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# {Bis[2-(3,5-dimethylpyrazol-1-yl-$\kappa N^2$)-ethyl]amine-$\kappa N$}chloridopalladium(II) chloride 0.25-hydrate

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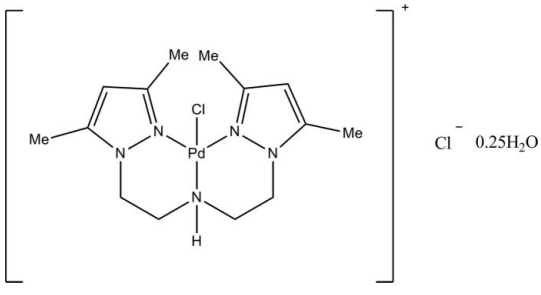
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(Pd–N) = 0.006 Å; H-atom completeness 98%; disorder in main residue; $R$ factor = 0.023; $wR$ factor = 0.057; data-to-parameter ratio = 12.5.

The title compound, $[PdCl(C_{14}H_{23}N_5)]Cl\cdot0.25H_2O$, is a pseudopolymorph of the previously reported compound $[PdCl(C_{14}H_{23}N_5)]Cl\cdot2H_2O$ [de Mendoza *et al.* (2006). *Acta Cryst.* E**62**, m2934–m2936]. The cationic complex and chloride anion are disordered over two positions each in a 0.584 (4):0.416 (4) ratio. The geometry about the Pd atom is distorted square-planar. The pyrazole rings are almost perpendicular, forming a dihedral angle of 86.6 (6)° to each other, to mitigate steric conflict between their methyl groups.

## Related literature

For the previously reported pseudopolymorph, see: de Mendoza *et al.* (2006). For the use of bis(pyrazolyl)alkylamines as ligands in metal complexes, see: Kunrath *et al.* (2003); Ajellal *et al.* (2006); Zhang *et al.* (2008); John *et al.* (2010). For geometrical parameter checks, see: Bruno *et al.* (2004); Allen (2002).




## Experimental

### Crystal data

$[PdCl(C_{14}H_{23}N_5)]Cl\cdot0.25H_2O$
$M_r$ = 443.68
Monoclinic, $P2_1/n$
$a$ = 10.5995 (8) Å
$b$ = 12.4740 (9) Å
$c$ = 13.8168 (10) Å
$\beta$ = 99.865 (1)°
$V$ = 1799.8 (2) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 1.33 mm$^{-1}$
$T$ = 100 K
0.27 × 0.27 × 0.19 mm

### Data collection

Bruker CCD 1000 area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min}$ = 0.715, $T_{max}$ = 0.786
26455 measured reflections
5182 independent reflections
4450 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.029

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.057
$S$ = 1.01
5182 reflections
415 parameters
691 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.44 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.28 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N3—H3···Cl2 | 0.93 | 2.24 | 3.162 (12) | 174 |
| N3$A$—H3$B$···Cl2$A$ | 0.93 | 2.17 | 3.088 (15) | 170 |

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT-Plus* (Bruker, 2007); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008) and *FCF_filter* (Guzei, 2007); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *DIAMOND* (Brandenburg, 2009); software used to prepare material for publication: *SHELXTL*, *publCIF* (Westrip, 2010) and *modiCIFer* (Guzei, 2007).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2207).

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# supporting information

*Acta Cryst.* (2010). E**66**, m1243 [doi:10.1107/S1600536810035427]

# {Bis[2-(3,5-dimethylpyrazol-1-yl-$\kappa N^2$)ethyl]amine-$\kappa N$}chloridopalladium(II) chloride 0.25-hydrate

**Ilia A. Guzei, Lara C. Spencer, Nangamso Miti and James Darkwa**

## S1. Comment

Bis(pyrazolyl)alkylamines are frequently used as N^N^N ligands in metal complexes (Kunrath *et al.*, 2003, Ajellal *et al.*, 2006, Zhang *et al.*, 2008), although bis(pyrazolyl)arylamines can act as bidentate N^N ligands (John *et al.*, 2010).

Palladium dichloride reacts with bis(3,5-dimethylpyrazolyl)alkylamine to afford the title compound, in which the ligand acts as a tridentate N^N^N donor. It is a pseudopolymorph of the previously reported complex $[PdCl(C_{14}H_{23}N_5]Cl.2H_2O$, which contains two solvent water molecules per ionic complex (de Mendoza *et al.*, 2006).

The title compound consists of discrete $[PdCl(C_{14}H_{23}N_5)]$ cations and chloride anions (Fig. 1). The lattice also contains one quarter of a solvent water molecule per ionic complex. The geometry about the central palladium atom is slightly distorted square planar. This distortion is observed in the bond angles about the palladium atom and the deviation from planarity by the palladium and its four coordinating atoms (average r.m.s. of 0.07 (6) Å). The pyrazole rings are almost perpendicular to each other forming an average dihedral angle of 86.6 (6)° required to mitigate steric conflict between the methyl groups C1 and C14. The pyrazole rings are tilted av. 47.2 (11)° relative to the Pd coordination plane. The bond distances and angles are typical, as confirmed by a *Mogul* structural check (Bruno *et al.*, 2004) and by comparing the values in the title compound to six similar compounds found in the Cambridge Structural Database (CSD, version 5.31, last update May 2010; Allen, 2002).

The cationic complex exhibits a "whole molecule disorder" over two positions, and the chloride anion is also disordered over two positions. The major components of the disordered moieties are present 58.4 (4)% of the time. There is one strong intermolecular hydrogen bond of the type N—H···Cl present in the ionic compound (Table 1). It is likely that when the solvent water molecule is present it participates in a hydrogen bond with atom Cl2A as indicated by the distance of 3.034 (5) Å between the two atoms. Since the hydrogen atoms on the solvent water molecule could not be located, no further information about a possible hydrogen bond can be obtained. The solvent water molecule cannot be present when atom Cl2, the major component of the disordered chloride anion, is present as it would place the O and Cl atoms in prohibitively close proximity.

