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Crystal structure of bis(acetonitrile-κN)(4,4′-di-*tert*-butyl-2,2′-bipyridine-$\kappa^2 N,N'$)platinum(II) bis(tetrafluoridoborate) packing as head-to-head dimers

Chris Joseph,[a] Vladimir N. Nesterov[b] and Bradley W. Smucker[a]*

[a]Austin College, 900 N Grand, Sherman, TX 75090-4400, USA, and [b]University of North Texas, 1155 Union Circle, Denton, TX 76203-5070, USA. *Correspondence e-mail: bsmucker@austincollege.edu

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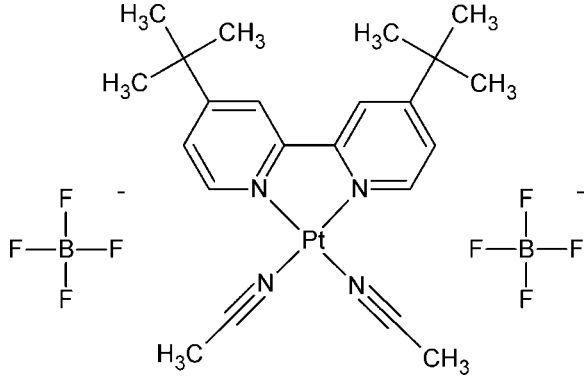
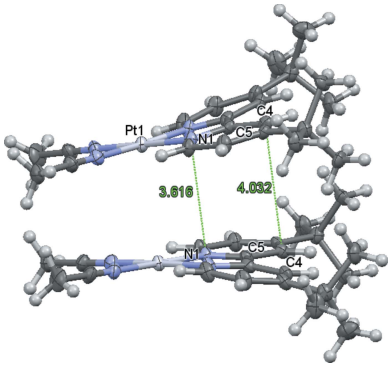
The crystal structure of a platinum(II) supramolecular building block, [Pt(dbbpy)$(NCCH_3)_2$]$(BF_4)_2$ (dbbpy = 4,4′-di-*tert*-butyl-2,2′-bipyridine, $C_{18}H_{24}N_2$) is an example of a rare head-to-head dimer, even with the bulky *tert*-butyl groups of the bipyridine. This packing motif still enables significant π–π interactions between two pyridyl groups, and may result from the close proximity of the tetrafluoridoborate ions to the platinum(II) complexes, resulting in intramolecular H···F distances between 2.156 and 2.573 Å.

1. Chemical context

The title compound is soluble in a diverse range of solvents and possesses exchangeable acetonitrile ligands for facile incorporation of novel ligands to develop new and diverse behaviors of platinum(II) complexes. The solubility and apt geometry of the (dbbpy)platinum(II) complex make it a desirable building block for coordination-driven self-assembly of homo-metallic (Zhang, *et al.*, 2017) and hetero-metallic (Bera *et al.*, 2001) supramolecular complexes. This platinum(II) diimine can also be combined with dithiolene ligands to study methylation kinetics (Stace, *et al.*, 2016), generate charge-transfer materials (Smucker, *et al.*, 2003), or make model complexes for examining photophysical properties (Lazarides, *et al.*, 2011; Yang *et al.*, 2014).





2. Structural commentary

The platinum–nitrogen distances for the bipyridyl N1 and N2 of the +2 cation are 1.994 (4) and 1.995 (4) Å, respectively, with a bond angle of 80.5 (2)°. These are shorter than those affected by the stronger *trans*-influence of chloride in two

structures of the neutral (dbbpy)$PtCl_2$ molecule: one with Pt—N distances of 2.013 (2) and 2.011 (2) Å and a 79.79 (6)° N—Pt—N angle (Day, 2009), and the other having Pt—N distances of 2.010 (12) and 2.019 (10) Å and a 78.7 (5)° N—Pt—N angle (Achar & Catalano, 1997). The Pt—N distances of the title compound are longer than those having the weaker *trans*-influence of water in the +2 cation of [(dbbpy)Pt(OH_2)$_2$]$(OTf)_2$ (Singh *et al.*, 2008), which exhibits Pt—N distances of 1.966 (5) and 1.974 (5) Å and the resulting wider bond angle of 81.1 (2)° for N—Pt—N. The *trans*-influence of the ligand is, indeed, on par with that of the related monocation [(dbbpy)Pt($NCCH_3$)(Ph)] [BAr'$_4$], containing a Pt—N distance of 2.000 (4) Å, located *trans* to the acetonitrile, while the phenyl ligand causes an elongation to 2.092 (4) Å for the other Pt—N bond (McKeown, *et al.*, 2011).

