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(η^5-Cyclopentadienyl)(2-naphthylethynyl)(triphenylphosphine-κP)nickel(II)

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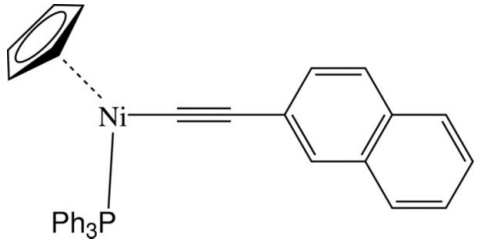
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.004 Å; R factor = 0.048; wR factor = 0.120; data-to-parameter ratio = 17.1.

The title compound, $[Ni(C_5H_5)(C_{12}H_7)(C_{18}H_{15}P)]$, does not contain strong hydrogen-bond donors or acceptors and the primary interactions are limited to those of the weak C—H$\cdots\pi$(arene) type and mainly involving the arene rings.

Related literature

For related literature, see: Butler *et al.* (1998, 2005); Gallagher *et al.* (1998, 2002); Orpen *et al.* (1994); Whittal, Humphrey & Hockless (1998); Whittal, McDonagh *et al.* (1998).



Experimental

Crystal data

$[Ni(C_5H_5)(C_{12}H_7)(C_{18}H_{15}P)]$
M_r = 537.25
Monoclinic, $P2_1/n$
a = 14.4455 (4) Å
b = 12.7392 (5) Å
c = 15.2816 (4) Å
β = 108.439 (2)°
V = 2667.80 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.81 mm^{-1}
T = 150 (1) K
0.16 × 0.15 × 0.11 mm

Data collection

Nonius KappaCCD area-detector diffractometer
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.813, T_{max} = 0.954
8684 measured reflections
5695 independent reflections
3173 reflections with $I > 2\sigma(I)$
R_{int} = 0.083

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.120
S = 0.98
5695 reflections
334 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.61 e Å^{-3}

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

Cg1, Cg2, Cg3 and Cg4 are the centroids of the rings C41–C46, C21–C26, C31–C36 and C11–C15, respectively.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C3—H3$\cdots Cg1$	0.95	2.84	3.760 (4)	164
C6—H6$\cdots Cg2^{i}$	0.95	2.74	3.549 (4)	144
C25—H25$\cdots Cg3^{ii}$	0.95	2.83	3.722 (3)	157
C23—H23$\cdots Cg4^{iii}$	0.95	3.04	3.797 (4)	138

Symmetry codes: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x, -y, -z+1$; (iii) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$.

Data collection: *KappaCCD Server Software* (Nonius, 1997); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PREP8* (Ferguson, 1998).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2154).

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supplementary materials

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(η^5-Cyclopentadienyl)(2-naphthylethynyl)(triphenylphosphine-κP)nickel(II)

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Comment

The acetylide linkage in Ni(η^5-C_5H_5)(PPh_3)-C≡C–*X* complexes allows facile electronic communication between the electron-rich Ni(η^5-C_5H_5)(PPh_3) moiety and the *X* group (*X* is alkyl or arene), thus affecting the characteristic chemistry of both *X* and the acetylide linkage (Gallagher *et al.*, 2002). However, if *X* is an electron-withdrawing group, the molecule is a donor–π-acceptor (D–π-A) system which may have nonlinear optical (NLO) properties (Whittal *et al.*, 1998*a*,b), although the phenyl derivative (*X* = C_6H_5) does not appear to be particularly effective. We have

demonstrated that polycylic hydrocarbons containing one to five aromatic rings

can act as an electron-donor endgroup in D–π-A systems in the presence of suitable acceptors, and have examined their behaviour attached to the Ni(η^5-C_5H_5)(PPh_3) donor moiety (Butler *et al.*, 2005). The spectroscopic and electrochemical evidence suggests limited communication between either end of these Ni(η^5-C_5H_5)(PPh_3)-C≡C–*X* systems, at least in the ground state, and is not sufficient to influence significant changes in the geometric data from diffraction measurements. Here, we present the title 2-naphthyl derivative, (I) (where *X* = $C_{10}H_7$).

