JACS

JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

J. Am. Chem. Soc., 1997, 119(48), 11620-11627, DOI:10.1021/ja9723803

Table S1. Crystal and Intensity Collection Data for Pt(bpy)(bdt)

Formula: $PtC_{16}H_{12}N_2S_2$	Formula Weight: 491.49
Crystal Color: red	Habit: needle
Crystal Size: 0.15 x 0.18 x 0.26 mm	ρ_{calcd} = 2.18 g cm^{-3}
Crystal System: monoclinic	Space group: $P2_1/n$ (no. 14)
a = 8.206(2) Å	
b = 11.456(4) Å	β = 103.14(2)°
c = 16.350(4) Å	
V = 1496.8(7) Å^3	Z = 4
Lattice parameters: 25 reflections,	$6 \le \theta \le 11°$
μ = 97.33 cm^{-1}	Absorption correction: Ψ scans
Enraf-Nonius Cad-4 diffractometer	ω scans
MoKα, λ = 0.7107 Å	Graphite monochromator
2θ range: 2 - 50°	$-9 \le h \le 9, -13 \le k \le 13, 0 \le l \le 19$
T = 297 K	
Number of reflections measured: 5743	Number of independent reflections: 2634
Number with $F_o^2 > 0$: 2469	Number with $F_o^2 > 3\sigma(F_o^2)$: 2087
Standard reflections: 3 every 150 min.	Variation: within counting statistics
GOF_{merge}: 1.11 for 2500 multiples	R_{merge}: 0.024 for 2127 duplicates
Number used in refinement: 2634	Criterion: All reflections used

Final R on F: 0.033 for 2469 reflections with $F_o^2 > 0$

Final R on F: 0.024 for 2087 reflections with $F_o^2 > 3\sigma(F_o^2)$

Final weighted R_w on F_o^2: 0.053

Final GOF: 1.37 for 190 parameters and 2634 reflections

$(\Delta/\sigma)_{max}$ in final least squares cycle: < 0.005

$\Delta\rho_{max}$: 1.3 e Å^{-3}, $\Delta\rho_{min}$: -1.2 e Å^{-3} in final difference map

Definitions:

$GOF = \left(\sum w\left(F_o^2 - F_c^2\right)^2 / (n-p)\right)^{1/2}$ where n is the number of data and p is the number of parameters refined.

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

Table S2. Final Heavy Atom Parameters for Pt(bpy)(bdt)

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

Atom	x	y	z	U_{eq}
Pt	1425(.3)	1917(.2)	4101(.1)	367(.4)
S1	3055(2)	1221(1)	3281(1)	493(4)
S2	3139(2)	3469(1)	4398(1)	557(4)
N1	−313(6)	605(4)	3837(3)	417(11)
N2	−146(6)	2415(4)	4848(3)	443(12)
C1	−325(8)	−259(5)	3284(4)	513(15)
C2	−1582(9)	−1089(6)	3122(4)	616(18)
C3	−2838(9)	−1031(6)	3542(5)	642(19)
C4	−2839(8)	−157(6)	4113(4)	595(18)
C5	−1561(7)	667(5)	4248(4)	435(14)
C6	−1492(7)	1666(5)	4813(4)	481(15)
C7	−2675(8)	1925(7)	5277(4)	632(18)
C8	−2481(10)	2908(8)	5774(4)	733(22)
C9	−1136(10)	3602(7)	5820(4)	683(20)
C10	18(9)	3341(5)	5355(4)	588(17)
C11	4598(7)	2299(5)	3309(4)	431(14)
C12	5837(8)	2129(5)	2845(4)	529(16)
C13	7058(8)	2982(7)	2857(4)	636(19)
C14	7032(9)	3979(7)	3330(4)	704(21)
C15	5846(9)	4144(6)	3786(4)	611(18)

Table S2. (Cont.)

Atom	x	y	z	U_{eq}
C16	4620(7)	3293(5)	3781(4)	444(14)

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

Table S3. Assigned H Atom Parameters for Pt(bpy)(bdt)

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

Atom	x	y	z	B
H1	554	−303	2995	6.0
H2	−1570	−1691	2724	6.0
H3	−3710	−1595	3439	6.0
H4	−3701	−113	4413	6.0
H7	−3610	1427	5250	6.0
H8	−3293	3097	6085	6.0
H9	−986	4271	6172	6.0
H10	962	3837	5396	6.0
H12	5839	1436	2526	6.0
H13	7892	2879	2544	6.0
H14	7858	4563	3339	6.0
H15	5853	4836	4106	6.0

Table S4. Anisotropic Displacement Parameters for Pt(bpy)(bdt)

