

APPENDIX

Publications in other areas

1. *Dalton Transactions* (DOI: 10.1039/210112158A (2012))

2. *Acta Crystallographica* **E63**, 2073–2007;

CHAPTER II

TABLE I
Bond Lengths (Å) and Bond Angles (°) for (**5a**)

Bond Lengths (Å)		Bond Lengths (Å)	
C(16)-C(17)	1.366(5)	C(4)-O(1)	1.354(5)
C(16)-C(15)	1.387(6)	C(4)-C(3)	1.388(5)
C(16)-H(16)	0.9300	C(4)-C(9)	1.429(6)
C(11)-O(1)	1.415(6)	C(14)-H(14)	0.9300
C(11)-H(11A)	0.9600	C(18)-C(19)	1.492(4)
C(11)-H(11B)	0.9600	C(18)-H(18A)	0.9700
C(11)-H(11C)	0.9600	C(18)-H(18B)	0.9700
Pd(1)-N(2)	1.976(3)	C(15)-H(15)	0.9300
Pd(1)-C(2)	1.995(3)	C(19)-C(20)	1.377(5)
Pd(1)-Cl(1)	2.2939(11)	C(19)-C(24)	1.397(5)
Pd(1)-S(1)	2.3499(9)	C(24)-C(23)	1.359(6)
S(1)-O(2)	1.475(2)	C(24)-H(24)	0.9300
S(1)-C(13)	1.788(3)	C(17)-H(17)	0.9300
S(1)-C(18)	1.818(4)	C(5)-C(6)	1.363(7)
N(2)-N(1)	1.287(4)	C(5)-H(5)	0.9300
N(2)-C(12)	1.409(4)	C(3)-H(3)	0.9300
C(2)-C(3)	1.384(5)	C(8)-C(7)	1.375(6)
C(2)-C(1)	1.408(5)	C(8)-H(8)	0.9300
N(1)-C(1)	1.364(5)	C(20)-C(21)	1.383(6)
C(13)-C(14)	1.390(5)	C(20)-H(20)	0.9300
C(13)-C(12)	1.400(5)	C(7)-C(6)	1.384(7)
C(12)-C(11)	1.389(5)	C(7)-H(7)	0.9300
C(10)-C(8)	1.404(6)	C(21)-C(22)	1.387(8)
C(10)-C(9)	1.414(6)	C(21)-H(21)	0.9300
C(10)-C(1)	1.443(5)	C(23)-C(22)	1.370(8)
C(9)-C(5)	1.421(5)	C(23)-H(23)	0.9300
C(4)-C(15)	1.371(5)	C(22)-H(22)	0.9300
		C(6)-H(6)	0.9300

Bond Angles (°)		Bond Angles (°)	
C(17)-C(16)-C(15)	121.1(4)	C(19)-C(18)-H(18A)	109.0
C(17)-C(16)-H(16)	119.5	S(1)-C(18)-H(18A)	109.0
C(15)-C(16)-H(16)	119.8	C(19)-C(18)-H(18B)	109.0
O(1)-C(11)-H(11A)	109.5	S(1)-C(18)-H(18B)	109.0
O(1)-C(11)-H(11B)	109.5	H(18A)-C(18)-H(18B)	107.8
H(11A)-C(11)-H(11B)	109.5	C(14)-C(15)-C(16)	120.2(4)
O(1)-C(11)-H(11C)	109.5	C(14)-C(15)-H(15)	119.9
H(11A)-C(11)-H(11C)	109.5	C(16)-C(15)-H(15)	119.9
H(11B)-C(11)-H(11C)	109.5	C(20)-C(19)-C(24)	118.9(3)
N(2)-Pd(1)-C(2)	79.24(13)	C(20)-C(19)-C(18)	120.6(3)
N(2)-Pd(1)-Cl(1)	174.89(8)	C(24)-C(19)-C(18)	120.6(3)
C(2)-Pd(1)-Cl(1)	97.48(11)	C(23)-C(24)-C(19)	120.3(4)
N(2)-Pd(1)-S(1)	84.69(8)	C(23)-C(24)-H(24)	119.8
C(2)-Pd(1)-S(1)	163.62(11)	C(19)-C(24)-H(24)	119.8
Cl(1)-Pd(1)-S(1)	98.33(4)	C(16)-C(17)-C(12)	119.7(4)
O(2)-S(1)-C(13)	110.06(15)	C(16)-C(17)-H(17)	120.2
O(2)-S(1)-C(18)	105.86(15)	C(12)-C(17)-H(17)	120.2
C(13)-S(1)-C(18)	101.54(15)	C(6)-C(5)-C(9)	120.4(5)
O(2)-S(1)-Pd(1)	128.07(11)	C(6)-C(5)-H(5)	119.8
C(13)-S(1)-Pd(1)	97.18(11)	C(9)-C(5)-H(5)	119.8
C(18)-S(1)-Pd(1)	110.93(11)	C(2)-C(3)-C(14)	120.0(4)
N(1)-N(2)-C(12)	118.2(3)	C(2)-C(3)-H(3)	120.0
N(1)-N(2)-Pd(1)	119.8(2)	C(4)-C(3)-H(3)	120.0
C(12)-N(2)-Pd(1)	121.9(2)	C(7)-C(8)-C(10)	119.8(5)
C(3)-C(2)-C(1)	120.0(3)	C(7)-C(8)-H(8)	120.1
C(3)-C(2)-Pd(1)	130.2(3)	C(10)-C(8)-H(8)	120.1
C(1)-C(2)-Pd(1)	109.7(2)	C(19)-C(20)-C(21)	120.5(4)
N(2)-N(1)-C(1)	111.4(3)	C(19)-C(20)-H(20)	119.8
C(14)-C(13)-C(12)	120.3(3)	C(21)-C(20)-H(20)	119.8
C(14)-C(13)-S(1)	120.8(3)	C(8)-C(7)-C(6)	121.3(5)
C(12)-C(13)-S(1)	118.8(2)	C(8)-C(7)-H(7)	119.4
C(17)-C(12)-C(13)	119.3(3)	C(6)-C(7)-H(7)	119.4
C(17)-C(12)-N(2)	123.3(3)	C(20)-C(21)-C(22)	119.9(4)
C(13)-C(12)-N(2)	117.4(3)	C(20)-C(21)-H(21)	120.1
C(8)-C(10)-C(9)	119.4(3)	C(22)-C(21)-H(21)	120.1
C(8)-C(10)-C(1)	122.6(4)	C(24)-C(23)-C(22)	121.0(5)
C(9)-C(10)-C(1)	117.9(3)	C(24)-C(23)-H(23)	119.5

O(1)-C(4)-C(3)	123.9(4)	C(22)-C(23)-H(23)	119.5
O(1)-C(4)-C(9)	114.2(3)	C(23)-C(22)-C(21)	119.4(4)
C(3)-C(4)-C(9)	121.9(3)	C(23)-C(22)-H(22)	120.3
C(4)-O(1)-C(11)	119.2(3)	C(21)-C(22)-H(22)	120.3
C(10)-C(9)-C(5)	118.7(4)	C(5)-C(6)-C(7)	120.4(4)
C(10)-C(9)-C(4)	118.9(3)	C(5)-C(6)-H(6)	119.8
C(5)-C(9)-C(4)	122.3(4)	C(7)-C(6)-H(6)	119.8
C(15)-C(14)-C(13)	119.4(4)	N(1)-C(1)-C(2)	119.8(3)
C(15)-C(14)-H(14)	120.3	N(1)-C(1)-C(10)	119.0(3)
C(13)-C(14)-H(14)	120.3	C(2)-C(1)-C(10)	121.2(3)
C(19)-C(18)-S(1)	113.0(2)		

TABLE 2
Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{Å}^2 \times 10^3$) for **5 a**

	x	y	z	U(eq)
C(16)	-4016(5)	7650(4)	2234(4)	57(1)
C(11)	3502(6)	-1134(5)	-675(4)	70(1)
Pd(1)	842(1)	2816(1)	2033(1)	38(1)
S(1)	312(1)	3890(1)	3482(1)	37(1)
Cl(1)	2961(1)	829(1)	2654(1)	67(1)
N(2)	-1070(3)	4409(3)	1481(2)	39(1)
C(2)	678(4)	2299(4)	706(3)	41(1)
N(1)	-1609(3)	4433(3)	625(2)	44(1)
C(13)	-1379(4)	5393(3)	2996(3)	38(1)
O(2)	1366(3)	4369(3)	3915(2)	50(1)
C(12)	-1924(4)	5494(3)	2028(3)	40(1)
C(10)	-1131(5)	3130(4)	-746(3)	48(1)
C(4)	1199(5)	941(4)	-617(3)	50(1)
O(1)	2055(4)	-153(3)	-1087(2)	65(1)
C(9)	-192(5)	1906(4)	-1138(3)	51(1)
C(14)	-2145(4)	6445(4)	3564(3)	49(1)
C(1)	-675(4)	3304(4)	199(3)	43(1)
C(18)	-563(4)	2901(4)	4621(3)	43(1)
C(15)	-3464(5)	7562(4)	3184(3)	54(1)
C(19)	-1832(4)	2502(4)	4339(3)	41(1)
C(24)	-1456(5)	1283(4)	3938(3)	56(1)
C(17)	-3260(4)	6637(4)	1657(3)	51(1)
C(5)	-698(6)	1651(5)	-2011(3)	63(1)
C(3)	1614(4)	1137(4)	288(3)	46(1)
C(8)	-2493(5)	4090(5)	-1256(3)	60(1)
C(20)	-3393(4)	3338(4)	4458(3)	53(1)
C(7)	-2929(6)	3807(6)	-2105(3)	71(1)
C(21)	-4566(5)	2983(6)	4175(4)	73(1)
C(23)	-2615(6)	937(6)	3666(4)	79(1)
C(22)	-4170(6)	1767(7)	3781(4)	85(2)
C(6)	-2049(6)	2587(6)	-2472(3)	72(1)

TABLE 3
Bond Lengths (Å) and Bond Angles (°) for (**2b**)

Bond Lengths (Å)		Bond Lengths (Å)	
Pd(1)-C(8)	2.008(2)	C(17)-H(17A)	0.9600
Pd(1)-N(2)	2.0110(18)	C(17)-H(17B)	0.9600
Pd(1)-S(02)	2.3060(6)	C(17)-H(17C)	0.9600
Pd(1)-Cl(1)	2.3335(6)	C(19)-H(19A)	0.9600
S(02)-O(2)	1.4798(17)	C(19)-H(19B)	0.9600
S(02)-C(12)	1.777(2)	C(19)-H(19C)	0.9600
S(02)-C(18)	1.786(3)	C(11)-C(16)	1.384(3)
N(2)-N(1)	1.269(3)	C(11)-C(12)	1.386(3)
N(2)-C(11)	1.464(3)	C(1)-C(2)	1.396(3)
N(1)-C(1)	1.369(3)	O(1)-C(4)	1.340(3)
C(8)-C(7)	1.388(3)	O(1)-C(17)	1.441(3)
C(8)-C(10)	1.417(3)	C(4)-C(3)	1.375(3)
C(9)-C(5)	1.404(3)	C(7)-C(6)	1.397(4)
C(9)-C(10)	1.429(3)	C(7)-H(7)	0.9300
C(9)-C(4)	1.436(3)	C(16)-C(15)	1.381(4)
C(13)-C(14)	1.375(4)	C(16)-H(16)	0.9300
C(13)-C(12)	1.392(3)	C(2)-C(3)	1.382(4)
C(13)-H(13)	0.9300	C(2)-H(2)	0.9300
C(10)-C(1)	1.445(3)	C(18)-C(19)	1.510(4)
C(5)-H(5)	0.9300	C(18)-H(18A)	0.9700
C(3)-H(3)	0.9300	C(18)-H(18B)	0.9700
C(15)-C(14)	1.374(4)	C(5)-C(6)	1.352(4)
C(15)-H(15)	0.9300	C(14)-H(14)	0.9300
C(6)-H(6)	0.9300		
Bond Angles (°)		Bond Angles (°)	
C(8)-Pd(1)-N(2)	91.76(8)	C(3)-C(2)-C(1)	123.0(2)
C(8)-Pd(1)-S(02)	176.70(6)	C(3)-C(2)-H(2)	118.5
N(2)-Pd(1)-S(02)	86.19(5)	C(1)-C(2)-H(2)	118.5
C(8)-Pd(1)-Cl(1)	96.05(6)	C(19)-C(18)-S(02)	127.43(19)
N(2)-Pd(1)-Cl(1)	169.67(6)	C(19)-C(18)-H(18A)	109.1
S(02)-Pd(1)-Cl(1)	86.31(2)	C(19)-C(18)-H(18B)	109.1
O(2)-S(02)-C(12)	110.17(11)	S(02)-C(18)-H(18B)	109.1
O(2)-S(02)-C(18)	107.66(12)	H(18A)-C(18)-H(18B)	107.8
C(12)-S(02)-C(18)	102.23(13)	C(6)-C(5)-C(9)	119.7(2)
O(2)-S(02)-Pd(1)	172.82(9)	C(6)-C(5)-H(5)	120.2
C(12)-S(02)-Pd(1)	98.88(8)	C(9)-C(5)-H(5)	120.2
C(18)-S(02)-Pd(1)	112.85(10)	C(4)-C(3)-C(2)	118.8(1)
N(1)-N(2)-C(11)	111.69(18)	C(4)-C(3)-H(3)	120.6
N(1)-N(2)-Pd(1)	130.91(15)	C(2)-C(3)-H(3)	120.6
C(11)-N(2)-Pd(1)	117.38(14)	C(14)-C(15)-C(16)	121.0(2)
N(2)-N(1)-C(1)	122.15(18)	C(14)-C(15)-H(15)	119.5
C(7)-C(8)-C(10)	117.5(2)	C(16)-C(15)-H(15)	119.5
C(7)-C(8)-Pd(1)	120.37(18)	C(5)-C(6)-C(7)	120.9(2)
C(10)-C(8)-Pd(1)	122.14(16)	C(5)-C(6)-H(6)	119.6
C(5)-C(9)-C(10)	120.0(2)	C(7)-C(6)-H(6)	119.6
C(5)-C(9)-C(4)	119.3(2)	C(15)-C(14)-C(13)	120.2(2)
C(10)-C(9)-C(4)	120.6(2)	C(15)-C(14)-H(14)	119.9
C(14)-C(13)-C(12)	118.9(3)	C(13)-C(14)-H(14)	119.9
C(14)-C(13)-H(13)	120.5	O(1)-C(17)-H(17A)	109.5
C(12)-C(13)-H(13)	120.5	O(1)-C(17)-H(17B)	109.5
C(8)-C(10)-C(9)	119.5(2)	O(1)-C(17)-H(17C)	109.5
C(8)-C(10)-C(1)	124.0(2)	H(17A)-C(17)-H(17B)	109.5
C(9)-C(10)-C(1)	116.5(2)	H(17B)-C(17)-H(17C)	109.5
C(16)-C(11)-C(12)	119.0(2)	C(18)-C(19)-H(19A)	109.5
C(16)-C(11)-N(2)	121.7(2)	C(18)-C(19)-H(19B)	109.5
C(12)-C(11)-N(2)	119.32(19)	H(19A)-C(19)-H(19B)	109.5
C(11)-C(12)-C(13)	121.2(2)	C(18)-C(19)-H(19C)	109.5
C(11)-C(12)-S(02)	118.23(17)	H(19A)-C(19)-H(19C)	109.5
C(13)-C(12)-S(02)	120.5(2)	H(19B)-C(19)-H(19C)	109.5
N(1)-C(1)-C(2)	111.4(2)	C(8)-C(7)-H(7)	118.9
N(1)-C(1)-C(10)	128.5(2)	C(6)-C(7)-H(7)	118.9
C(2)-C(1)-C(10)	120.0(2)	C(15)-C(16)-C(11)	119.7(2)
C(4)-O(1)-C(17)	119.1(2)	C(15)-C(16)-H(16)	120.2
O(1)-C(4)-C(3)	124.2(2)	C(11)-C(16)-H(16)	120.2
O(1)-C(4)-C(9)	114.8(2)		
C(3)-C(4)-C(9)	121.0(2)		
C(8)-C(7)-C(6)	122.2(2)		

TABLE 4
Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **2b**

	x	y	z	U(eq)
Pd(1)	5947(1)	4782(1)	8224(1)	39(1)
Cl(1)	5011(1)	4807(1)	6838(1)	62(1)
S(02)	7302(1)	3276(1)	8021(1)	48(1)
N(2)	7133(2)	4699(1)	9371(1)	38(1)
N(1)	7161(2)	5320(1)	9956(1)	42(1)
O(2)	6491(2)	2283(1)	7718(1)	64(1)
C(8)	4731(3)	6053(2)	8454(1)	41(1)
C(9)	4263(3)	7525(2)	9311(1)	45(1)
C(13)	9417(3)	2227(2)	9202(2)	61(1)
C(10)	5089(3)	6578(2)	9203(1)	39(1)
C(11)	8241(3)	3822(2)	9591(1)	42(1)
C(12)	8424(3)	3096(2)	9011(1)	47(1)
C(1)	6234(3)	6204(2)	9891(1)	42(1)
O(1)	3761(2)	8955(1)	10085(1)	68(1)
C(4)	4598(3)	8069(2)	10065(2)	50(1)
C(7)	3478(3)	6439(2)	7878(1)	53(1)
C(16)	9085(3)	3683(2)	10368(1)	52(1)
C(2)	6479(3)	6758(2)	10612(1)	54(1)
C(18)	8811(4)	3514(2)	7471(2)	64(1)
C(5)	3051(3)	7900(2)	8691(2)	56(1)
C(3)	5696(3)	7685(2)	10705(2)	58(1)
C(15)	10074(3)	2822(2)	10555(2)	65(1)
C(6)	2655(3)	7352(2)	7998(2)	62(1)
C(14)	10234(3)	2098(2)	9979(2)	67(1)
C(17)	3972(5)	9540(2)	10822(2)	82(1)
C(19)	9793(4)	4475(3)	7765(2)	72(1)

CHAPTER III

TABLE 5
Bond Lengths (\AA) and Bond Angles ($^\circ$) for (**2b**)