3. Supramolecular features

Most platinum(II) compounds containing the bulky dbbpy ligand pack as head-to-tail dimers, such as the aforementioned (dbbpy)$PtCl_2$ (Day, 2009; Achar & Catalano, 1997), [(dbbpy)-Pt(OH_2)$_2$]$(OTf)_2$ (Singh *et al.*, 2008), [(dbbpy)Pt($NCCH_3$)-(Ph)][BAr$'_4$] (Ar$'$ = 3,5-bis(trifluoromethyl)phenyl; McKeown *et al.*, 2011), and (dbbpy)Pt(dmid) (dmid = 1,3-dithiole-2-one-4,5-dithiolate; Smucker *et al.*, 2003). The cations in the title compound, however, pack as head-to-head dimers (Figs. 1 and 2). In these dimers, the molecules are offset (translation by half a molecule)and slightly canted [the planes composed of all non-H atoms except the *tert*-butly groups for the (dbbpy)Pt($NCCH_3$)$_2$ cation and its corresponding dimer ($-x$, y, $\frac{1}{2}-z$) are at an angle of 10.82°], both of which accommodate the bulky *tert*-butyl groups of the dbbpy ligands. The intramolecular Pt—Pt distance is quite long at 4.5123 (3) Å, yet the pyridyl rings of the dbbpy are positioned for π–π interactions with distances between 3.616 (5) Å (N1···N1^{i}) and 4.032 (7) Å (C4···C4^{i}) [symmetry code: (i) $-x$, y, $\frac{1}{2}-z$]

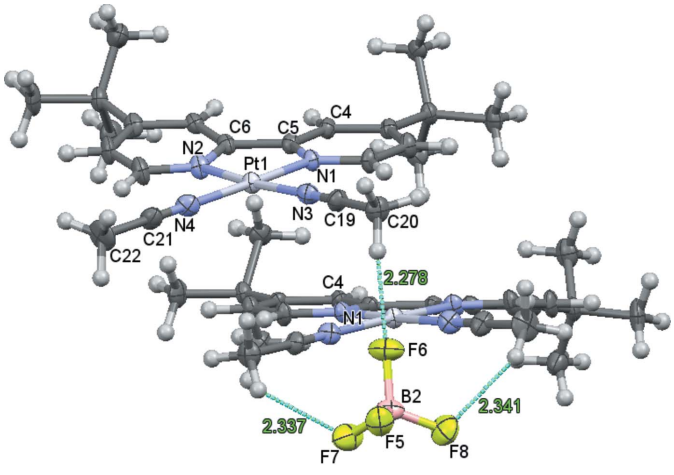


Figure 1
Displacement ellipsoid plot (50% probability of all non-H atoms), illustrating the head-to-head dimer with selected H···F intermolecular distances (Å) between a BF_4^- anion and acetonitrile molecules on adjacent molecules.

Table 1
Intermolecular H···F distances (Å) between all eight fluorine atoms of the two BF_4^- anions.

F1···H1*A*	2.16	F5^{iii}···H7*A*^{iv}	2.30
F1···H20*B*	2.43	F5^{iii}···H4*A*^{iv}	2.35
F2···H9*A*^{ii}	2.43	F6^{iii}···H20*C*^{i}	2.28
F3···H9*A*^{ii}	2.57	F7^{iii}···H20*A*	2.34
F4···H2*A*	2.43 (4)	F8^{iii}···H22*C*	2.34

