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# *cis*-Dichlorido[4,4,5,5-tetramethyl-2-(2-pyridyl)-2-imidazoline-1-oxyl]-palladium(II) tetrahydrofuran hemisolvate

**Sihem Badeche,[a]* Djamil Azzedine Rouag,[a] Sabrina Benmebarek,[a] Salah-Eddine Bouaoud[a] and Stéphane Golhen[b]**

[a]Laboratoire de Chimie Moléculaire, du Contrôle de l'Environnement et de Mesures Physico-Chimiques, Département de Chimie, Université Frères Mentouri, Constantine, Algeria, and [b]Sciences Chimiques de Rennes, UMR 6226, CNRS–Université de Rennes 1, 263 Avenue du Général Leclerc, CS 74205, 35042 Rennes Cedex, France
Correspondence e-mail: s_badeche@yahoo.fr

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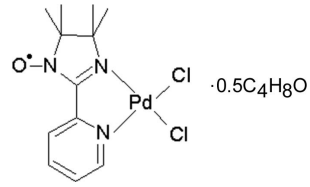
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.013 Å; $R$ factor = 0.057; $wR$ factor = 0.153; data-to-parameter ratio = 15.4.

The asymmetric unit of the title complex, $[PdCl_2(C_{12}H_{16}N_3O)]\cdot0.5C_4H_8O$, consists of one palladium complex in a general position and one half tetrahydrofuran (THF) solvent molecule, with the O atom lying on a twofold rotation axis. The $Pd^{II}$ atom is bound to one chelating imino nitroxide radical through two N atoms, one from the pyridyl ring and the other from the imidazoline ring. The coordination of the metal centre is completed by two Cl atoms in a *cis* configuration, leading to a quasi-square-planar coordination of the metal centre. The four atoms that define the $Pd^{II}$ coordination environment and the eight atoms that belong to the pyridylimine fragment are coplanar, with no deviation larger than 0.087 (5) Å. In the crystal structure, intermolecular interactions shorter than the corresponding van der Waals radii sum are observed only between $Pd^{II}$ complexes, and no short contact is observed around the THF molecule. Weak C—H···O and C—H···Cl interactions yield a two-dimensional network of complexes in the (101) plane.

## Related literature

For related literature, see: Caneschi *et al.* (1991); Davis *et al.* (1972); Evans *et al.* (1968); Fettouhi *et al.* (2003); Li *et al.* (2004); Ma *et al.* (2006, 2007); Oshio *et al.* (1996); Ueda *et al.* (2003, 2005); Ullman & Holm (1970); Xu *et al.* (2007).




## Experimental

### Crystal data

$[PdCl_2(C_{12}H_{16}N_3O)]\cdot0.5C_4H_8O$
$M_r$ = 431.65
Monoclinic, $C2/c$
$a$ = 19.1398 (10) Å
$b$ = 15.2061 (12) Å
$c$ = 13.8291 (10) Å
$\beta$ = 123.415 (3)°
$V$ = 3359.6 (4) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 1.43 mm$^{-1}$
$T$ = 293 (2) K
0.7 × 0.3 × 0.3 mm

### Data collection

Nonius KappaCCD diffractometer
Absorption correction: none
5707 measured reflections
3065 independent reflections
2049 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.059

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.152
$S$ = 1.03
3065 reflections
199 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.61 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.95 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C4—H4···O1$^{i}$ | 0.93 | 2.61 | 3.307 (8) | 132 |
| C10—H10$B$···Cl1$^{ii}$ | 0.96 | 2.77 | 3.691 (7) | 160 |

Symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *HKL DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2318).

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# supporting information

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## *cis*-Dichlorido[4,4,5,5-tetramethyl-2-(2-pyridyl)-2-imidazoline-1-oxyl]palladium(II) tetrahydrofuran hemisolvate

**Sihem Badeche, Djamil Azzedine Rouag, Sabrina Benmebarek, Salah-Eddine Bouaoud and Stéphane Golhen**

### S1. Comment

Organic nitronyl nitroxide radicals have attracted much attention for their magnetic properties in general and ferromagnetism in particular. Then several transition metal complexes with stable nitronyl nitroxide radical ligands have been prepared and extensively investigated (Ma *et al.*, 2007; Xu *et al.*, 2007; Ma *et al.*, 2006; Ueda *et al.*, 2005; Li *et al.*, 2004; Ueda *et al.*, 2003; Oshio *et al.*, 1996; Caneschi *et al.*, 1991). Our contribution in this field is the synthesis (see Scheme 1) and structure characterization of the title compound.

