

Dichlorido[[2-(diphenylphosphino)-phenyliminomethyl]ferrocene-κ²N,P]-platinum(II) dichloromethane hemisolvate

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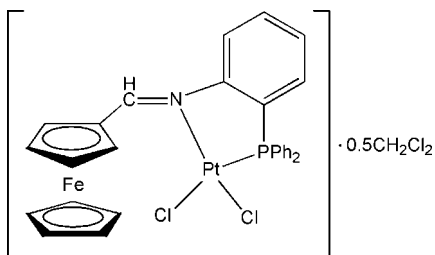
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Key indicators: single-crystal X-ray study; *T* = 293 K; mean σ (C–C) = 0.008 Å; disorder in solvent or counterion; *R* factor = 0.043; *wR* factor = 0.116; data-to-parameter ratio = 17.1.

In the title compound, [FePt(C₅H₅)(C₂₄H₁₉NP)Cl₂]-0.5CH₂Cl₂, the Pt^{II} atom adopts a distorted square-planar geometry defined by one P atom and one N atom from the bidentate [2-(diphenylphosphino)phenyliminomethyl]ferrocene ligand and two Cl atoms. Two disordered dichloromethane solvent molecules are each 0.25-occupied on a twofold rotation axis.

Related literature

For general background, see: Cullen & Woolins (1981); Farrell *et al.* (2002); Gul *et al.* (2002); Wu *et al.* (2001). For the ligand synthesis, see: Gong *et al.* (2006); Zhang *et al.* (2006).



Experimental

Crystal data

[FePt(C₅H₅)(C₂₄H₁₉NP)Cl₂]-0.5CH₂Cl₂

M_r = 781.75
Orthorhombic, *P*2₁2₁2

a = 19.5045 (11) Å
b = 12.0182 (7) Å
c = 12.9800 (8) Å
V = 3042.6 (3) Å³
Z = 4

Mo *K*α radiation
 μ = 5.40 mm⁻¹
T = 293 (2) K
0.3 × 0.1 × 0.1 mm

Data collection

Siemens SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
*T*_{min} = 0.532, *T*_{max} = 0.588

19964 measured reflections
5902 independent reflections
4954 reflections with *I* > 2σ(*I*)
*R*_{int} = 0.058

Refinement

R [*F*² > 2σ(*F*²)] = 0.043
wR (*F*²) = 0.116
S = 1.04
5902 reflections
345 parameters
24 restraints

H-atom parameters constrained
 $\Delta\rho_{\text{max}}$ = 1.18 e Å⁻³
 $\Delta\rho_{\text{min}}$ = -0.93 e Å⁻³
Absolute structure: Flack (1983), 856 Friedel pairs
Flack parameter: 0.002 (11)

Table 1

Selected bond lengths (Å).

| | | | |
|------|-------------|--------|-------------|
| Pt–N | 2.031 (3) | Pt–Cl1 | 2.2996 (13) |
| Pt–P | 2.2089 (10) | Pt–Cl2 | 2.3673 (11) |

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINTE* (Siemens, 1996); data reduction: *SAINTE*; 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2171).

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supplementary materials

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Dichlorido{[2-(diphenylphosphino)phenyliminomethyl]ferrocene- κ^2N,P }platinum(II) dichloromethane hemisolvate

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Comment

Ferrocene derivatives containing heteroatoms with good donor abilities have attracted great interest during the last few years in organometallic chemistry, since the coordination of a metal to these heteroatoms produces polymetallic molecules (Cullen & Woolins, 1981). Some examples showing the utility of these polymetallic compounds in homogeneous catalysis (Farrell *et al.*, 2002; Wu *et al.*, 2001) or for the design of new materials with outstanding properties (Gul *et al.*, 2002) have been described. Here we report a new bimetallic platinum(II) complex with a ferrocenyliminophosphine ligand.

In the title compound, the Pt^{II} atom adopts a distorted square planar geometry, defined by one P atom and one N atom from the bidentate ferrocenyliminophosphine ligand (*L*) and two Cl atoms (Fig. 1), with N—Pt—Cl1 = 176.29 (9)° and P—Pt—Cl2 = 170.19 (4)°. The difference between the Pt—Cl bond lengths [2.2996 (13) and 2.3673 (11) Å] (Table 1) reflects the stronger *trans* influence of the tertiary phosphine compared with the imino group. The ligand *L* adopts a five-membered chelating ring. The benzene ring and the cyclopentadienyl ring are *trans*, with respect to the C11—N double bond.

