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Dibromido[*N*-(1-diethylamino-1-oxo-3-phenylpropan-2-yl)-*N*′-(pyridin-2-yl)imidazol-2-ylidene]palladium(II) dichloromethane monosolvate

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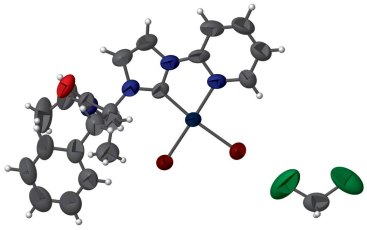
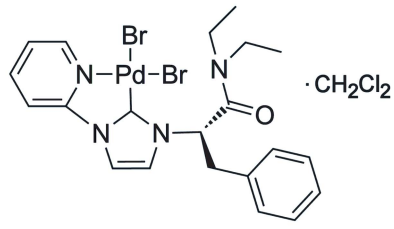
In the molecule of the title *N*,*N*′-disubstituted imidazol-2-ylidene palladium(II) complex, $[PdBr_2(C_{21}H_{24}N_4O)]\cdot CH_2Cl_2$, the palladium(II) atom adopts a slightly distorted square-planar coordination (r.m.s. deviation = 0.0145 Å), and the five-membered chelate ring is almost planar [maximum displacement = 0.015 (8) Å]. The molecular conformation is enforced by intramolecular C—H···Br hydrogen bonds. In the crystal, complex molecules and dichloromethane molecules are linked into a three-dimensional network by C—H···O and C—H···Br hydrogen bonds.

3D view



Chemical scheme



Structure description

N-Heterocyclic carbenes (NHCs) have been widely used as ancillary ligands in coordination chemistry and organic catalysis since the successful isolation and characterization of the first stable NHC by Arduengo (Arduengo *et al.*, 1991). Chelating NHC metal complexes containing heteroatom donors, such as P, N, O and S, have been synthesized, characterized and employed extensively as catalysts for organic transformations (Ahrens *et al.*, 2006; Bierenstiel & Cross, 2011; Meyer *et al.*, 2012; Peris & Crabtree, 2004). Our group has developed an efficient procedure for the synthesis of chiral imidazole derivatives carrying hydroxyalkyl or amide functional groups (Mao *et al.*, 2010). Through simple quaternization by 2-bromopyridine or 2-chloropyrimidine, hetero-difunctionalized imidazolium salts were obtained. Direct metallation of the hetero-difunctionalized imidazolium salts by $Pd(OAc)_2$ under mild reaction condition produced the C_{NHC},N-chelating palladium complexes smoothly (Yang *et al.*, 2015; Yang, Zhang, Xiao & Mao, 2016; Yang, Zhang, Yuan *et al.*, 2016). As part of our work on the synthesis

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···Br2^{i}	0.93	2.77	3.540 (7)	141
C9—H9···Br2	0.98	2.57	3.381 (12)	141
C16—H16···Br2	0.93	2.92	3.678 (9)	140
C22—H22A···Br1^{ii}	0.97	2.91	3.836 (19)	160
C22—H22B···O1^{iii}	0.97	2.46	3.40 (2)	164

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

and application of chiral chelating NHC palladium complexes, we report here the crystal structure of the title *N,N′*-disubstituted imidazol-2-ylidene palladium(II) complex.

In the title complex (Fig. 1), the palladium(II) atom adopts a slightly distorted square-planar coordination bonded to C6, N1, Br1, and Br2 (r.m.s. deviation = 0.0145 Å). The Pd1—C6, Pd1—N1, Pd1—Br1 and Pd1—Br2 bond lengths are 1.986 (9), 2.052 (5), 2.4678 (12) and 2.3849 (12) Å, respectively. The five-membered chelate ring (C6/Pd1/N1/C5/N2) is almost planar [maximum displacement = 0.015 (8) Å for atom C5]. The N1—C5—N2—C6 torsion angle is 1.3 (13)°. A pair of intramolecular C—H···Br hydrogen bonds (Table 1) stabilizes the molecular conformation. In the crystal, complex molecules and dichloromethane molecules are linked into a three-dimensional network by C—H···O and C—H···Br hydrogen bonds (Table 1).