The molecular structure of the complex [Pd(I$M_2$py)$Cl_2$] 0.5THF(I) is shown in Fig. 1 while selected geometric parameters are given in Table 1. Focusing the coordination square of $Pd^{II}$, one can notice that Cl2 atom deviates significantly from the phane defined with atoms N3/N1/Pd1/Cl1 by 0.0843 (23) Å. The mean bond distance of Pd—Cl 2.277 Å is in agreement with the values observed in a similar complex while the average bond length of Pd—N 2.045 Å is slightly longer than seen previously (Fettouhi *et al.*, 2003). Due to a chelation of the iminonitroxide radical with $Pd^{II}$ ion, the four atoms which define the $Pd^{II}$ coordination plane and the eight atoms which belong to both pyridyl ring and imino fragment are coplanar, the larger deviation to the plane is equal to 0.087 (5) and -0.064 (5) Å for O1 and N3 respectively. Only $sp^3$ carbon C7 and C8 from imino and methyl carbon C9, C10, C11 and C12 deviate significantly from the mean plane.

In the packing, one can notice that intermolecular interactions shorter than the corresponding van-der-Waals radii are only observed between $Pd^{II}$ complexes, no short contact are observed around THF molecule. Centrosymetric contacts take place between imino and pyridyl ring (O1—H4) of one neighbouring complex as well as contacts between chlorine Cl1 and H10B atom of methylene group (Table 1). These contacts yield a two-dimensional network of interacting complexes along the (101) plane (Fig. 2). Another short contact is observed between two adjacent 2-D networks thanks to a van-der-Waals interaction between two C1 atoms of pyridyl rings of two neighbouring molecules with C1—C1 3.393 (16) Å. The shortest distance between two palladium take place between ions from two adjacent planes (Pd1—Pd1 = 3.648 (2) Å), onto a plane, the shorter Pd1—Pd1 distance is 8.7834 (7) Å. THF solvent molecules are lying between two planes. A contact O1s—H1 of 2.7445 Å is observed with pyridyl ring.

### S2. Experimental

Dichlorobis benzonitrile palladium(II) $PdCl_2(PhCN)_2$ and 2-(*ortho*- pyridyl)-4,4,5,5-tetramethyl imidazoline-1-oxyl-3-oxyde (NIT2Py) were synthesized according to literature method (Evans *et al.*, 1968; Ullman & Holm, 1970; Davis *et al.*, 1972). The complex Pd(I$M_2$py)$Cl_2$ was synthesized as follows: The reaction was performed under a dry nitrogen atmosphere using standard schlenk technique. All solvents used were distilled under nitrogen. To a solution of

$PdCl_2(PhCN)_2$ (0.1 g;0.26 mmol) in 30 ml of toluene was added with stirring a solution of the radical NIT2Py (0.12 g;0.52 mmol) in 20 ml of toluene. After 2 h of stirring at room temperature, the mixture was filtered and the solvent removed under reduced pressure. Parallelepipedic brown crystals of complex (I) suitable for *x*-ray crystallographic analysis were obtained by slow diffusion of hexane in THF solution of complex (I).

### S3. Refinement

All H atoms were placed in calculated positions and treated as riding model with C—H ranging from 0.93 Å [$U_{iso}$(H) = 1.2Ueq(C)] for pyridyl ring to 0.96—0.97 Å with $U_{iso}$(H) = 1.5Ueq(C)—1.2Ueq(C)) for methyl and methylene respectively.

