Supplementary Material (ESI) for Dalton Transactions

Supplementary Information

Synthesis and Preliminary DNA-Binding Studies of Diimineplatinum(II) Complexes Containing 3- or 4-Pyridineboronic Acid

H. Y. Vincent Ching,[a] Jack K. Clegg,[b] and Louis M. Rendina[a]*

[a] *School of Chemistry, The University of Sydney, Sydney, NSW 2006, Australia.*

[b] *Crystal Structure Analysis Facility, School of Chemistry, The University of Sydney, Sydney, NSW 2006, Australia.*

X-ray Diffraction Study: Analysis of Crystal Packing

The $[Pt(phen)(py)_2]^{2+}$ cations in **7** pack closely together in the structure, forming an infinite three-dimensional network of π-π stacking interactions. These interactions are shown in Figures S1 and S2. Figure S1 shows a view down the crystallographic *a*-axis of a portion of the crystal packing. Each of the phen ligands is sandwiched between two adjacent molecules and participates in offset face-to-face π-π stacking reflected in C–C distances ranging from 3.3 Å to 3.7 Å, forming infinite one-dimensional chains. Each of these chains interacts with adjacent chains *via* edge-to-face π-π stacking. These are reflected in CH-C distances ranging from 2.9 Å to 3.6 Å. These interactions are present between pyridine rings and phen ligands in a herring-bone type of arrangement to form an infinite 3D network.

Figure S2 depicts a "top view" of the one-dimensional chains described above. The chains depicted in blue are rotated by approximately 60° from the green chains resulting in the herring-bone type arrangement. Each of the green chains interacts with adjacent green and blue chains *via* π-π stacking. Each blue chain similarly interacts with each adjacent green and blue chain. Voids throughout the lattice are filled with the PF_6^- anions.