Synthesis and crystallization

A mixture of (*S*)-*N*-(1-(diethylamino)-1-oxo-3-phenylpropan-2-yl)-*N′*-(pyridin-2-yl)-1H-imidazolium bromide (1 mmol, 0.43 g) and $Pd(OAc)_2$ (1 mmol, 0.22 g) was stirred in anhydrous dichloromethane (10 mL) at room temperature for 12 h. The reaction mixture was then evaporated. Purification of the residue by column chromatography (silica, CH_2Cl_2/acetone, gradient elution, 15:1–8:1 *v*/*v*) produced the title NHC palladium complex as a yellow solid (0.24 g, 39%). Crystallization of the solid from CH_2Cl_2/hexane (1:1 *v*/*v*) afforded the title complex as yellow crystals.

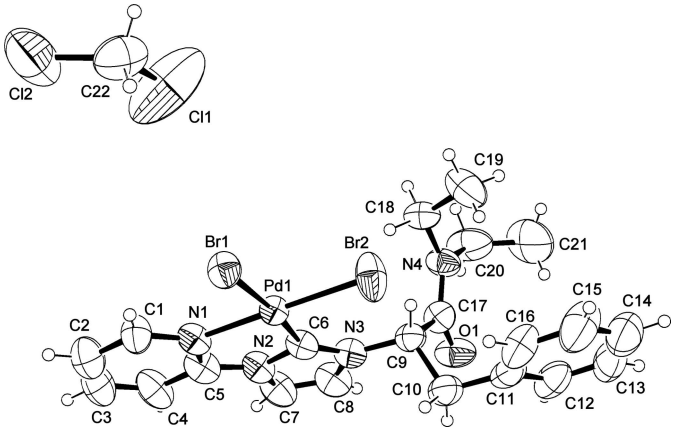


Figure 1
The asymmetric unit of the title compound, showing 40% probability displacement ellipsoids.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[PdBr_2(C_{21}H_{24}N_4O)]\cdot CH_2Cl_2$
M_r	699.59
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	293
a, b, c (Å)	17.6670 (4), 12.8871 (3), 11.7476 (3)
V (Å^3)	2674.65 (11)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	11.11
Crystal size (mm)	0.33 × 0.17 × 0.07
Data collection	
Diffractometer	Agilent Xcalibur Eos Gemini
Absorption correction	Gaussian (*CrysAlis PRO*; Agilent, 2014)
T_{min}, T_{max}	0.149, 0.607
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7177, 4332, 3852
R_{int}	0.039
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.597
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.049, 0.138, 1.03
No. of reflections	4332
No. of parameters	267
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.01, −0.44
Absolute structure	Flack x determined using 1279 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	−0.009 (13)

Computer programs: *CrysAlis PRO* (Agilent, 2014), *SUPERFLIP* (Palatinus & Chapuis, 2007; Palatinus & van der Lee, 2008; Palatinus *et al.*, 2012), *SHELXL* (Sheldrick, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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full crystallographic data

IUCrData (2019). **4**, x190899 [https://doi.org/10.1107/S241431461900899X]

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Crystal data

$[PdBr_2(C_{21}H_{24}N_4O)]\cdot CH_2Cl_2$
M_r = 699.59
Orthorhombic, $P2_12_12_1$
a = 17.6670 (4) Å
b = 12.8871 (3) Å
c = 11.7476 (3) Å
V = 2674.65 (11) Å^3
Z = 4
$F(000)$ = 1376
D_x = 1.737 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 2891 reflections
θ = 3.8–70.6°
μ = 11.11 mm^{-1}
T = 293 K
, light yellow
0.33 × 0.17 × 0.07 mm