Experimental

The ligand *L* was prepared by literature method (Gong *et al.*, 2006; Zhang *et al.*, 2006). The title compound was prepared by reacting equal molar K₂PtCl₄ and *L* in CH₂Cl₂ (yield 83%). Brown needle crystals suitable for X-ray analysis were obtained by vapor diffusion of diethyl ether into a solution of the title compound in CH₂Cl₂. Analysis calculated for C_{29.5}H₂₅Cl₃FeNPt: C 45.32, H 3.22, N 1.79%; found: C 45.61, H 3.33, N 1.70%.

Refinement

H atoms were positioned geometrically and treated as riding, with C—H = 0.98 (cyclopentadienyl), 0.93 (phenyl) and 0.96 (CH₂) Å and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The highest residual electron density was found 0.67 Å from atom Cl4 and the deepest hole 0.79 Å from atom Pt. The disordered dichloromethane solvent molecules are each 0.25-occupied on a twofold rotation axis.

Figures

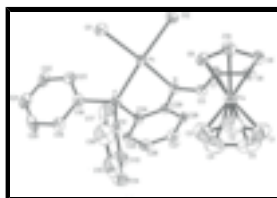


Fig. 1. The molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. H atoms and disordered dichloromethane solvent molecules have been omitted for clarity.

Dichlorido{[2-(diphenylphosphino)phenyliminomethyl]ferrocene- κ^2N,P }platinum(II) dichloromethane hemisolvate

Crystal data

| | |
|---|--|
| $[\text{FePt}(\text{C}_5\text{H}_5)(\text{C}_{24}\text{H}_{19}\text{NP})\text{Cl}_2] \cdot 0.5\text{CH}_2\text{Cl}_2$ | $F_{000} = 1516$ |
| $M_r = 781.75$ | $D_x = 1.707 \text{ Mg m}^{-3}$ |
| Orthorhombic, $P2_12_12$ | Mo $K\alpha$ radiation |
| Hall symbol: P 2 2ab | $\lambda = 0.71073 \text{ \AA}$ |
| $a = 19.5045 (11) \text{ \AA}$ | Cell parameters from 892 reflections |
| $b = 12.0182 (7) \text{ \AA}$ | $\theta = 3.2\text{--}25.8^\circ$ |
| $c = 12.9800 (8) \text{ \AA}$ | $\mu = 5.40 \text{ mm}^{-1}$ |
| $V = 3042.6 (3) \text{ \AA}^3$ | $T = 293 (2) \text{ K}$ |
| $Z = 4$ | Needle, brown–yellow |
| | $0.3 \times 0.1 \times 0.1 \text{ mm}$ |

Data collection

| | |
|---|--|
| Siemens SMART CCD diffractometer | 5902 independent reflections |
| Radiation source: fine-focus sealed tube | 4954 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{\text{int}} = 0.058$ |
| $T = 293(2) \text{ K}$ | $\theta_{\text{max}} = 26.0^\circ$ |
| ω scans | $\theta_{\text{min}} = 1.9^\circ$ |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996) | $h = -23 \rightarrow 24$ |
| $T_{\text{min}} = 0.532, T_{\text{max}} = 0.588$ | $k = -14 \rightarrow 14$ |
| 19964 measured reflections | $l = -16 \rightarrow 15$ |

Refinement

| | |
|--|--|
| Refinement on F^2 | Hydrogen site location: inferred from neighbouring sites |
| Least-squares matrix: full | H-atom parameters constrained |
| $R[F^2 > 2\sigma(F^2)] = 0.043$ | $w = 1/[\sigma^2(F_o^2) + (0.05P)^2]$ |
| $wR(F^2) = 0.116$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.04$ | $(\Delta/\sigma)_{\text{max}} = 0.024$ |
| 5902 reflections | $\Delta\rho_{\text{max}} = 1.18 \text{ e \AA}^{-3}$ |
| 345 parameters | $\Delta\rho_{\text{min}} = -0.93 \text{ e \AA}^{-3}$ |
| 24 restraints | Extinction correction: none |
| Primary atom site location: structure-invariant direct methods | Absolute structure: Flack (1983), 856 Friedel pairs |
| Secondary atom site location: difference Fourier map | Flack parameter: 0.002 (11) |