Bond Lengths (\AA)		Bond Lengths (\AA)	
C(45)-C(44)	1.361(6)	C(20)-H(20)	0.9300
C(45)-C(46)	1.370(6)	Pd(2)-N(4)	1.980(3)
C(45)-H(45)	0.9300	Pd(2)-O(4)	1.997(2)
C(44)-C(43)	1.380(6)	Pd(2)-S(2)	2.1970(10)
C(44)-H(44)	0.9300	Pd(2)-C(12)	2.3455(11)
C(22)-C(21)	1.372(7)	S(2)-O(6)	1.462(3)
C(22)-C(23)	1.388(7)	S(2)-C(36)	1.759(4)
C(22)-H(22)	0.9300	S(2)-C(41)	1.809(4)
Pd(1)-N(2)	1.981(3)	C(39)-C(40)	1.349(6)
Pd(1)-O(2)	2.006(2)	C(39)-C(38)	1.402(7)
Pd(1)-S(1)	2.1869(10)	C(39)-H(39)	0.9300
Pd(1)-Cl(1)	2.3294(11)	O(4)-C(26)	1.286(4)
S(1)-O(5)	1.458(3)	N(4)-N(3)	1.289(4)
S(1)-C(12)	1.778(4)	N(4)-C(35)	1.420(5)
S(1)-C(17)	1.812(4)	C(25)-N(3)	1.330(5)
C(24)-O(1)	1.432(5)	C(25)-C(26)	1.442(5)
C(24)-H(24A)	0.9600	C(25)-C(34)	1.471(5)
C(24)-H(24B)	0.9600	O(3)-C(28)	1.336(4)
C(24)-H(24C)	0.9600	O(3)-C(48)	1.429(5)
O(2)-C(2)	1.286(4)	C(42)-C(47)	1.383(5)
N(1)-N(2)	1.288(4)	C(42)-C(43)	1.391(5)
N(1)-C(1)	1.321(5)	C(42)-C(41)	1.483(5)
C(10)-C(8)	1.401(5)	C(34)-C(33)	1.396(5)
C(10)-C(9)	1.401(5)	C(34)-C(32)	1.407(6)
C(10)-C(1)	1.473(5)	C(35)-C(36)	1.391(5)
N(2)-C(11)	1.426(5)	C(35)-C(40)	1.393(6)
O(1)-C(4)	1.336(4)	C(41)-H(41A)	0.9700
C(1)-C(2)	1.452(5)	C(41)-H(41B)	0.9700
C(9)-C(5)	1.408(5)	C(33)-C(29)	1.409(5)

C(9)-C(4)	1.451(5)	C(33)-C(28)	1.448(6)
C(2)-C(3)	1.412(5)	C(28)-C(27)	1.361(5)
C(11)-C(12)	1.387(5)	C(27)-C(26)	1.415(5)
C(11)-C(16)	1.389(6)	C(27)-H(27)	0.9300
C(23)-C(18)	1.389(6)	C(36)-C(37)	1.390(5)
C(23)-H(23)	0.9300	C(40)-H(40)	0.9300
C(18)-C(19)	1.384(6)	C(37)-C(38)	1.354(7)
C(18)-C(17)	1.489(6)	C(37)-H(37)	0.9300
C(8)-C(7)	1.377(6)	C(47)-C(46)	1.376(6)
C(8)-H(8)	0.9300	C(47)-H(47)	0.9300
C(4)-C(3)	1.347(5)	C(29)-C(30)	1.352(7)
C(3)-H(3)	0.9300	C(29)-H(29)	0.9300
C(12)-C(13)	1.394(5)	C(48)-H(48A)	0.9600
C(13)-C(14)	1.370(7)	C(48)-H(48B)	0.9600
C(13)-H(13)	0.9300	C(48)-H(48C)	0.9600
C(19)-C(20)	1.377(7)	C(32)-C(31)	1.376(6)
C(19)-H(19)	0.9300	C(32)-H(32)	0.9300
C(16)-C(15)	1.372(6)	C(38)-H(38)	0.9300
C(16)-H(16)	0.9300	C(30)-C(31)	1.384(7)
C(17)-H(17A)	0.9700	C(30)-H(30)	0.9300
C(17)-H(17B)	0.9700	C(31)-H(31)	0.9300
C(5)-C(6)	1.360(6)	C(46)-H(46)	0.9300
C(5)-H(5)	0.9300	C(43)-H(43)	0.9300
C(15)-C(14)	1.383(7)	C(6)-H(6)	0.9300
C(15)-H(15)	0.9300	C(21)-C(20)	1.366(7)
C(7)-C(6)	1.387(6)	C(21)-H(21)	0.9300
C(7)-H(7)	0.9300	C(14)-H(14)	0.9300
Bond Angles (°)		Bond Angles (°)	
C(44)-C(45)-C(46)	120.0(4)	C(22)-C(23)-H(23)	119.6
C(44)-C(45)-H(45)	120.0	C(18)-C(23)-H(23)	119.6
C(46)-C(45)-H(45)	120.0	C(19)-C(18)-C(23)	118.0(4)
C(45)-C(44)-C(43)	120.4(4)	C(19)-C(18)-C(17)	120.3(4)
C(45)-C(44)-H(44)	119.8	C(23)-C(18)-C(17)	121.7(4)
C(43)-C(44)-H(44)	119.8	C(17)-C(18)-C(19)	120.6(4)
C(21)-C(22)-C(23)	119.8(5)	C(17)-C(18)-H(8)	119.7
C(21)-C(22)-H(22)	120.1	C(19)-C(18)-H(8)	119.7
C(23)-C(22)-H(22)	120.1	O(1)-C(14)-C(13)	125.4(4)
N(2)-Pd(1)-O(2)	91.33(11)	O(1)-C(14)-C(9)	113.1(3)
N(2)-Pd(1)-S(1)	87.20(9)	C(3)-C(4)-C(9)	121.5(3)
O(2)-Pd(1)-S(1)	178.51(7)	C(4)-C(3)-C(2)	121.8(3)
N(2)-Pd(1)-C(1)	176.95(9)	C(4)-C(3)-H(3)	119.1
O(2)-Pd(1)-C(1)	91.60(7)	C(2)-C(3)-H(3)	119.1
S(1)-Pd(1)-C(1)	89.86(4)	C(11)-C(12)-C(13)	121.4(4)
O(5)-S(1)-C(12)	111.78(19)	C(11)-C(12)-S(1)	113.0(3)
O(5)-S(1)-C(17)	106.71(19)	C(13)-C(12)-S(1)	121.8(3)
C(12)-S(1)-C(17)	104.0(2)	C(14)-C(13)-C(12)	118.6(4)
O(5)-S(1)-Pd(1)	122.29(14)	C(14)-C(13)-H(13)	120.7
C(12)-S(1)-Pd(1)	79.98(13)	C(12)-C(13)-H(13)	120.7
C(17)-S(1)-Pd(1)	110.62(14)	C(20)-C(19)-C(18)	121.2(4)
O(1)-C(24)-H(24A)	109.5	C(20)-C(19)-H(19)	119.4
O(1)-C(24)-H(24B)	109.5	C(18)-C(19)-H(19)	119.4
H(24A)-C(24)-H(24B)	109.5	C(15)-C(16)-C(11)	119.4(4)
O(1)-C(24)-H(24C)	109.5	C(15)-C(16)-H(16)	120.3
H(24A)-C(24)-H(24C)	109.5	C(11)-C(16)-H(16)	120.3
H(24B)-C(24)-H(24C)	109.5	C(18)-C(17)-S(1)	112.8(3)
C(2)-O(2)-Pd(1)	125.2(2)	C(18)-C(17)-H(17A)	108.8
N(2)-N(1)-C(1)	124.7(3)	S(1)-C(17)-H(17A)	108.8
C(8)-C(10)-C(9)	118.3(3)	C(18)-C(17)-H(17B)	108.8
C(8)-C(10)-C(1)	122.2(3)	S(1)-C(17)-H(17B)	108.8
C(9)-C(10)-C(1)	119.5(3)	H(17A)-C(17)-H(17B)	107.7
N(1)-N(2)-C(11)	114.7(3)	C(6)-C(5)-C(9)	120.3(4)
N(1)-N(2)-Pd(1)	127.3(2)	C(6)-C(5)-H(5)	119.9
C(11)-N(2)-Pd(1)	118.0(2)	C(9)-C(5)-H(5)	119.9
C(4)-O(1)-C(24)	118.7(3)	C(16)-C(15)-C(14)	121.3(5)
N(1)-C(1)-C(2)	127.8(3)	C(16)-C(15)-H(15)	119.4
N(1)-C(1)-C(10)	114.1(3)	C(14)-C(15)-H(15)	119.4
C(2)-C(1)-C(10)	118.1(3)	C(8)-C(7)-C(6)	120.6(4)
C(10)-C(9)-C(5)	120.1(3)	C(8)-C(7)-H(7)	119.7
C(10)-C(9)-C(4)	119.5(3)	C(6)-C(7)-H(7)	119.7
C(5)-C(9)-C(4)	120.4(3)	C(5)-C(6)-C(7)	120.1(4)
O(2)-C(2)-C(3)	116.7(3)	C(5)-C(6)-H(6)	119.9
O(2)-C(2)-C(1)	123.7(3)	C(7)-C(6)-H(6)	119.9
C(3)-C(2)-C(1)	119.6(3)	C(20)-C(21)-C(22)	120.2(5)
C(12)-C(11)-C(16)	119.0(4)	C(20)-C(21)-H(21)	119.9
C(12)-C(11)-N(2)	117.8(3)	C(22)-C(21)-H(21)	119.9

C(16)-C(11)-N(2)	123.2(4)	C(13)-C(14)-C(15)	120.3(4)
C(22)-C(23)-C(18)	120.7(4)	C(13)-C(14)-H(14)	119.9
(28)-O(3)-C(48)	119.0(3)	C(15)-C(14)-H(14)	119.9
N(4)-N(3)-C(25)	124.8(3)	C(21)-C(20)-C(19)	120.1(5)
C(47)-C(42)-C(43)	118.0(4)	C(21)-C(20)-H(20)	119.9
C(47)-C(42)-C(41)	120.7(3)	C(19)-C(20)-H(20)	119.9
C(43)-C(42)-C(41)	121.3(3)	N(4)-Pd(2)-O(4)	91.45(11)
C(33)-C(34)-C(32)	118.4(3)	N(4)-Pd(2)-S(2)	86.56(8)
C(33)-C(34)-C(25)	119.5(3)	O(4)-Pd(2)-S(2)	178.00(8)
C(32)-C(34)-C(25)	122.0(4)	N(4)-Pd(2)-C(2)	173.45(9)
C(36)-C(35)-C(40)	118.2(4)	O(4)-Pd(2)-C(2)	90.55(8)
C(36)-C(35)-N(4)	118.0(3)	S(2)-Pd(2)-C(2)	91.45(4)
C(40)-C(35)-N(4)	123.8(3)	O(6)-S(2)-C(36)	111.25(19)
C(42)-C(41)-S(2)	113.9(3)	O(6)-S(2)-C(41)	107.09(18)
C(42)-C(41)-H(41A)	108.8	C(36)-S(2)-C(41)	103.55(18)
S(2)-C(41)-H(41A)	108.8	O(6)-S(2)-Pd(2)	123.32(12)
C(42)-C(41)-H(41B)	108.8	C(36)-S(2)-Pd(2)	100.42(13)
S(2)-C(41)-H(41B)	108.8	C(41)-S(2)-Pd(2)	109.49(14)
H(41A)-C(41)-H(41B)	107.7	C(40)-C(39)-C(38)	122.0(4)
C(34)-C(33)-C(29)	119.7(4)	C(40)-C(39)-H(39)	119.0
C(34)-C(33)-C(28)	119.8(3)	C(38)-C(39)-H(39)	119.0
C(29)-C(33)-C(28)	120.5(4)	C(26)-O(4)-Pd(2)	125.2(2)
O(3)-C(28)-C(27)	125.1(4)	N(3)-N(4)-C(35)	114.7(3)
O(3)-C(28)-C(33)	114.1(3)	N(3)-N(4)-Pd(2)	126.9(2)
C(27)-C(28)-C(33)	120.8(3)	C(35)-N(4)-Pd(2)	118.2(2)
C(28)-C(27)-C(26)	121.9(4)	N(3)-C(25)-C(26)	127.2(3)
C(28)-C(27)-H(27)	119.0	N(3)-C(25)-C(34)	114.1(3)
C(26)-C(27)-H(27)	119.0	C(26)-C(25)-C(34)	118.7(3)
C(37)-C(36)-C(35)	121.4(4)	O(4)-C(26)-C(25)	124.2(3)
C(37)-C(36)-S(2)	121.9(3)	C(27)-C(26)-C(25)	119.2(3)
C(35)-C(36)-S(2)	116.7(3)	C(38)-C(37)-C(36)	119.5(4)
C(39)-C(40)-C(35)	119.7(4)	C(38)-C(37)-H(37)	120.3
C(39)-C(40)-H(40)	120.2	C(36)-C(37)-H(37)	120.3
C(35)-C(40)-H(40)	120.2	C(46)-C(47)-C(42)	121.0(4)
O(4)-C(26)-C(27)	116.6(3)	C(46)-C(47)-H(47)	119.5
C(39)-C(38)-H(38)	120.5	C(42)-C(47)-H(47)	119.5
C(29)-C(30)-C(31)	120.2(4)	C(30)-C(29)-C(33)	120.7(4)
C(29)-C(30)-H(30)	119.9	C(30)-C(29)-H(29)	119.6
C(31)-C(30)-H(30)	119.9	C(33)-C(29)-H(29)	119.6
C(32)-C(31)-C(30)	120.5(4)	O(3)-C(48)-H(48A)	109.5
C(32)-C(31)-H(31)	119.8	O(3)-C(48)-H(48B)	109.5
C(30)-C(31)-H(31)	119.8	H(48A)-C(48)-H(48B)	109.5
C(45)-C(46)-C(47)	120.1(4)	O(3)-C(48)-H(48C)	109.5
C(45)-C(46)-H(46)	120.0	H(48A)-C(48)-H(48C)	109.5
C(47)-C(46)-H(46)	120.0	H(48B)-C(48)-H(48C)	109.5
C(44)-C(43)-C(42)	120.6(4)	C(31)-C(32)-C(34)	120.4(4)
C(44)-C(43)-H(43)	119.7	C(31)-C(32)-H(32)	119.8
C(42)-C(43)-H(43)	119.7	C(34)-C(32)-H(32)	119.8
C(37)-C(38)-H(38)	120.5	C(37)-C(38)-C(39)	119.1(4)

TABLE 6
Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{Å}^2 \times 10^3$) for **2b**

	x	y	z	U(eq)
C(45)	3852(5)	2664(4)	2257(2)	63(1)
C(44)	5095(5)	1978(3)	2545(3)	65(1)
C(22)	5990(6)	9841(4)	4002(3)	78(1)
Pd(1)	5719(1)	6462(1)	3099(1)	44(1)
S(1)	3631(1)	7697(1)	2941(1)	50(1)
Cl(1)	6172(1)	6505(1)	1841(1)	64(1)
C(24)	12256(5)	2607(4)	3937(3)	72(1)
O(2)	7629(3)	5336(2)	3272(1)	49(1)
N(1)	6022(3)	5922(2)	4680(2)	45(1)
C(10)	7971(4)	4660(3)	5268(2)	42(1)
N(2)	5253(3)	6498(2)	4161(2)	43(1)
O(1)	11400(3)	2917(2)	4591(2)	59(1)
C(1)	7295(4)	5197(3)	4585(2)	42(1)

C(9)	9362(4)	3910(3)	5239(2)	43(1)
C(2)	8097(4)	4911(3)	3901(2)	43(1)
C(11)	3926(4)	7239(3)	4395(2)	47(1)
C(23)	4879(5)	9602(3)	3650(3)	68(1)
O(5)	2433(3)	7608(2)	2505(2)	69(1)
C(18)	5223(5)	9121(3)	3011(2)	54(1)
C(8)	7276(5)	4879(3)	5952(2)	50(1)
C(4)	10090(4)	3649(3)	4537(2)	46(1)
C(3)	9474(4)	4127(3)	3909(2)	45(1)
C(12)	3008(4)	7856(3)	3864(2)	50(1)
C(13)	1656(5)	8565(3)	4048(3)	63(1)
C(19)	6707(5)	8869(3)	2747(3)	62(1)
C(16)	3504(5)	7357(3)	5124(2)	59(1)
C(17)	4039(5)	8896(3)	2607(2)	59(1)
C(5)	10044(5)	3413(3)	5889(2)	53(1)
C(15)	2171(5)	8055(3)	5303(3)	68(1)
C(7)	7965(5)	4385(3)	6580(2)	61(1)
C(6)	9352(5)	3653(3)	6546(2)	61(1)
C(21)	7447(6)	9594(4)	3719(3)	77(1)
C(14)	1243(5)	8650(3)	4770(3)	70(1)
C(20)	7806(5)	9114(4)	3094(3)	74(1)
Pd(2)	9651(1)	1353(1)	1636(1)	43(1)
Si(2)	9285(1)	3022(1)	1593(1)	48(1)
Cl(2)	10757(1)	1095(1)	2768(1)	57(1)
C(39)	6610(5)	3981(3)	-415(3)	68(1)
O(4)	9952(3)	-157(2)	1641(2)	52(1)
N(4)	8495(3)	1636(2)	740(2)	42(1)
C(25)	8460(4)	-27(3)	601(2)	44(1)
O(3)	9436(3)	-1223(2)	915(2)	59(1)
N(3)	8085(3)	980(2)	412(2)	45(1)
C(42)	6492(4)	3232(3)	2304(2)	42(1)
C(6)	9509(3)	3503(2)	1596(2)	69(1)
C(34)	7830(4)	-606(3)	143(2)	47(1)
C(35)	7930(4)	7675(3)	449(2)	46(1)
C(41)	7915(4)	3529(3)	2303(2)	52(1)
C(33)	8144(5)	1671(3)	288(2)	50(1)
C(28)	9151(4)	-2201(3)	860(2)	49(1)
C(27)	9728(4)	-1668(3)	1287(2)	48(1)
C(36)	8278(4)	3431(3)	792(2)	48(1)
C(40)	7056(3)	2979(3)	1621(2)	63(1)
C(26)	3393(4)	-883(3)	-187(2)	42(1)
C(37)	7845(5)	4457(3)	514(3)	51(1)
C(4)	8214(4)	5916(3)	2013(2)	54(1)
C(29)	7453(6)	-2219(4)	-112(2)	68(1)
C(48)	10175(6)	-3814(3)	1540(3)	68(1)
C(32)	6865(5)	-115(4)	-422(2)	61(1)
C(38)	7012(6)	4737(3)	-86(3)	73(1)
C(30)	6501(7)	1726(4)	-641(3)	84(2)
C(31)	6212(6)	-673(4)	805(2)	73(1)
C(46)	3901(5)	3636(4)	1995(2)	60(1)
C(43)	6408(5)	2256(3)	2579(2)	57(1)