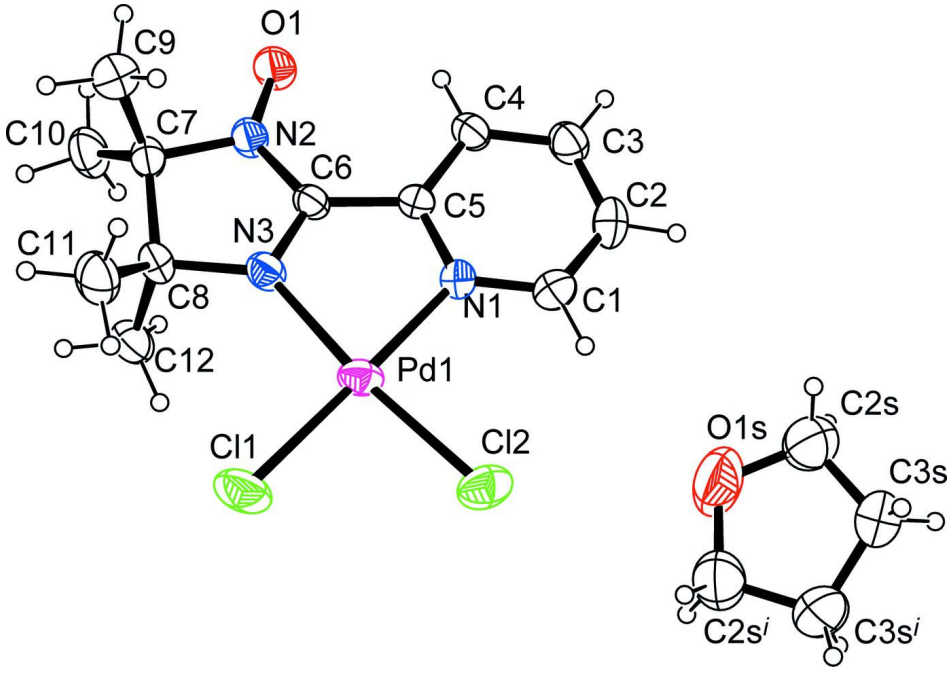


**Figure 1**

An *ORTEP* drawing of title compound showing 30% probability displacement ellipsoids and the atom-numbering scheme. The labels of the H atoms have been omitted for clarity. [Symmetry codes: (i) -*x* + 1, *y*, -*z* + 1.5]

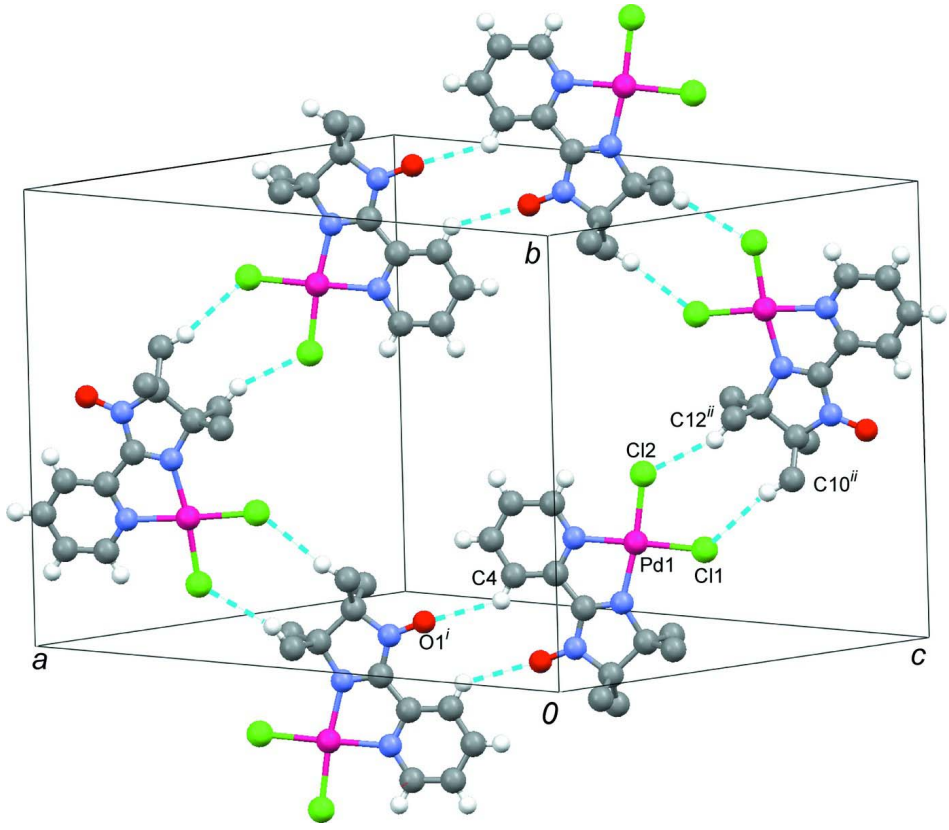


**Figure 2**

Partial packing view showing the formation of a two-dimensionnal network through C—H···O and C—H···Cl intermolecular interactions. H bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted for clarity. [Symmetry codes: (i) -*x* –+1, -*y*, -*z* + 1; (ii) 1/2 - *x*, *y* + 1/2, 3/2 - *z*]

