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Bis[1,3-bis(diphenylphosphino)propane-κ^2P,P']-nickel(0)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.036
wR factor = 0.092
Data-to-parameter ratio = 17.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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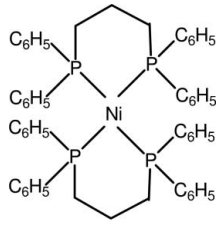
The neutral title complex, $[Ni(C_{27}H_{26}P_2)_2]$, contains a distorted tetrahedrally coordinated Ni^0 atom lying on a twofold rotation axis. The bridging propane groups of the ligands are twisted by approximately 90° with respect to each other.

Comment

As part of our ongoing studies to synthesize nickel compounds relevant to the structure and function of the microbial nickel-containing enzyme acetyl–CoA synthase, a range of new starting materials is required (Duff *et al.*, 2005; Evans, 2005). The title compound, (I), was obtained as a minor product from the attempted methylation of $[NiCl_2(dppp)]$, where dppp is 1,3-bis(diphenylphosphino)propane. Nickel(0) diphosphine (diphos) compounds of the type $[Ni(diphos)_2]$ were first prepared 45 years ago by Chatt & Hart (1960). Compound (I) has since been prepared by various methods (van Hecke & Horrocks, 1966; Giannoccaro & Vasapollo, 1983; Fisher & Alyea, 1989; Bricout *et al.*, 1995), but its structure has not been reported until now.



(I)

In (I), the Ni atom, which lies on a twofold rotation axis, displays a distorted tetrahedral coordination geometry; bond lengths to the P atoms are as expected, while the P—Ni—P angles range from 99.52 (2)° within one dppp ligand to 120.49 (3)° between the ligands (see Table 1). The ligands are arranged unsymmetrically about the Ni atom, with P—Ni—P angles between the ligands of 106.38 (3) and 115.43 (3)°. The P atoms are also distorted tetrahedral, with angles ranging from 98.58 (9) to 122.21 (6)°; the trend is for angles involving the Ni atom and the ligating phenyl C atoms to be the largest and the angles involving the bridging C atoms and the ligating phenyl C atoms to be the smallest. The P—C—C and C—C—C angles about the bridging C atoms are also distorted, being slightly larger than the ideal tetrahedral value (see Table 1). Dimensions within the phenyl rings are not unusual.

Each molecule is arranged with the bridging propane groups twisted by approximately 90° with respect to each other, the angle between the normals to the NiP_2 planes being 92.44 (2)°. When viewed along the twofold rotation axis, three

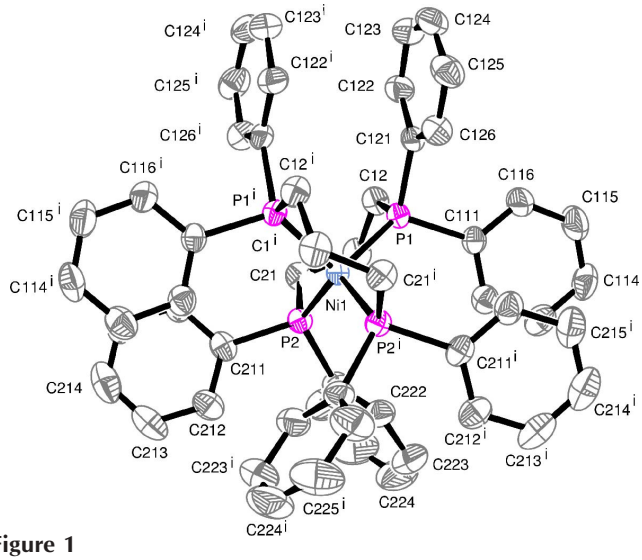


Figure 1
A view of (I), with displacement ellipsoids drawn at the 50% probability level. H atoms have been omitted for clarity. [Symmetry code: (i) $-x, y, \frac{1}{2}-z$.]