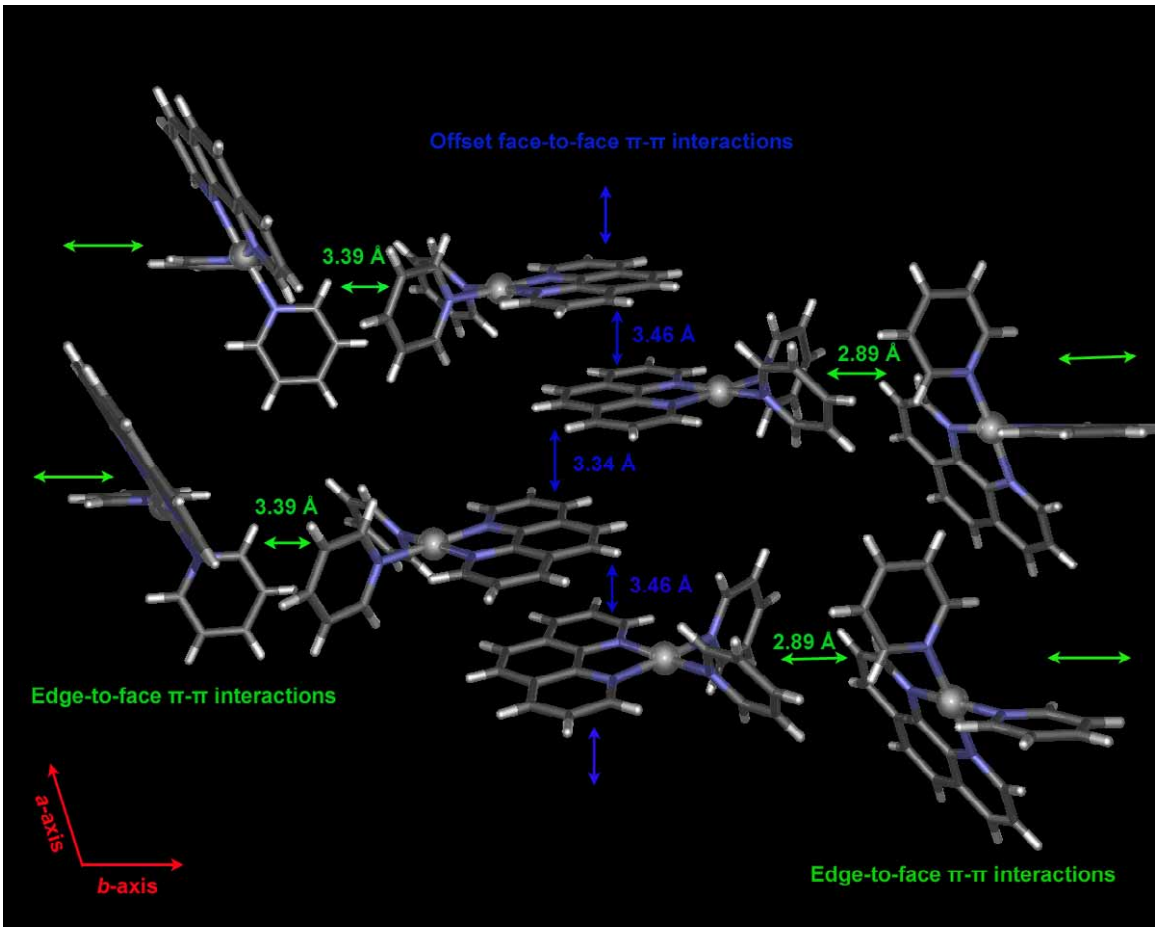

Figure S1. A schematic diagram of part of the crystal packing of $[Pt(phen)(py)_2](PF_6)_2$. Anions are omitted for clarity.

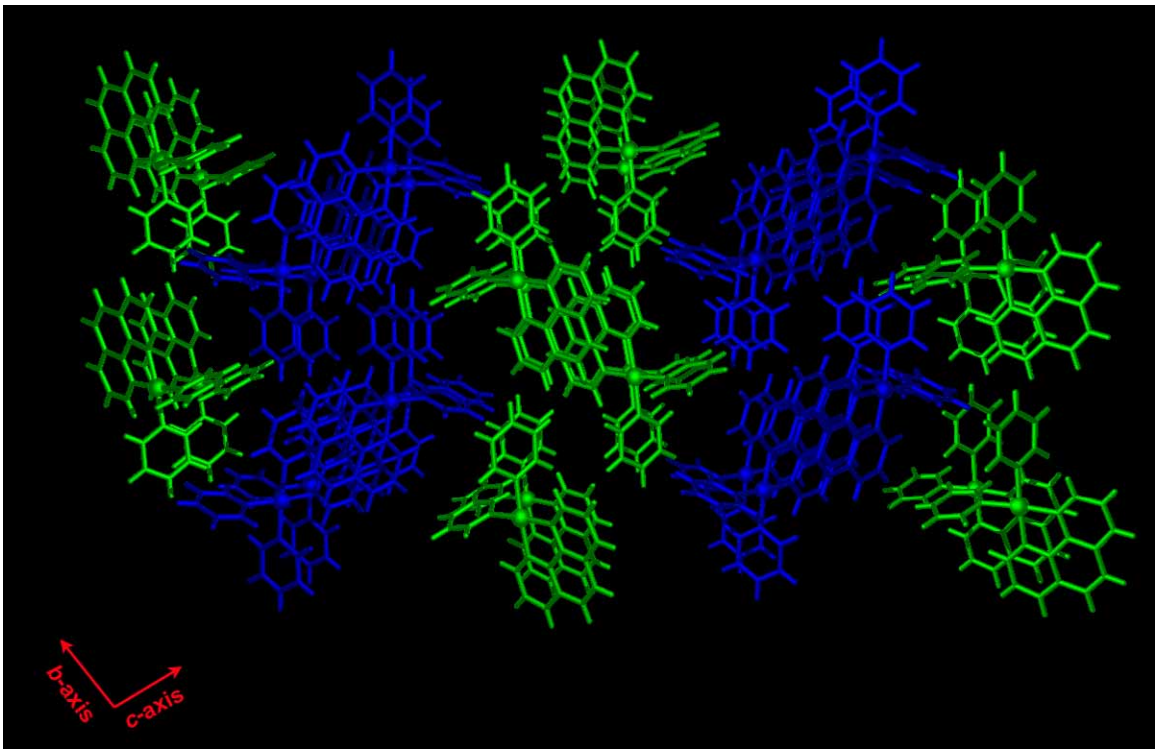

Figure S2. A representation of the crystal packing viewed down the crystallographic *a*-axis. Those molecules shown in blue are rotated by approximately 60° compared to those in green. Anions are omitted for clarity.