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Pt	385(1)	341(1)	367(1)	32(1)	67(1)	−37(1)
S1	504(9)	432(9)	575(10)	−6(7)	188(8)	−95(7)
S2	582(10)	454(9)	659(11)	−72(8)	192(9)	−169(8)
N1	438(28)	406(27)	389(26)	3(22)	56(22)	18(23)
N2	461(29)	457(28)	376(27)	126(25)	23(22)	7(23)
C1	531(39)	501(37)	487(36)	−60(30)	77(30)	−82(31)
C2	600(44)	552(42)	607(42)	−107(34)	−46(36)	−103(34)
C3	570(44)	614(46)	661(46)	−161(35)	−28(37)	58(38)
C4	445(37)	715(47)	615(42)	−14(35)	98(32)	141(38)
C5	368(32)	474(35)	430(33)	58(27)	20(26)	110(29)
C6	429(35)	580(42)	415(33)	156(30)	57(27)	90(30)
C7	542(40)	828(50)	570(40)	144(39)	221(33)	144(41)
C8	660(50)	1044(66)	530(43)	352(46)	211(38)	20(45)
C9	765(56)	738(49)	561(44)	286(41)	181(40)	−51(38)
C10	709(46)	528(42)	539(39)	120(33)	164(35)	−141(32)
C11	351(31)	510(37)	429(33)	42(26)	81(26)	78(28)
C12	579(39)	564(41)	433(35)	56(32)	89(30)	110(30)
C13	443(38)	952(58)	505(38)	−82(39)	90(30)	180(41)
C14	683(49)	825(55)	557(44)	−285(42)	42(38)	176(41)
C15	647(45)	590(43)	554(40)	−146(36)	47(34)	19(35)
C16	433(33)	475(37)	400(31)	6(28)	44(26)	28(28)

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

The form of the displacement factor is:

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

Table S5. Complete Distances and Angles for Pt(bpy)(bdt)

	Distance(Å)		Distance(Å)
Pt –S1	2.244(2)	C7 –C8	1.376(11)
Pt –S2	2.250(2)	C7 –H7	0.950
Pt –N1	2.050(4)	C8 –C9	1.349(11)
Pt –N2	2.049(5)	C8 –H8	0.950
S1 –C11	1.762(6)	C9 –C10	1.375(10)
S2 –C16	1.759(6)	C9 –H9	0.950
N1 –C1	1.338(7)	C10 –H10	0.950
N1 –C5	1.348(7)	C11 –C12	1.413(8)
N2 –C6	1.389(8)	C11 –C16	1.373(8)
N2 –C10	1.334(8)	C12 –C13	1.397(9)
C1 –C2	1.383(9)	C12 –H12	0.950
C1 –H1	0.950	C13 –C14	1.383(10)
C2 –C3	1.364(10)	C13 –H13	0.950
C2 –H2	0.950	C14 –C15	1.367(10)
C3 –C4	1.369(10)	C14 –H14	0.950
C3 –H3	0.950	C15 –C16	1.399(9)
C4 –C5	1.390(9)	C15 –H15	0.950
C4 –H4	0.950	S1 –H1	2.653
C5 –C6	1.464(8)	S2 –H10	2.712
C6 –C7	1.393(9)	H4 –H7	2.224

Table S5. (Cont.)

			Angle(°)				Angle(°)
S1	–Pt	–S2	89.0(1)	C4	–C3	–C2	119.8(6)
S1	–Pt	–N1	95.4(1)	H3	–C3	–C2	120.1
S1	–Pt	–N2	175.2(1)	H3	–C3	–C4	120.1
S2	–Pt	–N1	174.7(1)	C5	–C4	–C3	119.2(6)
S2	–Pt	–N2	95.7(1)	H4	–C4	–C3	120.4
N1	–Pt	–N2	80.1(2)	H4	–C4	–C5	120.4
Pt	–S1	–C11	104.9(2)	C4	–C5	–N1	121.1(5)
Pt	–S2	–C16	105.3(2)	C6	–C5	–N1	115.5(5)
Pt	–N1	–C1	125.6(4)	C6	–C5	–C4	123.4(5)
Pt	–N1	–C5	115.3(4)	C5	–C6	–N2	115.2(5)
Pt	–N2	–C10	127.1(4)	C7	–C6	–N2	119.4(5)
Pt	–N2	–C6	113.9(4)	C7	–C6	–C5	125.4(6)
C5	–N1	–C1	119.0(5)	C8	–C7	–C6	119.7(6)
C10	–N2	–C6	119.0(5)	H7	–C7	–C6	120.2
C2	–C1	–N1	121.9(6)	H7	–C7	–C8	120.2
H1	–C1	–N1	119.1	C9	–C8	–C7	119.9(7)
H1	–C1	–C2	119.1	H8	–C8	–C7	120.1
C3	–C2	–C1	119.1(6)	H8	–C8	–C9	120.1
H2	–C2	–C1	120.5	C10	–C9	–C8	120.0(7)
H2	–C2	–C3	120.5	H9	–C9	–C8	120.0

Table S5. (Cont.)

	Angle(°)		Angle(°)
H9 –C9 –C10	120.0	C15 –C16 –S2	120.4(5)
C9 –C10 –N2	122.1(6)	C15 –C16 –C11	119.9(5)
H10 –C10 –N2	119.0		
H10 –C10 –C9	119.0		
C12 –C11 –S1	119.3(4)		
C16 –C11 –S1	120.9(4)		
C16 –C11 –C12	119.8(5)		
C13 –C12 –C11	119.8(6)		
H12 –C12 –C11	120.1		
H12 –C12 –C13	120.1		
C14 –C13 –C12	118.9(6)		
H13 –C13 –C12	120.6		
H13 –C13 –C14	120.6		
C15 –C14 –C13	121.5(7)		
H14 –C14 –C13	119.3		
H14 –C14 –C15	119.3		
C16 –C15 –C14	120.1(6)		
H15 –C15 –C14	120.0		
H15 –C15 –C16	120.0		
C11 –C16 –S2	119.7(4)		

