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# Chlorido{1-[(dimethylamino)methyl]-ferrocenyl-$\kappa^2C^2,N$}(triphenylstibine-$\kappa Sb$)palladium(II)

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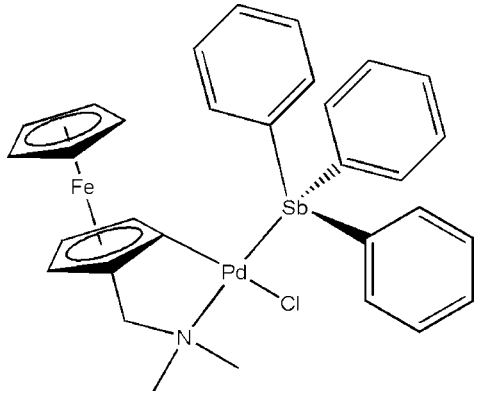
Key indicators: single-crystal X-ray study; $T$ = 291 K; mean $\sigma$(C–C) = 0.007 Å; $R$ factor = 0.032; $wR$ factor = 0.063; data-to-parameter ratio = 15.2.

In the title compound, [FePdCl($C_5H_5$)($C_8H_{11}N$)($C_{18}H_{15}Sb$)], obtained by reaction of diphenyl(*N*,*N*-dimethylaminomethylferrocenyl)stibine with sodium tetrachloridopalladate(II) in acetone, the $Pd^{II}$ atom is coordinated in a slightly distorted square-planar geometry by a C atom of the ferrocenyl ring, and by N, Cl and Sb atoms. The Sb and N atoms are *trans* to each other.

## Related literature

For the use of 1,2-disubstituted ferrocenylphosphines as catalytic precursors, see: Sokolov *et al.* (2005); Zirakzadeh *et al.* (2012). For Pd—Sb bond lengths in related compounds, see: Mentes & Fawcett (2005).




## Experimental

### Crystal data

[FePdCl($C_5H_5$)($C_8H_{11}N$)-($C_{18}H_{15}Sb$)]
$M_r$ = 737.02
Monoclinic, $P2_1/c$
$a$ = 10.3138 (6) Å
$b$ = 19.8865 (12) Å
$c$ = 13.7584 (9) Å
$\beta$ = 92.984 (1)°
$V$ = 2818.1 (3) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 2.21 mm$^{-1}$
$T$ = 291 K
0.36 × 0.12 × 0.10 mm

### Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: analytical (*SADABS*; Bruker, 2007)
$T_{min}$ = 0.490, $T_{max}$ = 0.797
23494 measured reflections
5158 independent reflections
4107 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.048

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.063
$S$ = 0.93
4963 reflections
327 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.77 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.31 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Sb1—C14 | 2.127 (4) | Pd1—C1 | 1.973 (4) |
| Sb1—C20 | 2.120 (4) | Pd1—Cl1 | 2.3952 (10) |
| Sb1—C26 | 2.119 (4) | Pd1—N1 | 2.174 (3) |
| Sb1—Pd1 | 2.4853 (4) | | |

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: VN2072).

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# supporting information

*Acta Cryst.* (2013). E**69**, m372 [https://doi.org/10.1107/S1600536813015109]

# Chlorido{1-[(dimethylamino)methyl]ferrocenyl-$\kappa^2C^2,N$}(triphenylstibine-$\kappa Sb$)palladium(II)

**Diego Pérez, Pankaj Sharma, Manju Sharma and Simón Hernández**

## S1. Comment

1,2-disubstituted ferrocenylphosphines are used as catalytic precursors (Sokolov *et al.*, 2005; Zirakzadeh *et al.*, 2012). In an attempt to synthesize *cis*-dichloro[diphenyl(2-*N*,*N*-dimethylaminomethyl ferrocenyl)-stibino-N,Sb)]palladium(II), [PdCl($C_{10}H_8Fe$)($C_3H_8N$)($C_{18}H_{15}Sb$)] was obtained. This paper describes the crystal structure of a new compound *viz*. chloro-(2-*N*,*N*-dimethylaminomethylferrocenyl)-(triphenylstibino) palladium (II), (Fig. 1), which was grown from $CHCl_3$ and hexane at room temperature. In the crystal structure, palladium is in a slightly distorted square-planar environment bound to a chlorine, the antimony, the nitrogen and the C(1) atom of the ferocenyl unit. The compound contains a bicyclic system, which is formed by the substituted pentagonal ring of the ferrocenyl fragment and a five-membered palladacycle which has an envelope-like conformation. The Pd—Sb bond length in this compound is 2.4853 (4) Å which compares well with the literature values for similar complexes of palladium (Mentes & Fawcett, 2005). The *cis* angles at Pd are close to the expected value of 90°, with the most noticeable distortion being the N—Pd—Cl angle of 93.71 (7)°, as a result of chelation (Fig. 1). The distance between the Fe and the Pd is 3.4836 (7)° for this compound, thus suggesting that there is interaction between the two metals. The two pentagonal rings of the ferrocenyl moiety are nearly parallel (tilt angle 1.74°).