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

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ | Occ. (<1) |
|------|--------------|---------------|---------------|----------------------------------|-----------|
| Pt | 0.270357 (7) | 0.911967 (14) | 0.143789 (12) | 0.03558 (4) | |
| Fe | 0.34183 (3) | 0.52770 (6) | 0.19921 (5) | 0.04447 (19) | |
| Cl1 | 0.32009 (6) | 1.06905 (11) | 0.21198 (10) | 0.0568 (4) | |
| Cl2 | 0.35362 (5) | 0.90898 (12) | 0.01112 (9) | 0.0538 (3) | |
| Cl3 | 0.4874 (2) | 0.8826 (5) | 0.3249 (4) | 0.167 (2) | 0.50 |
| Cl4 | 0.06774 (11) | 0.54821 (19) | 0.23620 (19) | 0.0506 (7) | 0.50 |
| P | 0.17978 (5) | 0.91268 (11) | 0.24594 (8) | 0.0378 (3) | |
| N | 0.22282 (15) | 0.7723 (3) | 0.0921 (2) | 0.0337 (9) | |
| C1 | 0.3477 (4) | 0.3728 (6) | 0.2664 (5) | 0.097 (3) | |
| H1A | 0.3771 | 0.3110 | 0.2447 | 0.117* | |
| C2 | 0.3629 (4) | 0.4509 (6) | 0.3371 (4) | 0.096 (3) | |
| H2A | 0.4066 | 0.4563 | 0.3742 | 0.115* | |
| C3 | 0.3087 (4) | 0.5257 (7) | 0.3468 (5) | 0.102 (2) | |
| H3A | 0.3067 | 0.5896 | 0.3936 | 0.123* | |
| C4 | 0.2585 (4) | 0.4921 (8) | 0.2825 (6) | 0.112 (2) | |
| H4A | 0.2137 | 0.5282 | 0.2749 | 0.135* | |
| C5 | 0.2797 (4) | 0.3974 (6) | 0.2289 (6) | 0.110 (3) | |
| H5A | 0.2530 | 0.3543 | 0.1789 | 0.132* | |
| C6 | 0.3711 (2) | 0.6848 (4) | 0.1581 (3) | 0.0451 (13) | |
| H6A | 0.3666 | 0.7517 | 0.2007 | 0.054* | |
| C7 | 0.3221 (2) | 0.6444 (4) | 0.0886 (3) | 0.0402 (12) | |
| C8 | 0.3478 (2) | 0.5451 (4) | 0.0462 (3) | 0.0442 (13) | |
| H8A | 0.3246 | 0.4984 | -0.0050 | 0.053* | |
| C9 | 0.4145 (2) | 0.5275 (4) | 0.0860 (4) | 0.0482 (13) | |
| H9A | 0.4452 | 0.4658 | 0.0686 | 0.058* | |
| C10 | 0.4278 (2) | 0.6129 (4) | 0.1561 (4) | 0.0539 (15) | |
| H10A | 0.4696 | 0.6210 | 0.1973 | 0.065* | |
| C11 | 0.25027 (18) | 0.6757 (4) | 0.0722 (3) | 0.0360 (11) | |
| H11A | 0.2215 | 0.6215 | 0.0449 | 0.043* | |
| C12 | 0.1890 (2) | 0.8272 (4) | 0.3601 (4) | 0.0516 (13) | |
| C13 | 0.1388 (3) | 0.7539 (5) | 0.3915 (4) | 0.0752 (19) | |
| H13A | 0.0985 | 0.7462 | 0.3539 | 0.090* | |
| C14 | 0.1495 (4) | 0.6915 (6) | 0.4806 (4) | 0.090 (2) | |
| H14A | 0.1174 | 0.6392 | 0.5022 | 0.108* | |
| C15 | 0.2068 (3) | 0.7088 (6) | 0.5338 (5) | 0.092 (2) | |
| H15A | 0.2139 | 0.6660 | 0.5925 | 0.111* | |
| C16 | 0.2540 (3) | 0.7823 (6) | 0.5090 (5) | 0.0902 (19) | |
| H16A | 0.2923 | 0.7946 | 0.5502 | 0.108* | |
| C17 | 0.2437 (3) | 0.8398 (6) | 0.4191 (4) | 0.086 (2) | |
| H17A | 0.2770 | 0.8904 | 0.3985 | 0.104* | |
| C18 | 0.1426 (2) | 1.0435 (4) | 0.2854 (3) | 0.0443 (13) | |
| C19 | 0.1014 (3) | 1.0460 (5) | 0.3785 (4) | 0.0586 (16) | |
| H19A | 0.0966 | 0.9831 | 0.4195 | 0.070* | |
| C20 | 0.0699 (3) | 1.1442 (5) | 0.4040 (5) | 0.0793 (19) | |
| H20A | 0.0416 | 1.1462 | 0.4617 | 0.095* | |