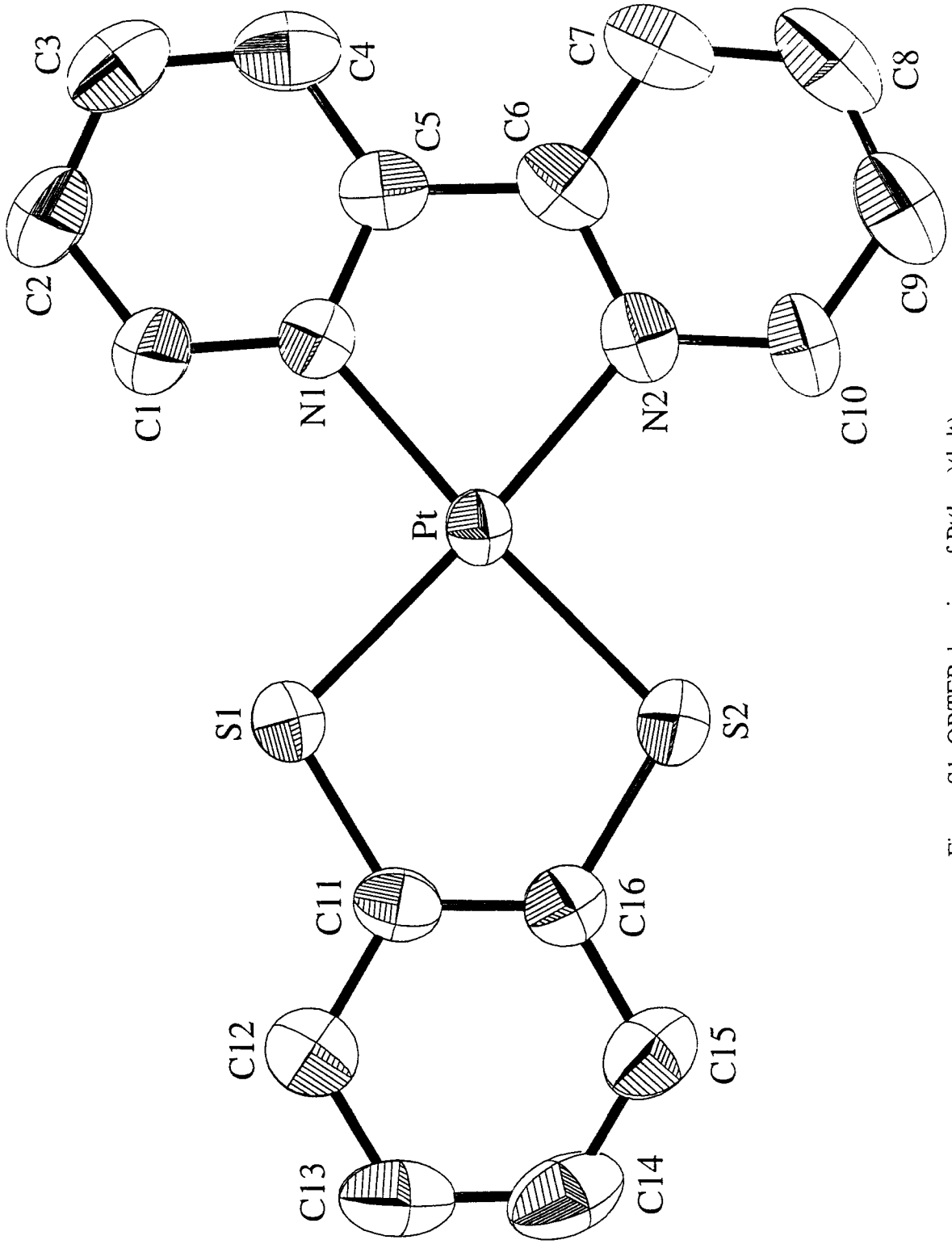

Figure S1. ORTEP drawing of Pt(bpy)(bdt)

Table S6. Crystal and Intensity Collection Data for Pt(bpy)($bdtO_2$)

Formula: $PtC_{16}H_{12}N_2O_{2.28}S_2$	Formula Weight: 527.96
Crystal Color: orange	Habit: needle
Crystal Size: 0.05 x 0.05 x 0.50 mm	ρ_{calcd} = 2.28 g cm^{-3}
Crystal System: monoclinic	Space group: $P2_1/c$ (no. 14)
a = 8.045(2) Å	
b = 14.629(3) Å	β = 101.71(2)°
c = 13.342(4) Å	
V = 1537.5(7) Å^3	Z = 4
Lattice parameters: 25 reflections.	$10 \le \theta \le 13°$
μ = 94.93 cm^{-1}	Absorption correction: Gaussian quadrature
Enraf-Nonius Cad-4 diffractometer	ω scans
MoKα, λ = 0.7107 Å	Graphite monochromator
2θ range: 2 - 50°	$0 \le h \le 9$, $-17 \le k \le 17$, $-15 \le l \le 15$
T = 293 K	
Number of reflections measured: 6125	Number of independent reflections: 2704
Number with $F_o^2 > 0$: 2493	Number with $F_o^2 > 3\sigma(F_o^2)$: 1993
Standard reflections: 3 every 150 min.	Variation: within counting statistics
GOF_{merge}: 0.97 for 2596 multiples	R_{merge}: 0.025 for 2078 duplicates
Number used in refinement: 2704	Criterion: All reflections used

Final R on F: 0.034 for 2493 reflections with $F_o^2 > 0$

Final R on F: 0.022 for 1993 reflections with $F_o^2 > 3\sigma(F_o^2)$

Final weighted R_w on F_o^2: 0.050

Final GOF: 1.19 for 228 parameters and 2704 reflections

$(\Delta/\sigma)_{max}$ in final least squares cycle: < 0.005

$\Delta\rho_{max}$: 0.9 e Å^{-3}, $\Delta\rho_{min}$: -0.9 e Å^{-3} in final difference map

Definitions:

$GOF = \left(\sum w\left(F_o^2 - F_c^2\right)^2 / (n-p)\right)^{1/2}$ where n is the number of data and p is the number of parameters refined.