## S2. Experimental

The title compound was obtained as follows: a solution of sodium tetrachloropalladate (0.294 g, 1 mmol) in acetone-water mixture (5 ml, 50–50%) is added to a solution of diphenyl(*N*,*N*-dimethyl aminomethylferrocenyl)stibine (0.519 g, 1 mmol) in acetone(10 ml). The mixture was stirred overnight. A red powder was obtained, which after recrystallization from a chloroform-hexane solvent mixture afforded chloro-(2-*N*,*N*-dimethylaminomethylferrocenyl)(triphenylstibino) palladium (II) as red crystals in 40% yield.

## S3. Refinement

The H-atoms were placed geometrically (C—H = 0.93–0.98 Å), and refined using a riding model with $U_{iso}$(H) = 1.2$U_{eq}$ of the carrier atom.

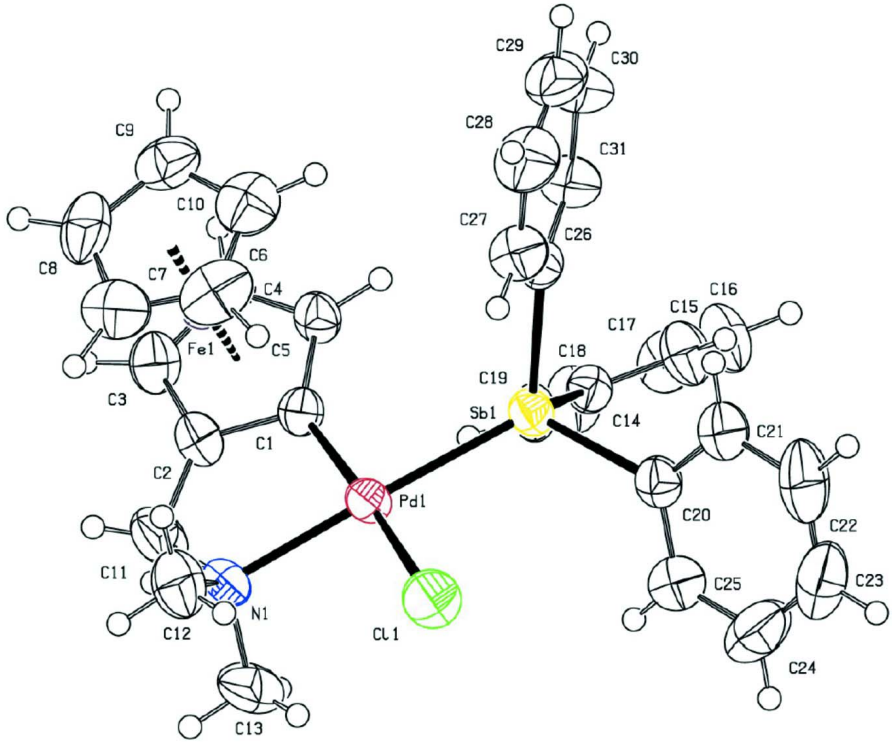


**Figure 1**

The title molecule with numbering scheme. The displacement ellipsoids are shown at the 50% probability level.

**Chlorido{1-[(dimethylamino)methyl]ferrocenyl-$\kappa^2C^1,N$}(triphenylstibine-$\kappa Sb$)palladium(II)**

*Crystal data*

$[FePdCl(C_5H_5)(C_8H_{11}N)(C_{18}H_{15}Sb)]$
$M_r$ = 737.02
Monoclinic, $P2_1/c$
$a$ = 10.3138 (6) Å
$b$ = 19.8865 (12) Å
$c$ = 13.7584 (9) Å
$\beta$ = 92.984 (1)°
$V$ = 2818.1 (3) Å$^3$
$Z$ = 4
$F(000)$ = 1456
$D_x$ = 1.737 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 5485 reflections
$\theta$ = 2.2–30.8°
$\mu$ = 2.21 mm$^{-1}$
$T$ = 291 K
Prism, red
0.36 × 0.12 × 0.10 mm

*Data collection*

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 0.83 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: analytical (*SADABS*; Bruker, 2007)
$T_{min}$ = 0.490, $T_{max}$ = 0.797
23494 measured reflections
5158 independent reflections
4107 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.048
$\theta_{max}$ = 25.4°, $\theta_{min}$ = 1.8°
$h$ = −12→12
$k$ = −23→23
$l$ = −16→16

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.063$
$S = 0.93$
4963 reflections
327 parameters
0 restraints

