe & Cie, 2025), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *XP* in *SHELXTL* (Sheldrick, 2008) and *publCIF* (Westrip, 2010).

^{1}H NMR: (300 MHz, CD_2Cl_2) δ 8.59 (*ddd*, J = 4.8, 1.9, 1.0 Hz, 1H), 7.49 (*tt*, J = 7.7, 2.0 Hz, 1H), 7.45–7.36 (*m*, 2H), 7.32 (*ddt*, J = 7.7, 5.1, 1.3 Hz, 2H), 7.21–7.15 (*m*, 1H), 7.08 (*dddd*, J = 7.5, 4.8, 1.3, 0.6 Hz, 1H), 6.86 (*q*, 2H), 1.18 (*d*, J = 12.0 Hz, 10H), 1.11 (*dd*, J = 12.5, 2.0 Hz, 19H). ^{13}C{^{1}H}-NMR: (75 MHz, CD_2Cl_2) δ 165.3 (*s*), 149.1 (*d*, J_{PC} = 10.2 Hz), 141.7 (*d*, J_{PC} = 3 Hz), 135.0 (*d*, J_{PC} = 3 Hz), 131.1 (*m*), 130.7 (*m*), 128.1, (*d*, J_{PC} = 19 Hz), 127.7 (*d*, J_{PC} = 5.5 Hz), 127.7 (*s*), 121.1 (*s*), 118.1 (*d*, J_{PC} = 3.6 Hz), 117.9 (*d*, J_{PC} = 4.7 Hz), 32.8 (*d*, J_{PC} = 17.6 Hz), 32.4 (*d*, J_{PC} = 11.7 Hz), 30.2 (*d*, J_{PC} = 8.3 Hz), 30.1 (*d*, J_{PC} = 8.6 Hz), 28.3 (*d*, J_{PC} = 13.9 Hz). ^{31}P{^{1}H}-NMR: (122 MHz, CD_2Cl_2) δ 4.45 (*d*, J^5_{PP} = 12.2 Hz), −12.35 (*d*, J^5_{PP} = 12.2 Hz). HRMS analysis calculated for $C_{27}H_{38}N_2P_2$: 453.2583; found: 453.2593.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

Acknowledgements

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full crystallographic data

IUCrData (2026). **11**, x261132 [https://doi.org/10.1107/S2414314626011326]

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Crystal data

$C_{27}H_{38}N_2P_2$
M_r = 452.53
Triclinic, $P\overline{1}$
a = 7.5484 (2) Å
b = 13.1146 (3) Å
c = 14.3570 (3) Å
α = 71.552 (2)°
β = 79.486 (2)°
γ = 86.193 (2)°
V = 1325.53 (6) Å^3
Z = 2
$F(000)$ = 488
D_x = 1.134 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 35896 reflections
θ = 1.5–29.7°
μ = 0.18 mm^{-1}
T = 150 K
Block, colourless
0.31 × 0.26 × 0.16 mm

