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**Table S1. Crystal and Intensity Collection Data for
Pt(bpm)Cl₂·0.5(nmp) (3)**

Formula: C ₈ Cl ₂ H ₆ N ₄ Pt·0.5(C ₅ H ₉ NO)	Formula weight: 473.72
Crystal color: Red	Habit: Short needle
Crystal Size: 0.10 x 0.19 x 0.31 mm	$\rho_{\text{calc}} = 2.38 \text{ g cm}^{-3}$
Crystal System: Monoclinic	Space group: <i>C2/m</i> (no. 12)
$a = 12.668(4) \text{ \AA}$	
$b = 15.618(6) \text{ \AA}$	$\beta = 93.43(3)^\circ$
$c = 6.704(3) \text{ \AA}$	
$V = 1324.0(8) \text{ \AA}^3$	$Z = 4$
Lattice parameters: 25 reflections,	$10^\circ \leq \theta \leq 15^\circ$
$\mu = 112.1 \text{ cm}^{-1}$	Absorption correction: none
Enraf-Nonius Cad-4 diffractometer	ω scans
MoK α , $\lambda = 0.7107 \text{ \AA}$	Graphite monochromator
2θ range: 2 – 50°	$-15 \leq h \leq 15, -18 \leq k \leq 18, 0 \leq l \leq 7$
T = 294 K	
Number of reflections measured: 2539	Number of independent reflections: 978
Number with $F_o^2 > 0$: 900	Number with $F_o^2 > 3\sigma(F_o^2)$: 793
Standard reflections: 2 every 150 min.	Variation: within counting statistics
GOF _{merge} : 1.30 for 978 multiples	R _{merge} : 0.035 for 778 duplicates
Number used in refinement: 978	Criterion: All reflections used
Final R on F: 0.031 for 793 reflections with $F_o^2 > 3\sigma(F_o^2)$	
Final R on F: 0.038 for 900 reflections with $F_o^2 > 0$	
Final weighted R _w on F ² : 0.069	
Final GOF: 1.55 for 83 parameters and 978 reflections	
$(\Delta/\sigma)_{\text{max}}$ in final least squares cycle: < 0.005	
$\Delta\rho_{\text{max}}$: 1.97 eÅ ⁻³ , $\Delta\rho_{\text{min}}$: -1.46 eÅ ⁻³ in final difference map	
Secondary extinction parameter: 0.11(1) x 10 ⁻⁶ (Larson, A. C. <i>Acta Cryst.</i> 1967, 23, 644)	

Definitions:

$$R = \frac{\sum |F_o - |F_c||}{\sum F_o}; \quad R_w = \left\{ \frac{\sum w(F_o^2 - F_c^2)^2}{\sum w(F_o^2)^2} \right\}^{\frac{1}{2}}$$

$$GOF = \left\{ \frac{\sum w(F_o^2 - F_c^2)^2}{n-p} \right\}^{\frac{1}{2}}, \text{ where } n = \text{number of data, } p = \text{number of parameters refined.}$$

**Table S2. Final Heavy Atom Parameters for
Pt(bpm)Cl₂·0.5(nmp) (3)**

<i>x, y, z and $U_{eq}^a \times 10^4$</i>					
Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U_{eq}</i> or <i>B</i>	Multiplicity [†]
Pt	5203(.4)	0	2508(.8)	267(1)	4.0
Cl	6488(2)	1035(2)	2487(4)	438(7)	8.0
N(1)	3991(6)	825(5)	2526(11)	299(19)	8.0
N(2)	2123(6)	897(5)	2397(15)	486(23)	8.0
C(1)	3028(8)	468(6)	2446(13)	339(23)	8.0
C(2)	4046(8)	1696(6)	2609(17)	442(27)	8.0
C(3)	3144(9)	2158(6)	2602(18)	481(28)	8.0
C(4)	2186(9)	1748(7)	2490(20)	556(31)	8.0
O	70(17)	1468(9)	5383(25)	0.3(3) *	2.0
C(5)	-134	751	4610	3.0 *	2.0
C(6)	-615(20)	487(18)	2814(45)	6.5(7) *	4.0
C(8)	-34	-721	4697	3.0 *	2.0
N(3)	215(19)	61(65)	5714(37)	4.1(8) *	2.0
C(9)	663	151	7743	4.0 *	2.0

$$^a U_{eq} = \frac{1}{3} \sum_i \sum_j [U_{ij}(a_i^* a_j^*) (\vec{a}_i \cdot \vec{a}_j)]$$

* Isotropic displacement parameter, *B*

† Number of atoms in the unit cell

Note: Since atom C(7) is related to C(6) by a mirror plane, it was removed from the calculations and C(6) was given double weight.

**Table S3. Assigned Hydrogen Atom Parameters for
Pt(bpm)Cl₂·0.5(nmp) (3)**

x, y and $z \times 10^4$

Atom	x	y	z	B
H2	4714	1974	2670	6.0
H3	3174	2764	2675	7.0
H4	1556	2076	2481	8.0
H6A	-212	726	1719	7.0
H6B	-1309	726	2631	7.0
H8A	602	-1019	4468	7.0
H8B	-464	-1065	5489	7.0

**Table S4. Anisotropic Displacement Parameters for
Pt(bpm)Cl₂·0.5(nmp) (3)**

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Pt	284(4)	211(3)	308(3)	0	37(2)	0
Cl	382(16)	394(16)	542(17)	-131(12)	52(12)	-25(13)
N(1)	261(49)	328(46)	310(43)	79(36)	30(32)	31(36)
N(2)	418(54)	385(47)	659(64)	106(41)	63(45)	-13(47)
C(1)	426(66)	267(48)	325(55)	-26(46)	25(42)	-37(44)
C(2)	497(69)	268(49)	564(70)	-51(46)	60(52)	-37(52)
C(3)	591(75)	269(49)	588(74)	86(55)	70(56)	8(53)
C(4)	515(75)	419(61)	740(86)	145(56)	78(60)	27(63)

$U_{i,j}$ values have been multiplied by 10^4

The form of the displacement factor is:

$$\exp -2\pi^2(U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}l^2c^{*2} + 2U_{12}hka^*b^* + 2U_{13}hla^*c^* + 2U_{23}klb^*c^*)$$

**Table S5. Complete Distances and Angles for
Pt(bpm)Cl₂·0.5(nmp) (3)**

		Distance(Å)			Angle(°)
Pt	-Cl	2.294(3)	N(1)	-Pt -Cl	95.2(2)
Pt	-N(1)	2.006(8)	Pt	-N(1) -C(1)	115.4(6)
N(1)	-C(1)	1.339(12)	Pt	-N(1) -C(2)	127.1(6)
N(1)	-C(2)	1.362(13)	C(2)	-N(1) -C(1)	117.5(8)
N(2)	-C(1)	1.327(13)	C(4)	-N(2) -C(1)	116.9(9)
N(2)	-C(4)	1.333(15)	N(2)	-C(1) -N(1)	125.1(9)
C(1)	-C(1)	1.463(13)	C(1)	-C(1) -N(1)	114.6(8)
C(2)	-C(3)	1.352(15)	C(1)	-C(1) -N(2)	120.3(8)
C(3)	-C(4)	1.370(16)	C(3)	-C(2) -N(1)	119.4(9)
O	-C(5)	1.255	C(4)	-C(3) -C(2)	119.8(10)
C(6)	-C(5)	1.380	C(3)	-C(4) -N(2)	121.3(11)
C(6)	-C(6)	1.52(4)	C(6)	-C(6) -C(5)	107.4
C(6)	-C(8)	1.469	C(8)	-N(3) -C(5)	111.2
N(3)	-C(5)	1.365	C(9)	-N(3) -C(5)	121.9
N(3)	-C(8)	1.425	C(9)	-N(3) -C(8)	126.5
N(3)	-C(9)	1.449	C(6)	-C(5) -O	134.2
C(2)	-H2	0.949	N(3)	-C(5) -O	115.4
C(3)	-H3	0.949	N(3)	-C(5) -C(6)	110.4
C(4)	-H4	0.947	N(3)	-C(8) -C(6)	106.4
C(6)	-H6A	0.992	H2	-C(2) -N(1)	120.2
C(6)	-H6B	0.957	H2	-C(2) -C(3)	120.4
C(8)	-H8A	0.950	H3	-C(3) -C(2)	120.1
C(8)	-H8B	0.950	H3	-C(3) -C(4)	120.2
			H4	-C(4) -N(2)	119.4
			H4	-C(4) -C(3)	119.3
			H6A	-C(6) -C(5)	108.3
			H6B	-C(6) -C(5)	110.5
			H6B	-C(6) -H6A	105.5
			C(6)	-C(6) -H6A	112.1
			C(6)	-C(6) -H6B	113.0
			H8A	-C(8) -C(6)	111.7
			H8B	-C(8) -C(6)	110.3
			H8A	-C(8) -N(3)	109.4
			H8B	-C(8) -N(3)	109.6
			H8B	-C(8) -H8A	109.5