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.027P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.77$ e Å$^{-3}$
$\Delta\rho_{min} = -0.31$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Sb1 | 0.76605 (2) | 0.06765 (2) | 0.80847 (2) | 0.03930 (8) |
| Pd1 | 0.63076 (3) | 0.12392 (2) | 0.67766 (2) | 0.03893 (9) |
| Fe1 | 0.83892 (6) | 0.11299 (3) | 0.48685 (4) | 0.04535 (15) |
| Cl1 | 0.55085 (11) | 0.20492 (5) | 0.78865 (8) | 0.0617 (3) |
| N1 | 0.5010 (3) | 0.15681 (15) | 0.5573 (2) | 0.0436 (8) |
| C1 | 0.7077 (4) | 0.06914 (18) | 0.5758 (3) | 0.0404 (9) |
| C2 | 0.6501 (4) | 0.08030 (19) | 0.4804 (3) | 0.0468 (10) |
| C3 | 0.7239 (4) | 0.0457 (2) | 0.4126 (3) | 0.0539 (11) |
| H3 | 0.7062 | 0.0447 | 0.3419 | 0.065* |
| C4 | 0.8258 (4) | 0.01262 (19) | 0.4639 (3) | 0.0525 (11) |
| H4 | 0.8918 | −0.0156 | 0.4353 | 0.063* |
| C5 | 0.8176 (4) | 0.02703 (18) | 0.5641 (3) | 0.0442 (10) |
| H5 | 0.8773 | 0.0107 | 0.6166 | 0.053* |
| C6 | 0.8900 (5) | 0.2057 (2) | 0.5419 (4) | 0.0734 (14) |
| H6 | 0.8525 | 0.2275 | 0.5978 | 0.088* |
| C7 | 0.8440 (5) | 0.2115 (2) | 0.4449 (4) | 0.0740 (15) |
| H7 | 0.7699 | 0.2386 | 0.4204 | 0.089* |
| C8 | 0.9262 (5) | 0.1721 (2) | 0.3882 (3) | 0.0718 (14) |
| H8 | 0.9191 | 0.1669 | 0.3173 | 0.086* |
| C9 | 1.0205 (4) | 0.1429 (2) | 0.4515 (4) | 0.0644 (13) |
| H9 | 1.0911 | 0.1133 | 0.4329 | 0.077* |
| C10 | 0.9961 (5) | 0.1630 (2) | 0.5460 (4) | 0.0690 (13) |
| H10 | 1.0469 | 0.1499 | 0.6052 | 0.083* |
| C11 | 0.5280 (4) | 0.1194 (2) | 0.4671 (3) | 0.0677 (13) |
| H11A | 0.4564 | 0.0892 | 0.4506 | 0.081* |
| H11B | 0.5352 | 0.1509 | 0.4138 | 0.081* |
| C12 | 0.5130 (5) | 0.2297 (2) | 0.5424 (3) | 0.0702 (13) |

| | | | | |
|---|---|---|---|---|
| H12A | 0.5993 | 0.2400 | 0.5240 | 0.105* |
| H12B | 0.4962 | 0.2528 | 0.6017 | 0.105* |
| H12C | 0.4514 | 0.2438 | 0.4918 | 0.105* |
| C13 | 0.3667 (4) | 0.1431 (3) | 0.5849 (4) | 0.0756 (14) |
| H13A | 0.3515 | 0.1652 | 0.6452 | 0.113* |
| H13B | 0.3550 | 0.0955 | 0.5924 | 0.113* |
| H13C | 0.3064 | 0.1596 | 0.5350 | 0.113* |
| C14 | 0.7714 (4) | −0.03917 (18) | 0.8157 (3) | 0.0402 (9) |
| C15 | 0.8309 (4) | −0.0706 (2) | 0.8955 (3) | 0.0578 (12) |
| H15 | 0.8687 | −0.0448 | 0.9457 | 0.069* |
| C16 | 0.8350 (5) | −0.1400 (2) | 0.9019 (3) | 0.0670 (13) |
| H16 | 0.8766 | −0.1608 | 0.9554 | 0.080* |
| C17 | 0.7766 (4) | −0.1780 (2) | 0.8279 (3) | 0.0637 (13) |
| H17 | 0.7804 | −0.2247 | 0.8311 | 0.076* |
| C18 | 0.7138 (4) | −0.1479 (2) | 0.7506 (3) | 0.0611 (12) |
| H18 | 0.6717 | −0.1739 | 0.7024 | 0.073* |
| C19 | 0.7122 (4) | −0.07832 (19) | 0.7435 (3) | 0.0498 (10) |
| H19 | 0.6709 | −0.0579 | 0.6895 | 0.060* |
| C20 | 0.7170 (4) | 0.08795 (19) | 0.9533 (3) | 0.0446 (10) |
| C21 | 0.8071 (4) | 0.1086 (2) | 1.0237 (3) | 0.0597 (12) |
| H21 | 0.8938 | 0.1127 | 1.0092 | 0.072* |
| C22 | 0.7691 (7) | 0.1234 (2) | 1.1168 (3) | 0.0816 (16) |
| H22 | 0.8306 | 0.1384 | 1.1637 | 0.098* |
| C23 | 0.6431 (7) | 0.1163 (3) | 1.1405 (4) | 0.0837 (18) |
| H23 | 0.6187 | 0.1259 | 1.2031 | 0.100* |
| C24 | 0.5537 (6) | 0.0950 (3) | 1.0711 (4) | 0.0837 (16) |
| H24 | 0.4677 | 0.0896 | 1.0868 | 0.100* |
| C25 | 0.5888 (4) | 0.0814 (2) | 0.9785 (3) | 0.0634 (12) |
| H25 | 0.5260 | 0.0675 | 0.9318 | 0.076* |
| C26 | 0.9668 (4) | 0.09096 (19) | 0.8159 (3) | 0.0405 (9) |
| C27 | 1.0016 (4) | 0.1584 (2) | 0.8228 (3) | 0.0579 (11) |
| H27 | 0.9374 | 0.1913 | 0.8220 | 0.069* |
| C28 | 1.1312 (5) | 0.1770 (2) | 0.8310 (3) | 0.0716 (14) |
| H28 | 1.1536 | 0.2222 | 0.8363 | 0.086* |
| C29 | 1.2254 (5) | 0.1295 (3) | 0.8311 (3) | 0.0741 (14) |
| H29 | 1.3123 | 0.1422 | 0.8366 | 0.089* |
| C30 | 1.1933 (4) | 0.0630 (3) | 0.8233 (4) | 0.0746 (14) |
| H30 | 1.2584 | 0.0306 | 0.8236 | 0.090* |
| C31 | 1.0645 (4) | 0.0436 (2) | 0.8149 (3) | 0.0592 (12) |
| H31 | 1.0435 | −0.0017 | 0.8086 | 0.071* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Sb1 | 0.03905 (15) | 0.04112 (15) | 0.03734 (15) | 0.00225 (12) | −0.00182 (11) | −0.00163 (12) |
| Pd1 | 0.03648 (17) | 0.04065 (17) | 0.03923 (17) | 0.00368 (14) | −0.00218 (13) | −0.00211 (14) |
| Fe1 | 0.0529 (4) | 0.0395 (3) | 0.0439 (3) | 0.0023 (3) | 0.0053 (3) | 0.0017 (3) |
| Cl1 | 0.0681 (7) | 0.0604 (7) | 0.0565 (7) | 0.0136 (6) | 0.0026 (6) | −0.0131 (5) |