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

occurring between the two rings (Fig. 2). This atypical head-to-head packing may be partly explained through the favorable non-polar interactions between the *tert*-butyl groups. Another viable explanation comes through the intermolecular interactions between fluorine atoms of the BF_4^- ions and the hydrogen atoms on the pyridine and acetonitrile ligands on multiple cations. Indeed, all eight fluorine atoms of the two unique BF_4^- anions are in close proximity to hydrogen atoms on the cation with intermolecular H···F distances between 2.16 and 2.57 Å (Fig. 1 and Table 1). Changing the anion in related bis(acetonitrile)(diimine) platinum(II) cations seems to have a significant influence, as observed in the structures of 2,2′-bipyridine in [(bpy)Pt($NCCH_3$)$_2$]$(OTf)_2$ (Field *et al.*, 2003) or 1,10-phenanthroline in [(phen)Pt($NCCh_3$)$_2$]$(ClO_4)_2$ (Ha, 2010), which do not form dimers as the positions of the triflate or perchlorate anions minimize the close proximity of the two platinum-containing cations.

4. Synthesis

The synthesis of the title compound used a method which replaced the chloride from Pt(dbbpy)Cl_2 (Tzeng *et al.*, 2001)

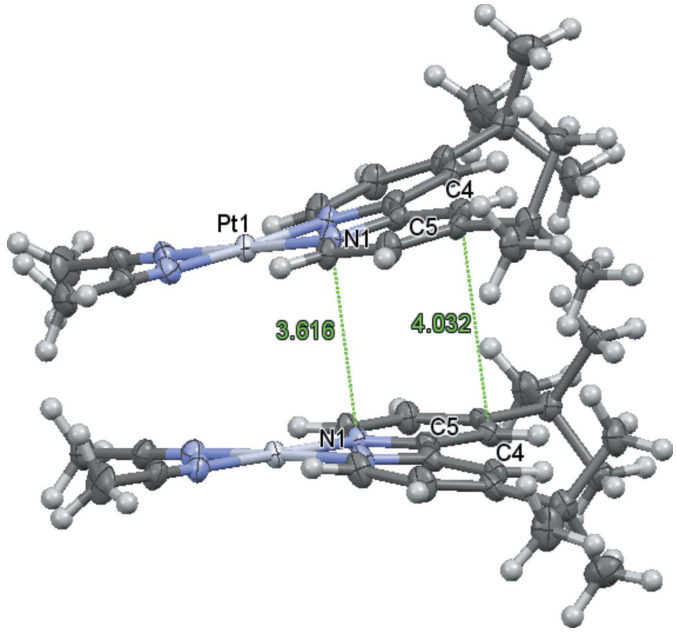


Figure 2
Displacement ellipsoid plot (50% probability of all non-H atoms), illustrating the slightly canted head-to-head dimer with selected intramolecular distances shown.

with acetonitrile using excess $AgBF_4$ by following the general syntheses of (dbbpy)$Pt(SO_3CF_3)_2$ (Hill *et al.*, 1996) and $[Pt(NCCH_3)_4](BF_4)_2$ (de Renzi *et al.*, 1976).

$[Pt(dbbpy)(NCCH_3)_2](BF_4)_2$ A solution containing 25 mL of acetonitrile, 200.7 mg (0.2500 mmol) of Pt(dbbpy)Cl_2, and 164 mg (0.8425 mmol) of $AgBF_4$ was refluxed under stirring until a yellow solution formed. The solution was isolated, *via* cannula, from the AgCl precipitate and condensed under reduced pressure until ∼5 mL of orange solution remained. This was combined with 25 ml of Et_2O and the resulting precipitate was washed with 3 × 20 mL Et_2O to give 206.9 mg (83.8% yield) of product. UV–vis λmax (ε $Lmol^{-1}cm^{-1}$): 211 (4.6×10^4), 249 (4.2×10^4), 306 (2.0×10^4), 319 (2.4×10^4) and 346 (6.0×10^3) nm.

Yellow crystals of the title compound were grown from liquid diffusion of hexanes into a dilute acetone solution.

