Supplementary Material (ESI) for Chemical Communications

Exciplex quenching of a luminescent cyclometallated Platinum complex by extremely poor Lewis bases

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Supplementary Information

Experimental details:

Synthesis:

Synthesis was performed according to a method previously reported.[1, 2] All materials were purchased from Sigma-Aldrich and used without further purification. All synthetic procedures were carried out in inert gas atmosphere. The 2-phenyl-5-nitropyridine ligand was prepared by Suzuki coupling reaction with commercially available phenylboronic acid and 2-bromo-5-nitropyridine. The mononuclear cyclometalated Pt(II) chloro precursor complex[2] was prepared by heating K_2PtCl_4 salt with 2-2.5 equiv of cyclometalating ligand in a 3:1 mixture of 2-ethoxyethanol (Aldrich) and water to 80 °C for 16 h. The chloro complex was isolated in water and subsequently reacted with 3 equiv of the chelating diketone derivative and 10 equiv of Na_2CO_3 in 2-ethoxyethanol at 100 °C for 16 h. The solvent was removed under reduced pressure, and the compound was purified by flash chromatography using dichloromethane. The product was further purified by sublimation (yield = 23%). Crystals were grown by slow diffusion of hexane into a concentrated solution of NPt into dichloroethane.

^{1}H NMR (400 MHz, CDCl3), ppm: 9.74 (s, 1H), 8.39 (d, 1H, J = 8.94 Hz), 7.50 (m, 2H), 7.32 (d, 1H, J = 7.21 Hz), 7.18 (d, 1H, J = 8.53 Hz), 7.03 (m, 2H), 5.42 (s, 1H), 1.99 (s, 3H), 1.96 (s, 3H). ^{13}C NMR (400MHz, $CDCl_3$), ppm: 186.36; 184.19; 173.62; 143.73; 142.66; 141.96;

141.39; 132.95; 131.62; 130.92; 125.24; 123.91; 117.47; 102.67; 28.26; 26.96. MS: m/z = 493 [M^+]; 394 [M-acac$^+$] Anal. for $C_{16}H_{14}N_2O_4Pt$: found C 39.47, H 2.85, N 5.35, calcd C 38.95, H 2.86, N 5.68.

Quenching measurements

Luminescence quenching studies were conducted on dilute solutions (1×10^{-5} M) in cyclohexane that were degassed for ten minutes with N_2. The quencher concentration was determined volumetrically. Quantum yield and lifetimes were measured after each addition of quencher. All solvents were purchased from Sigma-Aldrich.

Instrumentation

UV-vis spectra were recorded using an Agilent 8453 UV-Vis spectrometer. Photoluminescent spectra were measured using a Photon Technology International QuantaMaster C-60SE spectrofluorometer. Emission lifetime measurements were performed using time-resolved single photon counting on an IBH photon timing instrument connected to an IBH model TBX-04 PMT detector. Quantum efficiency measurements were carried out using a calibrated integrating sphere equipped with a xenon lamp and Hamamatsu Model C10027 photonic multi-channel analyzer. The quantum efficiency data was processed using the U6039-05 software package provided by Hamamatsu. The error in the quantum efficiency measurements is $\pm$ 5%. Cyclic voltammetry and differential pulse voltammetry were performed using an EG&G potentiostat/galvanostat model 28. Anhydrous dichloromethane was used as the solvent under a nitrogen atmosphere, and 0.1 M tetra(*n*-butyl)ammonium hexafluorophosphate was used as the supporting electrolyte. A Pt wire acted as the counter electrode, Ag wire was used as the pseudo reference electrode, and the working electrode was glassy carbon. The redox

potentials are based on values measured from differential pulse voltammetry and reported relative to an internal ferrocenium/ferrocene (Cp_2Fe^+/Cp_2Fe) reference.

Computational Details

The HOMO-LUMO energies and electronic potential surfaces (B3LYP method with a LACVP** basis set) were determined using the Titan (version 1.0.7) software package (Wavefunction, Inc.). Electronic structure calculations of the singlet ground states (SGS) were performed using the density functional theory (DFT) method using the Gaussian-03 software package.[3] For all calculations the B3LYP functional consisting of Becke's three-parameter equation[4] and Lee, Yang, and Parr's non-local hybrid functional[5] was used with the LANL2DZ basis set, which uses the Dunning-Hay split valence double-ζ for C,H,N atoms (D95) and Hay-Wadt double-ζ with Los Alamos National Laboratories relativistic effective core potential (ECP) for heavy atoms.[6] The lowest SGS structure was obtained by optimizing the geometry in the gas phase without any dihedral constraints. Time-dependent (TD) DFT calculations were performed on the gas phase SGS geometries. A total of ten singlet and ten triplet states were calculated for each structure. Singlet and triplet vertical transition energies were calculated in the gas phase and in solvent shells. Solvent calculations were performed in hexanes using the conductor-like polarizable continuum model (CPCM)[7] in conjunction with TDDFT routine.