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

Table S7. Final Heavy Atom Parameters for

$Pt(bpy)(bdtO_2)$

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

Atom	x	y	z	U_{eq}
Pt	2328(.3)	58(.1)	3681(.1)	309
N1	2445(5)	−65(3)	5242(3)	386(10)
N2	1269(6)	1288(3)	4004(4)	385(11)
S1	2127(2)	303(1)	2016(1)	395(3)
S2	3596(2)	−1291(1)	3502(1)	460(4)
O1[b]	2987(6)	1143(3)	1818(4)	525(12)
O2[b]	407(6)	230(3)	1443(3)	564(13)
O3[c]	4937(23)	−1478(14)	4156(14)	563(59)
O4[c]	2100(22)	−2034(12)	3382(15)	543(53)
C1	3012(8)	−800(4)	5815(5)	514(17)
C2	3060(9)	−816(5)	6859(5)	543(18)
C3	2508(8)	−79(5)	7313(5)	610(19)
C4	1930(8)	681(5)	6729(5)	509(17)
C5	1906(7)	676(4)	5694(4)	405(14)
C6	1334(7)	1449(4)	5010(5)	417(14)
C7	851(9)	2293(5)	5325(5)	599(18)
C8	268(9)	2964(4)	4639(6)	651(21)
C9	106(8)	2779(4)	3621(6)	566(18)
C10	648(8)	1943(4)	3320(5)	494(16)
C11	3941(7)	−1277(4)	2238(4)	386(14)

Table S7. (Cont.)

Atom	x	y	z	U_{eq}
C12	4904(8)	−1972(4)	1884(5)	489(16)
C13	5095(9)	−1969(5)	891(6)	608(19)
C14	4372(9)	−1289(5)	205(5)	598(18)
C15	3453(9)	−603(4)	548(5)	488(16)
C16	3270(7)	−591(3)	1561(4)	371(13)

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

[b] Refined to 92.8% occupancy.

[c] Refined to 22.5% occupancy.

Table S8. Assigned Hydrogen Atom Parameters for $Pt(bpy)(bdtO_2)$

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

Atom	x	y	z	B
H1	3388	−1320	5497	4.7
H2	3476	−1340	7252	4.9
H3	2517	−84	8027	5.5
H4	1552	1205	7040	4.6
H7	929	2405	6034	5.4
H8	−20	3549	4863	5.9
H9	−376	3219	3123	5.1
H10	581	1828	2612	4.5
H12	5418	−2439	2337	4.4
H13	5735	−2442	660	5.5
H14	4511	−1299	−486	5.4
H15	2944	−137	90	4.4

Table S9. Anisotropic Displacement Parameters for Pt(bpy)(bdtO$_4$)·(H$_2$O)

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Pt	309(1)	304(1)	319(1)	6(1)	75(1)	2(1)
N1	311(24)	489(27)	356(24)	−11(25)	62(20)	0(25)
N2	295(26)	366(25)	500(30)	−2(20)	98(24)	−28(22)
S1	418(9)	386(7)	394(8)	31(6)	112(7)	32(6)
S2	578(11)	360(8)	461(9)	73(7)	148(9)	46(7)
O1[a]	642(34)	366(25)	607(32)	−3(22)	219(27)	34(21)
O2[a]	414(28)	807(35)	460(27)	102(24)	66(22)	−12(24)
O3[b]	407(125)	861(149)	422(120)	99(101)	87(100)	125(98)
O4[b]	396(121)	499(109)	771(146)	−138(88)	204(108)	11(94)
C1	473(41)	568(39)	482(40)	37(32)	50(34)	76(31)
C2	475(42)	754(46)	406(39)	51(35)	105(33)	114(33)
C3	447(37)	1031(56)	359(32)	−108(43)	101(29)	3(40)
C4	379(38)	728(44)	428(38)	−8(33)	104(32)	−120(32)
C5	317(34)	455(33)	441(36)	−85(27)	70(29)	−109(27)
C6	304(32)	433(32)	534(39)	−37(26)	131(30)	−126(28)
C7	547(44)	607(42)	664(46)	25(35)	171(38)	−217(36)
C8	578(49)	458(38)	935(60)	108(34)	196(44)	−134(38)
C9	427(40)	477(36)	823(53)	121(30)	198(38)	35(35)
C10	470(41)	460(34)	568(41)	75(30)	143(34)	25(30)
C11	313(32)	341(29)	517(37)	−67(25)	115(28)	−66(26)
C12	384(37)	401(32)	688(46)	−3(27)	121(34)	−100(30)
C13	488(45)	568(42)	835(56)	−61(33)	296(42)	−336(38)
C14	689(49)	614(42)	573(44)	−14(38)	321(39)	−121(34)
C15	652(45)	440(34)	412(36)	−29(32)	205(34)	13(27)
C16	336(32)	315(28)	496(36)	−83(24)	163(28)	−50(25)

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

The form of the displacement factor is:

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

[a] Refined to 92.8% occupancy.

[b] Refined to 22.5% occupancy.