supplementary materials

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|------|--------------|------------|-------------|-------------|------|
| C21 | 0.0784 (3) | 1.2379 (4) | 0.3481 (5) | 0.0659 (17) | |
| H21A | 0.0579 | 1.3039 | 0.3693 | 0.079* | |
| C22 | 0.1165 (3) | 1.2358 (5) | 0.2618 (5) | 0.0641 (17) | |
| H22A | 0.1198 | 1.2999 | 0.2219 | 0.077* | |
| C23 | 0.1507 (2) | 1.1413 (4) | 0.2307 (4) | 0.0505 (14) | |
| H23A | 0.1792 | 1.1434 | 0.1732 | 0.061* | |
| C24 | 0.1200 (2) | 0.8442 (4) | 0.1607 (3) | 0.0378 (11) | |
| C25 | 0.0481 (2) | 0.8598 (4) | 0.1615 (3) | 0.0404 (12) | |
| H25A | 0.0273 | 0.9038 | 0.2115 | 0.049* | |
| C26 | 0.0092 (2) | 0.8074 (4) | 0.0854 (4) | 0.0536 (15) | |
| H26A | -0.0381 | 0.8164 | 0.0841 | 0.064* | |
| C27 | 0.0420 (2) | 0.7399 (4) | 0.0095 (3) | 0.0506 (14) | |
| H27A | 0.0159 | 0.7044 | -0.0406 | 0.061* | |
| C28 | 0.1120 (2) | 0.7269 (4) | 0.0100 (3) | 0.0410 (12) | |
| H28A | 0.1336 | 0.6825 | -0.0389 | 0.049* | |
| C29 | 0.14973 (19) | 0.7811 (3) | 0.0845 (3) | 0.0372 (11) | |
| C30 | 0.5000 | 1.0000 | 0.2754 (18) | 0.104 (8) | 0.50 |
| H30A | 0.5386 | 0.9885 | 0.2308 | 0.125* | 0.50 |
| C31 | 0.0000 | 0.5000 | 0.1697 (9) | 0.051 (4) | 0.50 |
| H31A | -0.0159 | 0.5590 | 0.1260 | 0.061* | 0.50 |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|-------------|--------------|--------------|
| Pt | 0.03605 (6) | 0.03424 (7) | 0.03646 (7) | 0.00216 (7) | -0.00032 (7) | 0.00005 (8) |
| Fe | 0.0432 (3) | 0.0405 (4) | 0.0497 (4) | 0.0021 (3) | 0.0018 (3) | -0.0005 (3) |
| Cl1 | 0.0584 (6) | 0.0514 (7) | 0.0608 (7) | -0.0109 (6) | 0.0017 (5) | -0.0103 (6) |
| Cl2 | 0.0508 (5) | 0.0506 (6) | 0.0598 (6) | 0.0014 (6) | 0.0200 (5) | 0.0055 (6) |
| Cl3 | 0.131 (3) | 0.146 (5) | 0.223 (5) | -0.030 (3) | -0.087 (3) | 0.041 (4) |
| Cl4 | 0.0373 (10) | 0.0439 (13) | 0.0706 (14) | -0.0113 (9) | -0.0071 (10) | -0.0009 (11) |
| P | 0.0425 (5) | 0.0380 (6) | 0.0329 (5) | 0.0046 (6) | 0.0017 (4) | 0.0009 (5) |
| N | 0.0341 (15) | 0.0340 (17) | 0.0331 (15) | 0.0043 (15) | 0.0016 (14) | -0.0008 (14) |
| C1 | 0.132 (5) | 0.060 (4) | 0.100 (5) | -0.006 (4) | 0.029 (4) | 0.016 (3) |
| C2 | 0.119 (5) | 0.115 (6) | 0.054 (3) | -0.001 (4) | 0.009 (3) | 0.029 (3) |
| C3 | 0.124 (4) | 0.104 (4) | 0.078 (3) | 0.008 (3) | 0.032 (3) | -0.005 (3) |
| C4 | 0.097 (4) | 0.117 (4) | 0.123 (4) | 0.006 (3) | 0.030 (3) | 0.021 (4) |
| C5 | 0.123 (5) | 0.113 (5) | 0.095 (5) | -0.060 (5) | -0.009 (4) | 0.023 (4) |
| C6 | 0.046 (2) | 0.038 (2) | 0.051 (3) | -0.004 (2) | -0.010 (2) | -0.004 (2) |
| C7 | 0.051 (2) | 0.031 (2) | 0.039 (2) | 0.009 (2) | 0.001 (2) | -0.0032 (19) |
| C8 | 0.038 (2) | 0.045 (3) | 0.049 (2) | 0.004 (2) | -0.0016 (19) | -0.003 (2) |
| C9 | 0.036 (2) | 0.042 (3) | 0.066 (3) | 0.005 (2) | 0.002 (2) | -0.006 (2) |
| C10 | 0.0300 (18) | 0.065 (3) | 0.067 (3) | 0.004 (2) | -0.006 (2) | -0.011 (3) |
| C11 | 0.0337 (19) | 0.044 (2) | 0.0302 (19) | 0.0036 (17) | -0.0006 (16) | 0.0032 (19) |
| C12 | 0.063 (2) | 0.047 (3) | 0.044 (2) | 0.020 (2) | 0.016 (2) | -0.005 (2) |
| C13 | 0.095 (4) | 0.068 (4) | 0.063 (3) | 0.015 (3) | 0.018 (3) | 0.018 (3) |
| C14 | 0.129 (5) | 0.075 (4) | 0.067 (3) | 0.004 (4) | 0.045 (3) | 0.023 (3) |
| C15 | 0.121 (4) | 0.087 (4) | 0.069 (3) | 0.035 (3) | 0.006 (3) | 0.011 (3) |
| C16 | 0.093 (3) | 0.095 (4) | 0.083 (3) | 0.028 (3) | -0.014 (3) | 0.018 (3) |

