# metal-organic compounds

# Bromido{dicyclohexyl[2′-(dimethylamino)biphenyl-2-yl]phosphine-κP}-[2-(4,6-dimethylpyrimidin-2-yl)ferrocenyl-κ²C¹,N]palladium(II) dichloromethane solvate

## Xin-Qi Hao,[a] Hong-Mei Li,[b] Hui Jiang,[a] Yong-Tao Ma[a] and Mao-Ping Song[a]*

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In the title compound, $[FePdBr(C_5H_5)(C_{11}H_{10}N_2)(C_{26}H_{36}NP)]\cdot CH_2Cl_2$, the Pd atom displays a distorted square-planar coordination environment. The five-membered metallacycle adopts an envelope conformation with the coordinated cyclopentadienyl C atom 0.4222 (4) Å out of plane. The dihedral angle between the pyrimidinyl ring and substituted cyclopentadienyl ring is 21.47 (2)°. In the crystal structure, the dimeric unit is generated through the C—H⋯$\pi$ contact *via* a crystallographic inversion centre, while the C—H⋯Cl contacts in the dimeric centre link the dichlormethane molecules with the Pd complex molecules.

## Related literature

For historical background of cyclopalladated compounds, see: Cope & Sickman (1965). For the properties of cyclopalladated compounds, see: Dupont *et al.* (2005); Gong *et al.* (2007); Xu *et al.* (2007). For related structures, see: Xu *et al.* (2008, 2009).
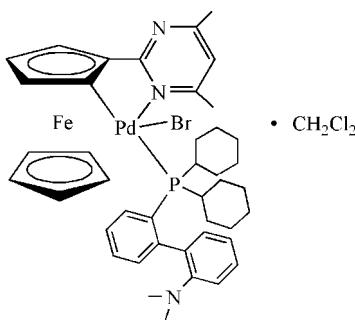


## Experimental

### Crystal data

| | |
|---|---|
| $[FePdBr(C_5H_5)(C_{11}H_{10}N_2)(C_{26}H_{36}NP)]\cdot CH_2Cl_2$ | $\beta$ = 76.590 (1)° |
| $M_r$ = 955.91 | $\gamma$ = 72.647 (1)° |
| Triclinic, $P\bar{1}$ | $V$ = 2141.9 (3) Å³ |
| $a$ = 10.2059 (9) Å | $Z$ = 2 |
| $b$ = 10.3637 (9) Å | Mo $K\alpha$ radiation |
| $c$ = 21.900 (2) Å | $\mu$ = 1.89 mm⁻¹ |
| $\alpha$ = 81.195 (1)° | $T$ = 293 K |
| | 0.37 × 0.24 × 0.21 mm |

### Data collection

| | |
|---|---|
| Bruker SMART APEX CCD area-detector diffractometer | 16458 measured reflections |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) | 7919 independent reflections |
| $T_{min}$ = 0.540, $T_{max}$ = 0.697 | 6716 reflections with $I > 2\sigma(I)$ |
| | $R_{int}$ = 0.017 |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)]$ = 0.038 | 473 parameters |
| $wR(F^2)$ = 0.099 | H-atom parameters constrained |
| $S$ = 1.08 | $\Delta\rho_{max}$ = 1.03 e Å⁻³ |
| 7919 reflections | $\Delta\rho_{min}$ = −0.69 e Å⁻³ |

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Pd1—C1 | 1.997 (3) | Pd1—P1 | 2.2654 (9) |
| Pd1—N1 | 2.192 (3) | Pd1—Br1 | 2.6585 (6) |
| N1—Pd1—P1 | 173.00 (9) | C1—Pd1—Br1 | 160.40 (10) |

**Table 2**
Hydrogen-bond geometry (Å, °).

| $D$—H⋯$A$ | $D$—H | H⋯$A$ | $D$⋯$A$ | $D$—H⋯$A$ |
|---|---|---|---|---|
| C3—H3⋯Cl2ⁱ | 0.98 | 2.78 | 3.671 (5) | 151 |
| C16—H16C⋯Cg1ⁱⁱ | 0.96 | 2.68 | 3.544 (6) | 151 |

Symmetry codes: (i) $-x + 1, -y + 1, -z$; (ii) $-x + 1, -y + 2, -z$. Cg1 is the centroid of the C6–C10 Cp ring.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

## References

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# supporting information

# Bromido{dicyclohexyl[2′-(dimethylamino)biphenyl-2-yl]phosphine-*κP*}[2-(4,6-dimethylpyrimidin-2-yl)ferrocenyl-*κ²C¹,N*]palladium(II) dichloromethane solvate

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## S1. Comment

Cyclopalladated compounds containing a Pd—C bond intramolecularly stabilized by one donor atom were first reported in the middle 1960's (Cope & Sickman, 1965). Forty years later, the chemistry of these compound has developed into one of the most fruitful fields in organometallic chemistry (Dupont *et al.*, 2005). In the palladium-catalyzed coupling reactions, palladacycles have shown enormous superiority in many respects (Gong *et al.*, 2007; Xu *et al.*, 2007).

  The Pd atom in the title complex is in a distorted square-planar environment bonded to the atoms shown in Fig. 1: the Br atom,the pyrimidinyl nitrogen atom and the carbon atom of the ferrocenyl moiety. The Pd—C1 (N1,P1,Br1) bond lengths and the P1—Pd1—N1 and C1—Pd1—Br1 bond angles (Table 1) are within comparable ranges of 162.08 (7) ° - 174.76 (7) ° and 162.27 (9) ° - 166.04 (8) ° (C—Pd—Cl), respectively (Xu *et al.*, 2009). The five-membered metallacycle (containing atoms C1/C2/C11/N1/Pd1) adopts an envelope conformation, with the C1 atom 0.4222 (4) Å out of plane. The dihedral angle between the pyrimidinyl ring and substituted cyclopentadienyl ring is 21.47 (2)°. In the crystal structure, the dimeric unit (Fig.2) is generated through the C—H···$\pi$ contacts *via* a crystallographic inversion centre, and the C—H···Cl contact (Table 2) connects a symmetry-related dichlormethane molecule with the Pd complex (Table 2).This hydrogen bonding motif is different from those of related cyclopalladated ferrocene derivatives (Xu *et al.*, 2008; Xu *et al.*, 2009), in which C—H···Cl hydrogen bonds construct the one-dimensional chain structures.

## S2. Experimental

The title compound was prepared as described in literature (Xu *et al.*, 2009), using $Li_2PdBr_4$ instead of $Li_2PdCl_4$ and recrystallized from dichloromethane-petroleum ether solution at room temperature to give the desired product as red crystals suitable for single-crystal X-ray diffraction.

## S3. Refinement

H atoms attached to C atoms of the title compound were placed in geometrically idealized positions and treated as riding with C—H distances constrained to 0.93–0.96 Å, and with $U_{iso}(H)=1.2U_{eq}(C)$ (1.5$U_{eq}$ for methyl H).
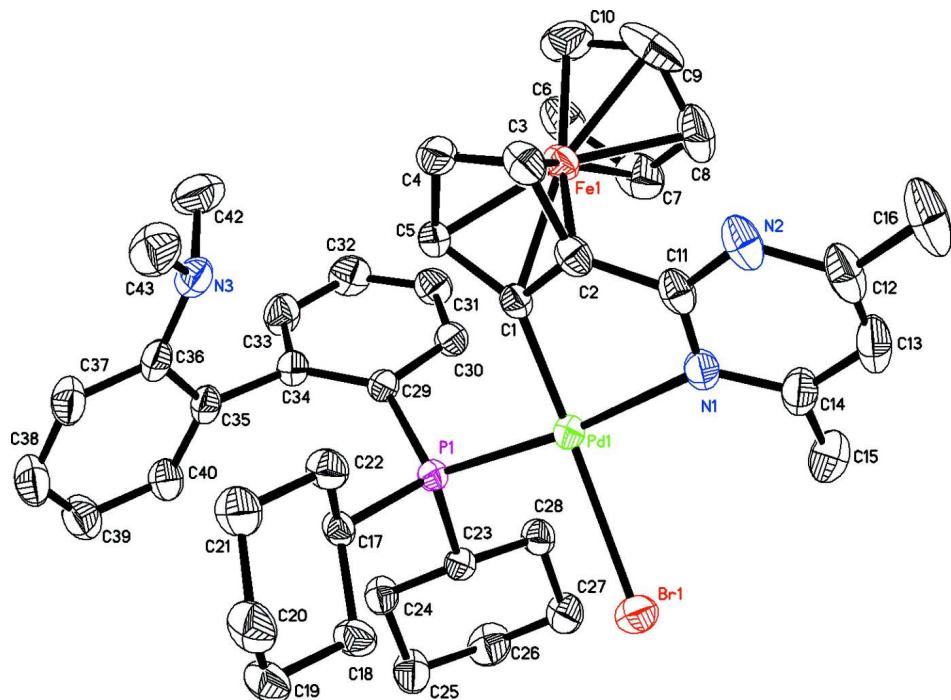
**Figure 1**