Data collection

Stoe IPDS II diffractometer
Radiation source: microfocus
ω scans
Absorption correction: multi-scan (*LANA*; Stoe & Cie, 2025)
T_{min} = 0.95, T_{max} = 0.97
21892 measured reflections
7053 independent reflections
6547 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 29.0°, θ_{min} = 1.6°
h = −10→10
k = −17→17
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.105
S = 1.05
7053 reflections
289 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.065P)^2 + 0.2453P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.80441 (13)	0.21146 (7)	0.22220 (7)	0.02534 (18)
C2	0.94913 (14)	0.27417 (8)	0.16379 (8)	0.0296 (2)
H2	1.047794	0.251351	0.123438	0.035*
C3	0.92480 (14)	0.37736 (8)	0.17452 (8)	0.0294 (2)
H3	1.004114	0.436207	0.142222	0.035*
C4	0.76581 (13)	0.37897 (7)	0.24007 (7)	0.02521 (18)
C5	0.95132 (13)	0.00170 (8)	0.26292 (7)	0.02675 (18)
C6	1.07711 (16)	0.03685 (9)	0.30567 (10)	0.0384 (2)
H6	1.064669	0.106128	0.314058	0.046*
C7	1.22044 (16)	−0.02935 (10)	0.33595 (11)	0.0428 (3)
H7	1.306671	−0.006335	0.365492	0.051*
C8	1.23548 (16)	−0.12934 (10)	0.32235 (10)	0.0396 (2)
H8	1.332060	−0.176799	0.342061	0.048*
C9	1.10558 (17)	−0.15823 (10)	0.27915 (10)	0.0425 (3)
H9	1.116890	−0.226730	0.269104	0.051*
C10	0.71074 (16)	0.07960 (8)	0.11127 (8)	0.0319 (2)
C11	0.8746 (2)	0.11840 (11)	0.03039 (9)	0.0475 (3)
H11A	0.980302	0.075078	0.050179	0.071*
H11B	0.896516	0.194036	0.021308	0.071*
H11C	0.852361	0.111025	−0.032310	0.071*
C12	0.5498 (2)	0.15621 (11)	0.08882 (10)	0.0481 (3)
H12A	0.581628	0.228672	0.085517	0.072*
H12B	0.445928	0.130960	0.141782	0.072*
H12C	0.519388	0.157838	0.024867	0.072*
C13	0.65784 (18)	−0.03326 (9)	0.11583 (9)	0.0387 (2)
H13A	0.631243	−0.031281	0.050971	0.058*
H13B	0.550879	−0.056843	0.167022	0.058*
H13C	0.757661	−0.083610	0.132410	0.058*
C14	0.81431 (15)	0.51416 (9)	0.35734 (9)	0.0341 (2)
C15	0.80473 (18)	0.41654 (12)	0.45210 (9)	0.0456 (3)
H15A	0.834431	0.350950	0.433419	0.068*
H15B	0.682691	0.411042	0.490910	0.068*
H15C	0.890969	0.425461	0.492289	0.068*
C16	1.01121 (15)	0.52961 (10)	0.30548 (10)	0.0398 (2)
H16A	1.019515	0.590127	0.243756	0.060*
H16B	1.056346	0.464090	0.289819	0.060*
H16C	1.083775	0.544493	0.349687	0.060*
C17	0.74836 (19)	0.61433 (12)	0.38788 (12)	0.0505 (3)
H17A	0.817144	0.621562	0.437082	0.076*
H17B	0.620110	0.606976	0.416992	0.076*
H17C	0.765788	0.678294	0.329030	0.076*
C18	0.61935 (16)	0.59512 (8)	0.17323 (9)	0.0352 (2)
C19	0.5273 (3)	0.54573 (11)	0.11094 (12)	0.0567 (4)
H19A	0.495923	0.602751	0.053076	0.085*
H19B	0.417543	0.508802	0.151742	0.085*