| | | | | | | |
|-----|-------------|------------|------------|--------------|--------------|--------------|
| C17 | 0.108 (4) | 0.114 (5) | 0.037 (2) | 0.045 (4) | -0.034 (3) | -0.007 (3) |
| C18 | 0.040 (2) | 0.049 (3) | 0.044 (2) | 0.013 (2) | -0.0078 (19) | -0.007 (2) |
| C19 | 0.065 (3) | 0.058 (3) | 0.053 (3) | -0.002 (3) | 0.011 (2) | -0.011 (2) |
| C20 | 0.070 (3) | 0.093 (4) | 0.075 (3) | 0.038 (3) | 0.015 (3) | -0.029 (3) |
| C21 | 0.071 (3) | 0.037 (3) | 0.090 (4) | 0.016 (2) | -0.010 (3) | -0.006 (3) |
| C22 | 0.064 (3) | 0.042 (3) | 0.085 (4) | 0.010 (3) | -0.007 (3) | -0.017 (3) |
| C23 | 0.052 (2) | 0.048 (3) | 0.051 (3) | -0.003 (2) | -0.007 (2) | 0.002 (2) |
| C24 | 0.048 (2) | 0.039 (2) | 0.026 (2) | 0.0119 (19) | 0.0011 (18) | 0.0000 (18) |
| C25 | 0.0375 (19) | 0.042 (2) | 0.042 (2) | -0.0011 (19) | 0.0028 (18) | 0.003 (2) |
| C26 | 0.039 (2) | 0.056 (3) | 0.065 (3) | 0.005 (2) | -0.004 (2) | 0.017 (3) |
| C27 | 0.047 (2) | 0.051 (3) | 0.054 (3) | 0.003 (2) | -0.018 (2) | 0.001 (2) |
| C28 | 0.040 (2) | 0.028 (2) | 0.055 (3) | 0.0042 (19) | 0.003 (2) | -0.0047 (19) |
| C29 | 0.0346 (18) | 0.029 (2) | 0.048 (2) | 0.0037 (18) | 0.0009 (18) | 0.0088 (19) |
| C30 | 0.017 (6) | 0.121 (17) | 0.174 (19) | 0.001 (8) | 0.000 | 0.000 |
| C31 | 0.093 (9) | 0.020 (6) | 0.040 (7) | -0.019 (7) | 0.000 | 0.000 |