Table 1. Non-Hydrogen Atom Coordinates, Isotropic Thermal Parameters and Occupancies

atom	x	y	z	U_{eq}(Å^2)	Occ
C(1)	0.1324(13)	0.4671(5)	0.2325(9)	0.030(3)	1
C(2)	0.0550(12)	0.5115(5)	0.2589(10)	0.030(3)	1
C(3)	0.0843(14)	0.5324(5)	0.3667(11)	0.036(3)	1
C(4)	0.1922(13)	0.5084(4)	0.4489(10)	0.029(3)	1
C(5)	0.2672(12)	0.4636(4)	0.4145(9)	0.024(2)	1
C(6)	0.2342(14)	0.5268(5)	0.5639(11)	0.037(3)	1
C(7)	0.3402(14)	0.5009(6)	0.6388(10)	0.038(3)	1
C(8)	0.4144(13)	0.4553(5)	0.6053(10)	0.031(3)	1
C(9)	0.5245(14)	0.4265(6)	0.6784(10)	0.037(3)	1
C(10)	0.5899(15)	0.3835(6)	0.6372(11)	0.043(3)	1
C(11)	0.5432(14)	0.3676(5)	0.5242(10)	0.035(3)	1
C(12)	0.3740(12)	0.4367(4)	0.4934(9)	0.023(2)	1
C(13)	0.2201(15)	0.3319(5)	0.0707(12)	0.040(3)	1
C(14)	0.1726(17)	0.3290(6)	-0.0464(13)	0.048(4)	1
C(15)	0.2011(15)	0.3681(6)	-0.1155(12)	0.045(4)	1
C(16)	0.2772(14)	0.4116(6)	-0.0698(10)	0.037(3)	1
C(17)	0.3234(13)	0.4126(5)	0.0466(10)	0.031(3)	1
C(18)	0.4569(17)	0.2719(5)	0.3294(13)	0.045(3)	1
C(19)	0.555(2)	0.2298(6)	0.3421(16)	0.061(5)	1
C(20)	0.6957(18)	0.2332(6)	0.3042(13)	0.051(4)	1
C(21)	0.7394(17)	0.2770(6)	0.2509(13)	0.051(4)	1
C(22)	0.6396(14)	0.3187(5)	0.2423(10)	0.034(3)	1
N(1)	0.2371(10)	0.4439(3)	0.3065(7)	0.0219(19)	1
N(2)	0.4407(10)	0.3936(3)	0.4543(7)	0.023(2)	1
N(3)	0.2952(10)	0.3732(3)	0.1162(7)	0.025(2)	1
N(4)	0.4991(10)	0.3159(4)	0.2806(8)	0.027(2)	1
F(1)	0.8121(9)	0.4007(4)	-0.1118(6)	0.053(2)	1
F(2)	0.7075(10)	0.4385(3)	0.1252(6)	0.052(2)	1
F(3)	0.6354(9)	0.4581(3)	-0.0607(6)	0.0440(19)	1
F(4)	0.8886(10)	0.4645(4)	0.0135(7)	0.060(2)	1
F(5)	0.6350(9)	0.3752(3)	-0.0008(7)	0.0478(19)	1
F(6)	0.8857(9)	0.3825(3)	0.0772(6)	0.049(2)	1
F(7)	0.1436(11)	0.1317(4)	0.0794(11)	0.088(4)	1
F(8)	-0.0540(13)	0.1645(4)	0.1502(10)	0.087(4)	1
F(9)	-0.0586(14)	0.2313(4)	0.0230(10)	0.093(4)	1
F(10)	0.1334(19)	0.1973(5)	-0.0495(14)	0.141(7)	1
F(11)	-0.079(2)	0.1503(6)	-0.0318(11)	0.138(6)	1
F(12)	0.1479(18)	0.2126(5)	0.1396(13)	0.134(6)	1
P(1)	0.7619(4)	0.41978(13)	0.0069(3)	0.0303(7)	1
P(2)	0.0418(4)	0.18181(14)	0.0493(3)	0.0414(8)	1
Pt(1)	0.36678(5)	0.380170(17)	0.28666(4)	0.02618(13)	1