The molecule of (I) has a half-sandwich structure and contains the σ-bonded ethynyl-2-naphthyl ligand, the η^5-C_5 ring and triphenyl phosphine bonded to the central Ni^{II} atom. A view of the molecule with the atomic numbering scheme is presented in Fig. 1 (with selected dimensions in Table 2). The principal Ni–ligand dimensions include Ni1—P1 [2.1484 (9) Å], Ni1—C1 [1.843 (4) Å] and P1—Ni1—C1 [89.04 (9)°], and these are similar to data in related derivatives (Gallagher *et al.*, 1998, 2002; Butler *et al.*, 1998, 2005). The acetylide C≡C and C*sp*—C_{ar} bond lengths are 1.211 (4) and 1.433 (5) Å, respectively. The former is slightly longer than the expected value of 1.18 (1) Å for C≡C (Orpen *et al.*, 1994), while the latter is as expected. The bond angles of the Ni—C≡C—C chain deviate slightly from linearity, with Ni—C≡C = 176.8 (3)° and C≡C—C = 173.0 (3)°.

The η^5-C_5H_5 ring is orthogonal to the P1/Ni1/C1 plane [88.70 (12)°] and to the naphthyl ring [73.83 (10)°]. The naphthyl ring is twisted by 24.23 (9)° from the P1/Ni1/C1 plane.

The closest intramolecular contact to Ni1 involves H42, with H42···Ni1 = 3.11 Å and C42—H42···Ni1 = 113° [C42 is the closest PPh_3 *ortho*-C atom to Ni1, at 3.586 (3) Å]. Although the three Ni1—P—C angles vary, at 111.85 (10), 114.48 (10) and 118.63 (10)°, there is little asymmetry in the PPh_3 ligand, with all six P—C—C angles in the range 119.1 (2)–122.6 (3)° and three P—C_{ipso}···C_{para} angles of 177.20 (18), 177.42 (16) and 178.25 (18)°.

In the absence of strong hydrogen-bond donors or acceptors, C—H···π(arene) interactions involving the phosphine arene rings arise, with C···*Cg* in the range 3.549 (4)–3.797 (4) Å and with C—H···*Cg* angles in the range 138–164° (details in Table 2), where *Cg* is an aromatic ring centroid (Fig. 2).

Experimental

Compound (I) was prepared according to literature methods (Butler *et al.*, 2005) and is compound 1 d in the aforementioned paper.

Refinement

H atoms were treated as riding, with C—H distances of 0.95 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

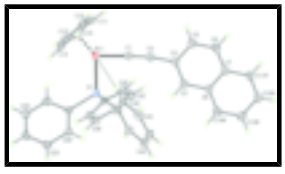

Fig. 1. A view of (I), with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. The dashed line indicates the intramolecular H42···Ni1 contact.

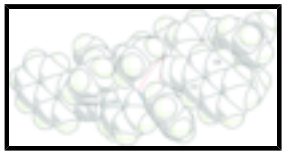

Fig. 2. A view of the weak interactions in the crystal structure of (I), with atoms shown as their van der Waals spheres. Three of the C—H···π(arene) interactions have labels.

(η^5-Cyclopentadienyl)(2-naphthylethynyl)(triphenylphosphine-κ*P*)nickel(II)

Crystal data

$[Ni(C_5H_5)(C_{12}H_7)(C_{18}H_{15}P)]$	$F_{000} = 1120$
$M_r = 537.25$	? #Insert any comments here.
Monoclinic, $P2_1/n$	$D_x = 1.338$ Mg m^{-3}
Hall symbol: -p 2yn	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 14.4455$ (4) Å	Cell parameters from 17521 reflections
$b = 12.7392$ (5) Å	$\theta = 2.6$–27.5º
$c = 15.2816$ (4) Å	$\mu = 0.81$ mm^{-1}
$\beta = 108.439$ (2)º	$T = 150$ (1) K
$V = 2667.80$ (15) Å^3	Block, green
$Z = 4$	0.16 × 0.15 × 0.11 mm

Data collection

Nonius KappaCCD area-detector diffractometer	5695 independent reflections
Radiation source: fine-focus sealed X-ray tube	3173 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.083$
$T = 150$(1) K	$\theta_{max} = 27.5$º
φ and ω scans with κ offsets	$\theta_{min} = 2.8$º
Absorption correction: multi-scan	$h = -18 \rightarrow 15$

(SORTAV; Blessing, 1995)

T_{min} = 0.813, T_{max} = 0.954

8684 measured reflections

k = −16→16

l = −19→19

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.048

$wR(F^2)$ = 0.120

S = 0.98

5695 reflections

334 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0504P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max}$ = 0.54 e Å^{-3}