## S2. Experimental

A solution of $[PdCl_2(NCMe)_2]$ (0.10 g, 0.39 mmol) and bis(3,5-dimethylpyrazolyl)ethylamine (0.10 g, 0.39 mmol) in dichloromethane (20 ml) was stirred at 233 K for 24 h. The resultant yellowish-orange solution was stored at 269 K for several days to form orange crystals. Yield: 0.06 g (35%). $^1$H NMR ($CDCl_3$): 2.49 (s, 12H, $CH_3$, pz), 3.62 (t, $^3J_{H—H}$ = 12.3 Hz, 4H, $CH_2$-pz), 4.00 (t, $^3J_{H—H}$ = 12.3 Hz, 4H, $CH_2$—NH), 5.26 (s, 2H, CH, pz).

### S3. Refinement

The cationic palladium complex and chloride anion are disordered over two positions in a 0.584 (4):0.416 (4) ratio. The complexes were refined with similarity restraints. There is also one quarter molecule of a solvent water per molecule of complex. The H-atoms of this solvent water could not be located. All the other H-atoms were placed in idealized locations and refined as riding: N-H = 0.93 Å, C-H = 0.95, 0.99 and 0.98 Å for CH, $CH_2$ and $CH_3$ H-atoms, respectively, with $U_{iso}$(H) = k × $U_{eq}$(bearing atom), where k = 1.5 methyl H-atoms and k = 1.2 for all other H–atoms.

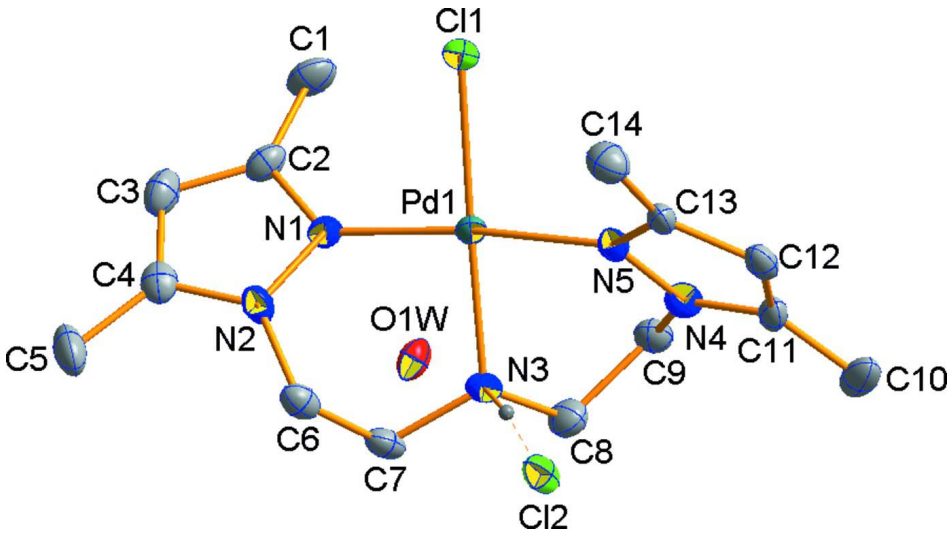


**Figure 1**

Molecular structure of the title compond. The thermal ellipsoids are shown at the 50% probability level. All hydrogen atoms connected to carbon atoms and the minor components of disordered atoms were omitted for clarity. The intermolecular hydrogen bond is shown as a dashed line. The solvent water molecule has an ocupancy of 25%.

**{Bis[2-(3,5-dimethylpyrazol-1-yl-$\kappa N^2$)ethyl]amine- $\kappa N$}chloridopalladium(II) chloride 0.25-hydrate**

*Crystal data*

$[PdCl(C_{14}H_{23}N_5)]Cl·0.25H_2O$
$M_r$ = 443.68
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a$ = 10.5995 (8) Å
$b$ = 12.4740 (9) Å
$c$ = 13.8168 (10) Å
$\beta$ = 99.865 (1)°
$V$ = 1799.8 (2) Å$^3$
$Z$ = 4
$F(000)$ = 898
$D_x$ = 1.636 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 11031 reflections
$\theta$ = 2.2–30.0°
$\mu$ = 1.33 mm$^{-1}$
$T$ = 100 K
Block, yellow
0.27 × 0.27 × 0.19 mm

*Data collection*

Bruker CCD 1000 area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
0.30° $\omega$ and 0.4 ° $\varphi$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min}$ = 0.715, $T_{max}$ = 0.786
26455 measured reflections
5182 independent reflections
4450 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.029
$\theta_{max}$ = 30.0°, $\theta_{min}$ = 2.2°
$h$ = −14→14
$k$ = −17→17
$l$ = −18→19