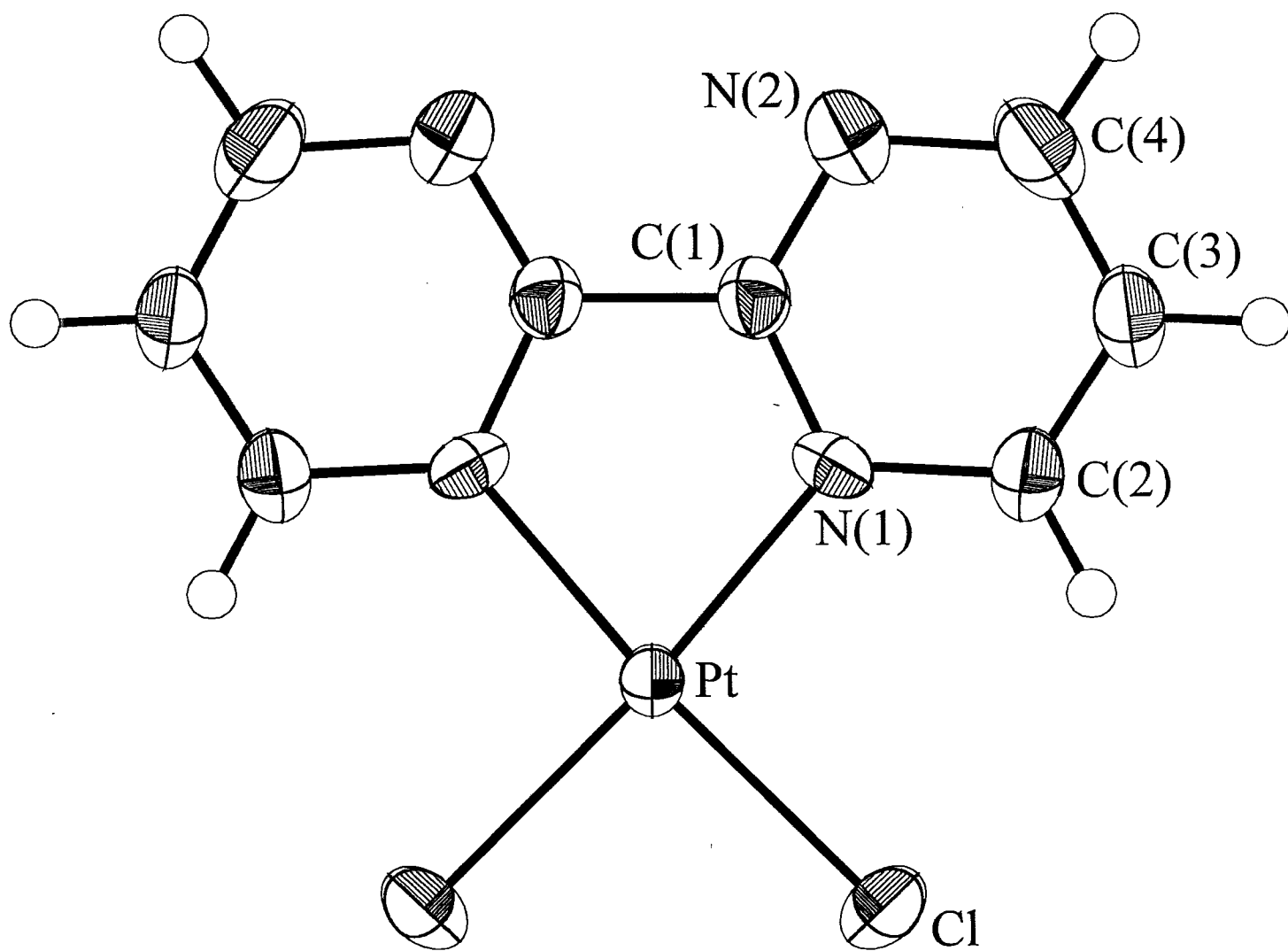


Fig. S1

**Table S6. Crystal and Intensity Collection Data for
Pt(phen)(CN)₂ (6)**

Formula: C ₁₄ H ₈ N ₄ Pt	Formula weight: 427.32
Crystal color: Violet	Habit: Thin needle
Crystal Size: 0.02 x 0.06 x 0.20 mm	$\rho_{\text{calc}} = 2.38 \text{ g cm}^{-3}$
Crystal System: Orthorhombic	Space group: <i>Pbca</i> (no. 61)
$a = 38.731(13) \text{ \AA}$	
$b = 18.569(3) \text{ \AA}$	
$c = 6.628(1) \text{ \AA}$	
$V = 4766(2) \text{ \AA}^3$	$Z = 16$
Lattice parameters: 25 reflections, $\mu = 118.9 \text{ cm}^{-1}$	$8.3^\circ \leq \theta \leq 10.1^\circ$
Enraf-Nonius Cad-4 diffractometer	Relative transmission: 0.83 – 1.09
MoK α , $\lambda = 0.7107 \text{ \AA}$	ω scans
2θ range: 2 – 40°	Graphite monochromator
T = 294 K	$-37 \leq h \leq 37, -17 \leq k \leq 17, 0 \leq l \leq 6$
Number of reflections measured: 10428	Number of independent reflections: 2213
Number with $F_o^2 > 0$: 1754	Number with $F_o^2 > 3\sigma(F_o^2)$: 1221
Standard reflections: 3 every 90 min.	Variation: within counting statistics
GOF _{merge} : 0.98 for 2213 multiples	R _{merge} : 0.0326 for 78 duplicates
Number used in refinement: 2213	Criterion: All reflections used
Final R on F: 0.041 for 1221 reflections with $F_o^2 > 3\sigma(F_o^2)$	
Final R on F: 0.069 for 1754 reflections with $F_o^2 > 0$	
Final weighted R _w on F ² : 0.086	
Final GOF: 1.61 for 164 parameters and 2213 reflections	
$(\Delta/\sigma)_{\text{max}}$ in final least squares cycle: 0.01	
$\Delta\rho_{\text{max}}$: 3.46 e \AA^{-3} , $\Delta\rho_{\text{min}}$: -2.65 e \AA^{-3} in final difference map	
Secondary extinction parameter: 0.0039(11) x 10 ⁻⁶ (Larson, A. C. <i>Acta Cryst.</i> 1967, 23, 644)	

Definitions:

$$R = \frac{\sum |F_o - |F_c||}{\sum F_o}; \quad R_w = \left\{ \frac{\sum w(F_o^2 - F_c^2)^2}{\sum w(F_o^2)^2} \right\}^{\frac{1}{2}}$$

$$GOF = \left\{ \frac{\sum w(F_o^2 - F_c^2)^2}{n-p} \right\}^{\frac{1}{2}}, \text{ where } n = \text{number of data, } p = \text{number of parameters refined.}$$