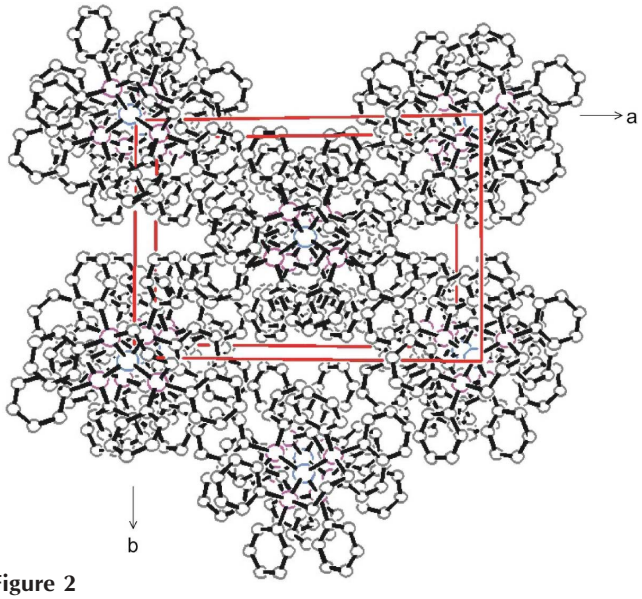


Figure 2
Packing diagram of (I), viewed along the crystallographic *c* axis. Atoms are represented by arbitrary spheres. H atoms have been omitted.

of the phenyl rings of each dppp ligand lie with their normals at approximately right angles to the crystallographic *b* axis. The normal to the fourth phenyl ring in each ligand is approximately parallel to the crystallographic *b* axis. The molecules are arranged in chains parallel to the crystallographic *c* axis, with four chains enclosing a channel parallel to the *c* axis with normal van der Waals contacts binding the molecules within and across the rows (see Fig. 2).

The structure of the related compound [Ni(dppe)$_2$], (II), where dppe is 1,2-bis(diphenylphosphino)ethane, has been reported previously (Hartung *et al.*, 1989). The distorted tetrahedral coordination about the Ni atom is similar in both molecules, with bond lengths to the Ni atom in (II) lying in the range 2.152 (3)–2.177 (3) Å. Bond angles are slightly different in the two, due to the steric effects of an ethyl rather than a propyl bridging group; in complex (II), the P—Ni—P angles within ligands are 90.8 (1) and 90.1 (1)°, while interligand P—Ni—P angles lie between 113.8 (1) and 129.3 (1)°.

Experimental

To a stirred slurry of [NiCl$_2$(dppp)] (0.20 g, 0.37 mmol) in tetrahydrofuran (13 ml) was added a solution of methyl magnesium iodide in diethyl ether (3 *M* solution, 1.6 ml, 4.8 mmol) and additional tetrahydrofuran (20 ml). After 2 d, the mixture was filtered, and the filtrate was allowed to stand for two weeks; the solvent was then removed *in vacuo*. The solid residue was washed with diethyl ether to give a mixture of a brown solid and orange crystals of (I).

