Supplementary Information

Exploring Excited States of Pt(II) Diimine Catecholates for Photoinduced Charge Separation

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Part 1.

X-ray crystallographic data for compound 2, {(COO^{i}Pr)$_2$bpy}Pt(pCat).

CCDC 1028956, Compound Name **{(COO^{i}Pr)$_2$bpy}Pt(pCat) (2)**

Formula: C24 H24 N2 O6 Pt1,H2 O1; Unit Cell Parameters: a 6.6241(3) b 10.9966(4) c 17.2394(7) P-1

Table 1. Crystal data and structure refinement for ch1jw252p-1 (**{(COO^{i}Pr)$_2$bpy}Pt(pCat)**).

Identification code	ch1jw252p-1	
Empirical formula	C24 H26 N2 O7 Pt	
Formula weight	649.56	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 6.6241(3) Å	α= 100.0200(10)°.
	b = 10.9966(4) Å	β= 95.6330(10)°.
	c = 17.2394(7) Å	γ = 101.8470(10)°.
Volume	1198.53(8) Å^3	
Z	2	
Density (calculated)	1.800 Mg/m^3	
Absorption coefficient	5.900 mm^{-1}	
F(000)	636	
Crystal size	0.43 x 0.21 x 0.11 mm^3	

Theta range for data collection	1.21 to 27.47°.
Index ranges	-8<=h<=8, -11<=k<=14, -22<=l<=22
Reflections collected	15762
Independent reflections	5273 [R(int) = 0.0276]
Completeness to theta = 27.47°	96.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.5630 and 0.1858
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5273 / 0 / 311
Goodness-of-fit on F^2	1.146
Final R indices [I>2sigma(I)]	R1 = 0.0213, wR2 = 0.0633
R indices (all data)	R1 = 0.0232, wR2 = 0.0699
Largest diff. peak and hole	0.973 and -2.068 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for ch1jw252p-1 (**{(COO^{i}Pr)$_2$bpy}Pt(pCat))**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pt(1)	2681(1)	10290(1)	4558(1)	10(1)
O(1)	855(4)	6451(2)	7246(1)	17(1)
O(2)	-1574(4)	5201(2)	6259(2)	22(1)
O(3)	6076(5)	14071(3)	8382(2)	28(1)
O(4)	4240(4)	12222(2)	8594(1)	20(1)
O(5)	1660(4)	9254(2)	3474(1)	15(1)
O(6)	3659(4)	11684(2)	3979(2)	15(1)
N(1)	1746(4)	8903(3)	5129(2)	10(1)
N(2)	3549(4)	11256(3)	5674(2)	10(1)
C(1)	752(5)	7700(3)	4768(2)	15(1)
C(2)	74(5)	6799(3)	5206(2)	15(1)
C(3)	511(5)	7113(3)	6032(2)	14(1)
C(4)	-202(5)	6142(3)	6514(2)	16(1)
C(5)	165(6)	5644(3)	7811(2)	20(1)
C(6)	862(8)	4414(4)	7631(3)	35(1)
C(7)	1126(7)	6435(4)	8618(2)	30(1)

C(8)	1561(5)	8338(3)	6402(2)	14(1)
C(9)	2118(5)	9216(3)	5936(2)	12(1)
C(10)	3119(5)	10570(3)	6240(2)	13(1)
C(11)	4488(5)	12501(3)	5900(2)	16(1)
C(12)	4997(5)	13086(3)	6694(2)	16(1)
C(13)	4533(5)	12381(3)	7276(2)	14(1)
C(14)	3587(5)	11092(3)	7048(2)	13(1)
C(15)	5061(5)	13005(3)	8140(2)	17(1)
C(16)	4694(6)	12645(4)	9459(2)	24(1)
C(17)	3112(7)	13371(4)	9739(2)	33(1)
C(18)	4642(7)	11447(4)	9769(2)	33(1)
C(19)	1996(6)	9980(4)	2926(2)	17(1)
C(20)	3068(6)	11258(4)	3189(2)	17(1)
C(21)	3478(6)	12036(4)	2636(2)	22(1)
C(22)	2773(6)	11555(4)	1828(2)	27(1)
C(23)	1695(6)	10307(4)	1573(2)	27(1)
C(24)	1291(6)	9517(4)	2111(2)	23(1)
O(1S)	5756(5)	14281(3)	4325(2)	33(1)

Table 3. Bond lengths [Å] and angles [°] for ch1jw252p-1 (**{(COO^{i}Pr)$_2$bpy}Pt(pCat)**).

Pt(1)-N(1)	1.983(3)
Pt(1)-O(5)	1.986(2)
Pt(1)-N(2)	1.994(3)
Pt(1)-O(6)	2.005(2)
O(1)-C(4)	1.332(4)
O(1)-C(5)	1.471(4)
O(2)-C(4)	1.212(4)
O(3)-C(15)	1.205(4)
O(4)-C(15)	1.333(4)
O(4)-C(16)	1.464(4)
O(5)-C(19)	1.345(4)
O(6)-C(20)	1.350(4)
N(1)-C(9)	1.358(4)
N(1)-C(1)	1.359(4)
N(2)-C(10)	1.351(5)
N(2)-C(11)	1.353(5)
C(1)-C(2)	1.378(5)
C(1)-H(20)	0.9300
C(2)-C(3)	1.392(5)
C(2)-H(19)	0.9300
C(3)-C(8)	1.391(5)
C(3)-C(4)	1.494(5)
C(5)-C(7)	1.508(5)
C(5)-C(6)	1.509(6)
C(5)-H(7)	0.9800
C(6)-H(1)	0.9600
C(6)-H(3)	0.9600
C(6)-H(2)	0.9600
C(7)-H(4)	0.9600
C(7)-H(6)	0.9600
C(7)-H(5)	0.9600
C(8)-C(9)	1.378(5)
C(8)-H(18)	0.9300
C(9)-C(10)	1.479(5)

C(10)-C(14)	1.389(5)
C(11)-C(12)	1.384(5)
C(11)-H(8)	0.9300
C(12)-C(13)	1.392(4)
C(12)-H(17)	0.9300
C(13)-C(14)	1.396(5)
C(13)-C(15)	1.501(5)
C(14)-H(9)	0.9300
C(16)-C(18)	1.500(5)
C(16)-C(17)	1.509(6)
C(16)-H(10)	0.9800
C(17)-H(11)	0.9600
C(17)-H(12)	0.9600
C(17)-H(13)	0.9600
C(18)-H(15)	0.9600
C(18)-H(14)	0.9600
C(18)-H(16)	0.9600
C(19)-C(24)	1.406(5)
C(19)-C(20)	1.410(5)
C(20)-C(21)	1.399(5)
C(21)-C(22)	1.398(5)
C(21)-H(24)	0.9300
C(22)-C(23)	1.382(6)
C(22)-H(23)	0.9300
C(23)-C(24)	1.386(6)
C(23)-H(22)	0.9300
C(24)-H(21)	0.9300
O(1S)-H(1S1)	0.8500
O(1S)-H(2S2)	0.8501

N(1)-Pt(1)-O(5)	95.68(11)
N(1)-Pt(1)-N(2)	80.97(12)
O(5)-Pt(1)-N(2)	176.11(9)
N(1)-Pt(1)-O(6)	179.28(9)
O(5)-Pt(1)-O(6)	84.22(10)
N(2)-Pt(1)-O(6)	99.16(11)

C(4)-O(1)-C(5)	117.1(3)
C(15)-O(4)-C(16)	118.3(3)
C(19)-O(5)-Pt(1)	110.1(2)
C(20)-O(6)-Pt(1)	109.5(2)
C(9)-N(1)-C(1)	119.5(3)
C(9)-N(1)-Pt(1)	116.1(2)
C(1)-N(1)-Pt(1)	124.5(2)
C(10)-N(2)-C(11)	118.9(3)
C(10)-N(2)-Pt(1)	114.9(2)
C(11)-N(2)-Pt(1)	126.2(2)
N(1)-C(1)-C(2)	121.1(3)
N(1)-C(1)-H(20)	119.4
C(2)-C(1)-H(20)	119.4
C(1)-C(2)-C(3)	119.2(3)
C(1)-C(2)-H(19)	120.4
C(3)-C(2)-H(19)	120.4
C(8)-C(3)-C(2)	119.7(3)
C(8)-C(3)-C(4)	120.5(3)
C(2)-C(3)-C(4)	119.8(3)
O(2)-C(4)-O(1)	125.4(3)
O(2)-C(4)-C(3)	123.2(3)
O(1)-C(4)-C(3)	111.5(3)
O(1)-C(5)-C(7)	104.6(3)
O(1)-C(5)-C(6)	110.2(3)
C(7)-C(5)-C(6)	113.0(3)
O(1)-C(5)-H(7)	109.6
C(7)-C(5)-H(7)	109.6
C(6)-C(5)-H(7)	109.6
C(5)-C(6)-H(1)	109.5
C(5)-C(6)-H(3)	109.5
H(1)-C(6)-H(3)	109.5
C(5)-C(6)-H(2)	109.5
H(1)-C(6)-H(2)	109.5
H(3)-C(6)-H(2)	109.5
C(5)-C(7)-H(4)	109.5
C(5)-C(7)-H(6)	109.5