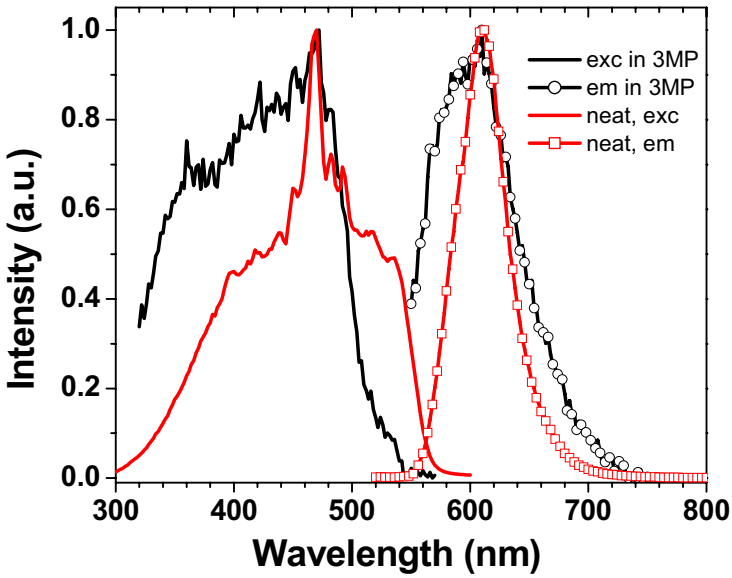
X-ray Crystallography

Diffraction data for *NPt* was collected at T = -163º C (110K) on a Bruker SMART APEX CCD diffractometer with graphite-monochromated Mo Kα radiation (λ = 0.71073 Å). The cell parameters for the Pt complex were obtained from the least-squares refinement of the spots (from 60 collected frames) using the SMART program. A hemisphere of the crystal data was collected up to a resolution of 0.75 Å, and the intensity data was processed using the Saint Plus program.

All calculations for structure determination were carried out using the SHELXTL package (version 5.1). Initial atomic positions were located by Patterson methods using XS, and the structure was refined by least-squares methods using SHELX with 7063 independent reflections and within the range of Φ = 1.61–27.51º (completeness 93.8%). Absorption corrections were applied by using SADABS. Calculated hydrogen positions were input and refined in a riding manner along with the attached carbons.

Figure S1: Excitation and emission spectra at 77K in 3-methylpentane (3MP) and for the neat solid (a), and at 77K in 2-methyltetrahydrofuran and methanol-ethanol (b).

(a)



(b)

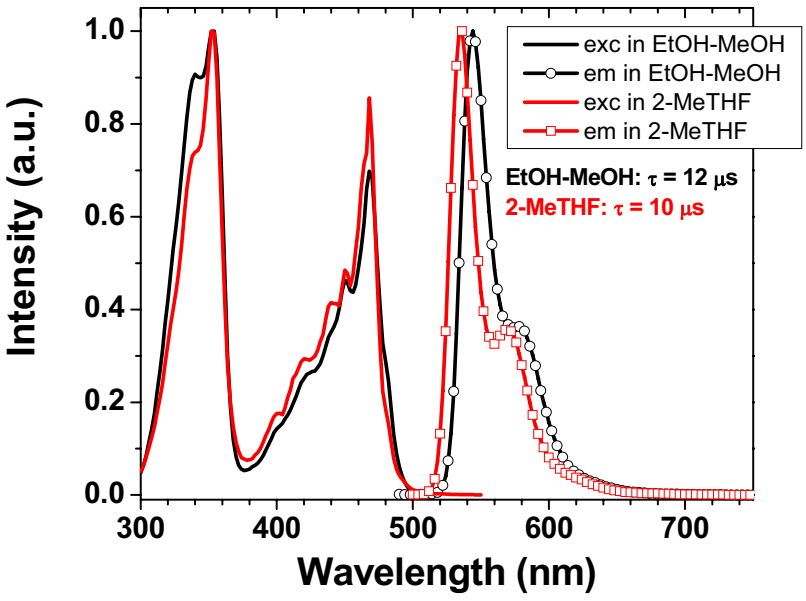
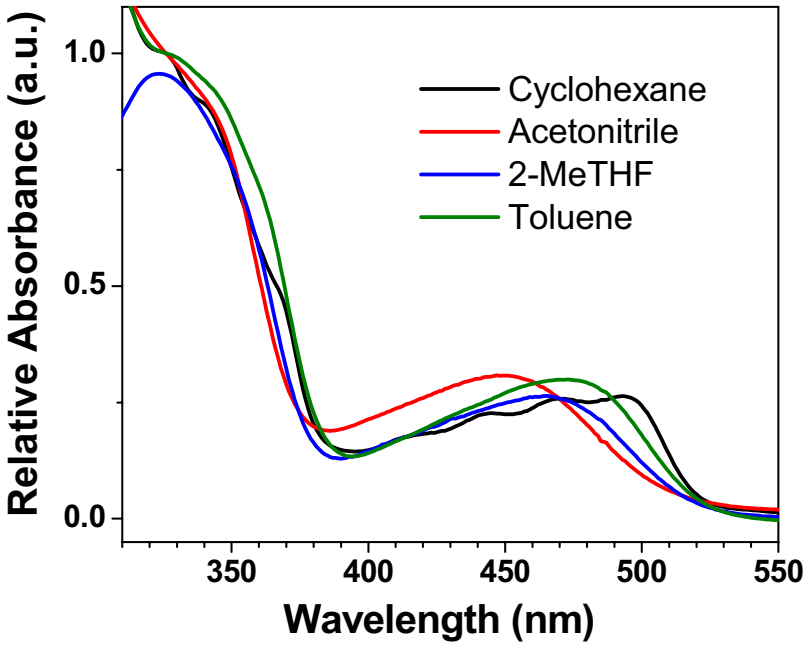


Figure S2: Absorption spectra showing the negative solvatochromic effect for *NPt* (a) and ppyPt(acac) (b).