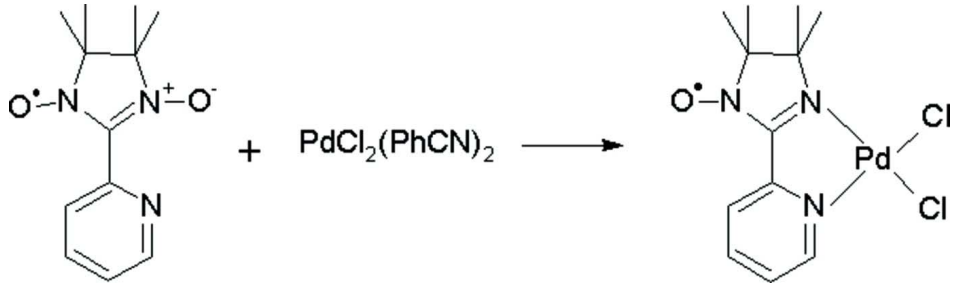


**Figure 3**

The formation of the title compound.

**_cis_-Dichlorido[4,4,5,5-tetramethyl-2-(2-pyridyl)-2-imidazoline-1- oxyl]palladium(II) tetrahydrofuran hemisolvate**

*Crystal data*

$[PdCl_2(C_{12}H_{16}N_3O)]\cdot 0.5C_4H_8O$
$M_r = 431.65$
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
$a = 19.1398\ (10)$ Å
$b = 15.2061\ (12)$ Å
$c = 13.8291\ (10)$ Å
$\beta = 123.415\ (3)°$
$V = 3359.6\ (4)$ Å$^3$
$Z = 8$
$F(000) = 1736$
$D_x = 1.707$ Mg m$^{-3}$

Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 2981 reflections
$\theta$ = 2.6–25.4°
$\mu$ = 1.43 mm$^{-1}$
$T$ = 293 K
Thick plate, brown
0.7 × 0.3 × 0.3 mm

*Data collection*

Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
5707 measured reflections
3065 independent reflections
2049 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.059
$\theta_{max}$ = 25.4°, $\theta_{min}$ = 3.0°
$h$ = −22→22
$k$ = −17→18
$l$ = −16→16

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.152
$S$ = 1.03
3065 reflections
199 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
$w = 1/[\sigma^2(F_o^2) + (0.0709P)^2 + 4.5052P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.61 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.95 e Å$^{-3}$

*Special details*

**Experimental**. Multiscan absorption correction methods did not yield a better refinement agreement, then no correction was applied.

**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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.4332 (5) | 0.2973 (4) | 0.6038 (6) | 0.0604 (18) |
| H1 | 0.4196 | 0.3511 | 0.6214 | 0.073* |
| C2 | 0.4905 (5) | 0.2955 (5) | 0.5741 (8) | 0.072 (2) |
| H2 | 0.5154 | 0.3475 | 0.5723 | 0.087* |
| C3 | 0.5113 (5) | 0.2173 (5) | 0.5470 (6) | 0.0603 (18) |
| H3 | 0.5497 | 0.2151 | 0.5258 | 0.072* |
| C4 | 0.4733 (5) | 0.1419 (4) | 0.5520 (6) | 0.0558 (18) |
| H4 | 0.4851 | 0.0877 | 0.5330 | 0.067* |
| C5 | 0.4172 (4) | 0.1475 (4) | 0.5858 (5) | 0.0443 (14) |
| C6 | 0.3741 (4) | 0.0747 (4) | 0.5988 (5) | 0.0445 (14) |
| C7 | 0.3264 (5) | −0.0669 (4) | 0.6000 (6) | 0.0560 (17) |