**Table S7. Final Heavy Atom Parameters for
Pt(phen)(CN)₂ (6)**

x, y, z and $U_{eq}^a \times 10^4$

Atom	x	y	z	U_{eq} or B
Pt1	379(.3)	2407(1)	3109(1)	295(3)
Pt2	2878(.3)	2393(1)	2970(1)	264(2)
N1	221(7)	3476(12)	2929(30)	2.9(5)*
N2	853(5)	2897(9)	3396(31)	2.7(4)*
N3	-369(14)	1813(15)	2669(27)	3.8(6)*
N4	691(7)	865(12)	3272(37)	4.2(5)*
C1	-96(11)	3751(19)	2667(31)	2.7(8)*
C2	-133(11)	4499(20)	2495(28)	2.6(8)*
C3	139(11)	4921(20)	2602(33)	3.2(8)*
C4	459(8)	4700(15)	2997(40)	3.3(6)*
C5	500(8)	3941(14)	3121(43)	3.3(6)*
C6	832(7)	3642(12)	3383(41)	2.6(5)*
C7	1128(7)	4073(13)	3565(39)	3.7(6)*
C8	1442(8)	3728(15)	3965(43)	4.9(7)*
C9	1454(8)	3008(15)	3978(43)	5.4(7)*
C10	1171(6)	2593(13)	3684(32)	3.5(5)*
C11	771(8)	5118(15)	3245(51)	4.5(6)*
C12	1073(8)	4855(13)	3471(44)	4.1(6)*
C13	-88(9)	2025(15)	2836(35)	2.5(6)*
C14	562(8)	1436(14)	3238(44)	3.3(5)*

Table 7. (Cont.)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U_{eq}</i> or <i>B</i>
N5	2734(7)	3451(12)	2851(28)	2.6(5)*
N6	3337(5)	2870(9)	3252(29)	2.8(4)*
N7	2146(14)	1801(16)	2619(29)	4.4(7)*
N8	3187(6)	862(11)	3212(35)	3.7(5)*
C15	2426(11)	3705(19)	2617(30)	2.3(7)*
C16	2345(12)	4435(22)	2614(34)	3.7(9)*
C17	2621(10)	4946(20)	2790(38)	3.6(8)*
C18	2957(8)	4668(14)	3070(40)	3.1(5)*
C19	3005(8)	3924(13)	3035(40)	2.4(5)*
C20	3330(7)	3612(11)	3254(40)	2.9(5)*
C21	3631(8)	4037(13)	3550(40)	4.0(6)*
C22	3946(8)	3705(15)	3829(43)	4.8(7)*
C23	3967(8)	2987(15)	3814(42)	4.9(7)*
C24	3659(6)	2571(14)	3530(34)	3.9(5)*
C25	3264(7)	5111(13)	3221(46)	3.7(5)*
C26	3577(9)	4804(14)	3479(46)	4.9(6)*
C27	2430(11)	2008(18)	2717(34)	3.4(8)*
C28	3053(8)	1420(15)	3115(46)	3.8(6)*

$$^a U_{eq} = \frac{1}{3} \sum_i \sum_j [U_{ij} (a_i^* a_j^*) (\vec{a}_i \cdot \vec{a}_j)]$$

* Isotropic displacement parameter, *B*

**Table S8. Assigned Hydrogen Atom Parameters for
Pt(phen)(CN)₂ (6)** x, y and $z \times 10^4$

Atom	x	y	z	B
H1	-292	3445	2600	3.1
H2	-355	4702	2298	3.0
H3	104	5421	2383	3.7
H8	1644	4002	4224	5.7
H9	1669	2779	4204	6.2
H10	1193	2083	3678	4.0
H11	749	5628	3239	5.1
H12	1266	5170	3581	4.7
H15	2243	3371	2434	2.7
H16	2112	4592	2498	4.3
H17	2580	5450	2722	4.1
H22	4148	3987	4031	5.5
H23	4184	2754	3990	5.6
H24	3678	2061	3532	4.5
H25	3245	5621	3137	4.3
H26	3772	5110	3621	5.6

Table S9. Platinum Atom Anisotropic Displacement Parameters for Pt(phen)(CN)₂ (6)

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Pt1	326(7)	268(7)	292(5)	16(5)	24(7)	10(6)
Pt2	296(7)	219(6)	277(5)	11(5)	5(6)	-12(5)

$U_{i,j}$ values have been multiplied by 10^4

The form of the displacement factor is:

$$\exp -2\pi^2(U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}l^2c^{*2} + 2U_{12}hka^*b^* + 2U_{13}hla^*c^* + 2U_{23}klb^*c^*)$$

**Table S10. Complete Distances and Angles for
Pt(phen)(CN)₂ (6)**

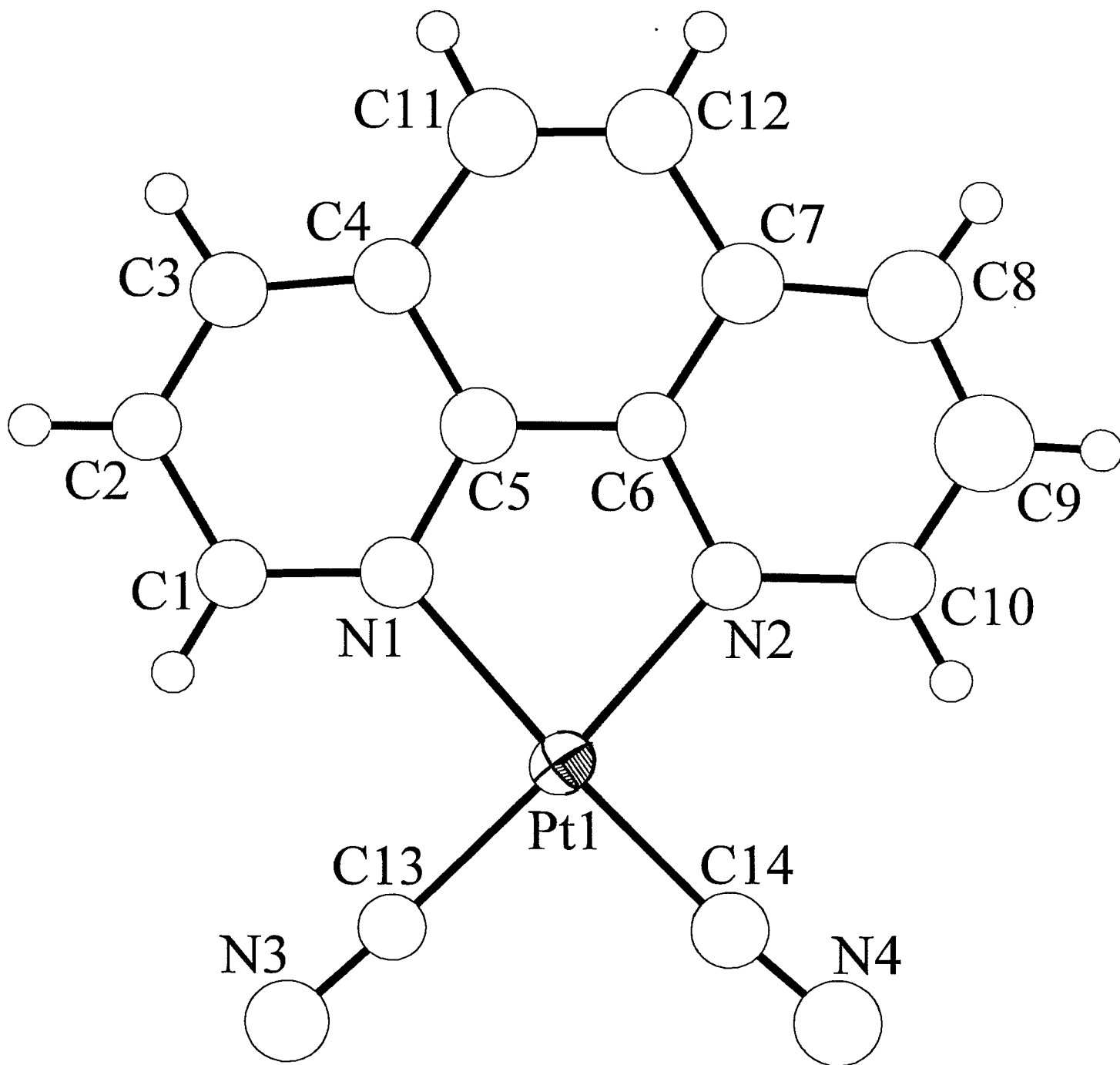
	Distance(Å)		Distance(Å)
Pt1 -N1	2.08(2)	C22 -C23	1.34(4)
Pt1 -N2	2.06(2)	C23 -C24	1.44(4)
Pt1 -C13	1.95(3)	C25 -C26	1.35(4)
Pt1 -C14	1.94(3)		
Pt2 -N5	2.04(2)		
Pt2 -N6	1.99(2)		
Pt2 -C27	1.89(3)		
Pt2 -C28	1.93(3)		
N1 -C1	1.34(4)		
N1 -C5	1.39(4)		
N2 -C6	1.39(3)		
N2 -C10	1.37(3)		
N3 -C13	1.16(4)		
N4 -C14	1.17(4)		
C1 -C2	1.40(5)		
C2 -C3	1.31(5)		
C3 -C4	1.33(4)		
C4 -C5	1.42(4)		
C4 -C11	1.45(4)		
C5 -C6	1.41(4)		
C6 -C7	1.40(4)		
C7 -C8	1.40(4)		
C7 -C12	1.47(4)		
C8 -C9	1.34(4)		
C9 -C10	1.35(4)		
C11 -C12	1.28(4)		
N5 -C15	1.29(4)		
N5 -C19	1.38(4)		
N6 -C20	1.38(3)		
N6 -C24	1.38(3)		
N7 -C27	1.17(5)		
N8 -C28	1.16(4)		
C15 -C16	1.39(5)		
C16 -C17	1.43(5)		
C17 -C18	1.41(4)		
C18 -C19	1.39(4)		
C18 -C25	1.45(4)		
C19 -C20	1.39(4)		
C20 -C21	1.42(4)		
C21 -C22	1.38(4)		
C21 -C26	1.44(4)		