Table S10. Complete Distances and Angles for $Pt(bpy)(bdtO_2)$

	Distance(Å)		Distance(Å)
Pt –N1	2.074(4)	C14 –H14	0.950
Pt –N2	2.075(4)	C15 –C16	1.390(8)
Pt –S1	2.223(1)	C15 –H15	0.950
Pt –S2	2.256(2)		
S1 –C11	2.717(6)		
S2 –C16	2.747(6)		
N1 –C1	1.345(8)		
N1 –C5	1.354(7)		
N2 –C6	1.352(7)		
N2 –C10	1.347(8)		
S1 –O1	1.460(5)		
S1 –O2	1.442(5)		
S2 –O3	1.272(19)		
S2 –O4	1.605(18)		
C1 –C2	1.385(9)		
C1 –H1	0.950		
C2 –C3	1.356(9)		
C2 –H2	0.950		
C3 –C4	1.384(9)		
C3 –H3	0.950		
C4 –C5	1.376(9)		
C4 –H4	0.950		
C5 –C6	1.468(8)		
C6 –C7	1.385(9)		
C7 –C8	1.359(10)		
C7 –H7	0.950		
C8 –C9	1.365(10)		
C8 –H8	0.950		
C9 –C10	1.385(9)		
C9 –H9	0.950		
C10 –H10	0.950		
C11 –C12	1.416(8)		
C11 –C16	1.385(8)		
C12 –C13	1.364(9)		
C12 –H12	0.950		
C13 –C14	1.396(10)		
C13 –H13	0.950		
C14 –C15	1.379(9)		

Table S10. (Cont.)

			Angle(°)				Angle(°)
N1	-Pt	-N2	78.6(2)	C7	-C6	-N2	119.9(5)
S1	-Pt	-S2	88.8(1)	C7	-C6	-C5	124.7(5)
S1	-Pt	-N1	175.4(1)	C8	-C7	-C6	121.3(6)
S1	-Pt	-N2	96.8(1)	H7	-C7	-C6	119.3
S2	-Pt	-N1	95.8(1)	H7	-C7	-C8	119.3
S2	-Pt	-N2	174.1(1)	C9	-C8	-C7	118.4(7)
Pt	-S1	-C11	79.9(1)	H8	-C8	-C7	120.8
Pt	-S1	-O1	112.0(2)	H8	-C8	-C9	120.8
Pt	-S1	-O2	112.6(2)	C10	-C9	-C8	119.5(6)
C11	-S1	-O1	118.2(2)	H9	-C9	-C8	120.3
C11	-S1	-O2	115.6(2)	H9	-C9	-C10	120.3
O1	-S1	-O2	113.9(3)	C9	-C10	-N2	121.8(6)
Pt	-S2	-C16	79.3(1)	H10	-C10	-N2	119.1
Pt	-S2	-O3	116.9(9)	H10	-C10	-C9	119.1
Pt	-S2	-O4	104.9(7)	C16	-C11	-C12	118.0(5)
C16	-S2	-O3	129.2(9)	C13	-C12	-C11	120.0(6)
C16	-S2	-O4	103.4(7)	H12	-C12	-C11	120.0
O3	-S2	-O4	115.9(11)	H12	-C12	-C13	120.0
C5	-N1	-C1	119.2(5)	C14	-C13	-C12	121.7(6)
C10	-N2	-C6	118.9(5)	H13	-C13	-C12	119.2
O2	-S1	-O1	113.9(3)	H13	-C13	-C14	119.2
O4	-S2	-O3	115.9(11)	C15	-C14	-C13	118.8(6)
C2	-C1	-N1	121.5(6)	H14	-C14	-C13	120.6
H1	-C1	-N1	119.2	H14	-C14	-C15	120.6
H1	-C1	-C2	119.2	C16	-C15	-C14	120.1(6)
C3	-C2	-C1	119.4(6)	H15	-C15	-C14	119.9
H2	-C2	-C1	120.3	H15	-C15	-C16	119.9
H2	-C2	-C3	120.3	C15	-C16	-C11	121.4(5)
C4	-C3	-C2	119.4(6)				
H3	-C3	-C2	120.3				
H3	-C3	-C4	120.3				
C5	-C4	-C3	119.7(6)				
H4	-C4	-C3	120.2				
H4	-C4	-C5	120.2				
C4	-C5	-N1	120.8(5)				
C6	-C5	-N1	115.3(5)				
C6	-C5	-C4	123.9(5)				
C5	-C6	-N2	115.3(5)				