| | | | | |
|---|---|---|---|---|
| C8 | 0.2934 (4) | 0.0028 (4) | 0.6501 (6) | 0.0498 (16) |
| C9 | 0.2604 (6) | −0.0980 (6) | 0.4783 (7) | 0.081 (2) |
| H9A | 0.2328 | −0.0479 | 0.4294 | 0.122* |
| H9B | 0.2201 | −0.1339 | 0.4806 | 0.122* |
| H9C | 0.2867 | −0.1317 | 0.4480 | 0.122* |
| C10 | 0.3725 (5) | −0.1451 (5) | 0.6789 (8) | 0.078 (2) |
| H10A | 0.3899 | −0.1843 | 0.6415 | 0.117* |
| H10B | 0.3359 | −0.1757 | 0.6946 | 0.117* |
| H10C | 0.4208 | −0.1246 | 0.7503 | 0.117* |
| C11 | 0.1983 (5) | 0.0032 (5) | 0.5897 (7) | 0.076 (2) |
| H11A | 0.1824 | 0.0501 | 0.6202 | 0.114* |
| H11B | 0.1805 | −0.0520 | 0.6030 | 0.114* |
| H11C | 0.1723 | 0.0116 | 0.5080 | 0.114* |
| C12 | 0.3364 (5) | −0.0032 (5) | 0.7811 (6) | 0.067 (2) |
| H12A | 0.3951 | −0.0143 | 0.8167 | 0.101* |
| H12B | 0.3121 | −0.0502 | 0.7994 | 0.101* |
| H12C | 0.3292 | 0.0513 | 0.8098 | 0.101* |
| N1 | 0.3961 (3) | 0.2250 (3) | 0.6084 (5) | 0.0470 (12) |
| N2 | 0.3857 (4) | −0.0129 (3) | 0.5888 (5) | 0.0512 (13) |
| N3 | 0.3211 (3) | 0.0884 (3) | 0.6270 (5) | 0.0509 (13) |
| O1 | 0.4363 (3) | −0.0447 (3) | 0.5657 (5) | 0.0687 (14) |
| Cl1 | 0.21890 (16) | 0.20499 (14) | 0.7093 (2) | 0.0865 (7) |
| Cl2 | 0.30744 (14) | 0.36626 (13) | 0.67356 (19) | 0.0761 (6) |
| Pd1 | 0.30983 (3) | 0.21827 (3) | 0.65241 (5) | 0.0534 (2) |
| O1S | 0.5000 | 0.4980 (7) | 0.7500 | 0.177 (7) |
| C2S | 0.5251 (8) | 0.5487 (7) | 0.6926 (10) | 0.108 (3) |
| H2S1 | 0.4949 | 0.5319 | 0.6116 | 0.130* |
| H2S2 | 0.5845 | 0.5408 | 0.7263 | 0.130* |
| C3S | 0.5078 (9) | 0.6386 (6) | 0.7032 (11) | 0.118 (4) |
| H3S1 | 0.4590 | 0.6595 | 0.6312 | 0.142* |
| H3S2 | 0.5552 | 0.6758 | 0.7235 | 0.142* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.069 (5) | 0.050 (4) | 0.066 (5) | 0.003 (3) | 0.040 (4) | −0.004 (3) |
| C2 | 0.077 (6) | 0.059 (5) | 0.091 (6) | −0.023 (4) | 0.052 (5) | −0.002 (4) |
| C3 | 0.060 (4) | 0.068 (5) | 0.065 (5) | −0.006 (4) | 0.041 (4) | 0.000 (4) |
| C4 | 0.071 (5) | 0.053 (4) | 0.064 (5) | 0.003 (3) | 0.050 (4) | 0.003 (3) |
| C5 | 0.050 (4) | 0.045 (3) | 0.039 (3) | −0.002 (3) | 0.026 (3) | −0.002 (3) |
| C6 | 0.050 (4) | 0.046 (3) | 0.048 (4) | 0.004 (3) | 0.034 (3) | 0.003 (3) |
| C7 | 0.068 (5) | 0.046 (3) | 0.073 (5) | −0.006 (3) | 0.050 (4) | 0.001 (3) |
| C8 | 0.050 (4) | 0.053 (4) | 0.054 (4) | 0.000 (3) | 0.034 (4) | 0.008 (3) |
| C9 | 0.095 (7) | 0.079 (5) | 0.083 (6) | −0.018 (5) | 0.057 (6) | −0.017 (5) |
| C10 | 0.100 (7) | 0.060 (5) | 0.105 (7) | 0.009 (4) | 0.075 (6) | 0.022 (4) |
| C11 | 0.061 (5) | 0.085 (6) | 0.091 (6) | −0.010 (4) | 0.048 (5) | 0.000 (5) |