$\Delta\rho_{min}$ = −0.61 e Å^{-3}

Extinction correction: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ni1	0.07764 (3)	0.09838 (3)	0.27091 (3)	0.02909 (14)
P1	0.18440 (6)	0.08760 (7)	0.40539 (5)	0.0265 (2)
C1	0.1713 (2)	0.0554 (3)	0.2201 (2)	0.0309 (8)
C2	0.2363 (2)	0.0278 (2)	0.1910 (2)	0.0313 (8)
C3	0.4134 (2)	0.0207 (3)	0.2268 (2)	0.0324 (8)
C4	0.3212 (2)	−0.0016 (2)	0.1674 (2)	0.0313 (8)
C5	0.3134 (2)	−0.0539 (3)	0.0825 (2)	0.0339 (8)
C6	0.3948 (2)	−0.0804 (3)	0.0611 (2)	0.0349 (8)
C7	0.4892 (2)	−0.0577 (3)	0.1204 (2)	0.0307 (8)
C8	0.4987 (2)	−0.0065 (2)	0.2054 (2)	0.0292 (8)
C11A	0.5747 (2)	−0.0834 (3)	0.0985 (2)	0.0362 (8)
C12A	0.6643 (3)	−0.0598 (3)	0.1573 (2)	0.0403 (9)
C13A	0.6735 (3)	−0.0100 (3)	0.2418 (2)	0.0421 (9)
C14A	0.5928 (2)	0.0161 (3)	0.2657 (2)	0.0371 (9)
C11	−0.0315 (2)	0.1281 (3)	0.1477 (2)	0.0460 (10)
C12	−0.0613 (2)	0.0393 (3)	0.1885 (2)	0.0430 (9)
C13	−0.0665 (2)	0.0694 (3)	0.2737 (2)	0.0415 (9)
C14	−0.0426 (2)	0.1787 (3)	0.2848 (2)	0.0412 (9)
C15	−0.0263 (2)	0.2162 (3)	0.2053 (3)	0.0478 (10)
C21	0.1570 (2)	0.1480 (2)	0.5034 (2)	0.0276 (7)
C22	0.2256 (2)	0.2058 (3)	0.5702 (2)	0.0327 (8)
C23	0.2028 (2)	0.2488 (3)	0.6449 (2)	0.0359 (8)
C24	0.1112 (2)	0.2351 (3)	0.6528 (2)	0.0359 (8)
C25	0.0422 (2)	0.1784 (3)	0.5873 (2)	0.0384 (9)
C26	0.0648 (2)	0.1347 (3)	0.5127 (2)	0.0363 (8)
C31	0.2103 (2)	−0.0496 (2)	0.4429 (2)	0.0276 (7)
C32	0.2333 (2)	−0.1217 (3)	0.3845 (2)	0.0388 (9)

C33	0.2494 (3)	−0.2259 (3)	0.4093 (2)	0.0428 (9)
C34	0.2427 (2)	−0.2602 (3)	0.4926 (2)	0.0375 (9)
C35	0.2215 (2)	−0.1900 (3)	0.5520 (2)	0.0384 (9)
C36	0.2052 (2)	−0.0857 (3)	0.5267 (2)	0.0346 (8)
C41	0.3034 (2)	0.1433 (2)	0.4134 (2)	0.0270 (7)
C42	0.3077 (2)	0.2302 (3)	0.3603 (2)	0.0330 (8)
C43	0.3962 (2)	0.2780 (3)	0.3678 (2)	0.0406 (9)
C44	0.4815 (2)	0.2370 (3)	0.4286 (2)	0.0408 (9)
C45	0.4781 (2)	0.1507 (3)	0.4819 (2)	0.0384 (9)
C46	0.3893 (2)	0.1032 (3)	0.4742 (2)	0.0319 (8)
H3	0.4195	0.0552	0.2835	0.039*
H5	0.2509	−0.0701	0.0407	0.041*
H6	0.3878	−0.1152	0.0044	0.042*
H11A	0.5692	−0.1176	0.0419	0.043*
H12A	0.7209	−0.0770	0.1415	0.048*
H13A	0.7366	0.0058	0.2827	0.051*
H14A	0.6002	0.0495	0.3231	0.045*
H11	−0.0175	0.1283	0.0910	0.055*
H12	−0.0751	−0.0287	0.1619	0.052*
H13	−0.0830	0.0257	0.3169	0.050*
H14	−0.0385	0.2192	0.3381	0.049*
H15	−0.0142	0.2869	0.1924	0.057*
H22	0.2888	0.2162	0.5650	0.039*
H23	0.2507	0.2876	0.6904	0.043*
H24	0.0958	0.2648	0.7035	0.043*
H25	−0.0210	0.1689	0.5927	0.046*
H26	0.0167	0.0955	0.4677	0.044*
H32	0.2379	−0.0989	0.3269	0.047*
H33	0.2653	−0.2741	0.3688	0.051*
H34	0.2527	−0.3323	0.5090	0.045*
H35	0.2180	−0.2131	0.6101	0.046*
H36	0.1902	−0.0377	0.5678	0.042*
H42	0.2493	0.2574	0.3182	0.040*
H43	0.3985	0.3382	0.3318	0.049*
H44	0.5425	0.2686	0.4335	0.049*
H45	0.5366	0.1235	0.5239	0.046*
H46	0.3872	0.0433	0.5106	0.038*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0241 (3)	0.0308 (3)	0.0317 (2)	0.00182 (19)	0.00784 (18)	−0.00069 (19)
P1	0.0234 (5)	0.0257 (5)	0.0306 (4)	0.0002 (4)	0.0086 (4)	−0.0009 (4)
C1	0.032 (2)	0.0265 (19)	0.0322 (17)	−0.0016 (15)	0.0065 (16)	0.0011 (15)
C2	0.034 (2)	0.0252 (19)	0.0358 (18)	−0.0035 (16)	0.0128 (16)	−0.0022 (15)
C3	0.036 (2)	0.0290 (19)	0.0361 (18)	−0.0009 (16)	0.0173 (16)	−0.0010 (15)
C4	0.038 (2)	0.0245 (19)	0.0358 (18)	−0.0002 (16)	0.0175 (17)	0.0039 (15)
C5	0.033 (2)	0.032 (2)	0.0362 (18)	−0.0044 (16)	0.0108 (16)	−0.0012 (15)

