

APPENDIX

APPENDIX

Publications in other areas

1. *Molecular Crystals & Liquid Crystals*, **501**, 53 (2009).
2. *Liquid Crystals*, **35**, 895 (2008).
3. *Transition Met. Chem.*, **31**, 495 (2006).

Table 1.Bond lengths (Å) and bond angles (°) for [Pd(L³)Cl] (3)

Bond lengths	(Å)	Bond lengths	(Å)
Pd(1)-N(2)	1.975(2)	C(7)-H(7)	0.9300
Pd(1)-O(1)	1.992(2)	C(8)-C(9)	1.400(4)
Pd(1)-S(1)	2.2413(9)	C(8)-H(8)	0.9300
Pd(1)-Cl(1)	2.3250(10)	C(9)-C(10)	1.412(4)
S(1)-C(12)	1.774(2)	C(11)-C(12)	1.387(3)
S(1)-C(17)	1.826(3)	C(11)-C(16)	1.390(3)
O(1)-C(2)	1.281(3)	C(12)-C(13)	1.395(3)
N(1)-N(2)	1.274(3)	C(13)-C(14)	1.376(4)
N(1)-C(1)	1.347(3)	C(13)-H(13)	0.9300
N(2)-C(11)	1.435(3)	C(14)-C(15)	1.377(4)
C(1)-C(2)	1.438(3)	C(14)-H(14)	0.9300
C(1)-C(9)	1.461(3)	C(15)-C(16)	1.369(4)
C(2)-C(3)	1.434(4)	C(15)-H(15)	0.9300
C(3)-C(4)	1.338(4)	C(16)-H(16)	0.9300
C(3)-H(3)	0.9300	C(17)-C(18)	1.505(4)
C(4)-C(10)	1.418(4)	C(17)-H(17A)	0.9700
C(4)-H(4)	0.9300	C(17)-H(17B)	0.9700
C(5)-C(6)	1.356(4)	C(18)-C(19)	1.494(5)
C(5)-C(10)	1.410(4)	C(18)-H(18A)	0.9700
C(5)-H(5)	0.9300	C(18)-H(18B)	0.9700
C(6)-C(7)	1.380(4)	C(19)-H(19A)	0.9600
C(6)-H(6)	0.9300	C(19)-H(19B)	0.9600
C(7)-C(8)	1.376(4)	C(19)-H(19C)	0.9600

Bond angles	(°)	Bond lengths	(°)
N(2)-Pd(1)-O(1)	91.74(7)	C(8)-C(7)-C(6)	121.4(3)
N(2)-Pd(1)-S(1)	87.53(6)	C(8)-C(7)-H(7)	119.3
O(1)-Pd(1)-S(1)	178.35(6)	C(6)-C(7)-H(7)	119.3
N(2)-Pd(1)-Cl(1)	177.08(6)	C(7)-C(8)-C(9)	120.7(3)
O(1)-Pd(1)-Cl(1)	91.18(5)	C(7)-C(8)-H(8)	119.7
S(1)-Pd(1)-Cl(1)	89.55(2)	C(9)-C(8)-H(8)	119.7
C(12)-S(1)-C(17)	102.75(11)	C(8)-C(9)-C(10)	118.0(2)
C(12)-S(1)-Pd(1)	97.71(8)	C(8)-C(9)-C(1)	122.2(2)
C(17)-S(1)-Pd(1)	108.13(10)	C(10)-C(9)-C(1)	119.8(2)
C(2)-O(1)-Pd(1)	123.71(16)	C(5)-C(10)-C(9)	119.3(3)
N(2)-N(1)-C(1)	124.2(2)	C(5)-C(10)-C(4)	122.3(3)
N(1)-N(2)-C(11)	114.7(2)	C(9)-C(10)-C(4)	118.4(2)
N(1)-N(2)-Pd(1)	127.71(16)	C(12)-C(11)-C(16)	119.0(2)
C(11)-N(2)-Pd(1)	117.58(15)	C(12)-C(11)-N(2)	117.7(2)
N(1)-C(1)-C(2)	126.2(2)	C(16)-C(11)-N(2)	123.4(2)
N(1)-C(1)-C(9)	114.2(2)	C(11)-C(12)-C(13)	120.7(2)
C(2)-C(1)-C(9)	119.5(2)	C(11)-C(12)-S(1)	118.81(18)
O(1)-C(2)-C(1)	116.9(2)	C(13)-C(12)-S(1)	120.43(19)
O(1)-C(2)-C(1)	125.9(2)	C(14)-C(13)-C(12)	119.3(2)
C(3)-C(2)-C(1)	117.3(2)	C(13)-C(14)-C(15)	119.8(2)
C(4)-C(3)-C(2)	122.3(3)	C(16)-C(15)-C(14)	121.3(2)
C(3)-C(4)-C(10)	122.8(3)	C(15)-C(16)-C(11)	119.8(2)
C(6)-C(5)-C(10)	121.4(3)	C(18)-C(17)-S(1)	114.9(2)
C(5)-C(6)-C(7)	119.3(3)	C(19)-C(18)-C(17)	113.0(3)

Table 2.

Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for $[\text{Pd}(\text{L}^3)\text{Cl}]$ (**3**)

	x	y	z	U(eq)
Pd(1)	752(1)	4451(1)	3503(1)	40(1)
Cl(1)	-491(1)	4344(1)	3548(1)	60(1)
S(1)	757(1)	2592(1)	2835(1)	42(1)
O(1)	763(1)	6071(2)	4117(1)	54(1)
N(1)	2248(1)	5215(2)	3754(1)	39(1)
N(2)	1807(1)	4461(2)	3433(1)	37(1)
C(1)	2056(1)	6181(2)	4202(1)	39(1)
C(2)	1335(1)	6585(3)	4366(1)	46(1)
C(3)	1248(2)	7672(3)	4845(1)	60(1)
C(4)	1807(2)	8295(3)	5135(1)	58(1)
C(5)	3112(2)	8605(3)	5298(1)	57(1)
C(6)	3797(2)	8240(3)	5157(1)	61(1)
C(7)	3923(2)	7191(3)	4707(1)	57(1)
C(8)	3369(1)	6506(3)	4398(1)	48(1)
C(9)	2657(1)	6866(3)	4530(1)	42(1)
C(10)	2527(2)	7933(3)	4994(1)	49(1)
C(11)	2131(1)	3506(2)	2977(1)	36(1)
C(12)	1684(1)	2596(3)	2642(1)	40(1)
C(13)	1961(1)	1660(3)	2181(1)	49(1)
C(14)	2685(1)	1656(3)	2055(1)	54(1)
C(15)	3129(1)	2546(3)	2397(1)	54(1)
C(16)	2863(1)	3453(3)	2857(1)	46(1)
C(17)	344(1)	3087(3)	2049(1)	51(1)
C(18)	603(2)	4441(3)	1765(2)	70(1)
C(19)	224(2)	4838(5)	1140(2)	89(1)

Table 3.

Bond lengths (\AA) and bond angles ($^\circ$) for $[\text{Pd}(\text{L}^6)\text{Cl}]$ (**6**)

Bond lengths	(\AA)	Bond lengths	(\AA)
Pd(1)-N(2)	1.977(5)	C(16)-C(15)	1.375(9)
Pd(1)-O(1)	1.990(4)	C(16)-H(16)	0.9300
Pd(1)-S(1)	2.2300(15)	C(5)-C(6)	1.352(11)
Pd(1)-Cl(1)	2.3109(16)	C(5)-H(5)	0.9300
S(1)-C(12)	1.774(6)	C(8)-C(7)	1.373(9)
S(1)-C(17)	1.810(7)	C(8)-H(8)	0.9300
N(2)-N(1)	1.258(6)	C(17)-H(17A)	0.9600
N(2)-C(11)	1.434(7)	C(17)-H(17B)	0.9600
O(1)-C(1)	1.282(7)	C(17)-H(17C)	0.9600
N(1)-C(2)	1.363(8)	C(13)-C(14)	1.376(9)
C(11)-C(16)	1.390(8)	C(13)-H(13)	0.9300
C(11)-C(12)	1.394(8)	C(15)-C(14)	1.382(10)
C(2)-C(3)	1.425(8)	C(15)-H(15)	0.9300
C(2)-C(1)	1.440(9)	C(14)-H(14)	0.9300
C(1)-C(10)	1.459(8)	C(3)-H(3)	0.9300
C(10)-C(8)	1.391(9)	C(6)-C(7)	1.389(10)
C(10)-C(9)	1.405(8)	C(6)-H(6)	0.9300
C(12)-C(13)	1.379(8)	C(7)-H(7)	0.9300
C(4)-C(3)	1.327(9)	C(4)-H(4)	0.9300
C(4)-C(9)	1.423(10)	C(9)-C(5)	1.400(9)
Bond angles	($^\circ$)	Bond lengths	($^\circ$)
N(2)-Pd(1)-O(1)	92.75(18)	C(9)-C(5)-H(5)	119.0
N(2)-Pd(1)-S(1)	86.97(14)	C(7)-C(8)-C(10)	120.9(7)
O(1)-Pd(1)-S(1)	176.56(13)	C(7)-C(8)-H(8)	119.6