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.023$
$wR(F^2) = 0.057$
$S = 1.01$
5182 reflections
415 parameters
691 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
$w = 1/[\sigma^2(F_o^2) + (0.0271P)^2 + 0.7513P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.44$ e Å$^{-3}$
$\Delta\rho_{min} = -0.28$ 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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Pd1 | 0.80405 (12) | 0.79001 (8) | 1.01257 (6) | 0.01812 (12) | 0.584 (4) |
| Cl1 | 0.72843 (17) | 0.72421 (12) | 1.14792 (8) | 0.0288 (3) | 0.584 (4) |
| Cl2 | 0.67632 (16) | 0.72034 (5) | 0.71803 (7) | 0.0260 (3) | 0.584 (4) |
| N1 | 0.7742 (3) | 0.9419 (3) | 1.0504 (3) | 0.0226 (6) | 0.584 (4) |
| N2 | 0.7043 (4) | 1.0067 (3) | 0.9815 (3) | 0.0227 (7) | 0.584 (4) |
| N3 | 0.8628 (7) | 0.8406 (9) | 0.8864 (7) | 0.0196 (12) | 0.584 (4) |
| H3 | 0.8127 | 0.8008 | 0.8374 | 0.024* | 0.584 (4) |
| N4 | 0.9397 (10) | 0.6260 (7) | 0.9251 (9) | 0.0213 (12) | 0.584 (4) |
| N5 | 0.8247 (14) | 0.6423 (8) | 0.9573 (12) | 0.0211 (18) | 0.584 (4) |
| C1 | 0.8615 (4) | 0.9538 (4) | 1.2288 (3) | 0.0343 (8) | 0.584 (4) |
| H1A | 0.8131 | 0.8997 | 1.2586 | 0.051* | 0.584 (4) |
| H1B | 0.8834 | 1.0134 | 1.2748 | 0.051* | 0.584 (4) |
| H1C | 0.9402 | 0.9217 | 1.2137 | 0.051* | 0.584 (4) |
| C2 | 0.7825 (4) | 0.9942 (4) | 1.1371 (3) | 0.0245 (8) | 0.584 (4) |
| C3 | 0.7174 (5) | 1.0910 (5) | 1.1218 (4) | 0.0304 (9) | 0.584 (4) |
| H3A | 0.7074 | 1.1427 | 1.1704 | 0.036* | 0.584 (4) |
| C4 | 0.6704 (5) | 1.0979 (4) | 1.0231 (4) | 0.0266 (8) | 0.584 (4) |
| C5 | 0.5964 (6) | 1.1848 (5) | 0.9651 (5) | 0.0409 (11) | 0.584 (4) |
| H5A | 0.6469 | 1.2144 | 0.9182 | 0.061* | 0.584 (4) |
| H5B | 0.5777 | 1.2416 | 1.0095 | 0.061* | 0.584 (4) |
| H5C | 0.5160 | 1.1556 | 0.9292 | 0.061* | 0.584 (4) |
| C6 | 0.7008 (4) | 0.9829 (4) | 0.8770 (4) | 0.0238 (9) | 0.584 (4) |
| H6A | 0.6694 | 1.0465 | 0.8372 | 0.029* | 0.584 (4) |
| H6B | 0.6405 | 0.9231 | 0.8570 | 0.029* | 0.584 (4) |
| C7 | 0.8313 (5) | 0.9530 (5) | 0.8579 (4) | 0.0235 (9) | 0.584 (4) |

| | | | | | |
|---|---|---|---|---|---|
| H7A | 0.8344 | 0.9625 | 0.7872 | 0.028* | 0.584 (4) |
| H7B | 0.8959 | 1.0013 | 0.8956 | 0.028* | 0.584 (4) |
| C8 | 0.9946 (5) | 0.8097 (5) | 0.8785 (4) | 0.0286 (10) | 0.584 (4) |
| H8A | 1.0532 | 0.8700 | 0.9008 | 0.034* | 0.584 (4) |
| H8B | 0.9996 | 0.7950 | 0.8088 | 0.034* | 0.584 (4) |
| C9 | 1.0378 (8) | 0.7104 (5) | 0.9401 (6) | 0.0259 (12) | 0.584 (4) |
| H9A | 1.1180 | 0.6826 | 0.9218 | 0.031* | 0.584 (4) |
| H9B | 1.0558 | 0.7304 | 1.0104 | 0.031* | 0.584 (4) |
| C10 | 1.0477 (4) | 0.4927 (4) | 0.8342 (2) | 0.0369 (8) | 0.584 (4) |
| H10A | 1.0551 | 0.5399 | 0.7787 | 0.055* | 0.584 (4) |
| H10B | 1.0302 | 0.4193 | 0.8102 | 0.055* | 0.584 (4) |
| H10C | 1.1281 | 0.4940 | 0.8813 | 0.055* | 0.584 (4) |
| C11 | 0.9421 (5) | 0.5300 (4) | 0.8827 (4) | 0.0218 (9) | 0.584 (4) |
| C12 | 0.8283 (4) | 0.4817 (4) | 0.8913 (3) | 0.0233 (7) | 0.584 (4) |
| H12 | 0.8009 | 0.4123 | 0.8685 | 0.028* | 0.584 (4) |
| C13 | 0.7602 (7) | 0.5541 (6) | 0.9401 (5) | 0.0233 (11) | 0.584 (4) |
| C14 | 0.6270 (4) | 0.5440 (4) | 0.9603 (3) | 0.0325 (8) | 0.584 (4) |
| H14A | 0.6253 | 0.5644 | 1.0286 | 0.049* | 0.584 (4) |
| H14B | 0.5982 | 0.4696 | 0.9498 | 0.049* | 0.584 (4) |
| H14C | 0.5701 | 0.5912 | 0.9160 | 0.049* | 0.584 (4) |
| Pd1A | 0.77404 (15) | 0.77658 (11) | 1.00983 (9) | 0.01597 (15) | 0.416 (4) |
| Cl1A | 0.68638 (18) | 0.69209 (17) | 1.13068 (12) | 0.0258 (3) | 0.416 (4) |
| Cl2A | 0.7350 (3) | 0.72156 (8) | 0.69987 (10) | 0.0311 (5) | 0.416 (4) |
| N1A | 0.7336 (4) | 0.9221 (4) | 1.0594 (4) | 0.0195 (8) | 0.416 (4) |
| N2A | 0.6665 (5) | 0.9933 (5) | 0.9944 (4) | 0.0219 (9) | 0.416 (4) |
| N3A | 0.8351 (11) | 0.8443 (12) | 0.8917 (9) | 0.0164 (12) | 0.416 (4) |
| H3B | 0.7974 | 0.8038 | 0.8379 | 0.020* | 0.416 (4) |
| N4A | 0.9562 (12) | 0.6458 (9) | 0.9264 (12) | 0.0152 (14) | 0.416 (4) |
| N5A | 0.8447 (19) | 0.6399 (11) | 0.9623 (16) | 0.0165 (17) | 0.416 (4) |
| C1A | 0.8271 (5) | 0.9143 (4) | 1.2373 (4) | 0.0289 (10) | 0.416 (4) |
| H1D | 0.7743 | 0.8595 | 1.2619 | 0.043* | 0.416 (4) |
| H1E | 0.8529 | 0.9682 | 1.2885 | 0.043* | 0.416 (4) |
| H1F | 0.9036 | 0.8806 | 1.2197 | 0.043* | 0.416 (4) |
| C2A | 0.7510 (5) | 0.9674 (5) | 1.1478 (4) | 0.0212 (10) | 0.416 (4) |
| C3A | 0.6937 (7) | 1.0679 (6) | 1.1386 (6) | 0.0252 (11) | 0.416 (4) |
| H3C | 0.6909 | 1.1175 | 1.1904 | 0.030* | 0.416 (4) |
| C4A | 0.6421 (6) | 1.0829 (5) | 1.0422 (5) | 0.0238 (11) | 0.416 (4) |
| C5A | 0.5703 (9) | 1.1756 (7) | 0.9907 (6) | 0.0428 (16) | 0.416 (4) |
| H5D | 0.6213 | 1.2085 | 0.9457 | 0.064* | 0.416 (4) |
| H5E | 0.5539 | 1.2288 | 1.0392 | 0.064* | 0.416 (4) |
| H5F | 0.4887 | 1.1504 | 0.9533 | 0.064* | 0.416 (4) |
| C6A | 0.6608 (6) | 0.9767 (6) | 0.8892 (5) | 0.0198 (11) | 0.416 (4) |
| H6C | 0.6234 | 1.0407 | 0.8527 | 0.024* | 0.416 (4) |
| H6D | 0.6053 | 0.9144 | 0.8672 | 0.024* | 0.416 (4) |
| C7A | 0.7925 (6) | 0.9571 (6) | 0.8680 (6) | 0.0190 (12) | 0.416 (4) |
| H7C | 0.8533 | 1.0073 | 0.9072 | 0.023* | 0.416 (4) |
| H7D | 0.7936 | 0.9714 | 0.7976 | 0.023* | 0.416 (4) |
| C8A | 0.9775 (8) | 0.8360 (6) | 0.8929 (6) | 0.0229 (12) | 0.416 (4) |