(a)



(b)

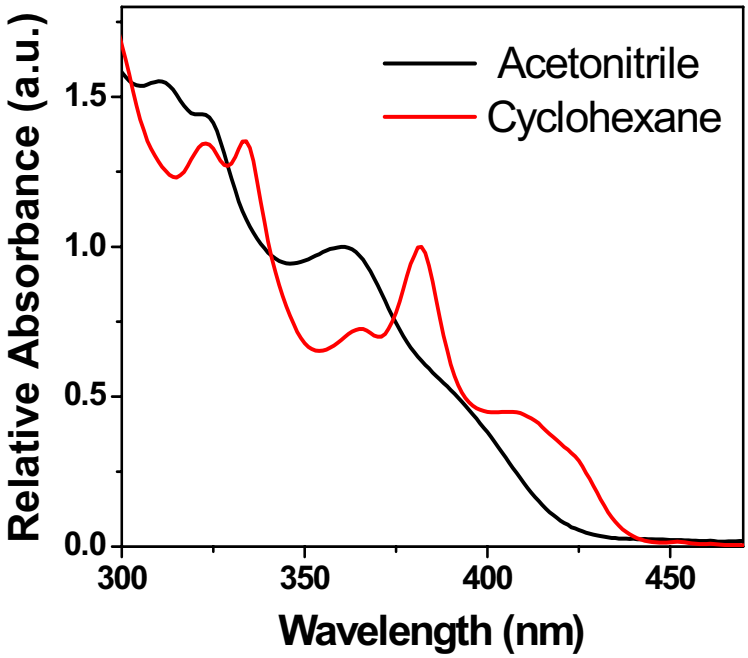


Figure S3: Cyclic voltammogram of *NPt* recorded in dichloromethane with 0.1 M TBAPF.

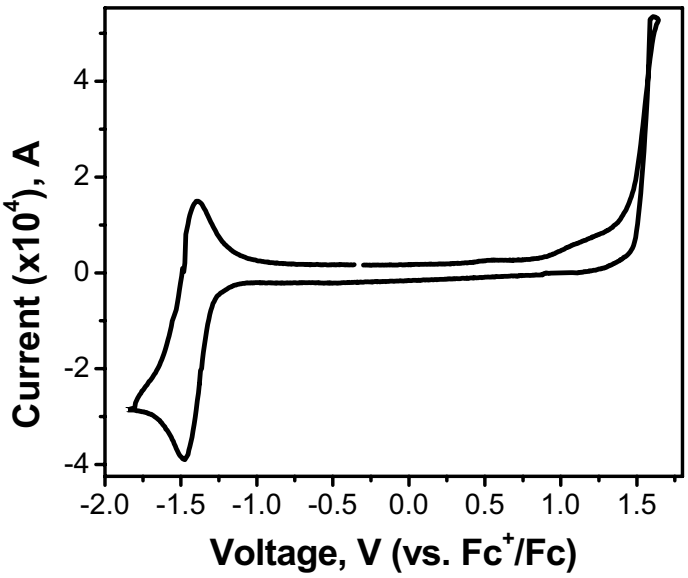


Figure S4: Second-order fit to Stern-Volmer data using toluene as quencher.

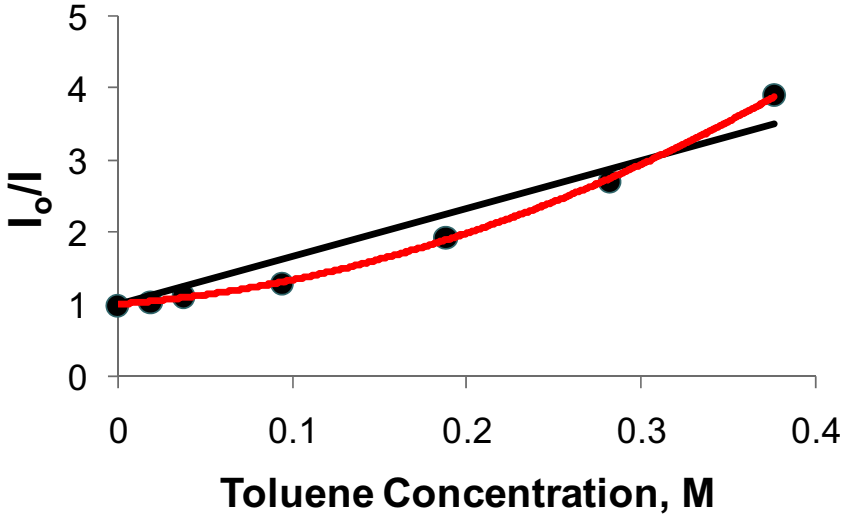


Figure S5: ORTEP diagram for one unique *NPt* molecule from the asymmetric unit cell. Thermal ellipsoids are for 50% probability and hydrogen atoms are not included.