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms were attached to C atoms and ideally positioned (C—H = 0.95–0.98 Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(CH)$ or $U_{iso}(H) = 1.2U_{eq}(CH_3)$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Pt(C_{18}H_{24}N_2)(C_2H_3N)_2](BF_4)_2$
M_r	719.21
Crystal system, space group	Orthorhombic, *Pbcn*
Temperature (K)	100
a, *b*, *c* (Å)	16.3409 (10), 13.0447 (8), 25.1105 (16)
V (Å^3)	5352.6 (6)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	5.32
Crystal size (mm)	0.14 × 0.14 × 0.08
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2001)
T_{min}, T_{max}	0.515, 0.682
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	61655, 5919, 4823
R_{int}	0.048
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.641
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.033, 0.113, 1.01
No. of reflections	5919
No. of parameters	342
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.39, −1.56

Computer programs: *APEX2* (Bruker, 2007), *SHELXS97* (Sheldrick, 2008), *SHELXL97* (Sheldrick, 2008), *SHELXTL* (Sheldrick, 2008) and *Mercury* (Macrae *et al.*, 2006).

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X-ray data were collected at the University of North Texas using a Bruker APEXII CCD diffractometer.

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Crystal structure of bis(acetonitrile-κN)(4,4′-di-*tert*-butyl-2,2′-bipyridine-$\kappa^2 N,N'$)platinum(II) bis(tetrafluoridoborate) packing as head-to-head dimers

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Computing details

Data collection: *APEX2* (Bruker, 2007); cell refinement: *APEX2* (Bruker, 2007); data reduction: *APEX2* (Bruker, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008) and *Mercury* (Macrae *et al.*, 2006).

Bis(acetonitrile-κN)(4,4′-di-*tert*-butyl-2,2′-bipyridine-$\kappa^2 N,N'$)platinum(II) bis(tetrafluoridoborate)

Crystal data

$[Pt(C_{18}H_{24}N_2)(C_2H_3N)_2](BF_4)_2$
$M_r = 719.21$
Orthorhombic, *Pbcn*
Hall symbol: -P 2n 2ab
$a = 16.3409$ (10) Å
$b = 13.0447$ (8) Å
$c = 25.1105$ (16) Å
$V = 5352.6$ (6) Å^3
$Z = 8$
$F(000) = 2800$
$D_x = 1.785$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9946 reflections
$\theta = 2.2$–$27.1°$
$\mu = 5.32$ mm^{-1}
$T = 100$ K
Plate, yellow
0.14 × 0.14 × 0.08 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2001)
$T_{min} = 0.515$, $T_{max} = 0.682$
61655 measured reflections
5919 independent reflections
4823 reflections with $I > 2\sigma(I)$
$R_{int} = 0.048$
$\theta_{max} = 27.1°$, $\theta_{min} = 1.6°$
$h = -20 \rightarrow 20$
$k = -16 \rightarrow 16$
$l = -32 \rightarrow 32$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.113$
$S = 1.01$
5919 reflections
342 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
$w = 1/[\sigma^2(F_o^2) + (0.080P)^2 + 5.P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.39$ e Å^{-3}
$\Delta\rho_{min} = -1.55$ e Å^{-3}