| | | | | | | |
|---|---|---|---|---|---|---|
| N1 | 0.0372 (18) | 0.0446 (19) | 0.048 (2) | 0.0038 (15) | −0.0076 (15) | 0.0045 (16) |
| C1 | 0.044 (2) | 0.040 (2) | 0.038 (2) | −0.0006 (18) | 0.0023 (18) | −0.0011 (18) |
| C2 | 0.052 (3) | 0.042 (2) | 0.045 (2) | 0.002 (2) | −0.008 (2) | −0.0012 (19) |
| C3 | 0.070 (3) | 0.050 (3) | 0.042 (2) | −0.003 (2) | −0.004 (2) | −0.011 (2) |
| C4 | 0.063 (3) | 0.036 (2) | 0.059 (3) | 0.007 (2) | 0.013 (2) | −0.001 (2) |
| C5 | 0.051 (2) | 0.037 (2) | 0.045 (2) | 0.0072 (19) | 0.0011 (19) | 0.0036 (18) |
| C6 | 0.084 (4) | 0.047 (3) | 0.092 (4) | −0.013 (3) | 0.026 (3) | −0.011 (3) |
| C7 | 0.067 (3) | 0.044 (3) | 0.112 (5) | 0.000 (2) | 0.014 (3) | 0.027 (3) |
| C8 | 0.094 (4) | 0.067 (3) | 0.055 (3) | −0.019 (3) | 0.010 (3) | 0.019 (3) |
| C9 | 0.059 (3) | 0.056 (3) | 0.080 (4) | −0.004 (2) | 0.021 (3) | 0.005 (3) |
| C10 | 0.070 (3) | 0.063 (3) | 0.075 (4) | −0.018 (3) | 0.004 (3) | −0.004 (3) |
| C11 | 0.063 (3) | 0.084 (3) | 0.054 (3) | 0.018 (3) | −0.017 (2) | −0.014 (3) |
| C12 | 0.084 (4) | 0.059 (3) | 0.067 (3) | 0.003 (3) | −0.006 (3) | 0.016 (2) |
| C13 | 0.040 (3) | 0.098 (4) | 0.088 (4) | −0.007 (3) | −0.011 (2) | 0.006 (3) |
| C14 | 0.042 (2) | 0.041 (2) | 0.038 (2) | −0.0042 (19) | 0.0008 (18) | 0.0003 (18) |
| C15 | 0.069 (3) | 0.050 (3) | 0.053 (3) | −0.006 (2) | −0.017 (2) | 0.000 (2) |
| C16 | 0.079 (3) | 0.055 (3) | 0.064 (3) | −0.003 (3) | −0.019 (3) | 0.017 (2) |
| C17 | 0.078 (3) | 0.041 (2) | 0.073 (3) | −0.003 (2) | 0.011 (3) | 0.006 (2) |
| C18 | 0.080 (3) | 0.047 (3) | 0.055 (3) | −0.008 (2) | −0.007 (2) | −0.005 (2) |
| C19 | 0.059 (3) | 0.050 (3) | 0.040 (2) | −0.007 (2) | −0.005 (2) | 0.004 (2) |
| C20 | 0.052 (3) | 0.040 (2) | 0.042 (2) | 0.007 (2) | 0.001 (2) | −0.0006 (18) |
| C21 | 0.062 (3) | 0.069 (3) | 0.048 (3) | 0.000 (2) | −0.002 (2) | 0.001 (2) |
| C22 | 0.129 (5) | 0.073 (4) | 0.041 (3) | 0.006 (4) | −0.015 (3) | −0.006 (3) |
| C23 | 0.131 (6) | 0.072 (4) | 0.050 (3) | 0.031 (4) | 0.024 (4) | 0.011 (3) |
| C24 | 0.090 (4) | 0.082 (4) | 0.083 (4) | 0.017 (3) | 0.044 (4) | 0.013 (3) |
| C25 | 0.057 (3) | 0.073 (3) | 0.061 (3) | 0.002 (2) | 0.006 (2) | 0.001 (2) |
| C26 | 0.042 (2) | 0.046 (2) | 0.033 (2) | −0.005 (2) | 0.0040 (17) | 0.0003 (18) |
| C27 | 0.059 (3) | 0.050 (3) | 0.065 (3) | −0.002 (2) | 0.008 (2) | 0.000 (2) |
| C28 | 0.075 (4) | 0.060 (3) | 0.080 (4) | −0.029 (3) | 0.006 (3) | 0.002 (3) |
| C29 | 0.052 (3) | 0.106 (4) | 0.065 (3) | −0.021 (3) | 0.008 (2) | −0.001 (3) |
| C30 | 0.044 (3) | 0.086 (4) | 0.094 (4) | 0.010 (3) | 0.005 (3) | −0.006 (3) |
| C31 | 0.050 (3) | 0.053 (3) | 0.074 (3) | 0.000 (2) | 0.002 (2) | −0.003 (2) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Sb1—C14 | 2.127 (4) | C11—H11B | 0.9700 |
| Sb1—C20 | 2.120 (4) | C12—H12A | 0.9600 |
| Sb1—C26 | 2.119 (4) | C12—H12B | 0.9600 |
| Sb1—Pd1 | 2.4853 (4) | C12—H12C | 0.9600 |
| Pd1—C1 | 1.973 (4) | C13—H13A | 0.9600 |
| Pd1—Cl1 | 2.3952 (10) | C13—H13B | 0.9600 |
| Pd1—N1 | 2.174 (3) | C13—H13C | 0.9600 |
| Fe1—C4 | 2.024 (4) | C14—C15 | 1.378 (5) |
| Fe1—C3 | 2.029 (4) | C14—C19 | 1.380 (5) |
| Fe1—C5 | 2.031 (4) | C15—C16 | 1.383 (6) |
| Fe1—C10 | 2.035 (5) | C15—H15 | 0.9300 |
| Fe1—C8 | 2.040 (4) | C16—C17 | 1.380 (6) |
| Fe1—C7 | 2.044 (4) | C16—H16 | 0.9300 |