H19C	0.609555	0.494110	0.088230	0.085*
C20	0.78762 (19)	0.65587 (10)	0.10935 (11)	0.0497 (3)
H20A	0.874535	0.605341	0.088048	0.074*
H20B	0.841887	0.690583	0.148437	0.074*
H20C	0.754322	0.710634	0.050600	0.074*
C21	0.48592 (18)	0.67560 (9)	0.20672 (11)	0.0454 (3)
H21A	0.544299	0.712522	0.242483	0.068*
H21B	0.380146	0.637106	0.250863	0.068*
H21C	0.448268	0.728487	0.148178	0.068*
C22	0.53262 (12)	0.24124 (7)	0.33952 (7)	0.02313 (17)
C23	0.36548 (13)	0.27146 (8)	0.31240 (8)	0.02822 (19)
H23	0.356784	0.313626	0.246031	0.034*
C24	0.21050 (14)	0.23975 (9)	0.38281 (9)	0.0335 (2)
H24	0.095547	0.261290	0.364818	0.040*
C25	0.22310 (15)	0.17681 (9)	0.47918 (9)	0.0377 (2)
H25	0.116981	0.155445	0.527276	0.045*
C26	0.39048 (17)	0.14515 (10)	0.50522 (8)	0.0406 (3)
H26	0.399040	0.101068	0.571020	0.049*
C27	0.54613 (14)	0.17754 (9)	0.43554 (8)	0.0323 (2)
H27	0.661068	0.156149	0.453612	0.039*
N1	0.69371 (10)	0.27646 (6)	0.26849 (5)	0.02275 (16)
N2	0.96496 (14)	−0.09621 (8)	0.25050 (8)	0.0370 (2)
P1	0.73955 (3)	0.07500 (2)	0.23985 (2)	0.02393 (7)
P2	0.64532 (3)	0.48100 (2)	0.28947 (2)	0.02566 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0283 (4)	0.0203 (4)	0.0269 (4)	−0.0006 (3)	−0.0007 (3)	−0.0089 (3)
C2	0.0302 (5)	0.0246 (4)	0.0321 (5)	−0.0026 (3)	0.0041 (4)	−0.0110 (4)
C3	0.0306 (5)	0.0222 (4)	0.0328 (5)	−0.0042 (3)	0.0033 (4)	−0.0091 (4)
C4	0.0278 (4)	0.0192 (4)	0.0275 (4)	−0.0023 (3)	−0.0012 (3)	−0.0073 (3)
C5	0.0279 (4)	0.0224 (4)	0.0289 (4)	−0.0002 (3)	−0.0020 (3)	−0.0081 (3)
C6	0.0366 (5)	0.0280 (5)	0.0555 (7)	0.0012 (4)	−0.0160 (5)	−0.0156 (5)
C7	0.0343 (6)	0.0385 (6)	0.0583 (7)	0.0007 (4)	−0.0161 (5)	−0.0142 (5)
C8	0.0308 (5)	0.0381 (6)	0.0474 (6)	0.0082 (4)	−0.0057 (4)	−0.0121 (5)
C9	0.0435 (6)	0.0332 (5)	0.0563 (7)	0.0115 (5)	−0.0124 (5)	−0.0216 (5)
C10	0.0433 (6)	0.0258 (4)	0.0291 (5)	−0.0012 (4)	−0.0085 (4)	−0.0105 (4)
C11	0.0670 (9)	0.0453 (7)	0.0306 (5)	−0.0155 (6)	0.0040 (5)	−0.0164 (5)
C12	0.0663 (9)	0.0381 (6)	0.0463 (7)	0.0135 (6)	−0.0293 (6)	−0.0138 (5)
C13	0.0493 (6)	0.0309 (5)	0.0429 (6)	−0.0034 (4)	−0.0154 (5)	−0.0167 (4)
C14	0.0305 (5)	0.0370 (5)	0.0404 (5)	−0.0041 (4)	−0.0015 (4)	−0.0215 (4)
C15	0.0424 (6)	0.0601 (8)	0.0359 (6)	−0.0044 (6)	−0.0064 (5)	−0.0164 (5)
C16	0.0300 (5)	0.0434 (6)	0.0519 (7)	−0.0063 (4)	−0.0030 (5)	−0.0242 (5)
C17	0.0427 (7)	0.0556 (8)	0.0698 (9)	−0.0026 (6)	−0.0030 (6)	−0.0458 (7)
C18	0.0397 (6)	0.0219 (4)	0.0392 (5)	0.0022 (4)	−0.0022 (4)	−0.0056 (4)
C19	0.0845 (11)	0.0376 (6)	0.0524 (8)	0.0085 (7)	−0.0349 (8)	−0.0092 (6)
C20	0.0487 (7)	0.0321 (6)	0.0490 (7)	0.0035 (5)	0.0103 (6)	0.0031 (5)