C6	0.046 (2)	0.027 (2)	0.0365 (18)	−0.0049 (16)	0.0195 (17)	−0.0055 (15)
C7	0.035 (2)	0.0245 (18)	0.0360 (18)	−0.0004 (15)	0.0159 (16)	0.0037 (15)
C8	0.033 (2)	0.0225 (18)	0.0340 (18)	0.0025 (15)	0.0133 (16)	0.0049 (14)
C11A	0.037 (2)	0.038 (2)	0.0390 (18)	0.0019 (17)	0.0201 (17)	0.0023 (17)
C12A	0.040 (2)	0.040 (2)	0.047 (2)	0.0039 (17)	0.0234 (19)	0.0039 (17)
C13A	0.032 (2)	0.050 (2)	0.044 (2)	−0.0004 (18)	0.0104 (17)	0.0050 (18)
C14A	0.037 (2)	0.039 (2)	0.0338 (18)	0.0021 (17)	0.0099 (17)	0.0001 (16)
C11	0.023 (2)	0.077 (3)	0.0326 (19)	0.0067 (19)	0.0015 (16)	0.006 (2)
C12	0.025 (2)	0.052 (3)	0.048 (2)	−0.0013 (18)	0.0047 (17)	−0.010 (2)
C13	0.0239 (19)	0.053 (3)	0.048 (2)	0.0009 (17)	0.0112 (16)	0.0022 (19)
C14	0.0228 (19)	0.048 (2)	0.049 (2)	0.0098 (17)	0.0070 (16)	−0.0032 (19)
C15	0.037 (2)	0.044 (2)	0.057 (2)	0.0111 (19)	0.0085 (19)	0.012 (2)
C21	0.0261 (18)	0.0245 (18)	0.0317 (17)	0.0017 (14)	0.0084 (14)	−0.0014 (14)
C22	0.0244 (18)	0.035 (2)	0.0370 (18)	0.0006 (15)	0.0072 (15)	−0.0007 (16)
C23	0.037 (2)	0.033 (2)	0.0333 (18)	−0.0006 (16)	0.0051 (16)	−0.0065 (16)
C24	0.042 (2)	0.034 (2)	0.0343 (18)	0.0070 (17)	0.0156 (17)	−0.0035 (16)
C25	0.034 (2)	0.041 (2)	0.042 (2)	−0.0020 (17)	0.0154 (17)	−0.0062 (17)
C26	0.033 (2)	0.036 (2)	0.0381 (19)	−0.0050 (16)	0.0088 (16)	−0.0063 (16)
C31	0.0206 (17)	0.0260 (18)	0.0346 (17)	0.0001 (14)	0.0065 (14)	−0.0025 (15)
C32	0.049 (2)	0.033 (2)	0.0388 (19)	0.0055 (17)	0.0202 (17)	0.0009 (16)
C33	0.057 (2)	0.032 (2)	0.045 (2)	0.0059 (18)	0.0220 (19)	−0.0022 (17)
C34	0.035 (2)	0.027 (2)	0.047 (2)	−0.0010 (16)	0.0076 (17)	0.0030 (17)
C35	0.044 (2)	0.036 (2)	0.0373 (19)	−0.0028 (17)	0.0148 (17)	0.0013 (17)
C36	0.037 (2)	0.034 (2)	0.0335 (18)	0.0012 (16)	0.0124 (15)	−0.0006 (16)
C41	0.0235 (18)	0.0245 (18)	0.0334 (17)	0.0002 (14)	0.0095 (15)	−0.0055 (15)
C42	0.029 (2)	0.0294 (19)	0.0387 (19)	0.0000 (15)	0.0083 (15)	−0.0019 (16)
C43	0.040 (2)	0.031 (2)	0.055 (2)	−0.0044 (17)	0.0203 (19)	0.0004 (17)
C44	0.028 (2)	0.036 (2)	0.060 (2)	−0.0044 (17)	0.0171 (18)	−0.0079 (19)
C45	0.026 (2)	0.036 (2)	0.050 (2)	0.0030 (16)	0.0084 (16)	−0.0024 (18)
C46	0.0298 (19)	0.0293 (19)	0.0360 (17)	0.0000 (16)	0.0093 (15)	0.0015 (15)