H(4)-C(7)-H(6)	109.5
C(5)-C(7)-H(5)	109.5
H(4)-C(7)-H(5)	109.5
H(6)-C(7)-H(5)	109.5
C(9)-C(8)-C(3)	118.6(3)
C(9)-C(8)-H(18)	120.7
C(3)-C(8)-H(18)	120.7
N(1)-C(9)-C(8)	121.8(3)
N(1)-C(9)-C(10)	113.1(3)
C(8)-C(9)-C(10)	125.1(3)
N(2)-C(10)-C(14)	122.7(3)
N(2)-C(10)-C(9)	115.0(3)
C(14)-C(10)-C(9)	122.3(3)
N(2)-C(11)-C(12)	121.6(3)
N(2)-C(11)-H(8)	119.2
C(12)-C(11)-H(8)	119.2
C(11)-C(12)-C(13)	119.4(3)
C(11)-C(12)-H(17)	120.3
C(13)-C(12)-H(17)	120.3
C(12)-C(13)-C(14)	119.3(3)
C(12)-C(13)-C(15)	120.0(3)
C(14)-C(13)-C(15)	120.7(3)
C(10)-C(14)-C(13)	118.0(3)
C(10)-C(14)-H(9)	121.0
C(13)-C(14)-H(9)	121.0
O(3)-C(15)-O(4)	125.2(3)
O(3)-C(15)-C(13)	124.2(3)
O(4)-C(15)-C(13)	110.7(3)
O(4)-C(16)-C(18)	104.4(3)
O(4)-C(16)-C(17)	109.0(3)
C(18)-C(16)-C(17)	114.6(3)
O(4)-C(16)-H(10)	109.6
C(18)-C(16)-H(10)	109.6
C(17)-C(16)-H(10)	109.6
C(16)-C(17)-H(11)	109.5
C(16)-C(17)-H(12)	109.5

H(11)-C(17)-H(12)	109.5
C(16)-C(17)-H(13)	109.5
H(11)-C(17)-H(13)	109.5
H(12)-C(17)-H(13)	109.5
C(16)-C(18)-H(15)	109.5
C(16)-C(18)-H(14)	109.5
H(15)-C(18)-H(14)	109.5
C(16)-C(18)-H(16)	109.5
H(15)-C(18)-H(16)	109.5
H(14)-C(18)-H(16)	109.5
O(5)-C(19)-C(24)	122.4(3)
O(5)-C(19)-C(20)	118.1(3)
C(24)-C(19)-C(20)	119.4(3)
O(6)-C(20)-C(21)	122.3(4)
O(6)-C(20)-C(19)	117.9(3)
C(21)-C(20)-C(19)	119.7(3)
C(22)-C(21)-C(20)	119.9(4)
C(22)-C(21)-H(24)	120.0
C(20)-C(21)-H(24)	120.0
C(23)-C(22)-C(21)	120.2(3)
C(23)-C(22)-H(23)	119.9
C(21)-C(22)-H(23)	119.9
C(22)-C(23)-C(24)	120.8(3)
C(22)-C(23)-H(22)	119.6
C(24)-C(23)-H(22)	119.6
C(23)-C(24)-C(19)	119.9(4)
C(23)-C(24)-H(21)	120.1
C(19)-C(24)-H(21)	120.1
H(1S1)-O(1S)-H(2S2)	107.7

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for ch1jw252p-1 (**{(COO^{i}Pr)$_2$bpy}Pt(pCat)**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt(1)	10(1)	12(1)	10(1)	2(1)	4(1)	4(1)
O(1)	19(1)	15(1)	16(1)	4(1)	3(1)	1(1)
O(2)	24(1)	16(1)	22(1)	5(1)	0(1)	-5(1)
O(3)	37(2)	20(1)	18(1)	-1(1)	4(1)	-10(1)
O(4)	29(1)	16(1)	11(1)	1(1)	4(1)	-2(1)
O(5)	18(1)	17(1)	9(1)	2(1)	2(1)	4(1)
O(6)	17(1)	16(1)	14(1)	6(1)	4(1)	4(1)
N(1)	8(1)	13(1)	11(1)	4(1)	1(1)	4(1)
N(2)	10(1)	12(1)	9(1)	0(1)	2(1)	4(1)
C(1)	14(2)	13(2)	17(2)	-1(1)	3(1)	5(1)
C(2)	17(2)	13(2)	17(2)	2(1)	4(1)	5(1)
C(3)	12(1)	14(2)	16(2)	2(1)	3(1)	6(1)
C(4)	14(2)	14(2)	20(2)	2(1)	6(1)	6(1)
C(5)	23(2)	16(2)	19(2)	7(1)	3(1)	0(1)
C(6)	55(3)	25(2)	30(2)	9(2)	6(2)	18(2)
C(7)	39(2)	27(2)	21(2)	4(2)	4(2)	4(2)
C(8)	11(1)	14(2)	15(2)	1(1)	4(1)	3(1)
C(9)	8(1)	12(2)	15(2)	0(1)	2(1)	1(1)
C(10)	9(1)	14(2)	17(2)	3(1)	4(1)	4(1)
C(11)	16(2)	15(2)	18(2)	6(1)	6(1)	2(1)
C(12)	17(2)	13(2)	18(2)	3(1)	5(1)	0(1)
C(13)	13(1)	14(2)	14(2)	2(1)	5(1)	2(1)
C(14)	13(2)	14(2)	14(2)	5(1)	5(1)	3(1)
C(15)	19(2)	17(2)	16(2)	3(1)	5(1)	3(1)
C(16)	35(2)	21(2)	12(2)	0(1)	4(1)	0(2)
C(17)	48(3)	32(2)	21(2)	0(2)	9(2)	12(2)
C(18)	53(3)	30(2)	17(2)	8(2)	7(2)	9(2)
C(19)	18(2)	22(2)	15(2)	6(1)	8(1)	8(2)
C(20)	16(2)	24(2)	14(2)	3(1)	6(1)	9(2)
C(21)	23(2)	25(2)	21(2)	8(2)	10(2)	7(2)
C(22)	30(2)	39(2)	18(2)	17(2)	8(2)	12(2)

C(23)	31(2)	42(2)	11(2)	5(2)	1(1)	13(2)
C(24)	23(2)	28(2)	16(2)	-1(2)	3(1)	6(2)
O(1S)	34(2)	22(2)	40(2)	1(1)	-4(1)	5(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for ch1jw252p-1 (**{(COO^{i}Pr)$_2$bpy}Pt(pCat)**).

	x	y	z	U(eq)
H(20)	526	7481	4215	18
H(19)	-668	5991	4953	18
H(7)	-1357	5467	7773	23
H(1)	150	3930	7125	52
H(3)	542	3938	8038	52
H(2)	2337	4592	7616	52
H(4)	2616	6576	8661	45
H(6)	646	5997	9024	45
H(5)	729	7235	8682	45
H(18)	1880	8559	6953	16
H(8)	4798	12975	5512	19
H(17)	5644	13943	6837	20
H(9)	3280	10597	7425	16
H(10)	6094	13196	9602	29
H(11)	3200	14098	9495	50
H(12)	3390	13644	10307	50
H(13)	1740	12834	9593	50
H(15)	3280	10898	9617	49
H(14)	4958	11649	10339	49
H(16)	5655	11028	9550	49
H(24)	4219	12872	2805	27
H(23)	3029	12075	1460	32
H(22)	1235	9995	1034	33
H(21)	554	8681	1933	27
H(1S1)	5231	13488	4221	40
H(2S2)	4759	14658	4307	40_

Part 2.

X-ray crystallographic data for compound **{(COO^{i}Pr)$_2$bpy}PtCl$_2$, CCDC** 1028955.

Table 6. Crystal data and structure refinement for ch1jw241_0m ({(COO^{i}Pr)$_2$bpy}PtCl$_2$).