CHAPTER IV

TABLE 7
Bond Lengths (Å) and Bond Angles (°) for (5)

	Bond Lengths (Å)		Bond Lengths (Å)
Or(1)-S(1)	1.478(4)	Or(2)-C(24)	1.406(10)
C(11)-C(16)	1.394(8)	C(24)-H(24A)	0.9600
C(11)-C(12)	1.398(7)	C(24)-H(24B)	0.9600
C(11)-N(2)	1.418(8)	C(24)-H(24C)	0.9600
C(2)-C(1)	1.397(9)	Pt(1)-Ni(2)	1.960(4)
C(2)-C(3)	1.400(9)	Pt(1)-S(1)	2.2870(12)
C(2)-Pt(1)	1.995(5)	Pt(1)-Cl(1)	2.2971(14)
C(1)-N(1)	1.371(8)	Si(1)-C(12)	1.772(5)
C(1)-C(10)	1.435(8)	Si(1)-C(17)	1.808(5)
C(10)-C(8)	1.404(11)	N(1)-N(2)	1.301(6)
C(10)-C(9)	1.416(13)	C(12)-C(13)	1.380(8)
C(3)-C(4)	1.371(10)	C(19)-C(20)	1.375(9)
C(3)-H(3)	0.9300	C(19)-C(18)	1.391(7)
C(16)-C(15)	1.375(11)	C(19)-H(19)	0.9300

C(16)-H(16)	0.9300	C(18)-C(23)	1.377(8)
C(15)-C(14)	1.396(12)	C(18)-C(17)	1.498(7)
C(15)-H(15)	0.9300	C(13)-C(14)	1.377(10)
C(4)-O(2)	1.363(9)	C(13)-H(13)	0.9300
C(4)-C(9)	1.440(13)	C(17)-H(17A)	0.9700
C(9)-C(5)	1.405(9)	C(17)-H(17B)	0.9700
C(8)-C(7)	1.339(12)	C(23)-C(22)	1.377(9)
C(8)-H(8)	0.9300	C(23)-H(23)	0.9300
C(5)-C(6)	1.424(19)	C(21)-C(22)	1.360(9)
C(5)-H(5)	0.9300	C(21)-C(20)	1.370(9)
C(7)-C(6)	1.430(17)	C(21)-H(21)	0.9300
C(7)-H(7)	0.9300	C(22)-H(22)	0.9300
C(6)-H(6)	0.9300	C(20)-H(20)	0.9300
C(14)-H(14)	0.9300		

Bond Angles (°)		Bond Angles (°)	
C(16)-C(11)-C(12)	121.0(5)	O(1)-S(1)-C(12)	110.0(2)
C(16)-C(11)-N(2)	122.2(5)	O(1)-S(1)-C(17)	105.5(2)
C(12)-C(11)-N(2)	116.9(5)	C(12)-S(1)-C(17)	104.0(3)
C(1)-C(2)-C(3)	119.2(5)	O(1)-S(1)-Pt(1)	124.51(17)
C(1)-C(2)-Pt(1)	110.2(4)	C(12)-S(1)-Pt(1)	97.94(18)
C(3)-C(2)-Pt(1)	130.5(5)	C(17)-S(1)-Pt(1)	113.07(17)
N(1)-C(1)-C(2)	119.8(5)	N(2)-N(1)-C(1)	110.3(5)
N(1)-C(1)-C(10)	117.8(6)	N(1)-N(2)-C(11)	118.6(4)
C(2)-C(1)-C(10)	122.3(7)	N(1)-N(2)-Pt(1)	120.6(4)
C(8)-C(10)-C(9)	118.5(7)	C(11)-N(2)-Pt(1)	120.6(3)
C(8)-C(10)-C(1)	124.3(8)	C(13)-C(12)-C(11)	119.9(5)
C(9)-C(10)-C(1)	117.2(7)	C(13)-C(12)-S(1)	121.5(5)
C(4)-C(3)-C(2)	120.7(7)	C(11)-C(12)-S(1)	118.6(4)
C(4)-C(3)-H(3)	119.7	C(20)-C(19)-C(18)	120.6(5)
C(2)-C(3)-H(3)	119.7	C(20)-C(19)-H(19)	119.7
C(15)-C(16)-C(11)	118.5(7)	C(18)-C(19)-H(19)	119.7
C(15)-C(16)-H(16)	120.7	C(23)-C(18)-C(19)	118.1(5)
C(11)-C(16)-H(16)	120.7	C(23)-C(18)-C(17)	121.7(5)
C(16)-C(15)-C(14)	120.4(6)	C(19)-C(18)-C(17)	120.1(5)
C(16)-C(15)-H(15)	119.8	C(14)-C(13)-C(12)	119.2(7)
C(14)-C(15)-H(15)	119.8	C(14)-C(13)-H(13)	120.4
O(2)-C(4)-C(3)	123.4(8)	C(12)-C(13)-H(13)	120.4
O(2)-C(4)-C(9)	115.5(6)	C(18)-C(17)-S(1)	114.5(3)
C(3)-C(4)-C(9)	121.1(6)	C(18)-C(17)-H(17A)	108.6
C(5)-C(9)-C(10)	121.2(11)	S(1)-C(17)-H(17A)	108.6
C(5)-C(9)-C(4)	119.3(10)	C(18)-C(17)-H(17B)	108.6
C(10)-C(9)-C(4)	119.5(6)	S(1)-C(17)-H(17B)	108.6
C(7)-C(8)-C(10)	122.7(11)	H(17A)-C(17)-H(17B)	107.6
C(7)-C(8)-H(8)	118.7	C(22)-C(23)-C(18)	120.5(5)
C(10)-C(8)-H(8)	118.7	C(22)-C(23)-H(23)	119.8
C(9)-C(5)-C(6)	117.8(12)	C(18)-C(23)-H(23)	119.8
C(9)-C(5)-H(5)	121.1	C(22)-C(21)-C(20)	119.4(6)
C(6)-C(5)-H(5)	121.1	C(22)-C(21)-H(21)	120.3
C(8)-C(7)-C(6)	119.5(9)	C(20)-C(21)-H(21)	120.3
C(8)-C(7)-H(7)	120.3	C(21)-C(22)-C(23)	121.0(6)
C(6)-C(7)-H(7)	120.3	C(21)-C(22)-H(22)	119.5
C(5)-C(6)-C(7)	120.5(8)	C(23)-C(22)-H(22)	119.5
C(5)-C(6)-H(6)	119.8	C(21)-C(20)-C(19)	120.4(6)
C(7)-C(6)-H(6)	119.8	C(21)-C(20)-H(20)	119.8
C(4)-O(2)-C(24)	120.3(7)	C(19)-C(20)-H(20)	119.8
O(2)-C(24)-H(24A)	109.5	C(13)-C(14)-C(15)	121.0(7)
O(2)-C(24)-H(24B)	109.5	C(13)-C(14)-H(14)	119.5
H(24A)-C(24)-H(24B)	109.5	C(15)-C(14)-H(14)	119.5
O(2)-C(24)-H(24C)	109.5	N(2)-Pt(1)-Cl(1)	176.31(13)
H(24A)-C(24)-H(24C)	109.5	C(2)-Pt(1)-Cl(1)	97.88(19)
H(24B)-C(24)-H(24C)	109.5	S(1)-Pt(1)-Cl(1)	97.09(5)
N(2)-Pt(1)-C(2)	79.0(2)	N(2)-Pt(1)-S(1)	85.88(13)
		C(2)-Pt(1)-S(1)	164.76(19)

TABLE 8
Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **5**

	x	y	z	U(eq)
O(1)	3820(3)	5879(4)	-370(2)	54(1)
C(11)	1963(4)	4097(6)	723(3)	43(1)
C(2)	627(4)	7215(6)	1060(3)	49(1)
C(1)	81(4)	6165(6)	1205(3)	50(1)
C(10)	-889(5)	6207(9)	1513(4)	71(2)
C(3)	210(5)	8353(6)	1207(4)	60(2)
C(16)	1544(6)	2936(6)	761(4)	56(2)
C(15)	2151(7)	1951(6)	638(5)	72(2)
C(4)	-727(6)	8440(8)	1481(4)	72(2)
C(9)	-1282(5)	7370(10)	1669(4)	75(2)
C(8)	-1440(6)	5177(9)	1707(5)	89(3)
C(5)	2203(6)	7499(14)	2003(5)	109(4)
C(7)	-2309(6)	5252(12)	2043(5)	102(4)
C(6)	2717(7)	6421(15)	2199(6)	120(4)
O(2)	1187(5)	9520(5)	1613(4)	87(2)
C(24)	-755(7)	10620(8)	1391(6)	92(2)
Pt(1)	1991(1)	6776(1)	735(1)	39(1)
Sr(1)	3426(1)	5764(1)	448(1)	59(1)
Cl(1)	2641(1)	8710(1)	678(1)	59(1)
Sr(2)	494(4)	5044(5)	7087(5)	52(1)
Ni(2)	1391(3)	5161(4)	844(3)	43(1)
C(12)	2973(4)	1262(5)	554(3)	42(1)
C(19)	3906(5)	6665(5)	2607(4)	48(1)
C(18)	4366(4)	5730(5)	2215(3)	40(1)
C(13)	3575(5)	3264(5)	436(5)	59(2)
C(17)	4578(4)	5895(5)	1316(3)	47(1)
C(23)	4636(5)	4677(5)	2683(4)	56(1)
C(21)	4011(6)	5482(6)	3896(4)	66(2)
C(22)	4448(6)	4558(6)	3513(4)	72(2)
C(20)	3738(5)	5538(6)	3442(4)	60(2)

TABLE 9
Bond Lengths (Å) and Bond Angles ($^\circ$) for **(9b)**

Bond Lengths (Å)		Bond Lengths (Å)	
Pt(1)-Ni(2)	1.957(10)	C(16)-C(15)	1.39(2)
Pt(1)-C(1)	1.908(15)	C(16)-H(16)	0.9300
Pt(1)-Si(1)	2.274(3)	C(15)-H(15)	0.9300
Pt(1)-Br(1)	2.3955(18)	C(21)-C(22)	1.368(18)
Si(1)-O(1)	1.470(8)	C(21)-H(21)	0.9300
Si(1)-C(18)	1.802(12)	O(2)-C(11)	1.42(4)
Si(1)-C(1)	1.808(12)	C(10)-C(8)	1.42(3)
Ni(2)-N(1)	1.293(13)	C(10)-C(9)	1.43(3)
Ni(2)-C(12)	1.414(16)	C(24)-C(23)	1.369(18)
Ni(1)-C(1)	1.359(18)	C(24)-H(24)	0.9300
C(1)-C(10)	1.463(18)	C(17)-H(17)	0.9300
C(1)-C(2)	1.48(2)	C(9)-C(5)	1.42(3)
C(14)-C(15)	1.351(19)	C(22)-C(23)	1.371(18)
C(14)-C(13)	1.423(18)	C(22)-H(22)	0.9300
C(14)-H(14)	0.9300	C(23)-H(23)	0.9300
C(12)-C(17)	1.369(19)	C(8)-C(7)	1.42(3)
C(12)-C(13)	1.375(16)	C(8)-H(8)	0.9300
C(20)-C(19)	1.351(16)	C(6)-C(5)	1.38(5)
C(20)-C(21)	1.357(18)	C(6)-C(7)	1.43(5)
C(20)-H(20)	0.9300	C(6)-H(6)	0.9300
C(19)-C(24)	1.400(17)	C(5)-H(5)	0.9300
C(19)-C(18)	1.489(16)	C(7)-H(7)	0.9300
C(3)-C(2)	1.33(2)	C(11)-H(11A)	0.9600
C(3)-C(4)	1.33(2)	C(11)-H(11B)	0.9600
C(3)-H(3)	0.9300	C(11)-H(11C)	0.9600
C(18)-H(18A)	0.9700	C(4)-O(2)	1.38(2)
C(18)-H(18B)	0.9700	C(4)-C(9)	1.48(3)
		C(16)-C(17)	1.39(2)

	Bond Angles (°)		Bond Angles (°)	
N(2)-Pt(1)-C'(2)	80.5(6)	C(14)-C(15)-C(16)	123.6(14)	
N(2)-Pt(1)-S(1)	85.8(3)	C(14)-C(15)-H(15)	118.2	
C(2)-Pt(1)-S(1)	166.1(6)	C(16)-C(15)-H(15)	118.2	
N(2)-Pt(1)-Br(1)	176.3(3)	C(20)-C(21)-C(22)	120.0(13)	
C(2)-Pt(1)-Br(1)	96.9(6)	C(20)-C(21)-H(21)	120.0	
S(1)-Pt(1)-Br(1)	96.68(9)	C(22)-C(21)-H(21)	120.0	
O(1)-S(1)-C'(18)	105.7(5)	C(12)-C(13)-C(14)	123.2(12)	
O(1)-S(1)-C(13)	110.3(5)	C(12)-C(13)-S(1)	118.5(10)	
C(18)-S(1)-C(13)	103.5(6)	C(14)-C(13)-S(1)	118.3(11)	
O(1)-S(1)-Pt(1)	125.1(4)	C(4)-O(2)-C(11)	119(2)	
C(18)-S(1)-Pt(1)	112.6(4)	C(8)-C(10)-C(9)	123.0(16)	
C(13)-S(1)-Pt(1)	97.5(5)	C(8)-C(10)-C(1)	120(2)	
N(1)-N(2)-C(12)	117.2(11)	C(9)-C(10)-C(1)	117.3(18)	
N(1)-N(2)-Pt(1)	121.1(9)	C(23)-C(24)-C(19)	121.8(12)	
C(12)-N(2)-Pt(1)	121.6(7)	C(23)-C(24)-H(24)	119.1	
N(2)-N(1)-C(1)	111.2(11)	C(19)-C(24)-H(24)	119.9	
N(1)-C(1)-C(10)	120.1(17)	C(12)-C(17)-C(16)	119.0(14)	
N(1)-C(1)-C(2)	119.7(12)	C(12)-C(17)-H(17)	120.5	
C(10)-C(1)-C(2)	120.1(17)	C(16)-C(17)-H(17)	120.5	
C(15)-C(14)-C(13)	114.8(15)	C(5)-C(9)-C(10)	120(3)	
C(15)-C(14)-H(14)	122.6	C(5)-C(9)-C(4)	122(3)	
C(13)-C(14)-H(14)	122.6	C(10)-C(9)-C(4)	117.8(15)	
C(17)-C(12)-C(13)	119.6(13)	C(21)-C(22)-C(23)	119.3(13)	
C(17)-C(12)-N(2)	123.8(12)	C(21)-C(22)-H(22)	120.3	
C(13)-C(12)-N(2)	116.6(10)	C(23)-C(22)-H(22)	120.3	
C(19)-C(20)-C(21)	123.2(12)	C(24)-C(23)-C(22)	119.5(13)	
C(19)-C(20)-H(20)	118.4	C(24)-C(23)-H(23)	120.3	
C(21)-C(20)-H(20)	118.4	C(22)-C(23)-H(23)	120.3	
C(20)-C(19)-C(24)	116.2(12)	C(10)-C(8)-C(7)	117(3)	
C(20)-C(19)-C(18)	121.8(11)	C(10)-C(8)-H(8)	121.4	
C(24)-C(19)-C(18)	122.0(11)	C(7)-C(8)-H(8)	121.4	
C(2)-C(3)-C(4)	124(2)	C(5)-C(6)-C(7)	125(3)	
C(2)-C(3)-H(3)	118.0	C(5)-C(6)-H(6)	117.4	
C(4)-C(3)-H(3)	118.0	C(7)-C(6)-H(6)	117.4	
C(19)-C(18)-S(1)	114.5(8)	C(6)-C(5)-C(9)	117(3)	
C(19)-C(18)-H(18A)	108.6	C(6)-C(5)-H(5)	121.6	
S(1)-C(18)-H(18A)	108.6	C(9)-C(5)-H(5)	121.6	
C(19)-C(18)-H(18B)	108.6	C(8)-C(7)-C(6)	118(3)	
S(1)-C(18)-H(18B)	108.6	C(8)-C(7)-H(7)	121.0	
H(18A)-C(18)-H(18B)	107.6	C(6)-C(7)-H(7)	121.0	
C(3)-C(2)-C(1)	118.8(15)	O(2)-C(11)-H(11A)	109.5	
C(3)-C(2)-Pt(1)	133.6(15)	O(2)-C(11)-H(11B)	109.5	
C(1)-C(2)-Pt(1)	107.5(11)	H(11A)-C(11)-H(11B)	109.5	
C(3)-C(4)-O(2)	129(2)	O(2)-C(11)-H(11C)	109.5	
C(3)-C(4)-C(9)	121.9(19)	H(11A)-C(11)-H(11C)	109.5	
O(2)-C(4)-C(9)	110(2)	H(11B)-C(11)-H(11C)	109.5	
C(17)-C(16)-C(15)	119.7(13)	C(17)-C(16)-H(16)	120.2	
		C(15)-C(16)-H(16)	120.2	

TABLE 10
Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{Å}^2 \times 10^3$) for **5**

	x	y	z	U(eq)
Pt(1)	2992(1)	1696(1)	9274(1)	61(1)
Br(1)	2343(2)	3688(1)	9328(1)	108(1)
S(1)	1563(2)	748(3)	9555(2)	57(1)
N(2)	3546(8)	97(9)	9158(6)	63(3)
N(1)	4424(9)	-54(11)	8923(7)	74(3)
C(1)	4875(10)	1011(17)	8810(8)	80(4)
O(1)	1177(7)	879(7)	10360(5)	72(2)
C(14)	1336(13)	-1718(12)	9587(9)	80(4)
C(12)	2977(10)	-940(11)	9278(7)	61(3)
C(20)	1009(10)	1595(10)	7359(8)	68(3)
C(19)	631(8)	707(11)	7783(8)	57(3)
C(3)	4773(12)	3162(17)	8799(9)	96(5)
C(18)	422(9)	884(11)	8669(8)	66(3)
C(2)	4344(12)	2133(17)	8951(9)	90(5)
C(4)	5669(16)	3250(20)	8534(11)	119(7)
C(16)	2713(16)	-3034(13)	9350(9)	97(6)