| | | | | | |
|---|---|---|---|---|---|
| H8C | 1.0202 | 0.9013 | 0.9233 | 0.027* | 0.416 (4) |
| H8D | 0.9939 | 0.8315 | 0.8246 | 0.027* | 0.416 (4) |
| C9A | 1.0336 (11) | 0.7383 (7) | 0.9498 (9) | 0.0220 (15) | 0.416 (4) |
| H9C | 1.1202 | 0.7243 | 0.9348 | 0.026* | 0.416 (4) |
| H9D | 1.0424 | 0.7530 | 1.0211 | 0.026* | 0.416 (4) |
| C10A | 1.0903 (4) | 0.5384 (4) | 0.8307 (3) | 0.0243 (8) | 0.416 (4) |
| H10D | 1.0891 | 0.5889 | 0.7762 | 0.036* | 0.416 (4) |
| H10E | 1.0908 | 0.4648 | 0.8059 | 0.036* | 0.416 (4) |
| H10F | 1.1673 | 0.5505 | 0.8799 | 0.036* | 0.416 (4) |
| C11A | 0.9752 (7) | 0.5549 (6) | 0.8762 (5) | 0.0184 (11) | 0.416 (4) |
| C12A | 0.8706 (6) | 0.4902 (5) | 0.8755 (4) | 0.0197 (10) | 0.416 (4) |
| H12A | 0.8595 | 0.4204 | 0.8478 | 0.024* | 0.416 (4) |
| C13A | 0.7836 (8) | 0.5442 (8) | 0.9224 (7) | 0.0197 (14) | 0.416 (4) |
| C14A | 0.6521 (5) | 0.5147 (5) | 0.9364 (4) | 0.0298 (11) | 0.416 (4) |
| H14D | 0.6495 | 0.5092 | 1.0068 | 0.045* | 0.416 (4) |
| H14E | 0.6285 | 0.4456 | 0.9047 | 0.045* | 0.416 (4) |
| H14F | 0.5917 | 0.5699 | 0.9070 | 0.045* | 0.416 (4) |
| O1W | 0.5114 (4) | 0.7644 (3) | 0.8052 (3) | 0.0239 (8) | 0.25 |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Pd1 | 0.0221 (3) | 0.0185 (2) | 0.01357 (11) | 0.00310 (19) | 0.0024 (2) | 0.00027 (12) |
| Cl1 | 0.0386 (6) | 0.0284 (5) | 0.0217 (4) | 0.0100 (4) | 0.0115 (4) | 0.0077 (3) |
| Cl2 | 0.0367 (6) | 0.0176 (3) | 0.0212 (3) | −0.0021 (3) | −0.0023 (3) | −0.0008 (2) |
| N1 | 0.0281 (18) | 0.0243 (14) | 0.0150 (11) | 0.0044 (12) | 0.0020 (12) | −0.0012 (9) |
| N2 | 0.025 (2) | 0.0190 (14) | 0.0216 (15) | 0.0028 (13) | −0.0026 (12) | 0.0003 (10) |
| N3 | 0.019 (3) | 0.0227 (17) | 0.0169 (13) | −0.001 (2) | 0.0025 (16) | 0.0033 (11) |
| N4 | 0.021 (2) | 0.022 (3) | 0.0189 (14) | −0.0030 (17) | −0.0023 (15) | −0.002 (2) |
| N5 | 0.018 (4) | 0.0246 (19) | 0.020 (2) | 0.0068 (17) | 0.002 (3) | 0.0044 (14) |
| C1 | 0.0361 (19) | 0.048 (3) | 0.0175 (13) | −0.0009 (15) | 0.0020 (12) | −0.0069 (15) |
| C2 | 0.0242 (19) | 0.029 (2) | 0.0202 (15) | −0.0046 (13) | 0.0044 (12) | −0.0081 (13) |
| C3 | 0.031 (2) | 0.023 (2) | 0.039 (2) | −0.0032 (15) | 0.0121 (15) | −0.0087 (16) |
| C4 | 0.022 (2) | 0.0230 (18) | 0.037 (2) | −0.0017 (13) | 0.0088 (14) | 0.0004 (14) |
| C5 | 0.040 (2) | 0.0256 (18) | 0.061 (3) | 0.0132 (15) | 0.0178 (19) | 0.009 (2) |
| C6 | 0.028 (3) | 0.0209 (14) | 0.0195 (16) | −0.0031 (18) | −0.0034 (16) | 0.0009 (11) |
| C7 | 0.032 (3) | 0.0215 (15) | 0.0156 (16) | −0.0040 (19) | −0.0001 (16) | 0.0030 (11) |
| C8 | 0.0254 (19) | 0.033 (3) | 0.028 (2) | 0.0020 (18) | 0.0088 (13) | 0.0016 (17) |
| C9 | 0.0310 (17) | 0.027 (3) | 0.0191 (19) | 0.002 (2) | 0.0020 (13) | 0.002 (2) |
| C10 | 0.0388 (19) | 0.053 (2) | 0.0182 (12) | 0.0216 (16) | 0.0019 (12) | −0.0002 (14) |
| C11 | 0.025 (3) | 0.022 (3) | 0.0175 (14) | 0.0099 (17) | 0.0012 (16) | −0.0002 (16) |
| C12 | 0.031 (2) | 0.0193 (15) | 0.0172 (16) | 0.0045 (16) | −0.0035 (13) | 0.0013 (12) |
| C13 | 0.034 (3) | 0.0192 (16) | 0.017 (2) | 0.0105 (16) | 0.0048 (14) | 0.0032 (14) |
| C14 | 0.0299 (18) | 0.033 (2) | 0.034 (2) | −0.0002 (14) | 0.0056 (13) | 0.0060 (14) |
| Pd1A | 0.0168 (4) | 0.0158 (3) | 0.01479 (16) | 0.0016 (2) | 0.0015 (2) | 0.00192 (15) |
| Cl1A | 0.0246 (6) | 0.0282 (7) | 0.0266 (5) | 0.0077 (5) | 0.0097 (5) | 0.0115 (5) |
| Cl2A | 0.0471 (11) | 0.0213 (5) | 0.0215 (5) | 0.0048 (5) | −0.0038 (5) | −0.0035 (3) |
| N1A | 0.016 (2) | 0.025 (2) | 0.0169 (15) | 0.0068 (14) | 0.0022 (14) | 0.0038 (13) |