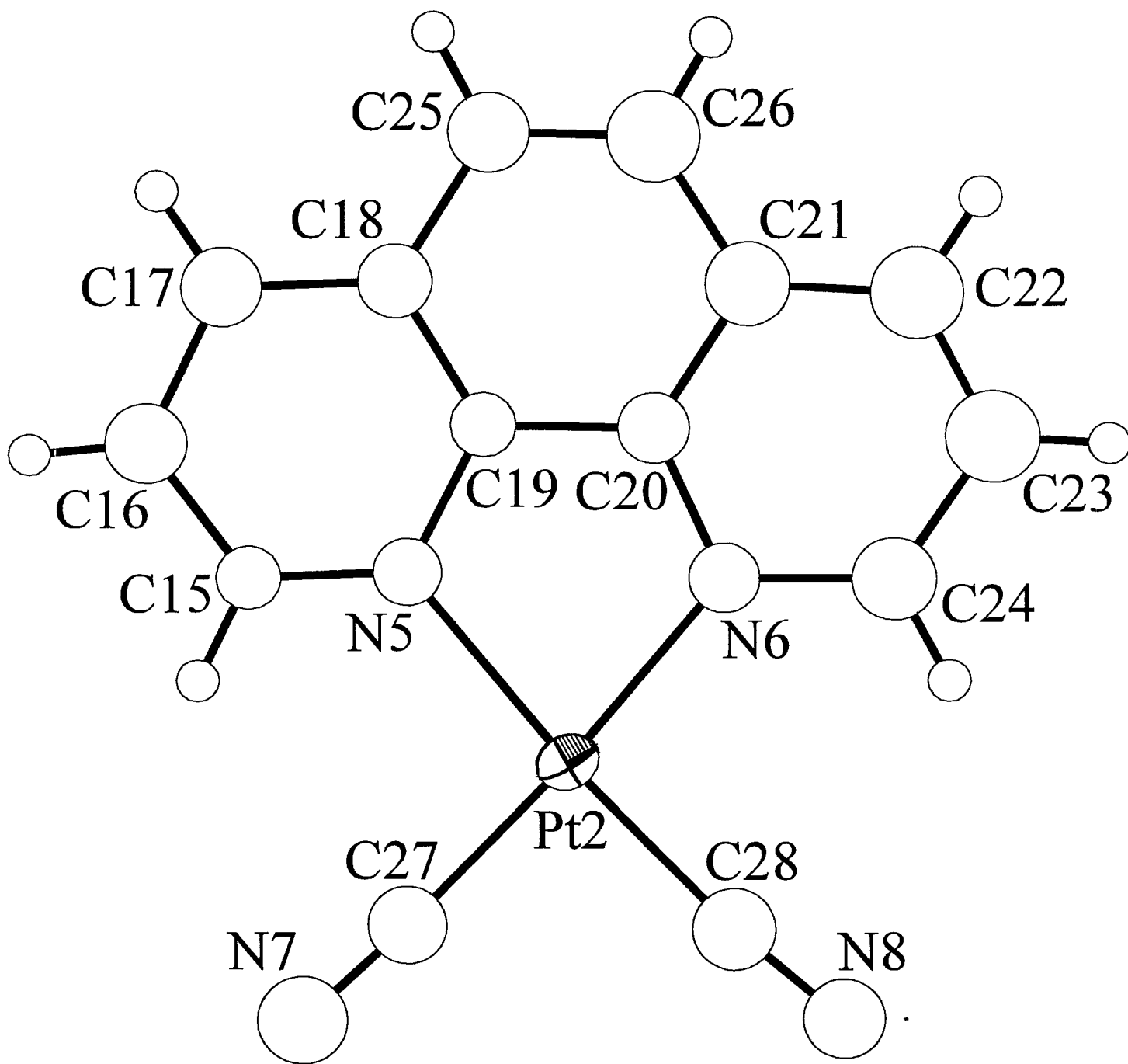
Table 10. (Cont.)