Crystal data

[Ni($C_{27}H_{26}P_2$)$_2$]
M_r = 883.55
Monoclinic, $C2/c$
a = 18.303 (6) Å
b = 13.212 (2) Å
c = 20.023 (4) Å
β = 109.67 (2)°
V = 4559 (2) Å^3
Z = 4
D_x = 1.287 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 10–11°
μ = 0.60 mm^{-1}
T = 293 (2) K
Rhomb, orange
0.67 × 0.52 × 0.24 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω/θ scans
Absorption correction: ψ scan (*EMPABS*; Sheldrick *et al.*, 1977)
T_{min} = 0.823, T_{max} = 0.865
7286 measured reflections
6631 independent reflections
4569 reflections with $I > 2\sigma(I)$
R_{int} = 0.008
θ_{max} = 30°
$h = -1 \rightarrow 25$
$k = -1 \rightarrow 18$
$l = -28 \rightarrow 28$
3 standard reflections
frequency: 167 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.092
S = 1.07
6631 reflections
371 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.033P)^2 + 0.7751P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—P1	2.1752 (6)	P1—C111	1.8449 (18)
Ni1—P1^i	2.1753 (6)	P1—C12	1.8484 (19)
Ni1—P2	2.1790 (6)	P2—C21	1.8473 (19)
Ni1—P2^i	2.1790 (6)	P2—C211	1.8486 (19)
P1—C121	1.8413 (18)	P2—C221	1.8552 (19)
P1—Ni1—P1^i	106.38 (3)	C12—P1—Ni1	115.31 (7)
P1—Ni1—P2	99.52 (2)	C21—P2—C211	98.92 (9)
P1^i—Ni1—P2	115.43 (3)	C21—P2—C221	98.58 (9)
P1—Ni1—P2^i	115.43 (3)	C211—P2—C221	99.78 (9)
P1^i—Ni1—P2^i	99.51 (2)	C21—P2—Ni1	112.49 (7)
P2—Ni1—P2^i	120.49 (3)	C211—P2—Ni1	122.21 (6)
C121—P1—C111	100.36 (8)	C221—P2—Ni1	120.47 (7)
C121—P1—C12	100.74 (9)	C1—C12—P1	113.75 (14)
C111—P1—C12	98.71 (9)	C12—C1—C21	113.54 (17)
C121—P1—Ni1	118.59 (6)	C1—C21—P2	113.02 (13)
C111—P1—Ni1	119.59 (6)		
Ni1—P1—C12—C1	−46.88 (17)	C12—C1—C21—P2	−78.6 (2)
P1—C12—C1—C21	73.0 (2)	C1—C21—P2—Ni1	55.34 (16)

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

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1992); cell refinement: *CAD-4 EXPRESS*; data reduction: *CAD-4 Processing Program* (Hursthouse, 1976); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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supporting information

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$Z = 4$
$F(000) = 1856$
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Mo_ $K\alpha$ radiation, $\lambda = 0.71069$ Å
Cell parameters from 25 reflections
$\theta = 10$–11°
$\mu = 0.60$ mm^{-1}
$T = 293$ K
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0.67 × 0.52 × 0.24 mm

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$\theta_{max} = 30°$, $\theta_{min} = 1.5°$
$h = -1 \rightarrow 25$
$k = -1 \rightarrow 18$
$l = -28 \rightarrow 28$
3 standard reflections every 167 min
intensity decay: none

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.092$
$S = 1.07$
6631 reflections
371 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
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.033P)^2 + 0.7751P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.003$
$\Delta\rho_{max} = 0.38$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-3}

Special details

Experimental. Data were corrected for Lorentz polarization effects (Hursthouse, 1976), absorption by semiempirical ψ-scan methods (Sheldrick *et al.*, 1977) and negative intensities by Bayesian statistics (French & Wilson, 1978).
French, S. & Wilson, K. (1978). Acta Cryst. A34, 517–525.