Identification code	ch1jw241_0m ({(COO^{i}Pr)$_2$bpy}PtCl$_2$)	
Empirical formula	C40 H50 Cl4 N4 O9 Pt2	
Formula weight	1262.82	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 13.6896(8) Å	α= 90.066(3)°.
	b = 14.3617(8) Å	β= 91.336(3)°.
	c = 23.8509(12) Å	γ = 104.659(3)°.
Volume	4535.2(4) Å^3	
Z	4	
Density (calculated)	1.849 Mg/m^3	
Absorption coefficient	6.454 mm^{-1}	
F(000)	2456	
Crystal size	0.43 x 0.12 x 0.12 mm^3	
Theta range for data collection	0.85 to 27.66°.	
Index ranges	-17<=h<=17, -18<=k<=18, -30<=l<=30	
Reflections collected	87085	
Independent reflections	20800 [R(int) = 0.0785]	
Completeness to theta = 27.66°	98.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.5114 and 0.1679	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	20800 / 0 / 1083	
Goodness-of-fit on F^2	1.011	
Final R indices [I>2sigma(I)]	R1 = 0.0409, wR2 = 0.0775	
R indices (all data)	R1 = 0.0660, wR2 = 0.0876	
Largest diff. peak and hole	1.377 and -2.041 e.Å^{-3}	

Table 7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for ch1jw241_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pt(1)	-884(1)	1309(1)	5078(1)	16(1)
Pt(2)	-843(1)	3285(1)	10072(1)	19(1)
Pt(3)	10816(1)	1716(1)	-213(1)	16(1)
Pt(4)	10635(1)	3665(1)	4798(1)	15(1)
Cl(1)	-1572(1)	2558(1)	10871(1)	26(1)
Cl(2)	-2379(1)	2815(1)	9611(1)	28(1)
Cl(3)	12195(1)	3883(1)	5224(1)	21(1)
Cl(4)	11311(1)	3300(1)	3981(1)	22(1)
Cl(5)	-2412(1)	1049(1)	4609(1)	24(1)
Cl(6)	-1629(1)	1669(1)	5875(1)	23(1)
Cl(7)	12376(1)	2201(1)	221(1)	22(1)
Cl(8)	11515(1)	2420(1)	-1022(1)	23(1)
N(1)	488(3)	1487(3)	5441(2)	15(1)
N(2)	-138(3)	980(3)	4421(2)	15(1)
N(3)	536(3)	3769(3)	10425(2)	19(1)
N(4)	-104(3)	3976(3)	9412(2)	16(1)
N(5)	10117(3)	1083(3)	471(2)	15(1)
N(6)	9421(3)	1203(3)	-543(2)	16(1)
N(7)	9948(3)	3979(3)	5485(2)	13(1)
N(8)	9234(3)	3524(3)	4474(2)	16(1)
O(1)	4079(3)	1502(3)	5734(1)	23(1)
O(2)	3733(3)	2068(3)	6564(1)	28(1)
O(3)	2620(3)	431(2)	3265(1)	20(1)
O(4)	1286(3)	-27(3)	2667(1)	23(1)
O(5)	4114(3)	5517(3)	10718(1)	24(1)
O(6)	3791(3)	4743(3)	11538(1)	29(1)
O(7)	2616(3)	5904(2)	8242(1)	18(1)
O(8)	1257(3)	5659(3)	7653(1)	24(1)
O(9)	7432(3)	-652(3)	1732(1)	21(1)
O(10)	8785(3)	-238(3)	2313(2)	40(1)
O(11)	5837(3)	-573(3)	-757(1)	23(1)

O(12)	6088(3)	215(3)	-1577(1)	27(1)
O(13)	7300(3)	4276(3)	6810(1)	22(1)
O(14)	8718(3)	4756(3)	7331(1)	29(1)
O(15)	5663(3)	3648(3)	4244(1)	22(1)
O(16)	5925(3)	2967(3)	3431(1)	28(1)
C(1)	753(4)	1774(4)	5974(2)	22(1)
C(2)	1708(4)	1877(4)	6192(2)	20(1)
C(3)	2433(4)	1650(3)	5860(2)	17(1)
C(4)	2167(4)	1340(3)	5305(2)	16(1)
C(5)	1211(4)	1281(3)	5108(2)	15(1)
C(6)	846(4)	1001(3)	4530(2)	16(1)
C(7)	1450(4)	774(3)	4116(2)	15(1)
C(8)	1039(4)	531(3)	3586(2)	16(1)
C(9)	40(4)	505(3)	3482(2)	19(1)
C(10)	-528(4)	742(3)	3901(2)	20(1)
C(11)	3483(4)	1774(4)	6100(2)	18(1)
C(12)	5117(4)	1556(4)	5914(2)	24(1)
C(13)	5773(5)	2526(4)	5782(3)	41(2)
C(14)	5411(5)	733(4)	5611(3)	42(2)
C(15)	1644(4)	263(3)	3118(2)	16(1)
C(16)	3290(4)	182(4)	2842(2)	22(1)
C(17)	4326(4)	803(4)	2982(2)	31(2)
C(18)	3205(4)	-889(4)	2869(2)	30(1)
C(19)	801(4)	3597(4)	10955(2)	21(1)
C(20)	1769(4)	3961(4)	11168(2)	23(1)
C(21)	2492(4)	4532(4)	10839(2)	19(1)
C(22)	2215(4)	4731(3)	10291(2)	17(1)
C(23)	1243(4)	4317(4)	10089(2)	16(1)
C(24)	885(4)	4437(3)	9519(2)	17(1)
C(25)	1470(4)	4959(3)	9104(2)	14(1)
C(26)	1050(4)	5009(4)	8574(2)	17(1)
C(27)	39(4)	4538(4)	8470(2)	21(1)
C(28)	-503(4)	4036(4)	8900(2)	20(1)
C(29)	1637(4)	5560(3)	8101(2)	16(1)
C(30)	3244(4)	6484(4)	7811(2)	23(1)
C(31)	3103(5)	7490(4)	7831(2)	33(2)

C(32)	4296(4)	6422(4)	7937(2)	35(2)
C(33)	3529(4)	4931(4)	11071(2)	20(1)
C(34)	5147(4)	5996(4)	10913(2)	27(1)
C(35)	5407(5)	6948(5)	10608(3)	49(2)
C(36)	5841(5)	5374(5)	10782(3)	48(2)
C(37)	10524(4)	1087(4)	985(2)	20(1)
C(38)	9993(4)	644(4)	1430(2)	17(1)
C(39)	8982(4)	183(3)	1353(2)	16(1)
C(40)	8550(4)	152(3)	821(2)	18(1)
C(41)	9126(4)	616(3)	383(2)	16(1)
C(42)	8736(4)	684(3)	-189(2)	16(1)
C(43)	7747(4)	263(3)	-368(2)	16(1)
C(44)	7455(4)	419(4)	-918(2)	18(1)
C(45)	8146(4)	946(4)	-1270(2)	24(1)
C(46)	9135(4)	1329(4)	-1078(2)	19(1)
C(47)	6397(4)	26(4)	-1128(2)	21(1)
C(48)	4797(4)	-1055(4)	-924(2)	25(1)
C(49)	4121(4)	-417(5)	-769(3)	40(2)
C(50)	4547(5)	-1998(5)	-622(2)	41(2)
C(51)	8393(4)	-263(4)	1854(2)	18(1)
C(52)	6801(4)	-1059(4)	2210(2)	29(1)
C(53)	6024(5)	-1915(5)	1964(3)	62(2)
C(54)	6375(5)	-307(5)	2452(3)	62(2)
C(55)	10384(4)	4181(4)	5991(2)	20(1)
C(56)	9864(4)	4375(3)	6444(2)	18(1)
C(57)	8846(4)	4340(4)	6378(2)	17(1)
C(58)	8390(4)	4146(3)	5848(2)	16(1)
C(59)	8959(4)	3962(3)	5413(2)	16(1)
C(60)	8554(4)	3718(4)	4835(2)	17(1)
C(61)	7578(4)	3684(3)	4656(2)	18(1)
C(62)	7275(4)	3407(4)	4108(2)	18(1)
C(63)	7974(4)	3199(4)	3751(2)	20(1)
C(64)	8938(4)	3267(4)	3940(2)	22(1)
C(65)	6223(4)	3308(4)	3887(2)	22(1)
C(66)	4611(4)	3599(4)	4065(2)	24(1)
C(67)	4371(4)	4481(4)	4311(2)	32(2)

C(68)	3942(4)	2672(4)	4267(3)	36(2)
C(69)	8294(4)	4496(4)	6889(2)	19(1)
C(70)	6707(4)	4299(4)	7314(2)	26(1)
C(71)	6645(5)	3381(4)	7638(3)	44(2)
C(72)	5688(4)	4406(5)	7122(2)	46(2)
O(1S)	1606(3)	2349(3)	2141(2)	31(1)
O(2S)	1411(3)	3397(3)	7139(2)	34(1)
C(1S)	3062(4)	1981(4)	1753(2)	35(2)
C(2S)	2659(4)	2437(4)	2241(2)	33(2)
C(3S)	1177(5)	2724(4)	2572(2)	39(2)
C(4S)	39(6)	2565(6)	2465(3)	63(2)
C(5S)	2939(5)	4419(4)	6785(2)	39(2)
C(6S)	2463(5)	3755(4)	7255(2)	41(2)
C(7S)	929(6)	2756(5)	7554(2)	48(2)
C(8S)	-212(6)	2494(5)	7440(2)	53(2)

Table 8. Bond lengths [Å] and angles [°] for ch1jw241_0m.