Geometric parameters (Å, °)

Ni1—P1	2.1484 (9)	C33—C34	1.378 (5)
Ni1—C1	1.843 (4)	C34—C35	1.376 (5)
Ni1—C11	2.073 (3)	C35—C36	1.383 (5)
Ni1—C12	2.141 (3)	C41—C42	1.386 (4)
Ni1—C13	2.129 (3)	C41—C46	1.391 (4)
Ni1—C14	2.084 (3)	C42—C43	1.388 (4)
Ni1—C15	2.136 (3)	C43—C44	1.389 (5)
P1—C21	1.835 (3)	C44—C45	1.378 (5)
P1—C31	1.841 (3)	C45—C46	1.390 (4)
P1—C41	1.828 (3)	C3—H3	0.9500
C1—C2	1.211 (4)	C5—H5	0.9500
C2—C4	1.433 (5)	C6—H6	0.9500
C3—C4	1.384 (4)	C11A—H11A	0.9500
C3—C8	1.414 (4)	C12A—H12A	0.9500
C4—C5	1.431 (4)	C13A—H13A	0.9500
C5—C6	1.359 (4)	C14A—H14A	0.9500

C6—C7	1.408 (4)	C11—H11	0.9500
C7—C11A	1.416 (4)	C12—H12	0.9500
C7—C8	1.422 (4)	C13—H13	0.9500
C8—C14A	1.410 (4)	C14—H14	0.9500
C11A—C12A	1.355 (4)	C15—H15	0.9500
C12A—C13A	1.406 (5)	C22—H22	0.9500
C13A—C14A	1.369 (5)	C23—H23	0.9500
C11—C15	1.414 (5)	C24—H24	0.9500
C11—C12	1.422 (5)	C25—H25	0.9500
C12—C13	1.382 (5)	C26—H26	0.9500
C13—C14	1.431 (5)	C32—H32	0.9500
C14—C15	1.393 (5)	C33—H33	0.9500
C21—C22	1.387 (4)	C34—H34	0.9500
C21—C26	1.393 (4)	C35—H35	0.9500
C22—C23	1.397 (4)	C36—H36	0.9500
C23—C24	1.378 (4)	C42—H42	0.9500
C24—C25	1.373 (4)	C43—H43	0.9500
C25—C26	1.397 (5)	C44—H44	0.9500
C31—C36	1.385 (4)	C45—H45	0.9500
C31—C32	1.392 (4)	C46—H46	0.9500
C32—C33	1.379 (5)		
C1—Ni1—C11	96.95 (14)	C14—C15—C11	106.3 (3)
C1—Ni1—C14	159.31 (14)	C14—C15—Ni1	68.71 (19)
C11—Ni1—C14	65.39 (14)	C11—C15—Ni1	67.98 (19)
C1—Ni1—C13	144.11 (14)	C22—C21—C26	118.3 (3)
C11—Ni1—C13	65.26 (14)	C22—C21—P1	122.3 (2)
C14—Ni1—C13	39.69 (13)	C26—C21—P1	119.5 (2)
C1—Ni1—C15	120.81 (14)	C21—C22—C23	120.7 (3)
C11—Ni1—C15	39.21 (14)	C24—C23—C22	120.2 (3)
C14—Ni1—C15	38.54 (13)	C25—C24—C23	119.9 (3)
C13—Ni1—C15	65.41 (14)	C24—C25—C26	120.1 (3)
C1—Ni1—C12	108.92 (14)	C21—C26—C25	120.8 (3)
C11—Ni1—C12	39.42 (14)	C36—C31—C32	117.8 (3)
C14—Ni1—C12	64.91 (14)	C36—C31—P1	122.6 (2)
C13—Ni1—C12	37.78 (13)	C32—C31—P1	119.6 (2)
C15—Ni1—C12	65.28 (15)	C33—C32—C31	120.9 (3)
C11—Ni1—P1	171.96 (12)	C34—C33—C32	120.2 (3)
C14—Ni1—P1	107.64 (10)	C35—C34—C33	119.9 (3)
C13—Ni1—P1	112.38 (10)	C34—C35—C36	119.6 (3)
C15—Ni1—P1	132.79 (11)	C35—C36—C31	121.6 (3)
C12—Ni1—P1	142.77 (11)	C42—C41—C46	119.3 (3)
C41—P1—C21	102.95 (14)	C42—C41—P1	119.1 (2)
C41—P1—C31	104.70 (14)	C46—C41—P1	121.6 (2)
C21—P1—C31	102.64 (14)	C41—C42—C43	120.9 (3)
Ni1—P1—C21	118.63 (10)	C42—C43—C44	119.3 (3)
Ni1—P1—C31	111.85 (10)	C45—C44—C43	120.4 (3)
Ni1—P1—C41	114.48 (10)	C44—C45—C46	120.1 (3)
P1—Ni1—C1	89.04 (9)	C45—C46—C41	120.1 (3)
Ni1—C1—C2	176.8 (3)	C4—C3—H3	119.1