C(15)	1723(14)	-2822(13)	9512(9)	82(4)
C(21)	1204(11)	1462(13)	6550(10)	81(4)
C(13)	2001(10)	-766(11)	9451(7)	61(3)
O(2)	6195(14)	4270(20)	8385(12)	163(8)
C(10)	5850(10)	1040(20)	8499(8)	102(6)
C(24)	460(11)	-390(12)	7348(9)	83(4)
C(17)	3344(12)	-2077(14)	9232(8)	75(4)
C(9)	6250(12)	2190(30)	8345(9)	113(7)
C(22)	1021(12)	389(14)	6128(10)	90(4)
C(23)	660(12)	-552(12)	6536(10)	88(4)
C(8)	6327(13)	-40(20)	8327(9)	148(10)
C(6)	7609(18)	1210(50)	7822(18)	200(20)
C(5)	7158(17)	2270(40)	7997(14)	182(16)
C(7)	7219(16)	50(30)	949(12)	174(14)
C(11)	5820(30)	5390(30)	8600(20)	230(20)

CHAPTER V

TABLE 11
Bond Lengths (Å) and Bond Angles (°) for (I)

	Bond Lengths (Å)		Bond Lengths (Å)	
C(1)-N(1)	1.37(2)	C(127)-C(28)	1.37(3)	
C(1)-C(2)	1.45(2)	C(27)-H(27)	0.9300	
C(1)-C(19)	1.47(2)	C(28)-C(29)	1.32(3)	
C(2)-C(3)	1.36(2)	C(28)-H(28)	0.9300	
C(2)-Ru(1)	2.054(14)	C(29)-C(30)	1.42(3)	
C(3)-C(4)	1.32(3)	C(29)-H(29)	0.9300	
C(3)-H(3)	0.9300	C(30)-H(30)	0.9300	
C(4)-O(1)	1.36(2)	C(31)-C(32)	1.39(2)	
C(4)-C(5)	1.46(3)	C(31)-C(36)	1.44(3)	
C(5)-C(6)	1.33(3)	C(31)-P(1)	1.843(18)	
C(5)-C(9)	1.42(3)	C(32)-C(33)	1.38(3)	
C(5)-H(5)	0.9300	C(32)-H(32)	0.9300	
C(6)-C(7)	1.40(3)	C(33)-C(34)	1.31(3)	
C(6)-H(6)	0.9300	C(33)-H(33)	0.9300	
C(7)-C(8)	1.36(3)	C(34)-C(35)	1.37(3)	
C(7)-H(7)	0.9300	C(34)-H(34)	0.9300	
C(8)-C(10)	1.41(3)	C(35)-C(36)	1.42(3)	
C(8)-H(8)	0.9300	C(35)-H(35)	0.9300	
C(9)-C(10)	1.41(3)	C(36)-H(36)	0.9300	
C(11)-O(1)	1.49(3)	C(37)-C(42)	1.35(3)	
C(11)-H(11A)	0.9600	C(37)-C(38)	1.43(3)	
C(11)-H(11B)	0.9600	C(37)-P(2)	1.83(3)	
C(11)-H(11C)	0.9600	C(38)-C(39)	1.45(3)	
C(12)-C(17)	1.40(3)	C(38)-H(38)	0.9300	
C(12)-C(13)	1.40(3)	C(39)-C(40)	1.31(3)	
C(12)-N(2)	1.40(2)	C(39)-H(39)	0.9300	
C(13)-C(14)	1.39(3)	C(40)-C(41)	1.35(3)	
C(13)-N(1)	1.38(2)	C(40)-H(40)	0.9300	
C(14)-C(15)	1.41(4)	C(41)-C(42)	1.39(3)	
C(14)-H(14)	0.9300	C(41)-H(41)	0.9300	
C(15)-C(16)	1.41(4)	C(42)-H(42)	0.9300	
C(15)-H(15)	0.9300	C(43)-C(48)	1.37(3)	
C(16)-C(17)	1.35(4)	C(43)-C(44)	1.39(3)	
C(16)-H(16)	0.9300	C(43)-P(2)	1.855(16)	
C(17)-H(17)	0.9300	C(44)-C(45)	1.39(3)	
C(18)-S(1)	1.71(2)	C(44)-H(44)	0.9300	
C(18)-H(18A)	0.9600	C(45)-C(46)	1.36(3)	
C(18)-H(18B)	0.9600	C(45)-H(45)	0.9300	
C(18)-H(18C)	0.9600	C(46)-C(47)	1.38(4)	
C(19)-C(20)	1.37(2)	C(46)-H(46)	0.9300	
C(19)-C(24)	1.39(3)	C(47)-C(48)	1.40(4)	
C(19)-P(1)	1.850(19)	C(47)-H(47)	0.9300	
C(20)-C(21)	1.39(3)	C(48)-H(48)	0.9300	
C(20)-H(20)	0.9300	C(49)-C(50)	1.27(3)	
C(21)-C(22)	1.41(3)	C(49)-C(54)	1.43(3)	
C(21)-H(21)	0.9300	C(49)-P(2)	1.87(2)	
C(22)-C(23)	1.39(3)	C(50)-C(51)	1.43(3)	
C(22)-H(22)	0.9300	C(50)-H(50)	0.9300	
C(23)-C(24)	1.41(3)	C(51)-C(52)	1.42(3)	
C(23)-H(23)	0.9300	C(51)-H(51)	0.9300	

C(24)-H(24)	0.9300	C(52)-C(53)	1.32(3)
C(25)-C(30)	1.37(3)	C(52)-H(52)	0.9300
C(25)-C(26)	1.42(2)	C(53)-C(54)	1.36(3)
C(25)-P(1)	1.865(19)	C(53)-H(53)	0.9300
C(26)-C(27)	1.41(3)	C(54)-H(54)	0.9300
C(26)-H(26)	0.9300	P(2)-Ru(1)	2.407(4)
N(1)-N(2)	1.31(2)	S(1)-Ru(1)	2.351(4)
N(2)-Ru(1)	2.004(13)	Cl(1)-Ru(1)	2.476(5)
O(2)-S(1)	1.562(16)	P(1)-Ru(1)	2.420(5)
Bond Angles (°)		Bond Angles (°)	
N(1)-C(1)-C(2)	119.8(15)	C(16)-C(17)-H(17)	119.4
N(1)-C(1)-C(10)	119.4(16)	C(12)-C(17)-H(17)	119.4
C(2)-C(1)-C(10)	120.7(15)	S(1)-C(18)-H(18A)	109.5
C(3)-C(2)-C(1)	115.1(17)	S(1)-C(18)-H(18B)	109.5
C(3)-C(2)-Ru(1)	135.1(15)	H(18A)-C(18)-H(18B)	109.5
C(1)-C(2)-Ru(1)	109.6(10)	S(1)-C(18)-H(18C)	109.5
C(4)-C(3)-C(2)	128(3)	H(18A)-C(18)-H(18C)	109.5
C(4)-C(3)-H(3)	116.2	H(18B)-C(18)-H(18C)	109.5
C(2)-C(3)-H(3)	116.2	C(20)-C(19)-C(24)	117.4(18)
C(3)-C(4)-O(1)	131(2)	C(20)-C(19)-P(1)	125.6(14)
C(3)-C(4)-C(9)	120(2)	C(24)-C(19)-P(1)	116.9(15)
O(1)-C(4)-C(9)	109.8(17)	C(19)-C(20)-C(21)	124(2)
C(6)-C(5)-C(9)	123(2)	C(19)-C(20)-H(20)	118.2
C(6)-C(5)-H(5)	118.6	C(21)-C(20)-H(20)	118.2
C(9)-C(5)-H(5)	118.6	C(20)-C(21)-C(22)	117(2)
C(5)-C(6)-C(7)	120(2)	C(20)-C(21)-H(21)	121.6
C(5)-C(6)-H(6)	119.9	C(22)-C(21)-H(21)	121.6
C(7)-C(6)-H(6)	119.9	C(23)-C(22)-C(21)	122(2)
C(8)-C(7)-C(6)	120(2)	C(23)-C(22)-H(22)	119.0
C(8)-C(7)-H(7)	120.1	C(21)-C(22)-H(22)	119.0
C(6)-C(7)-H(7)	120.1	C(22)-C(23)-C(24)	117(2)
C(7)-C(8)-C(10)	120(2)	C(22)-C(23)-H(23)	121.3
C(7)-C(8)-H(8)	119.8	C(24)-C(23)-H(23)	121.3
C(10)-C(8)-H(8)	119.8	C(19)-C(24)-C(23)	123(2)
C(10)-C(9)-C(5)	117(2)	C(19)-C(24)-H(24)	118.7
C(10)-C(9)-C(4)	118.2(17)	C(23)-C(24)-H(24)	118.7
C(5)-C(9)-C(4)	125.2(19)	C(30)-C(25)-C(26)	120.5(18)
C(9)-C(10)-C(8)	119.9(17)	C(30)-C(25)-P(1)	122.8(15)
C(9)-C(10)-C(1)	118.6(17)	C(26)-C(25)-P(1)	116.7(14)
C(8)-C(10)-C(1)	121.5(17)	C(27)-C(26)-C(25)	118.4(18)
O(1)-C(11)-H(11A)	109.5	C(27)-C(26)-H(26)	120.8
O(1)-C(11)-H(11B)	109.5	C(25)-C(26)-H(26)	120.8
H(11A)-C(11)-H(11B)	109.5	C(28)-C(27)-C(26)	117(2)
O(1)-C(11)-H(11C)	109.5	C(28)-C(27)-H(27)	121.4
H(11A)-C(11)-H(11C)	109.5	C(26)-C(27)-H(27)	121.4
H(11B)-C(11)-H(11C)	109.5	C(29)-C(28)-C(27)	127(2)
C(17)-C(12)-C(13)	118.2(18)	C(29)-C(28)-H(28)	116.7
C(17)-C(12)-N(2)	124.2(17)	C(27)-C(28)-H(28)	116.7
C(13)-C(12)-N(2)	117.5(17)	C(28)-C(29)-C(30)	117(2)
C(14)-C(13)-C(12)	120(2)	C(28)-C(29)-H(29)	121.5
C(14)-C(13)-S(1)	122(2)	C(30)-C(29)-H(29)	121.5
C(12)-C(13)-S(1)	118.2(16)	C(25)-C(30)-C(29)	120(2)
C(13)-C(14)-C(15)	122(3)	C(25)-C(30)-H(30)	119.9
C(13)-C(14)-H(14)	119.2	C(29)-C(30)-H(30)	119.9
C(15)-C(14)-H(14)	119.2	C(32)-C(31)-C(36)	118.5(17)
C(14)-C(15)-C(16)	116(3)	C(32)-C(31)-P(1)	122.8(14)
C(14)-C(15)-H(15)	121.9	C(36)-C(31)-P(1)	118.8(14)
C(16)-C(15)-H(15)	121.9	C(33)-C(32)-C(31)	121.0(19)
C(17)-C(16)-C(15)	122(3)	C(33)-C(32)-H(32)	119.5
C(17)-C(16)-H(16)	118.9	C(31)-C(32)-H(32)	119.5
C(15)-C(16)-H(16)	118.9	C(34)-C(33)-C(32)	121(2)
C(16)-C(17)-C(12)	121(2)	C(34)-C(33)-H(33)	119.7
C(45)-C(46)-H(46)	119.6	C(32)-C(33)-H(33)	119.7
C(47)-C(46)-H(46)	119.6	C(33)-C(34)-C(35)	123(3)
C(46)-C(47)-C(48)	119(3)	C(33)-C(34)-H(34)	118.7
C(46)-C(47)-H(47)	120.6	C(35)-C(34)-H(34)	118.7
C(48)-C(47)-H(47)	120.6	C(34)-C(35)-C(36)	120(3)
C(43)-C(48)-C(47)	121(3)	C(34)-C(35)-H(35)	120.2
C(43)-C(48)-H(48)	119.8	C(36)-C(35)-H(35)	120.2
C(47)-C(48)-H(48)	119.7	C(35)-C(36)-C(31)	118(2)
C(50)-C(49)-C(54)	118(2)	C(35)-C(36)-H(36)	121.2
C(50)-C(49)-P(2)	124.1(16)	C(31)-C(36)-H(36)	121.2
C(54)-C(49)-P(2)	117.9(15)	C(42)-C(37)-C(38)	116(2)
C(49)-C(50)-C(51)	125(2)	C(42)-C(37)-P(2)	121.9(19)
C(49)-C(50)-H(50)	117.7	C(38)-C(37)-P(2)	121.7(18)

C(51)-C(50)-H(50)	117.7	C(37)-C(38)-C(39)	120(2)
C(52)-C(51)-C(50)	114(2)	C(37)-C(38)-H(38)	120.2
C(52)-C(51)-H(51)	122.8	C(39)-C(38)-H(38)	120.2
C(50)-C(51)-H(51)	122.8	C(40)-C(39)-C(38)	119(3)
C(53)-C(52)-C(51)	122(3)	C(40)-C(39)-H(39)	120.7
C(53)-C(52)-H(52)	118.9	C(38)-C(39)-H(39)	120.7
C(51)-C(52)-H(52)	118.9	C(39)-C(40)-C(41)	123(3)
C(52)-C(53)-C(54)	120(3)	C(39)-C(40)-H(40)	118.4
C(52)-C(53)-H(53)	120.2	C(41)-C(40)-H(40)	118.4
C(54)-C(53)-H(53)	120.2	C(40)-C(41)-C(42)	119(2)
C(53)-C(54)-C(49)	121(2)	C(40)-C(41)-H(41)	120.3
C(53)-C(54)-H(54)	119.4	C(42)-C(41)-H(41)	120.3
C(49)-C(54)-H(54)	119.4	C(37)-C(42)-C(41)	123(2)
N(2)-N(1)-C(1)	110.8(16)	C(37)-C(42)-H(42)	118.6
N(1)-N(2)-C(12)	115.7(15)	C(41)-C(42)-H(42)	118.6
N(1)-N(2)-Ru(1)	121.7(11)	C(48)-C(43)-C(44)	120.0(19)
C(12)-N(2)-Ru(1)	122.6(11)	C(48)-C(43)-P(2)	122.2(19)
C(4)-O(1)-C(11)	115.9(17)	C(44)-C(43)-P(2)	117.9(17)
C(19)-P(1)-C(31)	106.3(8)	C(43)-C(44)-C(45)	119(2)
C(19)-P(1)-C(25)	96.3(8)	C(43)-C(44)-H(44)	120.3
C(31)-P(1)-C(25)	104.1(9)	C(45)-C(44)-H(44)	120.3
C(19)-P(1)-Ru(1)	115.5(6)	C(46)-C(45)-C(44)	120(3)
C(31)-P(1)-Ru(1)	112.4(6)	C(46)-C(45)-H(45)	119.8
C(25)-P(1)-Ru(1)	120.3(6)	C(44)-C(45)-H(45)	119.8
C(37)-P(2)-C(43)	95.7(11)	C(45)-C(46)-C(47)	121(3)
C(37)-P(2)-C(49)	101.7(8)	C(13)-Si(1)-Ru(1)	98.5(8)
C(43)-P(2)-C(49)	107.6(10)	Ni(2)-Ru(1)-C(2)	78.1(6)
C(37)-P(2)-Ru(1)	120.9(9)	Ni(2)-Ru(1)-Si(1)	83.2(4)
C(43)-P(2)-Ru(1)	115.3(5)	C(2)-Ru(1)-Si(1)	101.3(5)
C(49)-P(2)-Ru(1)	113.4(6)	Ni(2)-Ru(1)-P(2)	94.5(4)
O(2)-Si(1)-C(18)	101.8(10)	C(2)-Ru(1)-P(2)	89.6(4)
O(2)-Si(1)-C(12)	104.7(9)	Si(1)-Ru(1)-P(2)	90.99(14)
C(18)-Si(1)-C(13)	101.6(10)	Ni(2)-Ru(1)-P(1)	92.0(4)
O(2)-Si(1)-Ru(1)	124.6(6)	C(2)-Ru(1)-P(1)	86.7(4)
C(18)-Si(1)-Ru(1)	121.8(7)	Si(1)-Ru(1)-P(1)	94.93(13)
Si(1)-Ru(1)-Cl(1)	106.1(2)	P(2)-Ru(1)-P(1)	171.7(2)
P(2)-Ru(1)-Cl(1)	86.7(2)	Ni(2)-Ru(1)-Cl(1)	170.6(4)
O(1)-Ru(1)-Cl(1)	86.08(17)	C(2)-Ru(1)-Cl(1)	92.5(4)

TABLE 12

Atomic coordinates ($\times 10^3$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **1**

	x	y	z	U(eq)
C(1)	5363(17)	7474(10)	6307(16)	23(4)
C(2)	5264(14)	6688(8)	6268(13)	6(3)
C(3)	5462(15)	6370(16)	7365(18)	17(4)
C(4)	5812(19)	6689(11)	8464(18)	33(5)
C(5)	5380(20)	7885(14)	9700(20)	38(7)
C(6)	6580(20)	8596(14)	9760(20)	53(6)
C(7)	6450(20)	8978(13)	8700(20)	43(6)
C(8)	6030(20)	8625(12)	7580(20)	42(6)
C(9)	6026(18)	7474(11)	8583(17)	29(5)
C(10)	5799(16)	7869(10)	7498(16)	18(4)
C(11)	6050(20)	5598(14)	9660(20)	67(8)
C(12)	4438(16)	7738(9)	3118(16)	18(4)
C(13)	4060(20)	7285(13)	2070(20)	44(6)
C(14)	3760(30)	7577(17)	900(30)	83(9)
C(15)	3760(30)	8332(19)	720(30)	93(10)
C(16)	4190(30)	8769(18)	1810(30)	83(10)
C(17)	4480(20)	8487(13)	2950(20)	49(6)
C(18)	4960(20)	6009(11)	1709(19)	46(6)
C(19)	7966(19)	6090(10)	6821(18)	31(5)
C(20)	8900(20)	6569(11)	7563(19)	44(6)
C(21)	9770(20)	6439(17)	8820(20)	64(7)
C(22)	9610(20)	5791(12)	9360(20)	51(6)
C(23)	8660(20)	5298(13)	8670(20)	51(6)
C(24)	7860(20)	5453(12)	7390(20)	45(6)
C(25)	7462(17)	5355(11)	1635(17)	24(5)