Pt(1)-N(1)	2.005(4)
Pt(1)-N(2)	2.010(4)
Pt(1)-Cl(5)	2.2947(13)
Pt(1)-Cl(6)	2.2968(12)
Pt(2)-N(3)	2.003(4)
Pt(2)-N(4)	2.016(4)
Pt(2)-Cl(2)	2.2934(14)
Pt(2)-Cl(1)	2.2975(13)
Pt(3)-N(6)	2.008(4)
Pt(3)-N(5)	2.008(4)
Pt(3)-Cl(7)	2.2925(13)
Pt(3)-Cl(8)	2.2945(12)
Pt(4)-N(8)	2.014(4)
Pt(4)-N(7)	2.015(4)
Pt(4)-Cl(3)	2.2907(13)
Pt(4)-Cl(4)	2.2930(12)
N(1)-C(1)	1.347(6)

N(1)-C(5)	1.373(6)
N(2)-C(10)	1.348(6)
N(2)-C(6)	1.359(6)
N(3)-C(19)	1.349(6)
N(3)-C(23)	1.360(6)
N(4)-C(28)	1.338(6)
N(4)-C(24)	1.366(6)
N(5)-C(37)	1.334(6)
N(5)-C(41)	1.364(6)
N(6)-C(46)	1.351(6)
N(6)-C(42)	1.354(6)
N(7)-C(55)	1.333(6)
N(7)-C(59)	1.355(6)
N(8)-C(64)	1.349(6)
N(8)-C(60)	1.361(6)
O(1)-C(11)	1.332(6)
O(1)-C(12)	1.458(6)
O(2)-C(11)	1.195(6)
O(3)-C(15)	1.335(6)
O(3)-C(16)	1.481(5)
O(4)-C(15)	1.200(6)
O(5)-C(33)	1.322(6)
O(5)-C(34)	1.472(6)
O(6)-C(33)	1.214(6)
O(7)-C(29)	1.340(6)
O(7)-C(30)	1.475(6)
O(8)-C(29)	1.202(6)
O(9)-C(51)	1.318(6)
O(9)-C(52)	1.478(6)
O(10)-C(51)	1.204(6)
O(11)-C(47)	1.345(6)
O(11)-C(48)	1.463(6)
O(12)-C(47)	1.200(6)
O(13)-C(69)	1.326(6)
O(13)-C(70)	1.473(6)
O(14)-C(69)	1.203(6)

O(15)-C(65)	1.332(6)
O(15)-C(66)	1.476(6)
O(16)-C(65)	1.209(6)
C(1)-C(2)	1.369(7)
C(1)-H(1)	0.9500
C(2)-C(3)	1.385(7)
C(2)-H(2)	0.9500
C(3)-C(4)	1.406(7)
C(3)-C(11)	1.502(7)
C(4)-C(5)	1.362(7)
C(4)-H(4)	0.9500
C(5)-C(6)	1.475(7)
C(6)-C(7)	1.392(6)
C(7)-C(8)	1.379(7)
C(7)-H(7)	0.9500
C(8)-C(9)	1.375(7)
C(8)-C(15)	1.511(7)
C(9)-C(10)	1.374(7)
C(9)-H(9)	0.9500
C(10)-H(10)	0.9500
C(12)-C(13)	1.492(7)
C(12)-C(14)	1.528(7)
C(12)-H(12)	1.0000
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(16)-C(17)	1.502(7)
C(16)-C(18)	1.516(7)
C(16)-H(16)	1.0000
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-H(18A)	0.9800

C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-C(20)	1.380(7)
C(19)-H(19)	0.9500
C(20)-C(21)	1.375(7)
C(20)-H(20)	0.9500
C(21)-C(22)	1.402(7)
C(21)-C(33)	1.483(7)
C(22)-C(23)	1.388(7)
C(22)-H(22)	0.9500
C(23)-C(24)	1.460(7)
C(24)-C(25)	1.385(7)
C(25)-C(26)	1.386(6)
C(25)-H(25)	0.9500
C(26)-C(27)	1.394(7)
C(26)-C(29)	1.505(7)
C(27)-C(28)	1.373(7)
C(27)-H(27)	0.9500
C(28)-H(28)	0.9500
C(30)-C(32)	1.490(7)
C(30)-C(31)	1.506(7)
C(30)-H(30)	1.0000
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(34)-C(36)	1.498(8)
C(34)-C(35)	1.514(8)
C(34)-H(34)	1.0000
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
C(36)-H(36A)	0.9800
C(36)-H(36B)	0.9800

C(36)-H(36C)	0.9800
C(37)-C(38)	1.366(7)
C(37)-H(37)	0.9500
C(38)-C(39)	1.382(7)
C(38)-H(38)	0.9500
C(39)-C(40)	1.383(7)
C(39)-C(51)	1.506(7)
C(40)-C(41)	1.390(7)
C(40)-H(40)	0.9500
C(41)-C(42)	1.466(7)
C(42)-C(43)	1.393(7)
C(43)-C(44)	1.397(6)
C(43)-H(43)	0.9500
C(44)-C(45)	1.360(7)
C(44)-C(47)	1.490(7)
C(45)-C(46)	1.393(7)
C(45)-H(45)	0.9500
C(46)-H(46)	0.9500
C(48)-C(50)	1.501(7)
C(48)-C(49)	1.508(8)
C(48)-H(48)	1.0000
C(49)-H(49A)	0.9800
C(49)-H(49B)	0.9800
C(49)-H(49C)	0.9800
C(50)-H(50A)	0.9800
C(50)-H(50B)	0.9800
C(50)-H(50C)	0.9800
C(52)-C(54)	1.474(8)
C(52)-C(53)	1.515(8)
C(52)-H(52)	1.0000
C(53)-H(53A)	0.9800
C(53)-H(53B)	0.9800
C(53)-H(53C)	0.9800
C(54)-H(54A)	0.9800
C(54)-H(54B)	0.9800
C(54)-H(54C)	0.9800

C(55)-C(56)	1.373(7)
C(55)-H(55)	0.9500
C(56)-C(57)	1.388(7)
C(56)-H(56)	0.9500
C(57)-C(58)	1.392(6)
C(57)-C(69)	1.495(7)
C(58)-C(59)	1.378(6)
C(58)-H(58)	0.9500
C(59)-C(60)	1.481(6)
C(60)-C(61)	1.383(7)
C(61)-C(62)	1.390(7)
C(61)-H(61)	0.9500
C(62)-C(63)	1.382(7)
C(62)-C(65)	1.494(7)
C(63)-C(64)	1.365(7)
C(63)-H(63)	0.9500
C(64)-H(64)	0.9500
C(66)-C(68)	1.499(7)
C(66)-C(67)	1.509(7)
C(66)-H(66)	1.0000
C(67)-H(67A)	0.9800
C(67)-H(67B)	0.9800
C(67)-H(67C)	0.9800
C(68)-H(68A)	0.9800
C(68)-H(68B)	0.9800
C(68)-H(68C)	0.9800
C(70)-C(72)	1.502(7)
C(70)-C(71)	1.514(7)
C(70)-H(70)	1.0000
C(71)-H(71A)	0.9800
C(71)-H(71B)	0.9800
C(71)-H(71C)	0.9800
C(72)-H(72A)	0.9800
C(72)-H(72B)	0.9800
C(72)-H(72C)	0.9800
O(1S)-C(3S)	1.372(6)