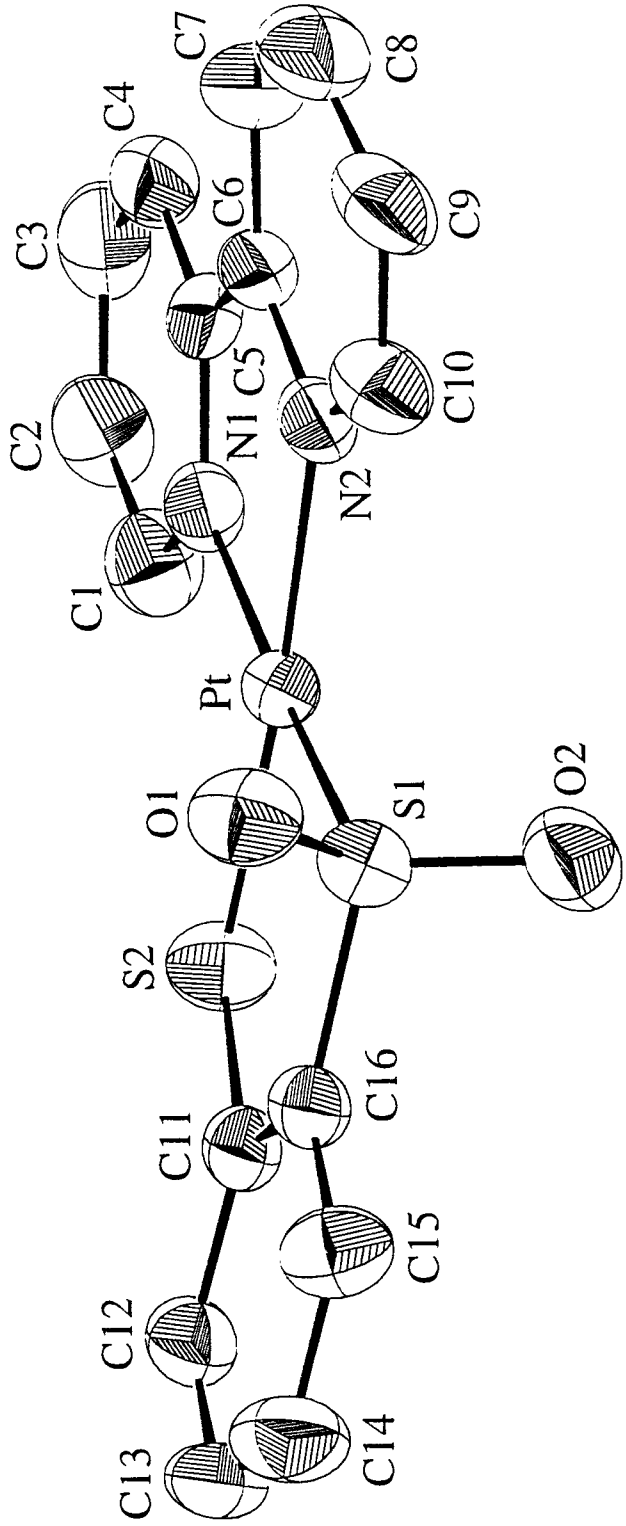

Figure S2. ORTEP drawing of Pt(bpy)(bdtO$_2$)

Table S11. Crystal and Intensity Collection Data for $Pt(bpy)(bdtO_4)\cdot H_2O$

Formula: $PtC_{16}H_{12}N_2O_4S_2\cdot H_2O$	Formula Weight: 573.50
Crystal Color: yellow	Habit: plate
Crystal Size: 0.2 x 0.5 x 1.0 mm	$\rho_{calcd} = 2.28$ g cm^{-3}
Crystal System: monoclinic	Space group: $P2_1/c$ (no. 14)
$a = 11.513(2)$ Å	
$b = 7.103(1)$ Å	$\beta = 101.64(1)^\circ$
$c = 20.865(3)$ Å	
V = 1670.5(4) Å^3	$Z = 4$
Lattice parameters: 25 reflections.	$11 \le \theta \le 13^\circ$
$\mu = 87.58$ cm^{-1}	Absorption correction: Ψ scans
Enraf-Nonius Cad-4 diffractometer	ω scans
MoKα, $\lambda = 0.7107$ Å	Graphite monochromator
2θ range: 2 - 50°	$0 \le h \le 13$, $-8 \le k \le 8$, $-24 \le l \le 24$
T = 293 K	
Number of reflections measured: 6449	Number of independent reflections: 2943
Number with $F_o^2 > 0$: 2151	Number with $F_o^2 > 3\sigma(F_o^2)$: 2775
Standard reflections: 3 every 150 min.	Variation: within counting statistics
GOF_{merge}: 1.34 for 2671 multiples	R_{merge}: 0.040 for 2199 duplicates
Number used in refinement: 2943	Criterion: All reflections used

Final R on F: 0.055 for 2775 reflections with $F_o^2 > 0$

Final R on F: 0.039 for 2151 reflections with $F_o^2 > 3\sigma(F_o^2)$

Final weighted R_w on F_o^2: 0.082

Final GOF: 1.71 for 235 parameters and 2943 reflections

$(\Delta/\sigma)_{max}$ in final least squares cycle: < 0.005

$\Delta\rho_{max}$: 1.3 e Å^{-3}, $\Delta\rho_{min}$: -1.6 e Å^{-3} in final difference map

Definitions:

$GOF = \left(\sum w\left(F_o^2 - F_c^2\right)^2 / (n-p)\right)^{1/2}$ where n is the number of data and p is the number of parameters refined.

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

Table S12. Final Heavy Atom Parameters for $Pt(bpy)(bdtO_4)\cdot H_2O$

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

Atom	x	y	z	U_{eq}
Pt	1275(.4)	2134(.5)	1010(.2)	294(1)
S1	1757(2)	2178(4)	2103(1)	412(6)
S2	3170(3)	1654(4)	987(1)	400(7)
O1	1586(7)	4043(12)	2366(3)	620(24)
O2	1222(8)	676(13)	2398(4)	715(28)
O3	3693(7)	3204(11)	687(4)	633(23)
O4	3375(8)	−174(11)	702(4)	630(23)
N1	−510(7)	2630(11)	957(4)	381(21)
N2	668(10)	2210(12)	3(4)	529(32)
C1	−1091(10)	2735(17)	1458(5)	490(29)
C2	−2271(10)	3164(16)	1372(5)	513(30)
C3	−2925(10)	3492(16)	765(6)	551(35)
C4	−2340(11)	3378(14)	241(5)	489(31)
C5	−1180(9)	2932(14)	343(4)	340(22)
C6	−489(10)	2701(14)	−192(4)	410(29)
C7	−1013(11)	2944(16)	−846(5)	539(31)
C8	−347(11)	2666(16)	−1307(5)	538(32)
C9	868(12)	2162(16)	−1123(5)	545(31)
C10	1291(9)	1941(14)	−463(5)	400(25)

Table S12. (Cont.)