The molecular structure of the title compound with displacement ellipsoids at the 30% probability level. The dichloromethane molecule is omitted for clarity.
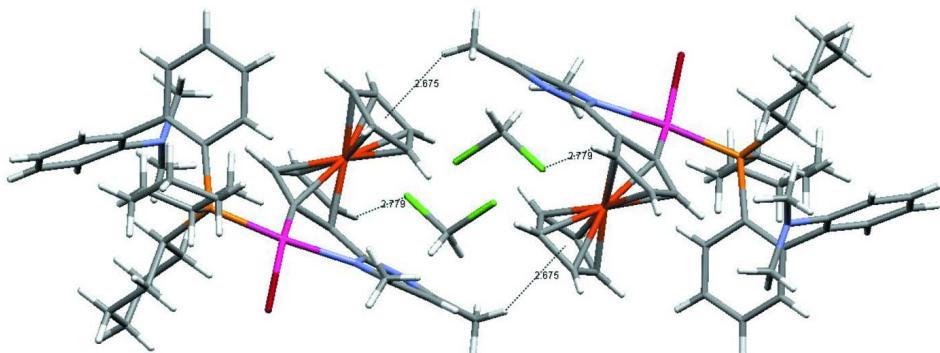


**Figure 2**

The dimeric unit of the title compound formed by the intermolecular C—H···Cl hydrogen bonds and C—H···$\pi$ interactions. $Cg$1 is the centroid of the Cp ring C6—C10, symmetry code ii: 1 - $x$, 2 - $y$, -$z$.

**Bromido{dicyclohexyl[2′-(dimethylamino)biphenyl-2-yl]phosphine-$\kappa P$}[2- (4,6-dimethylpyrimidin-2-yl)ferrocenyl-$\kappa^2 C^1$,$N$]palladium(II) dichloromethane solvate**

*Crystal data*

| | |
|---|---|
| [FePdBr($C_5H_5$)($C_{11}H_{10}N_2$)($C_{26}H_{36}NP$)]·$CH_2Cl_2$ | $\alpha = 81.195\ (1)°$ |
| $M_r = 955.91$ | $\beta = 76.590\ (1)°$ |
| Triclinic, $P\bar{1}$ | $\gamma = 72.647\ (1)°$ |
| $a = 10.2059\ (9)$ Å | $V = 2141.9\ (3)$ Å$^3$ |
| $b = 10.3637\ (9)$ Å | $Z = 2$ |
| $c = 21.900\ (2)$ Å | $F(000) = 976$ |

$D_x = 1.482$ Mg m$^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 7107 reflections

$\theta = 2.5–27.1°$

$\mu = 1.89$ mm$^{-1}$

$T = 293$ K

Block, red

$0.37 \times 0.24 \times 0.21$ mm

*Data collection*

Bruker SMART APEX CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\varphi$ and $\omega$ scans

Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)

$T_{min} = 0.540$, $T_{max} = 0.697$

16458 measured reflections

7919 independent reflections

6716 reflections with $I > 2\sigma(I)$

$R_{int} = 0.017$

$\theta_{max} = 25.5°$, $\theta_{min} = 2.5°$

$h = -12 \rightarrow 10$

$k = -12 \rightarrow 12$

$l = -26 \rightarrow 26$

*Refinement*

Refinement on $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.038$

$wR(F^2) = 0.099$

$S = 1.08$

7919 reflections

473 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

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0421P)^2 + 2.3428P]$ where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max} = 1.03$ e Å$^{-3}$

$\Delta\rho_{min} = -0.69$ e Å$^{-3}$

*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 $F^2 > \sigma(F^2)$ 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$^2$)*

|     | $x$ | $y$ | $z$ | $U_{iso}*/U_{eq}$ |
|-----|-----|-----|-----|-------------------|
| Pd1 | 0.29216 (3) | 0.66381 (3) | 0.217306 (12) | 0.03942 (9) |
| Fe1 | 0.63058 (6) | 0.70760 (5) | 0.12158 (2) | 0.04439 (14) |
| P1 | 0.33910 (9) | 0.56740 (8) | 0.31270 (4) | 0.03503 (19) |
| Br1 | 0.02020 (5) | 0.68171 (6) | 0.25105 (2) | 0.07101 (15) |
| Cl2 | 0.1066 (2) | 0.5000 (3) | 0.07189 (12) | 0.1586 (9) |
| Cl3 | 0.2456 (4) | 0.2376 (3) | 0.12552 (12) | 0.1980 (14) |
| N1 | 0.2744 (3) | 0.7531 (3) | 0.12117 (14) | 0.0477 (7) |
| N2 | 0.3968 (4) | 0.7000 (3) | 0.01637 (15) | 0.0592 (9) |
| N3 | 0.7663 (3) | 0.2896 (3) | 0.29096 (16) | 0.0565 (8) |
| C1 | 0.4926 (4) | 0.6039 (3) | 0.17412 (16) | 0.0395 (7) |

| | | | |
|---|---|---|---|
| C2 | 0.5018 (4) | 0.6044 (3) | 0.10732 (16) | 0.0443 (8) |
| C3 | 0.6430 (4) | 0.5430 (4) | 0.07875 (18) | 0.0537 (10) |
| H3 | 0.6788 | 0.5297 | 0.0339 | 0.064* |
| C4 | 0.7212 (4) | 0.5024 (4) | 0.1271 (2) | 0.0544 (10) |
| H4 | 0.8219 | 0.4579 | 0.1214 | 0.065* |
| C5 | 0.6299 (4) | 0.5404 (3) | 0.18529 (18) | 0.0449 (8) |
| H5 | 0.6578 | 0.5268 | 0.2262 | 0.054* |
| C6 | 0.6949 (6) | 0.8426 (5) | 0.1587 (2) | 0.0754 (14) |
| H6 | 0.7205 | 0.8302 | 0.2001 | 0.091* |
| C7 | 0.5625 (6) | 0.9016 (4) | 0.1460 (3) | 0.0746 (14) |
| H7 | 0.4782 | 0.9384 | 0.1771 | 0.090* |
| C8 | 0.5682 (7) | 0.9016 (5) | 0.0818 (3) | 0.0812 (16) |
| H8 | 0.4892 | 0.9383 | 0.0601 | 0.097* |
| C9 | 0.7057 (8) | 0.8393 (6) | 0.0538 (3) | 0.096 (2) |
| H9 | 0.7411 | 0.8256 | 0.0090 | 0.115* |
| C10 | 0.7859 (5) | 0.8021 (5) | 0.1023 (3) | 0.0872 (17) |
| H10 | 0.8866 | 0.7577 | 0.0970 | 0.105* |
| C11 | 0.3860 (4) | 0.6874 (4) | 0.07887 (17) | 0.0477 (9) |
| C12 | 0.2921 (6) | 0.7939 (5) | −0.0063 (2) | 0.0674 (13) |
| C13 | 0.1860 (6) | 0.8765 (5) | 0.0328 (2) | 0.0724 (13) |
| H13 | 0.1202 | 0.9473 | 0.0159 | 0.087* |
| C14 | 0.1768 (5) | 0.8542 (4) | 0.0977 (2) | 0.0618 (11) |
| C15 | 0.0679 (5) | 0.9476 (5) | 0.1408 (3) | 0.0829 (15) |
| H15A | −0.0102 | 0.9103 | 0.1570 | 0.124* |
| H15B | 0.0371 | 1.0344 | 0.1180 | 0.124* |
| H15C | 0.1064 | 0.9585 | 0.1751 | 0.124* |
| C16 | 0.3020 (7) | 0.8073 (5) | −0.0767 (2) | 0.0927 (19) |
| H16A | 0.2361 | 0.7675 | −0.0862 | 0.139* |
| H16B | 0.3951 | 0.7613 | −0.0967 | 0.139* |
| H16C | 0.2812 | 0.9016 | −0.0921 | 0.139* |
| C17 | 0.3460 (4) | 0.3850 (3) | 0.32533 (16) | 0.0397 (8) |
| H17 | 0.3978 | 0.3440 | 0.3592 | 0.048* |
| C18 | 0.2011 (4) | 0.3582 (4) | 0.3453 (2) | 0.0540 (10) |
| H18A | 0.1514 | 0.3996 | 0.3839 | 0.065* |
| H18B | 0.1467 | 0.3982 | 0.3128 | 0.065* |
| C19 | 0.2181 (5) | 0.2047 (4) | 0.3555 (2) | 0.0662 (12) |
| H19A | 0.2673 | 0.1663 | 0.3899 | 0.079* |
| H19B | 0.1264 | 0.1885 | 0.3674 | 0.079* |
| C20 | 0.2977 (5) | 0.1351 (4) | 0.2974 (2) | 0.0716 (13) |
| H20A | 0.2446 | 0.1673 | 0.2640 | 0.086* |
| H20B | 0.3099 | 0.0380 | 0.3062 | 0.086* |
| C21 | 0.4392 (5) | 0.1628 (4) | 0.2760 (2) | 0.0682 (12) |
| H21A | 0.4859 | 0.1223 | 0.2368 | 0.082* |
| H21B | 0.4962 | 0.1206 | 0.3073 | 0.082* |
| C22 | 0.4266 (4) | 0.3154 (4) | 0.26618 (19) | 0.0518 (9) |
| H22A | 0.5194 | 0.3291 | 0.2551 | 0.062* |
| H22B | 0.3789 | 0.3559 | 0.2315 | 0.062* |
| C23 | 0.1984 (4) | 0.6508 (3) | 0.37623 (16) | 0.0409 (8) |