| | | | | | | |
|---|---|---|---|---|---|---|
| N2A | 0.020 (2) | 0.023 (2) | 0.0231 (19) | 0.0004 (17) | 0.0029 (16) | 0.0017 (14) |
| N3A | 0.014 (4) | 0.0178 (19) | 0.016 (2) | 0.000 (2) | −0.0004 (19) | −0.0007 (15) |
| N4A | 0.016 (3) | 0.015 (3) | 0.0155 (19) | 0.001 (2) | 0.005 (2) | −0.004 (2) |
| N5A | 0.012 (4) | 0.015 (2) | 0.021 (3) | 0.0065 (18) | −0.003 (3) | 0.0012 (17) |
| C1A | 0.035 (3) | 0.033 (3) | 0.0186 (17) | 0.0070 (18) | 0.0032 (17) | −0.0008 (18) |
| C2A | 0.021 (2) | 0.023 (3) | 0.0217 (18) | 0.0015 (17) | 0.0075 (16) | 0.0012 (16) |
| C3A | 0.028 (3) | 0.022 (3) | 0.028 (2) | −0.0028 (19) | 0.0124 (18) | −0.0037 (18) |
| C4A | 0.022 (3) | 0.016 (2) | 0.037 (3) | 0.0018 (18) | 0.0167 (18) | 0.0000 (18) |
| C5A | 0.056 (4) | 0.031 (3) | 0.048 (4) | 0.021 (3) | 0.028 (3) | 0.013 (2) |
| C6A | 0.018 (3) | 0.019 (2) | 0.021 (2) | 0.0039 (19) | 0.0006 (18) | 0.0056 (14) |
| C7A | 0.024 (4) | 0.0173 (19) | 0.015 (2) | −0.003 (2) | 0.002 (2) | 0.0025 (14) |
| C8A | 0.032 (3) | 0.017 (3) | 0.020 (2) | 0.0082 (19) | 0.0079 (18) | 0.0021 (18) |
| C9A | 0.022 (2) | 0.016 (3) | 0.026 (3) | −0.002 (2) | −0.0006 (17) | −0.004 (2) |
| C10A | 0.025 (2) | 0.027 (2) | 0.0230 (17) | 0.0089 (15) | 0.0092 (14) | 0.0037 (15) |
| C11A | 0.024 (3) | 0.017 (3) | 0.0131 (17) | −0.0023 (17) | −0.0006 (18) | 0.0052 (16) |
| C12A | 0.026 (3) | 0.017 (2) | 0.0171 (19) | 0.003 (2) | 0.0065 (19) | 0.0016 (14) |
| C13A | 0.019 (3) | 0.024 (3) | 0.016 (3) | −0.001 (2) | 0.0010 (19) | 0.001 (2) |
| C14A | 0.025 (2) | 0.036 (3) | 0.028 (3) | −0.0013 (19) | 0.0044 (17) | 0.0051 (19) |
| O1W | 0.0207 (18) | 0.024 (2) | 0.028 (2) | −0.0029 (14) | 0.0055 (15) | −0.0101 (15) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Pd1—N1 | 2.005 (4) | Pd1A—N1A | 2.013 (5) |
| Pd1—N5 | 2.021 (8) | Pd1A—N5A | 2.017 (10) |
| Pd1—N3 | 2.048 (6) | Pd1A—N3A | 2.039 (8) |
| Pd1—Cl1 | 2.3079 (12) | Pd1A—Cl1A | 2.3009 (16) |
| N1—C2 | 1.353 (5) | N1A—C2A | 1.328 (8) |
| N1—N2 | 1.367 (6) | N1A—N2A | 1.372 (8) |
| N2—C4 | 1.350 (7) | N2A—C4A | 1.345 (10) |
| N2—C6 | 1.468 (6) | N2A—C6A | 1.460 (9) |
| N3—C8 | 1.471 (7) | N3A—C7A | 1.497 (14) |
| N3—C7 | 1.479 (11) | N3A—C8A | 1.511 (11) |
| N3—H3 | 0.9300 | N3A—H3B | 0.9300 |
| N4—C11 | 1.335 (9) | N4A—N5A | 1.360 (19) |
| N4—N5 | 1.381 (14) | N4A—C11A | 1.362 (13) |
| N4—C9 | 1.470 (9) | N4A—C9A | 1.421 (12) |
| N5—C13 | 1.296 (14) | N5A—C13A | 1.423 (17) |
| C1—C2 | 1.483 (6) | C1A—C2A | 1.510 (8) |
| C1—H1A | 0.9800 | C1A—H1D | 0.9800 |
| C1—H1B | 0.9800 | C1A—H1E | 0.9800 |
| C1—H1C | 0.9800 | C1A—H1F | 0.9800 |
| C2—C3 | 1.388 (8) | C2A—C3A | 1.390 (10) |
| C3—C4 | 1.372 (8) | C3A—C4A | 1.364 (11) |
| C3—H3A | 0.9500 | C3A—H3C | 0.9500 |
| C4—C5 | 1.489 (8) | C4A—C5A | 1.496 (11) |
| C5—H5A | 0.9800 | C5A—H5D | 0.9800 |
| C5—H5B | 0.9800 | C5A—H5E | 0.9800 |
| C5—H5C | 0.9800 | C5A—H5F | 0.9800 |