Table 2. Hydrogen Atom Coordinates, Isotropic Thermal Parameters and Occupancies

atom	x	y	z	U_{eq}(Å^2)	Occ
H(1)	0.1091	0.4527	0.1578	0.036	1
H(2)	-0.0183	0.5274	0.2024	0.037	1
H(3)	0.0318	0.5629	0.3854	0.043	1
H(6)	0.1875	0.5575	0.5880	0.045	1
H(7)	0.3651	0.5135	0.7149	0.045	1
H(9)	0.5530	0.4370	0.7557	0.044	1
H(10)	0.6666	0.3644	0.6850	0.051	1
H(11)	0.5871	0.3370	0.4971	0.043	1
H(13)	0.1986	0.3040	0.1189	0.048	1
H(14)	0.1195	0.2992	-0.0778	0.058	1
H(15)	0.1689	0.3659	-0.1957	0.054	1
H(16)	0.2972	0.4399	-0.1172	0.045	1
H(17)	0.3771	0.4422	0.0793	0.037	1
H(18)	0.3572	0.2699	0.3555	0.054	1
H(19)	0.5239	0.1989	0.3769	0.074	1
H(20)	0.7658	0.2048	0.3145	0.061	1
H(21)	0.8364	0.2786	0.2207	0.061	1
H(22)	0.6702	0.3498	0.2087	0.041	1

Table 3. Anisotropic Thermal Parameters ($Å^2$)

atom	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
C(1)	0.025(5)	0.039(7)	0.024(6)	0.004(5)	-0.001(5)	0.000(5)
C(2)	0.016(5)	0.045(8)	0.031(6)	0.007(5)	0.008(4)	0.006(5)
C(3)	0.029(6)	0.027(7)	0.053(8)	0.003(5)	0.017(6)	0.004(6)
C(4)	0.027(6)	0.025(6)	0.036(6)	-0.005(5)	0.016(5)	-0.001(5)
C(5)	0.018(5)	0.029(6)	0.027(5)	-0.007(4)	0.007(4)	0.002(5)
C(6)	0.028(6)	0.044(8)	0.044(7)	-0.010(6)	0.017(5)	-0.015(6)
C(7)	0.034(7)	0.061(9)	0.022(6)	-0.017(6)	0.016(5)	-0.013(6)
C(8)	0.024(6)	0.044(8)	0.026(6)	-0.010(5)	0.010(5)	0.000(5)
C(9)	0.025(6)	0.064(9)	0.020(5)	-0.016(6)	-0.004(4)	0.004(6)
C(10)	0.033(6)	0.056(9)	0.038(7)	-0.007(7)	-0.001(5)	0.013(7)
C(11)	0.032(6)	0.042(8)	0.033(6)	0.002(5)	0.007(5)	0.011(5)
C(12)	0.016(5)	0.032(6)	0.022(5)	-0.007(4)	0.009(4)	-0.001(4)
C(13)	0.036(7)	0.032(7)	0.052(8)	0.002(6)	-0.001(6)	-0.011(6)
C(14)	0.043(8)	0.042(8)	0.056(9)	0.001(6)	-0.013(7)	-0.018(7)
C(15)	0.029(7)	0.064(11)	0.039(7)	0.015(6)	-0.008(5)	-0.011(7)
C(16)	0.024(6)	0.059(9)	0.028(6)	0.010(6)	0.003(5)	0.006(6)
C(17)	0.024(6)	0.034(7)	0.034(6)	0.003(5)	0.004(5)	-0.002(5)
C(18)	0.043(8)	0.024(7)	0.070(10)	0.002(6)	0.010(7)	0.009(7)
C(19)	0.068(11)	0.028(8)	0.086(13)	0.003(7)	0.002(9)	0.013(8)
C(20)	0.049(9)	0.034(8)	0.066(10)	0.017(7)	-0.007(7)	-0.008(7)
C(21)	0.038(8)	0.056(10)	0.060(10)	0.002(7)	0.013(7)	-0.011(8)
C(22)	0.038(7)	0.036(7)	0.031(6)	0.007(6)	0.013(5)	0.003(5)
N(1)	0.016(4)	0.026(5)	0.024(4)	-0.002(4)	0.004(3)	-0.008(4)
N(2)	0.019(4)	0.028(5)	0.023(4)	0.004(4)	0.005(3)	0.006(4)
N(3)	0.029(5)	0.020(5)	0.025(4)	0.006(4)	-0.001(4)	-0.003(4)
N(4)	0.020(5)	0.029(5)	0.033(5)	0.005(4)	0.005(4)	-0.007(4)
F(1)	0.045(5)	0.081(6)	0.036(4)	0.006(4)	0.012(3)	0.001(4)
F(2)	0.070(6)	0.058(5)	0.029(4)	-0.001(4)	0.008(4)	-0.012(4)
F(3)	0.044(4)	0.042(5)	0.042(4)	0.005(4)	-0.010(3)	-0.003(3)
F(4)	0.051(5)	0.073(6)	0.052(5)	-0.037(5)	-0.009(4)	0.009(4)
F(5)	0.042(4)	0.041(5)	0.061(5)	-0.016(4)	0.010(4)	-0.007(4)
F(6)	0.051(5)	0.068(6)	0.026(3)	0.015(4)	-0.005(3)	0.014(4)
F(7)	0.060(6)	0.058(7)	0.158(11)	0.030(5)	0.056(7)	0.031(7)
F(8)	0.082(8)	0.094(8)	0.094(8)	0.024(6)	0.043(6)	0.029(7)
F(9)	0.097(9)	0.077(8)	0.104(9)	0.043(7)	0.007(7)	0.025(7)
F(10)	0.191(15)	0.076(8)	0.191(15)	0.030(9)	0.161(13)	0.045(9)
F(11)	0.196(16)	0.112(11)	0.088(9)	-0.073(11)	-0.054(9)	0.017(8)
F(12)	0.167(14)	0.065(8)	0.145(12)	-0.035(8)	-0.081(11)	0.031(8)
P(1)	0.0263(15)	0.0393(18)	0.0246(14)	-0.0059(13)	0.0004(12)	0.0006(13)
P(2)	0.043(2)	0.036(2)	0.046(2)	0.0066(16)	0.0100(16)	0.0055(16)
Pt(1)	0.0267(2)	0.0255(2)	0.0266(2)	0.0019(2)	0.00429(14)	0.0017(2)