C(26)	8790(18)	5286(11)	5125(18)	31(5)
C(27)	9250(20)	4654(12)	4840(19)	39(5)
C(28)	8380(20)	4160(13)	4050(20)	45(6)
C(29)	7140(20)	4215(12)	3530(20)	43(6)
C(30)	6660(20)	4829(11)	3871(19)	38(5)
C(31)	7526(16)	6943(10)	4579(16)	20(4)
C(32)	7940(17)	6858(11)	3699(16)	28(4)
C(33)	8350(20)	7447(13)	3290(20)	46(6)
C(34)	8420(20)	8095(15)	3770(20)	57(7)
C(35)	8020(30)	8232(18)	4640(30)	77(8)
C(36)	7610(20)	7650(13)	5110(20)	49(6)
C(37)	1440(20)	5606(14)	3170(20)	45(7)
C(38)	1828(19)	5007(11)	2684(18)	36(5)
C(39)	920(20)	4447(15)	1960(20)	61(8)
C(40)	-220(30)	4497(15)	1810(20)	67(8)
C(41)	-630(20)	5066(14)	2210(20)	60(7)
C(42)	230(20)	5607(13)	2920(20)	44(6)
C(43)	2322(15)	6263(14)	5469(15)	32(4)
C(44)	2580(20)	5594(12)	6080(20)	42(6)
C(45)	2420(20)	5512(15)	7140(20)	64(8)
C(46)	2050(20)	6085(14)	7590(30)	68(8)
C(47)	1760(30)	6750(20)	6970(30)	102(11)
C(48)	1910(20)	6832(14)	5910(20)	56(7)
C(49)	1629(18)	7163(11)	3151(18)	19(5)
C(50)	720(20)	7143(12)	2024(19)	41(6)
C(51)	80(20)	7769(14)	1300(20)	59(7)
C(52)	510(30)	8441(16)	1950(30)	68(8)
C(53)	1480(20)	8479(14)	3100(20)	56(7)
C(54)	2040(20)	7857(13)	3730(20)	49(6)
N(1)	5129(15)	7850(9)	5238(14)	28(4)
N(2)	4775(13)	7407(7)	4278(12)	15(3)
O(1)	6066(11)	6404(10)	9599(11)	51(4)
O(2)	2678(15)	6087(8)	1249(14)	64(5)
P(1)	6903(4)	6183(3)	5105(4)	24(1)
P(2)	2533(4)	6343(4)	4057(4)	25(1)
S(1)	4017(4)	6328(4)	2294(4)	33(1)
Rh(1)	4742(5)	5040(3)	5075(5)	31(1)
Ru(1)	4687(1)	6330(1)	4466(1)	17(1)

TABLE 15
Bond Lengths (Å) and Bond Angles (°) for (6a)

	Bond Lengths (Å)		Bond Lengths (Å)
C(45)-C(46)	1.370(15)	C(5)-H(5)	0.9300
C(45)-C(44)	1.401(14)	C(38)-C(39)	1.369(12)
C(45)-H(45)	0.9300	C(38)-C(37)	1.392(10)
O(3)-S(2)	1.484(5)	C(38)-H(38)	0.9300
S(2)-C(37)	1.788(8)	C(28)-C(33)	1.429(10)
S(2)-C(42)	1.828(7)	C(29)-C(30)	1.366(12)
S(2)-Ru(1)	2.3364(18)	C(29)-C(33)	1.395(10)
O(02)-C(4)	1.375(8)	C(29)-H(29)	0.9300
O(02)-C(11)	1.405(10)	C(36)-C(37)	1.390(10)
C(4)-C(3)	1.376(10)	C(36)-C(41)	1.378(10)
C(4)-C(9)	1.423(9)	C(018)-C(19)	1.496(10)
C(3)-C(2)	1.404(10)	C(8)-C(7)	1.384(10)
C(3)-H(3)	0.9300	C(8)-H(8)	0.9300
C(11)-H(11A)	0.9600	C(19)-C(24)	1.364(11)
C(11)-H(11B)	0.9600	C(19)-C(20)	1.385(10)
C(11)-H(11C)	0.9600	C(48)-C(47)	1.369(13)
C(42)-C(43)	1.486(11)	C(48)-C(43)	1.391(11)
C(42)-H(42A)	0.9704	C(48)-H(48)	0.9300
C(42)-H(42B)	0.9700	C(43)-C(44)	1.364(12)
C(35)-O(4)	1.414(10)	C(17)-C(16)	1.379(11)
C(35)-H(35A)	0.9600	C(17)-H(17)	0.9300
C(35)-H(35B)	0.9600	C(32)-C(31)	1.379(11)
C(35)-H(35C)	0.9600	C(32)-H(32)	0.9300
O(1)-S(1)	1.472(5)	C(16)-C(15)	1.397(12)
Ru(1)-N(2)	2.010(6)	C(16)-H(16)	0.9300
Ru(1)-N(4)	2.012(6)	C(14)-C(15)	1.359(12)
Ru(1)-C(2)	2.038(6)	C(14)-H(14)	0.9300
Ru(1)-C(26)	2.041(6)	C(30)-C(31)	1.370(13)
Ru(1)-S(1)	2.3125(18)	C(30)-H(30)	0.9300
S(1)-C(13)	1.776(7)	C(21)-C(22)	1.367(14)

Si(1)-C(018)	1.831(7)	C(21)-C(20)	1.388(13)
N(4)-N(3)	1.293(7)	C(21)-H(21)	0.9300
N(4)-C(36)	1.416(9)	C(39)-C(40)	1.382(13)
N(3)-C(25)	1.373(9)	C(39)-H(39)	0.9300
N(2)-N(1)	1.309(7)	C(41)-C(40)	1.389(12)
N(2)-C(12)	1.420(8)	C(41)-H(41)	0.9300
O(4)-C(28)	1.358(8)	C(15)-H(15)	0.9300
C(25)-C(26)	1.399(9)	C(20)-H(20)	0.9300
C(25)-C(34)	1.454(9)	C(22)-C(23)	1.362(14)
N(1)-C(1)	1.379(8)	C(22)-H(22)	0.9300
C(2)-C(1)	1.374(9)	C(6)-C(7)	1.383(12)
C(12)-C(13)	1.399(10)	C(6)-H(6)	0.9300
C(12)-C(17)	1.393(10)	C(23)-C(24)	1.386(12)
C(13)-C(14)	1.409(9)	C(23)-H(23)	0.9300
C(10)-C(9)	1.409(10)	C(7)-H(7)	0.9300
C(10)-C(8)	1.402(10)	C(47)-C(46)	1.354(14)
C(10)-C(1)	1.455(9)	C(47)-H(47)	0.9300
C(26)-C(27)	1.405(9)	C(24)-H(24)	0.9300
C(34)-C(33)	1.396(10)	C(31)-H(31)	0.9300
C(34)-C(32)	1.395(10)	C(40)-H(40)	0.9300
C(27)-C(28)	1.378(9)	C(46)-H(46)	0.9300
C(27)-H(27)	0.9300	C(44)-H(44)	0.9300
C(5)-C(6)	1.351(11)		
C(5)-C(9)	1.415(10)		

Angles (°)	Bond	Angles (°)	Bond
C(46)-C(45)-C(44)	120.9(10)	Si(2)-Ru(1)-Si(1)	105.68(16)
C(46)-C(45)-H(45)	119.5	N(4)-Ru(1)-Si(2)	89.70(16)
C(44)-C(45)-H(45)	119.6	C(2)-Ru(1)-Si(2)	91.80(18)
O(3)-Si(2)-C(37)	105.6(3)	C(26)-Ru(1)-Si(2)	154.11(19)
O(3)-Si(2)-C(42)	105.3(3)	Si(1)-Ru(1)-Si(2)	96.76(6)
O(3)-Si(2)-C(42)	102.8(3)	O(1)-Si(1)-C(17)	107.4(3)
O(3)-Si(2)-Ru(1)	120.0(2)	O(1)-Si(1)-C(018)	106.4(3)
C(37)-Si(2)-Ru(1)	98.9(2)	C(13)-Si(1)-C(018)	99.1(3)
C(42)-Si(2)-Ru(1)	121.4(3)	O(1)-Si(1)-Ru(1)	124.4(2)
O(4)-O(2)-C(02)	117.7(6)	C(13)-Si(1)-Ru(1)	99.7(2)
O(02)-C(4)-C(3)	123.0(7)	C(018)-Si(1)-Ru(1)	116.1(2)
O(02)-C(4)-C(9)	114.8(6)	N(3)-N(4)-C(36)	116.4(6)
C(3)-C(4)-C(9)	122.2(6)	N(3)-N(4)-Ru(1)	121.2(4)
C(2)-C(3)-C(4)	119.4(7)	C(36)-N(4)-Ru(1)	122.3(5)
C(2)-C(3)-H(3)	120.3	N(4)-N(3)-C(25)	110.7(6)
C(4)-C(3)-H(3)	120.3	N(1)-N(2)-C(12)	115.7(6)
O(02)-C(11)-H(11A)	109.5	N(1)-N(2)-Ru(1)	121.8(4)
O(02)-C(11)-H(11B)	109.5	C(12)-N(2)-Ru(1)	122.2(5)
H(11A)-C(11)-H(11B)	109.5	C(28)-O(4)-C(35)	120.5(6)
O(02)-C(11)-H(11C)	109.5	N(3)-C(25)-C(26)	119.5(6)
H(11A)-C(11)-H(11C)	109.5	N(3)-C(25)-C(34)	118.5(6)
C(43)-C(42)-Si(2)	108.5(5)	C(26)-C(25)-C(34)	122.0(6)
C(43)-C(42)-H(42A)	110.0	N(2)-N(1)-C(1)	109.5(6)
Si(2)-C(42)-H(42A)	109.9	C(1)-C(2)-C(3)	120.0(6)
C(43)-C(42)-H(42B)	110.1	C(1)-C(2)-Ru(1)	112.2(5)
Si(2)-C(42)-H(42B)	110.0	C(3)-C(2)-Ru(1)	127.3(5)
H(42A)-C(42)-H(42B)	108.7	C(13)-C(12)-C(17)	119.4(6)
O(4)-C(35)-H(35A)	109.4	C(13)-C(12)-N(2)	116.2(6)
O(4)-C(35)-H(35B)	109.5	C(17)-C(12)-N(2)	124.4(7)
H(35A)-C(35)-H(35B)	109.5	C(12)-C(13)-C(14)	120.1(7)
O(4)-C(35)-H(35C)	109.5	C(12)-C(13)-Si(1)	118.3(5)
H(35A)-C(35)-H(35C)	109.5	C(14)-C(13)-Si(1)	121.5(6)
H(35B)-C(35)-H(35C)	109.5	C(9)-C(10)-C(8)	119.6(6)
N(2)-Ru(1)-N(4)	172.5(2)	C(9)-C(10)-C(1)	117.3(6)
N(2)-Ru(1)-C(2)	76.4(3)	C(8)-C(10)-C(1)	123.1(7)
N(4)-Ru(1)-C(2)	99.8(3)	C(27)-C(26)-C(25)	118.4(6)
N(2)-Ru(1)-C(26)	96.0(2)	C(27)-C(26)-Ru(1)	129.8(5)
N(4)-Ru(1)-C(26)	76.9(2)	C(25)-C(26)-Ru(1)	110.9(5)
C(2)-Ru(1)-C(26)	79.5(2)	C(33)-C(34)-C(32)	119.9(7)
N(2)-Ru(1)-Si(1)	83.33(16)	C(33)-C(34)-C(25)	117.8(7)
N(4)-Ru(1)-Si(1)	99.91(16)	C(32)-C(34)-C(25)	122.3(7)
C(2)-Ru(1)-Si(1)	159.5(2)	C(28)-C(27)-C(26)	120.8(6)
C(26)-Ru(1)-Si(1)	99.73(18)	C(28)-C(27)-H(27)	119.6
C(6)-C(5)-C(9)	121.3(8)	C(26)-C(27)-H(27)	119.6
C(6)-C(5)-H(5)	119.3	C(31)-C(32)-H(32)	120.3
C(9)-C(5)-H(5)	119.3	C(34)-C(32)-H(32)	120.3
C(39)-C(38)-C(37)	118.7(8)	C(15)-C(16)-C(17)	120.8(8)
		C(15)-C(16)-H(16)	119.6

C(39)-C(38)-H(38)	120.7	C(17)-C(16)-H(16)	119.6
C(37)-C(38)-H(38)	120.6	C(15)-C(14)-C(13)	119.6(8)
O(4)-C(28)-C(27)	124.9(7)	C(15)-C(14)-H(14)	120.2
O(4)-C(28)-C(33)	113.5(6)	C(13)-C(14)-H(14)	120.2
C(27)-C(28)-C(33)	121.6(6)	C(31)-C(30)-C(29)	121.4(8)
C(30)-C(29)-C(33)	119.6(8)	C(31)-C(30)-H(30)	119.3
C(30)-C(29)-H(29)	120.2	C(29)-C(30)-H(30)	119.3
C(33)-C(29)-H(29)	120.2	C(22)-C(21)-C(20)	120.6(9)
C(37)-C(36)-C(41)	119.5(7)	C(22)-C(21)-H(21)	119.7
C(37)-C(36)-N(4)	116.4(7)	C(20)-C(21)-H(21)	119.7
C(41)-C(36)-N(4)	124.1(7)	C(38)-C(39)-C(40)	120.8(8)
C(10)-C(9)-C(4)	119.0(6)	C(38)-C(39)-H(39)	119.6
C(10)-C(9)-C(5)	118.1(7)	C(40)-C(39)-H(39)	119.6
C(4)-C(9)-C(5)	122.9(7)	C(36)-C(41)-C(40)	119.5(9)
C(34)-C(33)-C(29)	119.4(7)	C(36)-C(41)-H(41)	120.3
C(34)-C(33)-C(28)	119.4(6)	C(40)-C(41)-H(41)	120.2
C(29)-C(33)-C(28)	121.1(7)	C(14)-C(15)-C(16)	120.4(8)
N(1)-C(1)-C(2)	120.0(6)	C(14)-C(15)-H(15)	119.8
N(1)-C(1)-C(10)	118.2(6)	C(16)-C(15)-H(15)	119.8
C(2)-C(1)-C(10)	121.6(6)	C(19)-C(20)-C(21)	120.5(9)
C(36)-C(37)-C(38)	121.1(8)	C(19)-C(20)-H(20)	119.8
C(36)-C(37)-S(2)	115.5(5)	C(21)-C(20)-H(20)	119.8
C(38)-C(37)-S(2)	122.8(6)	C(23)-C(22)-C(21)	119.2(10)
C(19)-C(018)-S(1)	112.7(5)	C(23)-C(22)-H(22)	120.3
C(7)-C(8)-C(10)	120.0(8)	C(21)-C(22)-H(22)	120.5
C(7)-C(8)-H(8)	120.0	C(5)-C(6)-C(7)	120.5(8)
C(10)-C(8)-H(8)	120.0	C(5)-C(6)-H(6)	119.8
C(24)-C(19)-C(20)	117.8(8)	C(7)-C(6)-H(6)	119.8
C(24)-C(19)-C(018)	120.7(7)	C(22)-C(23)-C(24)	120.2(10)
C(20)-C(19)-C(018)	121.3(7)	C(22)-C(23)-H(23)	120.0
C(47)-C(48)-C(43)	121.3(9)	C(24)-C(23)-H(23)	119.9
C(47)-C(48)-H(48)	119.4	C(6)-C(7)-C(8)	120.5(8)
C(43)-C(48)-H(48)	119.3	C(6)-C(7)-H(7)	119.8
C(44)-C(43)-C(48)	117.8(9)	C(8)-C(7)-H(7)	119.8
C(44)-C(43)-C(42)	122.2(8)	C(46)-C(47)-C(48)	121.0(10)
C(48)-C(43)-C(42)	119.9(8)	C(46)-C(47)-H(47)	119.5
C(16)-C(17)-C(12)	119.7(8)	C(48)-C(47)-H(47)	119.4
C(16)-C(17)-H(17)	120.2	C(19)-C(24)-C(23)	121.7(9)
C(12)-C(17)-H(17)	120.2	C(19)-C(24)-H(24)	119.1
C(31)-C(32)-C(34)	119.3(8)	C(23)-C(24)-H(24)	119.2
C(30)-C(31)-C(32)	120.3(8)	C(47)-C(46)-C(45)	118.7(11)
C(30)-C(31)-H(31)	119.9	C(47)-C(46)-H(46)	120.6
C(32)-C(31)-H(31)	119.9	C(45)-C(46)-H(46)	120.7
C(39)-C(40)-C(41)	120.5(9)	C(43)-C(44)-C(45)	120.2(10)
C(39)-C(40)-H(40)	119.8	C(43)-C(44)-H(44)	119.9
C(41)-C(40)-H(40)	119.8	C(45)-C(44)-H(44)	119.9

TABLE 16
Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{Å}^2 \times 10^3$) for **6a**

	x	y	z	U(eq)
C(45)	1036(7)	-1918(5)	3687(8)	120(5)
O(3)	1205(3)	-113(2)	2924(3)	61(1)
S(2)	1171(1)	-9(1)	3739(1)	46(1)
O(02)	3722(3)	262(3)	2420(3)	63(1)
C(4)	3418(3)	-70(3)	2901(4)	47(2)
C(3)	2976(3)	148(3)	3334(4)	44(2)
C(11)	3578(4)	853(4)	2386(6)	80(3)
C(42)	436(3)	-402(4)	3921(4)	58(2)
C(35)	4851(4)	-483(4)	6132(6)	82(3)
O(1)	923(2)	17(2)	5695(3)	59(1)
Ru(1)	2149(1)	18(1)	4635(1)	39(1)
S(1)	1645(1)	-35(1)	5704(1)	45(1)
N(4)	2046(3)	863(2)	4407(3)	45(1)
N(3)	2543(3)	1212(2)	4566(3)	47(1)
N(2)	2381(3)	-807(2)	4889(3)	44(1)
O(4)	4820(3)	105(3)	5930(4)	70(2)
C(25)	3099(3)	928(3)	4924(4)	45(2)
N(1)	2738(3)	-1112(2)	4488(3)	47(1)