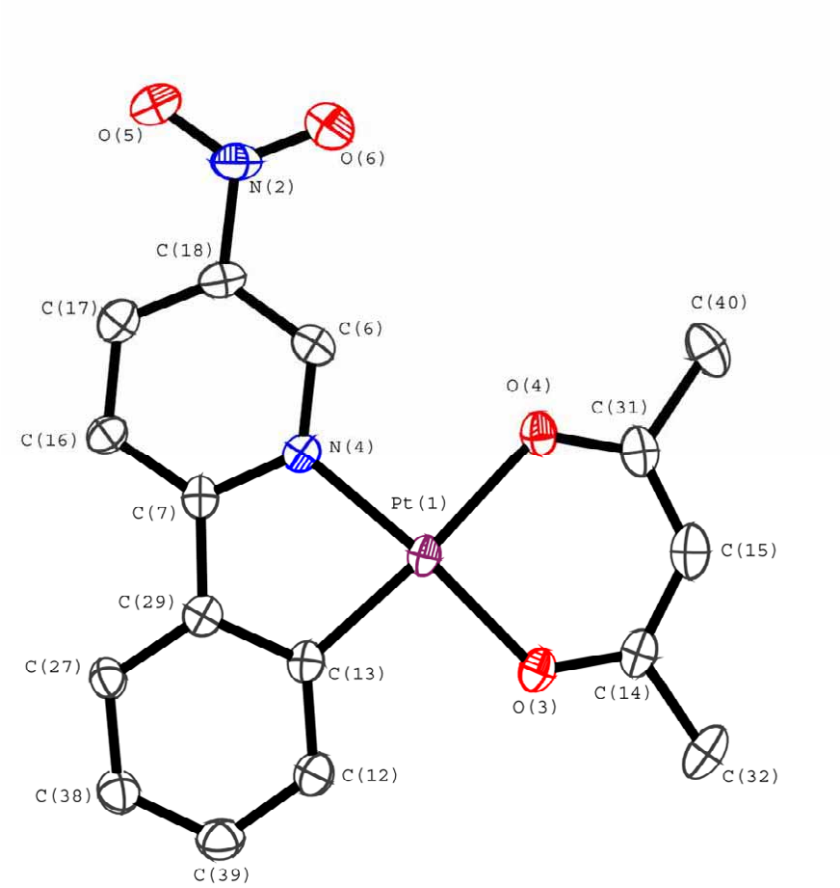
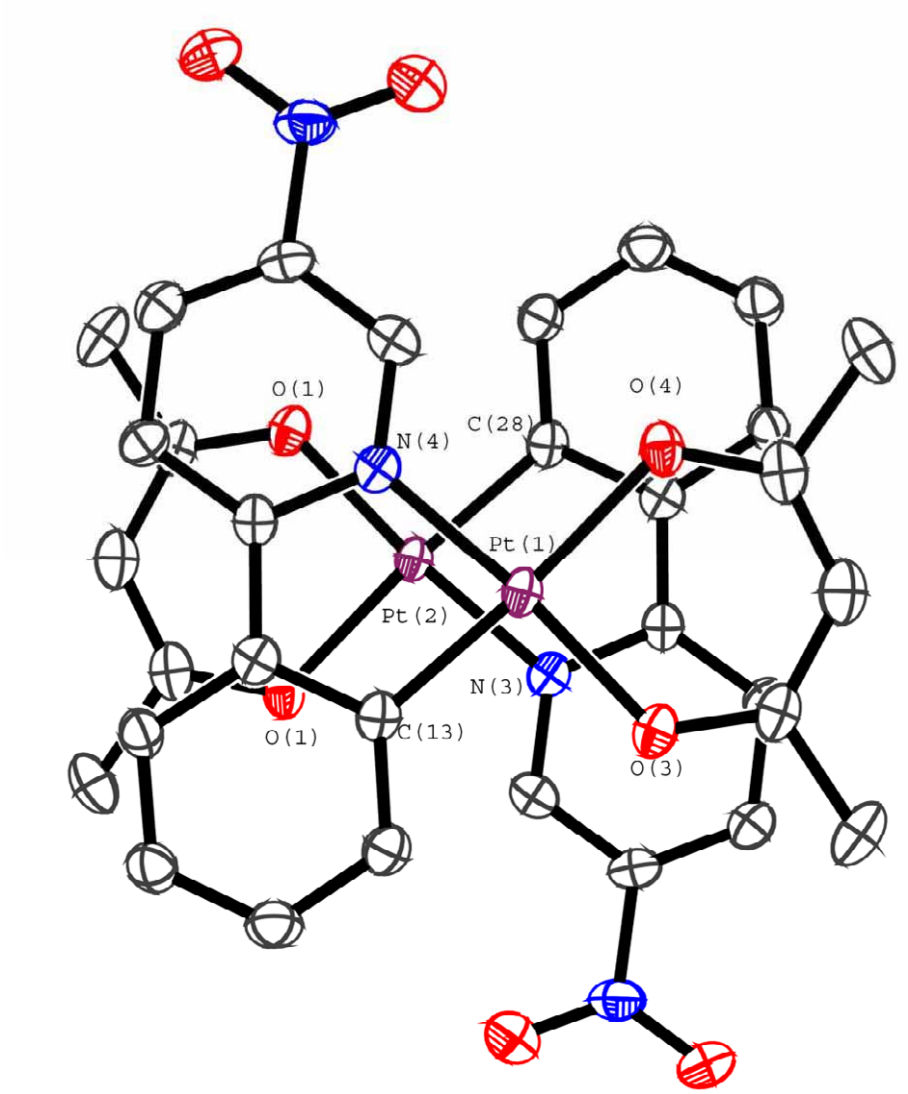
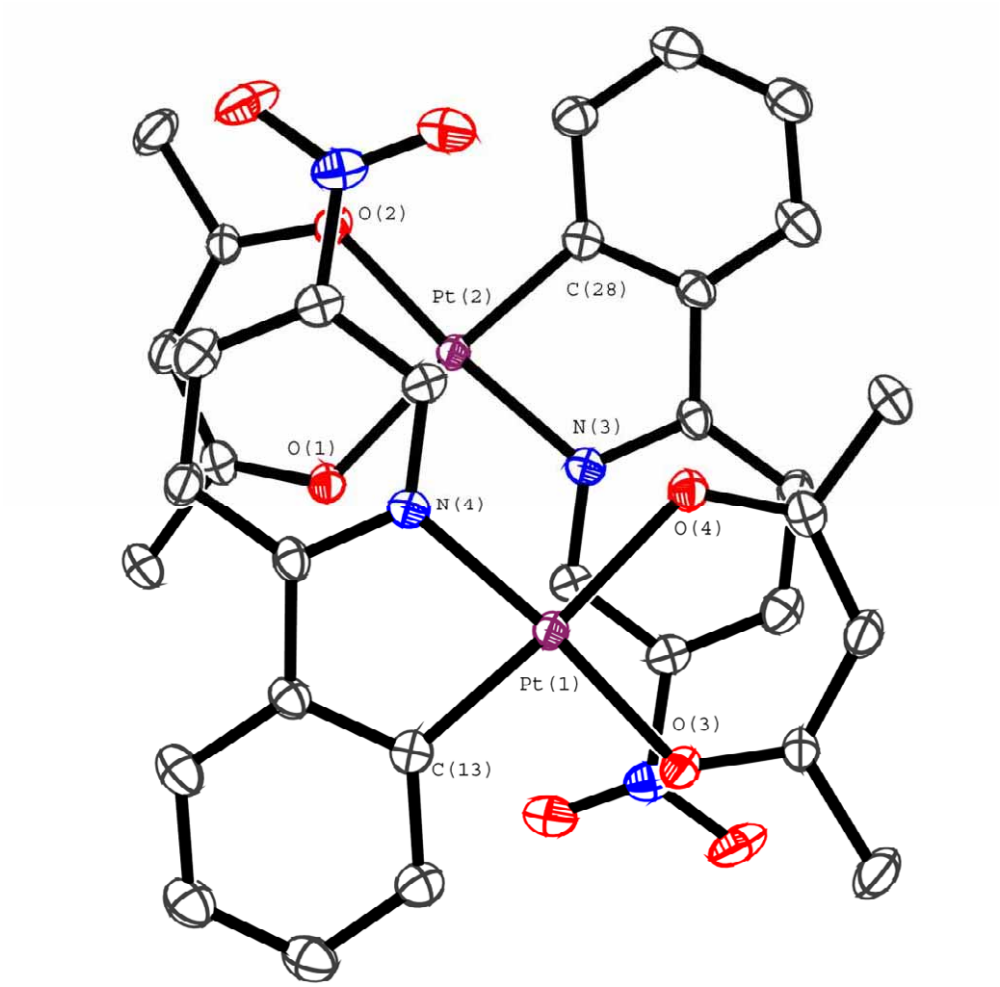