| | | | |
|---|---|---|---|
| H23 | 0.1134 | 0.6308 | 0.3716 | 0.049* |
| C24 | 0.2157 (4) | 0.5979 (4) | 0.44399 (17) | 0.0508 (9) |
| H24A | 0.2947 | 0.6205 | 0.4527 | 0.061* |
| H24B | 0.2339 | 0.4999 | 0.4491 | 0.061* |
| C25 | 0.0821 (5) | 0.6618 (5) | 0.4903 (2) | 0.0681 (13) |
| H25A | 0.0948 | 0.6303 | 0.5331 | 0.082* |
| H25B | 0.0047 | 0.6332 | 0.4835 | 0.082* |
| C26 | 0.0467 (5) | 0.8173 (5) | 0.4817 (2) | 0.0737 (13) |
| H26A | −0.0408 | 0.8554 | 0.5098 | 0.088* |
| H26B | 0.1196 | 0.8466 | 0.4926 | 0.088* |
| C27 | 0.0340 (5) | 0.8691 (4) | 0.4137 (2) | 0.0623 (11) |
| H27A | −0.0448 | 0.8474 | 0.4042 | 0.075* |
| H27B | 0.0166 | 0.9670 | 0.4085 | 0.075* |
| C28 | 0.1661 (4) | 0.8057 (4) | 0.36824 (19) | 0.0503 (9) |
| H28A | 0.2440 | 0.8324 | 0.3758 | 0.060* |
| H28B | 0.1547 | 0.8385 | 0.3254 | 0.060* |
| C29 | 0.4941 (3) | 0.5949 (3) | 0.33234 (15) | 0.0372 (7) |
| C30 | 0.5028 (4) | 0.7283 (3) | 0.31298 (17) | 0.0443 (8) |
| H30 | 0.4448 | 0.7823 | 0.2864 | 0.053* |
| C31 | 0.5932 (4) | 0.7823 (4) | 0.3316 (2) | 0.0554 (10) |
| H31 | 0.5953 | 0.8713 | 0.3178 | 0.066* |
| C32 | 0.6802 (5) | 0.7048 (5) | 0.3703 (2) | 0.0632 (11) |
| H32 | 0.7396 | 0.7413 | 0.3845 | 0.076* |
| C33 | 0.6785 (5) | 0.5717 (4) | 0.3881 (2) | 0.0609 (11) |
| H33 | 0.7388 | 0.5194 | 0.4140 | 0.073* |
| C34 | 0.5909 (4) | 0.5118 (4) | 0.36905 (17) | 0.0438 (8) |
| C35 | 0.6087 (4) | 0.3642 (4) | 0.39042 (18) | 0.0460 (8) |
| C36 | 0.6959 (4) | 0.2591 (4) | 0.3527 (2) | 0.0526 (9) |
| C37 | 0.7073 (5) | 0.1256 (4) | 0.3780 (2) | 0.0662 (12) |
| H37 | 0.7620 | 0.0554 | 0.3536 | 0.079* |
| C38 | 0.6395 (6) | 0.0938 (5) | 0.4387 (3) | 0.0771 (14) |
| H38 | 0.6486 | 0.0035 | 0.4542 | 0.092* |
| C39 | 0.5598 (5) | 0.1945 (5) | 0.4756 (2) | 0.0699 (12) |
| H39 | 0.5159 | 0.1734 | 0.5165 | 0.084* |
| C40 | 0.5445 (4) | 0.3289 (4) | 0.45172 (19) | 0.0553 (10) |
| H40 | 0.4900 | 0.3973 | 0.4772 | 0.066* |
| C42 | 0.8764 (5) | 0.3547 (6) | 0.2856 (3) | 0.0867 (16) |
| H42A | 0.8416 | 0.4319 | 0.3099 | 0.130* |
| H42B | 0.9064 | 0.3839 | 0.2422 | 0.130* |
| H42C | 0.9541 | 0.2915 | 0.3012 | 0.130* |
| C43 | 0.8130 (6) | 0.1821 (5) | 0.2488 (3) | 0.0862 (16) |
| H43A | 0.8887 | 0.1117 | 0.2625 | 0.129* |
| H43B | 0.8445 | 0.2183 | 0.2068 | 0.129* |
| H43C | 0.7368 | 0.1453 | 0.2495 | 0.129* |
| C44 | 0.2410 (10) | 0.4080 (8) | 0.1087 (4) | 0.138 (3) |
| H44A | 0.2313 | 0.4467 | 0.1477 | 0.166* |
| H44B | 0.3292 | 0.4154 | 0.0820 | 0.166* |