Geometric parameters (Å, °)

| | | | |
|---------|-------------|----------|------------|
| Pt—N | 2.031 (3) | C9—H9A | 0.9800 |
| Pt—P | 2.2089 (10) | C10—H10A | 0.9800 |
| Pt—Cl1 | 2.2996 (13) | C11—H11A | 0.9300 |
| Pt—Cl2 | 2.3673 (11) | C12—C17 | 1.323 (7) |
| Fe—C1 | 2.059 (7) | C12—C13 | 1.379 (8) |
| Fe—C2 | 2.055 (6) | C13—C14 | 1.394 (8) |
| Fe—C3 | 2.022 (7) | C13—H13A | 0.9300 |
| Fe—C4 | 1.998 (8) | C14—C15 | 1.330 (9) |
| Fe—C5 | 2.017 (7) | C14—H14A | 0.9300 |
| Fe—C6 | 2.043 (5) | C15—C16 | 1.317 (10) |
| Fe—C7 | 2.044 (4) | C15—H15A | 0.9300 |
| Fe—C8 | 2.000 (5) | C16—C17 | 1.371 (9) |
| Fe—C9 | 2.041 (5) | C16—H16A | 0.9300 |
| Fe—C10 | 2.042 (5) | C17—H17A | 0.9300 |
| Cl3—C30 | 1.570 (11) | C18—C23 | 1.382 (7) |
| Cl4—C31 | 1.681 (6) | C18—C19 | 1.451 (6) |
| P—C18 | 1.806 (5) | C19—C20 | 1.371 (8) |
| P—C24 | 1.806 (4) | C19—H19A | 0.9300 |
| P—C12 | 1.812 (5) | C20—C21 | 1.350 (8) |
| N—C11 | 1.304 (5) | C20—H20A | 0.9300 |
| N—C29 | 1.433 (5) | C21—C22 | 1.345 (8) |
| C1—C2 | 1.346 (10) | C21—H21A | 0.9300 |
| C1—C5 | 1.443 (10) | C22—C23 | 1.378 (7) |
| C1—H1A | 0.9800 | C22—H22A | 0.9300 |
| C2—C3 | 1.393 (10) | C23—H23A | 0.9300 |
| C2—H2A | 0.9800 | C24—C29 | 1.375 (6) |
| C3—C4 | 1.348 (11) | C24—C25 | 1.413 (6) |
| C3—H3A | 0.9800 | C25—C26 | 1.397 (6) |
| C4—C5 | 1.396 (11) | C25—H25A | 0.9300 |
| C4—H4A | 0.9800 | C26—C27 | 1.427 (7) |
| C5—H5A | 0.9800 | C26—H26A | 0.9300 |