| | | | |
|---|---|---|---|
| Fe1—C9 | 2.048 (4) | C17—C18 | 1.356 (6) |
| Fe1—C2 | 2.051 (4) | C17—H17 | 0.9300 |
| Fe1—C6 | 2.051 (4) | C18—C19 | 1.387 (5) |
| Fe1—C1 | 2.065 (4) | C18—H18 | 0.9300 |
| N1—C12 | 1.470 (5) | C19—H19 | 0.9300 |
| N1—C13 | 1.481 (5) | C20—C21 | 1.370 (5) |
| N1—C11 | 1.485 (5) | C20—C25 | 1.391 (6) |
| C1—C5 | 1.426 (5) | C21—C22 | 1.391 (6) |
| C1—C2 | 1.429 (5) | C21—H21 | 0.9300 |
| C2—C3 | 1.413 (5) | C22—C23 | 1.363 (7) |
| C2—C11 | 1.484 (5) | C22—H22 | 0.9300 |
| C3—C4 | 1.400 (5) | C23—C24 | 1.360 (7) |
| C3—H3 | 0.9800 | C23—H23 | 0.9300 |
| C4—C5 | 1.414 (5) | C24—C25 | 1.370 (6) |
| C4—H4 | 0.9800 | C24—H24 | 0.9300 |
| C5—H5 | 0.9800 | C25—H25 | 0.9300 |
| C6—C10 | 1.384 (6) | C26—C31 | 1.380 (5) |
| C6—C7 | 1.398 (7) | C26—C27 | 1.391 (5) |
| C6—H6 | 0.9800 | C27—C28 | 1.385 (6) |
| C7—C8 | 1.418 (6) | C27—H27 | 0.9300 |
| C7—H7 | 0.9800 | C28—C29 | 1.356 (6) |
| C8—C9 | 1.398 (6) | C28—H28 | 0.9300 |
| C8—H8 | 0.9800 | C29—C30 | 1.366 (6) |
| C9—C10 | 1.395 (6) | C29—H29 | 0.9300 |
| C9—H9 | 0.9800 | C30—C31 | 1.382 (6) |
| C10—H10 | 0.9800 | C30—H30 | 0.9300 |
| C11—H11A | 0.9700 | C31—H31 | 0.9300 |