C1—C2—C4	173.0 (3)	C8—C3—H3	119.1
C4—C3—C8	121.7 (3)	C6—C5—H5	119.7
C3—C4—C5	118.3 (3)	C4—C5—H5	119.7
C3—C4—C2	120.2 (3)	C5—C6—H6	119.0
C5—C4—C2	121.5 (3)	C7—C6—H6	119.0
C6—C5—C4	120.6 (3)	C12A—C11A—H11A	119.6
C5—C6—C7	122.0 (3)	C7—C11A—H11A	119.6
C6—C7—C11A	122.7 (3)	C11A—C12A—H12A	119.9
C6—C7—C8	118.4 (3)	C13A—C12A—H12A	119.9
C11A—C7—C8	118.9 (3)	C14A—C13A—H13A	119.6
C14A—C8—C3	122.0 (3)	C12A—C13A—H13A	119.6
C14A—C8—C7	119.0 (3)	C13A—C14A—H14A	119.9
C3—C8—C7	119.0 (3)	C8—C14A—H14A	119.9
C12A—C11A—C7	120.9 (3)	C15—C11—H11	125.6
C11A—C12A—C13A	120.2 (3)	C12—C11—H11	125.6
C14A—C13A—C12A	120.8 (3)	Ni1—C11—H11	120.5
C13A—C14A—C8	120.2 (3)	C13—C12—H12	126.1
C15—C11—C12	108.8 (3)	C11—C12—H12	126.1
C15—C11—Ni1	72.80 (19)	Ni1—C12—H12	127.1
C12—C11—Ni1	72.86 (19)	C12—C13—H13	126.3
C13—C12—C11	107.8 (3)	C14—C13—H13	126.3
C13—C12—Ni1	70.64 (19)	Ni1—C13—H13	125.2
C11—C12—Ni1	67.72 (19)	C15—C14—H14	125.3
C12—C13—C14	107.4 (3)	C13—C14—H14	125.3
C12—C13—Ni1	71.6 (2)	Ni1—C14—H14	121.7
C14—C13—Ni1	68.47 (19)	C14—C15—H15	126.9
C15—C14—C13	109.3 (3)	C11—C15—H15	126.9
C15—C14—Ni1	72.8 (2)	Ni1—C15—H15	127.9
C13—C14—Ni1	71.84 (19)		
C1—Ni1—P1—C41	44.41 (15)	Ni1—C13—C14—C15	63.5 (2)
C14—Ni1—P1—C41	−123.13 (16)	C12—C13—C14—Ni1	−61.3 (2)
C13—Ni1—P1—C41	−165.20 (15)	C1—Ni1—C14—C15	−4.2 (5)
C15—Ni1—P1—C41	−88.62 (18)	C11—Ni1—C14—C15	−37.5 (2)
C12—Ni1—P1—C41	165.3 (2)	C13—Ni1—C14—C15	−117.8 (3)
C1—Ni1—P1—C21	166.35 (16)	C12—Ni1—C14—C15	−81.2 (2)
C14—Ni1—P1—C21	−1.19 (17)	P1—Ni1—C14—C15	138.1 (2)
C13—Ni1—P1—C21	−43.26 (17)	C1—Ni1—C14—C13	113.6 (4)
C15—Ni1—P1—C21	33.32 (19)	C11—Ni1—C14—C13	80.3 (2)
C12—Ni1—P1—C21	−72.7 (2)	C15—Ni1—C14—C13	117.8 (3)
C1—Ni1—P1—C31	−74.47 (15)	C12—Ni1—C14—C13	36.6 (2)
C14—Ni1—P1—C31	117.99 (15)	P1—Ni1—C14—C13	−104.03 (19)
C13—Ni1—P1—C31	75.91 (16)	C13—C14—C15—C11	−5.1 (4)
C15—Ni1—P1—C31	152.49 (18)	Ni1—C14—C15—C11	57.8 (2)
C12—Ni1—P1—C31	46.5 (2)	C13—C14—C15—Ni1	−62.9 (2)
C8—C3—C4—C5	0.2 (5)	C12—C11—C15—C14	6.2 (4)
C8—C3—C4—C2	−179.5 (3)	Ni1—C11—C15—C14	−58.3 (2)
C3—C4—C5—C6	−0.2 (5)	C12—C11—C15—Ni1	64.4 (2)
C2—C4—C5—C6	179.5 (3)	C1—Ni1—C15—C14	178.3 (2)
C4—C5—C6—C7	−0.2 (5)	C11—Ni1—C15—C14	118.8 (3)