N(2)-Pd(1)-Cl(1)	175.22(14)	C(10)-C(8)-H(8)	119.6
O(1)-Pd(1)-Cl(1)	91.13(13)	S(1)-C(17)-H(17A)	109.5
S(1)-Pd(1)-Cl(1)	89.33(6)	S(1)-C(17)-H(17B)	109.5
C(12)-S(1)-C(17)	102.7(3)	H(17A)-C(17)-H(17B)	109.5
C(12)-S(1)-Pd(1)	98.7(2)	S(1)-C(17)-H(17C)	109.5
C(17)-S(1)-Pd(1)	108.3(3)	H(17A)-C(17)-H(17C)	109.5
N(1)-N(2)-C(11)	113.7(5)	H(17B)-C(17)-H(17C)	109.5
N(1)-N(2)-Pd(1)	127.7(4)	C(14)-C(13)-C(12)	119.9(6)
C(11)-N(2)-Pd(1)	118.5(4)	C(14)-C(13)-H(13)	120.1
C(1)-O(1)-Pd(1)	123.3(4)	C(12)-C(13)-H(13)	120.1
N(2)-N(1)-C(2)	123.3(5)	C(16)-C(15)-C(14)	121.4(6)
C(16)-C(11)-C(12)	118.2(5)	C(16)-C(15)-H(15)	119.3
C(16)-C(11)-N(2)	124.7(5)	C(14)-C(15)-H(15)	119.3
C(12)-C(11)-N(2)	117.0(5)	C(13)-C(14)-C(15)	119.2(6)
N(1)-C(2)-C(3)	113.7(6)	C(13)-C(14)-H(14)	120.4
N(1)-C(2)-C(1)	127.5(5)	C(15)-C(14)-H(14)	120.4
C(3)-C(2)-C(1)	118.7(6)	C(4)-C(3)-C(2)	123.1(7)
O(1)-C(1)-C(2)	125.3(5)	C(4)-C(3)-H(3)	118.5
O(1)-C(1)-C(10)	117.2(6)	C(2)-C(3)-H(3)	118.5
C(2)-C(1)-C(10)	117.5(5)	C(5)-C(6)-C(7)	120.1(7)
C(8)-C(10)-C(9)	119.5(6)	C(5)-C(6)-H(6)	119.9
C(8)-C(10)-C(1)	120.2(6)	C(7)-C(6)-H(6)	119.9
C(9)-C(10)-C(1)	120.3(6)	C(8)-C(7)-C(6)	119.6(7)
C(13)-C(12)-C(11)	121.3(5)	C(8)-C(7)-H(7)	120.2
C(13)-C(12)-S(1)	120.3(5)	C(6)-C(7)-H(7)	120.2
C(11)-C(12)-S(1)	118.3(4)	C(15)-C(16)-C(11)	120.0(6)
C(3)-C(4)-C(9)	120.8(6)	C(15)-C(16)-H(16)	120.0
C(3)-C(4)-H(4)	119.6	C(11)-C(16)-H(16)	120.0
C(9)-C(4)-H(4)	119.6	C(6)-C(5)-C(9)	121.9(7)
C(5)-C(9)-C(10)	117.9(7)	C(6)-C(5)-H(5)	119.0
C(5)-C(9)-C(4)	122.5(6)	C(10)-C(9)-C(4)	119.6(6)

Table 4.

Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for $[\text{Pd}(\text{L}^6)\text{Cl}]$ (**6**)

	x	y	z	U(eq)
Pd(1)	9308(1)	9749(1)	1311(1)	38(1)
S(1)	10771(2)	8495(1)	2047(1)	45(1)
Cl(1)	9000(6)	8181(5)	779(2)	41(1)
O(1)	8145(5)	10881(4)	631(2)	49(1)
N(1)	8280(6)	8097(5)	220(2)	45(1)
C(11)	9575(7)	6960(5)	1050(3)	42(1)
C(2)	7581(8)	9133(6)	-118(3)	45(1)
C(1)	7507(7)	10457(6)	89(3)	44(1)
C(10)	6643(8)	11396(6)	-356(3)	46(1)
C(12)	10419(8)	6977(5)	1665(3)	42(1)
C(4)	5984(9)	9670(7)	-1131(3)	59(2)
C(9)	5891(8)	10997(7)	-957(3)	51(2)
C(16)	9334(9)	5773(6)	746(3)	56(2)
C(5)	5117(9)	11943(8)	-1370(3)	61(2)
C(8)	6533(8)	12691(7)	-185(3)	56(2)
C(17)	9384(11)	8366(7)	2705(3)	70(2)
C(13)	11026(9)	5854(6)	1965(3)	54(2)
C(15)	9908(10)	4655(6)	1055(4)	66(2)
C(14)	10756(10)	4682(7)	1663(4)	65(2)
C(3)	6783(9)	8807(7)	-734(3)	55(2)
C(6)	5038(10)	13201(8)	-1200(4)	68(2)
C(7)	5754(10)	13591(7)	-602(4)	66(2)

Table 5.Bond lengths (Å) and bond angles (°) for [Pt(L³)C1] (**3**)

Bond lengths	(Å)	Bond lengths	(Å)
Pt(1)-N(2)	1.954(3)	C(18)-C(17)	1.496(5)
Pt(1)-O(1)	1.993(2)	C(18)-C(19)	1.519(6)
Pt(1)-S(1)	2.2266(10)	C(18)-H(18A)	0.9700
Pt(1)-Cl(1)	2.3194(9)	C(18)-H(18B)	0.9700
S(1)-C(12)	1.771(4)	C(5)-C(6)	1.365(6)
N(1)-N(2)	1.293(4)	C(5)-C(9)	1.398(5)
N(1)-C(1)	1.350(4)	C(5)-H(5)	0.9300
N(2)-C(11)	1.441(4)	C(17)-S(1)	1.828(4)
O(1)-C(2)	1.291(4)	C(17)-H(17A)	0.9700
C(1)-C(2)	1.431(4)	C(17)-H(17B)	0.9700
C(1)-C(10)	1.469(5)	C(7)-C(8)	1.374(5)
C(3)-C(4)	1.350(5)	C(7)-C(6)	1.386(6)
C(3)-C(2)	1.425(5)	C(7)-H(7)	0.9300
C(3)-H(3)	0.9300	C(13)-C(14)	1.367(6)
C(11)-C(12)	1.382(5)	C(13)-C(12)	1.399(5)
C(11)-C(16)	1.394(5)	C(13)-H(13)	0.9300
C(10)-C(8)	1.400(5)	C(6)-H(6)	0.9300
C(10)-C(9)	1.408(5)	C(14)-C(15)	1.381(6)
C(9)-C(4)	1.426(5)	C(14)-H(14)	0.9300
C(4)-H(4)	0.9300	C(19)-H(19A)	0.9600
C(16)-H(16)	0.9300	C(19)-H(19B)	0.9600
C(8)-H(8)	0.9300	C(19)-H(19C)	0.9600
		C(15)-C(16)	1.380(6)
Bond angles	(°)	Bond lengths	(°)
C(17)-C(18)-C(19)	110.9(3)	C(8)-C(7)-C(6)	120.9(4)
C(17)-C(18)-H(18A)	109.5	C(8)-C(7)-H(7)	119.5
C(19)-C(18)-H(18A)	109.5	C(6)-C(7)-H(7)	119.5
C(17)-C(18)-H(18B)	109.5	C(14)-C(13)-C(12)	118.9(4)
C(19)-C(18)-H(18B)	109.5	C(14)-C(13)-H(13)	120.6
H(18A)-C(18)-H(18B)	108.0	C(12)-C(13)-H(13)	120.6
C(6)-C(5)-C(9)	120.6(4)	C(5)-C(6)-C(7)	119.8(4)
C(6)-C(5)-H(5)	119.7	C(5)-C(6)-H(6)	120.1
C(9)-C(5)-H(5)	119.7	C(7)-C(6)-H(6)	120.1
C(18)-C(17)-S(1)	116.1(3)	C(13)-C(14)-C(15)	120.8(4)
C(18)-C(17)-H(17A)	108.3	C(13)-C(14)-H(14)	119.6
S(1)-C(17)-H(17A)	108.3	C(15)-C(14)-H(14)	119.6
C(18)-C(17)-H(17B)	108.3	C(18)-C(19)-H(19A)	109.5
S(1)-C(17)-H(17B)	108.3	C(18)-C(19)-H(19B)	109.5
H(17A)-C(17)-H(17B)	107.4	H(19A)-C(19)-H(19B)	109.5
O(1)-Pt(1)-S(1)	178.54(7)	C(18)-C(19)-H(19C)	109.5
N(2)-Pt(1)-Cl(1)	177.95(8)	H(19A)-C(19)-H(19C)	109.5
O(1)-Pt(1)-Cl(1)	88.49(7)	H(19B)-C(19)-H(19C)	109.5
S(1)-Pt(1)-Cl(1)	90.98(4)	C(16)-C(15)-C(14)	120.8(4)
C(12)-S(1)-C(17)	102.81(17)	C(16)-C(15)-H(15)	119.6
C(12)-S(1)-Pt(1)	98.40(12)	C(14)-C(15)-H(15)	119.6
C(17)-S(1)-Pt(1)	106.70(13)	N(2)-Pt(1)-O(1)	92.99(10)
N(2)-N(1)-C(1)	123.1(3)	N(2)-Pt(1)-S(1)	87.58(8)
N(1)-N(2)-C(1)	114.0(3)	C(4)-C(3)-C(2)	122.5(3)
N(1)-N(2)-Pt(1)	127.7(2)	C(12)-C(11)-C(16)	119.8(3)
C(11)-N(2)-Pt(1)	118.3(2)	C(12)-C(11)-N(2)	117.3(3)
C(2)-O(1)-Pt(1)	122.9(2)	C(16)-C(11)-N(2)	122.8(3)
N(1)-C(1)-C(2)	127.5(3)	O(1)-C(2)-C(3)	116.1(3)
N(1)-C(1)-C(10)	113.4(3)	O(1)-C(2)-C(1)	125.8(3)
C(2)-C(1)-C(10)	119.1(3)	C(3)-C(2)-C(1)	118.1(3)
C(3)-C(4)-H(4)	119.2	C(8)-C(10)-C(9)	118.3(3)
C(9)-C(4)-H(4)	119.2	C(8)-C(10)-C(1)	122.1(3)
C(15)-C(16)-C(11)	119.0(4)	C(9)-C(10)-C(1)	119.6(3)
C(7)-C(8)-C(10)	120.4(4)	C(5)-C(9)-C(10)	120.0(4)
C(11)-C(12)-C(13)	120.7(4)	C(5)-C(9)-C(4)	121.0(4)
C(11)-C(12)-S(1)	118.4(3)	C(10)-C(9)-C(4)	119.0(3)
C(13)-C(12)-S(1)	120.8(3)	C(3)-C(4)-C(9)	121.6(3)