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| C26—Sb1—C20 | 101.15 (15) | Fe1—C6—H6 | 125.7 |
| C26—Sb1—C14 | 101.14 (14) | C6—C7—C8 | 107.3 (5) |
| C20—Sb1—C14 | 98.81 (14) | C6—C7—Fe1 | 70.3 (3) |
| C26—Sb1—Pd1 | 116.53 (10) | C8—C7—Fe1 | 69.5 (2) |
| C20—Sb1—Pd1 | 116.27 (10) | C6—C7—H7 | 126.4 |
| C14—Sb1—Pd1 | 119.72 (10) | C8—C7—H7 | 126.4 |
| C1—Pd1—N1 | 83.09 (14) | Fe1—C7—H7 | 126.4 |
| C1—Pd1—Cl1 | 171.20 (11) | C9—C8—C7 | 107.7 (4) |
| N1—Pd1—Cl1 | 93.71 (9) | C9—C8—Fe1 | 70.3 (3) |
| C1—Pd1—Sb1 | 91.96 (11) | C7—C8—Fe1 | 69.9 (3) |
| N1—Pd1—Sb1 | 170.67 (8) | C9—C8—H8 | 126.2 |
| Cl1—Pd1—Sb1 | 92.29 (3) | C7—C8—H8 | 126.2 |
| C4—Fe1—C3 | 40.42 (15) | Fe1—C8—H8 | 126.2 |
| C4—Fe1—C5 | 40.83 (14) | C10—C9—C8 | 107.9 (4) |
| C3—Fe1—C5 | 68.41 (16) | C10—C9—Fe1 | 69.5 (3) |
| C4—Fe1—C10 | 126.1 (2) | C8—C9—Fe1 | 69.7 (3) |
| C3—Fe1—C10 | 163.0 (2) | C10—C9—H9 | 126.0 |
| C5—Fe1—C10 | 107.91 (18) | C8—C9—H9 | 126.0 |
| C4—Fe1—C8 | 119.50 (19) | Fe1—C9—H9 | 126.0 |
| C3—Fe1—C8 | 108.15 (18) | C6—C10—C9 | 108.6 (5) |