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. 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 $F^2 > 2\text{sigma}(F^2)$ 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}
Pt1	0.098683 (11)	0.487050 (15)	0.187162 (8)	0.02001 (9)
N1	0.1092 (2)	0.3711 (3)	0.23845 (16)	0.0200 (8)
C1	0.1088 (3)	0.3805 (4)	0.29169 (19)	0.0230 (10)
H1A	0.1042	0.4469	0.3070	0.028*
N2	0.1029 (2)	0.3703 (3)	0.13593 (17)	0.0227 (9)
C2	0.1149 (3)	0.2965 (4)	0.3246 (2)	0.0261 (11)
H2A	0.1140	0.3054	0.3622	0.031*
N3	0.1005 (2)	0.5974 (3)	0.24244 (18)	0.0247 (9)
C3	0.1223 (3)	0.1981 (4)	0.30320 (17)	0.0188 (9)
N4	0.0870 (2)	0.5961 (3)	0.13214 (18)	0.0261 (9)
C4	0.1233 (3)	0.1908 (3)	0.24737 (17)	0.0203 (9)
H4A	0.1280	0.1254	0.2310	0.024*
C5	0.1174 (3)	0.2771 (4)	0.21635 (17)	0.0197 (9)
C6	0.1182 (3)	0.2775 (4)	0.15764 (18)	0.0214 (10)
C7	0.1341 (3)	0.1931 (3)	0.12624 (17)	0.0197 (9)
H7A	0.1449	0.1288	0.1425	0.024*
C8	0.1346 (3)	0.2010 (4)	0.07074 (18)	0.0235 (10)
C9	0.1159 (3)	0.2968 (4)	0.0501 (2)	0.0282 (11)
H9A	0.1142	0.3057	0.0125	0.034*
C10	0.0999 (3)	0.3787 (4)	0.08242 (19)	0.0281 (12)
H10A	0.0864	0.4429	0.0669	0.034*
C11	0.1265 (3)	0.1023 (4)	0.33750 (18)	0.0224 (10)
C12	0.2078 (3)	0.0461 (4)	0.32623 (19)	0.0261 (10)
H12A	0.2115	0.0299	0.2882	0.039*
H12B	0.2099	−0.0174	0.3470	0.039*
H12C	0.2538	0.0903	0.3364	0.039*
C13	0.0557 (3)	0.0306 (4)	0.3229 (2)	0.0274 (11)
H13A	0.0624	0.0069	0.2861	0.041*
H13B	0.0038	0.0675	0.3263	0.041*
H13C	0.0557	−0.0285	0.3470	0.041*
C14	0.1207 (3)	0.1287 (4)	0.39695 (19)	0.0315 (12)
H14A	0.0716	0.1698	0.4034	0.047*
H14B	0.1693	0.1677	0.4076	0.047*
H14C	0.1177	0.0653	0.4178	0.047*
C15	0.1569 (3)	0.1088 (4)	0.03663 (18)	0.0249 (10)

C16	0.0911 (4)	0.0262 (4)	0.0438 (2)	0.0344 (13)
H16A	0.0875	0.0072	0.0815	0.052*
H16B	0.1057	−0.0344	0.0227	0.052*
H16C	0.0382	0.0528	0.0317	0.052*
C17	0.2397 (3)	0.0657 (5)	0.0539 (2)	0.0389 (13)
H17A	0.2383	0.0504	0.0921	0.058*
H17B	0.2826	0.1163	0.0468	0.058*
H17C	0.2512	0.0027	0.0340	0.058*
C18	0.1638 (4)	0.1369 (4)	−0.02260 (19)	0.0379 (14)
H18A	0.1101	0.1584	−0.0359	0.057*
H18B	0.1826	0.0771	−0.0428	0.057*
H18C	0.2029	0.1932	−0.0269	0.057*
C19	0.1018 (3)	0.6625 (4)	0.2714 (2)	0.0249 (11)
C20	0.1019 (3)	0.7449 (5)	0.3107 (2)	0.0320 (13)
H20A	0.1448	0.7945	0.3019	0.048*
H20B	0.1124	0.7162	0.3461	0.048*
H20C	0.0486	0.7793	0.3106	0.048*
C21	0.0799 (3)	0.6560 (4)	0.1006 (2)	0.0282 (11)
C22	0.0702 (4)	0.7321 (4)	0.0583 (2)	0.0435 (15)
H22B	0.0863	0.7018	0.0241	0.065*
H22C	0.1049	0.7916	0.0659	0.065*
H22A	0.0129	0.7538	0.0565	0.065*
F5	0.3387 (3)	0.4742 (3)	0.18538 (12)	0.0439 (9)
F1	0.0964 (2)	0.5412 (3)	0.37735 (13)	0.0444 (9)
F6	0.4162 (2)	0.3323 (3)	0.18232 (14)	0.0466 (9)
F7	0.2907 (2)	0.3270 (3)	0.22056 (14)	0.0499 (9)
F8	0.3013 (2)	0.3445 (3)	0.13080 (14)	0.0481 (9)
F2	0.0499 (2)	0.5587 (3)	0.46122 (13)	0.0498 (9)
F3	0.1841 (2)	0.5745 (3)	0.44502 (13)	0.0519 (10)
F4	0.1237 (3)	0.4179 (3)	0.43888 (16)	0.0742 (14)
B1	0.1145 (5)	0.5186 (6)	0.4330 (2)	0.0345 (16)
B2	0.3361 (4)	0.3695 (5)	0.1792 (2)	0.0293 (13)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pt1	0.02479 (13)	0.01503 (13)	0.02021 (13)	−0.00068 (6)	−0.00068 (7)	0.00112 (6)
N1	0.025 (2)	0.018 (2)	0.018 (2)	−0.0017 (15)	−0.0023 (15)	−0.0012 (15)
C1	0.034 (3)	0.018 (2)	0.017 (2)	−0.0026 (19)	−0.0004 (19)	−0.0040 (19)
N2	0.031 (2)	0.016 (2)	0.022 (2)	−0.0061 (15)	−0.0026 (16)	0.0006 (16)
C2	0.037 (3)	0.023 (3)	0.019 (2)	−0.001 (2)	−0.003 (2)	−0.002 (2)
N3	0.026 (2)	0.021 (2)	0.028 (2)	0.0024 (15)	−0.0013 (16)	0.0027 (18)
C3	0.021 (2)	0.018 (2)	0.018 (2)	−0.0039 (18)	0.0009 (18)	0.0024 (17)
N4	0.030 (2)	0.018 (2)	0.031 (2)	0.0031 (16)	−0.0006 (17)	−0.0011 (18)
C4	0.023 (2)	0.022 (2)	0.016 (2)	−0.0032 (18)	−0.0004 (18)	−0.0033 (18)
C5	0.022 (2)	0.019 (2)	0.018 (2)	−0.0040 (17)	0.0009 (18)	−0.0023 (17)
C6	0.022 (2)	0.022 (2)	0.020 (2)	−0.0055 (18)	−0.0032 (18)	0.0021 (18)
C7	0.023 (2)	0.017 (2)	0.019 (2)	−0.0040 (18)	−0.0039 (18)	0.0020 (17)