Table 6.

Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for $[\text{Pt}(\text{L}^3)\text{Cl}]$ (**3**)

	x	y	z	U(eq)
C(18)	9576(3)	10820(4)	2222(2)	61(1)
C(5)	13511(3)	4108(5)	224(3)	65(1)
C(17)	8552(3)	10049(4)	2328(2)	61(1)
C(7)	12479(4)	5817(5)	-778(2)	72(1)
C(13)	7163(3)	9980(4)	303(3)	69(1)
C(6)	13363(4)	4800(5)	-492(3)	76(1)
C(14)	7148(4)	10383(5)	-450(3)	78(1)
C(19)	9987(5)	12064(5)	2831(3)	83(1)
C(15)	7965(4)	9846(5)	-771(2)	75(1)
Pt(1)	9538(1)	6847(1)	1950(1)	42(1)
S(1)	8049(1)	8396(1)	1709(1)	54(1)
Cl(1)	9409(1)	6301(1)	3209(1)	60(1)
N(1)	10364(3)	6895(3)	558(2)	45(1)
N(2)	9639(2)	7383(3)	898(2)	43(1)
O(1)	10844(2)	5417(3)	2166(1)	51(1)
C(1)	11177(3)	5870(3)	897(2)	43(1)
C(3)	12284(3)	4081(4)	1894(2)	56(1)
C(11)	8821(3)	8435(4)	420(2)	48(1)
C(2)	11391(3)	5165(3)	1660(2)	45(1)
C(10)	11908(3)	5497(4)	403(2)	47(1)
C(9)	12795(3)	4444(4)	683(2)	53(1)
C(4)	12943(3)	3728(4)	1433(2)	58(1)
C(16)	8802(3)	8867(4)	-345(2)	58(1)
C(8)	11758(3)	6164(4)	-342(2)	59(1)
C(12)	8018(3)	9007(4)	745(2)	51(1)

Table 7.

Bond lengths (\AA) and bond angles ($^\circ$) for $[\text{Pt}(\text{L}^9)\text{Cl}]$ (**9**)

Bond lengths	(\AA)	Bond lengths	(\AA)
Pt(1)-N(2)	1.968(4)	C(12)-C(11)	1.391(7)
Pt(1)-O(1)	2.003(3)	C(18)-C(19)	1.510(8)
Pt(1)-S(1)	2.2241(13)	C(18)-C(17)	1.513(7)
Pt(1)-Cl(1)	2.3200(15)	C(10)-C(9)	1.415(7)
S(1)-C(12)	1.777(5)	C(10)-C(1)	1.450(7)
S(1)-C(17)	1.831(5)	C(13)-C(14)	1.377(7)
N(2)-N(1)	1.281(5)	C(14)-C(15)	1.383(7)
N(2)-C(11)	1.448(6)	C(4)-C(3)	1.347(7)
O(1)-C(1)	1.301(6)	C(4)-C(9)	1.427(7)
N(1)-C(2)	1.355(6)	C(6)-C(7)	1.385(8)
C(2)-C(1)	1.426(7)	C(6)-C(5)	1.385(8)
C(2)-C(3)	1.430(7)	C(9)-C(5)	1.418(7)
C(8)-C(7)	1.376(7)	C(19)-C(20)	1.507(8)
C(8)-C(10)	1.400(7)	C(19)-H(19A)	0.9700
C(12)-C(13)	1.388(7)	C(19)-H(19B)	0.9700
C(16)-C(15)	1.386(7)	C(11)-C(16)	1.387(7)
Bond angles	($^\circ$)	Bond lengths	($^\circ$)
N(2)-Pt(1)-O(1)	92.94(15)	C(14)-C(15)-H(15)	119.5
N(2)-Pt(1)-S(1)	87.29(12)	C(16)-C(15)-H(15)	119.5
O(1)-Pt(1)-S(1)	176.50(10)	C(19)-C(20)-H(20A)	109.5
N(2)-Pt(1)-Cl(1)	178.40(12)	C(19)-C(20)-H(20B)	109.5
O(1)-Pt(1)-Cl(1)	88.55(10)	H(20A)-C(20)-H(20B)	109.5
S(1)-Pt(1)-Cl(1)	91.25(5)	C(19)-C(20)-H(20C)	109.5
C(12)-S(1)-C(17)	104.9(2)	H(20A)-C(20)-H(20C)	109.5
C(12)-S(1)-Pt(1)	98.94(17)	H(20B)-C(20)-H(20C)	109.5

C(17)-S(1)-Pt(1)	111.17(17)	C(9)-C(4)-H(4)	119.7
N(1)-N(2)-C(11)	114.2(4)	C(7)-C(6)-C(5)	120.6(5)
N(1)-N(2)-Pt(1)	127.8(3)	C(7)-C(6)-H(6)	119.7
C(11)-N(2)-Pt(1)	118.0(3)	C(5)-C(6)-H(6)	119.7
C(1)-O(1)-Pt(1)	122.4(3)	C(10)-C(9)-C(5)	119.2(5)
N(2)-N(1)-C(2)	122.6(4)	C(10)-C(9)-C(4)	119.4(5)
N(1)-C(2)-C(1)	128.6(5)	C(5)-C(9)-C(4)	121.4(5)
N(1)-C(2)-C(3)	112.4(5)	C(8)-C(7)-C(6)	120.0(5)
C(1)-C(2)-C(3)	119.0(5)	C(8)-C(7)-H(7)	120.0
C(7)-C(8)-C(10)	121.5(5)	C(6)-C(7)-H(7)	120.0
C(7)-C(8)-H(8)	119.2	C(20)-C(19)-C(18)	113.3(5)
C(10)-C(8)-H(8)	119.2	C(20)-C(19)-H(19A)	108.9
C(13)-C(12)-C(11)	120.3(5)	C(18)-C(19)-H(19A)	108.9
C(13)-C(12)-S(1)	121.9(4)	C(20)-C(19)-H(19B)	108.9
C(11)-C(12)-S(1)	117.6(4)	C(18)-C(19)-H(19B)	108.9
C(19)-C(18)-C(17)	111.1(4)	H(19A)-C(19)-H(19B)	107.7
C(19)-C(18)-H(18A)	109.4	C(16)-C(11)-C(12)	120.4(5)
C(17)-C(18)-H(18A)	109.4	C(16)-C(11)-N(2)	122.1(5)
C(19)-C(18)-H(18B)	109.4	C(12)-C(11)-N(2)	117.5(4)
C(17)-C(18)-H(18B)	109.4	C(6)-C(5)-C(9)	120.0(5)
H(18A)-C(18)-H(18B)	108.0	C(6)-C(5)-H(5)	120.0
C(8)-C(10)-C(9)	118.6(4)	C(9)-C(5)-H(5)	120.0
C(8)-C(10)-C(1)	121.1(4)	C(15)-C(16)-C(11)	118.6(5)
C(9)-C(10)-C(1)	120.2(4)	C(15)-C(16)-H(16)	120.7
C(14)-C(13)-C(12)	119.1(5)	C(11)-C(16)-H(16)	120.7
C(14)-C(13)-H(13)	120.4	C(4)-C(3)-C(2)	122.4(5)
C(12)-C(13)-H(13)	120.4	C(4)-C(3)-H(3)	118.8
O(1)-C(1)-C(2)	125.3(5)	C(2)-C(3)-H(3)	118.8
O(1)-C(1)-C(10)	116.3(4)	C(14)-C(15)-C(16)	120.9(5)
C(2)-C(1)-C(10)	118.3(4)	H(17A)-C(17)-H(17B)	107.2
C(18)-C(17)-S(1)	117.7(4)	C(13)-C(14)-C(15)	120.5(5)
C(18)-C(17)-H(17A)	107.9	C(13)-C(14)-H(14)	119.7
S(1)-C(17)-H(17A)	107.9	C(15)-C(14)-H(14)	119.7
C(18)-C(17)-H(17B)	107.9	C(3)-C(4)-C(9)	120.6(5)
S(1)-C(17)-H(17B)	107.9	C(3)-C(4)-H(4)	119.7

Table 8.

Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{Å}^2 \times 10^3$] for $[\text{Pt}(\text{L}^9)\text{Cl}]$ (9)

	x	y	z	U(eq)
Pt(1)	6994(1)	8305(1)	6071(1)	22(1)
S(1)	6539(1)	10144(1)	6773(1)	26(1)
Cl(1)	8952(1)	8309(1)	6682(1)	30(1)
N(2)	5320(4)	8326(4)	5578(2)	22(1)
O(1)	7434(3)	6745(3)	5400(2)	26(1)
N(1)	4836(4)	7575(5)	5017(2)	27(1)
C(2)	5456(5)	6618(5)	4668(3)	26(1)
C(8)	8357(4)	4821(5)	4502(3)	28(1)
C(12)	4975(4)	10164(5)	6471(3)	26(1)
C(18)	5949(5)	8347(5)	7922(3)	32(1)
C(10)	7156(4)	5221(5)	4365(3)	24(1)
C(13)	4242(5)	11098(6)	6782(3)	34(1)
C(1)	6686(4)	6248(5)	4840(3)	25(1)
C(17)	6757(4)	9557(6)	7725(3)	29(1)
C(14)	3050(5)	11155(7)	6484(3)	36(1)
C(4)	5178(4)	5016(6)	3597(3)	33(1)
C(6)	8081(5)	3263(5)	3444(3)	33(1)
C(9)	6405(4)	4621(5)	3745(3)	28(1)
C(7)	8813(5)	3856(6)	4051(3)	32(1)
C(19)	6219(5)	8026(6)	8728(3)	36(1)

C(11)	4508(4)	9285(5)	5871(3)	26(1)
C(5)	6888(5)	3637(6)	3282(3)	32(1)
C(16)	3310(4)	9357(6)	5567(3)	31(1)
C(3)	4734(5)	5957(6)	4041(3)	34(1)
C(15)	2589(5)	10300(6)	5880(3)	34(1)
C(20)	5280(5)	7088(6)	8979(3)	42(1)

Table 9.

Bond lengths (Å) and bond angles (°) for [Pt(L³)II] (13)

Bond lengths	(Å)	Bond lengths	(Å)
Pt(1)-N(2)	1.980(6)	C(4)-H(4)	0.9300
Pt(1)-O(1)	2.003(5)	C(3)-H(3)	0.9300
Pt(1)-S(1)	2.222(2)	C(6)-C(7)	1.354(14)
Pt(1)-I(1)	2.6007(8)	C(6)-H(6)	0.9300
S(1)-C(12)	1.794(9)	C(8)-C(7)	1.377(11)
S(1)-C(17)	1.831(9)	C(8)-H(8)	0.9300
O(1)-C(2)	1.284(8)	C(18)-C(19)	1.504(15)
N(2)-N(1)	1.261(8)	C(18)-C(17)	1.533(12)
N(2)-C(11)	1.429(10)	C(18)-H(18A)	0.9700
N(1)-C(1)	1.369(9)	C(18)-H(18B)	0.9700
C(11)-C(12)	1.339(11)	C(15)-C(14)	1.337(12)
C(11)-C(16)	1.387(11)	C(15)-H(15)	0.9300
C(16)-C(15)	1.383(11)	C(5)-H(5)	0.9300
C(16)-H(16)	0.9300	C(17)-H(17A)	0.9700
C(1)-C(2)	1.408(10)	C(17)-H(17B)	0.9700
C(1)-C(10)	1.444(10)	C(13)-C(14)	1.349(13)
C(10)-C(8)	1.416(12)	C(13)-H(13)	0.9300
C(10)-C(9)	1.445(11)	C(14)-H(14)	0.9300
C(2)-C(3)	1.452(11)	C(7)-H(7)	0.9300
C(9)-C(5)	1.373(11)	C(19)-H(19A)	0.9600
C(9)-C(4)	1.395(12)	C(19)-H(19B)	0.9600
C(12)-C(13)	1.450(12)	C(19)-H(19C)	0.9600
C(4)-C(3)	1.351(12)		

Bond angles	(°)	Bond lengths	(°)
N(2)-Pt(1)-O(1)	92.4(2)	C(19)-C(18)-C(17)	111.2(8)
N(2)-Pt(1)-S(1)	87.17(18)	C(19)-C(18)-H(18A)	109.4
O(1)-Pt(1)-S(1)	177.76(16)	C(17)-C(18)-H(18A)	109.4
N(2)-Pt(1)-I(1)	176.97(18)	C(19)-C(18)-H(18B)	109.4
O(1)-Pt(1)-I(1)	89.03(15)	C(17)-C(18)-H(18B)	109.4
S(1)-Pt(1)-I(1)	91.54(6)	H(18A)-C(18)-H(18B)	108.0
C(12)-S(1)-C(17)	100.8(4)	C(14)-C(15)-C(16)	122.9(10)
C(12)-S(1)-Pt(1)	97.8(3)	C(14)-C(15)-H(15)	118.5
C(17)-S(1)-Pt(1)	108.6(3)	C(16)-C(15)-H(15)	118.5
C(2)-O(1)-Pt(1)	121.6(5)	C(6)-C(5)-C(9)	122.9(9)
N(1)-N(2)-C(11)	114.5(6)	C(6)-C(5)-H(5)	118.5
N(1)-N(2)-Pt(1)	127.7(5)	C(9)-C(5)-H(5)	118.5
C(11)-N(2)-Pt(1)	117.7(5)	C(18)-C(17)-S(1)	114.9(6)
N(2)-N(1)-C(1)	124.0(7)	C(18)-C(17)-H(17A)	108.5
C(12)-C(11)-C(16)	119.7(8)	S(1)-C(17)-H(17A)	108.5
C(12)-C(11)-N(2)	118.2(8)	C(18)-C(17)-H(17B)	108.5
C(16)-C(11)-N(2)	122.0(7)	S(1)-C(17)-H(17B)	108.5
C(15)-C(16)-C(11)	118.4(8)	H(17A)-C(17)-H(17B)	107.5
C(15)-C(16)-H(16)	120.8	C(14)-C(13)-C(12)	118.5(9)
C(11)-C(16)-H(16)	120.8	C(14)-C(13)-H(13)	120.8
N(1)-C(1)-C(2)	125.6(6)	C(12)-C(13)-H(13)	120.8
N(1)-C(1)-C(10)	113.2(7)	C(15)-C(14)-C(13)	120.0(10)
C(2)-C(1)-C(10)	121.1(7)	C(15)-C(14)-H(14)	120.0
C(8)-C(10)-C(1)	122.9(7)	C(13)-C(14)-H(14)	120.0
C(8)-C(10)-C(9)	117.8(7)	C(6)-C(7)-C(8)	122.9(11)
C(1)-C(10)-C(9)	119.3(7)	C(6)-C(7)-H(7)	118.6
O(1)-C(2)-C(1)	128.4(7)	C(8)-C(7)-H(7)	118.6
O(1)-C(2)-C(3)	114.5(7)	C(18)-C(19)-H(19A)	109.5
C(1)-C(2)-C(3)	117.0(7)	C(18)-C(19)-H(19B)	109.5

C(5)-C(9)-C(4)	123.4(8)	H(19A)-C(19)-H(19B)	109.5
C(5)-C(9)-C(10)	118.8(9)	C(18)-C(19)-H(19C)	109.5
C(4)-C(9)-C(10)	117.8(7)	H(19A)-C(19)-H(19C)	109.5
C(11)-C(12)-C(13)	120.5(9)	H(19B)-C(19)-H(19C)	109.5
C(11)-C(12)-S(1)	119.1(7)	C(5)-C(6)-H(6)	120.7
C(13)-C(12)-S(1)	120.5(7)	C(7)-C(6)-H(6)	120.7
C(3)-C(4)-C(9)	123.2(8)	C(7)-C(8)-C(10)	118.9(9)
C(3)-C(4)-H(4)	118.4	C(7)-C(8)-H(8)	120.6
C(9)-C(4)-H(4)	118.4	C(10)-C(8)-H(8)	120.6
C(4)-C(3)-C(2)	121.6(8)	C(2)-C(3)-H(3)	119.2
C(4)-C(3)-H(3)	119.2	C(5)-C(6)-C(7)	118.5(9)

Table 10.

Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for [Pt(L³)I] (**13**)

	x	y	z	U(eq)
Pt(1)	5377(1)	1497(1)	8006(1)	51(1)
I(1)	5578(1)	862(1)	6534(1)	74(1)
S(1)	6760(1)	2979(3)	8328(2)	61(1)
O(1)	4164(4)	101(6)	7746(3)	57(1)
N(2)	5208(4)	2090(7)	9106(4)	45(1)
N(1)	4513(5)	1677(7)	9414(4)	56(2)
C(11)	5941(6)	3123(8)	9622(5)	53(2)
C(16)	5888(6)	3605(9)	10402(5)	57(2)
C(1)	3736(5)	696(8)	9023(5)	47(2)
C(10)	3024(6)	429(9)	9498(5)	55(2)
C(2)	3632(5)	-65(9)	8258(5)	53(2)
C(9)	2188(6)	-628(10)	9177(6)	61(2)
C(12)	6700(6)	3626(9)	9336(5)	61(2)
C(4)	2123(6)	-1375(10)	8425(6)	65(2)
C(3)	2775(6)	-1112(9)	7970(6)	65(2)
C(6)	1558(7)	-95(13)	10344(7)	86(3)
C(8)	3108(7)	1156(11)	10275(6)	72(2)
C(18)	5415(7)	5439(12)	7727(7)	86(3)
C(15)	6627(7)	4607(12)	10863(6)	80(3)
C(5)	1490(6)	-830(11)	9615(7)	74(3)
C(17)	6411(6)	4674(10)	7690(6)	68(2)
C(13)	7473(7)	4658(12)	9841(7)	89(3)
C(14)	7399(7)	5112(12)	10595(7)	82(3)
C(7)	2383(7)	851(13)	10677(7)	90(3)
C(19)	5184(11)	6807(12)	7179(9)	115(4)

Table 11.

Bond lengths (Å) and bond angles (°) for [Rh(L')(PPh₃)₂] (1-Rh)

Bond lengths	(Å)	Bond lengths	(Å)
O(2)-C(2)	1.300(4)	C(20)-H(20)	0.9300
O(2)-Rh(1)	2.192(3)	C(54)-C(53)	1.379(16)
C(23)-C(24)	1.381(6)	C(54)-H(54A)	0.9600
C(23)-C(28)	1.388(6)	C(54)-H(54B)	0.9600
C(23)-P(1)	1.827(4)	C(54)-H(54C)	0.9600
C(29)-C(34)	1.368(6)	N(3)-C(53)	1.050(14)
C(29)-C(30)	1.379(5)	Rh(1)-N(1)	1.985(3)
C(29)-P(1)	1.834(4)	Rh(1)-C(12)	2.006(4)
C(16)-C(15)	1.376(7)	Rh(1)-P(2)	2.3769(12)
C(16)-C(11)	1.394(6)	Rh(1)-P(1)	2.3806(12)
C(16)-H(16)	0.9300	Rh(1)-C(11)	2.3915(13)
C(17)-C(18)	1.383(6)	P(2)-C(35)	1.829(4)
C(17)-C(22)	1.383(6)	P(2)-C(41)	1.830(4)
C(17)-P(1)	1.830(4)	P(2)-C(47)	1.835(4)
C(22)-C(21)	1.375(7)	C(11)-N(2)	1.403(5)
C(22)-H(22)	0.9300	C(11)-C(12)	1.411(6)
C(24)-C(25)	1.400(6)	N(2)-N(1)	1.290(4)
C(24)-H(24)	0.9300	C(35)-C(40)	1.379(6)
C(31)-C(32)	1.368(7)	C(35)-C(36)	1.386(5)
C(31)-C(30)	1.379(6)	C(41)-C(46)	1.384(6)
C(31)-H(31)	0.9300	C(41)-C(42)	1.392(6)
C(30)-H(30)	0.9300	C(47)-C(48)	1.364(6)
C(28)-C(27)	1.377(6)	C(47)-C(52)	1.383(5)
C(28)-H(28)	0.9300	C(2)-C(1)	1.414(5)
C(7)-C(8)	1.367(6)	C(2)-C(3)	1.428(5)
C(7)-C(6)	1.377(8)	C(9)-C(5)	1.405(6)
C(7)-H(7)	0.9300	C(9)-C(10)	1.418(6)
C(25)-C(26)	1.371(7)	C(9)-C(4)	1.425(6)
C(25)-H(25)	0.9300	C(3)-C(4)	1.349(6)
C(15)-C(14)	1.362(7)	C(3)-H(3)	0.9300
C(15)-H(15)	0.9300	N(1)-C(1)	1.381(5)
C(18)-C(19)	1.380(7)	C(36)-C(37)	1.381(7)
C(18)-H(18)	0.9300	C(36)-H(36)	0.9300
C(34)-C(33)	1.385(6)	C(4)-H(4)	0.9300
C(34)-H(34)	0.9300	C(1)-C(10)	1.443(5)
C(27)-C(26)	1.362(7)	C(8)-C(10)	1.417(6)
C(27)-H(27)	0.9300	C(8)-H(8)	0.9300
C(26)-H(26)	0.9300	C(42)-H(42)	0.9300
C(45)-C(44)	1.381(7)	C(48)-C(49)	1.384(6)
C(45)-C(46)	1.397(6)	C(48)-H(48)	0.9300
C(45)-H(45)	0.9300	C(5)-H(5)	0.9300
C(43)-C(44)	1.362(8)	C(52)-C(51)	1.383(6)
C(43)-C(42)	1.381(6)	C(52)-H(52)	0.9300
C(43)-H(43)	0.9300	C(37)-H(37)	0.9300
C(13)-C(12)	1.379(6)	C(46)-H(46)	0.9300
C(13)-C(14)	1.402(6)	C(51)-C(50)	1.363(7)
C(13)-H(13)	0.9300	C(51)-H(51)	0.9300
C(14)-H(14)	0.9300	C(40)-H(40)	0.9300
C(44)-H(44)	0.9300	C(50)-C(49)	1.373(7)
C(6)-C(5)	1.371(8)	C(50)-H(50)	0.9300
C(6)-H(6)	0.9300	C(49)-H(49)	0.9300
C(21)-C(20)	1.382(9)	C(19)-C(20)	1.373(9)
C(21)-H(21)	0.9300	C(19)-H(19)	0.9300
C(33)-C(32)	1.371(7)	C(38)-C(37)	1.371(9)
C(33)-H(33)	0.9300	C(38)-H(38)	0.9300
C(39)-C(38)	1.370(9)	C(32)-H(32)	0.9300
C(39)-C(40)	1.385(7)	C(39)-H(39)	0.9300
Bond angles	(°)	Bond lengths	(°)
C(2)-O(2)-Rh(1)	107.9(2)	N(2)-N(1)-C(1)	123.6(3)
C(24)-C(23)-C(28)	119.3(4)	N(2)-N(1)-Rh(1)	118.8(3)
C(24)-C(23)-P(1)	118.1(3)	C(1)-N(1)-Rh(1)	117.7(2)
C(28)-C(23)-P(1)	122.5(3)	C(37)-C(36)-C(35)	120.5(5)