Atom	x	y	z	U_{eq}
C11	3313(10)	1764(13)	2302(5)	391(28)
C12	3916(10)	1723(14)	2958(5)	446(28)
C13	5124(11)	1487(15)	3104(5)	491(31)
C14	5738(10)	1278(16)	2605(6)	517(32)
C15	5152(10)	1308(15)	1957(5)	454(28)
C16	3964(9)	1570(13)	1813(5)	355(25)
OW	4424(10)	1945(18)	9481(5)	1253(41)

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

Table S13. Assigned H Atom Parameters for $Pt(bpy)(bdtO_4)\cdot H_2O$

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

Atom	x	y	z	B
H1	−661	2501	1890	5.0
H2	−2637	3232	1741	5.0
H3	−3745	3787	699	5.0
H4	−2764	3617	−192	5.0
H7	−1823	3299	−969	5.0
H8	−698	2810	−1758	5.0
H9	1356	1990	−1435	5.0
H10	2095	1565	−327	5.0
H12	3489	1859	3300	5.0
H13	5535	1468	3547	5.0
H14	6574	1113	2707	5.0
H15	5580	1145	1616	5.0

Table S14. Anisotropic Displacement Parameters for $Pt(bpy)(bdtO_4)\cdot H_2O$

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Pt	314(2)	338(2)	234(2)	−32(2)	64(1)	−10(2)
S1	403(15)	590(17)	244(11)	−24(15)	71(10)	3(13)
S2	382(16)	489(19)	336(13)	−15(13)	88(12)	−30(11)
O3	635(60)	752(63)	552(48)	−149(49)	212(42)	134(42)
O4	619(62)	670(57)	602(51)	117(45)	129(44)	−258(41)
O1	553(59)	812(63)	491(47)	128(47)	96(41)	−174(41)
O2	495(60)	1116(75)	521(51)	−156(53)	75(43)	213(47)
OW	1087(92)	2090(126)	626(60)	508(92)	278(60)	285(72)
N1	429(53)	366(55)	324(41)	−57(42)	16(36)	14(36)
N2	1133(91)	281(46)	185(38)	−74(59)	160(48)	−3(37)
C1	426(74)	693(83)	363(53)	−71(66)	110(48)	−82(52)
C2	410(73)	619(84)	553(67)	−106(61)	202(55)	−121(58)
C3	325(70)	663(86)	604(75)	4(59)	−48(56)	−123(59)
C4	506(79)	428(75)	485(65)	−15(56)	−16(55)	28(48)
C5	345(59)	287(50)	377(51)	3(52)	45(42)	−43(46)
C6	614(78)	228(57)	338(51)	−45(56)	−25(49)	86(43)
C7	744(91)	455(63)	367(59)	−62(69)	−6(56)	87(51)
C8	629(83)	590(84)	351(56)	−139(67)	−7(54)	17(52)
C9	935(99)	464(64)	285(51)	−272(74)	237(57)	−63(50)
C10	374(62)	405(63)	420(56)	−40(55)	77(46)	−16(50)
C11	507(73)	280(67)	368(54)	−34(50)	45(49)	30(42)
C12	485(74)	478(76)	373(56)	−63(56)	82(50)	16(47)
C13	444(77)	469(71)	485(65)	−67(56)	−86(55)	7(50)
C14	391(74)	476(70)	645(77)	−7(58)	11(59)	20(58)
C15	470(77)	425(64)	486(64)	−52(56)	143(56)	−17(51)
C16	307(62)	336(62)	404(57)	−9(45)	31(46)	10(42)

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

The form of the displacement factor is:

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

Table S15. Complete Distances and Angles for

$Pt(bpy)(bdtO_4)\cdot H_2O$

	Distance(Å)		Distance(Å)
Pt –S1	2.235(3)	C7 –C8	1.361(16)
Pt –S2	2.218(3)	C8 –C9	1.420(16)
Pt –N1	2.065(8)	C9 –C10	1.373(15)
Pt –N2	2.076(9)	C11 –C12	1.404(14)
S1 –O1	1.462(8)	C11 –C16	1.388(14)
S1 –O2	1.430(9)	C12 –C13	1.373(15)
S1 –C11	1.780(10)	C13 –C14	1.379(16)
S2 –O3	1.455(8)	C14 –C15	1.383(16)
S2 –O4	1.467(9)	C15 –C16	1.353(15)
S2 –C16	1.781(10)		
N1 –C1	1.352(13)		
N1 –C5	1.372(12)		
N2 –C6	1.357(14)		
N2 –C10	1.333(14)		
C1 –C2	1.369(16)		
C2 –C3	1.357(16)		
C3 –C4	1.397(16)		
C4 –C5	1.348(15)		
C5 –C6	1.505(14)		
C6 –C7	1.385(15)		

Table S15. (Cont.)