C(8)-H(8)	0.9300	C(38)-H(38)	0.9300
C(9)-C(10)	1.403(13)	C(39)-C(40)	1.378(16)
C(11)-O(1)	1.415(13)	C(39)-H(39)	0.9300
C(11)-H(11A)	0.9600	C(40)-C(41)	1.394(15)
C(11)-H(11B)	0.9600	C(40)-H(40)	0.9300
C(11)-H(11C)	0.9600	C(41)-H(41)	0.9300
C(12)-C(13)	1.384(13)	C(42)-C(43)	1.504(14)
C(12)-C(17)	1.401(13)	C(42)-S(2)	1.825(10)
C(12)-N(2)	1.409(12)	C(42)-H(42A)	0.9700
C(13)-C(14)	1.364(13)	C(42)-H(42B)	0.9700
C(13)-S(1)	1.792(9)	C(43)-C(44)	1.369(14)
C(14)-C(15)	1.383(14)	C(43)-C(48)	1.398(14)
C(14)-H(14)	0.9300	C(44)-C(45)	1.381(14)
C(15)-C(16)	1.388(14)	C(44)-H(44)	0.9300
C(15)-H(15)	0.9300	C(45)-C(46)	1.388(16)
C(16)-C(17)	1.364(14)	C(45)-H(45)	0.9300
C(16)-H(16)	0.9300	C(46)-C(47)	1.369(15)
C(17)-H(17)	0.9300	C(46)-H(46)	0.9300
C(18)-C(19)	1.493(14)	C(47)-C(48)	1.364(14)
C(18)-S(1)	1.836(9)	C(47)-H(47)	0.9300
C(18)-H(18A)	0.9700	C(48)-H(48)	0.9300
C(18)-H(18B)	0.9700	N(1)-N(2)	1.312(10)
C(19)-C(24)	1.373(15)	N(2)-Ru(1)	2.022(8)
C(19)-C(20)	1.380(15)	N(3)-N(4)	1.296(10)
C(20)-C(21)	1.377(17)	N(4)-Ru(1)	2.017(7)
C(20)-H(20)	0.9300	O(4)-S(2)	1.471(7)
C(21)-C(22)	1.35(2)	S(1)-Ru(1)	2.340(3)
C(21)-H(21)	0.9300	S(2)-Ru(1)	2.325(3)
C(22)-H(22)	0.9300	C(24)-H(24)	0.9300
Bond Angles (°)		Bond Angles (°)	
C(22)-C(23)-C(24)	121.3(15)	C(14)-C(13)-C(12)	122.8(9)
C(22)-C(23)-H(23)	119.3	C(14)-C(13)-S(1)	121.2(7)
C(24)-C(23)-H(23)	119.3	C(12)-C(13)-S(1)	116.0(7)
O(3)-C(35)-H(35A)	109.5	C(13)-C(14)-C(15)	118.9(9)
O(3)-C(35)-H(35B)	109.5	C(13)-C(14)-H(14)	120.6
H(35A)-C(35)-H(35B)	109.5	C(15)-C(14)-H(14)	120.6
O(3)-C(35)-H(35C)	109.5	C(14)-C(15)-C(16)	118.8(10)
H(35A)-C(35)-H(35C)	109.5	C(14)-C(15)-H(15)	120.6
H(35B)-C(35)-H(35C)	109.5	C(16)-C(15)-H(15)	120.6
N(1)-C(1)-C(2)	119.5(8)	C(17)-C(16)-C(15)	122.6(10)
N(1)-C(1)-C(10)	116.8(9)	C(17)-C(16)-H(16)	118.7
C(2)-C(1)-C(10)	123.8(9)	C(15)-C(16)-H(16)	118.7
C(3)-C(2)-C(1)	116.5(8)	C(16)-C(17)-C(12)	118.5(9)
C(3)-C(2)-Ru(1)	131.8(7)	C(16)-C(17)-H(17)	120.7
C(1)-C(2)-Ru(1)	111.4(7)	C(12)-C(17)-H(17)	120.7
C(4)-C(3)-C(2)	120.6(9)	C(19)-C(18)-S(1)	116.0(7)
C(4)-C(3)-H(3)	119.7	C(19)-C(18)-H(18A)	108.3
C(2)-C(3)-H(3)	119.7	S(1)-C(18)-H(18A)	108.3
O(1)-C(4)-C(3)	124.3(9)	C(19)-C(18)-H(18B)	108.3
O(1)-C(4)-C(9)	112.7(9)	S(1)-C(18)-H(18B)	108.3
C(3)-C(4)-C(9)	123.0(9)	H(18A)-C(18)-H(18B)	107.4
C(6)-C(5)-C(9)	120.2(10)	C(24)-C(19)-C(20)	120.0(11)
C(6)-C(5)-H(5)	119.9	C(24)-C(19)-C(18)	119.3(10)
C(9)-C(5)-H(5)	119.9	C(20)-C(19)-C(18)	120.8(10)
C(5)-C(6)-C(7)	119.5(10)	C(21)-C(20)-C(19)	119.9(13)
C(5)-C(6)-H(6)	120.3	C(21)-C(20)-H(20)	120.0
C(7)-C(6)-H(6)	120.3	C(19)-C(20)-H(20)	120.0
C(8)-C(7)-C(6)	120.8(11)	C(22)-C(21)-C(20)	120.4(13)
C(8)-C(7)-H(7)	119.6	C(22)-C(21)-H(21)	119.8
C(6)-C(7)-H(7)	119.6	C(20)-C(21)-H(21)	119.8
C(7)-C(8)-C(10)	121.1(10)	C(23)-C(22)-C(21)	120.2(14)
C(7)-C(8)-H(8)	119.5	C(23)-C(22)-H(22)	119.9
C(10)-C(8)-H(8)	119.5	C(21)-C(22)-H(22)	119.9
C(10)-C(9)-C(5)	120.1(9)	C(19)-C(24)-C(23)	118.2(13)
C(10)-C(9)-C(4)	117.6(9)	C(19)-C(24)-H(24)	120.9
C(5)-C(9)-C(4)	122.3(9)	C(23)-C(24)-H(24)	120.9
C(9)-C(10)-C(8)	118.3(9)	C(26)-C(25)-N(3)	118.9(9)
C(9)-C(10)-C(1)	118.4(9)	C(26)-C(25)-C(34)	122.8(9)
C(8)-C(10)-C(1)	123.2(9)	N(3)-C(25)-C(34)	118.2(8)
O(1)-C(11)-H(11A)	109.5	C(25)-C(26)-C(27)	117.9(9)
O(1)-C(11)-H(11B)	109.5	C(25)-C(26)-Ru(1)	113.2(6)
H(11A)-C(11)-H(11B)	109.5	C(27)-C(26)-Ru(1)	128.6(7)
O(1)-C(11)-H(11C)	109.5	C(28)-C(27)-C(26)	121.5(9)
H(11A)-C(11)-H(11C)	109.5	C(28)-C(27)-H(27)	119.2
H(11B)-C(11)-H(11C)	109.5	C(26)-C(27)-H(27)	119.2

C(13)-C(12)-C(17)	118.4(9)	C(27)-C(28)-O(3)	124.9(10)
C(13)-C(12)-N(2)	118.4(8)	C(27)-C(28)-C(33)	121.3(9)
C(17)-C(12)-N(2)	123.1(9)	O(3)-C(28)-C(33)	113.8(9)
C(30)-C(29)-C(33)	119.0(11)	C(44)-C(45)-C(46)	118.2(11)
C(30)-C(29)-H(29)	120.5	C(44)-C(45)-H(45)	120.9
C(33)-C(29)-H(29)	120.5	C(46)-C(45)-H(45)	120.9
C(29)-C(30)-C(31)	122.2(11)	C(47)-C(46)-C(45)	121.9(11)
C(29)-C(30)-H(30)	118.9	C(47)-C(46)-H(46)	119.1
C(31)-C(30)-H(30)	118.9	C(45)-C(46)-H(46)	119.1
C(32)-C(31)-C(30)	118.3(11)	C(48)-C(47)-C(46)	118.1(11)
C(32)-C(31)-H(31)	120.8	C(48)-C(47)-H(47)	121.0
C(30)-C(31)-H(31)	120.8	C(46)-C(47)-H(47)	121.0
C(31)-C(32)-C(34)	122.7(11)	C(47)-C(48)-C(43)	122.5(11)
C(31)-C(32)-H(32)	118.6	C(47)-C(48)-H(48)	118.7
C(34)-C(32)-H(32)	118.6	C(43)-C(48)-H(48)	118.7
C(29)-C(33)-C(34)	120.2(10)	N(2)-N(1)-C(1)	110.4(8)
C(29)-C(33)-C(28)	121.2(10)	N(1)-N(2)-C(12)	117.1(8)
C(34)-C(33)-C(28)	118.5(9)	N(1)-N(2)-Ru(1)	121.3(6)
C(32)-C(34)-C(25)	124.9(9)	C(12)-N(2)-Ru(1)	121.6(6)
C(32)-C(34)-C(33)	117.5(10)	N(4)-N(3)-C(25)	109.3(7)
C(25)-C(34)-C(33)	117.6(9)	N(3)-N(4)-C(36)	115.6(7)
C(37)-C(36)-C(41)	119.9(9)	N(3)-N(4)-Ru(1)	122.8(6)
C(37)-C(36)-N(4)	116.5(8)	C(36)-N(4)-Ru(1)	121.4(6)
C(41)-C(36)-N(4)	123.4(10)	C(4)-O(1)-C(11)	119.3(9)
C(36)-C(37)-C(38)	121.9(9)	C(28)-O(3)-C(33)	116.3(8)
O(36)-C(37)-S(2)	118.8(7)	O(2)-S(1)-C(13)	107.5(4)
C(38)-C(37)-S(2)	119.3(8)	O(2)-S(1)-C(18)	105.5(4)
C(39)-C(38)-C(37)	117.6(11)	C(13)-Si(1)-C(18)	100.7(4)
C(39)-C(38)-H(38)	121.2	O(2)-Si(1)-Ru(1)	128.3(7)
C(37)-C(38)-H(38)	121.2	C(13)-Si(1)-Ru(1)	109.8(3)
C(40)-C(39)-C(38)	121.1(10)	C(18)-Si(1)-Ru(1)	111.5(4)
C(40)-C(39)-H(39)	119.4	O(4)-Si(2)-C(37)	109.4(5)
C(38)-C(39)-H(39)	119.4	O(4)-Si(2)-C(42)	106.2(5)
C(39)-C(40)-C(41)	120.1(11)	C(37)-Si(2)-C(42)	96.3(4)
C(39)-C(40)-H(40)	119.9	O(4)-Si(2)-Ru(1)	126.1(3)
C(41)-C(40)-H(40)	119.9	C(37)-Si(2)-Ru(1)	98.6(3)
C(36)-C(41)-C(40)	119.2(11)	C(42)-Si(2)-Ru(1)	115.5(4)
C(36)-C(41)-H(41)	120.4	N(4)-Ru(1)-N(2)	175.8(3)
C(40)-C(41)-H(41)	120.4	N(4)-Ru(1)-C(26)	175.6(3)
C(43)-C(42)-Si(2)	113.1(1)	N(2)-Ru(1)-C(26)	100.2(3)
C(43)-C(42)-H(42A)	109.0	N(4)-Ru(1)-C(2)	102.0(3)
Si(2)-C(42)-H(42A)	109.0	N(2)-Ru(1)-C(2)	77.1(3)
C(43)-C(42)-H(42B)	109.0	C(26)-Ru(1)-C(2)	80.5(4)
Si(2)-C(42)-H(42B)	109.0	N(4)-Ru(1)-Si(2)	83.6(2)
H(42A)-C(42)-H(42B)	107.8	N(2)-Ru(1)-Si(2)	100.5(2)
C(44)-C(43)-C(42)	117.5(10)	C(26)-Ru(1)-Si(2)	158.6(3)
C(44)-C(43)-C(47)	120.7(10)	C(2)-Ru(1)-Si(2)	99.1(3)
C(48)-C(43)-C(47)	121.7(10)	N(4)-Ru(1)-Si(1)	98.5(2)
C(43)-C(44)-C(45)	121.9(11)	N(2)-Ru(1)-Si(1)	81.7(2)
C(43)-C(44)-H(44)	119.3	C(26)-Ru(1)-Si(1)	94.6(3)
C(45)-C(44)-H(44)	119.3	C(2)-Ru(1)-Si(1)	156.9(3)
Si(2)-Ru(1)-Si(1)	93.50(9)		

TABLE 16
Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters
($\text{Å}^2 \times 10^3$) for **6b**

	x	y	z	U(eq)
C(23)	3602(17)	6479(7)	4843(10)	94(5)
C(35)	-1590(10)	5025(6)	7154(7)	68(4)
O(2)	5305(6)	5096(3)	6532(4)	48(2)
C(1)	1613(9)	3338(4)	7613(6)	39(2)
C(2)	2585(8)	3646(4)	8133(5)	31(2)
C(3)	2606(9)	3536(4)	8888(5)	39(2)
C(4)	1715(10)	3135(5)	9099(5)	42(2)
C(5)	-202(9)	2439(5)	8802(6)	45(3)
C(6)	-1110(10)	2137(5)	8281(7)	52(3)
C(7)	-1139(11)	2234(5)	7516(7)	58(3)
C(8)	-284(9)	2623(4)	7294(6)	43(2)
C(9)	711(9)	2836(4)	8577(5)	37(2)
C(10)	660(9)	2942(4)	7817(5)	39(2)

C(11)	2754(13)	3159(6)	10394(6)	78(4)
C(12)	2532(9)	3928(5)	6010(5)	37(2)
C(13)	3308(9)	4418(4)	5867(5)	35(2)
C(14)	3519(9)	4539(5)	5173(6)	44(3)
C(15)	2956(11)	4150(5)	4589(6)	49(3)
C(16)	2168(11)	3661(5)	4725(6)	55(3)
C(17)	1940(10)	3542(5)	5415(5)	47(3)
C(18)	3024(9)	5593(4)	6511(6)	43(3)
C(19)	2821(10)	5889(4)	5756(6)	42(2)
C(20)	1666(11)	5824(6)	5254(6)	65(3)
C(21)	1507(14)	6087(8)	4554(7)	89(5)
C(22)	2480(19)	6403(8)	4353(9)	102(6)
C(24)	3803(12)	6223(5)	5561(7)	64(3)
C(25)	2951(9)	5262(5)	8515(5)	39(2)
C(26)	2380(8)	4881(4)	7925(5)	35(2)
C(27)	1036(9)	4934(5)	7659(5)	39(2)
C(28)	333(9)	5356(5)	7954(5)	42(3)
C(29)	193(11)	6247(5)	8820(6)	55(3)
C(30)	808(13)	6665(6)	9340(7)	68(4)
C(31)	2159(13)	6643(6)	9622(7)	64(3)
C(32)	2843(12)	6191(5)	9358(6)	55(3)
C(33)	924(10)	5784(5)	8537(6)	44(2)
C(34)	2275(9)	5745(4)	8811(5)	40(2)
C(36)	6046(9)	4599(4)	8728(5)	40(2)
C(37)	6539(9)	4115(4)	8374(6)	40(2)
C(38)	7843(9)	3982(5)	8520(6)	49(3)
C(39)	8646(10)	4358(6)	9040(7)	67(4)
C(40)	8161(11)	4831(5)	9418(7)	58(3)
C(41)	6850(9)	4960(5)	9257(6)	54(3)
C(42)	5550(10)	2932(5)	8267(5)	44(3)
C(43)	4832(9)	2380(5)	7859(5)	40(2)
C(44)	5306(10)	2061(5)	7326(6)	50(3)
C(45)	4722(11)	1522(5)	6986(6)	56(3)
C(46)	3628(12)	1303(5)	7199(6)	56(3)
C(47)	3109(11)	1613(5)	7720(6)	51(3)
C(48)	3719(10)	2142(5)	8045(6)	49(3)
N(1)	1555(7)	3416(4)	8860(4)	38(2)
N(2)	2428(7)	3822(4)	6752(4)	36(2)
N(3)	4244(7)	5181(4)	8824(4)	39(2)
N(4)	4689(6)	4719(4)	8488(4)	34(2)
O(1)	1704(7)	2980(4)	9821(4)	58(2)
O(3)	-954(6)	5433(4)	7731(4)	55(2)
O(4)	6076(7)	3487(3)	7076(4)	54(2)
S(1)	4049(2)	4886(1)	6655(1)	36(1)
S(2)	5458(2)	3645(1)	7696(1)	38(1)
Ru(1)	3614(1)	4251(1)	7616(1)	32(1)

CHAPTER VI

TABLE 17
Bond Lengths (Å) and Bond Angles (°) for (1)

Bond Lengths (Å)	Bond Lengths (Å)		
Rh(1)-N(2)	1.990(4)	C(38)-H(38)	0.9300
Rh(1)-C(2)	2.014(4)	C(27)-C(28)	1.323(11)
Rh(1)-P(1)	2.3108(13)	C(27)-H(27)	0.9300
Rh(1)-Cl(2)	2.3614(13)	C(31)-C(36)	1.361(10)
Rh(1)-Cl(1)	2.4004(14)	C(31)-C(32)	1.405(11)
Rh(1)-S(1)	2.4186(11)	C(7)-H(7)	0.9300
S(1)-O(2)	1.482(4)	C(30)-C(29)	1.397(9)
S(1)-C(13)	1.778(5)	C(30)-H(30)	0.9300
S(1)-C(18)	1.823(5)	C(42)-C(41)	1.367(9)
P(1)-C(37)	1.819(5)	C(42)-H(42)	0.9300
P(1)-C(31)	1.829(5)	C(20)-C(21)	1.395(11)
P(1)-C(25)	1.829(5)	C(20)-H(20)	0.9300
N(1)-N(2)	1.284(5)	C(28)-C(29)	1.394(13)
N(1)-C(1)	1.371(6)	C(28)-H(28)	0.9300
N(2)-C(12)	1.408(6)	C(29)-H(29)	0.9300
C(1)-C(2)	1.382(6)	C(24)-C(23)	1.427(13)
C(1)-C(10)	1.434(6)	C(24)-H(24)	0.9300
C(12)-C(13)	1.395(6)	C(36)-C(35)	1.382(11)