C21	0.0409 (6)	0.0255 (5)	0.0605 (8)	0.0064 (4)	0.0012 (5)	−0.0070 (5)
C22	0.0246 (4)	0.0195 (4)	0.0248 (4)	−0.0022 (3)	−0.0012 (3)	−0.0074 (3)
C23	0.0271 (4)	0.0245 (4)	0.0327 (5)	−0.0008 (3)	−0.0057 (4)	−0.0080 (4)
C24	0.0248 (4)	0.0302 (5)	0.0467 (6)	−0.0015 (4)	−0.0024 (4)	−0.0155 (4)
C25	0.0324 (5)	0.0380 (6)	0.0393 (6)	−0.0086 (4)	0.0081 (4)	−0.0137 (4)
C26	0.0408 (6)	0.0453 (6)	0.0275 (5)	−0.0085 (5)	0.0018 (4)	−0.0026 (4)
C27	0.0304 (5)	0.0347 (5)	0.0273 (5)	−0.0022 (4)	−0.0040 (4)	−0.0036 (4)
N1	0.0245 (4)	0.0188 (3)	0.0243 (4)	−0.0013 (3)	−0.0014 (3)	−0.0070 (3)
N2	0.0395 (5)	0.0287 (4)	0.0490 (5)	0.0068 (4)	−0.0125 (4)	−0.0194 (4)
P1	0.02654 (13)	0.01878 (12)	0.02614 (13)	−0.00115 (8)	−0.00266 (9)	−0.00732 (9)
P2	0.02552 (13)	0.02012 (12)	0.03106 (13)	−0.00178 (9)	0.00038 (9)	−0.01014 (9)

Geometric parameters (Å, º)

C1—C2	1.3861 (13)	C14—P2	1.8870 (11)
C1—N1	1.3885 (11)	C15—H15A	0.9800
C1—P1	1.8141 (9)	C15—H15B	0.9800
C2—C3	1.4063 (13)	C15—H15C	0.9800
C2—H2	0.9500	C16—H16A	0.9800
C3—C4	1.3869 (13)	C16—H16B	0.9800
C3—H3	0.9500	C16—H16C	0.9800
C4—N1	1.3925 (11)	C17—H17A	0.9800
C4—P2	1.8232 (10)	C17—H17B	0.9800
C5—N2	1.3460 (13)	C17—H17C	0.9800
C5—C6	1.3931 (14)	C18—C20	1.5284 (17)
C5—P1	1.8376 (10)	C18—C19	1.5348 (19)
C6—C7	1.3862 (16)	C18—C21	1.5371 (16)
C6—H6	0.9500	C18—P2	1.8877 (11)
C7—C8	1.3801 (17)	C19—H19A	0.9800
C7—H7	0.9500	C19—H19B	0.9800
C8—C9	1.3819 (18)	C19—H19C	0.9800
C8—H8	0.9500	C20—H20A	0.9800
C9—N2	1.3381 (15)	C20—H20B	0.9800
C9—H9	0.9500	C20—H20C	0.9800
C10—C11	1.5240 (17)	C21—H21A	0.9800
C10—C13	1.5369 (14)	C21—H21B	0.9800
C10—C12	1.5377 (16)	C21—H21C	0.9800
C10—P1	1.8796 (10)	C22—C23	1.3841 (13)
C11—H11A	0.9800	C22—C27	1.3856 (13)
C11—H11B	0.9800	C22—N1	1.4338 (11)
C11—H11C	0.9800	C23—C24	1.3894 (14)
C12—H12A	0.9800	C23—H23	0.9500
C12—H12B	0.9800	C24—C25	1.3854 (17)
C12—H12C	0.9800	C24—H24	0.9500
C13—H13A	0.9800	C25—C26	1.3831 (18)
C13—H13B	0.9800	C25—H25	0.9500
C13—H13C	0.9800	C26—C27	1.3892 (15)
C14—C16	1.5313 (15)	C26—H26	0.9500