*Atomic displacement parameters (Å²)*

|  | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Pd1 | 0.03597 (15) | 0.04066 (15) | 0.04152 (15) | −0.01016 (11) | −0.01180 (11) | 0.00234 (11) |
| Fe1 | 0.0491 (3) | 0.0377 (3) | 0.0443 (3) | −0.0144 (2) | −0.0046 (2) | 0.0003 (2) |
| P1 | 0.0351 (4) | 0.0315 (4) | 0.0382 (4) | −0.0091 (3) | −0.0079 (3) | −0.0011 (3) |
| Br1 | 0.0486 (2) | 0.0991 (4) | 0.0643 (3) | −0.0267 (2) | −0.0149 (2) | 0.0144 (2) |
| Cl2 | 0.0879 (13) | 0.193 (2) | 0.161 (2) | −0.0153 (13) | 0.0182 (13) | −0.0262 (17) |
| Cl3 | 0.345 (5) | 0.142 (2) | 0.1273 (18) | −0.095 (2) | −0.063 (2) | 0.0086 (15) |
| N1 | 0.0528 (19) | 0.0448 (17) | 0.0487 (18) | −0.0164 (15) | −0.0190 (15) | 0.0061 (14) |
| N2 | 0.096 (3) | 0.0469 (19) | 0.0463 (19) | −0.0302 (19) | −0.0288 (18) | 0.0041 (15) |
| N3 | 0.0462 (18) | 0.0532 (19) | 0.062 (2) | −0.0014 (15) | −0.0091 (16) | −0.0063 (16) |
| C1 | 0.0429 (19) | 0.0334 (17) | 0.0402 (18) | −0.0112 (15) | −0.0069 (15) | 0.0024 (14) |
| C2 | 0.059 (2) | 0.0326 (17) | 0.0422 (19) | −0.0151 (16) | −0.0081 (17) | −0.0029 (15) |
| C3 | 0.070 (3) | 0.039 (2) | 0.045 (2) | −0.0119 (18) | 0.0007 (19) | −0.0070 (16) |
| C4 | 0.047 (2) | 0.041 (2) | 0.065 (3) | −0.0057 (17) | 0.0009 (19) | −0.0053 (18) |
| C5 | 0.043 (2) | 0.0377 (19) | 0.047 (2) | −0.0068 (15) | −0.0078 (16) | 0.0053 (15) |
| C6 | 0.107 (4) | 0.071 (3) | 0.069 (3) | −0.053 (3) | −0.028 (3) | 0.007 (2) |
| C7 | 0.094 (4) | 0.040 (2) | 0.089 (4) | −0.027 (2) | −0.003 (3) | −0.011 (2) |
| C8 | 0.117 (5) | 0.046 (3) | 0.093 (4) | −0.034 (3) | −0.050 (4) | 0.025 (3) |
| C9 | 0.159 (6) | 0.076 (4) | 0.058 (3) | −0.075 (4) | 0.020 (4) | −0.004 (3) |
| C10 | 0.057 (3) | 0.066 (3) | 0.136 (5) | −0.030 (2) | −0.002 (3) | −0.001 (3) |
| C11 | 0.069 (3) | 0.0349 (18) | 0.047 (2) | −0.0231 (18) | −0.0209 (19) | 0.0027 (16) |
| C12 | 0.112 (4) | 0.050 (2) | 0.060 (3) | −0.042 (3) | −0.045 (3) | 0.016 (2) |
| C13 | 0.092 (4) | 0.058 (3) | 0.078 (3) | −0.023 (3) | −0.052 (3) | 0.019 (2) |
| C14 | 0.063 (3) | 0.054 (2) | 0.074 (3) | −0.018 (2) | −0.034 (2) | 0.011 (2) |
| C15 | 0.067 (3) | 0.067 (3) | 0.100 (4) | 0.005 (2) | −0.025 (3) | 0.003 (3) |
| C16 | 0.177 (6) | 0.064 (3) | 0.063 (3) | −0.052 (4) | −0.066 (4) | 0.018 (2) |
| C17 | 0.0454 (19) | 0.0312 (17) | 0.0453 (19) | −0.0144 (15) | −0.0129 (15) | 0.0022 (14) |
| C18 | 0.056 (2) | 0.049 (2) | 0.062 (2) | −0.0258 (19) | −0.0076 (19) | −0.0030 (18) |
| C19 | 0.073 (3) | 0.053 (2) | 0.080 (3) | −0.036 (2) | −0.014 (2) | 0.006 (2) |
| C20 | 0.090 (3) | 0.042 (2) | 0.093 (4) | −0.030 (2) | −0.022 (3) | −0.008 (2) |
| C21 | 0.076 (3) | 0.038 (2) | 0.089 (3) | −0.015 (2) | −0.008 (3) | −0.013 (2) |
| C22 | 0.057 (2) | 0.040 (2) | 0.057 (2) | −0.0152 (17) | −0.0027 (18) | −0.0091 (17) |
| C23 | 0.0379 (18) | 0.0372 (18) | 0.0446 (19) | −0.0077 (14) | −0.0058 (15) | −0.0026 (15) |
| C24 | 0.055 (2) | 0.047 (2) | 0.043 (2) | −0.0045 (18) | −0.0075 (17) | −0.0050 (16) |
| C25 | 0.071 (3) | 0.067 (3) | 0.046 (2) | 0.003 (2) | −0.002 (2) | −0.003 (2) |
| C26 | 0.068 (3) | 0.069 (3) | 0.069 (3) | 0.001 (2) | 0.004 (2) | −0.025 (2) |
| C27 | 0.062 (3) | 0.037 (2) | 0.074 (3) | 0.0025 (18) | −0.002 (2) | −0.0109 (19) |
| C28 | 0.053 (2) | 0.0358 (19) | 0.057 (2) | −0.0084 (17) | −0.0060 (18) | −0.0027 (16) |
| C29 | 0.0369 (17) | 0.0375 (17) | 0.0375 (17) | −0.0094 (14) | −0.0087 (14) | −0.0040 (14) |
| C30 | 0.045 (2) | 0.0369 (18) | 0.052 (2) | −0.0125 (16) | −0.0096 (16) | −0.0033 (16) |
| C31 | 0.061 (2) | 0.046 (2) | 0.065 (3) | −0.0234 (19) | −0.012 (2) | −0.0048 (19) |
| C32 | 0.063 (3) | 0.063 (3) | 0.079 (3) | −0.030 (2) | −0.024 (2) | −0.013 (2) |
| C33 | 0.059 (3) | 0.063 (3) | 0.069 (3) | −0.018 (2) | −0.032 (2) | 0.001 (2) |
| C34 | 0.045 (2) | 0.0404 (19) | 0.045 (2) | −0.0093 (16) | −0.0131 (16) | −0.0013 (15) |
| C35 | 0.045 (2) | 0.042 (2) | 0.052 (2) | −0.0058 (16) | −0.0220 (17) | 0.0005 (16) |
| C36 | 0.045 (2) | 0.047 (2) | 0.062 (2) | −0.0005 (17) | −0.0219 (18) | 0.0005 (18) |

| C37 | 0.068 (3) | 0.045 (2) | 0.076 (3) | 0.001 (2) | −0.021 (2) | 0.000 (2) |
| C38 | 0.088 (4) | 0.047 (3) | 0.088 (4) | −0.009 (2) | −0.026 (3) | 0.012 (2) |
| C39 | 0.081 (3) | 0.065 (3) | 0.062 (3) | −0.022 (3) | −0.019 (2) | 0.011 (2) |
| C40 | 0.062 (3) | 0.054 (2) | 0.050 (2) | −0.013 (2) | −0.0198 (19) | 0.0008 (18) |
| C42 | 0.051 (3) | 0.109 (4) | 0.098 (4) | −0.023 (3) | −0.007 (3) | −0.011 (3) |
| C43 | 0.085 (4) | 0.076 (3) | 0.082 (4) | 0.000 (3) | −0.001 (3) | −0.025 (3) |
| C44 | 0.198 (9) | 0.139 (7) | 0.125 (6) | −0.101 (6) | −0.080 (6) | 0.033 (5) |

## Geometric parameters (Å, º)

| | | | |
|---|---|---|---|
| Pd1—C1 | 1.997 (3) | C18—H18A | 0.9700 |
| Pd1—N1 | 2.192 (3) | C18—H18B | 0.9700 |
| Pd1—P1 | 2.2654 (9) | C19—C20 | 1.501 (6) |
| Pd1—Br1 | 2.6585 (6) | C19—H19A | 0.9700 |
| Fe1—C2 | 2.025 (4) | C19—H19B | 0.9700 |
| Fe1—C3 | 2.028 (4) | C20—C21 | 1.510 (6) |
| Fe1—C9 | 2.032 (5) | C20—H20A | 0.9700 |
| Fe1—C7 | 2.034 (4) | C20—H20B | 0.9700 |
| Fe1—C10 | 2.035 (5) | C21—C22 | 1.533 (5) |
| Fe1—C8 | 2.041 (4) | C21—H21A | 0.9700 |
| Fe1—C4 | 2.047 (4) | C21—H21B | 0.9700 |
| Fe1—C6 | 2.047 (5) | C22—H22A | 0.9700 |
| Fe1—C5 | 2.053 (3) | C22—H22B | 0.9700 |
| Fe1—C1 | 2.058 (3) | C23—C28 | 1.530 (5) |
| P1—C29 | 1.841 (3) | C23—C24 | 1.532 (5) |
| P1—C17 | 1.851 (3) | C23—H23 | 0.9800 |
| P1—C23 | 1.857 (3) | C24—C25 | 1.533 (5) |
| Cl2—C44 | 1.715 (8) | C24—H24A | 0.9700 |
| Cl3—C44 | 1.737 (7) | C24—H24B | 0.9700 |
| N1—C14 | 1.343 (5) | C25—C26 | 1.535 (6) |
| N1—C11 | 1.364 (5) | C25—H25A | 0.9700 |
| N2—C11 | 1.337 (5) | C25—H25B | 0.9700 |
| N2—C12 | 1.346 (6) | C26—C27 | 1.525 (6) |
| N3—C36 | 1.414 (5) | C26—H26A | 0.9700 |
| N3—C42 | 1.449 (6) | C26—H26B | 0.9700 |
| N3—C43 | 1.454 (6) | C27—C28 | 1.513 (5) |
| C1—C5 | 1.420 (5) | C27—H27A | 0.9700 |
| C1—C2 | 1.443 (5) | C27—H27B | 0.9700 |
| C2—C3 | 1.425 (5) | C28—H28A | 0.9700 |
| C2—C11 | 1.448 (5) | C28—H28B | 0.9700 |
| C3—C4 | 1.411 (6) | C29—C30 | 1.405 (5) |
| C3—H3 | 0.9800 | C29—C34 | 1.419 (5) |
| C4—C5 | 1.425 (5) | C30—C31 | 1.372 (5) |
| C4—H4 | 0.9800 | C30—H30 | 0.9300 |
| C5—H5 | 0.9800 | C31—C32 | 1.368 (6) |
| C6—C7 | 1.381 (7) | C31—H31 | 0.9300 |
| C6—C10 | 1.398 (8) | C32—C33 | 1.379 (6) |
| C6—H6 | 0.9800 | C32—H32 | 0.9300 |