Angle(°)				Angle(°)			
N1 -Pt1 -N2	81.2(8)	C11 -C12 -C7	120.9(27)				
N1 -Pt1 -C13	93.8(11)	C19 -N5 -C15	118.9(24)				
N1 -Pt1 -C14	175.8(10)	C24 -N6 -C20	114.9(20)				
N2 -Pt1 -C13	175.0(10)	C16 -C15 -N5	124.3(30)				
N2 -Pt1 -C14	94.8(10)	C17 -C16 -C15	118.4(32)				
C13 -Pt1 -C14	90.2(12)	C18 -C17 -C16	117.1(30)				
N5 -Pt2 -N6	79.7(8)	C19 -C18 -C17	119.0(26)				
N5 -Pt2 -C27	96.2(12)	C25 -C18 -C17	123.8(26)				
N5 -Pt2 -C28	175.3(11)	C25 -C18 -C19	117.0(24)				
N6 -Pt2 -C27	175.8(11)	C18 -C19 -N5	122.1(24)				
N6 -Pt2 -C28	95.7(10)	C20 -C19 -N5	115.8(23)				
C27 -Pt2 -C28	88.5(13)	C20 -C19 -C18	122.1(25)				
Pt1 -N1 -C5	110.9(18)	C19 -C20 -N6	115.7(22)				
Pt1 -N2 -C6	112.9(15)	C21 -C20 -N6	122.7(22)				
Pt1 -C13 -N3	178.5(28)	C21 -C20 -C19	121.6(24)				
Pt1 -C14 -N4	175.8(25)	C22 -C21 -C20	119.7(25)				
Pt2 -N5 -C19	113.6(17)	C26 -C21 -C20	115.2(24)				
Pt2 -N6 -C20	115.3(15)	C26 -C21 -C22	125.1(26)				
Pt2 -C27 -N7	176.4(31)	C23 -C22 -C21	120.0(27)				
Pt2 -C28 -N8	174.1(26)	C24 -C23 -C22	119.1(26)				
C5 -N1 -C1	119.3(25)	C23 -C24 -N6	123.7(22)				
C10 -N2 -C6	117.8(19)	C26 -C25 -C18	120.3(26)				
C2 -C1 -N1	118.7(29)	C25 -C26 -C21	123.6(27)				
C3 -C2 -C1	120.5(31)	H1 -C1 -N1	120.7				
C4 -C3 -C2	124.9(32)	H1 -C1 -C2	120.7				
C5 -C4 -C3	114.9(27)	H2 -C2 -C1	119.8				
C11 -C4 -C3	129.4(28)	H2 -C2 -C3	119.8				
C11 -C4 -C5	115.7(26)	H3 -C3 -C2	117.6				
C4 -C5 -N1	121.5(25)	H3 -C3 -C4	117.6				
C6 -C5 -N1	118.5(24)	H8 -C8 -C7	120.4				
C6 -C5 -C4	120.0(25)	H8 -C8 -C9	120.4				
C5 -C6 -N2	116.6(22)	H9 -C9 -C8	118.6				
C7 -C6 -N2	121.3(22)	H9 -C9 -C10	118.6				
C7 -C6 -C5	122.1(24)	H10 -C10 -N2	119.6				
C8 -C7 -C6	117.8(24)	H10 -C10 -C9	119.6				
C12 -C7 -C6	116.3(23)	H11 -C11 -C4	117.5				
C12 -C7 -C8	125.8(24)	H11 -C11 -C12	117.5				
C9 -C8 -C7	119.1(27)	H12 -C12 -C7	119.5				
C10 -C9 -C8	122.8(27)	H12 -C12 -C11	119.5				
C9 -C10 -N2	120.8(23)	H15 -C15 -N5	117.8				
C12 -C11 -C4	125.0(29)	H15 -C15 -C16	117.8				

Table 10. (Cont.)

	Angle(°)
H16 -C16 -C15	120.8
H16 -C16 -C17	120.8
H17 -C17 -C16	121.4
H17 -C17 -C18	121.4
H22 -C22 -C21	120.0
H22 -C22 -C23	120.0
H23 -C23 -C22	120.5
H23 -C23 -C24	120.5
H24 -C24 -N6	118.2
H24 -C24 -C23	118.2
H25 -C25 -C18	119.8
H25 -C25 -C26	119.8
H26 -C26 -C21	118.2
H26 -C26 -C25	118.2





**Table S11. Crystal and Intensity Collection Data for
Pt(bpy)(NCS)₂ (7)**

Formula: C ₁₂ H ₈ N ₄ PtS ₂	Formula weight: 467.43
Crystal color: Red	Habit: Blade
Crystal Size: 0.03 x 0.06 x 0.41 mm	$\rho_{\text{calc}} = 2.29 \text{ g cm}^{-3}$
Crystal System: Orthorhombic	Space group: <i>Pbcm</i> (no. 57)
$a = 10.349(3) \text{ \AA}$	
$b = 19.927(5) \text{ \AA}$	
$c = 6.572(3) \text{ \AA}$	
$V = 1355.3(7) \text{ \AA}^3$	$Z = 4$
Lattice parameters: 25 reflections, $\mu = 107.4 \text{ cm}^{-1}$	$9^\circ \leq \theta \leq 11^\circ$
Enraf-Nonius Cad-4 diffractometer	Absorption correction: none
MoK α , $\lambda = 0.7107 \text{ \AA}$	ω scans
2θ range: 2 – 40°	Graphite monochromator
T = 294 K	$0 \leq h \leq 9, 0 \leq k \leq 19, -6 \leq l \leq 6$
Number of reflections measured: 1626	Number of independent reflections: 710
Number with $F_o^2 > 0$: 643	Number with $F_o^2 > 3\sigma(F_o^2)$: 565
Standard reflections: 3 every 150 min.	Variation: within counting statistics
GOF _{merge} : 1.06 for 709 multiples	R _{merge} : 0.019 for 629 duplicates
Number used in refinement: 710	Criterion: All reflections used
Final R on F: 0.044 for 565 reflections with $F_o^2 > 3\sigma(F_o^2)$	
Final R on F: 0.050 for 643 reflections with $F_o^2 > 0$	
Final weighted R _w on F ² : 0.099	
Final GOF: 2.80 for 67 parameters and 710 reflections	
$(\Delta/\sigma)_{\text{max}}$ in final least squares cycle: < 0.01	
$\Delta\rho_{\text{max}}$: 1.68 eÅ ⁻³ , $\Delta\rho_{\text{min}}$: -1.49 eÅ ⁻³ in final difference map	

Definitions:

$$R = \frac{\sum |F_o - |F_c||}{\sum F_o}; \quad R_w = \left\{ \frac{\sum w(F_o^2 - F_c^2)^2}{\sum w(F_o^2)^2} \right\}^{\frac{1}{2}}$$

$$GOF = \left\{ \frac{\sum w(F_o^2 - F_c^2)^2}{n-p} \right\}^{\frac{1}{2}}, \text{ where } n = \text{number of data, } p = \text{number of parameters refined.}$$

Table S12. Final Heavy Atom Parameters for**Pt(bpy)(NCS)₂ (7)***x, y, z* and $U_{eq}^a \times 10^4$

Atom	<i>x</i>	<i>y</i>	<i>z</i>	U_{eq} or <i>B</i>
Pt	1495(1)	2572(1)	2500	562(3)
N1	-219(22)	2964(10)	2500	4.9(5) *
C1	-1145(26)	3241(12)	2500	5.1(6) *
S1	-2572(10)	3645(4)	2500	1076(30)
N2	2286(26)	3546(12)	2500	6.2(6) *
C2	2850(30)	3982(14)	2500	5.7(7) *
S2	3615(10)	4659(4)	2500	1179(32)
N3	806(22)	1603(10)	2500	5.2(5) *
C3	-331(28)	1379(12)	2500	5.0(6) *
C4	-610(30)	725(13)	2500	5.9(7) *
C5	279(28)	290(12)	2500	5.4(6) *
C6	1576(28)	474(12)	2500	5.8(6) *
C7	1927(23)	1139(11)	2500	4.0(6) *
C8	3166(25)	1460(11)	2500	4.1(6) *
C9	4249(29)	1069(12)	2500	5.3(6) *
C10	5414(33)	1410(14)	2500	6.6(7) *
C11	5477(30)	2058(14)	2500	6.5(7) *
C12	4326(24)	2409(12)	2500	4.9(5) *
N4	3139(17)	2134(9)	2500	3.6(4) *

$$^a U_{eq} = \frac{1}{3} \sum_i \sum_j [U_{ij}(a_i^* a_j^*)(\vec{a}_i \cdot \vec{a}_j)]$$

* Isotropic displacement parameter, *B*

**Table S13. Assigned Hydrogen Atom Parameters for
Pt(bpy)(NCS)₂ (7)**

x, y and $z \times 10^4$

Atom	x	y	z	B
H3	-1057	1704	2500	6.1
H4	-1521	581	2500	6.7
H5	46	-182	2500	6.5
H6	2231	127	2500	6.4
H9	4253	577	2500	6.5
H10	6203	1150	2500	7.3
H11	6307	2283	2500	7.5
H12	4404	2895	2500	5.7

**Table S14. Anisotropic Displacement Parameters for
Pt(bpy)(NCS)₂ (7)**

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Pt	753(8)	498(7)	436(7)	24(8)	0	0
S1	940(71)	793(54)	1496(96)	67(52)	0	0
S2	1254(83)	737(50)	1546(97)	-72(60)	0	0