| | | | |
|---|---|---|---|
| C6—C7 | 1.500 (5) | C6A—C7A | 1.495 (7) |
| C6—H6A | 0.9900 | C6A—H6C | 0.9900 |
| C6—H6B | 0.9900 | C6A—H6D | 0.9900 |
| C7—H7A | 0.9900 | C7A—H7C | 0.9900 |
| C7—H7B | 0.9900 | C7A—H7D | 0.9900 |
| C8—C9 | 1.528 (9) | C8A—C9A | 1.515 (12) |
| C8—H8A | 0.9900 | C8A—H8C | 0.9900 |
| C8—H8B | 0.9900 | C8A—H8D | 0.9900 |
| C9—H9A | 0.9900 | C9A—H9C | 0.9900 |
| C9—H9B | 0.9900 | C9A—H9D | 0.9900 |
| C10—C11 | 1.476 (6) | C10A—C11A | 1.479 (8) |
| C10—H10A | 0.9800 | C10A—H10D | 0.9800 |
| C10—H10B | 0.9800 | C10A—H10E | 0.9800 |
| C10—H10C | 0.9800 | C10A—H10F | 0.9800 |
| C11—C12 | 1.372 (5) | C11A—C12A | 1.371 (6) |
| C12—C13 | 1.399 (5) | C12A—C13A | 1.389 (7) |
| C12—H12 | 0.9500 | C12A—H12A | 0.9500 |
| C13—C14 | 1.490 (7) | C13A—C14A | 1.486 (9) |
| C14—H14A | 0.9800 | C14A—H14D | 0.9800 |
| C14—H14B | 0.9800 | C14A—H14E | 0.9800 |
| C14—H14C | 0.9800 | C14A—H14F | 0.9800 |

| | | | |
|---|---|---|---|
| N1—Pd1—N5 | 172.9 (5) | C7A—N3A—C8A | 109.2 (9) |
| N1—Pd1—N3 | 90.9 (3) | C7A—N3A—Pd1A | 116.1 (6) |
| N5—Pd1—N3 | 83.7 (5) | C8A—N3A—Pd1A | 114.6 (7) |
| N1—Pd1—Cl1 | 91.86 (10) | C7A—N3A—H3B | 105.2 |
| N5—Pd1—Cl1 | 93.3 (4) | C8A—N3A—H3B | 105.2 |
| N3—Pd1—Cl1 | 175.9 (4) | Pd1A—N3A—H3B | 105.2 |
| C2—N1—N2 | 106.1 (4) | N5A—N4A—C11A | 110.8 (8) |
| C2—N1—Pd1 | 134.2 (3) | N5A—N4A—C9A | 117.7 (11) |
| N2—N1—Pd1 | 117.9 (3) | C11A—N4A—C9A | 131.4 (9) |
| C4—N2—N1 | 110.7 (4) | N4A—N5A—C13A | 105.7 (9) |
| C4—N2—C6 | 128.7 (4) | N4A—N5A—Pd1A | 117.8 (11) |
| N1—N2—C6 | 119.0 (4) | C13A—N5A—Pd1A | 131.7 (12) |
| C8—N3—C7 | 113.7 (6) | C2A—C1A—H1D | 109.5 |
| C8—N3—Pd1 | 114.5 (5) | C2A—C1A—H1E | 109.5 |
| C7—N3—Pd1 | 115.5 (5) | H1D—C1A—H1E | 109.5 |
| C8—N3—H3 | 103.7 | C2A—C1A—H1F | 109.5 |
| C7—N3—H3 | 103.7 | H1D—C1A—H1F | 109.5 |
| Pd1—N3—H3 | 103.7 | H1E—C1A—H1F | 109.5 |
| C11—N4—N5 | 110.9 (7) | N1A—C2A—C3A | 108.1 (6) |
| C11—N4—C9 | 129.6 (8) | N1A—C2A—C1A | 122.5 (5) |
| N5—N4—C9 | 119.5 (8) | C3A—C2A—C1A | 129.4 (6) |
| C13—N5—N4 | 106.5 (6) | C4A—C3A—C2A | 107.9 (7) |
| C13—N5—Pd1 | 139.0 (8) | C4A—C3A—H3C | 126.0 |
| N4—N5—Pd1 | 114.5 (8) | C2A—C3A—H3C | 126.0 |
| N1—C2—C3 | 109.2 (4) | N2A—C4A—C3A | 106.7 (7) |
| N1—C2—C1 | 122.3 (4) | N2A—C4A—C5A | 122.3 (7) |