| | | | |
|---|---|---|---|
| C7—C8 | 1.394 (7) | C33—C34 | 1.393 (5) |
| C7—H7 | 0.9800 | C33—H33 | 0.9300 |
| C8—C9 | 1.393 (8) | C34—C35 | 1.499 (5) |
| C8—H8 | 0.9800 | C35—C40 | 1.396 (5) |
| C9—C10 | 1.427 (8) | C35—C36 | 1.420 (5) |
| C9—H9 | 0.9800 | C36—C37 | 1.391 (6) |
| C10—H10 | 0.9800 | C37—C38 | 1.389 (7) |
| C12—C13 | 1.371 (7) | C37—H37 | 0.9300 |
| C12—C16 | 1.510 (6) | C38—C39 | 1.360 (7) |
| C13—C14 | 1.391 (6) | C38—H38 | 0.9300 |
| C13—H13 | 0.9300 | C39—C40 | 1.386 (6) |
| C14—C15 | 1.488 (7) | C39—H39 | 0.9300 |
| C15—H15A | 0.9600 | C40—H40 | 0.9300 |
| C15—H15B | 0.9600 | C42—H42A | 0.9600 |
| C15—H15C | 0.9600 | C42—H42B | 0.9600 |
| C16—H16A | 0.9600 | C42—H42C | 0.9600 |
| C16—H16B | 0.9600 | C43—H43A | 0.9600 |
| C16—H16C | 0.9600 | C43—H43B | 0.9600 |
| C17—C22 | 1.521 (5) | C43—H43C | 0.9600 |
| C17—C18 | 1.537 (5) | C44—H44A | 0.9700 |
| C17—H17 | 0.9800 | C44—H44B | 0.9700 |
| C18—C19 | 1.534 (5) | | |
| | | | |
| C1—Pd1—N1 | 80.12 (13) | C14—C15—H15B | 109.5 |
| C1—Pd1—P1 | 93.07 (10) | H15A—C15—H15B | 109.5 |
| N1—Pd1—P1 | 173.00 (9) | C14—C15—H15C | 109.5 |
| C1—Pd1—Br1 | 160.40 (10) | H15A—C15—H15C | 109.5 |
| N1—Pd1—Br1 | 92.84 (8) | H15B—C15—H15C | 109.5 |
| P1—Pd1—Br1 | 94.13 (3) | C12—C16—H16A | 109.5 |
| C2—Fe1—C3 | 41.18 (15) | C12—C16—H16B | 109.5 |
| C2—Fe1—C9 | 122.5 (2) | H16A—C16—H16B | 109.5 |
| C3—Fe1—C9 | 106.90 (19) | C12—C16—H16C | 109.5 |
| C2—Fe1—C7 | 123.4 (2) | H16A—C16—H16C | 109.5 |
| C3—Fe1—C7 | 159.1 (2) | H16B—C16—H16C | 109.5 |
| C9—Fe1—C7 | 67.4 (2) | C22—C17—C18 | 109.9 (3) |
| C2—Fe1—C10 | 159.3 (2) | C22—C17—P1 | 109.9 (2) |
| C3—Fe1—C10 | 122.8 (2) | C18—C17—P1 | 113.7 (2) |
| C9—Fe1—C10 | 41.1 (2) | C22—C17—H17 | 107.7 |
| C7—Fe1—C10 | 67.2 (2) | C18—C17—H17 | 107.7 |
| C2—Fe1—C8 | 107.86 (19) | P1—C17—H17 | 107.7 |
| C3—Fe1—C8 | 122.8 (2) | C19—C18—C17 | 109.7 (3) |
| C9—Fe1—C8 | 40.0 (2) | C19—C18—H18A | 109.7 |
| C7—Fe1—C8 | 40.0 (2) | C17—C18—H18A | 109.7 |
| C10—Fe1—C8 | 67.7 (2) | C19—C18—H18B | 109.7 |
| C2—Fe1—C4 | 68.24 (16) | C17—C18—H18B | 109.7 |
| C3—Fe1—C4 | 40.50 (17) | H18A—C18—H18B | 108.2 |
| C9—Fe1—C4 | 123.1 (2) | C20—C19—C18 | 111.8 (4) |
| C7—Fe1—C4 | 159.5 (2) | C20—C19—H19A | 109.3 |

| | | | |
|---|---|---|---|
| C10—Fe1—C4 | 108.1 (2) | C18—C19—H19A | 109.3 |
| C8—Fe1—C4 | 158.8 (2) | C20—C19—H19B | 109.3 |
| C2—Fe1—C6 | 158.8 (2) | C18—C19—H19B | 109.3 |
| C3—Fe1—C6 | 159.1 (2) | H19A—C19—H19B | 107.9 |
| C9—Fe1—C6 | 67.9 (2) | C19—C20—C21 | 110.7 (4) |
| C7—Fe1—C6 | 39.6 (2) | C19—C20—H20A | 109.5 |
| C10—Fe1—C6 | 40.1 (2) | C21—C20—H20A | 109.5 |
| C8—Fe1—C6 | 67.1 (2) | C19—C20—H20B | 109.5 |
| C4—Fe1—C6 | 124.0 (2) | C21—C20—H20B | 109.5 |
| C2—Fe1—C5 | 68.29 (15) | H20A—C20—H20B | 108.1 |
| C3—Fe1—C5 | 68.69 (16) | C20—C21—C22 | 111.7 (4) |
| C9—Fe1—C5 | 159.4 (3) | C20—C21—H21A | 109.3 |
| C7—Fe1—C5 | 123.73 (19) | C22—C21—H21A | 109.3 |
| C10—Fe1—C5 | 123.2 (2) | C20—C21—H21B | 109.3 |
| C8—Fe1—C5 | 159.2 (2) | C22—C21—H21B | 109.3 |
| C4—Fe1—C5 | 40.68 (15) | H21A—C21—H21B | 107.9 |
| C6—Fe1—C5 | 108.64 (18) | C17—C22—C21 | 111.2 (3) |
| C2—Fe1—C1 | 41.39 (14) | C17—C22—H22A | 109.4 |
| C3—Fe1—C1 | 69.73 (15) | C21—C22—H22A | 109.4 |
| C9—Fe1—C1 | 158.8 (3) | C17—C22—H22B | 109.4 |
| C7—Fe1—C1 | 107.86 (17) | C21—C22—H22B | 109.4 |
| C10—Fe1—C1 | 158.2 (2) | H22A—C22—H22B | 108.0 |
| C8—Fe1—C1 | 123.1 (2) | C28—C23—C24 | 110.0 (3) |
| C4—Fe1—C1 | 68.68 (14) | C28—C23—P1 | 113.1 (2) |
| C6—Fe1—C1 | 122.59 (18) | C24—C23—P1 | 116.3 (2) |
| C5—Fe1—C1 | 40.43 (14) | C28—C23—H23 | 105.5 |
| C29—P1—C17 | 110.59 (16) | C24—C23—H23 | 105.5 |
| C29—P1—C23 | 101.08 (16) | P1—C23—H23 | 105.5 |
| C17—P1—C23 | 106.19 (16) | C23—C24—C25 | 109.8 (3) |
| C29—P1—Pd1 | 115.27 (11) | C23—C24—H24A | 109.7 |
| C17—P1—Pd1 | 112.84 (12) | C25—C24—H24A | 109.7 |
| C23—P1—Pd1 | 109.86 (11) | C23—C24—H24B | 109.7 |
| C14—N1—C11 | 117.0 (3) | C25—C24—H24B | 109.7 |
| C14—N1—Pd1 | 132.7 (3) | H24A—C24—H24B | 108.2 |
| C11—N1—Pd1 | 110.3 (2) | C24—C25—C26 | 111.1 (4) |
| C11—N2—C12 | 116.1 (4) | C24—C25—H25A | 109.4 |
| C36—N3—C42 | 116.4 (4) | C26—C25—H25A | 109.4 |
| C36—N3—C43 | 116.8 (4) | C24—C25—H25B | 109.4 |
| C42—N3—C43 | 109.8 (4) | C26—C25—H25B | 109.4 |
| C5—C1—C2 | 106.1 (3) | H25A—C25—H25B | 108.0 |
| C5—C1—Pd1 | 142.9 (3) | C27—C26—C25 | 110.4 (4) |
| C2—C1—Pd1 | 109.9 (3) | C27—C26—H26A | 109.6 |
| C5—C1—Fe1 | 69.6 (2) | C25—C26—H26A | 109.6 |
| C2—C1—Fe1 | 68.06 (19) | C27—C26—H26B | 109.6 |
| Pd1—C1—Fe1 | 132.86 (17) | C25—C26—H26B | 109.6 |
| C3—C2—C1 | 109.1 (3) | H26A—C26—H26B | 108.1 |
| C3—C2—C11 | 130.0 (3) | C28—C27—C26 | 111.1 (3) |
| C1—C2—C11 | 119.3 (3) | C28—C27—H27A | 109.4 |