Figure S6: ORTEP diagram showing top view of *NPt* dimers with short (3.465 Å) (a), and long (4.476 Å) (b) Pt-Pt separations. Thermal ellipsoids are for 50% probability and hydrogen atoms are not included.

(a)



(b)



X-ray data

Table 1. Crystal data and structure refinement for C16H14ClN2O4Pt.

Identification code	ptn1m	
Empirical formula	C16.50 H15 Cl0.50 N2 O4 Pt	
Formula weight	518.12	
Temperature	110(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 11.7451(7) Å	α= 88.8210(10)°.
	b = 12.1959(7) Å	β= 86.7640(10)°.
	c = 12.6839(7) Å	γ = 64.3710(10)°.
Volume	1635.49(16) $Å^3$	
Z	4	
Density (calculated)	2.104 Mg/m^3	
Absorption coefficient	8.684 mm^{-1}	
F(000)	986	
Crystal size	0.30 x 0.25 x 0.09 mm^3	
Theta range for data collection	1.61 to 27.51°.	
Index ranges	-15<=h<=14, -15<=k<=8, -16<=l<=15	
Reflections collected	10116	
Independent reflections	7063 [R(int) = 0.0180]	
Completeness to theta = 27.51°	93.8 %	
Absorption correction	Semi-empirical	
Max. and min. transmission	0.5087 and 0.1804	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7063 / 0 / 437	
Goodness-of-fit on F^2	1.033	
Final R indices [I>2sigma(I)]	R1 = 0.0269, wR2 = 0.0679	
R indices (all data)	R1 = 0.0304, wR2 = 0.0698	
Largest diff. peak and hole	4.386 and -1.038 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for C16H14ClN2O4Pt. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pt(1)	1022(1)	855(1)	864(1)	16(1)
Pt(2)	10119(1)	3802(1)	5816(1)	20(1)
O(4)	-360(3)	2240(3)	28(2)	21(1)
O(3)	2350(3)	1386(3)	370(2)	22(1)
O(1)	11704(3)	2346(3)	5399(2)	26(1)
O(2)	9004(3)	3150(3)	5055(2)	25(1)
N(4)	-174(3)	212(3)	1457(3)	18(1)
N(3)	8638(3)	5303(3)	6319(3)	20(1)
C(6)	-1405(4)	677(4)	1237(3)	18(1)
C(7)	329(4)	-765(4)	2106(3)	19(1)
C(9)	8899(4)	6054(4)	6946(3)	20(1)
O(5)	-3881(3)	1600(3)	872(3)	38(1)
N(2)	-3489(4)	688(4)	1414(3)	27(1)
C(13)	2204(4)	-474(4)	1712(3)	19(1)
C(22)	7449(4)	5598(4)	6061(3)	23(1)
C(19)	10725(5)	6259(4)	7705(4)	25(1)
C(15)	967(4)	3189(4)	-531(4)	24(1)
C(16)	-433(4)	-1296(4)	2557(3)	22(1)
C(18)	-2166(4)	167(4)	1688(3)	20(1)
C(17)	-1688(4)	-825(4)	2340(4)	25(1)
C(14)	2127(4)	2366(4)	-152(3)	20(1)
C(20)	10239(4)	5620(4)	7109(3)	23(1)
C(21)	7928(4)	7140(4)	7343(3)	24(1)
C(12)	3487(4)	-785(4)	1830(3)	24(1)
O(6)	-4117(3)	160(3)	1746(3)	35(1)
N(1)	5189(4)	6975(4)	6144(3)	34(1)
O(7)	5034(4)	6262(4)	5575(4)	53(1)
C(25)	6682(5)	7446(5)	7095(4)	28(1)
C(26)	12034(5)	5784(5)	7787(4)	30(1)
C(27)	2380(5)	-2128(4)	2922(3)	26(1)
C(28)	11028(4)	4523(4)	6607(3)	21(1)