Table 4. Non Hydrogen Bond Lengths (Å)

atom	atom	Distance	atom	atom	Distance
C(1)	N(1)	1.316(14)	C(1)	C(2)	1.384(16)
C(2)	C(3)	1.371(17)	C(3)	C(4)	1.400(17)
C(4)	C(5)	1.411(16)	C(4)	C(6)	1.435(17)
C(5)	N(1)	1.361(13)	C(5)	C(12)	1.406(15)
C(6)	C(7)	1.363(19)	C(7)	C(8)	1.423(18)
C(8)	C(12)	1.402(15)	C(8)	C(9)	1.410(17)
C(9)	C(10)	1.37(2)	C(10)	C(11)	1.399(18)
C(11)	N(2)	1.314(14)	C(12)	N(2)	1.360(14)
C(13)	N(3)	1.327(15)	C(13)	C(14)	1.386(19)
C(14)	C(15)	1.34(2)	C(15)	C(16)	1.378(19)
C(16)	C(17)	1.376(16)	C(17)	N(3)	1.349(15)
C(18)	N(4)	1.346(16)	C(18)	C(19)	1.376(19)
C(19)	C(20)	1.35(2)	C(20)	C(21)	1.37(2)
C(21)	C(22)	1.375(19)	C(22)	N(4)	1.345(14)
N(1)	Pt(1)	2.024(9)	N(2)	Pt(1)	2.022(9)
N(3)	Pt(1)	2.027(9)	N(4)	Pt(1)	2.025(9)
F(1)	P(1)	1.590(8)	F(2)	P(1)	1.596(8)
F(3)	P(1)	1.608(8)	F(4)	P(1)	1.588(8)
F(5)	P(1)	1.586(8)	F(6)	P(1)	1.590(8)
F(7)	P(2)	1.582(9)	F(8)	P(2)	1.592(10)
F(9)	P(2)	1.557(10)	F(10)	P(2)	1.537(10)
F(11)	P(2)	1.554(12)	F(12)	P(2)	1.534(12)