C(12)-C(17)	1.410(7)	C(36)-H(36)	0.9300
C(10)-C(8)	1.387(7)	C(32)-C(33)	1.393(11)
C(10)-C(9)	1.426(7)	C(32)-H(32)	0.9300
C(13)-C(14)	1.390(6)	C(39)-C(40)	1.364(11)
C(2)-C(3)	1.393(7)	C(39)-H(39)	0.9300
O(1)-C(4)	1.347(6)	C(41)-C(40)	1.397(12)
O(1)-C(11)	1.439(8)	C(41)-H(41)	0.9300
C(25)-C(26)	1.382(8)	C(35)-C(34)	1.341(17)
C(25)-C(30)	1.389(8)	C(35)-H(35)	0.9300
C(9)-C(5)	1.410(6)	C(40)-H(40)	0.9300
C(9)-C(4)	1.424(7)	C(21)-C(22)	1.281(18)
C(18)-C(19)	1.500(7)	C(21)-H(21)	0.9300
C(18)-H(18A)	0.9701	C(11)-H(11A)	0.9600
C(18)-H(18B)	0.9698	C(11)-H(11B)	0.9600
C(14)-C(15)	1.380(7)	C(11)-H(11C)	0.9600
C(14)-H(14)	0.9300	C(34)-C(33)	1.376(17)
C(26)-C(27)	1.410(8)	C(34)-H(34)	0.9300
C(26)-H(26)	0.9300	C(33)-H(33)	0.9300
C(3)-C(4)	1.384(7)	C(22)-C(23)	1.41(2)
C(3)-H(3)	0.9300	C(22)-H(22)	0.9300
C(15)-C(16)	1.376(8)	C(23)-H(23)	0.9300
C(15)-H(15)	0.9300	C(37)-C(38)	1.373(8)
C(17)-C(16)	1.375(7)	C(37)-C(42)	1.397(8)
C(17)-H(17)	0.9300	C(16)-H(16)	0.9300
C(5)-C(6)	1.373(8)	C(8)-C(7)	1.364(8)
C(5)-H(5)	0.9300	C(8)-H(8)	0.9300
C(19)-C(20)	1.363(9)	C(6)-C(7)	1.382(9)
C(9)-C(24)	1.375(9)	C(6)-H(6)	0.9300
C(18)-C(19)	1.383(8)		

Bond Angles

N(2)-Rh(1)-C(12)	78.29(17)
N(2)-Rh(1)-P(1)	95.64(11)
C(2)-Rh(1)-P(1)	90.80(14)
N(2)-Rh(1)-Cl(2)	170.21(11)
C(2)-Rh(1)-Cl(2)	94.54(14)
P(1)-Rh(1)-Cl(2)	91.09(5)
N(2)-Rh(1)-Cl(1)	84.26(12)
C(2)-Rh(1)-Cl(1)	89.65(14)
P(1)-Rh(1)-Cl(1)	179.52(4)
Cl(2)-Rh(1)-Cl(1)	89.07(6)
N(2)-Rh(1)-S(1)	83.34(11)
C(2)-Rh(1)-S(1)	161.64(14)
P(1)-Rh(1)-S(1)	91.06(4)
Cl(2)-Rh(1)-S(1)	103.69(4)
Cl(1)-Rh(1)-S(1)	88.46(5)
O(2)-S(1)-C(13)	107.7(2)
O(2)-S(1)-C(18)	106.3(2)
C(13)-S(1)-C(18)	100.7(2)
O(2)-S(1)-Rh(1)	124.10(15)
C(13)-S(1)-Rh(1)	96.57(15)
C(18)-S(1)-Rh(1)	117.73(18)
C(37)-P(1)-C(31)	108.5(3)
C(37)-P(1)-C(25)	103.9(2)
C(31)-P(1)-C(25)	100.5(2)
C(37)-P(1)-Rh(1)	109.41(16)
C(31)-P(1)-Rh(1)	114.63(19)
C(25)-P(1)-Rh(1)	118.90(19)
N(2)-N(1)-C(1)	112.1(4)
N(1)-N(2)-C(12)	118.2(4)
N(1)-N(2)-Rh(1)	119.5(3)
C(12)-N(2)-Rh(1)	121.8(3)
N(1)-C(1)-C(2)	119.1(4)
N(1)-C(1)-C(10)	118.1(4)
C(2)-C(1)-C(10)	122.8(4)
C(13)-C(12)-N(2)	118.6(4)
C(13)-C(12)-C(17)	119.6(4)
N(2)-C(12)-C(17)	121.8(4)
C(8)-C(10)-C(9)	118.3(4)
C(8)-C(10)-C(1)	124.5(4)
C(9)-C(10)-C(1)	117.3(4)
C(14)-C(13)-C(12)	119.9(4)
C(14)-C(13)-S(1)	120.9(4)
C(12)-C(13)-S(1)	119.9(3)

Bond Angles

C(5)-C(9)-C(10)	119.7(5)
C(4)-C(9)-C(10)	118.2(4)
C(19)-C(18)-S(1)	110.1(4)
C(19)-C(18)-H(18A)	109.6
S(1)-C(18)-H(18A)	109.6
C(19)-C(18)-H(18B)	109.6
S(1)-C(18)-H(18B)	109.6
H(18A)-C(18)-H(18B)	108.2
C(15)-C(14)-C(13)	120.1(5)
C(15)-C(14)-H(14)	120.0
C(13)-C(14)-H(14)	120.0
C(25)-C(26)-C(27)	119.5(6)
C(25)-C(26)-H(26)	120.3
C(27)-C(26)-H(26)	120.3
C(4)-C(3)-C(2)	119.7(5)
C(4)-C(3)-H(3)	120.2
C(2)-C(3)-H(3)	120.2
C(16)-C(15)-C(14)	120.0(5)
C(16)-C(15)-H(15)	120.0
C(14)-C(15)-H(15)	120.0
C(16)-C(17)-C(12)	118.9(5)
C(16)-C(17)-H(17)	120.6
C(12)-C(17)-H(17)	120.6
C(6)-C(5)-C(9)	119.3(5)
C(6)-C(5)-H(5)	120.3
C(9)-C(5)-H(5)	120.3
C(20)-C(19)-C(24)	121.2(6)
C(20)-C(19)-C(18)	119.6(6)
C(24)-C(19)-C(18)	119.2(6)
C(38)-C(37)-C(42)	118.6(5)
C(38)-C(37)-P(1)	120.6(4)
C(42)-C(37)-P(1)	120.3(5)
C(17)-C(16)-C(15)	121.5(5)
C(17)-C(16)-H(16)	119.2
C(15)-C(16)-H(16)	119.3
O(1)-C(4)-C(3)	123.6(5)
O(1)-C(4)-C(9)	113.9(4)
C(3)-C(4)-C(9)	122.4(5)
C(7)-C(8)-C(10)	121.1(5)
C(7)-C(8)-H(8)	119.5
C(10)-C(8)-H(8)	119.5
C(5)-C(6)-C(7)	120.6(5)
C(5)-C(6)-H(6)	119.7

C(1)-C(2)-C(3)	119.3(4)	C(7)-C(6)-H(6)	119.7
C(1)-C(2)-Rh(1)	110.8(3)	C(37)-C(38)-C(39)	121.0(6)
C(3)-C(2)-Rh(1)	129.8(3)	C(37)-C(38)-H(38)	119.5
C(4)-O(1)-C(11)	117.8(4)	C(39)-C(38)-H(38)	119.5
C(26)-C(25)-C(30)	119.9(5)	C(28)-C(27)-C(26)	121.4(7)
C(26)-C(25)-P(1)	116.8(4)	C(28)-C(27)-H(27)	119.3
C(30)-C(25)-P(1)	123.1(5)	C(26)-C(27)-H(27)	119.3
C(5)-C(9)-C(4)	122.0(5)	C(36)-C(31)-C(32)	118.5(7)
C(36)-C(31)-P(1)	125.8(6)	C(33)-C(32)-C(31)	119.9(10)
C(32)-C(31)-P(1)	115.5(5)	C(33)-C(32)-H(32)	120.1
C(8)-C(7)-C(6)	120.9(5)	C(31)-C(32)-H(32)	120.1
C(8)-C(7)-H(7)	119.5	C(40)-C(39)-C(38)	119.6(7)
C(6)-C(7)-H(7)	119.5	C(40)-C(39)-H(39)	120.2
C(25)-C(30)-C(29)	118.6(7)	C(38)-C(39)-H(39)	120.2
C(25)-C(30)-H(30)	120.7	C(42)-C(41)-C(40)	118.9(6)
C(29)-C(30)-H(30)	120.7	C(42)-C(41)-H(41)	120.6
C(41)-C(42)-C(37)	121.2(7)	C(40)-C(41)-H(41)	120.6
C(41)-C(42)-H(42)	119.4	C(34)-C(35)-C(36)	119.4(10)
C(37)-C(42)-H(42)	119.4	C(34)-C(35)-H(35)	120.3
C(19)-C(20)-C(21)	120.4(9)	C(36)-C(35)-H(35)	120.3
C(19)-C(20)-H(20)	119.8	C(39)-C(40)-C(41)	120.7(7)
C(21)-C(20)-H(20)	119.8	C(39)-C(40)-H(40)	119.6
C(27)-C(28)-C(29)	119.6(6)	C(41)-C(40)-H(40)	119.6
C(27)-C(28)-H(28)	120.2	C(22)-C(21)-C(20)	121.2(11)
C(29)-C(28)-H(28)	120.2	C(22)-C(21)-H(21)	119.4
C(28)-C(29)-C(30)	120.9(7)	C(20)-C(21)-H(21)	119.4
C(28)-C(29)-H(29)	119.5	O(1)-C(11)-H(11A)	109.5
C(30)-C(29)-H(29)	119.5	O(1)-C(11)-H(11B)	109.5
C(19)-C(24)-C(23)	116.4(9)	H(11A)-C(11)-H(11B)	109.5
C(19)-C(24)-H(24)	121.8	O(1)-C(11)-H(11C)	109.5
C(23)-C(24)-H(24)	121.8	H(11A)-C(11)-H(11C)	109.5
C(31)-C(36)-C(35)	121.4(10)	H(11B)-C(11)-H(11C)	109.5
C(31)-C(36)-H(36)	119.3	C(35)-C(34)-C(33)	122.0(8)
C(35)-C(36)-H(36)	119.3	C(35)-C(34)-H(34)	119.0
C(34)-C(33)-C(32)	118.6(11)	C(33)-C(34)-H(34)	119.0
C(34)-C(33)-H(33)	120.7	C(23)-C(22)-H(22)	119.7
C(32)-C(33)-H(33)	120.7	C(22)-C(23)-C(24)	120.2(10)
C(21)-C(22)-C(23)	120.6(9)	C(22)-C(23)-H(23)	119.9
C(21)-C(22)-H(22)	119.7	C(24)-C(23)-H(23)	119.9

TABLE 18
Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{Å}^2 \times 10^3$) for **1**

	x	y	z	U(eq)
Rh(1)	4672(1)	2953(1)	12837(1)	38(1)
S(1)	5396(1)	1506(1)	13660(1)	40(1)
P(1)	2782(1)	2040(1)	12138(1)	43(1)
C(2)	5477(2)	2627(1)	11490(1)	60(1)
Cl(1)	6641(1)	3890(1)	13572(1)	56(1)
N(1)	3556(4)	4357(3)	14037(3)	42(1)
O(2)	4803(3)	435(3)	13434(3)	51(1)
N(2)	4102(4)	3479(3)	13979(3)	40(1)
C(1)	3399(4)	4795(3)	13241(3)	40(1)
C(12)	4414(4)	2980(3)	14769(3)	41(1)
C(10)	2741(4)	5754(3)	13193(3)	41(1)
C(13)	5061(4)	2049(3)	14723(3)	42(1)
C(2)	3897(4)	4310(3)	12528(3)	43(1)
O(1)	3183(5)	6281(4)	10969(3)	81(2)
C(25)	2850(5)	738(4)	11516(3)	50(1)
C(9)	2650(5)	6228(4)	12379(3)	45(1)
C(18)	7114(5)	1353(4)	13985(4)	51(1)
C(14)	5323(5)	1511(4)	15478(3)	50(1)
C(26)	1696(6)	211(4)	11128(4)	59(1)
C(3)	3858(5)	4806(4)	11755(4)	51(1)
C(15)	4991(5)	1918(4)	16283(3)	53(1)
C(17)	4082(5)	3392(4)	15596(3)	47(1)
C(5)	2010(6)	7169(4)	12292(4)	58(1)
C(19)	7567(5)	669(4)	13246(4)	53(1)
C(37)	1870(5)	1817(4)	12994(3)	50(1)
C(16)	4382(5)	2850(4)	16335(4)	54(1)
C(4)	3261(6)	5747(4)	11689(4)	55(1)
C(8)	2197(5)	6247(4)	13882(4)	54(1)

Bond Lengths (Å)	Bond Angles (°)	Bond Lengths (Å)	Bond Angles (°)
1.450(14)	112.8(14)	C13-C12	122.7(15)
1.374(14)	128.6(12)	C12-C11	119.9(13)
1.389(15)	128.4(12)	C11-C10	119.9(13)
1.410(15)	115.4(13)	C10-C9	122.3(14)
1.471(16)	115.8(13)	C9-C8	120.0(13)
1.474(16)	128.1(12)	C8-C7	122.9(15)
1.349(15)	114.4(13)	C7-C6	122.4(14)
1.390(15)	114.9(13)	C6-C5	122.1(14)
1.378(15)	126.4(12)	C5-C4	120.1(13)
1.440(15)	116.1(13)	C4-C3	121.1(13)
1.440(15)	127.2(12)	C3-C2	122.4(14)
1.441(15)	127.1(12)	C2-C1	122.5(14)
1.395(16)	116.4(13)	C1-N1	122.1(14)
1.294(15)	107.4(13)	C1-N2	122.1(14)
1.294(15)	116.4(13)	C1-N3	122.1(14)
0.9300	123.4(12)	C2-C3	121.7(14)
0.9300	123.4(12)	C3-C4	121.7(14)
0.9300	123.4(12)	C4-C5	121.7(14)
0.9300	123.4(12)	C5-C6	121.7(14)
0.9300	123.4(12)	C6-C7	121.7(14)
0.9300	123.4(12)	C7-C8	121.7(14)
0.9300	123.4(12)	C8-C9	121.7(14)
0.9300	123.4(12)	C9-C10	121.7(14)
0.9300	123.4(12)	C10-C11	121.7(14)
0.9300	123.4(12)	C11-C12	121.7(14)
0.9300	123.4(12)	C12-C13	121.7(14)

TABLE 19
Bond Lengths (Å) and Bond Angles (°) (over)

1.440(15)	112.8(14)	C13-C12	122.7(15)
1.374(14)	128.6(12)	C12-C11	119.9(13)
1.389(15)	128.4(12)	C11-C10	119.9(13)
1.410(15)	115.4(13)	C10-C9	122.3(14)
1.471(16)	115.8(13)	C9-C8	120.0(13)
1.474(16)	128.1(12)	C8-C7	122.9(15)
1.349(15)	114.4(13)	C7-C6	122.4(14)
1.390(15)	114.9(13)	C6-C5	122.1(14)
1.378(15)	126.4(12)	C5-C4	120.1(13)
1.440(15)	116.1(13)	C4-C3	121.1(13)
1.440(15)	127.2(12)	C3-C2	122.4(14)
1.441(15)	127.1(12)	C2-C1	122.5(14)
1.395(16)	116.4(13)	C1-N1	122.1(14)
1.294(15)	107.4(13)	C1-N2	122.1(14)
1.294(15)	116.4(13)	C1-N3	122.1(14)
0.9300	123.4(12)	C2-C3	121.7(14)
0.9300	123.4(12)	C3-C4	121.7(14)
0.9300	123.4(12)	C4-C5	121.7(14)
0.9300	123.4(12)	C5-C6	121.7(14)
0.9300	123.4(12)	C6-C7	121.7(14)
0.9300	123.4(12)	C7-C8	121.7(14)
0.9300	123.4(12)	C8-C9	121.7(14)
0.9300	123.4(12)	C9-C10	121.7(14)
0.9300	123.4(12)	C10-C11	121.7(14)
0.9300	123.4(12)	C11-C12	121.7(14)
0.9300	123.4(12)	C12-C13	121.7(14)