| C12 | 0.074 (5) | 0.078 (5) | 0.060 (5) | −0.003 (4) | 0.044 (4) | 0.005 (4) |
| N1 | 0.051 (3) | 0.043 (3) | 0.049 (3) | −0.002 (2) | 0.029 (3) | 0.002 (2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| N2 | 0.059 (3) | 0.043 (3) | 0.067 (4) | 0.006 (3) | 0.044 (3) | 0.006 (2) |
| N3 | 0.056 (3) | 0.052 (3) | 0.057 (3) | 0.006 (3) | 0.039 (3) | 0.005 (2) |
| O1 | 0.083 (4) | 0.052 (3) | 0.103 (4) | 0.014 (3) | 0.072 (4) | 0.004 (3) |
| Cl1 | 0.0970 (17) | 0.0960 (15) | 0.1066 (18) | 0.0216 (13) | 0.0814 (16) | 0.0034 (12) |
| Cl2 | 0.0873 (15) | 0.0578 (10) | 0.0865 (15) | 0.0200 (10) | 0.0499 (13) | −0.0037 (9) |
| Pd1 | 0.0586 (4) | 0.0552 (3) | 0.0549 (4) | 0.0116 (3) | 0.0366 (3) | −0.0002 (2) |
| O1S | 0.249 (17) | 0.068 (6) | 0.35 (2) | 0.000 | 0.246 (18) | 0.000 |
| C2S | 0.116 (9) | 0.094 (7) | 0.134 (10) | −0.007 (6) | 0.081 (8) | −0.014 (7) |
| C3S | 0.178 (12) | 0.073 (6) | 0.142 (10) | −0.025 (7) | 0.113 (10) | −0.009 (6) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—N1 | 1.329 (8) | C10—H10A | 0.9600 |
| C1—C2 | 1.367 (11) | C10—H10B | 0.9600 |
| C1—H1 | 0.9300 | C10—H10C | 0.9600 |
| C2—C3 | 1.370 (10) | C11—H11A | 0.9600 |
| C2—H2 | 0.9300 | C11—H11B | 0.9600 |
| C3—C4 | 1.381 (9) | C11—H11C | 0.9600 |
| C3—H3 | 0.9300 | C12—H12A | 0.9600 |
| C4—C5 | 1.388 (8) | C12—H12B | 0.9600 |
| C4—H4 | 0.9300 | C12—H12C | 0.9600 |
| C5—N1 | 1.338 (7) | N1—Pd1 | 2.052 (5) |
| C5—C6 | 1.451 (8) | N2—O1 | 1.269 (6) |
| C6—N3 | 1.289 (7) | N3—Pd1 | 2.037 (5) |
| C6—N2 | 1.370 (8) | Cl1—Pd1 | 2.280 (2) |
| C7—N2 | 1.476 (8) | Cl2—Pd1 | 2.273 (2) |
| C7—C9 | 1.520 (11) | O1S—C2S$^{i}$ | 1.370 (10) |
| C7—C10 | 1.524 (10) | O1S—C2S | 1.370 (10) |
| C7—C8 | 1.576 (9) | C2S—C3S | 1.433 (13) |
| C8—N3 | 1.505 (8) | C2S—H2S1 | 0.9700 |
| C8—C12 | 1.526 (9) | C2S—H2S2 | 0.9700 |
| C8—C11 | 1.529 (10) | C3S—C3S$^{i}$ | 1.479 (18) |
| C9—H9A | 0.9600 | C3S—H3S1 | 0.9700 |
| C9—H9B | 0.9600 | C3S—H3S2 | 0.9700 |
| C9—H9C | 0.9600 | | |
| | | | |
| N1—C1—C2 | 122.5 (6) | H10B—C10—H10C | 109.5 |
| N1—C1—H1 | 118.8 | C8—C11—H11A | 109.5 |
| C2—C1—H1 | 118.8 | C8—C11—H11B | 109.5 |
| C1—C2—C3 | 120.1 (7) | H11A—C11—H11B | 109.5 |
| C1—C2—H2 | 120.0 | C8—C11—H11C | 109.5 |
| C3—C2—H2 | 120.0 | H11A—C11—H11C | 109.5 |
| C2—C3—C4 | 117.9 (6) | H11B—C11—H11C | 109.5 |
| C2—C3—H3 | 121.1 | C8—C12—H12A | 109.5 |
| C4—C3—H3 | 121.1 | C8—C12—H12B | 109.5 |
| C3—C4—C5 | 119.4 (6) | H12A—C12—H12B | 109.5 |
| C3—C4—H4 | 120.3 | C8—C12—H12C | 109.5 |
| C5—C4—H4 | 120.3 | H12A—C12—H12C | 109.5 |