Symmetry Operators

□ (1) x, y, z (2) -x, y+1/2, -z+1/2 (3) -x, -y, -z

(4) x, -y-1/2, z-1/2

Table 5. Non Hydrogen Bond Angles (º)

atom	atom	atom	angle
N(1)	C(1)	C(2)	122.7(10)
C(3)	C(2)	C(1)	119.8(11)
C(2)	C(3)	C(4)	119.3(11)
C(3)	C(4)	C(5)	117.2(11)
C(3)	C(4)	C(6)	124.6(11)
C(5)	C(4)	C(6)	118.2(11)
N(1)	C(5)	C(12)	117.4(10)
N(1)	C(5)	C(4)	122.3(10)
C(12)	C(5)	C(4)	120.3(10)
C(7)	C(6)	C(4)	120.8(12)
C(6)	C(7)	C(8)	121.2(11)
C(12)	C(8)	C(9)	117.3(12)
C(12)	C(8)	C(7)	118.6(11)
C(9)	C(8)	C(7)	124.2(11)
C(10)	C(9)	C(8)	119.5(11)
C(9)	C(10)	C(11)	119.6(12)
N(2)	C(11)	C(10)	122.1(12)
N(2)	C(12)	C(5)	117.0(9)
N(2)	C(12)	C(8)	122.1(10)
C(5)	C(12)	C(8)	120.8(11)
N(3)	C(13)	C(14)	120.7(13)
C(15)	C(14)	C(13)	120.5(13)
C(14)	C(15)	C(16)	119.8(13)
C(17)	C(16)	C(15)	117.8(13)
N(3)	C(17)	C(16)	122.4(12)
N(4)	C(18)	C(19)	121.5(13)
C(20)	C(19)	C(18)	118.5(14)
C(19)	C(20)	C(21)	121.1(14)
C(22)	C(21)	C(20)	118.5(13)
N(4)	C(22)	C(21)	121.0(12)
C(1)	N(1)	C(5)	118.6(9)
C(1)	N(1)	Pt(1)	129.7(7)
C(5)	N(1)	Pt(1)	111.7(7)
C(11)	N(2)	C(12)	119.3(10)
C(11)	N(2)	Pt(1)	128.6(8)
C(12)	N(2)	Pt(1)	112.0(7)
C(13)	N(3)	C(17)	118.9(10)
C(13)	N(3)	Pt(1)	122.8(9)
C(17)	N(3)	Pt(1)	118.3(8)
C(18)	N(4)	C(22)	119.4(11)
C(18)	N(4)	Pt(1)	119.8(8)
C(22)	N(4)	Pt(1)	120.2(8)
F(5)	P(1)	F(4)	179.5(5)
F(5)	P(1)	F(1)	89.2(5)
F(4)	P(1)	F(1)	90.5(5)
F(5)	P(1)	F(2)	89.7(4)
F(4)	P(1)	F(2)	90.6(5)

F(1)	P(1)	F(2)	178.7(5)
F(5)	P(1)	F(6)	90.0(5)
F(4)	P(1)	F(6)	90.3(5)
F(1)	P(1)	F(6)	91.6(4)
F(2)	P(1)	F(6)	89.1(4)
F(5)	P(1)	F(3)	90.1(4)
F(4)	P(1)	F(3)	89.6(5)
F(1)	P(1)	F(3)	90.1(4)
F(2)	P(1)	F(3)	89.2(4)
F(6)	P(1)	F(3)	178.3(5)
F(12)	P(2)	F(10)	93.9(10)
F(12)	P(2)	F(11)	173.3(10)
F(10)	P(2)	F(11)	92.5(9)
F(12)	P(2)	F(9)	88.6(7)
F(10)	P(2)	F(9)	87.8(7)
F(11)	P(2)	F(9)	89.8(8)
F(12)	P(2)	F(7)	90.4(7)
F(10)	P(2)	F(7)	93.4(6)
F(11)	P(2)	F(7)	91.0(8)
F(9)	P(2)	F(7)	178.6(7)
F(12)	P(2)	F(8)	87.3(8)
F(10)	P(2)	F(8)	178.6(8)
F(11)	P(2)	F(8)	86.3(8)
F(9)	P(2)	F(8)	93.0(6)
F(7)	P(2)	F(8)	85.8(6)
N(3)	Pt(1)	N(2)	175.1(4)
N(3)	Pt(1)	N(4)	89.7(4)
N(2)	Pt(1)	N(4)	93.8(4)
N(3)	Pt(1)	N(1)	94.8(3)
N(2)	Pt(1)	N(1)	81.8(3)
N(4)	Pt(1)	N(1)	175.4(4)