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| C5—Fe1—C8 | 153.73 (19) | C6—C10—Fe1 | 70.8 (3) |
| C10—Fe1—C8 | 67.3 (2) | C9—C10—Fe1 | 70.5 (3) |
| C4—Fe1—C7 | 154.6 (2) | C6—C10—H10 | 125.7 |
| C3—Fe1—C7 | 120.8 (2) | C9—C10—H10 | 125.7 |
| C5—Fe1—C7 | 163.7 (2) | Fe1—C10—H10 | 125.7 |
| C10—Fe1—C7 | 67.2 (2) | C2—C11—N1 | 110.7 (3) |
| C8—Fe1—C7 | 40.63 (18) | C2—C11—H11A | 109.5 |
| C4—Fe1—C9 | 107.67 (17) | N1—C11—H11A | 109.5 |
| C3—Fe1—C9 | 126.17 (18) | C2—C11—H11B | 109.5 |
| C5—Fe1—C9 | 119.59 (18) | N1—C11—H11B | 109.5 |
| C10—Fe1—C9 | 39.96 (17) | H11A—C11—H11B | 108.1 |
| C8—Fe1—C9 | 40.01 (18) | N1—C12—H12A | 109.5 |
| C7—Fe1—C9 | 67.51 (19) | N1—C12—H12B | 109.5 |
| C4—Fe1—C2 | 67.99 (16) | H12A—C12—H12B | 109.5 |
| C3—Fe1—C2 | 40.53 (15) | N1—C12—H12C | 109.5 |
| C5—Fe1—C2 | 68.11 (15) | H12A—C12—H12C | 109.5 |
| C10—Fe1—C2 | 155.11 (18) | H12B—C12—H12C | 109.5 |
| C8—Fe1—C2 | 127.22 (19) | N1—C13—H13A | 109.5 |
| C7—Fe1—C2 | 109.27 (18) | N1—C13—H13B | 109.5 |
| C9—Fe1—C2 | 163.79 (19) | H13A—C13—H13B | 109.5 |
| C4—Fe1—C6 | 163.2 (2) | N1—C13—H13C | 109.5 |
| C3—Fe1—C6 | 155.6 (2) | H13A—C13—H13C | 109.5 |
| C5—Fe1—C6 | 126.6 (2) | H13B—C13—H13C | 109.5 |
| C10—Fe1—C6 | 39.61 (18) | C15—C14—C19 | 118.7 (4) |
| C8—Fe1—C6 | 67.3 (2) | C15—C14—Sb1 | 119.9 (3) |
| C7—Fe1—C6 | 39.92 (19) | C19—C14—Sb1 | 121.4 (3) |
| C9—Fe1—C6 | 66.82 (19) | C14—C15—C16 | 120.9 (4) |
| C2—Fe1—C6 | 121.72 (19) | C14—C15—H15 | 119.5 |
| C4—Fe1—C1 | 68.63 (15) | C16—C15—H15 | 119.5 |
| C3—Fe1—C1 | 68.64 (16) | C17—C16—C15 | 119.2 (4) |
| C5—Fe1—C1 | 40.73 (14) | C17—C16—H16 | 120.4 |
| C10—Fe1—C1 | 120.16 (17) | C15—C16—H16 | 120.4 |
| C8—Fe1—C1 | 164.44 (19) | C18—C17—C16 | 120.6 (4) |
| C7—Fe1—C1 | 126.83 (18) | C18—C17—H17 | 119.7 |
| C9—Fe1—C1 | 154.07 (18) | C16—C17—H17 | 119.7 |
| C2—Fe1—C1 | 40.64 (14) | C17—C18—C19 | 119.9 (4) |
| C6—Fe1—C1 | 108.92 (17) | C17—C18—H18 | 120.0 |
| C12—N1—C13 | 107.7 (3) | C19—C18—H18 | 120.0 |
| C12—N1—C11 | 110.8 (3) | C14—C19—C18 | 120.6 (4) |
| C13—N1—C11 | 109.9 (3) | C14—C19—H19 | 119.7 |
| C12—N1—Pd1 | 110.5 (2) | C18—C19—H19 | 119.7 |
| C13—N1—Pd1 | 107.2 (2) | C21—C20—C25 | 118.0 (4) |
| C11—N1—Pd1 | 110.6 (2) | C21—C20—Sb1 | 122.4 (3) |
| C5—C1—C2 | 106.4 (3) | C25—C20—Sb1 | 119.5 (3) |
| C5—C1—Pd1 | 139.1 (3) | C20—C21—C22 | 120.2 (5) |
| C2—C1—Pd1 | 113.8 (3) | C20—C21—H21 | 119.9 |
| C5—C1—Fe1 | 68.3 (2) | C22—C21—H21 | 119.9 |
| C2—C1—Fe1 | 69.1 (2) | C23—C22—C21 | 121.0 (5) |

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| Pd1—C1—Fe1 | 119.20 (17) | C23—C22—H22 | 119.5 |
| C3—C2—C1 | 108.6 (3) | C21—C22—H22 | 119.5 |
| C3—C2—C11 | 131.0 (4) | C24—C23—C22 | 119.0 (5) |
| C1—C2—C11 | 120.3 (4) | C24—C23—H23 | 120.5 |
| C3—C2—Fe1 | 68.9 (2) | C22—C23—H23 | 120.5 |
| C1—C2—Fe1 | 70.2 (2) | C23—C24—C25 | 120.8 (5) |
| C11—C2—Fe1 | 129.6 (3) | C23—C24—H24 | 119.6 |
| C4—C3—C2 | 108.2 (4) | C25—C24—H24 | 119.6 |
| C4—C3—Fe1 | 69.6 (2) | C24—C25—C20 | 120.9 (5) |
| C2—C3—Fe1 | 70.6 (2) | C24—C25—H25 | 119.5 |
| C4—C3—H3 | 125.9 | C20—C25—H25 | 119.5 |
| C2—C3—H3 | 125.9 | C31—C26—C27 | 118.2 (4) |
| Fe1—C3—H3 | 125.9 | C31—C26—Sb1 | 124.2 (3) |
| C3—C4—C5 | 108.3 (4) | C27—C26—Sb1 | 117.5 (3) |
| C3—C4—Fe1 | 70.0 (2) | C28—C27—C26 | 120.5 (4) |
| C5—C4—Fe1 | 69.8 (2) | C28—C27—H27 | 119.8 |
| C3—C4—H4 | 125.8 | C26—C27—H27 | 119.8 |
| C5—C4—H4 | 125.8 | C29—C28—C27 | 120.2 (4) |
| Fe1—C4—H4 | 125.8 | C29—C28—H28 | 119.9 |
| C4—C5—C1 | 108.5 (3) | C27—C28—H28 | 119.9 |
| C4—C5—Fe1 | 69.3 (2) | C28—C29—C30 | 120.3 (5) |
| C1—C5—Fe1 | 70.9 (2) | C28—C29—H29 | 119.9 |
| C4—C5—H5 | 125.7 | C30—C29—H29 | 119.9 |
| C1—C5—H5 | 125.7 | C29—C30—C31 | 120.3 (5) |
| Fe1—C5—H5 | 125.7 | C29—C30—H30 | 119.9 |
| C10—C6—C7 | 108.5 (5) | C31—C30—H30 | 119.9 |
| C10—C6—Fe1 | 69.5 (3) | C26—C31—C30 | 120.6 (4) |
| C7—C6—Fe1 | 69.8 (3) | C26—C31—H31 | 119.7 |
| C10—C6—H6 | 125.7 | C30—C31—H31 | 119.7 |
| C7—C6—H6 | 125.7 | | |