| | | | |
|---|---|---|---|
| C3—C2—C1 | 128.2 (4) | C3A—C4A—C5A | 131.0 (7) |
| C4—C3—C2 | 107.0 (5) | C4A—C5A—H5D | 109.5 |
| C4—C3—H3A | 126.5 | C4A—C5A—H5E | 109.5 |
| C2—C3—H3A | 126.5 | H5D—C5A—H5E | 109.5 |
| N2—C4—C3 | 107.0 (5) | C4A—C5A—H5F | 109.5 |
| N2—C4—C5 | 122.5 (5) | H5D—C5A—H5F | 109.5 |
| C3—C4—C5 | 130.5 (5) | H5E—C5A—H5F | 109.5 |
| N2—C6—C7 | 110.8 (4) | N2A—C6A—C7A | 109.7 (5) |
| N2—C6—H6A | 109.5 | N2A—C6A—H6C | 109.7 |
| C7—C6—H6A | 109.5 | C7A—C6A—H6C | 109.7 |
| N2—C6—H6B | 109.5 | N2A—C6A—H6D | 109.7 |
| C7—C6—H6B | 109.5 | C7A—C6A—H6D | 109.7 |
| H6A—C6—H6B | 108.1 | H6C—C6A—H6D | 108.2 |
| N3—C7—C6 | 111.2 (4) | C6A—C7A—N3A | 111.5 (6) |
| N3—C7—H7A | 109.4 | C6A—C7A—H7C | 109.3 |
| C6—C7—H7A | 109.4 | N3A—C7A—H7C | 109.3 |
| N3—C7—H7B | 109.4 | C6A—C7A—H7D | 109.3 |
| C6—C7—H7B | 109.4 | N3A—C7A—H7D | 109.3 |
| H7A—C7—H7B | 108.0 | H7C—C7A—H7D | 108.0 |
| N3—C8—C9 | 111.6 (6) | N3A—C8A—C9A | 111.3 (8) |
| N3—C8—H8A | 109.3 | N3A—C8A—H8C | 109.4 |
| C9—C8—H8A | 109.3 | C9A—C8A—H8C | 109.4 |
| N3—C8—H8B | 109.3 | N3A—C8A—H8D | 109.4 |
| C9—C8—H8B | 109.3 | C9A—C8A—H8D | 109.4 |
| H8A—C8—H8B | 108.0 | H8C—C8A—H8D | 108.0 |
| N4—C9—C8 | 111.4 (7) | N4A—C9A—C8A | 112.0 (10) |
| N4—C9—H9A | 109.3 | N4A—C9A—H9C | 109.2 |
| C8—C9—H9A | 109.3 | C8A—C9A—H9C | 109.2 |
| N4—C9—H9B | 109.3 | N4A—C9A—H9D | 109.2 |
| C8—C9—H9B | 109.3 | C8A—C9A—H9D | 109.2 |
| H9A—C9—H9B | 108.0 | H9C—C9A—H9D | 107.9 |
| N4—C11—C12 | 105.8 (5) | C11A—C10A—H10D | 109.5 |
| N4—C11—C10 | 123.8 (5) | C11A—C10A—H10E | 109.5 |
| C12—C11—C10 | 130.4 (4) | H10D—C10A—H10E | 109.5 |
| C11—C12—C13 | 107.0 (5) | C11A—C10A—H10F | 109.5 |
| C11—C12—H12 | 126.5 | H10D—C10A—H10F | 109.5 |
| C13—C12—H12 | 126.5 | H10E—C10A—H10F | 109.5 |
| N5—C13—C12 | 109.7 (6) | N4A—C11A—C12A | 107.7 (7) |
| N5—C13—C14 | 121.7 (6) | N4A—C11A—C10A | 122.5 (6) |
| C12—C13—C14 | 128.2 (6) | C12A—C11A—C10A | 129.8 (7) |
| N1A—Pd1A—N5A | 170.5 (6) | C11A—C12A—C13A | 108.2 (7) |
| N1A—Pd1A—N3A | 90.8 (4) | C11A—C12A—H12A | 125.9 |
| N5A—Pd1A—N3A | 84.5 (7) | C13A—C12A—H12A | 125.9 |
| N1A—Pd1A—Cl1A | 91.72 (13) | C12A—C13A—N5A | 107.1 (8) |
| N5A—Pd1A—Cl1A | 93.9 (6) | C12A—C13A—C14A | 130.8 (7) |
| N3A—Pd1A—Cl1A | 173.5 (4) | N5A—C13A—C14A | 122.1 (8) |
| C2A—N1A—N2A | 107.5 (5) | C13A—C14A—H14D | 109.5 |
| C2A—N1A—Pd1A | 133.8 (4) | C13A—C14A—H14E | 109.5 |