Symmetry Operators

□ (1) x, y, z (2) -x, y+1/2, -z+1/2 (3) -x, -y, -z

(4) x, -y-1/2, z-1/2

Table 6. Torsion Angles (º)

atom	atom	atom	atom	angle
N(1)	C(1)	C(2)	C(3)	-1.3(18)
C(1)	C(2)	C(3)	C(4)	-0.2(17)
C(2)	C(3)	C(4)	C(5)	0.9(16)
C(2)	C(3)	C(4)	C(6)	179.2(11)
C(3)	C(4)	C(5)	N(1)	-0.2(16)
C(6)	C(4)	C(5)	N(1)	-178.7(10)
C(3)	C(4)	C(5)	C(12)	-178.3(10)
C(6)	C(4)	C(5)	C(12)	3.2(15)
C(3)	C(4)	C(6)	C(7)	179.7(11)
C(5)	C(4)	C(6)	C(7)	-1.9(17)
C(4)	C(6)	C(7)	C(8)	0.9(18)
C(6)	C(7)	C(8)	C(12)	-1.2(17)
C(6)	C(7)	C(8)	C(9)	-179.8(11)
C(12)	C(8)	C(9)	C(10)	2.0(17)
C(7)	C(8)	C(9)	C(10)	-179.4(11)
C(8)	C(9)	C(10)	C(11)	-1.9(18)
C(9)	C(10)	C(11)	N(2)	1.9(19)
N(1)	C(5)	C(12)	N(2)	1.3(14)
C(4)	C(5)	C(12)	N(2)	179.4(9)
N(1)	C(5)	C(12)	C(8)	178.3(9)
C(4)	C(5)	C(12)	C(8)	-3.6(15)
C(9)	C(8)	C(12)	N(2)	-2.0(15)
C(7)	C(8)	C(12)	N(2)	179.3(10)
C(9)	C(8)	C(12)	C(5)	-178.8(10)
C(7)	C(8)	C(12)	C(5)	2.4(15)
N(3)	C(13)	C(14)	C(15)	0(2)
C(13)	C(14)	C(15)	C(16)	0(2)
C(14)	C(15)	C(16)	C(17)	0.9(19)
C(15)	C(16)	C(17)	N(3)	-0.7(17)
N(4)	C(18)	C(19)	C(20)	0(2)
C(18)	C(19)	C(20)	C(21)	-2(3)
C(19)	C(20)	C(21)	C(22)	3(2)
C(20)	C(21)	C(22)	N(4)	-3(2)
C(2)	C(1)	N(1)	C(5)	1.9(17)
C(2)	C(1)	N(1)	Pt(1)	-178.7(8)
C(12)	C(5)	N(1)	C(1)	177.0(10)
C(4)	C(5)	N(1)	C(1)	-1.1(15)
C(12)	C(5)	N(1)	Pt(1)	-2.5(11)
C(4)	C(5)	N(1)	Pt(1)	179.4(8)
C(10)	C(11)	N(2)	C(12)	-1.9(17)
C(10)	C(11)	N(2)	Pt(1)	176.1(9)
C(5)	C(12)	N(2)	C(11)	178.9(10)
C(8)	C(12)	N(2)	C(11)	1.9(15)
C(5)	C(12)	N(2)	Pt(1)	0.6(11)
C(8)	C(12)	N(2)	Pt(1)	-176.3(8)
C(14)	C(13)	N(3)	C(17)	0.6(18)
C(14)	C(13)	N(3)	Pt(1)	179.6(10)