118.8(3)	(37)-C(36)-H(36)	119.8	(37)-H(2)-C(47)	103.13(18)
118.8(3)	(34)-C(29)-H(30)	119.8	(35)-H(2)-C(47)	103.29(18)
121.4(3)	(34)-C(29)-H(1)	119.8(3)	(35)-H(2)-C(41)	103.29(18)
119.8(3)	(30)-C(29)-H(1)	119.8(3)	(29)-H(1)-Rb(1)	112.02(12)
118.2(4)	(15)-C(16)-C(11)	118.2(4)	(17)-H(1)-Rb(1)	114.16(12)
120.9	(15)-C(16)-H(16)	120.9	(23)-H(1)-Rb(1)	117.80(13)
118.2(4)	(11)-C(11)-C(16)	118.2(4)	(17)-H(1)-C(29)	103.13(18)
119.5	(11)-C(11)-H(11)	119.5	(23)-H(1)-C(29)	104.22(17)
121.0(5)	(12)-C(12)-C(17)	121.0(5)	(23)-H(1)-C(17)	103.93(17)
121.0(5)	(12)-C(12)-H(12)	118.7	P(1)-Rb(1)-C(11)	87.35(4)
118.7	(6)-C(7)-H(7)	118.7	P(2)-Rb(1)-C(11)	87.35(4)
122.6(5)	(8)-C(7)-H(7)	122.6(5)	O(2)-Rb(1)-C(11)	105.56(7)
119.9	(23)-C(28)-H(28)	119.9	N(1)-Rb(1)-C(11)	175.57(10)
120.0(5)	(26)-C(25)-C(24)	120.0(5)	P(2)-Rb(1)-P(1)	169.68(3)
120.0	(24)-C(25)-H(25)	120.0	O(2)-Rb(1)-P(1)	86.34(8)
120.4(4)	(30)-C(31)-H(31)	120.4(4)	(12)-Rb(1)-P(1)	94.79(13)
119.9	(29)-C(30)-C(31)	119.9	N(1)-Rb(1)-P(2)	93.10(10)
120.6(4)	(30)-C(30)-C(31)	120.6(4)	(12)-Rb(1)-O(2)	159.38(12)
120.0	(16)-C(15)-H(15)	120.0	N(1)-Rb(1)-O(2)	78.87(12)
120.4(4)	(14)-C(15)-C(16)	120.4(4)	N(1)-Rb(1)-C(1)	80.51(5)
120.0	(14)-C(15)-H(15)	120.0	(48)-C(49)-H(49)	119.9
120.4(4)	(34)-C(34)-H(34)	120.4(4)	(50)-C(49)-H(49)	119.9
119.7	(29)-C(34)-C(35)	119.7	(50)-C(49)-C(48)	120.2(4)
119.5	(17)-C(18)-H(18)	119.5	(11)-C(12)-Rb(1)	109.3(3)
119.5	(19)-C(18)-H(18)	119.5	(13)-C(12)-Rb(1)	133.2(3)
121.8(5)	(19)-C(18)-H(18)	121.8(5)	(13)-C(12)-C(11)	117.4(3)
120.0	(16)-C(15)-H(15)	120.0	(49)-C(50)-H(50)	120.2
120.4(4)	(14)-C(15)-C(16)	120.4(4)	(51)-C(50)-H(50)	120.2
120.0	(14)-C(15)-H(15)	120.0	(51)-C(50)-C(49)	119.6(4)
120.4(4)	(34)-C(34)-H(34)	120.4(4)	(39)-C(40)-H(40)	119.6
120.0	(24)-C(25)-H(25)	120.0	(35)-C(40)-C(39)	120.7(5)
120.0	(24)-C(25)-C(24)	120.0	(52)-C(51)-H(51)	119.8
120.4(4)	(30)-C(31)-H(31)	120.4(4)	(50)-C(51)-H(51)	119.8
120.0	(29)-C(30)-C(31)	120.0	(50)-C(51)-C(52)	120.3(4)
120.0	(24)-C(25)-H(25)	120.0	(45)-C(46)-H(46)	120.2
120.4(4)	(30)-C(31)-H(31)	120.4(4)	(41)-C(46)-H(46)	120.2
120.0	(24)-C(25)-H(25)	120.0	(41)-C(46)-C(45)	119.7(4)
120.0(5)	(26)-C(25)-C(24)	120.0(5)	(36)-C(37)-H(37)	119.8
118.7	(6)-C(7)-H(7)	118.7	(38)-C(37)-H(37)	119.8
118.7	(8)-C(7)-H(7)	118.7	(38)-C(37)-C(36)	120.3(5)
122.6(5)	(7)-C(6)-H(6)	122.6(5)	(47)-C(52)-H(52)	119.9
119.9	(23)-C(28)-H(28)	119.9	(51)-C(52)-H(52)	119.9
119.9	(27)-C(28)-H(28)	119.9	(51)-C(52)-C(47)	120.2(4)
120.2(4)	(27)-C(28)-C(23)	120.2(4)	(9)-C(5)-H(5)	119.4
119.7	(30)-C(30)-H(30)	119.7	(6)-C(5)-H(5)	119.4
120.6(4)	(29)-C(30)-C(31)	120.6(4)	(6)-C(5)-C(9)	121.2(5)
119.9	(30)-C(30)-C(31)	119.9	(49)-C(48)-H(48)	119.8
119.9	(30)-C(31)-H(31)	119.9	(47)-C(48)-H(48)	119.8
120.3(4)	(32)-C(31)-C(30)	120.3(4)	(47)-C(48)-C(49)	120.4(4)
120.2	(25)-C(24)-H(24)	120.2	(41)-C(42)-H(42)	119.8
119.6(4)	(23)-C(24)-H(24)	119.6(4)	(43)-C(42)-H(42)	119.8
119.5	(17)-C(17)-H(17)	119.5	(43)-C(42)-C(41)	120.4(4)
122.2(5)	(17)-C(17)-C(18)	122.2(5)	(9)-C(10)-C(1)	117.2(3)
118.2(4)	(15)-C(16)-H(16)	118.2(4)	(8)-C(10)-C(1)	125.4(4)
120.9	(15)-C(16)-H(16)	120.9	(8)-C(10)-C(9)	117.4(4)
118.2(4)	(15)-C(16)-C(11)	118.2(4)	(10)-C(8)-H(8)	119.9
119.8(3)	(30)-C(29)-H(1)	119.8(3)	(7)-C(8)-H(8)	119.9
121.4(3)	(34)-C(29)-H(1)	121.4(3)	(7)-C(8)-C(10)	120.2(4)
118.8(3)	(34)-C(29)-H(1)	118.8(3)	(2)-C(1)-C(10)	122.3(3)
118.8(3)	(34)-C(29)-H(1)	118.8(3)	N(1)-C(1)-C(10)	125.6(3)
118.8(3)	(34)-C(29)-H(1)	118.8(3)	N(1)-C(1)-C(2)	112.2(3)
118.8(3)	(34)-C(29)-H(1)	118.8(3)	(9)-C(4)-H(4)	118.9
118.8(3)	(34)-C(29)-H(1)	118.8(3)	(3)-C(4)-H(4)	118.9
118.8(3)	(34)-C(29)-H(1)	118.8(3)	(3)-C(4)-C(9)	122.3(4)
118.8(3)	(34)-C(29)-H(1)	118.8(3)	(35)-C(36)-H(36)	119.8

C(38)-C(39)-H(39)	120.0	C(41)-P(2)-C(47)	104.09(17)
C(40)-C(39)-H(39)	120.0	C(35)-P(2)-Rh(1)	114.20(12)
C(20)-C(19)-C(18)	119.3(5)	C(41)-P(2)-Rh(1)	118.03(13)
C(20)-C(19)-H(19)	120.4	C(47)-P(2)-Rh(1)	112.01(12)
C(18)-C(19)-H(19)	120.4	C(16)-C(11)-N(2)	118.1(4)
C(39)-C(38)-C(37)	119.8(5)	C(16)-C(11)-C(12)	122.6(4)
C(39)-C(38)-H(38)	120.1	N(2)-C(11)-C(12)	119.3(3)
C(37)-C(38)-H(38)	120.1	N(1)-N(2)-C(11)	112.1(3)
C(31)-C(32)-C(33)	119.5(4)	C(40)-C(35)-C(36)	118.6(4)
C(31)-C(32)-H(32)	120.3	C(40)-C(35)-P(2)	122.1(3)
C(33)-C(32)-H(32)	120.3	C(36)-C(35)-P(2)	119.4(3)
C(19)-C(20)-C(21)	120.3(5)	C(46)-C(41)-C(42)	119.2(4)
C(19)-C(20)-H(20)	119.8	C(46)-C(41)-P(2)	118.0(3)
C(21)-C(20)-H(20)	119.8	C(42)-C(41)-P(2)	122.8(3)
C(53)-C(54)-H(54A)	109.5	C(48)-C(47)-C(52)	119.2(3)
C(53)-C(54)-H(54B)	109.5	C(48)-C(47)-P(2)	121.3(3)
H(54A)-C(54)-H(54B)	109.5	C(52)-C(47)-P(2)	119.4(3)
C(53)-C(54)-H(54C)	109.5	O(2)-C(2)-C(1)	123.4(3)
H(54A)-C(54)-H(54C)	109.5	O(2)-C(2)-C(3)	118.9(3)
H(54B)-C(54)-H(54C)	109.5	C(1)-C(2)-C(3)	117.6(3)
N(3)-C(53)-C(54)	178(2)	C(5)-C(9)-C(10)	120.0(4)
C(4)-C(3)-C(2)	121.1(4)	C(5)-C(9)-C(4)	120.4(4)
C(4)-C(3)-H(3)	119.5	C(10)-C(9)-C(4)	119.6(3)
C(2)-C(3)-H(3)	119.5		

Table 12.

Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for $[\text{Rh}(\text{L}^*)(\text{PPh}_3)_2]$ (1-Rh)

	x	y	z	U(eq)
O(2)	5346(3)	5454(2)	6564(2)	39(1)
C(23)	5684(4)	1239(3)	6735(4)	42(1)
C(29)	7478(4)	2339(3)	7281(3)	40(1)
C(16)	2202(6)	3437(4)	4548(4)	56(1)
C(17)	4048(4)	3168(3)	8415(3)	41(1)
C(22)	2476(5)	3442(4)	8534(4)	55(1)
C(24)	6753(5)	666(4)	5668(4)	54(1)
C(31)	9365(5)	2992(4)	7519(4)	57(1)
C(30)	8050(5)	3243(4)	7208(4)	47(1)
C(28)	4678(5)	679(4)	7604(4)	56(1)
C(7)	-1951(5)	7115(5)	8226(5)	67(1)
C(25)	6791(6)	-458(4)	5470(5)	67(1)
C(15)	3048(6)	2571(4)	3684(5)	65(1)
C(18)	4340(6)	3273(5)	9417(4)	61(1)
C(34)	8263(6)	1182(4)	7640(5)	65(1)
C(27)	4742(6)	-432(4)	7396(5)	68(1)
C(26)	5786(7)	-994(4)	6340(5)	68(1)
C(45)	6796(6)	4356(5)	656(4)	67(1)
C(43)	4737(6)	6286(5)	677(4)	70(1)
C(13)	5559(6)	2543(4)	3655(4)	53(1)
C(14)	4682(7)	2138(5)	3250(5)	68(1)
C(44)	5784(7)	5230(5)	115(4)	70(1)
C(6)	-2276(6)	7927(5)	9042(5)	79(2)
C(21)	1238(6)	3790(5)	9623(5)	73(1)
C(33)	9590(7)	927(5)	7944(7)	90(2)
C(39)	3104(8)	9402(5)	4740(6)	89(2)
C(19)	3108(8)	3633(6)	10514(5)	87(2)
C(38)	1556(7)	9507(5)	4994(6)	87(2)
C(32)	10136(6)	1835(5)	7886(6)	74(2)
C(20)	1560(7)	3882(6)	10614(5)	86(2)
C(54)	1410(30)	10870(14)	1973(15)	330(16)
N(3)	1840(20)	9451(14)	574(14)	296(9)
C(53)	1640(20)	10078(11)	1173(11)	179(6)
Rh(1)	5483(1)	4240(1)	5350(1)	32(1)