C5—C6—C7—C11A	−179.1 (3)	C13—Ni1—C15—C14	38.4 (2)
C5—C6—C7—C8	0.7 (5)	C12—Ni1—C15—C14	80.1 (2)
C4—C3—C8—C14A	179.9 (3)	P1—Ni1—C15—C14	−60.0 (3)
C4—C3—C8—C7	0.3 (5)	C1—Ni1—C15—C11	59.5 (3)
C6—C7—C8—C14A	179.7 (3)	C14—Ni1—C15—C11	−118.8 (3)
C11A—C7—C8—C14A	−0.6 (5)	C13—Ni1—C15—C11	−80.4 (2)
C6—C7—C8—C3	−0.7 (5)	C12—Ni1—C15—C11	−38.6 (2)
C11A—C7—C8—C3	179.0 (3)	P1—Ni1—C15—C11	−178.84 (18)
C6—C7—C11A—C12A	179.7 (3)	C41—P1—C21—C22	−9.5 (3)
C8—C7—C11A—C12A	0.0 (5)	C31—P1—C21—C22	99.1 (3)
C7—C11A—C12A—C13A	0.5 (5)	Ni1—P1—C21—C22	−137.0 (2)
C11A—C12A—C13A—C14A	−0.4 (5)	C41—P1—C21—C26	171.5 (3)
C12A—C13A—C14A—C8	−0.2 (5)	C31—P1—C21—C26	−80.0 (3)
C3—C8—C14A—C13A	−178.9 (3)	Ni1—P1—C21—C26	43.9 (3)
C7—C8—C14A—C13A	0.7 (5)	C26—C21—C22—C23	0.4 (5)
C1—Ni1—C11—C15	−131.8 (2)	P1—C21—C22—C23	−178.7 (2)
C14—Ni1—C11—C15	36.9 (2)	C21—C22—C23—C24	−0.6 (5)
C13—Ni1—C11—C15	80.8 (2)	C22—C23—C24—C25	0.4 (5)
C12—Ni1—C11—C15	116.7 (3)	C23—C24—C25—C26	0.0 (5)
C1—Ni1—C11—C12	111.5 (2)	C22—C21—C26—C25	−0.1 (5)
C14—Ni1—C11—C12	−79.8 (2)	P1—C21—C26—C25	179.0 (3)
C13—Ni1—C11—C12	−35.9 (2)	C24—C25—C26—C21	−0.1 (5)
C15—Ni1—C11—C12	−116.7 (3)	C41—P1—C31—C36	108.2 (3)
C15—C11—C12—C13	−4.9 (4)	C21—P1—C31—C36	0.9 (3)
Ni1—C11—C12—C13	59.5 (2)	Ni1—P1—C31—C36	−127.3 (2)
C15—C11—C12—Ni1	−64.4 (2)	C41—P1—C31—C32	−73.7 (3)
C1—Ni1—C12—C13	162.9 (2)	C21—P1—C31—C32	179.1 (3)
C11—Ni1—C12—C13	−119.6 (3)	Ni1—P1—C31—C32	50.8 (3)
C14—Ni1—C12—C13	−38.5 (2)	C36—C31—C32—C33	0.7 (5)
C15—Ni1—C12—C13	−81.1 (2)	P1—C31—C32—C33	−177.6 (3)
P1—Ni1—C12—C13	47.9 (3)	C31—C32—C33—C34	0.2 (5)
C1—Ni1—C12—C11	−77.5 (2)	C32—C33—C34—C35	−1.2 (5)
C14—Ni1—C12—C11	81.1 (2)	C33—C34—C35—C36	1.3 (5)
C13—Ni1—C12—C11	119.6 (3)	C34—C35—C36—C31	−0.4 (5)
C15—Ni1—C12—C11	38.4 (2)	C32—C31—C36—C35	−0.6 (5)
P1—Ni1—C12—C11	167.50 (18)	P1—C31—C36—C35	177.6 (2)
C11—C12—C13—C14	1.7 (4)	C21—P1—C41—C42	−96.4 (3)
Ni1—C12—C13—C14	59.3 (2)	C31—P1—C41—C42	156.6 (2)
C11—C12—C13—Ni1	−57.7 (2)	Ni1—P1—C41—C42	33.7 (3)
C1—Ni1—C13—C12	−28.4 (4)	C21—P1—C41—C46	80.9 (3)
C11—Ni1—C13—C12	37.4 (2)	C31—P1—C41—C46	−26.1 (3)
C14—Ni1—C13—C12	118.1 (3)	Ni1—P1—C41—C46	−149.0 (2)
C15—Ni1—C13—C12	80.8 (2)	C46—C41—C42—C43	−0.7 (5)
P1—Ni1—C13—C12	−150.9 (2)	P1—C41—C42—C43	176.7 (3)
C1—Ni1—C13—C14	−146.5 (2)	C41—C42—C43—C44	0.9 (5)
C11—Ni1—C13—C14	−80.6 (2)	C42—C43—C44—C45	−1.0 (5)
C15—Ni1—C13—C14	−37.3 (2)	C43—C44—C45—C46	0.8 (5)
C12—Ni1—C13—C14	−118.1 (3)	C44—C45—C46—C41	−0.6 (5)
P1—Ni1—C13—C14	91.0 (2)	C42—C41—C46—C45	0.5 (5)