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}
Ni1	0.0000	−0.00211 (2)	0.2500	0.02603 (8)
P1	0.04468 (2)	−0.10075 (3)	0.34176 (2)	0.02942 (10)
P2	−0.08743 (2)	0.07975 (3)	0.28021 (2)	0.03126 (10)
C111	0.12759 (10)	−0.05877 (14)	0.41856 (9)	0.0344 (4)
C112	0.13913 (11)	0.04289 (16)	0.43062 (10)	0.0406 (4)
H112	0.1056 (13)	0.0891 (17)	0.3983 (12)	0.057 (7)*
C113	0.19995 (13)	0.07926 (18)	0.48799 (11)	0.0502 (5)
H113	0.2042 (14)	0.155 (2)	0.4927 (13)	0.074 (8)*
C114	0.25006 (13)	0.0130 (2)	0.53318 (11)	0.0570 (6)
H114	0.2924 (13)	0.0361 (17)	0.5729 (12)	0.057 (6)*
C115	0.23919 (15)	−0.0889 (2)	0.52262 (13)	0.0682 (7)
H115	0.2733 (16)	−0.141 (2)	0.5581 (14)	0.085 (8)*
C116	0.17854 (14)	−0.12530 (18)	0.46590 (12)	0.0567 (6)
H116	0.1697 (14)	−0.1929 (19)	0.4588 (12)	0.063 (7)*
C121	0.07722 (10)	−0.22882 (13)	0.32874 (8)	0.0333 (4)
C122	0.04587 (12)	−0.31772 (16)	0.34380 (11)	0.0457 (5)
H122	0.0055 (13)	−0.3146 (17)	0.3628 (12)	0.059 (7)*
C123	0.07029 (14)	−0.41097 (17)	0.32785 (13)	0.0565 (6)
H123	0.0494 (13)	−0.4704 (19)	0.3373 (12)	0.059 (7)*
C124	0.12711 (15)	−0.41724 (18)	0.29788 (12)	0.0570 (6)
H124	0.1449 (15)	−0.481 (2)	0.2875 (13)	0.075 (8)*
C125	0.16018 (14)	−0.33040 (18)	0.28383 (11)	0.0533 (5)
H125	0.1982 (14)	−0.3318 (19)	0.2608 (13)	0.073 (8)*
C126	0.13487 (12)	−0.23706 (16)	0.29849 (11)	0.0441 (4)
H126	0.1576 (12)	−0.1790 (16)	0.2872 (10)	0.049 (6)*
C12	−0.02427 (11)	−0.13028 (16)	0.38852 (10)	0.0387 (4)
H12A	−0.0594 (11)	−0.1765 (15)	0.3599 (10)	0.039 (5)*
H12B	0.0039 (12)	−0.1644 (16)	0.4323 (11)	0.051 (6)*
C1	−0.06657 (12)	−0.03820 (17)	0.40259 (10)	0.0419 (4)
H1A	−0.0319 (11)	0.0144 (14)	0.4246 (10)	0.033 (5)*
H1B	−0.0900 (12)	−0.0558 (15)	0.4353 (10)	0.045 (6)*
C21	−0.12839 (10)	0.00308 (16)	0.33623 (10)	0.0383 (4)
H21A	−0.1655 (12)	0.0442 (16)	0.3475 (10)	0.042 (5)*
H21B	−0.1575 (12)	−0.0511 (16)	0.3064 (11)	0.045 (6)*
C211	−0.17899 (10)	0.12446 (15)	0.21406 (9)	0.0381 (4)
C212	−0.19222 (13)	0.22572 (17)	0.19513 (12)	0.0478 (5)