| | | | |
|---|---|---|---|
| C3—C2—Fe1 | 69.5 (2) | C26—C27—H27A | 109.4 |
| C1—C2—Fe1 | 70.6 (2) | C28—C27—H27B | 109.4 |
| C11—C2—Fe1 | 114.3 (2) | C26—C27—H27B | 109.4 |
| C4—C3—C2 | 107.3 (3) | H27A—C27—H27B | 108.0 |
| C4—C3—Fe1 | 70.5 (2) | C27—C28—C23 | 110.7 (3) |
| C2—C3—Fe1 | 69.3 (2) | C27—C28—H28A | 109.5 |
| C4—C3—H3 | 126.3 | C23—C28—H28A | 109.5 |
| C2—C3—H3 | 126.3 | C27—C28—H28B | 109.5 |
| Fe1—C3—H3 | 126.3 | C23—C28—H28B | 109.5 |
| C3—C4—C5 | 108.6 (3) | H28A—C28—H28B | 108.1 |
| C3—C4—Fe1 | 69.0 (2) | C30—C29—C34 | 117.3 (3) |
| C5—C4—Fe1 | 69.9 (2) | C30—C29—P1 | 111.3 (3) |
| C3—C4—H4 | 125.7 | C34—C29—P1 | 131.0 (3) |
| C5—C4—H4 | 125.7 | C31—C30—C29 | 122.9 (4) |
| Fe1—C4—H4 | 125.7 | C31—C30—H30 | 118.6 |
| C1—C5—C4 | 109.0 (3) | C29—C30—H30 | 118.6 |
| C1—C5—Fe1 | 69.99 (19) | C32—C31—C30 | 119.7 (4) |
| C4—C5—Fe1 | 69.5 (2) | C32—C31—H31 | 120.1 |
| C1—C5—H5 | 125.5 | C30—C31—H31 | 120.1 |
| C4—C5—H5 | 125.5 | C31—C32—C33 | 118.9 (4) |
| Fe1—C5—H5 | 125.5 | C31—C32—H32 | 120.6 |
| C7—C6—C10 | 108.1 (5) | C33—C32—H32 | 120.6 |
| C7—C6—Fe1 | 69.7 (3) | C32—C33—C34 | 123.2 (4) |
| C10—C6—Fe1 | 69.5 (3) | C32—C33—H33 | 118.4 |
| C7—C6—H6 | 125.9 | C34—C33—H33 | 118.4 |
| C10—C6—H6 | 125.9 | C33—C34—C29 | 117.8 (3) |
| Fe1—C6—H6 | 125.9 | C33—C34—C35 | 115.7 (3) |
| C6—C7—C8 | 109.0 (5) | C29—C34—C35 | 126.5 (3) |
| C6—C7—Fe1 | 70.8 (3) | C40—C35—C36 | 118.7 (4) |
| C8—C7—Fe1 | 70.3 (3) | C40—C35—C34 | 118.3 (3) |
| C6—C7—H7 | 125.5 | C36—C35—C34 | 122.8 (3) |
| C8—C7—H7 | 125.5 | C37—C36—N3 | 121.2 (4) |
| Fe1—C7—H7 | 125.5 | C37—C36—C35 | 117.9 (4) |
| C9—C8—C7 | 108.1 (5) | N3—C36—C35 | 120.9 (3) |
| C9—C8—Fe1 | 69.7 (3) | C38—C37—C36 | 122.0 (4) |
| C7—C8—Fe1 | 69.7 (3) | C38—C37—H37 | 119.0 |
| C9—C8—H8 | 125.9 | C36—C37—H37 | 119.0 |
| C7—C8—H8 | 125.9 | C39—C38—C37 | 120.1 (4) |
| Fe1—C8—H8 | 125.9 | C39—C38—H38 | 119.9 |
| C8—C9—C10 | 107.2 (5) | C37—C38—H38 | 119.9 |
| C8—C9—Fe1 | 70.3 (3) | C38—C39—C40 | 119.6 (4) |
| C10—C9—Fe1 | 69.6 (3) | C38—C39—H39 | 120.2 |
| C8—C9—H9 | 126.4 | C40—C39—H39 | 120.2 |
| C10—C9—H9 | 126.4 | C39—C40—C35 | 121.7 (4) |
| Fe1—C9—H9 | 126.4 | C39—C40—H40 | 119.1 |
| C6—C10—C9 | 107.5 (5) | C35—C40—H40 | 119.1 |
| C6—C10—Fe1 | 70.4 (3) | N3—C42—H42A | 109.5 |
| C9—C10—Fe1 | 69.3 (3) | N3—C42—H42B | 109.5 |

| | | | |
|---|---|---|---|
| C6—C10—H10 | 126.3 | H42A—C42—H42B | 109.5 |
| C9—C10—H10 | 126.3 | N3—C42—H42C | 109.5 |
| Fe1—C10—H10 | 126.3 | H42A—C42—H42C | 109.5 |
| N2—C11—N1 | 125.8 (4) | H42B—C42—H42C | 109.5 |
| N2—C11—C2 | 120.5 (4) | N3—C43—H43A | 109.5 |
| N1—C11—C2 | 113.6 (3) | N3—C43—H43B | 109.5 |
| N2—C12—C13 | 121.1 (4) | H43A—C43—H43B | 109.5 |
| N2—C12—C16 | 116.5 (5) | N3—C43—H43C | 109.5 |
| C13—C12—C16 | 122.3 (5) | H43A—C43—H43C | 109.5 |
| C12—C13—C14 | 120.0 (4) | H43B—C43—H43C | 109.5 |
| C12—C13—H13 | 120.0 | Cl2—C44—Cl3 | 112.9 (4) |
| C14—C13—H13 | 120.0 | Cl2—C44—H44A | 109.0 |
| N1—C14—C13 | 119.2 (4) | Cl3—C44—H44A | 109.0 |
| N1—C14—C15 | 119.8 (4) | Cl2—C44—H44B | 109.0 |
| C13—C14—C15 | 120.8 (4) | Cl3—C44—H44B | 109.0 |
| C14—C15—H15A | 109.5 | H44A—C44—H44B | 107.8 |
| | | | |
| C1—Pd1—P1—C29 | 43.93 (15) | C10—C6—C7—Fe1 | 59.0 (3) |
| N1—Pd1—P1—C29 | 31.0 (7) | C2—Fe1—C7—C6 | 162.9 (3) |
| Br1—Pd1—P1—C29 | −154.31 (12) | C3—Fe1—C7—C6 | −160.3 (4) |
| C1—Pd1—P1—C17 | −84.43 (15) | C9—Fe1—C7—C6 | −82.1 (4) |
| N1—Pd1—P1—C17 | −97.3 (7) | C10—Fe1—C7—C6 | −37.4 (3) |
| Br1—Pd1—P1—C17 | 77.32 (12) | C8—Fe1—C7—C6 | −119.5 (5) |
| C1—Pd1—P1—C23 | 157.29 (15) | C4—Fe1—C7—C6 | 43.1 (7) |
| N1—Pd1—P1—C23 | 144.4 (7) | C5—Fe1—C7—C6 | 78.2 (3) |
| Br1—Pd1—P1—C23 | −40.96 (12) | C1—Fe1—C7—C6 | 119.9 (3) |
| C1—Pd1—N1—C14 | −159.6 (4) | C2—Fe1—C7—C8 | −77.6 (4) |
| P1—Pd1—N1—C14 | −146.5 (6) | C3—Fe1—C7—C8 | −40.8 (7) |
| Br1—Pd1—N1—C14 | 38.9 (4) | C9—Fe1—C7—C8 | 37.3 (4) |
| C1—Pd1—N1—C11 | 21.8 (2) | C10—Fe1—C7—C8 | 82.1 (4) |
| P1—Pd1—N1—C11 | 34.9 (8) | C4—Fe1—C7—C8 | 162.6 (5) |
| Br1—Pd1—N1—C11 | −139.8 (2) | C6—Fe1—C7—C8 | 119.5 (5) |
| N1—Pd1—C1—C5 | 172.1 (4) | C5—Fe1—C7—C8 | −162.3 (3) |
| P1—Pd1—C1—C5 | −6.3 (4) | C1—Fe1—C7—C8 | −120.6 (3) |
| Br1—Pd1—C1—C5 | −117.7 (4) | C6—C7—C8—C9 | 1.1 (5) |
| N1—Pd1—C1—C2 | −22.0 (2) | Fe1—C7—C8—C9 | −59.3 (3) |
| P1—Pd1—C1—C2 | 159.5 (2) | C6—C7—C8—Fe1 | 60.4 (3) |
| Br1—Pd1—C1—C2 | 48.1 (4) | C2—Fe1—C8—C9 | −119.6 (4) |
| N1—Pd1—C1—Fe1 | 56.1 (2) | C3—Fe1—C8—C9 | −76.7 (4) |
| P1—Pd1—C1—Fe1 | −122.3 (2) | C7—Fe1—C8—C9 | 119.4 (5) |
| Br1—Pd1—C1—Fe1 | 126.2 (2) | C10—Fe1—C8—C9 | 38.9 (3) |
| C2—Fe1—C1—C5 | 118.0 (3) | C4—Fe1—C8—C9 | −43.8 (7) |
| C3—Fe1—C1—C5 | 80.6 (2) | C6—Fe1—C8—C9 | 82.4 (4) |
| C9—Fe1—C1—C5 | 165.1 (5) | C5—Fe1—C8—C9 | 164.7 (5) |
| C7—Fe1—C1—C5 | −121.4 (3) | C1—Fe1—C8—C9 | −162.6 (3) |
| C10—Fe1—C1—C5 | −48.4 (6) | C2—Fe1—C8—C7 | 121.0 (3) |
| C8—Fe1—C1—C5 | −162.8 (3) | C3—Fe1—C8—C7 | 163.9 (3) |
| C4—Fe1—C1—C5 | 37.1 (2) | C9—Fe1—C8—C7 | −119.4 (5) |