Data collection

Agilent Xcalibur Eos Gemini diffractometer
Radiation source: Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 16.2312 pixels mm^{-1}
ω scans
Absorption correction: gaussian (CrysAlis PRO; Agilent, 2014)
T_{min} = 0.149, T_{max} = 0.607
7177 measured reflections
4332 independent reflections
3852 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 67.1°, θ_{min} = 4.3°
h = −10→21
k = −15→9
l = −12→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.138
S = 1.03
4332 reflections
267 parameters
0 restraints
Primary atom site location: iterative
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0803P)^2 + 0.2381P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.01 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}
Absolute structure: Flack x determined using 1279 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: −0.009 (13)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. All H atoms were placed geometrically and refined using a riding atom approximation, with C–H = 0.93-0.98 Å, and with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C) for methyl H atoms. A rotating model was used for the methyl groups.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.59851 (6)	0.56133 (8)	0.49147 (12)	0.0705 (3)
Br2	0.60329 (6)	0.82311 (9)	0.4899 (2)	0.0984 (6)
C5	0.3460 (3)	0.6459 (4)	0.4318 (7)	0.072 (3)
C4	0.2814 (3)	0.5863 (7)	0.4143 (9)	0.092 (4)
H4	0.2352	0.6185	0.4005	0.110*
C3	0.2860 (4)	0.4787 (6)	0.4174 (10)	0.099 (5)
H3	0.2428	0.4389	0.4056	0.119*
C2	0.3550 (5)	0.4306 (4)	0.4379 (9)	0.096 (4)
H2	0.3581	0.3586	0.4400	0.115*
C1	0.4196 (4)	0.4901 (5)	0.4554 (8)	0.081 (3)
H1	0.4658	0.4580	0.4692	0.098*
N1	0.4151 (3)	0.5978 (5)	0.4524 (6)	0.064 (2)
C6	0.4184 (5)	0.7990 (9)	0.4476 (8)	0.060 (2)
C7	0.2929 (7)	0.8202 (11)	0.4163 (13)	0.086 (4)
H7	0.2423	0.8042	0.4026	0.104*
C8	0.3227 (7)	0.9141 (11)	0.4248 (13)	0.083 (4)
H8	0.2966	0.9766	0.4203	0.100*
C9	0.4565 (7)	0.9878 (8)	0.4515 (9)	0.061 (2)
H9	0.5008	0.9641	0.4944	0.074*
C10	0.4826 (9)	1.0268 (10)	0.3327 (10)	0.081 (4)
H10A	0.5024	0.9687	0.2892	0.097*
H10B	0.4394	1.0546	0.2918	0.097*
C11	0.5431 (6)	1.1098 (6)	0.3424 (8)	0.083 (4)
C16	0.6182 (6)	1.0813 (6)	0.3583 (10)	0.104 (5)
H16	0.6317	1.0116	0.3589	0.125*
C15	0.6733 (5)	1.1572 (10)	0.3732 (12)	0.145 (9)
H15	0.7236	1.1381	0.3838	0.174*
C14	0.6532 (7)	1.2614 (9)	0.3722 (11)	0.124 (7)
H14	0.6901	1.3122	0.3822	0.149*
C13	0.5781 (8)	1.2899 (5)	0.3563 (9)	0.114 (6)
H13	0.5647	1.3597	0.3556	0.137*
C12	0.5230 (6)	1.2141 (7)	0.3414 (8)	0.096 (5)
H12	0.4727	1.2331	0.3307	0.116*
C17	0.4186 (7)	1.0784 (8)	0.5167 (11)	0.069 (3)
C18	0.4815 (7)	1.0208 (10)	0.6941 (9)	0.074 (3)
H18A	0.4820	0.9524	0.6597	0.089*