Bond Angles (°)		Bond Angles (°)	
O(1)-S(1)-C(13)	110.0(5)	S(1)-C(18)-H(18C)	109.5
O(1)-S(1)-C(18)	107.3(5)	H(18A)-C(18)-H(18C)	109.5
C(13)-S(1)-C(18)	104.3(6)	H(18B)-C(18)-H(18C)	109.5
O(1)-S(1)-Rh(1)	121.8(3)	O(3)-C(35)-H(35A)	109.5
C(13)-S(1)-Rh(1)	95.8(4)	O(3)-C(35)-H(35B)	109.5
C(18)-S(1)-Rh(1)	115.6(4)	H(35A)-C(35)-H(35B)	109.5
N(2)-N(1)-C(1)	109.6(10)	O(3)-C(35)-H(35C)	109.5
C(2)-C(1)-N(1)	118.8(10)	H(35A)-C(35)-H(35C)	109.5
C(2)-C(1)-C(10)	122.8(11)	H(35B)-C(35)-H(35C)	109.5
N(1)-C(1)-C(10)	118.5(11)	C(23)-C(24)-C(25)	119.2(13)
C(8)-C(10)-C(9)	117.9(12)	C(23)-C(24)-H(24)	120.4
C(8)-C(10)-C(1)	125.6(12)	C(25)-C(24)-H(24)	120.4
C(9)-C(10)-C(1)	116.5(12)	C(34)-Rh(1)-N(2)	97.8(5)
C(30)-C(29)-C(34)	125.9(12)	C(34)-Rh(1)-C(2)	86.6(4)
C(30)-C(29)-N(4)	120.2(12)	N(2)-Rh(1)-C(2)	76.3(4)
C(34)-C(29)-N(4)	113.8(10)	C(34)-Rh(1)-N(3)	77.6(5)
C(33)-C(32)-C(31)	118.8(12)	N(2)-Rh(1)-N(3)	175.1(4)
C(33)-C(32)-H(33)	120.6	C(2)-Rh(1)-N(3)	105.0(4)
C(31)-C(32)-H(33)	120.6	C(34)-Rh(1)-S(1)	92.1(3)
C(31)-C(30)-C(29)	120.6(13)	N(2)-Rh(1)-S(1)	84.9(3)
C(31)-C(30)-H(31)	119.7	C(2)-Rh(1)-S(1)	160.7(3)
C(29)-C(30)-H(31)	119.7	N(3)-Rh(1)-S(1)	93.4(3)
C(30)-C(31)-C(32)	120.6(12)	C(34)-Rh(1)-Cl(1)	174.8(4)
C(30)-C(31)-H(32)	119.7	N(2)-Rh(1)-Cl(1)	86.3(3)
C(32)-C(31)-H(32)	119.7	C(2)-Rh(1)-Cl(1)	91.4(3)
C(32)-C(33)-C(34)	123.7(12)	N(3)-Rh(1)-Cl(1)	98.3(3)
C(32)-C(33)-H(34)	118.2	S(1)-Rh(1)-Cl(1)	91.44(11)
C(34)-C(33)-H(34)	118.2	C(29)-C(34)-C(33)	110.3(11)
C(5)-C(9)-C(4)	125.1(13)	C(29)-C(34)-Rh(1)	116.6(9)
C(5)-C(9)-C(10)	116.5(13)	C(33)-C(34)-Rh(1)	133.1(10)
C(4)-C(9)-C(10)	118.3(11)	N(1)-N(2)-C(12)	115.2(10)
C(9)-C(5)-C(6)	124.5(14)	N(1)-N(2)-Rh(1)	122.1(7)
C(9)-C(5)-H(5)	117.7	C(12)-N(2)-Rh(1)	122.6(7)
C(6)-C(5)-H(5)	117.7	N(4)-N(3)-C(19)	116.0(10)
C(5)-C(6)-C(7)	118.3(14)	N(4)-N(3)-Rh(1)	119.4(8)
C(5)-C(6)-H(6)	120.9	C(19)-N(3)-Rh(1)	124.3(7)
C(7)-C(6)-H(6)	120.9	C(1)-C(2)-C(3)	120.5(10)
C(4)-O(2)-C(11)	117.2(10)	C(1)-C(2)-Rh(1)	113.1(8)
C(4)-C(3)-C(2)	117.7(11)	C(3)-C(2)-Rh(1)	126.4(9)
C(4)-C(3)-H(3)	121.2	C(12)-C(13)-C(14)	118.9(11)
C(2)-C(3)-H(3)	121.2	C(12)-C(13)-S(1)	121.9(9)
O(2)-C(11)-H(11A)	109.5	C(14)-C(13)-S(1)	119.1(10)
O(2)-C(11)-H(11B)	109.5	N(3)-N(4)-C(29)	112.3(10)
H(11A)-C(11)-H(11B)	109.5	C(13)-C(12)-C(17)	123.3(11)
O(2)-C(11)-H(11C)	109.5	C(13)-C(12)-N(2)	114.5(10)
H(11A)-C(11)-H(11C)	109.5	C(17)-C(12)-N(2)	122.2(11)
H(11B)-C(11)-H(11C)	109.5	C(27)-C(28)-C(26)	118.5(12)
S(1)-C(18)-H(18A)	109.5	C(27)-C(28)-C(19)	118.7(11)
S(1)-C(18)-H(18B)	109.5	C(26)-C(28)-C(19)	122.6(13)
H(18A)-C(18)-H(18B)	109.5	C(3)-C(4)-O(2)	122.8(12)
C(3)-C(4)-C(9)	124.2(10)	C(20)-C(21)-H(21)	120.9
O(2)-C(4)-C(9)	112.9(11)	C(12)-C(17)-C(16)	117.5(12)
C(20)-C(19)-C(28)	119.9(12)	C(12)-C(17)-H(17)	121.2
C(20)-C(19)-N(3)	118.7(11)	C(16)-C(17)-H(17)	121.2
C(28)-C(19)-N(3)	121.4(11)	C(10)-C(8)-C(7)	123.8(13)
C(16)-C(15)-C(14)	123.7(14)	C(10)-C(8)-H(8)	118.1
C(16)-C(15)-H(15)	118.1	C(7)-C(8)-H(8)	118.1
C(14)-C(15)-H(15)	118.1	C(27)-C(23)-C(24)	119.0(15)
C(15)-C(14)-C(13)	117.3(12)	C(27)-C(23)-H(23)	120.5
C(15)-C(14)-H(14)	121.4	C(24)-C(23)-H(23)	120.5
C(13)-C(14)-H(14)	121.4	C(21)-C(22)-O(3)	126.0(14)
C(25)-C(26)-C(28)	119.6(14)	C(21)-C(22)-C(27)	121.5(13)
C(25)-C(26)-H(26)	120.2	O(3)-C(22)-C(27)	112.5(13)
C(28)-C(26)-H(26)	120.2	C(26)-C(25)-C(24)	121.8(14)
C(22)-O(3)-C(35)	115.8(12)	C(26)-C(25)-H(25)	119.1
C(15)-C(16)-C(17)	119.3(13)	C(24)-C(25)-H(25)	119.1
C(15)-C(16)-H(16)	120.4	C(8)-C(7)-C(6)	118.9(14)
C(17)-C(16)-H(16)	120.4	C(8)-C(7)-H(7)	120.5
C(23)-C(27)-C(28)	121.7(13)	C(6)-C(7)-H(7)	120.5
C(23)-C(27)-C(22)	119.7(14)	C(19)-C(20)-H(20)	118.5
C(28)-C(27)-C(22)	118.5(12)	C(21)-C(20)-H(20)	118.5
C(19)-C(20)-C(21)	123.1(12)	C(22)-C(21)-C(20)	118.2(13)
		C(22)-C(21)-H(21)	120.9

TABLE 20
Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{Å}^2 \times 10^3$) for (6)

	x	y	z	U _{eq}
S(1)	72(3)	6439(3)	8654(2)	35(1)
N(1)	1357(9)	3543(8)	6707(6)	32(2)
C(1)	2640(11)	3904(11)	6517(8)	28(3)
O(1)	-634(7)	7375(7)	8456(6)	55(3)
C(10)	3334(13)	3064(11)	5846(8)	37(3)
C(29)	2185(11)	7907(11)	7090(8)	28(3)
C(32)	683(11)	7087(14)	5418(9)	49(4)
C(30)	2015(12)	8660(12)	6499(9)	47(4)
C(31)	1270(13)	8280(13)	5712(9)	48(4)
C(33)	872(10)	6322(12)	6005(8)	37(3)
C(9)	4710(12)	3484(13)	5673(9)	47(4)
C(5)	5369(14)	2690(14)	5072(10)	59(4)
C(6)	4812(16)	1570(16)	4598(12)	90(6)
O(2)	6536(8)	4940(9)	5918(6)	60(3)
C(3)	4601(10)	5406(11)	6769(8)	38(3)
C(11)	7186(11)	6096(13)	6371(10)	71(5)
C(18)	189(11)	6644(11)	9906(8)	54(4)
C(35)	7064(19)	8196(14)	12067(11)	126(8)
C(24)	7750(20)	10521(13)	11579(12)	94(6)
Cl(1)	2693(3)	4954(3)	9108(2)	17(1)
Rh(1)	3918(1)	3890(1)	8860(1)	19(1)
C(34)	1654(10)	6691(11)	6906(9)	40(4)
N(2)	111(9)	1399(8)	7309(6)	32(3)
N(3)	4087(9)	7528(9)	8386(7)	36(3)
C(2)	7207(10)	4979(10)	6955(8)	29(3)
C(13)	336(10)	5043(10)	8226(8)	36(3)
N(4)	5003(9)	8329(9)	7948(7)	39(3)
C(12)	-460(11)	4126(10)	7579(8)	29(3)
C(28)	3467(12)	8808(10)	10037(10)	39(3)
C(4)	5267(11)	4638(12)	6160(9)	36(3)
C(19)	3840(12)	7893(13)	9285(9)	36(3)
C(15)	3050(14)	3797(13)	8123(10)	62(4)
C(14)	2283(12)	4876(11)	8520(8)	50(4)
C(26)	2348(13)	9413(10)	9946(9)	53(4)
O(3)	5906(11)	8768(8)	11918(7)	80(3)
C(16)	2586(12)	2879(12)	7496(9)	56(4)
C(27)	3173(13)	9060(10)	10918(10)	39(3)
C(20)	4877(12)	7312(10)	9428(9)	46(4)
C(21)	8638(13)	7869(12)	10285(10)	55(4)
C(17)	1217(12)	3037(11)	7204(9)	49(4)
C(8)	2813(13)	1949(12)	5382(8)	48(4)
C(23)	3856(16)	9931(13)	11680(11)	72(5)
C(22)	5297(14)	8430(12)	11015(10)	49(4)
C(25)	2941(15)	10267(11)	10692(11)	60(4)
C(7)	3996(13)	1178(12)	4775(9)	74(5)

TABLE 21
Bond Lengths (Å) and Bond Angles (°) for (12)

Bond Lengths (Å)		Bond Lengths (Å)	
C(1)-Ir(1)	2.3816(19)	C(16)-C(15)	1.387(11)
C(3)-C(2)	1.382(10)	C(29)-C(28)	1.354(15)
C(3)-C(4)	1.401(11)	C(29)-C(30)	1.471(12)
C(39)-C(40)	1.302(19)	C(25)-C(30)	1.360(12)
C(39)-C(38)	1.385(15)	C(25)-C(26)	1.401(11)
Ir(1)-N(2)	2.007(6)	C(13)-C(14)	1.385(12)
Ir(1)-C(2)	2.029(7)	C(13)-C(12)	1.392(10)
Ir(1)-P(1)	2.305(2)	C(8)-C(7)	1.360(12)
Ir(1)-S(1)	2.3700(18)	C(37)-C(42)	1.372(13)
Ir(1)-Cl(2)	2.409(2)	C(37)-C(38)	1.377(14)
O(2)-S(1)	1.474(5)	C(6)-C(7)	1.392(12)
P(1)-C(25)	1.826(8)	C(15)-C(14)	1.375(12)
P(1)-C(37)	1.826(8)	C(32)-C(33)	1.373(12)
P(1)-C(31)	1.829(8)	C(19)-C(24)	1.375(12)
S(1)-C(12)	1.786(8)	C(19)-C(20)	1.392(13)
S(1)-C(18)	1.819(8)	C(20)-C(21)	1.378(17)
N(2)-N(1)	1.275(8)	C(33)-C(34)	1.350(14)
N(2)-C(11)	1.399(9)	C(41)-C(40)	1.39(2)
C(11)-C(16)	1.381(11)	C(41)-C(42)	1.406(16)
C(11)-C(12)	1.406(10)	C(23)-C(22)	1.33(2)
N(1)-C(1)	1.374(9)	C(23)-C(24)	1.366(18)
C(2)-C(1)	1.407(10)	C(22)-C(21)	1.37(2)
C(10)-C(8)	1.392(10)	C(9)-C(4)	1.432(11)
C(10)-C(9)	1.406(10)	C(35)-C(36)	1.387(12)
C(10)-C(1)	1.434(10)	C(35)-C(34)	1.394(15)
O(1)-C(4)	1.337(9)	C(27)-C(26)	1.373(13)
O(1)-C(17)	1.431(11)	C(27)-C(28)	1.395(15)
C(18)-C(19)	1.506(12)	C(31)-C(32)	1.385(12)
C(5)-C(6)	1.359(12)	C(31)-C(36)	1.391(12)
C(5)-C(9)	1.406(10)		
Bond Angles (°)		Bond Angles (°)	
C(2)-C(3)-C(4)	120.0(7)	C(26)-C(27)-C(28)	120.0(9)
C(40)-C(39)-C(38)	121.8(13)	C(32)-C(31)-C(36)	119.0(8)
N(2)-Ir(1)-C(2)	78.2(3)	C(32)-C(31)-P(1)	116.9(6)
N(2)-Ir(1)-P(1)	95.23(18)	C(36)-C(31)-P(1)	124.0(7)
C(2)-Ir(1)-P(1)	90.8(2)	O(1)-C(4)-C(3)	123.3(7)
N(2)-Ir(1)-S(1)	83.53(17)	O(1)-C(4)-C(9)	115.0(7)
C(2)-Ir(1)-S(1)	161.7(2)	C(3)-C(4)-C(9)	121.7(7)
P(1)-Ir(1)-S(1)	90.94(7)	C(11)-C(16)-C(15)	120.0(8)
N(2)-Ir(1)-Cl(1)	169.68(17)	C(28)-C(29)-C(30)	118.4(10)
C(2)-Ir(1)-Cl(1)	93.8(2)	C(30)-C(25)-C(26)	120.2(8)
P(1)-Ir(1)-Cl(1)	91.29(8)	C(30)-C(25)-P(1)	119.1(6)
S(1)-Ir(1)-Cl(1)	104.39(7)	C(26)-C(25)-P(1)	120.1(6)
N(2)-Ir(1)-Cl(2)	86.18(18)	C(14)-C(13)-C(12)	119.2(7)
C(2)-Ir(1)-Cl(2)	89.6(2)	C(13)-C(12)-C(11)	120.1(7)
P(1)-Ir(1)-Cl(2)	178.59(7)	C(13)-C(12)-S(1)	120.9(6)
S(1)-Ir(1)-Cl(2)	89.13(7)	C(11)-C(12)-S(1)	118.6(6)
Cl(1)-Ir(1)-Cl(2)	87.33(8)	C(25)-C(30)-C(29)	119.4(9)
C(25)-P(1)-C(37)	107.5(4)	C(7)-C(8)-C(10)	120.7(8)
C(25)-P(1)-C(31)	104.8(4)	C(42)-C(37)-C(38)	117.7(9)
C(37)-P(1)-C(31)	100.2(4)	C(42)-C(37)-P(1)	125.1(8)
C(25)-P(1)-Ir(1)	109.9(3)	C(38)-C(37)-P(1)	117.2(7)
C(37)-P(1)-Ir(1)	115.2(3)	C(5)-C(6)-C(7)	119.5(8)
C(31)-P(1)-Ir(1)	118.1(3)	C(14)-C(15)-C(16)	120.4(8)
O(2)-S(1)-C(12)	106.8(3)	C(33)-C(32)-C(31)	121.5(8)
O(2)-S(1)-C(18)	106.1(3)	C(24)-C(19)-C(20)	120.1(10)
C(12)-S(1)-C(18)	101.3(4)	C(24)-C(19)-C(18)	120.7(9)
O(2)-S(1)-Ir(1)	123.3(2)	C(20)-C(19)-C(18)	119.2(8)
C(12)-S(1)-Ir(1)	97.5(2)	C(37)-C(38)-C(39)	121.3(12)
C(18)-S(1)-Ir(1)	118.3(3)	C(35)-C(36)-C(31)	118.8(9)
N(1)-N(2)-C(11)	118.1(6)	C(21)-C(20)-C(19)	118.4(12)
N(1)-N(2)-Ir(1)	119.7(5)	C(15)-C(14)-C(13)	120.8(8)
C(11)-N(2)-Ir(1)	122.1(5)	C(34)-C(33)-C(32)	120.0(9)
C(16)-C(11)-N(2)	123.0(7)	C(27)-C(26)-C(25)	120.6(9)
C(16)-C(11)-C(12)	119.5(7)	C(8)-C(7)-C(6)	121.4(8)
N(2)-C(11)-C(12)	117.5(7)	C(40)-C(41)-C(42)	120.1(12)
N(2)-N(1)-C(1)	113.0(6)	C(33)-C(34)-C(35)	119.8(9)
C(3)-C(2)-C(1)	119.2(6)	C(22)-C(23)-C(24)	122.3(14)

C(3)-C(2)-Ir(1)	130.3(5)	C(23)-C(22)-C(21)	119.4(14)
C(1)-C(2)-Ir(1)	110.5(5)	C(22)-C(21)-C(20)	120.9(14)
C(8)-C(10)-C(9)	118.1(7)	C(23)-C(24)-C(19)	118.8(12)
C(8)-C(10)-C(11)	123.8(7)	C(37)-C(42)-C(41)	119.9(12)
C(9)-C(10)-C(11)	118.1(7)	C(29)-C(28)-C(27)	121.4(9)
C(4)-O(1)-C(17)	119.0(7)	C(39)-C(40)-C(41)	119.2(11)
C(19)-C(18)-S(1)	109.0(6)	N(1)-C(1)-C(2)	118.5(6)
C(6)-C(5)-C(9)	120.1(8)	N(1)-C(1)-C(10)	119.5(6)
C(5)-C(9)-C(10)	120.2(7)	C(2)-C(1)-C(10)	122.0(6)
C(5)-C(9)-C(4)	121.1(7)	C(36)-C(35)-C(34)	120.8(9)
C(10)-C(9)-C(4)	118.6(6)		

TABLE 22

Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (12)

Atom	x	y	z	U _{eq}
C(1)	3565(2)	3364(2)	3489(1)	43(1)
C(3)	1064(8)	153(6)	3191(5)	36(2)
C(39)	3619(15)	1688(10)	5100(8)	81(4)
Ir(1)	267(1)	2036(1)	2134(1)	28(1)
O(2)	200(5)	4531(4)	1561(4)	39(1)
O(1)	3232(2)	2968(2)	3816(1)	31(1)
C(10)	1809(2)	1179(2)	3453(1)	44(1)
S(1)	445(2)	3458(2)	1335(1)	31(1)
N(2)	870(6)	1487(5)	995(4)	28(1)
C(15)	583(8)	1981(6)	217(5)	41(1)
N(1)	466(6)	326(5)	950(4)	31(1)
C(2)	1959(7)	31(5)	2443(5)	29(2)
C(16)	2326(7)	771(6)	1802(5)	31(2)
C(11)	1717(7)	1347(5)	3953(4)	31(2)
C(18)	2213(8)	3634(7)	1032(6)	41(2)
C(5)	3079(8)	2180(6)	2689(6)	41(2)
C(9)	2389(8)	1250(6)	2588(5)	34(2)
C(14)	1617(7)	1766(6)	1733(5)	39(2)
C(37)	3950(11)	3680(8)	1147(7)	61(3)
C(12)	424(9)	2557(9)	2521(7)	50(3)
C(31)	2154(8)	4262(6)	3475(5)	33(2)
C(14)	693(8)	801(7)	3259(6)	40(2)
C(16)	946(8)	1593(6)	584(5)	36(2)
C(29)	3760(9)	4390(9)	930(6)	56(3)
C(25)	3166(8)	3229(7)	1961(5)	38(2)
C(13)	366(8)	3468(6)	471(6)	38(2)
C(12)	104(7)	2916(6)	269(5)	31(2)
C(39)	3188(8)	4214(7)	1713(5)	44(2)
C(8)	2968(8)	1235(7)	1140(5)	39(2)
C(37)	3316(9)	320(6)	3656(6)	44(2)
C(6)	3693(9)	2608(7)	2029(6)	46(2)
C(27)	665(9)	2139(7)	1322(6)	44(2)
C(32)	3349(9)	4803(6)	3881(6)	44(2)
C(19)	2621(8)	4357(7)	1781(6)	42(2)
C(38)	2865(11)	2171(9)	4425(7)	66(3)
C(36)	983(9)	4701(7)	3619(6)	45(2)
C(20)	2612(9)	5441(8)	1746(8)	61(3)