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| C6—C7 | 1.401 (6) | C27—C28 | 1.375 (6) |
| C6—C10 | 1.404 (6) | C27—H27A | 0.9300 |
| C6—H6A | 0.9800 | C28—C29 | 1.378 (6) |
| C7—C8 | 1.407 (6) | C28—H28A | 0.9300 |
| C7—C11 | 1.466 (6) | C30—C13 ⁱ | 1.570 (11) |
| C8—C9 | 1.415 (6) | C30—H30A | 0.9600 |
| C8—H8A | 0.9800 | C31—C14 ⁱⁱ | 1.681 (6) |
| C9—C10 | 1.396 (7) | C31—H31A | 0.9600 |
| N—Pt—P | 80.59 (9) | C10—C6—Fe | 69.9 (3) |
| N—Pt—C11 | 176.29 (9) | C7—C6—H6A | 125.9 |
| P—Pt—C11 | 95.92 (4) | C10—C6—H6A | 125.9 |
| N—Pt—C12 | 93.46 (9) | Fe—C6—H6A | 125.9 |
| P—Pt—C12 | 170.19 (4) | C6—C7—C8 | 107.6 (4) |
| C11—Pt—C12 | 90.17 (4) | C6—C7—C11 | 131.0 (4) |
| C4—Fe—C8 | 127.4 (3) | C8—C7—C11 | 120.1 (4) |
| C4—Fe—C5 | 40.7 (3) | C6—C7—Fe | 69.9 (3) |
| C8—Fe—C5 | 107.8 (3) | C8—C7—Fe | 68.0 (3) |
| C4—Fe—C3 | 39.2 (3) | C11—C7—Fe | 117.3 (3) |
| C8—Fe—C3 | 163.9 (2) | C7—C8—C9 | 108.2 (4) |
| C5—Fe—C3 | 67.5 (3) | C7—C8—Fe | 71.3 (3) |
| C4—Fe—C9 | 162.5 (3) | C9—C8—Fe | 71.1 (3) |
| C8—Fe—C9 | 40.96 (18) | C7—C8—H8A | 125.9 |
| C5—Fe—C9 | 123.6 (3) | C9—C8—H8A | 125.9 |
| C3—Fe—C9 | 154.7 (2) | Fe—C8—H8A | 125.9 |
| C4—Fe—C10 | 157.4 (3) | C10—C9—C8 | 107.4 (4) |
| C8—Fe—C10 | 68.14 (19) | C10—C9—Fe | 70.1 (3) |
| C5—Fe—C10 | 159.2 (3) | C8—C9—Fe | 68.0 (3) |
| C3—Fe—C10 | 121.9 (3) | C10—C9—H9A | 126.3 |
| C9—Fe—C10 | 39.98 (19) | C8—C9—H9A | 126.3 |
| C4—Fe—C6 | 124.5 (3) | Fe—C9—H9A | 126.3 |
| C8—Fe—C6 | 68.16 (18) | C9—C10—C6 | 108.6 (4) |
| C5—Fe—C6 | 159.2 (2) | C9—C10—Fe | 70.0 (3) |
| C3—Fe—C6 | 110.3 (3) | C6—C10—Fe | 69.9 (3) |
| C9—Fe—C6 | 67.63 (19) | C9—C10—H10A | 125.7 |
| C10—Fe—C6 | 40.19 (18) | C6—C10—H10A | 125.7 |
| C4—Fe—C7 | 111.9 (3) | Fe—C10—H10A | 125.7 |
| C8—Fe—C7 | 40.71 (18) | N—C11—C7 | 126.3 (4) |
| C5—Fe—C7 | 123.6 (2) | N—C11—H11A | 116.9 |
| C3—Fe—C7 | 127.8 (3) | C7—C11—H11A | 116.9 |
| C9—Fe—C7 | 68.04 (18) | C17—C12—C13 | 118.3 (5) |
| C10—Fe—C7 | 67.55 (18) | C17—C12—P | 119.3 (4) |
| C6—Fe—C7 | 40.09 (17) | C13—C12—P | 122.3 (4) |
| C4—Fe—C2 | 66.2 (3) | C12—C13—C14 | 118.9 (6) |
| C8—Fe—C2 | 154.1 (2) | C12—C13—H13A | 120.6 |
| C5—Fe—C2 | 66.8 (3) | C14—C13—H13A | 120.6 |
| C3—Fe—C2 | 40.0 (3) | C15—C14—C13 | 118.2 (6) |
| C9—Fe—C2 | 119.2 (2) | C15—C14—H14A | 120.9 |
| C10—Fe—C2 | 107.4 (3) | C13—C14—H14A | 120.9 |