$U_{i,j}$ values have been multiplied by 10^4

The form of the displacement factor is:

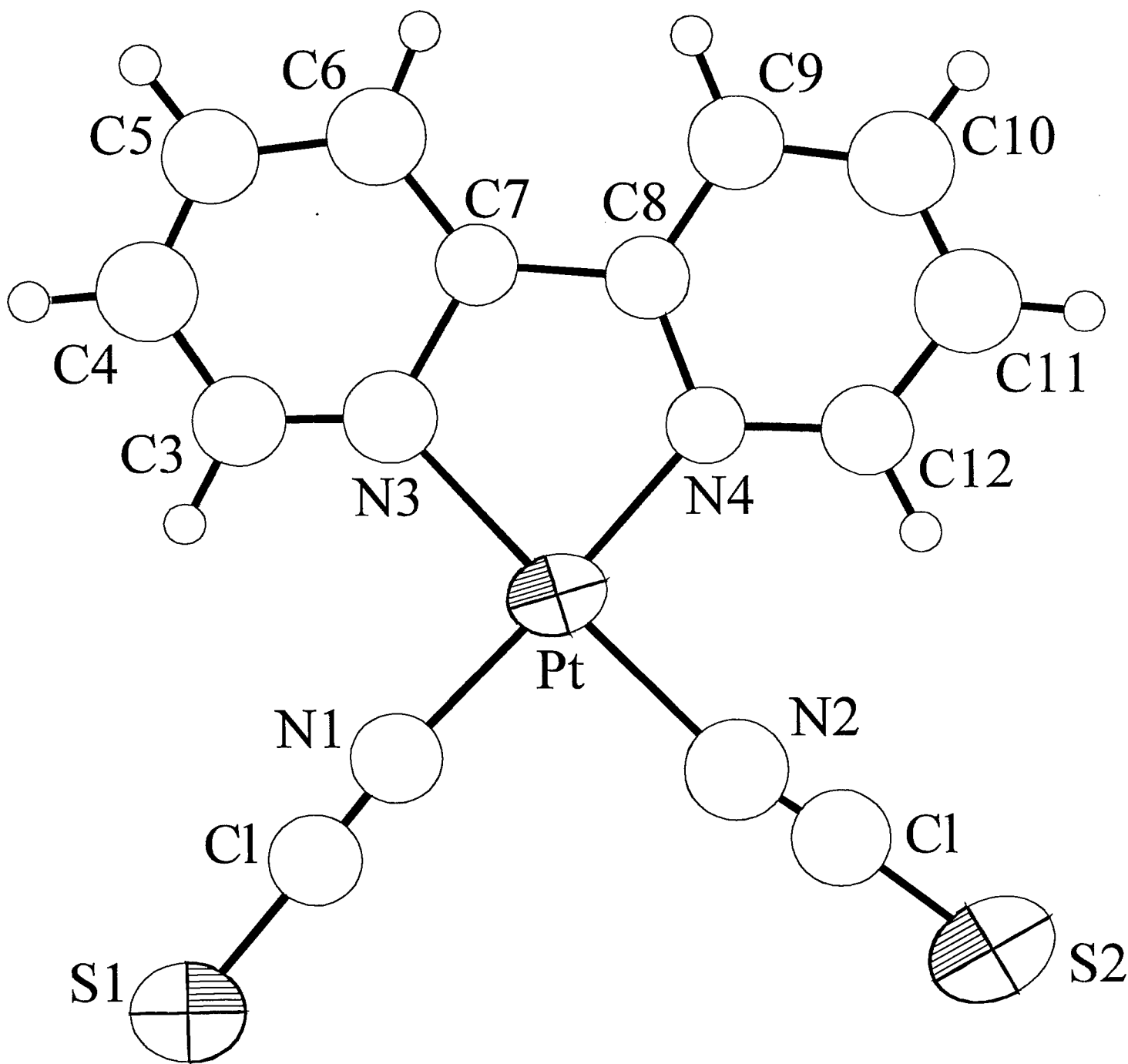
$$\exp -2\pi^2(U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}l^2c^{*2} + 2U_{12}hka^*b^* + 2U_{13}hla^*c^* + 2U_{23}klb^*c^*)$$

**Table S15. Complete Distances and Angles for
Pt(bpy)(NCS)₂ (7)**

		Distance(Å)			Angle(°)
Pt	-N1	1.94(2)	N1	-Pt -N2	89.1(9)
Pt	-N2	2.11(3)	N1	-Pt -N3	93.5(8)
Pt	-N3	2.06(2)	N1	-Pt -N4	176.6(8)
Pt	-N4	1.912(17)	N2	-Pt -N3	177.4(9)
N1	-C1	1.11(3)	N2	-Pt -N4	94.3(9)
C1	-S1	1.68(3)	N3	-Pt -N4	83.1(8)
N2	-C2	1.05(4)	Pt	-N1 -C1	173.8(21)
C2	-S2	1.57(3)	Pt	-N2 -C2	169.0(26)
N3	-C3	1.26(3)	Pt	-N3 -C3	131.1(19)
N3	-C7	1.48(3)	Pt	-N3 -C7	108.3(14)
C3	-C4	1.34(4)	Pt	-N4 -C8	118.3(15)
C4	-C5	1.26(4)	Pt	-N4 -C12	128.8(15)
C5	-C6	1.39(4)	S1	-C1 -N1	178.6(25)
C6	-C7	1.37(4)	S2	-C2 -N2	176.5(30)
C7	-C8	1.43(3)	C7	-N3 -C3	120.7(21)
C8	-C9	1.36(4)	C4	-C3 -N3	123.3(26)
C8	-N4	1.34(3)	C5	-C4 -C3	120.8(28)
C8	-C9	1.36(4)	C6	-C5 -C4	121.4(26)
C9	-C10	1.38(4)	C7	-C6 -C5	120.7(24)
C10	-C11	1.29(4)	C6	-C7 -N3	113.2(21)
C11	-C12	1.38(4)	C8	-C7 -N3	115.0(20)
C12	-N4	1.35(3)	C8	-C7 -C6	131.8(22)
C3	-H3	0.991	C9	-C8 -C7	118.7(22)
C4	-H4	0.985	N4	-C8 -C7	115.3(21)
C5	-H5	0.970	N4	-C8 -C9	126.0(23)
C6	-H6	0.969	C10	-C9 -C8	115.8(25)
C9	-H9	0.982	C11	-C10 -C9	122.3(29)
C10	-H10	0.968	C12	-C11 -C10	117.5(28)
C11	-H11	0.970	N4	-C12 -C11	125.5(23)
C12	-H12	0.973	C12	-N4 -C8	112.8(19)
			H3	-C3 -N3	118.4
			H3	-C3 -C4	118.3
			H4	-C4 -C3	119.4
			H4	-C4 -C5	119.8
			H5	-C5 -C4	118.9

Table 15. (Cont.)