H212	−0.1570 (11)	0.2741 (15)	0.2186 (10)	0.041 (6)*
C213	−0.26050 (16)	0.2561 (2)	0.14274 (13)	0.0605 (6)
H213	−0.2650 (15)	0.328 (2)	0.1318 (13)	0.074 (8)*
C214	−0.31584 (15)	0.1867 (2)	0.10910 (13)	0.0659 (7)
H214	−0.3636 (17)	0.204 (2)	0.0721 (15)	0.095 (9)*
C215	−0.30412 (14)	0.0864 (2)	0.12650 (13)	0.0610 (6)
H215	−0.3406 (16)	0.034 (2)	0.1062 (15)	0.084 (9)*
C216	−0.23574 (12)	0.05534 (18)	0.17845 (11)	0.0469 (5)
H216	−0.2283 (13)	−0.0155 (17)	0.1895 (11)	0.054 (7)*
C221	−0.06057 (11)	0.19386 (14)	0.33727 (10)	0.0407 (4)
C222	0.00923 (14)	0.24073 (16)	0.34617 (13)	0.0509 (5)
H222	0.0392 (14)	0.2186 (19)	0.3225 (13)	0.069 (8)*
C223	0.03409 (19)	0.3226 (2)	0.39189 (17)	0.0753 (8)
H223	0.0810 (16)	0.349 (2)	0.3959 (14)	0.078 (9)*
C224	−0.0111 (2)	0.3577 (2)	0.42868 (17)	0.0862 (10)
H224	0.0044 (18)	0.409 (2)	0.4578 (16)	0.094 (10)*
C225	−0.0812 (2)	0.3138 (2)	0.41992 (17)	0.0876 (10)
H225	−0.1124 (18)	0.341 (2)	0.4459 (16)	0.103 (10)*
C226	−0.10644 (17)	0.2326 (2)	0.37443 (15)	0.0663 (7)
H226	−0.1560 (15)	0.199 (2)	0.3690 (13)	0.082 (9)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.02445 (14)	0.02904 (15)	0.02616 (14)	0.000	0.01059 (11)	0.000
P1	0.0278 (2)	0.0329 (2)	0.0280 (2)	0.00107 (17)	0.00993 (16)	0.00261 (17)
P2	0.0289 (2)	0.0340 (2)	0.0336 (2)	0.00280 (17)	0.01413 (17)	−0.00095 (18)
C111	0.0335 (9)	0.0417 (10)	0.0273 (8)	0.0000 (7)	0.0093 (7)	0.0011 (7)
C112	0.0436 (10)	0.0457 (11)	0.0313 (9)	−0.0015 (9)	0.0110 (8)	0.0024 (8)
C113	0.0575 (13)	0.0526 (13)	0.0406 (10)	−0.0115 (11)	0.0167 (10)	−0.0071 (10)
C114	0.0456 (12)	0.0739 (17)	0.0404 (11)	−0.0060 (11)	0.0000 (9)	−0.0150 (11)
C115	0.0611 (15)	0.0683 (17)	0.0513 (13)	0.0150 (13)	−0.0124 (11)	−0.0063 (12)
C116	0.0598 (14)	0.0455 (12)	0.0473 (12)	0.0082 (11)	−0.0051 (10)	−0.0029 (10)
C121	0.0341 (9)	0.0337 (9)	0.0281 (8)	0.0029 (7)	0.0051 (7)	0.0021 (7)
C122	0.0453 (11)	0.0382 (10)	0.0521 (11)	0.0005 (9)	0.0144 (9)	0.0064 (9)
C123	0.0609 (14)	0.0353 (11)	0.0638 (14)	−0.0009 (10)	0.0085 (12)	0.0059 (10)
C124	0.0652 (15)	0.0409 (12)	0.0541 (13)	0.0170 (11)	0.0058 (11)	−0.0035 (10)
C125	0.0560 (13)	0.0559 (14)	0.0495 (12)	0.0181 (11)	0.0196 (10)	−0.0004 (10)
C126	0.0451 (11)	0.0450 (11)	0.0440 (10)	0.0027 (9)	0.0173 (9)	0.0016 (9)
C12	0.0372 (10)	0.0452 (11)	0.0372 (9)	−0.0001 (8)	0.0172 (8)	0.0089 (8)
C1	0.0436 (11)	0.0547 (12)	0.0346 (9)	0.0010 (9)	0.0227 (8)	0.0032 (9)
C21	0.0343 (9)	0.0457 (11)	0.0414 (9)	0.0031 (9)	0.0214 (8)	0.0014 (9)
C211	0.0342 (9)	0.0468 (11)	0.0377 (9)	0.0108 (8)	0.0180 (8)	0.0013 (8)
C212	0.0477 (12)	0.0490 (12)	0.0515 (12)	0.0092 (10)	0.0231 (10)	0.0072 (10)
C213	0.0672 (16)	0.0634 (16)	0.0570 (13)	0.0298 (13)	0.0291 (12)	0.0210 (12)
C214	0.0538 (14)	0.093 (2)	0.0480 (13)	0.0289 (14)	0.0132 (11)	0.0053 (13)
C215	0.0432 (12)	0.0832 (19)	0.0508 (12)	0.0117 (13)	0.0080 (10)	−0.0121 (13)
C216	0.0392 (10)	0.0542 (13)	0.0456 (11)	0.0085 (9)	0.0121 (9)	−0.0055 (10)