| | | | |
|---|---|---|---|
| N1—C5—C4 | 121.5 (6) | H12B—C12—H12C | 109.5 |
| N1—C5—C6 | 112.1 (5) | C1—N1—C5 | 118.6 (6) |
| C4—C5—C6 | 126.3 (6) | C1—N1—Pd1 | 126.5 (4) |
| N3—C6—N2 | 112.8 (5) | C5—N1—Pd1 | 114.9 (4) |
| N3—C6—C5 | 120.7 (5) | O1—N2—C6 | 125.7 (5) |
| N2—C6—C5 | 126.4 (5) | O1—N2—C7 | 123.5 (5) |
| N2—C7—C9 | 106.0 (6) | C6—N2—C7 | 110.6 (5) |
| N2—C7—C10 | 109.5 (6) | C6—N3—C8 | 110.5 (5) |
| C9—C7—C10 | 110.5 (7) | C6—N3—Pd1 | 112.6 (4) |
| N2—C7—C8 | 100.9 (5) | C8—N3—Pd1 | 136.0 (4) |
| C9—C7—C8 | 113.9 (6) | N3—Pd1—N1 | 79.58 (19) |
| C10—C7—C8 | 115.1 (6) | N3—Pd1—Cl2 | 173.28 (15) |
| N3—C8—C12 | 106.3 (5) | N1—Pd1—Cl2 | 93.72 (14) |
| N3—C8—C11 | 109.4 (5) | N3—Pd1—Cl1 | 98.44 (15) |
| C12—C8—C11 | 110.5 (5) | N1—Pd1—Cl1 | 176.70 (15) |
| N3—C8—C7 | 102.5 (4) | Cl2—Pd1—Cl1 | 88.28 (8) |
| C12—C8—C7 | 113.4 (6) | C2S$^{i}$—O1S—C2S | 111.5 (11) |
| C11—C8—C7 | 114.1 (6) | O1S—C2S—C3S | 107.6 (9) |
| C7—C9—H9A | 109.5 | O1S—C2S—H2S1 | 110.2 |
| C7—C9—H9B | 109.5 | C3S—C2S—H2S1 | 110.2 |
| H9A—C9—H9B | 109.5 | O1S—C2S—H2S2 | 110.2 |
| C7—C9—H9C | 109.5 | C3S—C2S—H2S2 | 110.2 |
| H9A—C9—H9C | 109.5 | H2S1—C2S—H2S2 | 108.5 |
| H9B—C9—H9C | 109.5 | C2S—C3S—C3S$^{i}$ | 105.0 (6) |
| C7—C10—H10A | 109.5 | C2S—C3S—H3S1 | 110.7 |
| C7—C10—H10B | 109.5 | C3S$^{i}$—C3S—H3S1 | 110.7 |
| H10A—C10—H10B | 109.5 | C2S—C3S—H3S2 | 110.7 |
| C7—C10—H10C | 109.5 | C3S$^{i}$—C3S—H3S2 | 110.7 |
| H10A—C10—H10C | 109.5 | H3S1—C3S—H3S2 | 108.8 |

Symmetry code: (i) $-x+1, y, -z+3/2$.

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C4—H4···O1$^{ii}$ | 0.93 | 2.61 | 3.307 (8) | 132 |
| C10—H10*B*···Cl1$^{iii}$ | 0.96 | 2.77 | 3.691 (7) | 160 |

Symmetry codes: (ii) $-x+1, -y, -z+1$; (iii) $-x+1/2, y-1/2, -z+3/2$.