H18B	0.4592	1.0140	0.7692	0.089*
C19	0.5616 (10)	1.0567 (14)	0.7076 (17)	0.118 (6)
H19A	0.5861	1.0570	0.6346	0.177*
H19B	0.5881	1.0105	0.7579	0.177*
H19C	0.5621	1.1255	0.7388	0.177*
C20	0.3960 (13)	1.1763 (13)	0.6898 (12)	0.120 (7)
H20A	0.3452	1.1870	0.6607	0.144*
H20B	0.3921	1.1579	0.7696	0.144*
C21	0.4391 (16)	1.2722 (13)	0.679 (2)	0.179 (13)
H21A	0.4528	1.2822	0.6003	0.269*
H21B	0.4840	1.2679	0.7242	0.269*
H21C	0.4087	1.3295	0.7038	0.269*
N2	0.3517 (5)	0.7504 (7)	0.4316 (8)	0.066 (2)
N3	0.4022 (5)	0.9018 (7)	0.4421 (8)	0.065 (2)
N4	0.4331 (6)	1.0885 (8)	0.6254 (8)	0.072 (3)
O1	0.3743 (6)	1.1351 (7)	0.4652 (7)	0.090 (3)
Pd1	0.50333 (3)	0.70009 (5)	0.46982 (5)	0.0533 (2)
C22	0.7655 (10)	0.3250 (16)	0.7695 (17)	0.121 (6)
H22A	0.8019	0.3344	0.8304	0.146*
H22B	0.7934	0.3225	0.6984	0.146*
Cl1	0.7074 (5)	0.4286 (8)	0.7666 (10)	0.253 (6)
Cl2	0.7195 (5)	0.2046 (6)	0.7892 (5)	0.186 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0626 (6)	0.0614 (6)	0.0876 (8)	0.0079 (4)	−0.0037 (6)	−0.0007 (5)
Br2	0.0518 (5)	0.0620 (6)	0.1813 (18)	−0.0015 (4)	−0.0171 (9)	0.0036 (9)
C5	0.039 (4)	0.099 (8)	0.076 (7)	0.001 (5)	0.012 (5)	−0.017 (6)
C4	0.058 (6)	0.111 (10)	0.107 (10)	−0.012 (6)	0.011 (7)	−0.037 (9)
C3	0.072 (7)	0.100 (10)	0.124 (12)	−0.028 (7)	0.009 (9)	−0.022 (9)
C2	0.085 (8)	0.087 (9)	0.115 (11)	−0.017 (7)	0.009 (9)	−0.012 (8)
C1	0.077 (7)	0.066 (7)	0.101 (9)	−0.010 (5)	−0.001 (7)	0.002 (6)
N1	0.047 (4)	0.079 (5)	0.066 (5)	−0.002 (4)	0.004 (4)	−0.013 (5)
C6	0.053 (4)	0.065 (6)	0.061 (5)	0.014 (4)	−0.001 (4)	−0.013 (5)
C7	0.055 (5)	0.095 (9)	0.109 (9)	0.013 (6)	−0.015 (7)	−0.024 (8)
C8	0.061 (6)	0.093 (9)	0.096 (9)	0.017 (6)	−0.007 (6)	−0.011 (7)
C9	0.072 (6)	0.056 (5)	0.057 (5)	0.011 (4)	−0.003 (5)	−0.001 (4)
C10	0.105 (10)	0.076 (7)	0.062 (6)	0.004 (7)	−0.001 (7)	0.000 (5)
C11	0.123 (11)	0.072 (7)	0.053 (5)	0.011 (7)	0.007 (7)	0.009 (5)
C16	0.100 (10)	0.094 (10)	0.117 (12)	0.003 (9)	0.023 (10)	0.035 (9)
C15	0.127 (16)	0.125 (15)	0.18 (2)	−0.003 (13)	0.004 (17)	0.065 (15)
C14	0.153 (18)	0.108 (14)	0.112 (13)	−0.026 (13)	0.022 (14)	0.012 (10)
C13	0.173 (19)	0.064 (8)	0.105 (11)	−0.010 (11)	0.020 (12)	0.005 (7)
C12	0.136 (13)	0.070 (8)	0.083 (7)	0.022 (8)	0.022 (8)	0.013 (6)
C17	0.069 (6)	0.065 (6)	0.073 (6)	0.011 (5)	0.005 (6)	−0.001 (5)
C18	0.079 (8)	0.088 (8)	0.055 (5)	0.015 (6)	−0.005 (5)	−0.005 (5)
C19	0.102 (12)	0.119 (13)	0.133 (15)	−0.005 (10)	−0.035 (12)	−0.031 (11)

C20	0.180 (19)	0.106 (12)	0.074 (8)	0.056 (13)	−0.009 (11)	−0.024 (8)
C21	0.30 (4)	0.072 (11)	0.17 (2)	0.039 (15)	−0.06 (2)	−0.043 (12)
N2	0.048 (4)	0.078 (6)	0.072 (5)	0.002 (4)	0.003 (4)	−0.011 (5)
N3	0.059 (4)	0.071 (5)	0.064 (5)	0.009 (4)	−0.001 (4)	−0.005 (4)
N4	0.082 (6)	0.073 (6)	0.061 (5)	0.016 (5)	−0.009 (5)	−0.015 (4)
O1	0.111 (7)	0.086 (5)	0.072 (5)	0.047 (5)	−0.018 (5)	−0.008 (4)
Pd1	0.0455 (3)	0.0578 (4)	0.0565 (3)	0.0016 (3)	0.0020 (3)	−0.0010 (3)
C22	0.089 (9)	0.174 (18)	0.101 (11)	−0.006 (11)	0.012 (9)	0.031 (12)
Cl1	0.186 (7)	0.284 (10)	0.290 (11)	0.124 (7)	0.111 (8)	0.154 (9)
Cl2	0.210 (7)	0.217 (7)	0.130 (4)	−0.105 (7)	0.024 (5)	−0.039 (4)

Geometric parameters (Å, º)