P(1)	5660(1)	2714(1)	6947(1)	35(1)
Cl(1)	8283(1)	3199(1)	4311(1)	49(1)
P(2)	5660(1)	5834(1)	3826(1)	35(1)
C(11)	3061(5)	3845(4)	4960(4)	43(1)
N(2)	2196(3)	4728(3)	5840(3)	41(1)
C(35)	4052(4)	7305(3)	4277(3)	40(1)
C(41)	5683(4)	5624(4)	2351(3)	43(1)
C(47)	7482(4)	6167(3)	3448(3)	41(1)
C(2)	3839(4)	6043(3)	7152(3)	35(1)
C(9)	580(5)	7385(4)	8493(4)	48(1)
C(3)	3423(5)	6901(3)	8010(3)	45(1)
N(1)	3125(4)	5029(3)	6143(3)	34(1)
C(36)	2478(5)	7421(4)	4548(4)	54(1)
C(4)	1876(5)	7531(4)	8643(4)	50(1)
C(1)	2572(4)	5879(3)	992(3)	36(1)
C(8)	-422(5)	6434(4)	7543(4)	53(1)
C(10)	908(4)	6546(3)	7659(3)	44(1)
C(42)	4680(5)	6496(4)	1786(4)	55(1)
C(48)	8258(6)	6531(5)	2296(4)	66(1)
C(5)	-1016(6)	8060(5)	9172(5)	66(1)
C(52)	8046(5)	6097(4)	4358(4)	47(1)
C(37)	1241(6)	8519(5)	4904(5)	41(1)
C(46)	6755(5)	4553(4)	1778(4)	53(1)
C(51)	-9367(5)	6409(4)	4101(4)	56(1)
C(40)	4349(6)	8304(4)	4380(5)	62(1)
C(50)	10133(6)	6775(6)	2949(5)	74(2)
C(12)	4753(5)	3411(3)	4520(3)	40(1)
C(49)	9589(7)	6830(7)	2041(5)	89(2)

Table 13.

Bond lengths (Å) and bond angles ($^{\circ}$) for $[\text{Rh}(\text{L}^*)(\text{PPh}_3)_2]$ (**2-Rh**)

Bond lengths	(Å)	Bond lengths	(Å)
Rh(1)-N(1)	1.941(8)	C(101)-C(102)	1.35(2)
Rh(1)-C(12)	1.988(9)	C(101)-H(101)	0.9300
Rh(1)-O(1)	2.230(7)	C(66)-H(66)	0.9300
Rh(1)-P(1)	2.353(3)	C(71)-H(71)	0.9300
Rh(1)-P(2)	2.366(3)	C(4)-H(4)	0.9300
Rh(1)-Cl(1)	2.380(3)	C(51)-C(50)	1.35(2)
Rh(2)-N(3)	1.939(8)	C(51)-H(51)	0.9300
Rh(2)-C(64)	1.991(10)	C(85)-H(85)	0.9300
Rh(2)-O(2)	2.225(7)	C(24)-C(25)	1.366(18)
Rh(2)-P(3)	2.354(3)	C(24)-H(24)	0.9300
Rh(2)-P(4)	2.363(3)	C(28)-C(27)	1.43(2)
Rh(2)-Cl(2)	2.381(3)	C(28)-H(28)	0.9300
P(2)-C(47)	1.814(11)	C(7)-C(6)	1.38(2)
P(2)-C(41)	1.831(10)	C(7)-H(7)	0.9300
P(2)-C(35)	1.852(10)	C(94)-C(95)	1.383(18)
P(4)-C(99)	1.827(11)	C(94)-H(94)	0.9300
P(4)-C(93)	1.839(10)	C(38)-C(37)	1.34(2)
P(4)-C(87)	1.844(10)	C(38)-H(38)	0.9300
P(1)-C(17)	1.812(10)	C(27)-C(26)	1.38(2)
P(1)-C(29)	1.835(10)	C(27)-H(27)	0.9300
P(1)-C(23)	1.834(12)	C(77)-C(78)	1.42(2)
P(3)-C(81)	1.818(10)	C(77)-C(76)	1.46(2)
P(3)-C(69)	1.826(10)	C(77)-H(77)	0.9300
P(3)-C(75)	1.844(12)	C(25)-C(26)	1.37(2)
N(3)-N(4)	1.302(11)	C(25)-H(25)	0.9300
N(3)-C(54)	1.376(13)	C(15)-H(15)	0.9300
N(1)-N(2)	1.310(11)	C(78)-C(79)	1.32(2)
N(1)-C(2)	1.367(13)	C(78)-H(78)	0.9300
O(1)-C(1)	1.274(12)	C(76)-H(76)	0.9300
O(2)-C(53)	1.298(12)	C(37)-H(37)	0.9300
N(2)-C(11)	1.416(14)	C(79)-H(79)	0.9300

N(4)-C(63)	1.417(14)	C(95)-H(95)	0.9300
C(64)-C(65)	1.403(15)	C(50)-C(49)	1.35(2)
C(64)-C(63)	1.414(15)	C(50)-H(50)	0.9300
C(12)-C(13)	1.380(15)	C(59)-C(58)	1.37(2)
C(12)-C(11)	1.423(15)	C(59)-H(59)	0.9300
C(53)-C(54)	1.383(14)	C(49)-H(49)	0.9300
C(53)-C(62)	1.464(15)	C(6)-C(5)	1.40(2)
C(81)-C(86)	1.388(15)	C(6)-H(6)	0.9300
C(81)-C(82)	1.405(15)	C(5)-H(5)	0.9300
C(1)-C(2)	1.437(13)	C(103)-C(102)	1.35(2)
C(1)-C(10)	1.442(15)	C(103)-H(103)	0.9300
C(93)-C(98)	1.358(16)	C(26)-H(26)	0.9300
C(93)-C(94)	1.373(17)	C(102)-H(102)	0.9300
C(54)-C(55)	1.432(14)	C(57)-C(58)	1.37(2)
C(35)-C(36)	1.356(16)	C(57)-H(57)	0.9300
C(35)-C(40)	1.367(16)	C(58)-H(58)	0.9300
C(17)-C(22)	1.377(16)	C(61)-C(56)	1.445(18)
C(17)-C(18)	1.404(16)	C(19)-C(20)	1.37(2)
C(87)-C(92)	1.369(14)	C(19)-H(19)	0.9300
C(87)-C(88)	1.395(16)	C(48)-C(49)	1.389(18)
C(2)-C(3)	1.415(14)	C(48)-H(48)	0.9300
C(99)-C(100)	1.371(16)	C(23)-C(28)	1.405(18)
C(99)-C(104)	1.398(17)	C(23)-C(24)	1.421(18)
C(41)-C(46)	1.384(15)	C(90)-C(89)	1.382(18)
C(41)-C(42)	1.399(15)	C(90)-H(90)	0.9300
C(30)-C(31)	1.373(16)	C(21)-C(20)	1.346(19)
C(30)-C(29)	1.404(15)	C(21)-C(22)	1.409(16)
C(30)-H(30)	0.9300	C(21)-H(21)	0.9300
C(69)-C(74)	1.382(15)	C(86)-C(85)	1.409(18)
C(69)-C(70)	1.393(16)	C(86)-H(86)	0.9300
C(29)-C(34)	1.385(15)	C(22)-H(22)	0.9300
C(62)-C(60)	1.384(16)	C(88)-C(89)	1.349(17)
C(62)-C(61)	1.406(15)	C(88)-H(88)	0.9300
C(11)-C(16)	1.384(16)	C(20)-H(20)	0.9300
C(63)-C(68)	1.374(16)	C(104)-C(103)	1.373(17)
C(70)-C(71)	1.390(18)	C(104)-H(104)	0.9300
C(70)-H(70)	0.9300	C(97)-C(96)	1.34(2)
C(100)-C(101)	1.400(18)	C(97)-H(97)	0.9300
C(100)-H(100)	0.9300	C(9)-C(5)	1.365(19)
C(92)-C(91)	1.390(16)	C(9)-C(4)	1.465(18)
C(92)-H(92)	0.9300	C(60)-C(59)	1.357(17)
C(98)-C(97)	1.386(18)	C(60)-H(60)	0.9300
C(98)-H(98)	0.9300	C(16)-C(15)	1.37(2)
C(82)-C(83)	1.382(16)	C(16)-H(16)	0.9300
C(82)-H(82)	0.9300	C(52)-C(51)	1.400(18)
C(43)-C(42)	1.357(17)	C(52)-H(52)	0.9300
C(43)-C(44)	1.366(18)	C(40)-C(39)	1.382(17)
C(43)-H(43)	0.9300	C(40)-H(40)	0.9300
C(44)-C(45)	1.389(18)	C(39)-C(38)	1.35(2)
C(44)-H(44)	0.9300	C(39)-H(39)	0.9300
C(18)-C(19)	1.377(17)	C(32)-C(31)	1.351(18)
C(18)-H(18)	0.9300	C(32)-C(33)	1.42(2)
C(42)-H(42)	0.9300	C(32)-H(32)	0.9300
C(10)-C(8)	1.390(16)	C(73)-C(72)	1.350(18)
C(10)-C(9)	1.418(15)	C(73)-C(74)	1.377(16)
C(13)-C(14)	1.404(17)	C(73)-H(73)	0.9300
C(13)-H(13)	0.9300	C(33)-H(33)	0.9300
C(91)-C(90)	1.351(17)	C(36)-C(37)	1.375(17)
C(91)-H(91)	0.9300	C(36)-H(36)	0.9300
C(47)-C(48)	1.382(16)	C(84)-C(83)	1.366(18)
C(47)-C(52)	1.396(16)	C(84)-C(85)	1.40(2)
C(65)-C(66)	1.369(17)	C(84)-H(84)	0.9300
C(65)-H(65)	0.9300	C(74)-H(74)	0.9300
C(34)-C(33)	1.397(18)	C(83)-H(83)	0.9300
C(34)-H(34)	0.9300	C(8)-C(7)	1.359(17)
C(46)-C(45)	1.375(16)	C(8)-H(8)	0.9300
C(46)-H(46)	0.9300	C(55)-C(56)	1.337(17)
C(68)-C(67)	1.37(2)	C(55)-H(80)	0.9300
C(68)-H(68)	0.9300	C(56)-H(56)	0.9300
C(61)-C(57)	1.403(19)	C(72)-C(71)	1.347(19)