C(29)	1670(4)	-1168(4)	2271(3)	19(1)
C(30)	9460(5)	2131(4)	4577(3)	27(1)
C(31)	-167(4)	3086(4)	-439(3)	23(1)
C(32)	3281(5)	2598(5)	-334(4)	32(1)
C(33)	11750(5)	1439(4)	4874(4)	27(1)
C(34)	10727(5)	1319(5)	4468(4)	32(1)
C(35)	12325(4)	4074(4)	6698(4)	26(1)
C(36)	6478(4)	6666(4)	6450(4)	26(1)
C(37)	12819(5)	4715(5)	7279(4)	32(1)
C(38)	3640(4)	-2413(4)	3034(4)	28(1)
C(39)	4189(4)	-1743(5)	2488(4)	29(1)
O(8)	4346(3)	7929(4)	6474(3)	44(1)
C(40)	-1302(5)	4039(5)	-937(4)	33(1)
C(41)	13049(5)	418(5)	4726(4)	37(1)
C(42)	8476(6)	1822(5)	4113(4)	36(1)
Cl(1)	5377(2)	5405(2)	8401(1)	47(1)
C(43)	5135(9)	4586(8)	9622(10)	108(4)

Table 3. Bond lengths [Å] and angles [°] for C16H14ClN2O4Pt.

Pt(1)-C(13)	1.965(4)
Pt(1)-N(4)	1.990(3)
Pt(1)-O(3)	1.998(3)
Pt(1)-O(4)	2.089(3)
Pt(2)-C(28)	1.971(5)
Pt(2)-N(3)	1.988(4)
Pt(2)-O(1)	1.992(3)
Pt(2)-O(2)	2.087(3)
O(4)-C(31)	1.276(5)
O(3)-C(14)	1.285(5)
O(1)-C(33)	1.283(6)
O(2)-C(30)	1.272(6)
N(4)-C(6)	1.349(5)
N(4)-C(7)	1.361(5)
N(3)-C(22)	1.341(6)
N(3)-C(9)	1.366(6)
C(6)-C(18)	1.385(6)
C(6)-H(6)	0.9500
C(7)-C(16)	1.406(6)
C(7)-C(29)	1.459(6)
C(9)-C(21)	1.401(6)
C(9)-C(20)	1.453(6)
O(5)-N(2)	1.218(5)
N(2)-O(6)	1.225(5)
N(2)-C(18)	1.462(6)
C(13)-C(12)	1.401(6)
C(13)-C(29)	1.413(6)
C(22)-C(36)	1.385(7)
C(22)-H(22)	0.9500
C(19)-C(26)	1.398(7)
C(19)-C(20)	1.401(6)
C(19)-H(19)	0.9500
C(15)-C(31)	1.390(6)
C(15)-C(14)	1.402(6)

C(15)-H(15)	0.9500
C(16)-C(17)	1.373(7)
C(16)-H(16)	0.9500
C(18)-C(17)	1.373(6)
C(17)-H(17)	0.9500
C(14)-C(32)	1.505(6)
C(20)-C(28)	1.396(6)
C(21)-C(25)	1.398(7)
C(21)-H(21)	0.9500
C(12)-C(39)	1.395(6)
C(12)-H(12)	0.9500
N(1)-O(8)	1.219(6)
N(1)-O(7)	1.220(6)
N(1)-C(36)	1.467(6)
C(25)-C(36)	1.372(7)
C(25)-H(25)	0.9500
C(26)-C(37)	1.376(7)
C(26)-H(26)	0.9500
C(27)-C(38)	1.381(7)
C(27)-C(29)	1.393(6)
C(27)-H(27)	0.9500
C(28)-C(35)	1.389(6)
C(30)-C(34)	1.387(7)
C(30)-C(42)	1.512(7)
C(31)-C(40)	1.500(6)
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-C(34)	1.398(7)
C(33)-C(41)	1.498(7)
C(34)-H(34)	0.9500
C(35)-C(37)	1.398(7)
C(35)-H(35)	0.9500
C(37)-H(37)	0.9500
C(38)-C(39)	1.394(7)
C(38)-H(38)	0.9500

C(39)-H(39)	0.9500
C(40)-H(40A)	0.9800
C(40)-H(40B)	0.9800
C(40)-H(40C)	0.9800
C(41)-H(41A)	0.9800
C(41)-H(41B)	0.9800
C(41)-H(41C)	0.9800
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800
Cl(1)-C(43)	1.899(12)
C(43)-C(43)#1	1.331(18)
C(43)-H(43A)	0.9900
C(43)-H(43B)	0.9900

C(13)-Pt(1)-N(4)	81.57(16)
C(13)-Pt(1)-O(3)	92.65(15)
N(4)-Pt(1)-O(3)	174.16(13)
C(13)-Pt(1)-O(4)	175.10(14)
N(4)-Pt(1)-O(4)	93.60(13)
O(3)-Pt(1)-O(4)	92.16(12)
C(28)-Pt(2)-N(3)	81.73(17)
C(28)-Pt(2)-O(1)	92.80(16)
N(3)-Pt(2)-O(1)	174.49(14)
C(28)-Pt(2)-O(2)	174.69(15)
N(3)-Pt(2)-O(2)	93.18(14)
O(1)-Pt(2)-O(2)	92.28(13)
C(31)-O(4)-Pt(1)	122.8(3)
C(14)-O(3)-Pt(1)	124.1(3)
C(33)-O(1)-Pt(2)	124.6(3)
C(30)-O(2)-Pt(2)	122.9(3)
C(6)-N(4)-C(7)	120.4(4)
C(6)-N(4)-Pt(1)	123.9(3)
C(7)-N(4)-Pt(1)	115.7(3)
C(22)-N(3)-C(9)	120.6(4)
C(22)-N(3)-Pt(2)	123.6(3)