			Angle(°)
H5	-C5	-C6	119.7
H6	-C6	-C5	119.1
H6	-C6	-C7	120.3
H9	-C9	-C8	125.1
H9	-C9	-C10	119.1
H10	-C10	-C9	118.3
H10	-C10	-C11	119.5
H11	-C11	-C10	120.6
H11	-C11	-C12	121.9
H12	-C12	-C11	115.7
H12	-C12	-N4	118.8



**Table S16. Crystal and Intensity Collection Data for
Pt(dmbpy)(NCO)₂ (1b)**

Formula: C ₁₄ H ₁₂ N ₄ O ₂ Pt	Formula weight: 463.36
Crystal color: Yellow	Habit: Rectangular prisms
Crystal Size: 0.11 x 0.14 x 0.22 mm	$\rho_{\text{calc}} = 2.22 \text{ g cm}^{-3}$
Crystal System: Monoclinic	Space group: <i>C2/c</i> (no. 15)
$a = 17.313(4) \text{ \AA}$	
$b = 12.263(3) \text{ \AA}$	$\beta = 114.00(2)^\circ$
$c = 14.291(4) \text{ \AA}$	
$V = 2771.8(11) \text{ \AA}^3$	$Z = 8$
Lattice parameters: 25 reflections, $\mu = 102.4 \text{ cm}^{-1}$	$4.5^\circ \leq \theta \leq 14.5^\circ$
Enraf-Nonius Cad-4 diffractometer	Relative transmission: 0.85 – 1.16
MoK α , $\lambda = 0.7107 \text{ \AA}$	$\theta - 2\theta$ scans
2θ range: 2 – 50°	Graphite monochromator
T = 294 K	$-16 \leq h \leq 16, -11 \leq k \leq 11, 0 \leq l \leq 13$
Number of reflections measured: 4737	Number of independent reflections: 2016
Number with $F_o^2 > 0$: 1920	Number with $F_o^2 > 3\sigma(F_o^2)$: 1605
Standard reflections: 3 every 150 min.	Variation: within counting statistics
GOF _{merge} : 1.07 for 1925 multiples	R _{merge} : 0.026 for 1652 duplicates
Number used in refinement: 2016	Criterion: All reflections used
Final R on F: 0.022 for 1605 reflections with $F_o^2 > 3\sigma(F_o^2)$	
Final R on F: 0.031 for 1920 reflections with $F_o^2 > 0$	
Final weighted R _w on F ² : 0.048	
Final GOF: 1.24 for 191 parameters and 2016 reflections	
$(\Delta/\sigma)_{\text{max}}$ in final least squares cycle: < 0.005	
$\Delta\rho_{\text{max}}$: 0.76 e \AA^{-3} , $\Delta\rho_{\text{min}}$: -0.72 e \AA^{-3} in final difference map	
Secondary extinction parameter: 0.083(4) x 10 ⁻⁶ (Larson, A. C. <i>Acta Cryst.</i> 1967, 23, 644)	

Definitions:

$$R = \frac{\sum |F_o - |F_c||}{\sum F_o}; \quad R_w = \left\{ \frac{\sum w(F_o^2 - F_c^2)^2}{\sum w(F_o^2)^2} \right\}^{\frac{1}{2}}$$

$$GOF = \left\{ \frac{\sum w(F_o^2 - F_c^2)^2}{n-p} \right\}^{\frac{1}{2}}, \text{ where } n = \text{number of data, } p = \text{number of parameters refined.}$$

**Table S17. Final Heavy Atom Parameters for
Pt(dmbpy)(NCO)₂ (1b)**

Atom	x, y, z and $U_{eq}^a \times 10^4$			
	x	y	z	U_{eq}
Pt	1361(.1)	93(.2)	1527(.2)	366(1)
N1	1841(3)	-1375(4)	1520(4)	542(15)
C1	2147(4)	-2086(6)	1283(5)	506(19)
O1	2458(3)	-2867(4)	1061(4)	827(16)
N2	2490(3)	766(4)	1806(5)	579(16)
C2	3183(5)	939(5)	2296(6)	563(20)
O2	3909(3)	1160(4)	2780(5)	977(21)
N3	204(3)	-464(4)	1274(3)	359(12)
C3	-28(4)	-1504(5)	1237(5)	437(17)
C4	-839(4)	-1806(5)	1090(5)	463(17)
C5	-1436(3)	-1013(5)	973(4)	405(16)
C6	-2330(4)	-1278(5)	798(6)	570(18)
C7	-1195(3)	65(5)	1005(4)	403(15)
C8	-387(3)	332(4)	1158(4)	326(13)
C9	-68(3)	1457(4)	1224(4)	346(15)
C10	-554(3)	2377(5)	1067(5)	407(16)
C11	-197(4)	3406(5)	1145(5)	458(17)
C12	-737(5)	4406(5)	940(6)	748(23)
C13	659(4)	3444(5)	1404(5)	564(19)
C14	1124(4)	2508(5)	1559(5)	462(17)

Table 17. (Cont.)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	U_{eq}
N4	784(3)	1522(4)	1467(4)	370(12)

$$^a U_{eq} = \frac{1}{3} \sum_i \sum_j [U_{ij}(a_i^* a_j^*)(\vec{a}_i \cdot \vec{a}_j)]$$

**Table S18. Assigned Hydrogen Atom Parameters for
Pt(dmbpy)(NCO)₂ (1b)**

Atom	x, y and $z \times 10^4$			B
	x	y	z	
H3	379	-2058	1313	3.8
H4	-985	-2555	1076	4.0
H6A	-2636	-615	737	5.0
H6B	-2586	-1685	185	5.0
H6C	-2334	-1685	1359	5.0
H6D	-2399	-2041	797	5.0
H6E	-2454	-959	1328	5.0
H6F	-2703	-983	156	5.0
H7	-1595	626	921	3.5
H10	-1142	2313	905	3.5
H12A	-388	5035	1029	6.5
H12B	-1151	4387	258	6.5
H12C	-998	4437	1405	6.5
H12D	-1302	4205	776	6.5
H12E	-535	4858	1533	6.5
H12F	-699	4797	383	6.5
H13	932	4131	1480	4.9
H14	1714	2566	1734	4.0

**Table S19. Anisotropic Displacement Parameters for
Pt(dmbpy)(NCO)₂ (1b)**

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Pt	309(1)	429(2)	353(2)	37(1)	128(1)	18(1)
N1	463(34)	519(35)	616(40)	222(27)	190(29)	22(29)
C1	435(40)	633(49)	433(43)	10(34)	159(32)	91(34)
O1	920(40)	811(38)	864(43)	343(32)	480(34)	-4(31)
N2	408(33)	689(39)	670(42)	-49(29)	249(31)	23(31)
C2	487(46)	422(39)	796(57)	6(32)	278(42)	-56(36)
O2	427(31)	736(36)	1520(61)	-73(25)	141(35)	-151(36)
N3	376(28)	421(29)	290(27)	1(21)	146(22)	-10(21)
C3	503(41)	366(37)	410(41)	-28(29)	153(32)	-37(28)
C4	535(43)	386(37)	471(42)	-97(30)	208(32)	-14(29)
C5	402(37)	438(40)	391(40)	-118(27)	178(30)	-43(27)
C6	462(40)	627(44)	660(50)	-159(32)	269(36)	-68(36)
C7	359(31)	509(41)	321(33)	25(30)	119(24)	27(27)
C8	336(32)	364(35)	315(33)	-7(23)	169(25)	8(24)
C9	333(37)	408(36)	305(36)	-1(26)	139(28)	-4(26)
C10	304(33)	438(38)	453(40)	42(26)	126(28)	11(28)
C11	485(41)	382(38)	511(43)	18(27)	206(33)	-28(29)
C12	738(51)	454(42)	1009(66)	50(37)	310(47)	47(42)
C13	618(46)	373(39)	723(53)	-85(31)	296(39)	-17(33)
C14	429(37)	452(41)	509(44)	-51(28)	194(32)	-6(30)
N4	343(30)	382(30)	399(32)	34(21)	165(23)	4(22)

$U_{i,j}$ values have been multiplied by 10^4

The form of the displacement factor is:

$$\exp -2\pi^2(U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}l^2c^{*2} + 2U_{12}hka^*b^* + 2U_{13}hla^*c^* + 2U_{23}klb^*c^*)$$

Table S20. Complete Distances and Angles for Pt(dmbpy)(NCO)₂ (1b)

	Distance(Å)	Distance(Å)
Pt -N1	1.985(6)	C12 -H12C 0.945
Pt -N2	2.007(6)	C12 -H12D 0.942
Pt -N3	2.005(5)	C12 -H12E 0.952
Pt -N4	2.001(5)	C12 -H12F 0.953
N1 -C1	1.141(9)	C13 -H13 0.950
C1 -O1	1.203(9)	C14 -H14 0.950
N2 -C2	1.136(9)	
C2 -O2	1.194(9)	
N3 -C3	1.332(8)	
N3 -C8	1.373(7)	
C3 -C4	1.384(9)	
C4 -C5	1.378(9)	
C5 -C6	1.500(9)	
C5 -C7	1.380(8)	
C7 -C8	1.365(8)	
C8 -C9	1.475(8)	
C9 -C10	1.371(8)	
C9 -N4	1.373(7)	
C10 -C11	1.389(9)	
C11 -C12	1.498(10)	
C11 -C13	1.374(9)	
C13 -C14	1.367(9)	
C14 -N4	1.327(8)	
C3 -H3	0.953	
C4 -H4	0.951	
C6 -H6A	0.955	
C6 -H6B	0.947	
C6 -H6C	0.946	
C6 -H6D	0.944	
C6 -H6E	0.951	
C6 -H6F	0.953	
C7 -H7	0.950	
C10 -H10	0.951	
C12 -H12A	0.956	
C12 -H12B	0.946	

Table 20. (Cont.)