C221	0.0448 (10)	0.0371 (10)	0.0412 (10)	0.0045 (8)	0.0158 (8)	−0.0046 (8)
C222	0.0527 (13)	0.0392 (11)	0.0606 (13)	−0.0006 (10)	0.0186 (11)	−0.0066 (10)
C223	0.0733 (18)	0.0480 (14)	0.095 (2)	−0.0121 (14)	0.0153 (16)	−0.0154 (14)
C224	0.117 (3)	0.0536 (17)	0.083 (2)	−0.0052 (18)	0.0271 (19)	−0.0309 (15)
C225	0.128 (3)	0.0631 (18)	0.090 (2)	0.0032 (19)	0.060 (2)	−0.0292 (16)
C226	0.0747 (17)	0.0596 (15)	0.0774 (17)	−0.0023 (13)	0.0426 (14)	−0.0234 (13)

Geometric parameters (Å, º)

Ni1—P1	2.1752 (6)	C126—H126	0.94 (2)
Ni1—P1^{i}	2.1753 (6)	C12—C1	1.519 (3)
Ni1—P2	2.1790 (6)	C12—H12A	0.93 (2)
Ni1—P2^{i}	2.1790 (6)	C12—H12B	0.97 (2)
P1—C121	1.8413 (18)	C1—C21	1.527 (3)
P1—C111	1.8449 (18)	C1—H1A	0.944 (19)
P1—C12	1.8484 (19)	C1—H1B	0.93 (2)
P2—C21	1.8473 (19)	C21—H21A	0.95 (2)
P2—C211	1.8486 (19)	C21—H21B	0.97 (2)
P2—C221	1.8552 (19)	C211—C216	1.387 (3)
C111—C112	1.369 (3)	C211—C212	1.389 (3)
C111—C116	1.395 (3)	C212—C213	1.393 (3)
C112—C113	1.389 (3)	C212—H212	0.92 (2)
C112—H112	0.95 (2)	C213—C214	1.364 (4)
C113—C114	1.366 (3)	C213—H213	0.97 (3)
C113—H113	1.00 (3)	C214—C215	1.369 (4)
C114—C115	1.368 (3)	C214—H214	0.96 (3)
C114—H114	0.95 (2)	C215—C216	1.393 (3)
C115—C116	1.380 (3)	C215—H215	0.95 (3)
C115—H115	1.03 (3)	C216—H216	0.96 (2)
C116—H116	0.91 (2)	C221—C222	1.376 (3)
C121—C122	1.384 (3)	C221—C226	1.393 (3)
C121—C126	1.386 (3)	C222—C223	1.390 (3)
C122—C123	1.384 (3)	C222—H222	0.89 (2)
C122—H122	0.94 (2)	C223—C224	1.361 (4)
C123—C124	1.367 (4)	C223—H223	0.91 (3)
C123—H123	0.92 (2)	C224—C225	1.365 (5)
C124—C125	1.370 (3)	C224—H224	0.87 (3)
C124—H124	0.95 (3)	C225—C226	1.381 (4)
C125—C126	1.383 (3)	C225—H225	0.96 (3)
C125—H125	0.95 (3)	C226—H226	0.98 (3)
P1—Ni1—P1^{i}	106.38 (3)	C1—C12—P1	113.75 (14)
P1—Ni1—P2	99.52 (2)	C1—C12—H12A	110.4 (12)
P1^{i}—Ni1—P2	115.43 (3)	P1—C12—H12A	106.0 (12)
P1—Ni1—P2^{i}	115.43 (3)	C1—C12—H12B	110.8 (12)
P1^{i}—Ni1—P2^{i}	99.51 (2)	P1—C12—H12B	108.1 (12)
P2—Ni1—P2^{i}	120.49 (3)	H12A—C12—H12B	107.5 (17)
C121—P1—C111	100.36 (8)	C12—C1—C21	113.54 (17)