C8	0.030 (3)	0.020 (2)	0.021 (2)	−0.0075 (19)	−0.002 (2)	0.0024 (18)
C9	0.044 (3)	0.027 (3)	0.013 (2)	−0.003 (2)	−0.003 (2)	0.0052 (19)
C10	0.043 (3)	0.023 (3)	0.018 (3)	−0.005 (2)	−0.008 (2)	0.0033 (19)
C11	0.029 (2)	0.022 (2)	0.017 (2)	0.002 (2)	−0.0029 (19)	0.0013 (18)
C12	0.029 (3)	0.024 (2)	0.026 (2)	0.007 (2)	0.003 (2)	0.009 (2)
C13	0.031 (3)	0.022 (2)	0.029 (3)	−0.006 (2)	0.001 (2)	0.007 (2)
C14	0.046 (3)	0.027 (3)	0.021 (3)	0.000 (2)	0.000 (2)	0.009 (2)
C15	0.034 (3)	0.025 (2)	0.016 (2)	−0.003 (2)	−0.0014 (19)	−0.0013 (19)
C16	0.049 (4)	0.024 (3)	0.030 (3)	0.001 (2)	−0.003 (2)	−0.007 (2)
C17	0.037 (3)	0.051 (4)	0.028 (3)	0.006 (3)	0.006 (2)	0.006 (3)
C18	0.066 (4)	0.035 (3)	0.013 (2)	0.006 (3)	−0.002 (2)	−0.003 (2)
C19	0.029 (3)	0.023 (3)	0.023 (3)	0.0030 (19)	0.002 (2)	−0.002 (2)
C20	0.041 (3)	0.022 (3)	0.032 (3)	0.001 (2)	0.000 (2)	−0.006 (2)
C21	0.032 (3)	0.023 (3)	0.029 (3)	0.008 (2)	0.005 (2)	0.005 (2)
C22	0.057 (4)	0.032 (3)	0.041 (4)	0.009 (3)	−0.006 (3)	0.022 (3)
F5	0.056 (2)	0.033 (2)	0.042 (2)	0.0095 (17)	0.0005 (15)	0.0018 (15)
F1	0.054 (2)	0.052 (2)	0.0273 (18)	0.0104 (16)	−0.0050 (14)	−0.0065 (17)
F6	0.0295 (17)	0.041 (2)	0.070 (3)	0.0038 (15)	0.0019 (15)	−0.0015 (17)
F7	0.0379 (19)	0.060 (2)	0.052 (2)	−0.0054 (16)	0.0043 (16)	0.0274 (19)
F8	0.049 (2)	0.049 (2)	0.046 (2)	−0.0100 (17)	−0.0084 (16)	−0.0111 (16)
F2	0.051 (2)	0.064 (3)	0.0348 (19)	−0.0122 (19)	0.0087 (16)	−0.0163 (17)
F3	0.046 (2)	0.074 (3)	0.0358 (19)	−0.0100 (19)	0.0048 (15)	−0.0153 (18)
F4	0.132 (4)	0.035 (2)	0.056 (3)	0.012 (2)	−0.024 (3)	−0.004 (2)
B1	0.035 (3)	0.046 (4)	0.023 (3)	0.014 (3)	−0.009 (3)	−0.026 (3)
B2	0.023 (3)	0.022 (3)	0.043 (4)	−0.005 (2)	0.003 (2)	0.005 (2)