C12—C13—C14—C15	2.2 (4)	P1—C41—C46—C45	−176.8 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···Cg1	0.95	2.84	3.760 (4)	164
C6—H6···Cg2^{i}	0.95	2.74	3.549 (4)	144
C25—H25···Cg3^{ii}	0.95	2.83	3.722 (3)	157
C23—H23···Cg4^{iii}	0.95	3.04	3.797 (4)	138

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

Fig. 1

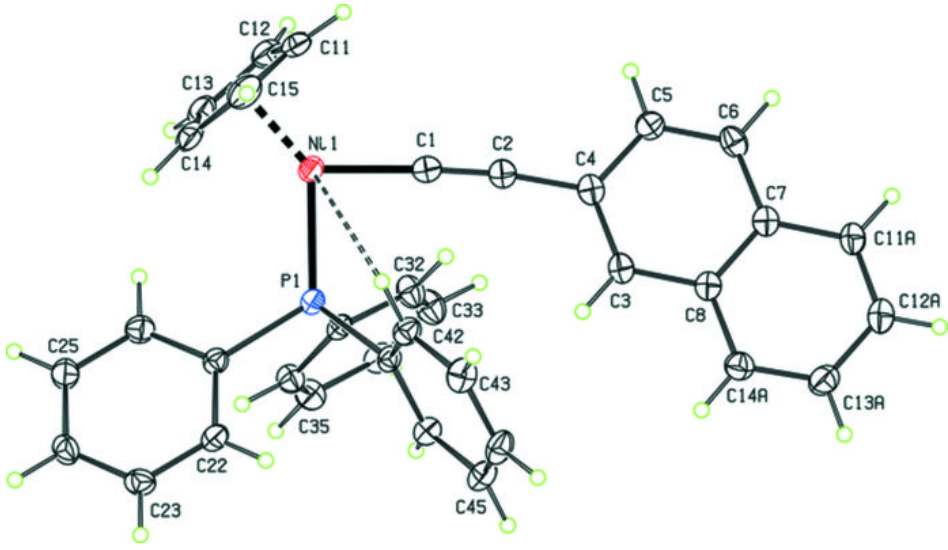
C12
C11
C13
C15
C14
NL1
C1
C2
C4
C5
C6
C7
C11A
C12A
C13A
C14A
C8
C3
P1
C32
C33
C42
C43
C35
C25
C22
C23
C45

Fig. 2