C121—P1—C12	100.74 (9)	C12—C1—H1A	111.8 (11)
C111—P1—C12	98.71 (9)	C21—C1—H1A	109.2 (11)
C121—P1—Ni1	118.59 (6)	C12—C1—H1B	108.5 (13)
C111—P1—Ni1	119.59 (6)	C21—C1—H1B	108.8 (13)
C12—P1—Ni1	115.31 (7)	H1A—C1—H1B	104.7 (17)
C21—P2—C211	98.92 (9)	C1—C21—P2	113.02 (13)
C21—P2—C221	98.58 (9)	C1—C21—H21A	112.1 (12)
C211—P2—C221	99.78 (9)	P2—C21—H21A	107.3 (12)
C21—P2—Ni1	112.49 (7)	C1—C21—H21B	111.4 (12)
C211—P2—Ni1	122.21 (6)	P2—C21—H21B	106.4 (12)
C221—P2—Ni1	120.47 (7)	H21A—C21—H21B	106.2 (17)
C112—C111—C116	118.06 (18)	C216—C211—C212	117.54 (19)
C112—C111—P1	118.49 (14)	C216—C211—P2	119.96 (15)
C116—C111—P1	123.44 (16)	C212—C211—P2	122.40 (16)
C111—C112—C113	121.25 (19)	C211—C212—C213	120.8 (2)
C111—C112—H112	119.0 (13)	C211—C212—H212	120.2 (13)
C113—C112—H112	119.7 (13)	C213—C212—H212	118.9 (13)
C114—C113—C112	119.9 (2)	C214—C213—C212	120.5 (2)
C114—C113—H113	124.1 (14)	C214—C213—H213	123.5 (15)
C112—C113—H113	116.0 (14)	C212—C213—H213	116.0 (16)
C113—C114—C115	119.9 (2)	C213—C214—C215	119.9 (2)
C113—C114—H114	121.5 (14)	C213—C214—H214	123.7 (18)
C115—C114—H114	118.6 (14)	C215—C214—H214	116.4 (18)
C114—C115—C116	120.3 (2)	C214—C215—C216	120.0 (3)
C114—C115—H115	121.5 (15)	C214—C215—H215	124.4 (17)
C116—C115—H115	118.0 (15)	C216—C215—H215	115.6 (17)
C115—C116—C111	120.6 (2)	C211—C216—C215	121.3 (2)
C115—C116—H116	121.4 (15)	C211—C216—H216	120.0 (13)
C111—C116—H116	118.0 (15)	C215—C216—H216	118.8 (13)
C122—C121—C126	117.44 (18)	C222—C221—C226	117.7 (2)
C122—C121—P1	124.83 (15)	C222—C221—P2	119.18 (15)
C126—C121—P1	117.65 (14)	C226—C221—P2	123.04 (17)
C123—C122—C121	121.0 (2)	C221—C222—C223	121.3 (2)
C123—C122—H122	119.4 (14)	C221—C222—H222	119.8 (16)
C121—C122—H122	119.5 (14)	C223—C222—H222	119.0 (17)
C124—C123—C122	120.5 (2)	C224—C223—C222	119.9 (3)
C124—C123—H123	117.9 (15)	C224—C223—H223	123.1 (18)
C122—C123—H123	121.5 (15)	C222—C223—H223	117.0 (18)
C123—C124—C125	119.6 (2)	C223—C224—C225	120.1 (3)
C123—C124—H124	121.2 (16)	C223—C224—H224	120 (2)
C125—C124—H124	119.3 (16)	C225—C224—H224	120 (2)
C124—C125—C126	120.0 (2)	C224—C225—C226	120.4 (3)
C124—C125—H125	121.8 (16)	C224—C225—H225	118.4 (19)
C126—C125—H125	118.0 (16)	C226—C225—H225	121.2 (19)
C125—C126—C121	121.4 (2)	C225—C226—C221	120.6 (3)
C125—C126—H126	118.1 (13)	C225—C226—H226	121.0 (16)
C121—C126—H126	120.5 (13)	C221—C226—H226	118.3 (16)

Ni1—P1—C12—C1	−46.88 (17)	C12—C1—C21—P2	−78.6 (2)
P1—C12—C1—C21	73.0 (2)	C1—C21—P2—Ni1	55.34 (16)

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