Br1—Pd1	2.4678 (12)	C11—C12	1.3900
Br2—Pd1	2.3849 (12)	C16—H16	0.9300
C5—C4	1.3900	C16—C15	1.3900
C5—N1	1.3900	C15—H15	0.9300
C5—N2	1.350 (11)	C15—C14	1.3900
C4—H4	0.9300	C14—H14	0.9300
C4—C3	1.3900	C14—C13	1.3900
C3—H3	0.9300	C13—H13	0.9300
C3—C2	1.3900	C13—C12	1.3900
C2—H2	0.9300	C12—H12	0.9300
C2—C1	1.3900	C17—N4	1.309 (16)
C1—H1	0.9300	C17—O1	1.229 (14)
C1—N1	1.3900	C18—H18A	0.9700
N1—Pd1	2.052 (5)	C18—H18B	0.9700
C6—N2	1.347 (13)	C18—C19	1.497 (19)
C6—N3	1.357 (14)	C18—N4	1.464 (15)
C6—Pd1	1.986 (9)	C19—H19A	0.9600
C7—H7	0.9300	C19—H19B	0.9600
C7—C8	1.323 (19)	C19—H19C	0.9600
C7—N2	1.387 (14)	C20—H20A	0.9700
C8—H8	0.9300	C20—H20B	0.9700
C8—N3	1.429 (14)	C20—C21	1.46 (3)
C9—H9	0.9800	C20—N4	1.511 (16)
C9—C10	1.554 (16)	C21—H21A	0.9600
C9—C17	1.549 (14)	C21—H21B	0.9600
C9—N3	1.469 (14)	C21—H21C	0.9600
C10—H10A	0.9700	C22—H22A	0.9700
C10—H10B	0.9700	C22—H22B	0.9700
C10—C11	1.516 (16)	C22—Cl1	1.684 (19)
C11—C16	1.3900	C22—Cl2	1.766 (19)
C4—C5—N1	120.0	C12—C13—H13	120.0
N2—C5—C4	127.7 (6)	C11—C12—H12	120.0
N2—C5—N1	112.3 (6)	C13—C12—C11	120.0
C5—C4—H4	120.0	C13—C12—H12	120.0

C3—C4—C5	120.0	N4—C17—C9	118.2 (10)
C3—C4—H4	120.0	O1—C17—C9	118.6 (11)
C4—C3—H3	120.0	O1—C17—N4	123.2 (11)
C4—C3—C2	120.0	H18A—C18—H18B	107.5
C2—C3—H3	120.0	C19—C18—H18A	108.5
C3—C2—H2	120.0	C19—C18—H18B	108.5
C1—C2—C3	120.0	N4—C18—H18A	108.5
C1—C2—H2	120.0	N4—C18—H18B	108.5
C2—C1—H1	120.0	N4—C18—C19	115.2 (13)
C2—C1—N1	120.0	C18—C19—H19A	109.5
N1—C1—H1	120.0	C18—C19—H19B	109.5
C5—N1—Pd1	113.4 (4)	C18—C19—H19C	109.5
C1—N1—C5	120.0	H19A—C19—H19B	109.5
C1—N1—Pd1	126.5 (4)	H19A—C19—H19C	109.5
N2—C6—N3	105.3 (9)	H19B—C19—H19C	109.5
N2—C6—Pd1	112.4 (8)	H20A—C20—H20B	108.0
N3—C6—Pd1	142.3 (8)	C21—C20—H20A	109.4
C8—C7—H7	126.7	C21—C20—H20B	109.4
C8—C7—N2	106.6 (11)	C21—C20—N4	111.3 (17)
N2—C7—H7	126.7	N4—C20—H20A	109.4
C7—C8—H8	126.2	N4—C20—H20B	109.4
C7—C8—N3	107.5 (11)	C20—C21—H21A	109.5
N3—C8—H8	126.2	C20—C21—H21B	109.5
C10—C9—H9	109.0	C20—C21—H21C	109.5
C17—C9—H9	109.0	H21A—C21—H21B	109.5
C17—C9—C10	109.2 (9)	H21A—C21—H21C	109.5
N3—C9—H9	109.0	H21B—C21—H21C	109.5
N3—C9—C10	111.7 (9)	C5—N2—C7	126.3 (9)
N3—C9—C17	108.9 (9)	C6—N2—C5	121.9 (9)
C9—C10—H10A	109.3	C6—N2—C7	111.8 (9)
C9—C10—H10B	109.3	C6—N3—C8	108.7 (10)
H10A—C10—H10B	107.9	C6—N3—C9	126.6 (9)
C11—C10—C9	111.7 (9)	C8—N3—C9	124.7 (10)
C11—C10—H10A	109.3	C17—N4—C18	126.4 (10)
C11—C10—H10B	109.3	C17—N4—C20	118.5 (11)
C16—C11—C10	119.8 (8)	C18—N4—C20	115.1 (10)
C16—C11—C12	120.0	Br2—Pd1—Br1	88.10 (4)
C12—C11—C10	120.1 (8)	N1—Pd1—Br1	93.58 (18)
C11—C16—H16	120.0	N1—Pd1—Br2	178.31 (18)
C15—C16—C11	120.0	C6—Pd1—Br1	173.4 (3)
C15—C16—H16	120.0	C6—Pd1—Br2	98.4 (3)
C16—C15—H15	120.0	C6—Pd1—N1	79.9 (4)
C16—C15—C14	120.0	H22A—C22—H22B	107.5
C14—C15—H15	120.0	Cl1—C22—H22A	108.6
C15—C14—H14	120.0	Cl1—C22—H22B	108.6
C13—C14—C15	120.0	Cl1—C22—Cl2	114.8 (10)
C13—C14—H14	120.0	Cl2—C22—H22A	108.6
C14—C13—H13	120.0	Cl2—C22—H22B	108.6