C14—C17	1.5375 (16)	C27—H27	0.9500
C14—C15	1.5392 (18)		
C2—C1—N1	106.48 (8)	C14—C16—H16B	109.5
C2—C1—P1	132.82 (7)	H16A—C16—H16B	109.5
N1—C1—P1	120.61 (7)	C14—C16—H16C	109.5
C1—C2—C3	108.27 (9)	H16A—C16—H16C	109.5
C1—C2—H2	125.9	H16B—C16—H16C	109.5
C3—C2—H2	125.9	C14—C17—H17A	109.5
C4—C3—C2	108.68 (8)	C14—C17—H17B	109.5
C4—C3—H3	125.7	H17A—C17—H17B	109.5
C2—C3—H3	125.7	C14—C17—H17C	109.5
C3—C4—N1	106.07 (8)	H17A—C17—H17C	109.5
C3—C4—P2	134.46 (7)	H17B—C17—H17C	109.5
N1—C4—P2	119.46 (7)	C20—C18—C19	109.90 (12)
N2—C5—C6	121.37 (9)	C20—C18—C21	108.58 (9)
N2—C5—P1	115.66 (8)	C19—C18—C21	107.59 (11)
C6—C5—P1	122.20 (8)	C20—C18—P2	118.59 (9)
C7—C6—C5	119.93 (10)	C19—C18—P2	105.23 (8)
C7—C6—H6	120.0	C21—C18—P2	106.43 (8)
C5—C6—H6	120.0	C18—C19—H19A	109.5
C8—C7—C6	118.72 (11)	C18—C19—H19B	109.5
C8—C7—H7	120.6	H19A—C19—H19B	109.5
C6—C7—H7	120.6	C18—C19—H19C	109.5
C7—C8—C9	117.88 (11)	H19A—C19—H19C	109.5
C7—C8—H8	121.1	H19B—C19—H19C	109.5
C9—C8—H8	121.1	C18—C20—H20A	109.5
N2—C9—C8	124.41 (11)	C18—C20—H20B	109.5
N2—C9—H9	117.8	H20A—C20—H20B	109.5
C8—C9—H9	117.8	C18—C20—H20C	109.5
C11—C10—C13	110.08 (9)	H20A—C20—H20C	109.5
C11—C10—C12	110.27 (11)	H20B—C20—H20C	109.5
C13—C10—C12	108.50 (10)	C18—C21—H21A	109.5
C11—C10—P1	115.05 (8)	C18—C21—H21B	109.5
C13—C10—P1	108.03 (7)	H21A—C21—H21B	109.5
C12—C10—P1	104.61 (8)	C18—C21—H21C	109.5
C10—C11—H11A	109.5	H21A—C21—H21C	109.5
C10—C11—H11B	109.5	H21B—C21—H21C	109.5
H11A—C11—H11B	109.5	C23—C22—C27	120.48 (9)
C10—C11—H11C	109.5	C23—C22—N1	120.16 (8)
H11A—C11—H11C	109.5	C27—C22—N1	119.36 (8)
H11B—C11—H11C	109.5	C22—C23—C24	119.60 (9)
C10—C12—H12A	109.5	C22—C23—H23	120.2
C10—C12—H12B	109.5	C24—C23—H23	120.2
H12A—C12—H12B	109.5	C25—C24—C23	120.20 (10)
C10—C12—H12C	109.5	C25—C24—H24	119.9
H12A—C12—H12C	109.5	C23—C24—H24	119.9
H12B—C12—H12C	109.5	C26—C25—C24	119.87 (10)