	Angle(°)		Angle(°)
S1 –Pt –S2	88.9(1)	C16 –S2 –O3	105.3(5)
N1 –Pt –N2	79.3(3)	C16 –S2 –O4	105.6(5)
N1 –Pt –S1	95.3(2)	C5 –N1 –C1	116.1(8)
N1 –Pt –S2	175.6(2)	C10 –N2 –C6	117.2(9)
N2 –Pt –S1	174.3(3)	C2 –C1 –N1	123.0(10)
N2 –Pt –S2	96.5(3)	C3 –C2 –C1	120.6(11)
Pt –S1 –C11	105.4(3)	C4 –C3 –C2	117.2(11)
Pt –S2 –C16	107.4(3)	C5 –C4 –C3	120.5(10)
Pt –N1 –C1	127.6(7)	C4 –C5 –N1	122.5(9)
Pt –N1 –C5	116.3(6)	C6 –C5 –N1	113.2(8)
Pt –N2 –C10	127.8(7)	C6 –C5 –C4	124.3(9)
Pt –N2 –C6	114.8(7)	C5 –C6 –N2	116.0(9)
Pt –S1 –O1	111.8(3)	C7 –C6 –N2	122.3(10)
Pt –S1 –O2	112.8(4)	C7 –C6 –C5	121.7(9)
Pt –S2 –O3	112.8(3)	C8 –C7 –C6	118.8(10)
Pt –S2 –O4	112.6(3)	C9 –C8 –C7	120.7(10)
O2 –S1 –O1	114.3(5)	C10 –C9 –C8	115.6(10)
C11 –S1 –O1	105.5(5)	C9 –C10 –N2	125.5(10)
C11 –S1 –O2	106.1(5)	C12 –C11 –S1	120.5(8)
O4 –S2 –O3	112.4(5)	C16 –C11 –S1	120.8(8)

Table S15. (Cont.)

	Angle(°)
C16 –C11 –C12	118.6(9)
C13 –C12 –C11	119.9(10)
C14 –C13 –C12	119.8(10)
C15 –C14 –C13	120.8(11)
C16 –C15 –C14	119.4(10)
C11 –C16 –S2	117.3(7)
C15 –C16 –S2	121.2(8)
C15 –C16 –C11	121.5(9)

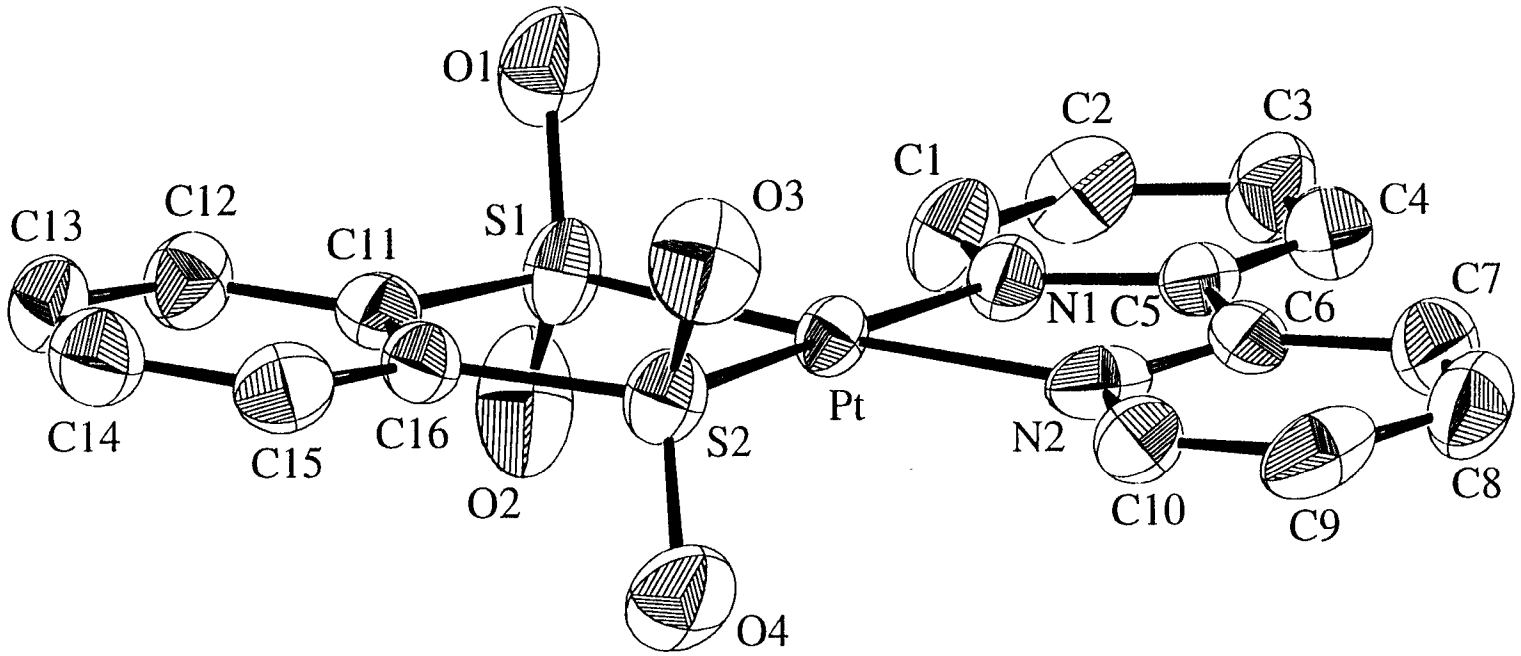

Figure S3. ORTEP drawing of Pt(bpy)($bdtO_4$)