Angle(°)				Angle(°)			
N1	-Pt	-N2	89.9(2)	H3	-C3	-C4	119.0
N1	-Pt	-N3	94.6(2)	H4	-C4	-C3	120.3
N1	-Pt	-N4	175.4(2)	H4	-C4	-C5	120.1
N2	-Pt	-N3	175.4(2)	H6A	-C6	-C5	109.1
N2	-Pt	-N4	94.4(2)	H6B	-C6	-C5	109.3
N3	-Pt	-N4	81.2(2)	H6C	-C6	-C5	109.6
Pt	-N1	-C1	160.2(6)	H6D	-C6	-C5	109.6
Pt	-N2	-C2	153.9(6)	H6E	-C6	-C5	109.3
Pt	-N3	-C3	126.6(4)	H6F	-C6	-C5	109.1
Pt	-N3	-C8	114.8(4)	H6B	-C6	-H6A	109.3
Pt	-N4	-C9	115.2(4)	H6C	-C6	-H6A	109.4
Pt	-N4	-C14	126.9(4)	H6C	-C6	-H6B	110.0
O1	-C1	-N1	176.9(8)	H6E	-C6	-H6D	109.9
O2	-C2	-N2	176.9(8)	H6F	-C6	-H6D	109.8
C8	-N3	-C3	118.6(5)	H6F	-C6	-H6E	109.1
C4	-C3	-N3	122.2(6)	H7	-C7	-C5	119.7
C5	-C4	-C3	119.6(6)	H7	-C7	-C8	119.6
C6	-C5	-C4	122.6(6)	H10	-C10	-C9	119.8
C7	-C5	-C4	118.0(6)	H10	-C10	-C11	119.5
C7	-C5	-C6	119.3(5)	H12A	-C12	-C11	108.9
C8	-C7	-C5	120.7(5)	H12B	-C12	-C11	109.4
C7	-C8	-N3	120.9(5)	H12C	-C12	-C11	109.6
C9	-C8	-N3	114.6(5)	H12D	-C12	-C11	109.7
C9	-C8	-C7	124.6(5)	H12E	-C12	-C11	109.1
C10	-C9	-C8	124.8(5)	H12F	-C12	-C11	109.0
N4	-C9	-C8	114.0(5)	H12B	-C12	-H12A	109.3
N4	-C9	-C10	121.2(5)	H12C	-C12	-H12A	109.4
C11	-C10	-C9	120.7(6)	H12C	-C12	-H12B	110.3
C12	-C11	-C10	120.4(6)	H12E	-C12	-H12D	110.0
C13	-C11	-C10	116.7(6)	H12F	-C12	-H12D	109.9
C13	-C11	-C12	122.9(6)	H12F	-C12	-H12E	109.0
C14	-C13	-C11	120.9(6)	H13	-C13	-C11	119.5
N4	-C14	-C13	122.7(6)	H13	-C13	-C14	119.5
C14	-N4	-C9	117.7(5)	H14	-C14	-C13	118.6
H3	-C3	-N3	118.8	H14	-C14	-N4	118.7

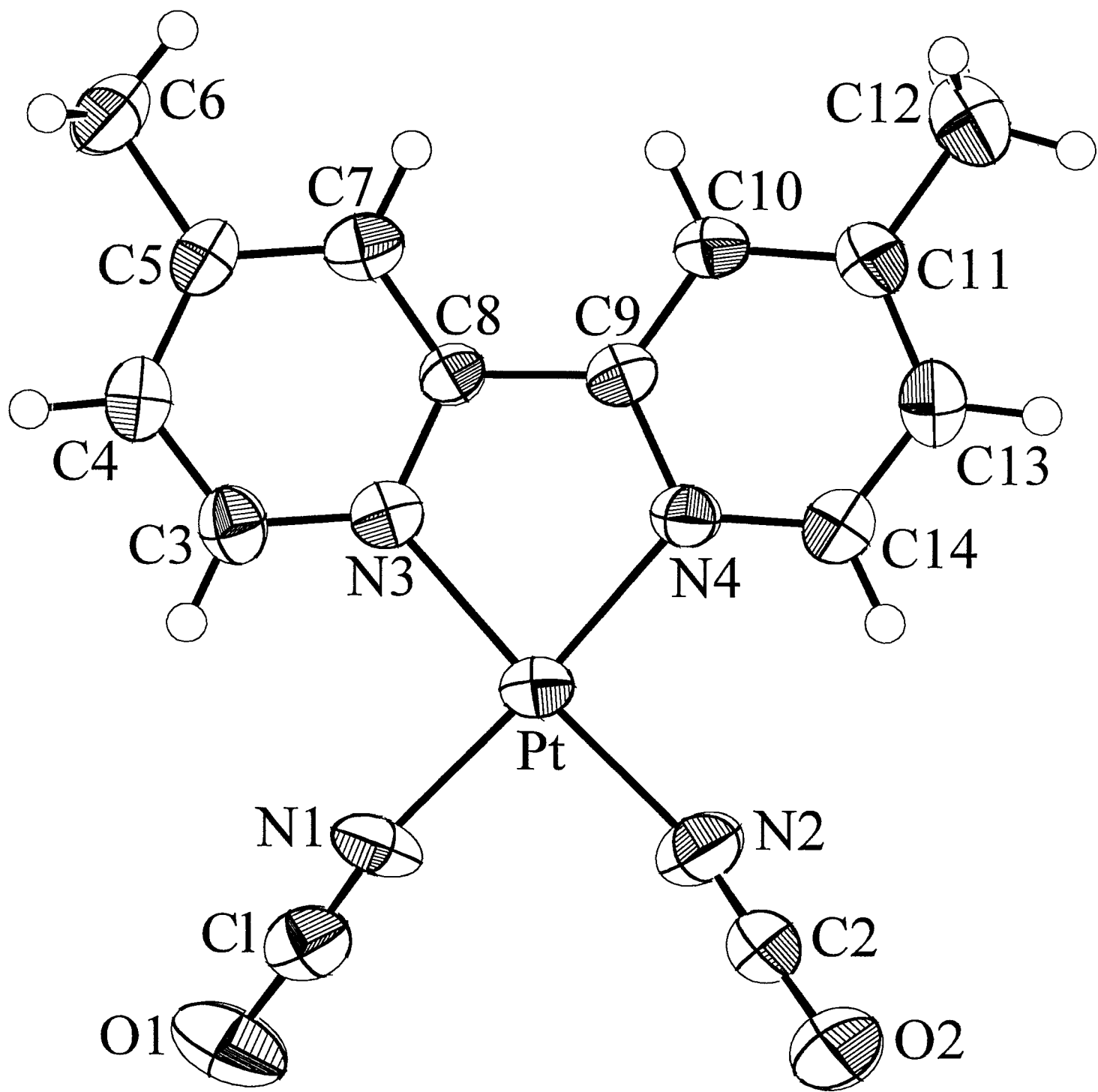


Fig. S5