C10—C13—H13A	109.5	C26—C25—H25	120.1
C10—C13—H13B	109.5	C24—C25—H25	120.1
H13A—C13—H13B	109.5	C25—C26—C27	120.27 (10)
C10—C13—H13C	109.5	C25—C26—H26	119.9
H13A—C13—H13C	109.5	C27—C26—H26	119.9
H13B—C13—H13C	109.5	C22—C27—C26	119.56 (10)
C16—C14—C17	109.14 (10)	C22—C27—H27	120.2
C16—C14—C15	108.28 (10)	C26—C27—H27	120.2
C17—C14—C15	108.60 (11)	C1—N1—C4	110.50 (7)
C16—C14—P2	118.29 (8)	C1—N1—C22	124.65 (7)
C17—C14—P2	108.89 (8)	C4—N1—C22	124.78 (7)
C15—C14—P2	103.18 (7)	C9—N2—C5	117.67 (10)
C14—C15—H15A	109.5	C1—P1—C5	101.12 (4)
C14—C15—H15B	109.5	C1—P1—C10	102.88 (4)
H15A—C15—H15B	109.5	C5—P1—C10	106.49 (5)
C14—C15—H15C	109.5	C4—P2—C14	101.97 (5)
H15A—C15—H15C	109.5	C4—P2—C18	102.93 (5)
H15B—C15—H15C	109.5	C14—P2—C18	111.33 (5)
C14—C16—H16A	109.5		

N1—C1—C2—C3	−0.36 (12)	P1—C5—N2—C9	−171.28 (9)
P1—C1—C2—C3	176.11 (8)	C2—C1—P1—C5	49.45 (11)
C1—C2—C3—C4	0.42 (12)	N1—C1—P1—C5	−134.50 (8)
C2—C3—C4—N1	−0.31 (12)	C2—C1—P1—C10	−60.54 (11)
C2—C3—C4—P2	−179.50 (9)	N1—C1—P1—C10	115.52 (8)
N2—C5—C6—C7	0.31 (18)	N2—C5—P1—C1	−161.39 (8)
P1—C5—C6—C7	169.84 (10)	C6—C5—P1—C1	28.52 (10)
C5—C6—C7—C8	0.3 (2)	N2—C5—P1—C10	−54.23 (9)
C6—C7—C8—C9	−0.1 (2)	C6—C5—P1—C10	135.68 (9)
C7—C8—C9—N2	−0.7 (2)	C11—C10—P1—C1	55.72 (9)
C27—C22—C23—C24	1.59 (15)	C13—C10—P1—C1	179.13 (8)
N1—C22—C23—C24	−177.89 (8)	C12—C10—P1—C1	−65.42 (9)
C22—C23—C24—C25	−1.04 (15)	C11—C10—P1—C5	−50.18 (10)
C23—C24—C25—C26	−0.24 (17)	C13—C10—P1—C5	73.23 (9)
C24—C25—C26—C27	0.97 (18)	C12—C10—P1—C5	−171.32 (8)
C23—C22—C27—C26	−0.87 (16)	C3—C4—P2—C14	−61.36 (12)
N1—C22—C27—C26	178.61 (10)	N1—C4—P2—C14	119.53 (8)
C25—C26—C27—C22	−0.42 (18)	C3—C4—P2—C18	54.12 (12)
C2—C1—N1—C4	0.17 (11)	N1—C4—P2—C18	−124.99 (8)
P1—C1—N1—C4	−176.82 (7)	C16—C14—P2—C4	44.44 (10)
C2—C1—N1—C22	−176.85 (8)	C17—C14—P2—C4	169.74 (9)
P1—C1—N1—C22	6.16 (12)	C15—C14—P2—C4	−75.03 (8)
C3—C4—N1—C1	0.09 (11)	C16—C14—P2—C18	−64.73 (10)
P2—C4—N1—C1	179.43 (7)	C17—C14—P2—C18	60.57 (10)
C3—C4—N1—C22	177.10 (8)	C15—C14—P2—C18	175.80 (7)
P2—C4—N1—C22	−3.56 (12)	C20—C18—P2—C4	−68.70 (10)
C23—C22—N1—C1	−105.95 (11)	C19—C18—P2—C4	54.68 (10)
C27—C22—N1—C1	74.57 (12)	C21—C18—P2—C4	168.68 (8)

C23—C22—N1—C4	77.45 (12)	C20—C18—P2—C14	39.85 (11)
C27—C22—N1—C4	−102.03 (11)	C19—C18—P2—C14	163.22 (9)
C8—C9—N2—C5	1.3 (2)	C21—C18—P2—C14	−82.77 (9)
C6—C5—N2—C9	−1.10 (17)		