C(9)-N(3)-Pt(2)	115.7(3)
N(4)-C(6)-C(18)	119.8(4)
N(4)-C(6)-H(6)	120.1
C(18)-C(6)-H(6)	120.1
N(4)-C(7)-C(16)	120.2(4)
N(4)-C(7)-C(29)	114.3(4)
C(16)-C(7)-C(29)	125.5(4)
N(3)-C(9)-C(21)	120.6(4)
N(3)-C(9)-C(20)	113.3(4)
C(21)-C(9)-C(20)	126.0(4)
O(5)-N(2)-O(6)	125.0(4)
O(5)-N(2)-C(18)	118.1(4)
O(6)-N(2)-C(18)	116.9(4)
C(12)-C(13)-C(29)	117.6(4)
C(12)-C(13)-Pt(1)	127.5(3)
C(29)-C(13)-Pt(1)	114.9(3)
N(3)-C(22)-C(36)	119.4(4)
N(3)-C(22)-H(22)	120.3
C(36)-C(22)-H(22)	120.3
C(26)-C(19)-C(20)	118.7(4)
C(26)-C(19)-H(19)	120.7
C(20)-C(19)-H(19)	120.7
C(31)-C(15)-C(14)	126.5(4)
C(31)-C(15)-H(15)	116.7
C(14)-C(15)-H(15)	116.7
C(17)-C(16)-C(7)	119.7(4)
C(17)-C(16)-H(16)	120.1
C(7)-C(16)-H(16)	120.1
C(17)-C(18)-C(6)	121.4(4)
C(17)-C(18)-N(2)	120.7(4)
C(6)-C(18)-N(2)	117.9(4)
C(16)-C(17)-C(18)	118.5(4)
C(16)-C(17)-H(17)	120.8
C(18)-C(17)-H(17)	120.8
O(3)-C(14)-C(15)	127.2(4)
O(3)-C(14)-C(32)	112.8(4)

C(15)-C(14)-C(32)	120.0(4)
C(28)-C(20)-C(19)	121.6(4)
C(28)-C(20)-C(9)	115.3(4)
C(19)-C(20)-C(9)	123.0(4)
C(25)-C(21)-C(9)	119.2(4)
C(25)-C(21)-H(21)	120.4
C(9)-C(21)-H(21)	120.4
C(39)-C(12)-C(13)	120.2(4)
C(39)-C(12)-H(12)	119.9
C(13)-C(12)-H(12)	119.9
O(8)-N(1)-O(7)	124.5(4)
O(8)-N(1)-C(36)	117.7(4)
O(7)-N(1)-C(36)	117.8(4)
C(36)-C(25)-C(21)	117.6(4)
C(36)-C(25)-H(25)	121.2
C(21)-C(25)-H(25)	121.2
C(37)-C(26)-C(19)	120.0(4)
C(37)-C(26)-H(26)	120.0
C(19)-C(26)-H(26)	120.0
C(38)-C(27)-C(29)	119.6(4)
C(38)-C(27)-H(27)	120.2
C(29)-C(27)-H(27)	120.2
C(35)-C(28)-C(20)	118.5(4)
C(35)-C(28)-Pt(2)	127.6(3)
C(20)-C(28)-Pt(2)	113.9(3)
C(27)-C(29)-C(13)	121.8(4)
C(27)-C(29)-C(7)	124.7(4)
C(13)-C(29)-C(7)	113.5(4)
O(2)-C(30)-C(34)	126.3(4)
O(2)-C(30)-C(42)	114.0(5)
C(34)-C(30)-C(42)	119.7(4)
O(4)-C(31)-C(15)	126.6(4)
O(4)-C(31)-C(40)	114.7(4)
C(15)-C(31)-C(40)	118.7(4)
C(14)-C(32)-H(32A)	109.5
C(14)-C(32)-H(32B)	109.5

H(32A)-C(32)-H(32B)	109.5
C(14)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
O(1)-C(33)-C(34)	126.6(5)
O(1)-C(33)-C(41)	114.2(4)
C(34)-C(33)-C(41)	119.2(5)
C(30)-C(34)-C(33)	127.3(5)
C(30)-C(34)-H(34)	116.4
C(33)-C(34)-H(34)	116.4
C(28)-C(35)-C(37)	120.3(4)
C(28)-C(35)-H(35)	119.9
C(37)-C(35)-H(35)	119.9
C(25)-C(36)-C(22)	122.5(4)
C(25)-C(36)-N(1)	119.2(4)
C(22)-C(36)-N(1)	118.3(4)
C(26)-C(37)-C(35)	120.8(5)
C(26)-C(37)-H(37)	119.6
C(35)-C(37)-H(37)	119.6
C(27)-C(38)-C(39)	119.6(4)
C(27)-C(38)-H(38)	120.2
C(39)-C(38)-H(38)	120.2
C(38)-C(39)-C(12)	121.2(4)
C(38)-C(39)-H(39)	119.4
C(12)-C(39)-H(39)	119.4
C(31)-C(40)-H(40A)	109.5
C(31)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
C(31)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
C(33)-C(41)-H(41A)	109.5
C(33)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	109.5
C(33)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5

H(41B)-C(41)-H(41C)	109.5
C(30)-C(42)-H(42A)	109.5
C(30)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(30)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
C(43)#1-C(43)-Cl(1)	102.5(9)
C(43)#1-C(43)-H(43A)	111.3
Cl(1)-C(43)-H(43A)	111.3
C(43)#1-C(43)-H(43B)	111.3
Cl(1)-C(43)-H(43B)	111.3
H(43A)-C(43)-H(43B)	109.2