Geometric parameters (Å, º)

Pt1—N4	1.992 (4)	C13—H13B	0.9800
Pt1—N1	1.994 (4)	C13—H13C	0.9800
Pt1—N2	1.995 (4)	C14—H14A	0.9800
Pt1—N3	2.000 (5)	C14—H14B	0.9800
N1—C1	1.343 (6)	C14—H14C	0.9800
N1—C5	1.353 (6)	C15—C17	1.528 (7)
C1—C2	1.377 (7)	C15—C16	1.533 (7)
C1—H1A	0.9500	C15—C18	1.536 (6)
N2—C10	1.349 (6)	C16—H16A	0.9800
N2—C6	1.350 (6)	C16—H16B	0.9800
C2—C3	1.396 (7)	C16—H16C	0.9800
C2—H2A	0.9500	C17—H17A	0.9800
N3—C19	1.118 (7)	C17—H17B	0.9800
C3—C4	1.405 (6)	C17—H17C	0.9800
C3—C11	1.520 (6)	C18—H18A	0.9800
N4—C21	1.119 (7)	C18—H18B	0.9800
C4—C5	1.372 (6)	C18—H18C	0.9800
C4—H4A	0.9500	C19—C20	1.460 (7)
C5—C6	1.474 (6)	C20—H20A	0.9800
C6—C7	1.379 (6)	C20—H20B	0.9800

C7—C8	1.398 (6)	C20—H20C	0.9800
C7—H7A	0.9500	C21—C22	1.462 (7)
C8—C9	1.386 (7)	C22—H22B	0.9800
C8—C15	1.521 (7)	C22—H22C	0.9800
C9—C10	1.368 (8)	C22—H22A	0.9800
C9—H9A	0.9500	F5—B2	1.375 (7)
C10—H10A	0.9500	F1—B1	1.459 (7)
C11—C13	1.532 (7)	F6—B2	1.398 (7)
C11—C14	1.535 (6)	F7—B2	1.392 (6)
C11—C12	1.544 (7)	F8—B2	1.381 (7)
C12—H12A	0.9800	F2—B1	1.374 (7)
C12—H12B	0.9800	F3—B1	1.385 (8)
C12—H12C	0.9800	F4—B1	1.330 (8)
C13—H13A	0.9800		