C12—C13—C14	120.0		
C5—C4—C3—C2	0.0	C16—C15—C14—C13	0.0
C4—C5—N1—C1	0.0	C15—C14—C13—C12	0.0
C4—C5—N1—Pd1	177.8 (5)	C14—C13—C12—C11	0.0
C4—C5—N2—C6	−178.7 (8)	C12—C11—C16—C15	0.0
C4—C5—N2—C7	1.6 (16)	C17—C9—C10—C11	63.9 (13)
C4—C3—C2—C1	0.0	C17—C9—N3—C6	−143.5 (10)
C3—C2—C1—N1	0.0	C17—C9—N3—C8	36.9 (15)
C2—C1—N1—C5	0.0	C19—C18—N4—C17	95.2 (16)
C2—C1—N1—Pd1	−177.5 (6)	C19—C18—N4—C20	−86.2 (17)
N1—C5—C4—C3	0.0	C21—C20—N4—C17	−85 (2)
N1—C5—N2—C6	1.3 (13)	C21—C20—N4—C18	96.5 (16)
N1—C5—N2—C7	−178.4 (11)	N2—C5—C4—C3	179.9 (9)
C7—C8—N3—C6	−2.1 (16)	N2—C5—N1—C1	−180.0 (8)
C7—C8—N3—C9	177.6 (11)	N2—C5—N1—Pd1	−2.1 (8)
C8—C7—N2—C5	178.6 (11)	N2—C6—N3—C8	1.4 (13)
C8—C7—N2—C6	−1.1 (16)	N2—C6—N3—C9	−178.3 (9)
C9—C10—C11—C16	82.4 (12)	N2—C7—C8—N3	1.9 (16)
C9—C10—C11—C12	−94.2 (11)	N3—C6—N2—C5	−179.9 (9)
C9—C17—N4—C18	−1.1 (19)	N3—C6—N2—C7	−0.2 (13)
C9—C17—N4—C20	−179.7 (13)	N3—C9—C10—C11	−175.6 (9)
C10—C9—C17—N4	−139.3 (12)	N3—C9—C17—N4	98.5 (12)
C10—C9—C17—O1	43.3 (15)	N3—C9—C17—O1	−79.0 (13)
C10—C9—N3—C6	95.8 (12)	O1—C17—N4—C18	176.2 (12)
C10—C9—N3—C8	−83.8 (14)	O1—C17—N4—C20	−2 (2)
C10—C11—C16—C15	−176.6 (9)	Pd1—C6—N2—C5	0.3 (13)
C10—C11—C12—C13	176.6 (9)	Pd1—C6—N2—C7	180.0 (9)
C11—C16—C15—C14	0.0	Pd1—C6—N3—C8	−178.9 (10)
C16—C11—C12—C13	0.0	Pd1—C6—N3—C9	1.4 (18)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···Br2^{i}	0.93	2.77	3.540 (7)	141
C9—H9···Br2	0.98	2.57	3.381 (12)	141
C16—H16···Br2	0.93	2.92	3.678 (9)	140
C22—H22*A*···Br1^{ii}	0.97	2.91	3.836 (19)	160
C22—H22*B*···O1^{iii}	0.97	2.46	3.40 (2)	164

Symmetry codes: (i) *x*−1/2, −*y*+3/2, −*z*+1; (ii) −*x*+3/2, −*y*+1, *z*+1/2; (iii) *x*+1/2, −*y*+3/2, −*z*+1.