O(1S)-C(2S)	1.428(6)
O(2S)-C(7S)	1.409(7)
O(2S)-C(6S)	1.422(7)
C(1S)-C(2S)	1.516(7)
C(1S)-H(1AA)	0.9800
C(1S)-H(1AB)	0.9800
C(1S)-H(1AC)	0.9800
C(2S)-H(2AA)	0.9900
C(2S)-H(2AB)	0.9900
C(3S)-C(4S)	1.531(9)
C(3S)-H(3AA)	0.9900
C(3S)-H(3AB)	0.9900
C(4S)-H(4AA)	0.9800
C(4S)-H(4AB)	0.9800
C(4S)-H(4AC)	0.9800
C(5S)-C(6S)	1.522(8)
C(5S)-H(5AA)	0.9800
C(5S)-H(5AB)	0.9800
C(5S)-H(5AC)	0.9800
C(6S)-H(6AA)	0.9900
C(6S)-H(6AB)	0.9900
C(7S)-C(8S)	1.529(9)
C(7S)-H(7AA)	0.9900
C(7S)-H(7AB)	0.9900
C(8S)-H(8AA)	0.9800
C(8S)-H(8AB)	0.9800
C(8S)-H(8AC)	0.9800

N(1)-Pt(1)-N(2)	80.76(16)
N(1)-Pt(1)-Cl(5)	175.73(12)
N(2)-Pt(1)-Cl(5)	95.08(12)
N(1)-Pt(1)-Cl(6)	94.77(12)
N(2)-Pt(1)-Cl(6)	175.35(12)
Cl(5)-Pt(1)-Cl(6)	89.36(5)
N(3)-Pt(2)-N(4)	80.41(16)
N(3)-Pt(2)-Cl(2)	175.39(12)

N(4)-Pt(2)-Cl(2)	95.12(12)
N(3)-Pt(2)-Cl(1)	94.98(12)
N(4)-Pt(2)-Cl(1)	175.30(13)
Cl(2)-Pt(2)-Cl(1)	89.47(5)
N(6)-Pt(3)-N(5)	80.72(16)
N(6)-Pt(3)-Cl(7)	175.13(12)
N(5)-Pt(3)-Cl(7)	94.84(12)
N(6)-Pt(3)-Cl(8)	95.59(12)
N(5)-Pt(3)-Cl(8)	176.27(12)
Cl(7)-Pt(3)-Cl(8)	88.87(5)
N(8)-Pt(4)-N(7)	80.42(16)
N(8)-Pt(4)-Cl(3)	175.70(11)
N(7)-Pt(4)-Cl(3)	95.42(12)
N(8)-Pt(4)-Cl(4)	95.44(11)
N(7)-Pt(4)-Cl(4)	175.86(12)
Cl(3)-Pt(4)-Cl(4)	88.71(5)
C(1)-N(1)-C(5)	118.1(4)
C(1)-N(1)-Pt(1)	126.4(3)
C(5)-N(1)-Pt(1)	115.5(3)
C(10)-N(2)-C(6)	119.1(4)
C(10)-N(2)-Pt(1)	126.0(4)
C(6)-N(2)-Pt(1)	114.9(3)
C(19)-N(3)-C(23)	119.1(5)
C(19)-N(3)-Pt(2)	125.4(3)
C(23)-N(3)-Pt(2)	115.4(3)
C(28)-N(4)-C(24)	119.1(4)
C(28)-N(4)-Pt(2)	126.0(4)
C(24)-N(4)-Pt(2)	114.9(3)
C(37)-N(5)-C(41)	118.8(4)
C(37)-N(5)-Pt(3)	126.6(3)
C(41)-N(5)-Pt(3)	114.6(3)
C(46)-N(6)-C(42)	119.4(4)
C(46)-N(6)-Pt(3)	125.4(3)
C(42)-N(6)-Pt(3)	115.2(3)
C(55)-N(7)-C(59)	119.2(4)
C(55)-N(7)-Pt(4)	125.3(4)

C(59)-N(7)-Pt(4)	115.5(3)
C(64)-N(8)-C(60)	119.4(5)
C(64)-N(8)-Pt(4)	125.3(4)
C(60)-N(8)-Pt(4)	115.3(3)
C(11)-O(1)-C(12)	117.6(4)
C(15)-O(3)-C(16)	116.3(4)
C(33)-O(5)-C(34)	117.5(4)
C(29)-O(7)-C(30)	115.5(4)
C(51)-O(9)-C(52)	115.6(4)
C(47)-O(11)-C(48)	117.6(4)
C(69)-O(13)-C(70)	115.7(4)
C(65)-O(15)-C(66)	116.9(4)
N(1)-C(1)-C(2)	123.0(5)
N(1)-C(1)-H(1)	118.5
C(2)-C(1)-H(1)	118.5
C(1)-C(2)-C(3)	119.0(5)
C(1)-C(2)-H(2)	120.5
C(3)-C(2)-H(2)	120.5
C(2)-C(3)-C(4)	118.7(5)
C(2)-C(3)-C(11)	118.9(5)
C(4)-C(3)-C(11)	122.4(5)
C(5)-C(4)-C(3)	119.3(5)
C(5)-C(4)-H(4)	120.3
C(3)-C(4)-H(4)	120.3
C(4)-C(5)-N(1)	121.8(5)
C(4)-C(5)-C(6)	124.8(5)
N(1)-C(5)-C(6)	113.4(4)
N(2)-C(6)-C(7)	121.1(4)
N(2)-C(6)-C(5)	115.3(4)
C(7)-C(6)-C(5)	123.6(5)
C(8)-C(7)-C(6)	119.1(5)
C(8)-C(7)-H(7)	120.5
C(6)-C(7)-H(7)	120.5
C(9)-C(8)-C(7)	119.2(5)
C(9)-C(8)-C(15)	118.7(4)
C(7)-C(8)-C(15)	122.0(5)

C(10)-C(9)-C(8)	119.9(5)
C(10)-C(9)-H(9)	120.0
C(8)-C(9)-H(9)	120.0
N(2)-C(10)-C(9)	121.6(5)
N(2)-C(10)-H(10)	119.2
C(9)-C(10)-H(10)	119.2
O(2)-C(11)-O(1)	125.2(5)
O(2)-C(11)-C(3)	123.4(5)
O(1)-C(11)-C(3)	111.4(4)
O(1)-C(12)-C(13)	109.5(5)
O(1)-C(12)-C(14)	105.8(4)
C(13)-C(12)-C(14)	113.6(5)
O(1)-C(12)-H(12)	109.3
C(13)-C(12)-H(12)	109.3
C(14)-C(12)-H(12)	109.3
C(12)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(12)-C(14)-H(14A)	109.5
C(12)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(12)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
O(4)-C(15)-O(3)	125.1(5)
O(4)-C(15)-C(8)	123.5(5)
O(3)-C(15)-C(8)	111.3(4)
O(3)-C(16)-C(17)	105.5(4)
O(3)-C(16)-C(18)	108.6(4)
C(17)-C(16)-C(18)	114.3(5)
O(3)-C(16)-H(16)	109.4
C(17)-C(16)-H(16)	109.4
C(18)-C(16)-H(16)	109.4

C(16)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(16)-C(18)-H(18A)	109.5
C(16)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(16)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
N(3)-C(19)-C(20)	121.9(5)
N(3)-C(19)-H(19)	119.1
C(20)-C(19)-H(19)	119.1
C(21)-C(20)-C(19)	120.1(5)
C(21)-C(20)-H(20)	120.0
C(19)-C(20)-H(20)	120.0
C(20)-C(21)-C(22)	118.3(5)
C(20)-C(21)-C(33)	119.9(5)
C(22)-C(21)-C(33)	121.8(5)
C(23)-C(22)-C(21)	119.5(5)
C(23)-C(22)-H(22)	120.2
C(21)-C(22)-H(22)	120.2
N(3)-C(23)-C(22)	121.0(5)
N(3)-C(23)-C(24)	114.7(5)
C(22)-C(23)-C(24)	124.3(5)
N(4)-C(24)-C(25)	120.6(5)
N(4)-C(24)-C(23)	114.5(4)
C(25)-C(24)-C(23)	124.9(5)
C(24)-C(25)-C(26)	119.7(5)
C(24)-C(25)-H(25)	120.1
C(26)-C(25)-H(25)	120.1
C(25)-C(26)-C(27)	119.1(5)
C(25)-C(26)-C(29)	122.8(5)
C(27)-C(26)-C(29)	118.1(5)

C(28)-C(27)-C(26)	118.4(5)
C(28)-C(27)-H(27)	120.8
C(26)-C(27)-H(27)	120.8
N(4)-C(28)-C(27)	123.0(5)
N(4)-C(28)-H(28)	118.5
C(27)-C(28)-H(28)	118.5
O(8)-C(29)-O(7)	125.4(5)
O(8)-C(29)-C(26)	122.8(5)
O(7)-C(29)-C(26)	111.8(4)
O(7)-C(30)-C(32)	105.8(4)
O(7)-C(30)-C(31)	108.7(4)
C(32)-C(30)-C(31)	114.4(5)
O(7)-C(30)-H(30)	109.3
C(32)-C(30)-H(30)	109.3
C(31)-C(30)-H(30)	109.3
C(30)-C(31)-H(31A)	109.5
C(30)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(30)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(30)-C(32)-H(32A)	109.5
C(30)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(30)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
O(6)-C(33)-O(5)	124.7(5)
O(6)-C(33)-C(21)	122.7(5)
O(5)-C(33)-C(21)	112.6(4)
O(5)-C(34)-C(36)	109.6(5)
O(5)-C(34)-C(35)	105.0(4)
C(36)-C(34)-C(35)	113.0(5)
O(5)-C(34)-H(34)	109.7
C(36)-C(34)-H(34)	109.7
C(35)-C(34)-H(34)	109.7