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| C6—Fe—C2 | 125.9 (2) | C16—C15—C14 | 124.5 (7) |
| C7—Fe—C2 | 163.2 (2) | C16—C15—H15A | 117.8 |
| C4—Fe—C1 | 67.8 (3) | C14—C15—H15A | 117.8 |
| C8—Fe—C1 | 120.8 (2) | C15—C16—C17 | 116.3 (6) |
| C5—Fe—C1 | 41.5 (3) | C15—C16—H16A | 121.8 |
| C3—Fe—C1 | 66.8 (3) | C17—C16—H16A | 121.8 |
| C9—Fe—C1 | 105.4 (2) | C12—C17—C16 | 123.7 (6) |
| C10—Fe—C1 | 121.6 (3) | C12—C17—H17A | 118.2 |
| C6—Fe—C1 | 158.5 (2) | C16—C17—H17A | 118.2 |
| C7—Fe—C1 | 158.2 (2) | C23—C18—C19 | 118.3 (4) |
| C2—Fe—C1 | 38.2 (3) | C23—C18—P | 123.3 (3) |
| C18—P—C24 | 108.1 (2) | C19—C18—P | 118.4 (4) |
| C18—P—C12 | 107.6 (2) | C20—C19—C18 | 117.9 (5) |
| C24—P—C12 | 107.9 (2) | C20—C19—H19A | 121.1 |
| C18—P—Pt | 119.65 (15) | C18—C19—H19A | 121.1 |
| C24—P—Pt | 98.46 (13) | C21—C20—C19 | 122.2 (5) |
| C12—P—Pt | 114.18 (15) | C21—C20—H20A | 118.9 |
| C11—N—C29 | 117.4 (3) | C19—C20—H20A | 118.9 |
| C11—N—Pt | 127.8 (3) | C22—C21—C20 | 120.0 (5) |
| C29—N—Pt | 114.6 (2) | C22—C21—H21A | 120.0 |
| C2—C1—C5 | 106.8 (7) | C20—C21—H21A | 120.0 |
| C2—C1—Fe | 70.7 (4) | C21—C22—C23 | 121.8 (5) |
| C5—C1—Fe | 67.7 (4) | C21—C22—H22A | 119.1 |
| C2—C1—H1A | 126.6 | C23—C22—H22A | 119.1 |
| C5—C1—H1A | 126.6 | C22—C23—C18 | 119.6 (5) |
| Fe—C1—H1A | 126.6 | C22—C23—H23A | 120.2 |
| C1—C2—C3 | 110.1 (7) | C18—C23—H23A | 120.2 |
| C1—C2—Fe | 71.1 (4) | C29—C24—C25 | 119.8 (4) |
| C3—C2—Fe | 68.7 (4) | C29—C24—P | 114.8 (3) |
| C1—C2—H2A | 124.9 | C25—C24—P | 125.1 (3) |
| C3—C2—H2A | 124.9 | C26—C25—C24 | 118.3 (4) |
| Fe—C2—H2A | 124.9 | C26—C25—H25A | 120.9 |
| C4—C3—C2 | 107.6 (7) | C24—C25—H25A | 120.9 |
| C4—C3—Fe | 69.5 (4) | C25—C26—C27 | 120.1 (4) |
| C2—C3—Fe | 71.3 (4) | C25—C26—H26A | 120.0 |
| C4—C3—H3A | 126.2 | C27—C26—H26A | 120.0 |
| C2—C3—H3A | 126.2 | C28—C27—C26 | 120.4 (4) |
| Fe—C3—H3A | 126.2 | C28—C27—H27A | 119.8 |
| C3—C4—C5 | 109.7 (7) | C26—C27—H27A | 119.8 |
| C3—C4—Fe | 71.3 (5) | C27—C28—C29 | 118.7 (4) |
| C5—C4—Fe | 70.4 (4) | C27—C28—H28A | 120.7 |
| C3—C4—H4A | 125.1 | C29—C28—H28A | 120.7 |
| C5—C4—H4A | 125.1 | C24—C29—C28 | 122.7 (4) |
| Fe—C4—H4A | 125.1 | C24—C29—N | 114.3 (4) |
| C4—C5—C1 | 105.7 (7) | C28—C29—N | 123.0 (4) |
| C4—C5—Fe | 68.9 (5) | Cl3 ⁱ —C30—Cl3 | 131.7 (16) |
| C1—C5—Fe | 70.8 (4) | Cl3 ⁱ —C30—H30A | 104.6 |
| C4—C5—H5A | 127.1 | Cl3—C30—H30A | 104.0 |

supplementary materials

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| C1—C5—H5A | 127.1 | C14—C31—C14 ⁱⁱ | 118.2 (7) |
| Fe—C5—H5A | 127.1 | C14—C31—H31A | 107.6 |
| C7—C6—C10 | 108.2 (4) | C14 ⁱⁱ —C31—H31A | 107.7 |
| C7—C6—Fe | 70.0 (3) | | |

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

Fig. 1