| | | | |
|---|---|---|---|
| N2A—N1A—Pd1A | 118.5 (4) | H14D—C14A—H14E | 109.5 |
| C4A—N2A—N1A | 109.8 (6) | C13A—C14A—H14F | 109.5 |
| C4A—N2A—C6A | 128.9 (6) | H14D—C14A—H14F | 109.5 |
| N1A—N2A—C6A | 119.3 (6) | H14E—C14A—H14F | 109.5 |
| | | | |
| N3—Pd1—N1—C2 | −148.4 (4) | N3A—Pd1A—N1A—C2A | −138.0 (6) |
| Cl1—Pd1—N1—C2 | 34.7 (4) | Cl1A—Pd1A—N1A—C2A | 48.0 (4) |
| N3—Pd1—N1—N2 | 49.4 (3) | N3A—Pd1A—N1A—N2A | 47.0 (5) |
| Cl1—Pd1—N1—N2 | −127.5 (2) | Cl1A—Pd1A—N1A—N2A | −127.0 (3) |
| C2—N1—N2—C4 | 0.6 (4) | C2A—N1A—N2A—C4A | 0.0 (5) |
| Pd1—N1—N2—C4 | 167.4 (2) | Pd1A—N1A—N2A—C4A | 176.2 (3) |
| C2—N1—N2—C6 | 167.5 (3) | C2A—N1A—N2A—C6A | 165.0 (4) |
| Pd1—N1—N2—C6 | −25.7 (4) | Pd1A—N1A—N2A—C6A | −18.7 (5) |
| N1—Pd1—N3—C8 | 120.0 (8) | N1A—Pd1A—N3A—C7A | −18.1 (9) |
| N5—Pd1—N3—C8 | −64.6 (9) | N5A—Pd1A—N3A—C7A | 170.2 (11) |
| N1—Pd1—N3—C7 | −15.0 (7) | N1A—Pd1A—N3A—C8A | 110.8 (9) |
| N5—Pd1—N3—C7 | 160.4 (8) | N5A—Pd1A—N3A—C8A | −60.9 (11) |
| C11—N4—N5—C13 | 3.8 (17) | C11A—N4A—N5A—C13A | −7 (2) |
| C9—N4—N5—C13 | −176.5 (11) | C9A—N4A—N5A—C13A | 176.1 (14) |
| C11—N4—N5—Pd1 | −175.1 (8) | C11A—N4A—N5A—Pd1A | −165.3 (12) |
| C9—N4—N5—Pd1 | 4.6 (18) | C9A—N4A—N5A—Pd1A | 18 (2) |
| N3—Pd1—N5—C13 | −129.7 (19) | N3A—Pd1A—N5A—N4A | 39.0 (17) |
| Cl1—Pd1—N5—C13 | 47.5 (18) | Cl1A—Pd1A—N5A—N4A | −147.3 (17) |
| N3—Pd1—N5—N4 | 48.7 (12) | N3A—Pd1A—N5A—C13A | −113 (2) |
| Cl1—Pd1—N5—N4 | −134.1 (12) | Cl1A—Pd1A—N5A—C13A | 61 (2) |
| N2—N1—C2—C3 | 0.2 (4) | N2A—N1A—C2A—C3A | 0.4 (5) |
| Pd1—N1—C2—C3 | −163.5 (3) | Pd1A—N1A—C2A—C3A | −175.0 (4) |
| N2—N1—C2—C1 | −174.3 (3) | N2A—N1A—C2A—C1A | −177.0 (4) |
| Pd1—N1—C2—C1 | 22.0 (5) | Pd1A—N1A—C2A—C1A | 7.6 (7) |
| N1—C2—C3—C4 | −0.9 (4) | N1A—C2A—C3A—C4A | −0.6 (6) |
| C1—C2—C3—C4 | 173.2 (4) | C1A—C2A—C3A—C4A | 176.5 (5) |
| N1—N2—C4—C3 | −1.2 (4) | N1A—N2A—C4A—C3A | −0.4 (6) |
| C6—N2—C4—C3 | −166.4 (4) | C6A—N2A—C4A—C3A | −163.6 (5) |
| N1—N2—C4—C5 | 178.4 (4) | N1A—N2A—C4A—C5A | 179.9 (5) |
| C6—N2—C4—C5 | 13.1 (6) | C6A—N2A—C4A—C5A | 16.7 (9) |
| C2—C3—C4—N2 | 1.2 (4) | C2A—C3A—C4A—N2A | 0.6 (6) |
| C2—C3—C4—C5 | −178.2 (4) | C2A—C3A—C4A—C5A | −179.7 (6) |
| C4—N2—C6—C7 | 121.7 (5) | C4A—N2A—C6A—C7A | 112.8 (7) |
| N1—N2—C6—C7 | −42.5 (5) | N1A—N2A—C6A—C7A | −49.0 (7) |
| C8—N3—C7—C6 | −174.3 (6) | N2A—C6A—C7A—N3A | 78.9 (9) |
| Pd1—N3—C7—C6 | −39.0 (8) | C8A—N3A—C7A—C6A | −166.3 (7) |
| N2—C6—C7—N3 | 79.1 (7) | Pd1A—N3A—C7A—C6A | −34.8 (11) |
| C7—N3—C8—C9 | 160.3 (6) | C7A—N3A—C8A—C9A | 160.0 (7) |
| Pd1—N3—C8—C9 | 24.4 (9) | Pd1A—N3A—C8A—C9A | 27.7 (12) |
| C11—N4—C9—C8 | 112.6 (12) | N5A—N4A—C9A—C8A | −73.7 (19) |
| N5—N4—C9—C8 | −67.0 (14) | C11A—N4A—C9A—C8A | 109.9 (16) |
| N3—C8—C9—N4 | 46.6 (9) | N3A—C8A—C9A—N4A | 44.1 (12) |
| N5—N4—C11—C12 | −2.5 (13) | N5A—N4A—C11A—C12A | 2.8 (18) |

| | | | |
|---|---|---|---|
| C9—N4—C11—C12 | 177.9 (11) | C9A—N4A—C11A—C12A | 179.4 (15) |
| N5—N4—C11—C10 | 175.0 (9) | N5A—N4A—C11A—C10A | −178.8 (13) |
| C9—N4—C11—C10 | −4.6 (16) | C9A—N4A—C11A—C10A | −2 (2) |
| N4—C11—C12—C13 | 0.3 (8) | N4A—C11A—C12A—C13A | 2.6 (11) |
| C10—C11—C12—C13 | −177.0 (5) | C10A—C11A—C12A—C13A | −175.7 (8) |
| N4—N5—C13—C12 | −3.6 (15) | C11A—C12A—C13A—N5A | −6.7 (14) |
| Pd1—N5—C13—C12 | 174.9 (14) | C11A—C12A—C13A—C14A | 175.5 (9) |
| N4—N5—C13—C14 | −176.6 (9) | N4A—N5A—C13A—C12A | 8 (2) |
| Pd1—N5—C13—C14 | 2 (2) | Pd1A—N5A—C13A—C12A | 162.4 (15) |
| C11—C12—C13—N5 | 2.2 (11) | N4A—N5A—C13A—C14A | −173.8 (13) |
| C11—C12—C13—C14 | 174.6 (6) | Pd1A—N5A—C13A—C14A | −20 (3) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N3—H3···Cl2 | 0.93 | 2.24 | 3.162 (12) | 174 |
| N3*A*—H3*B*···Cl2*A* | 0.93 | 2.17 | 3.088 (15) | 170 |