C(34)-C(35)-H(35A)	109.5
C(34)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(34)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(34)-C(36)-H(36A)	109.5
C(34)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(34)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
N(5)-C(37)-C(38)	123.0(5)
N(5)-C(37)-H(37)	118.5
C(38)-C(37)-H(37)	118.5
C(37)-C(38)-C(39)	119.2(5)
C(37)-C(38)-H(38)	120.4
C(39)-C(38)-H(38)	120.4
C(38)-C(39)-C(40)	118.8(5)
C(38)-C(39)-C(51)	118.6(4)
C(40)-C(39)-C(51)	122.6(5)
C(39)-C(40)-C(41)	119.6(5)
C(39)-C(40)-H(40)	120.2
C(41)-C(40)-H(40)	120.2
N(5)-C(41)-C(40)	120.6(5)
N(5)-C(41)-C(42)	114.8(4)
C(40)-C(41)-C(42)	124.5(5)
N(6)-C(42)-C(43)	121.2(5)
N(6)-C(42)-C(41)	114.5(4)
C(43)-C(42)-C(41)	124.2(5)
C(42)-C(43)-C(44)	118.8(5)
C(42)-C(43)-H(43)	120.6
C(44)-C(43)-H(43)	120.6
C(45)-C(44)-C(43)	119.6(5)
C(45)-C(44)-C(47)	119.0(5)
C(43)-C(44)-C(47)	121.4(5)

C(44)-C(45)-C(46)	119.7(5)
C(44)-C(45)-H(45)	120.1
C(46)-C(45)-H(45)	120.1
N(6)-C(46)-C(45)	121.3(5)
N(6)-C(46)-H(46)	119.4
C(45)-C(46)-H(46)	119.4
O(12)-C(47)-O(11)	124.3(5)
O(12)-C(47)-C(44)	123.8(5)
O(11)-C(47)-C(44)	111.9(4)
O(11)-C(48)-C(50)	106.2(4)
O(11)-C(48)-C(49)	108.8(5)
C(50)-C(48)-C(49)	112.8(5)
O(11)-C(48)-H(48)	109.7
C(50)-C(48)-H(48)	109.7
C(49)-C(48)-H(48)	109.7
C(48)-C(49)-H(49A)	109.5
C(48)-C(49)-H(49B)	109.5
H(49A)-C(49)-H(49B)	109.5
C(48)-C(49)-H(49C)	109.5
H(49A)-C(49)-H(49C)	109.5
H(49B)-C(49)-H(49C)	109.5
C(48)-C(50)-H(50A)	109.5
C(48)-C(50)-H(50B)	109.5
H(50A)-C(50)-H(50B)	109.5
C(48)-C(50)-H(50C)	109.5
H(50A)-C(50)-H(50C)	109.5
H(50B)-C(50)-H(50C)	109.5
O(10)-C(51)-O(9)	125.4(5)
O(10)-C(51)-C(39)	121.6(5)
O(9)-C(51)-C(39)	113.0(4)
C(54)-C(52)-O(9)	108.9(5)
C(54)-C(52)-C(53)	114.6(6)
O(9)-C(52)-C(53)	104.5(5)
C(54)-C(52)-H(52)	109.6
O(9)-C(52)-H(52)	109.6
C(53)-C(52)-H(52)	109.6

C(52)-C(53)-H(53A)	109.5
C(52)-C(53)-H(53B)	109.5
H(53A)-C(53)-H(53B)	109.5
C(52)-C(53)-H(53C)	109.5
H(53A)-C(53)-H(53C)	109.5
H(53B)-C(53)-H(53C)	109.5
C(52)-C(54)-H(54A)	109.5
C(52)-C(54)-H(54B)	109.5
H(54A)-C(54)-H(54B)	109.5
C(52)-C(54)-H(54C)	109.5
H(54A)-C(54)-H(54C)	109.5
H(54B)-C(54)-H(54C)	109.5
N(7)-C(55)-C(56)	122.2(5)
N(7)-C(55)-H(55)	118.9
C(56)-C(55)-H(55)	118.9
C(55)-C(56)-C(57)	119.2(5)
C(55)-C(56)-H(56)	120.4
C(57)-C(56)-H(56)	120.4
C(56)-C(57)-C(58)	118.9(4)
C(56)-C(57)-C(69)	117.4(4)
C(58)-C(57)-C(69)	123.7(5)
C(59)-C(58)-C(57)	118.7(5)
C(59)-C(58)-H(58)	120.6
C(57)-C(58)-H(58)	120.6
N(7)-C(59)-C(58)	121.8(4)
N(7)-C(59)-C(60)	114.4(4)
C(58)-C(59)-C(60)	123.8(5)
N(8)-C(60)-C(61)	120.8(4)
N(8)-C(60)-C(59)	114.4(4)
C(61)-C(60)-C(59)	124.9(5)
C(60)-C(61)-C(62)	119.5(5)
C(60)-C(61)-H(61)	120.2
C(62)-C(61)-H(61)	120.2
C(63)-C(62)-C(61)	118.6(5)
C(63)-C(62)-C(65)	118.3(5)
C(61)-C(62)-C(65)	123.1(5)

C(64)-C(63)-C(62)	120.0(5)
C(64)-C(63)-H(63)	120.0
C(62)-C(63)-H(63)	120.0
N(8)-C(64)-C(63)	121.7(5)
N(8)-C(64)-H(64)	119.2
C(63)-C(64)-H(64)	119.2
O(16)-C(65)-O(15)	124.3(5)
O(16)-C(65)-C(62)	123.4(5)
O(15)-C(65)-C(62)	112.3(4)
O(15)-C(66)-C(68)	108.8(4)
O(15)-C(66)-C(67)	105.8(4)
C(68)-C(66)-C(67)	113.6(5)
O(15)-C(66)-H(66)	109.5
C(68)-C(66)-H(66)	109.5
C(67)-C(66)-H(66)	109.5
C(66)-C(67)-H(67A)	109.5
C(66)-C(67)-H(67B)	109.5
H(67A)-C(67)-H(67B)	109.5
C(66)-C(67)-H(67C)	109.5
H(67A)-C(67)-H(67C)	109.5
H(67B)-C(67)-H(67C)	109.5
C(66)-C(68)-H(68A)	109.5
C(66)-C(68)-H(68B)	109.5
H(68A)-C(68)-H(68B)	109.5
C(66)-C(68)-H(68C)	109.5
H(68A)-C(68)-H(68C)	109.5
H(68B)-C(68)-H(68C)	109.5
O(14)-C(69)-O(13)	124.2(5)
O(14)-C(69)-C(57)	122.7(5)
O(13)-C(69)-C(57)	113.1(4)
O(13)-C(70)-C(72)	107.4(4)
O(13)-C(70)-C(71)	108.4(4)
C(72)-C(70)-C(71)	112.7(5)
O(13)-C(70)-H(70)	109.5
C(72)-C(70)-H(70)	109.5
C(71)-C(70)-H(70)	109.5

C(70)-C(71)-H(71A)	109.5
C(70)-C(71)-H(71B)	109.5
H(71A)-C(71)-H(71B)	109.5
C(70)-C(71)-H(71C)	109.5
H(71A)-C(71)-H(71C)	109.5
H(71B)-C(71)-H(71C)	109.5
C(70)-C(72)-H(72A)	109.5
C(70)-C(72)-H(72B)	109.5
H(72A)-C(72)-H(72B)	109.5
C(70)-C(72)-H(72C)	109.5
H(72A)-C(72)-H(72C)	109.5
H(72B)-C(72)-H(72C)	109.5
C(3S)-O(1S)-C(2S)	112.3(4)
C(7S)-O(2S)-C(6S)	112.3(5)
C(2S)-C(1S)-H(1AA)	109.5
C(2S)-C(1S)-H(1AB)	109.5
H(1AA)-C(1S)-H(1AB)	109.5
C(2S)-C(1S)-H(1AC)	109.5
H(1AA)-C(1S)-H(1AC)	109.5
H(1AB)-C(1S)-H(1AC)	109.5
O(1S)-C(2S)-C(1S)	108.7(4)
O(1S)-C(2S)-H(2AA)	110.0
C(1S)-C(2S)-H(2AA)	110.0
O(1S)-C(2S)-H(2AB)	110.0
C(1S)-C(2S)-H(2AB)	110.0
H(2AA)-C(2S)-H(2AB)	108.3
O(1S)-C(3S)-C(4S)	110.7(5)
O(1S)-C(3S)-H(3AA)	109.5
C(4S)-C(3S)-H(3AA)	109.5
O(1S)-C(3S)-H(3AB)	109.5
C(4S)-C(3S)-H(3AB)	109.5
H(3AA)-C(3S)-H(3AB)	108.1
C(3S)-C(4S)-H(4AA)	109.5
C(3S)-C(4S)-H(4AB)	109.5
H(4AA)-C(4S)-H(4AB)	109.5
C(3S)-C(4S)-H(4AC)	109.5