C(16)	C(17)	N(3)	C(13)	-0.1(17)
C(16)	C(17)	N(3)	Pt(1)	-179.1(9)
C(19)	C(18)	N(4)	C(22)	1(2)
C(19)	C(18)	N(4)	Pt(1)	-170.2(12)
C(21)	C(22)	N(4)	C(18)	0.8(19)
C(21)	C(22)	N(4)	Pt(1)	171.7(10)
C(13)	N(3)	Pt(1)	N(4)	59.6(9)
C(17)	N(3)	Pt(1)	N(4)	-121.4(8)
C(13)	N(3)	Pt(1)	N(1)	-119.3(9)
C(17)	N(3)	Pt(1)	N(1)	59.7(8)
C(11)	N(2)	Pt(1)	N(4)	1.8(10)
C(12)	N(2)	Pt(1)	N(4)	179.8(7)
C(11)	N(2)	Pt(1)	N(1)	-179.6(10)
C(12)	N(2)	Pt(1)	N(1)	-1.5(7)
C(18)	N(4)	Pt(1)	N(3)	-109.0(10)
C(22)	N(4)	Pt(1)	N(3)	80.2(9)
C(18)	N(4)	Pt(1)	N(2)	74.4(10)
C(22)	N(4)	Pt(1)	N(2)	-96.4(9)
C(1)	N(1)	Pt(1)	N(3)	6.3(10)
C(5)	N(1)	Pt(1)	N(3)	-174.3(7)
C(1)	N(1)	Pt(1)	N(2)	-177.3(10)
C(5)	N(1)	Pt(1)	N(2)	2.1(7)

Symmetry Operators

□ (1) x, y, z (2) -x, y+1/2, -z+1/2 (3) -x, -y, -z

(4) x, -y-1/2, z-1/2

Table 7. Hydrogen Bond Lengths (Å)

atom	atom	Distance	atom	atom	Distance
C(1)	H(1)	0.9500	C(2)	H(2)	0.9500
C(3)	H(3)	0.9500	C(6)	H(6)	0.9500
C(7)	H(7)	0.9500	C(9)	H(9)	0.9500
C(10)	H(10)	0.9500	C(11)	H(11)	0.9500
C(13)	H(13)	0.9500	C(14)	H(14)	0.9500
C(15)	H(15)	0.9500	C(16)	H(16)	0.9500
C(17)	H(17)	0.9500	C(18)	H(18)	0.9500
C(19)	H(19)	0.9500	C(20)	H(20)	0.9500
C(21)	H(21)	0.9500	C(22)	H(22)	0.9500

Symmetry Operators

 (1) x, y, z (2) -x, y+1/2, -z+1/2 (3) -x, -y, -z

(4) x, -y-1/2, z-1/2

Table 8. Hydrogen Bond Angles (º)

atom	atom	atom	angle
N(1)	C(1)	H(1)	118.6
C(2)	C(1)	H(1)	118.6
C(3)	C(2)	H(2)	120.1
C(1)	C(2)	H(2)	120.1
C(2)	C(3)	H(3)	120.4
C(4)	C(3)	H(3)	120.4
C(7)	C(6)	H(6)	119.6
C(4)	C(6)	H(6)	119.6
C(6)	C(7)	H(7)	119.4
C(8)	C(7)	H(7)	119.4
C(10)	C(9)	H(9)	120.3
C(8)	C(9)	H(9)	120.3
C(9)	C(10)	H(10)	120.2
C(11)	C(10)	H(10)	120.2
N(2)	C(11)	H(11)	118.9
C(10)	C(11)	H(11)	118.9
N(3)	C(13)	H(13)	119.7
C(14)	C(13)	H(13)	119.7
C(15)	C(14)	H(14)	119.8
C(13)	C(14)	H(14)	119.8
C(14)	C(15)	H(15)	120.1
C(16)	C(15)	H(15)	120.1
C(17)	C(16)	H(16)	121.1
C(15)	C(16)	H(16)	121.1
N(3)	C(17)	H(17)	118.8
C(16)	C(17)	H(17)	118.8
N(4)	C(18)	H(18)	119.3
C(19)	C(18)	H(18)	119.3
C(20)	C(19)	H(19)	120.8
C(18)	C(19)	H(19)	120.8
C(19)	C(20)	H(20)	119.4
C(21)	C(20)	H(20)	119.4
C(22)	C(21)	H(21)	120.8
C(20)	C(21)	H(21)	120.8
N(4)	C(22)	H(22)	119.5
C(21)	C(22)	H(22)	119.5

Symmetry Operators

□ (1) x, y, z (2) -x, y+1/2, -z+1/2 (3) -x, -y, -z

(4) x, -y-1/2, z-1/2