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| C5—C1—C2—C3 | −0.1 (4) | C7—C6—C10—Fe1 | −59.0 (3) |
| Pd1—C1—C2—C3 | 172.1 (3) | C8—C9—C10—C6 | −1.6 (5) |
| Fe1—C1—C2—C3 | 58.4 (3) | Fe1—C9—C10—C6 | −60.9 (3) |
| C5—C1—C2—C11 | 176.5 (4) | C8—C9—C10—Fe1 | 59.3 (3) |
| Pd1—C1—C2—C11 | −11.3 (5) | C3—C2—C11—N1 | −169.5 (4) |
| Fe1—C1—C2—C11 | −125.0 (4) | C1—C2—C11—N1 | 14.8 (6) |
| C5—C1—C2—Fe1 | −58.4 (2) | Fe1—C2—C11—N1 | −73.8 (5) |
| Pd1—C1—C2—Fe1 | 113.7 (2) | C12—N1—C11—C2 | 112.3 (4) |
| C1—C2—C3—C4 | 0.5 (5) | C13—N1—C11—C2 | −128.8 (4) |
| C11—C2—C3—C4 | −175.6 (4) | Pd1—N1—C11—C2 | −10.6 (4) |
| Fe1—C2—C3—C4 | 59.7 (3) | C19—C14—C15—C16 | 2.1 (6) |
| C1—C2—C3—Fe1 | −59.2 (3) | Sb1—C14—C15—C16 | 179.7 (3) |
| C11—C2—C3—Fe1 | 124.7 (5) | C14—C15—C16—C17 | −1.1 (7) |
| C2—C3—C4—C5 | −0.8 (5) | C15—C16—C17—C18 | −1.2 (7) |
| Fe1—C3—C4—C5 | 59.5 (3) | C16—C17—C18—C19 | 2.6 (7) |
| C2—C3—C4—Fe1 | −60.3 (3) | C15—C14—C19—C18 | −0.7 (6) |
| C3—C4—C5—C1 | 0.8 (4) | Sb1—C14—C19—C18 | −178.3 (3) |

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| Fe1—C4—C5—C1 | 60.3 (3) | C17—C18—C19—C14 | −1.6 (7) |
| C3—C4—C5—Fe1 | −59.6 (3) | C25—C20—C21—C22 | −1.1 (6) |
| C2—C1—C5—C4 | −0.4 (4) | Sb1—C20—C21—C22 | 177.9 (3) |
| Pd1—C1—C5—C4 | −169.4 (3) | C20—C21—C22—C23 | 1.5 (7) |
| Fe1—C1—C5—C4 | −59.4 (3) | C21—C22—C23—C24 | −0.6 (8) |
| C2—C1—C5—Fe1 | 58.9 (3) | C22—C23—C24—C25 | −0.6 (8) |
| Pd1—C1—C5—Fe1 | −110.1 (4) | C23—C24—C25—C20 | 1.0 (8) |
| C10—C6—C7—C8 | −1.1 (5) | C21—C20—C25—C24 | −0.2 (7) |
| Fe1—C6—C7—C8 | −60.0 (3) | Sb1—C20—C25—C24 | −179.1 (4) |
| C10—C6—C7—Fe1 | 58.9 (3) | C31—C26—C27—C28 | −1.6 (6) |
| C6—C7—C8—C9 | 0.1 (5) | Sb1—C26—C27—C28 | 178.0 (3) |
| Fe1—C7—C8—C9 | −60.4 (3) | C26—C27—C28—C29 | 0.8 (7) |
| C6—C7—C8—Fe1 | 60.5 (3) | C27—C28—C29—C30 | 0.0 (8) |
| C7—C8—C9—C10 | 0.9 (5) | C28—C29—C30—C31 | 0.1 (8) |
| Fe1—C8—C9—C10 | −59.2 (3) | C27—C26—C31—C30 | 1.7 (6) |
| C7—C8—C9—Fe1 | 60.1 (3) | Sb1—C26—C31—C30 | −177.8 (3) |
| C7—C6—C10—C9 | 1.7 (5) | C29—C30—C31—C26 | −1.0 (7) |
| Fe1—C6—C10—C9 | 60.7 (3) | | |