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| C6—Fe1—C1—C5 | −80.5 (3) | C10—Fe1—C8—C7 | −80.5 (4) |
| C3—Fe1—C1—C2 | −37.4 (2) | C4—Fe1—C8—C7 | −163.2 (5) |
| C9—Fe1—C1—C2 | 47.1 (6) | C6—Fe1—C8—C7 | −37.0 (3) |
| C7—Fe1—C1—C2 | 120.6 (3) | C5—Fe1—C8—C7 | 45.3 (7) |
| C10—Fe1—C1—C2 | −166.4 (5) | C1—Fe1—C8—C7 | 78.0 (4) |
| C8—Fe1—C1—C2 | 79.3 (3) | C7—C8—C9—C10 | −0.7 (5) |
| C4—Fe1—C1—C2 | −80.8 (2) | Fe1—C8—C9—C10 | −60.1 (3) |
| C6—Fe1—C1—C2 | 161.5 (3) | C7—C8—C9—Fe1 | 59.3 (3) |
| C5—Fe1—C1—C2 | −118.0 (3) | C2—Fe1—C9—C8 | 78.9 (4) |
| C2—Fe1—C1—Pd1 | −97.3 (3) | C3—Fe1—C9—C8 | 121.2 (3) |
| C3—Fe1—C1—Pd1 | −134.7 (3) | C7—Fe1—C9—C8 | −37.3 (3) |
| C9—Fe1—C1—Pd1 | −50.2 (6) | C10—Fe1—C9—C8 | −118.0 (5) |
| C7—Fe1—C1—Pd1 | 23.3 (3) | C4—Fe1—C9—C8 | 162.6 (3) |
| C10—Fe1—C1—Pd1 | 96.3 (5) | C6—Fe1—C9—C8 | −80.3 (4) |
| C8—Fe1—C1—Pd1 | −18.1 (3) | C5—Fe1—C9—C8 | −164.5 (5) |
| C4—Fe1—C1—Pd1 | −178.2 (3) | C1—Fe1—C9—C8 | 43.9 (7) |
| C6—Fe1—C1—Pd1 | 64.2 (3) | C2—Fe1—C9—C10 | −163.1 (3) |
| C5—Fe1—C1—Pd1 | 144.7 (4) | C3—Fe1—C9—C10 | −120.8 (3) |
| C5—C1—C2—C3 | −0.4 (4) | C7—Fe1—C9—C10 | 80.6 (4) |
| Pd1—C1—C2—C3 | −171.6 (2) | C8—Fe1—C9—C10 | 118.0 (5) |
| Fe1—C1—C2—C3 | 59.1 (3) | C4—Fe1—C9—C10 | −79.4 (4) |
| C5—C1—C2—C11 | −167.1 (3) | C6—Fe1—C9—C10 | 37.7 (3) |
| Pd1—C1—C2—C11 | 21.7 (4) | C5—Fe1—C9—C10 | −46.5 (7) |
| Fe1—C1—C2—C11 | −107.6 (3) | C1—Fe1—C9—C10 | 161.8 (4) |
| C5—C1—C2—Fe1 | −59.5 (2) | C7—C6—C10—C9 | 0.6 (5) |
| Pd1—C1—C2—Fe1 | 129.34 (18) | Fe1—C6—C10—C9 | 59.7 (3) |
| C9—Fe1—C2—C3 | 78.2 (3) | C7—C6—C10—Fe1 | −59.2 (3) |
| C7—Fe1—C2—C3 | 161.0 (3) | C8—C9—C10—C6 | 0.1 (5) |
| C10—Fe1—C2—C3 | 45.6 (6) | Fe1—C9—C10—C6 | −60.4 (3) |
| C8—Fe1—C2—C3 | 119.7 (3) | C8—C9—C10—Fe1 | 60.5 (3) |
| C4—Fe1—C2—C3 | −38.1 (2) | C2—Fe1—C10—C6 | 162.0 (5) |
| C6—Fe1—C2—C3 | −167.7 (5) | C3—Fe1—C10—C6 | −163.9 (3) |
| C5—Fe1—C2—C3 | −82.0 (2) | C9—Fe1—C10—C6 | 118.3 (5) |
| C1—Fe1—C2—C3 | −120.1 (3) | C7—Fe1—C10—C6 | 37.0 (3) |
| C3—Fe1—C2—C1 | 120.1 (3) | C8—Fe1—C10—C6 | 80.4 (4) |
| C9—Fe1—C2—C1 | −161.7 (3) | C4—Fe1—C10—C6 | −121.7 (3) |
| C7—Fe1—C2—C1 | −78.9 (3) | C5—Fe1—C10—C6 | −79.4 (4) |
| C10—Fe1—C2—C1 | 165.7 (5) | C1—Fe1—C10—C6 | −44.0 (6) |
| C8—Fe1—C2—C1 | −120.2 (3) | C2—Fe1—C10—C9 | 43.7 (7) |
| C4—Fe1—C2—C1 | 82.0 (2) | C3—Fe1—C10—C9 | 77.8 (4) |
| C6—Fe1—C2—C1 | −47.6 (6) | C7—Fe1—C10—C9 | −81.3 (4) |
| C5—Fe1—C2—C1 | 38.06 (19) | C8—Fe1—C10—C9 | −37.9 (3) |
| C3—Fe1—C2—C11 | −125.7 (4) | C4—Fe1—C10—C9 | 120.0 (3) |
| C9—Fe1—C2—C11 | −47.5 (4) | C6—Fe1—C10—C9 | −118.3 (5) |
| C7—Fe1—C2—C11 | 35.3 (4) | C5—Fe1—C10—C9 | 162.3 (3) |
| C10—Fe1—C2—C11 | −80.1 (6) | C1—Fe1—C10—C9 | −162.3 (4) |
| C8—Fe1—C2—C11 | −6.0 (3) | C12—N2—C11—N1 | 5.3 (6) |
| C4—Fe1—C2—C11 | −163.8 (3) | C12—N2—C11—C2 | −170.8 (3) |