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+2

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for C16H14ClN2O4Pt. 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)	16(1)	15(1)	16(1)	1(1)	0(1)	-8(1)
Pt(2)	25(1)	16(1)	18(1)	1(1)	1(1)	-9(1)
O(4)	22(2)	22(2)	20(1)	4(1)	-4(1)	-11(1)
O(3)	22(2)	25(2)	22(2)	2(1)	0(1)	-13(1)
O(1)	29(2)	20(2)	25(2)	0(1)	2(1)	-8(1)
O(2)	31(2)	24(2)	22(2)	-1(1)	3(1)	-16(1)
N(4)	18(2)	18(2)	18(2)	-2(1)	-1(1)	-7(2)
N(3)	24(2)	19(2)	17(2)	3(1)	1(1)	-9(2)
C(6)	18(2)	18(2)	20(2)	-2(2)	-1(2)	-8(2)
C(7)	22(2)	16(2)	15(2)	1(2)	0(2)	-6(2)
C(9)	30(2)	17(2)	13(2)	4(2)	0(2)	-11(2)
O(5)	23(2)	39(2)	51(2)	9(2)	-10(2)	-12(2)
N(2)	18(2)	30(2)	31(2)	-7(2)	1(2)	-9(2)
C(13)	20(2)	18(2)	17(2)	-4(2)	1(2)	-7(2)
C(22)	27(2)	28(2)	18(2)	4(2)	-3(2)	-16(2)
C(19)	30(2)	21(2)	24(2)	-5(2)	-2(2)	-10(2)
C(15)	26(2)	19(2)	29(2)	3(2)	3(2)	-13(2)
C(16)	24(2)	19(2)	22(2)	5(2)	3(2)	-9(2)
C(18)	19(2)	20(2)	22(2)	-6(2)	1(2)	-9(2)
C(17)	27(2)	24(2)	26(2)	-5(2)	7(2)	-15(2)
C(14)	24(2)	19(2)	20(2)	4(2)	-2(2)	-11(2)
C(20)	28(2)	23(2)	19(2)	4(2)	-1(2)	-12(2)
C(21)	25(2)	23(2)	23(2)	0(2)	-1(2)	-10(2)
C(12)	22(2)	21(2)	28(2)	-2(2)	2(2)	-10(2)
O(6)	22(2)	38(2)	50(2)	-7(2)	6(2)	-19(2)
N(1)	23(2)	39(3)	36(2)	2(2)	-7(2)	-10(2)
O(7)	36(2)	55(3)	66(3)	-21(2)	-11(2)	-15(2)
C(25)	27(2)	24(2)	28(2)	0(2)	4(2)	-6(2)
C(26)	35(3)	27(3)	28(2)	2(2)	-12(2)	-13(2)
C(27)	28(2)	24(2)	21(2)	4(2)	0(2)	-6(2)
C(28)	28(2)	16(2)	17(2)	6(2)	-2(2)	-9(2)

C(29)	18(2)	17(2)	18(2)	-1(2)	1(2)	-4(2)
C(30)	42(3)	26(2)	16(2)	2(2)	2(2)	-19(2)
C(31)	28(2)	18(2)	20(2)	1(2)	-3(2)	-9(2)
C(32)	29(3)	33(3)	38(3)	3(2)	5(2)	-19(2)
C(33)	34(3)	20(2)	23(2)	-2(2)	5(2)	-10(2)
C(34)	46(3)	24(2)	26(2)	-5(2)	3(2)	-15(2)
C(35)	28(2)	20(2)	26(2)	2(2)	-1(2)	-8(2)
C(36)	20(2)	29(2)	25(2)	5(2)	-1(2)	-8(2)
C(37)	23(2)	36(3)	33(3)	3(2)	-6(2)	-9(2)
C(38)	23(2)	21(2)	29(2)	3(2)	-1(2)	0(2)
C(39)	17(2)	35(3)	28(2)	-2(2)	-2(2)	-5(2)
O(8)	25(2)	37(2)	60(3)	-7(2)	-8(2)	-2(2)
C(40)	30(3)	28(3)	40(3)	15(2)	-10(2)	-12(2)
C(41)	40(3)	25(3)	36(3)	-3(2)	9(2)	-5(2)
C(42)	50(3)	34(3)	35(3)	-4(2)	-2(2)	-28(3)
Cl(1)	53(1)	52(1)	43(1)	13(1)	-7(1)	-29(1)
C(43)	58(5)	54(5)	226(14)	-30(6)	5(7)	-39(4)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for C16H14ClN2O4Pt.

	x	y	z	U(eq)
H(6)	-1749	1351	776	22
H(22)	7275	5078	5616	28
H(19)	10176	7001	8047	30
H(15)	956	3886	-887	28
H(16)	-81	-1978	3010	26
H(17)	-2214	-1177	2635	30
H(21)	8115	7662	7775	29
H(12)	3879	-343	1461	28
H(25)	6002	8168	7363	34
H(26)	12381	6199	8194	35
H(27)	2000	-2583	3287	32
H(32A)	3541	2762	343	48
H(32B)	3084	3302	-798	48
H(32C)	3970	1882	-666	48
H(34)	10922	601	4073	38
H(35)	12878	3329	6364	31
H(37)	13709	4407	7324	39
H(38)	4131	-3062	3480	34
H(39)	5056	-1942	2566	35
H(40A)	-1607	3657	-1453	49
H(40B)	-1068	4639	-1292	49
H(40C)	-1971	4445	-389	49
H(41A)	13673	751	4646	56
H(41B)	13095	-48	4092	56
H(41C)	13228	-116	5343	56
H(42A)	7771	1995	4635	54
H(42B)	8856	957	3924	54
H(42C)	8164	2313	3481	54
H(43A)	4428	4361	9550	129
H(43B)	5912	3844	9762	129

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