N4—Pt1—N1	176.23 (16)	C11—C13—H13C	109.5
N4—Pt1—N2	95.81 (18)	H13A—C13—H13C	109.5
N1—Pt1—N2	80.47 (18)	H13B—C13—H13C	109.5
N4—Pt1—N3	88.22 (19)	C11—C14—H14A	109.5
N1—Pt1—N3	95.53 (18)	C11—C14—H14B	109.5
N2—Pt1—N3	175.27 (16)	H14A—C14—H14B	109.5
C1—N1—C5	119.5 (4)	C11—C14—H14C	109.5
C1—N1—Pt1	125.0 (3)	H14A—C14—H14C	109.5
C5—N1—Pt1	115.6 (3)	H14B—C14—H14C	109.5
N1—C1—C2	121.7 (5)	C8—C15—C17	110.1 (4)
N1—C1—H1A	119.2	C8—C15—C16	108.8 (4)
C2—C1—H1A	119.2	C17—C15—C16	109.2 (4)
C10—N2—C6	118.8 (4)	C8—C15—C18	112.0 (4)
C10—N2—Pt1	125.4 (4)	C17—C15—C18	107.4 (4)
C6—N2—Pt1	115.5 (3)	C16—C15—C18	109.4 (4)
C1—C2—C3	120.4 (5)	C15—C16—H16A	109.5
C1—C2—H2A	119.8	C15—C16—H16B	109.5
C3—C2—H2A	119.8	H16A—C16—H16B	109.5
C19—N3—Pt1	176.6 (4)	C15—C16—H16C	109.5
C2—C3—C4	116.7 (4)	H16A—C16—H16C	109.5
C2—C3—C11	122.8 (4)	H16B—C16—H16C	109.5
C4—C3—C11	120.6 (4)	C15—C17—H17A	109.5
C21—N4—Pt1	178.7 (5)	C15—C17—H17B	109.5
C5—C4—C3	120.6 (4)	H17A—C17—H17B	109.5
C5—C4—H4A	119.7	C15—C17—H17C	109.5
C3—C4—H4A	119.7	H17A—C17—H17C	109.5
N1—C5—C4	121.2 (4)	H17B—C17—H17C	109.5
N1—C5—C6	114.0 (4)	C15—C18—H18A	109.5
C4—C5—C6	124.8 (4)	C15—C18—H18B	109.5
N2—C6—C7	121.3 (4)	H18A—C18—H18B	109.5
N2—C6—C5	114.0 (4)	C15—C18—H18C	109.5
C7—C6—C5	124.7 (4)	H18A—C18—H18C	109.5
C6—C7—C8	120.8 (4)	H18B—C18—H18C	109.5

C6—C7—H7A	119.6	N3—C19—C20	177.7 (6)
C8—C7—H7A	119.6	C19—C20—H20A	109.5
C9—C8—C7	116.0 (4)	C19—C20—H20B	109.5
C9—C8—C15	123.7 (4)	H20A—C20—H20B	109.5
C7—C8—C15	120.3 (4)	C19—C20—H20C	109.5
C10—C9—C8	121.6 (5)	H20A—C20—H20C	109.5
C10—C9—H9A	119.2	H20B—C20—H20C	109.5
C8—C9—H9A	119.2	N4—C21—C22	178.4 (6)
N2—C10—C9	121.4 (5)	C21—C22—H22B	109.5
N2—C10—H10A	119.3	C21—C22—H22C	109.5
C9—C10—H10A	119.3	H22B—C22—H22C	109.5
C3—C11—C13	109.4 (4)	C21—C22—H22A	109.5
C3—C11—C14	111.3 (4)	H22B—C22—H22A	109.5
C13—C11—C14	108.9 (4)	H22C—C22—H22A	109.5
C3—C11—C12	109.0 (4)	F4—B1—F2	113.9 (7)
C13—C11—C12	108.5 (4)	F4—B1—F3	113.8 (5)
C14—C11—C12	109.7 (4)	F2—B1—F3	108.6 (4)
C11—C12—H12A	109.5	F4—B1—F1	109.1 (5)
C11—C12—H12B	109.5	F2—B1—F1	105.1 (5)
H12A—C12—H12B	109.5	F3—B1—F1	105.6 (6)
C11—C12—H12C	109.5	F5—B2—F8	110.2 (5)
H12A—C12—H12C	109.5	F5—B2—F7	109.1 (5)
H12B—C12—H12C	109.5	F8—B2—F7	110.0 (4)
C11—C13—H13A	109.5	F5—B2—F6	108.0 (5)
C11—C13—H13B	109.5	F8—B2—F6	110.7 (5)
H13A—C13—H13B	109.5	F7—B2—F6	108.7 (5)