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| C6—Fe1—C2—C11 | 66.6 (6) | C14—N1—C11—N2 | −10.9 (5) |
| C5—Fe1—C2—C11 | 152.2 (3) | Pd1—N1—C11—N2 | 168.0 (3) |
| C1—Fe1—C2—C11 | 114.2 (3) | C14—N1—C11—C2 | 165.5 (3) |
| C1—C2—C3—C4 | 0.9 (4) | Pd1—N1—C11—C2 | −15.6 (4) |
| C11—C2—C3—C4 | 165.6 (4) | C3—C2—C11—N2 | 10.2 (6) |
| Fe1—C2—C3—C4 | 60.5 (3) | C1—C2—C11—N2 | 173.6 (3) |
| C1—C2—C3—Fe1 | −59.7 (2) | Fe1—C2—C11—N2 | 93.2 (4) |
| C11—C2—C3—Fe1 | 105.1 (4) | C3—C2—C11—N1 | −166.4 (4) |
| C2—Fe1—C3—C4 | −118.1 (3) | C1—C2—C11—N1 | −3.0 (5) |
| C9—Fe1—C3—C4 | 121.5 (3) | Fe1—C2—C11—N1 | −83.4 (3) |
| C7—Fe1—C3—C4 | −167.6 (5) | C11—N2—C12—C13 | 3.9 (6) |
| C10—Fe1—C3—C4 | 79.4 (3) | C11—N2—C12—C16 | −179.0 (4) |
| C8—Fe1—C3—C4 | 162.4 (3) | N2—C12—C13—C14 | −7.1 (7) |
| C6—Fe1—C3—C4 | 49.4 (6) | C16—C12—C13—C14 | 175.9 (4) |
| C5—Fe1—C3—C4 | −37.2 (2) | C11—N1—C14—C13 | 7.0 (6) |
| C1—Fe1—C3—C4 | −80.5 (2) | Pd1—N1—C14—C13 | −171.6 (3) |
| C9—Fe1—C3—C2 | −120.3 (3) | C11—N1—C14—C15 | −168.0 (4) |
| C7—Fe1—C3—C2 | −49.5 (6) | Pd1—N1—C14—C15 | 13.5 (6) |
| C10—Fe1—C3—C2 | −162.5 (3) | C12—C13—C14—N1 | 1.3 (7) |
| C8—Fe1—C3—C2 | −79.5 (3) | C12—C13—C14—C15 | 176.2 (5) |
| C4—Fe1—C3—C2 | 118.1 (3) | C29—P1—C17—C22 | −87.5 (3) |
| C6—Fe1—C3—C2 | 167.5 (5) | C23—P1—C17—C22 | 163.6 (3) |
| C5—Fe1—C3—C2 | 81.0 (2) | Pd1—P1—C17—C22 | 43.2 (3) |
| C1—Fe1—C3—C2 | 37.6 (2) | C29—P1—C17—C18 | 148.7 (3) |
| C2—C3—C4—C5 | −1.0 (4) | C23—P1—C17—C18 | 39.9 (3) |
| Fe1—C3—C4—C5 | 58.8 (3) | Pd1—P1—C17—C18 | −80.5 (3) |
| C2—C3—C4—Fe1 | −59.8 (2) | C22—C17—C18—C19 | 57.1 (4) |
| C2—Fe1—C4—C3 | 38.7 (2) | P1—C17—C18—C19 | −179.1 (3) |
| C9—Fe1—C4—C3 | −76.8 (3) | C17—C18—C19—C20 | −58.0 (5) |
| C7—Fe1—C4—C3 | 167.4 (5) | C18—C19—C20—C21 | 56.7 (5) |
| C10—Fe1—C4—C3 | −119.6 (3) | C19—C20—C21—C22 | −54.9 (5) |
| C8—Fe1—C4—C3 | −44.7 (6) | C18—C17—C22—C21 | −56.3 (4) |
| C6—Fe1—C4—C3 | −160.9 (3) | P1—C17—C22—C21 | 177.7 (3) |
| C5—Fe1—C4—C3 | 120.3 (3) | C20—C21—C22—C17 | 55.5 (5) |
| C1—Fe1—C4—C3 | 83.4 (2) | C29—P1—C23—C28 | 71.5 (3) |
| C2—Fe1—C4—C5 | −81.6 (2) | C17—P1—C23—C28 | −173.0 (3) |
| C3—Fe1—C4—C5 | −120.3 (3) | Pd1—P1—C23—C28 | −50.7 (3) |
| C9—Fe1—C4—C5 | 163.0 (3) | C29—P1—C23—C24 | −57.1 (3) |
| C7—Fe1—C4—C5 | 47.1 (6) | C17—P1—C23—C24 | 58.3 (3) |
| C10—Fe1—C4—C5 | 120.2 (3) | Pd1—P1—C23—C24 | −179.3 (2) |
| C8—Fe1—C4—C5 | −164.9 (5) | C28—C23—C24—C25 | 58.1 (4) |
| C6—Fe1—C4—C5 | 78.8 (3) | P1—C23—C24—C25 | −171.8 (3) |
| C1—Fe1—C4—C5 | −36.9 (2) | C23—C24—C25—C26 | −57.2 (5) |
| C2—C1—C5—C4 | −0.2 (4) | C24—C25—C26—C27 | 56.0 (5) |
| Pd1—C1—C5—C4 | 166.0 (3) | C25—C26—C27—C28 | −56.1 (5) |
| Fe1—C1—C5—C4 | −58.7 (3) | C26—C27—C28—C23 | 57.9 (5) |
| C2—C1—C5—Fe1 | 58.5 (2) | C24—C23—C28—C27 | −58.8 (4) |
| Pd1—C1—C5—Fe1 | −135.3 (4) | P1—C23—C28—C27 | 169.4 (3) |

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| C3—C4—C5—C1 | 0.7 (4) | C17—P1—C29—C30 | 169.9 (2) |
| Fe1—C4—C5—C1 | 59.0 (2) | C23—P1—C29—C30 | −78.0 (3) |
| C3—C4—C5—Fe1 | −58.3 (3) | Pd1—P1—C29—C30 | 40.4 (3) |
| C2—Fe1—C5—C1 | −38.9 (2) | C17—P1—C29—C34 | −18.8 (4) |
| C3—Fe1—C5—C1 | −83.4 (2) | C23—P1—C29—C34 | 93.4 (3) |
| C9—Fe1—C5—C1 | −164.6 (5) | Pd1—P1—C29—C34 | −148.2 (3) |
| C7—Fe1—C5—C1 | 77.6 (3) | C34—C29—C30—C31 | −4.5 (5) |
| C10—Fe1—C5—C1 | 160.6 (3) | P1—C29—C30—C31 | 168.2 (3) |
| C8—Fe1—C5—C1 | 44.3 (6) | C29—C30—C31—C32 | 0.4 (6) |
| C4—Fe1—C5—C1 | −120.4 (3) | C30—C31—C32—C33 | 2.3 (7) |
| C6—Fe1—C5—C1 | 118.7 (3) | C31—C32—C33—C34 | −0.8 (7) |
| C2—Fe1—C5—C4 | 81.4 (3) | C32—C33—C34—C29 | −3.4 (6) |
| C3—Fe1—C5—C4 | 37.0 (2) | C32—C33—C34—C35 | 177.1 (4) |
| C9—Fe1—C5—C4 | −44.3 (6) | C30—C29—C34—C33 | 5.8 (5) |
| C7—Fe1—C5—C4 | −162.0 (3) | P1—C29—C34—C33 | −165.1 (3) |
| C10—Fe1—C5—C4 | −79.0 (3) | C30—C29—C34—C35 | −174.8 (3) |
| C8—Fe1—C5—C4 | 164.6 (5) | P1—C29—C34—C35 | 14.3 (6) |
| C6—Fe1—C5—C4 | −120.9 (3) | C33—C34—C35—C40 | 80.8 (5) |
| C1—Fe1—C5—C4 | 120.4 (3) | C29—C34—C35—C40 | −98.7 (5) |
| C2—Fe1—C6—C7 | −42.9 (6) | C33—C34—C35—C36 | −94.5 (5) |
| C3—Fe1—C6—C7 | 160.3 (4) | C29—C34—C35—C36 | 86.0 (5) |
| C9—Fe1—C6—C7 | 80.9 (4) | C42—N3—C36—C37 | −113.7 (5) |
| C10—Fe1—C6—C7 | 119.5 (5) | C43—N3—C36—C37 | 18.8 (6) |
| C8—Fe1—C6—C7 | 37.4 (3) | C42—N3—C36—C35 | 67.7 (5) |
| C4—Fe1—C6—C7 | −163.2 (3) | C43—N3—C36—C35 | −159.8 (4) |
| C5—Fe1—C6—C7 | −120.8 (3) | C40—C35—C36—C37 | 3.1 (6) |
| C1—Fe1—C6—C7 | −78.3 (3) | C34—C35—C36—C37 | 178.4 (4) |
| C2—Fe1—C6—C10 | −162.4 (5) | C40—C35—C36—N3 | −178.3 (4) |
| C3—Fe1—C6—C10 | 40.7 (7) | C34—C35—C36—N3 | −3.0 (6) |
| C9—Fe1—C6—C10 | −38.7 (4) | N3—C36—C37—C38 | 179.6 (4) |
| C7—Fe1—C6—C10 | −119.5 (5) | C35—C36—C37—C38 | −1.7 (7) |
| C8—Fe1—C6—C10 | −82.1 (4) | C36—C37—C38—C39 | −0.5 (8) |
| C4—Fe1—C6—C10 | 77.3 (4) | C37—C38—C39—C40 | 1.3 (8) |
| C5—Fe1—C6—C10 | 119.7 (3) | C38—C39—C40—C35 | 0.1 (7) |
| C1—Fe1—C6—C10 | 162.2 (3) | C36—C35—C40—C39 | −2.3 (6) |
| C10—C6—C7—C8 | −1.0 (5) | C34—C35—C40—C39 | −177.9 (4) |
| Fe1—C6—C7—C8 | −60.1 (3) | | |

*Hydrogen-bond geometry (Å, °)*

| D—H···A | D—H | H···A | D···A | D—H···A |
|---|---|---|---|---|
| C3—H3···Cl2[i] | 0.98 | 2.78 | 3.671 (5) | 151 |
| C16—H16*C*···*Cg*1[ii] | 0.96 | 2.68 | 3.544 (6) | 151 |

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