H(4AA)-C(4S)-H(4AC)	109.5
H(4AB)-C(4S)-H(4AC)	109.5
C(6S)-C(5S)-H(5AA)	109.5
C(6S)-C(5S)-H(5AB)	109.5
H(5AA)-C(5S)-H(5AB)	109.5
C(6S)-C(5S)-H(5AC)	109.5
H(5AA)-C(5S)-H(5AC)	109.5
H(5AB)-C(5S)-H(5AC)	109.5
O(2S)-C(6S)-C(5S)	109.5(5)
O(2S)-C(6S)-H(6AA)	109.8
C(5S)-C(6S)-H(6AA)	109.8
O(2S)-C(6S)-H(6AB)	109.8
C(5S)-C(6S)-H(6AB)	109.8
H(6AA)-C(6S)-H(6AB)	108.2
O(2S)-C(7S)-C(8S)	109.4(5)
O(2S)-C(7S)-H(7AA)	109.8
C(8S)-C(7S)-H(7AA)	109.8
O(2S)-C(7S)-H(7AB)	109.8
C(8S)-C(7S)-H(7AB)	109.8
H(7AA)-C(7S)-H(7AB)	108.2
C(7S)-C(8S)-H(8AA)	109.5
C(7S)-C(8S)-H(8AB)	109.5
H(8AA)-C(8S)-H(8AB)	109.5
C(7S)-C(8S)-H(8AC)	109.5
H(8AA)-C(8S)-H(8AC)	109.5
H(8AB)-C(8S)-H(8AC)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 9. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for ch1jw241_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt(1)	15(1)	13(1)	22(1)	3(1)	5(1)	5(1)
Pt(2)	19(1)	12(1)	26(1)	0(1)	7(1)	4(1)
Pt(3)	18(1)	13(1)	17(1)	-1(1)	3(1)	4(1)
Pt(4)	17(1)	13(1)	16(1)	2(1)	2(1)	5(1)
Cl(1)	27(1)	17(1)	36(1)	4(1)	16(1)	4(1)
Cl(2)	17(1)	23(1)	42(1)	-2(1)	6(1)	2(1)
Cl(3)	18(1)	23(1)	23(1)	2(1)	1(1)	8(1)
Cl(4)	26(1)	22(1)	19(1)	-1(1)	5(1)	10(1)
Cl(5)	14(1)	26(1)	34(1)	3(1)	2(1)	7(1)
Cl(6)	23(1)	22(1)	28(1)	3(1)	10(1)	10(1)
Cl(7)	17(1)	24(1)	25(1)	-1(1)	2(1)	2(1)
Cl(8)	26(1)	21(1)	22(1)	4(1)	7(1)	5(1)
N(1)	14(3)	10(2)	22(2)	4(2)	4(2)	4(2)
N(2)	12(2)	15(2)	20(2)	-2(2)	2(2)	3(2)
N(3)	23(3)	16(2)	20(2)	-1(2)	10(2)	7(2)
N(4)	13(3)	13(2)	25(2)	2(2)	0(2)	9(2)
N(5)	8(2)	12(2)	24(2)	-3(2)	0(2)	4(2)
N(6)	19(3)	14(2)	17(2)	-3(2)	4(2)	5(2)
N(7)	12(2)	10(2)	16(2)	2(2)	3(2)	0(2)
N(8)	24(3)	10(2)	14(2)	1(2)	4(2)	6(2)
O(1)	17(2)	34(2)	15(2)	-7(2)	-1(2)	2(2)
O(2)	30(3)	39(2)	18(2)	-6(2)	-1(2)	12(2)
O(3)	17(2)	27(2)	14(2)	-2(2)	1(2)	6(2)
O(4)	20(2)	33(2)	18(2)	-7(2)	-6(2)	7(2)
O(5)	14(2)	38(2)	21(2)	5(2)	1(2)	7(2)
O(6)	33(3)	40(3)	15(2)	5(2)	-3(2)	11(2)
O(7)	11(2)	27(2)	13(2)	2(2)	2(1)	0(2)
O(8)	20(2)	31(2)	19(2)	0(2)	-6(2)	4(2)
O(9)	12(2)	30(2)	21(2)	6(2)	1(2)	5(2)
O(10)	23(3)	69(3)	17(2)	9(2)	-9(2)	-8(2)
O(11)	17(2)	31(2)	19(2)	5(2)	0(2)	5(2)

O(12)	25(2)	38(2)	18(2)	3(2)	-5(2)	9(2)
O(13)	17(2)	34(2)	16(2)	-7(2)	0(2)	8(2)
O(14)	20(2)	44(3)	20(2)	-3(2)	-4(2)	7(2)
O(15)	15(2)	33(2)	16(2)	-3(2)	-4(2)	3(2)
O(16)	24(2)	38(2)	18(2)	-7(2)	-3(2)	-1(2)
C(1)	29(4)	23(3)	16(3)	-3(2)	3(2)	9(3)
C(2)	25(3)	15(3)	19(3)	3(2)	4(2)	1(2)
C(3)	20(3)	14(3)	17(3)	4(2)	6(2)	3(2)
C(4)	14(3)	11(3)	20(3)	3(2)	5(2)	0(2)
C(5)	11(3)	10(3)	22(3)	2(2)	2(2)	0(2)
C(6)	15(3)	11(3)	20(3)	5(2)	4(2)	3(2)
C(7)	15(3)	9(3)	21(3)	1(2)	0(2)	1(2)
C(8)	15(3)	7(3)	23(3)	5(2)	2(2)	-2(2)
C(9)	17(3)	16(3)	23(3)	1(2)	-3(2)	4(2)
C(10)	24(3)	13(3)	25(3)	3(2)	-3(2)	8(2)
C(11)	18(3)	19(3)	17(3)	1(2)	3(2)	4(2)
C(12)	12(3)	37(4)	19(3)	-3(2)	-5(2)	2(3)
C(13)	27(4)	39(4)	50(4)	3(3)	-12(3)	-5(3)
C(14)	29(4)	53(5)	46(4)	-16(3)	2(3)	13(3)
C(15)	22(3)	12(3)	15(3)	4(2)	3(2)	3(2)
C(16)	25(3)	26(3)	17(3)	-1(2)	11(2)	11(3)
C(17)	23(4)	31(4)	40(4)	1(3)	10(3)	5(3)
C(18)	35(4)	32(4)	26(3)	3(3)	6(3)	15(3)
C(19)	22(3)	17(3)	23(3)	6(2)	8(2)	5(2)
C(20)	32(4)	25(3)	13(3)	2(2)	5(2)	9(3)
C(21)	20(3)	18(3)	20(3)	0(2)	4(2)	8(2)
C(22)	16(3)	14(3)	22(3)	1(2)	7(2)	8(2)
C(23)	18(3)	14(3)	19(3)	-1(2)	2(2)	9(2)
C(24)	18(3)	14(3)	22(3)	-4(2)	3(2)	10(2)
C(25)	16(3)	8(3)	21(3)	-3(2)	-1(2)	10(2)
C(26)	16(3)	17(3)	19(3)	0(2)	2(2)	5(2)
C(27)	25(3)	16(3)	23(3)	-6(2)	-8(2)	8(2)
C(28)	16(3)	17(3)	26(3)	-3(2)	-1(2)	4(2)
C(29)	17(3)	15(3)	18(3)	0(2)	0(2)	6(2)
C(30)	18(3)	31(3)	16(3)	2(2)	5(2)	0(3)
C(31)	40(4)	21(3)	33(3)	0(3)	7(3)	-1(3)

C(32)	18(4)	52(4)	32(3)	8(3)	5(3)	4(3)
C(33)	26(3)	17(3)	20(3)	1(2)	4(2)	10(3)
C(34)	15(3)	45(4)	16(3)	4(3)	1(2)	1(3)
C(35)	35(4)	61(5)	47(4)	25(4)	11(3)	3(4)
C(36)	32(4)	75(5)	45(4)	-15(4)	-7(3)	32(4)
C(37)	19(3)	21(3)	20(3)	-6(2)	-4(2)	7(2)
C(38)	18(3)	20(3)	16(3)	-2(2)	-3(2)	8(2)
C(39)	16(3)	15(3)	19(3)	0(2)	3(2)	5(2)
C(40)	21(3)	17(3)	20(3)	1(2)	1(2)	9(2)
C(41)	24(3)	12(3)	14(3)	-3(2)	0(2)	9(2)
C(42)	15(3)	14(3)	20(3)	0(2)	0(2)	8(2)
C(43)	16(3)	18(3)	14(3)	-3(2)	-1(2)	9(2)
C(44)	19(3)	20(3)	19(3)	0(2)	-2(2)	12(2)
C(45)	30(4)	26(3)	18(3)	1(2)	0(2)	13(3)
C(46)	21(3)	17(3)	20(3)	2(2)	7(2)	5(2)
C(47)	30(4)	24(3)	12(3)	-3(2)	2(2)	15(3)
C(48)	16(3)	41(4)	16(3)	-5(2)	-1(2)	2(3)
C(49)	19(4)	58(5)	46(4)	-7(3)	-3(3)	15(3)
C(50)	26(4)	54(5)	42(4)	18(3)	5(3)	8(3)
C(51)	19(3)	17(3)	19(3)	0(2)	2(2)	5(2)
C(52)	19(3)	41(4)	25(3)	15(3)	1(2)	4(3)
C(53)	46(5)	79(6)	38(4)	24(4)	-14(3)	-27(4)
C(54)	75(6)	86(6)	51(5)	37(4)	48(4)	63(5)
C(55)	17(3)	23(3)	20(3)	2(2)	-4(2)	8(2)
C(56)	24(3)	16(3)	15(3)	0(2)	-6(2)	6(2)
C(57)	21(3)	16(3)	14(3)	5(2)	1(2)	5(2)
C(58)	18(3)	7(3)	21(3)	1(2)	2(2)	1(2)
C(59)	21(3)	11(3)	16(3)	-2(2)	-4(2)	6(2)
C(60)	16(3)	16(3)	16(3)	1(2)	0(2)	-2(2)
C(61)	28(3)	7(3)	17(3)	0(2)	7(2)	0(2)
C(62)	12(3)	19(3)	21(3)	4(2)	-5(2)	0(2)
C(63)	23(3)	20(3)	13(3)	2(2)	-1(2)	0(2)
C(64)	30(4)	23(3)	13(3)	-2(2)	-2(2)	7(3)
C(65)	23(3)	22(3)	17(3)	3(2)	9(2)	0(3)
C(66)	13(3)	33(3)	23(3)	1(2)	-3(2)	2(3)
C(67)	19(3)	49(4)	30(3)	-6(3)	0(3)	11(3)

C(68)	21(4)	34(4)	51(4)	3(3)	-7(3)	1(3)
C(69)	16(3)	19(3)	22(3)	3(2)	-3(2)	7(2)
C(70)	20(3)	43(4)	16(3)	-7(3)	4(2)	11(3)
C(71)	40(4)	38(4)	56(4)	13(3)	28(3)	9(3)
C(72)	29(4)	87(6)	27(4)	-6(3)	5(3)	27(4)
O(1S)	39(3)	27(2)	28(2)	1(2)	-1(2)	10(2)
O(2S)	45(3)	29(2)	31(2)	-1(2)	-3(2)	13(2)
C(1S)	34(4)	34(4)	35(4)	0(3)	-5(3)	8(3)
C(2S)	36(4)	28(4)	33(4)	4(3)	-4(3)	5(3)
C(3S)	79(6)	22(3)	16(3)	7(2)	3(3)	12(3)
C(4S)	105(7)	92(6)	21(4)	6(4)	11(4)	78(6)
C(5S)	39(4)	31(4)	47(4)	-4(3)	-17(3)	10(3)
C(6S)	57(5)	38(4)	36(4)	-13(3)	-14(3)	26(4)
C(7S)	92(7)	45(4)	22(3)	4(3)	10(4)	41(4)
C(8S)	84(6)	42(4)	19(3)	2(3)	9(3)	-11(4)

Table 10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for ch1jw241_0m.

	x	y	z	U(eq)
H(1)	254	1910	6208	26
H(2)	1871	2101	6566	24
H(4)	2648	1174	5070	19
H(7)	2136	786	4197	18
H(9)	-256	324	3121	23
H(10)	-1213	738	3822	24
H(12)	5141	1451	6328	28
H(13A)	5755	2629	5376	62
H(13B)	6468	2564	5908	62
H(13C)	5525	3021	5974	62
H(14A)	4905	128	5678	63
H(14B)	6073	680	5753	63
H(14C)	5445	862	5207	63
H(16)	3073	348	2459	26
H(17A)	4303	1479	3000	47
H(17B)	4795	723	2693	47
H(17C)	4557	612	3346	47
H(18A)	3372	-1059	3251	44
H(18B)	3674	-1058	2607	44
H(18C)	2513	-1244	2768	44
H(19)	306	3214	11190	25
H(20)	1937	3817	11541	28
H(22)	2690	5146	10060	20
H(25)	2156	5281	9182	16
H(27)	-267	4564	8111	25
H(28)	-1192	3717	8830	24
H(30)	3023	6195	7433	27
H(31A)	2394	7471	7747	49
H(31B)	3532	7888	7553	49
H(31C)	3291	7765	8206	49

H(32A)	4527	6733	8299	52
H(32B)	4741	6746	7642	52
H(32C)	4313	5744	7953	52
H(34)	5157	6114	11327	32
H(35A)	5373	6829	10202	73
H(35B)	6091	7310	10719	73
H(35C)	4925	7320	10705	73
H(36A)	5624	4760	10979	72
H(36B)	6532	5700	10904	72
H(36C)	5823	5253	10377	72
H(37)	11215	1412	1044	24
H(38)	10314	652	1788	20
H(40)	7864	-183	756	22
H(43)	7280	-124	-121	19
H(45)	7954	1053	-1645	28
H(46)	9619	1684	-1328	23
H(48)	4752	-1173	-1338	30
H(49A)	4205	-262	-368	60
H(49B)	3416	-753	-854	60
H(49C)	4302	179	-986	60
H(50A)	5041	-2360	-712	62
H(50B)	3869	-2371	-739	62
H(50C)	4566	-1880	-216	62
H(52)	7225	-1285	2501	34
H(53A)	5541	-1688	1726	93
H(53B)	5665	-2306	2269	93
H(53C)	6363	-2306	1740	93
H(54A)	6923	213	2607	93
H(54B)	5913	-584	2751	93
H(54C)	6006	-50	2159	93
H(55)	11078	4191	6041	24
H(56)	10198	4530	6799	22
H(58)	7700	4140	5788	19
H(61)	7117	3848	4906	21
H(63)	7783	3010	3374	23
H(64)	9413	3129	3689	26

H(66)	4564	3622	3647	29
H(67A)	4382	4441	4722	48
H(67B)	3699	4517	4179	48
H(67C)	4875	5057	4194	48
H(68A)	4144	2130	4097	55
H(68B)	3239	2640	4160	55
H(68C)	4007	2640	4676	55
H(70)	7051	4865	7553	31
H(71A)	6295	2827	7407	67
H(71B)	6271	3393	7982	67
H(71C)	7328	3327	7735	67
H(72A)	5767	5022	6930	68
H(72B)	5260	4388	7448	68
H(72C)	5373	3879	6864	68
H(1AA)	2626	1335	1680	52
H(1AB)	3749	1934	1846	52
H(1AC)	3072	2378	1419	52
H(2AA)	2762	2110	2594	40
H(2AB)	3023	3124	2277	40
H(3AA)	1496	3422	2609	47
H(3AB)	1296	2412	2928	47
H(4AA)	-84	2766	2082	95
H(4AB)	-230	2946	2734	95
H(4AC)	-296	1881	2509	95
H(5AA)	2869	4053	6433	59
H(5AB)	3657	4693	6874	59
H(5AC)	2599	4940	6744	59
H(6AA)	2785	3212	7286	49
H(6AB)	2571	4111	7616	49
H(7AA)	1085	3060	7929	58
H(7AB)	1178	2166	7548	58
H(8AA)	-468	3066	7491	80
H(8AB)	-542	1994	7702	80
H(8AC)	-358	2254	7055	80