C(72)-H(72)	0.9300	C(80)-C(79)	1.370(19)
C(14)-C(15)	1.38(2)	C(80)-H(80A)	0.9300
C(14)-H(14)	0.9300	C(31)-H(31)	0.9300
C(67)-C(66)	1.40(2)	C(3)-C(4)	1.326(16)
C(67)-H(67)	0.9300	C(3)-H(3)	0.9300
C(75)-C(76)	1.405(19)	C(89)-H(89)	0.9300
C(75)-C(80)	1.414(18)	C(45)-H(45)	0.9300
C(96)-C(95)	1.35(2)	C(96)-H(96)	0.9300

Bond angles	(°)	Bond lengths	(°)
N(1)-Rh(1)-C(12)	80.3(4)	C(1)-O(1)-Rh(1)	107.2(6)
N(1)-Rh(1)-O(1)	78.8(3)	C(53)-O(2)-Rh(2)	106.1(6)
C(12)-Rh(1)-O(1)	159.1(4)	N(1)-N(2)-C(11)	109.2(9)
N(1)-Rh(1)-P(1)	93.8(3)	N(3)-N(4)-C(63)	110.0(9)
C(12)-Rh(1)-P(1)	92.9(3)	C(65)-C(64)-C(63)	117.2(10)
O(1)-Rh(1)-P(1)	87.8(2)	C(65)-C(64)-Rh(2)	132.1(9)
N(1)-Rh(1)-P(2)	91.7(3)	C(63)-C(64)-Rh(2)	110.6(8)
C(12)-Rh(1)-P(2)	90.4(3)	C(13)-C(12)-C(11)	117.3(9)
O(1)-Rh(1)-P(2)	90.9(2)	C(13)-C(12)-Rh(1)	132.8(9)
P(1)-Rh(1)-P(2)	173.96(9)	C(11)-C(12)-Rh(1)	109.9(7)
N(1)-Rh(1)-Cl(1)	177.7(3)	O(2)-C(53)-C(54)	123.7(10)
C(12)-Rh(1)-Cl(1)	97.5(3)	O(2)-C(53)-C(62)	118.7(9)
O(1)-Rh(1)-Cl(1)	103.43(16)	C(54)-C(53)-C(62)	117.6(10)
P(1)-Rh(1)-Cl(1)	86.59(10)	C(86)-C(81)-C(82)	115.9(10)
P(2)-Rh(1)-Cl(1)	88.00(10)	C(86)-C(81)-P(3)	122.3(9)
N(3)-Rh(2)-C(64)	79.9(4)	C(82)-C(81)-P(3)	121.8(8)
N(3)-Rh(2)-O(2)	78.7(3)	O(1)-C(1)-C(2)	122.4(10)
C(64)-Rh(2)-O(2)	158.7(4)	O(1)-C(1)-C(10)	120.7(9)
N(3)-Rh(2)-P(3)	94.2(3)	C(2)-C(1)-C(10)	116.9(9)
C(64)-Rh(2)-P(3)	93.0(3)	C(98)-C(93)-C(94)	118.9(11)
O(2)-Rh(2)-P(3)	87.7(2)	C(98)-C(93)-P(4)	120.9(9)
N(3)-Rh(2)-P(4)	91.3(3)	C(94)-C(93)-P(4)	120.0(9)
C(64)-Rh(2)-P(4)	90.5(3)	N(3)-C(54)-C(53)	113.1(9)
O(2)-Rh(2)-P(4)	90.9(2)	N(3)-C(54)-C(55)	124.0(9)
P(3)-Rh(2)-P(4)	173.96(10)	C(53)-C(54)-C(55)	122.8(10)
N(3)-Rh(2)-Cl(2)	177.7(3)	C(36)-C(35)-C(40)	119.1(11)
C(64)-Rh(2)-Cl(2)	97.9(3)	C(36)-C(35)-P(2)	120.1(9)
O(2)-Rh(2)-Cl(2)	103.49(17)	C(40)-C(35)-P(2)	120.5(9)
P(3)-Rh(2)-Cl(2)	86.67(10)	C(22)-C(17)-C(18)	118.3(10)
P(4)-Rh(2)-Cl(2)	87.96(10)	C(22)-C(17)-P(1)	120.4(9)
C(47)-P(2)-C(41)	106.4(5)	C(18)-C(17)-P(1)	121.2(9)
C(47)-P(2)-C(35)	103.3(5)	C(92)-C(87)-C(88)	118.4(10)
C(41)-P(2)-C(35)	102.4(5)	C(92)-C(87)-P(4)	118.3(8)
C(47)-P(2)-Rh(1)	112.8(4)	C(88)-C(87)-P(4)	123.2(8)
C(41)-P(2)-Rh(1)	116.0(4)	N(1)-C(2)-C(3)	124.3(9)
C(35)-P(2)-Rh(1)	114.6(4)	N(1)-C(2)-C(1)	112.7(9)
C(99)-P(4)-C(93)	103.3(5)	C(3)-C(2)-C(1)	122.5(10)
C(99)-P(4)-C(87)	106.0(5)	C(100)-C(99)-C(104)	119.3(11)
C(93)-P(4)-C(87)	102.5(5)	C(100)-C(99)-P(4)	119.7(10)
C(99)-P(4)-Rh(2)	112.7(4)	C(104)-C(99)-P(4)	120.8(9)
C(93)-P(4)-Rh(2)	114.7(4)	C(46)-C(41)-C(42)	118.0(10)
C(87)-P(4)-Rh(2)	116.2(4)	C(46)-C(41)-P(2)	118.8(8)
C(17)-P(1)-C(29)	102.7(5)	C(42)-C(41)-P(2)	123.0(8)
C(17)-P(1)-C(23)	103.4(5)	C(31)-C(30)-C(29)	120.7(11)
C(29)-P(1)-C(23)	106.4(5)	C(31)-C(30)-H(30)	119.6
C(17)-P(1)-Rh(1)	115.3(4)	C(29)-C(30)-H(30)	119.6
C(29)-P(1)-Rh(1)	114.3(4)	C(74)-C(69)-C(70)	119.5(10)
C(23)-P(1)-Rh(1)	113.4(4)	C(74)-C(69)-P(3)	120.2(9)
C(81)-P(3)-C(69)	102.7(5)	C(70)-C(69)-P(3)	120.3(8)
C(81)-P(3)-C(75)	106.9(5)	C(34)-C(29)-C(30)	116.8(10)
C(69)-P(3)-C(75)	103.0(5)	C(34)-C(29)-P(1)	122.6(9)
C(81)-P(3)-Rh(2)	114.6(3)	C(30)-C(29)-P(1)	120.6(8)
C(69)-P(3)-Rh(2)	115.1(4)	C(60)-C(62)-C(61)	118.1(10)
C(75)-P(3)-Rh(2)	113.3(4)	C(60)-C(62)-C(53)	122.5(9)
N(4)-N(3)-C(54)	120.3(8)	C(61)-C(62)-C(53)	119.3(10)
N(4)-N(3)-Rh(2)	121.5(7)	C(16)-C(11)-N(2)	119.3(11)
C(54)-N(3)-Rh(2)	118.2(6)	C(16)-C(11)-C(12)	121.9(11)
N(2)-N(1)-C(2)	119.7(8)	N(2)-C(11)-C(12)	118.8(9)
N(2)-N(1)-Rh(1)	121.6(7)	C(68)-C(63)-C(64)	121.4(11)
C(2)-N(1)-Rh(1)	118.5(6)	C(68)-C(63)-N(4)	120.8(11)

C(93)-C(98)-C(97)	119.7(13)	C(64)-C(63)-N(4)	117.9(9)
C(93)-C(98)-H(98)	120.1	C(71)-C(70)-C(69)	118.6(12)
C(97)-C(98)-H(98)	120.2	C(71)-C(70)-H(70)	120.7
C(83)-C(82)-C(81)	122.6(11)	C(69)-C(70)-H(70)	120.7
C(83)-C(82)-H(82)	118.7	C(99)-C(100)-C(101)	118.0(14)
C(81)-C(82)-H(82)	118.7	C(99)-C(100)-H(100)	121.0
C(42)-C(43)-C(44)	120.3(12)	C(101)-C(100)-H(100)	121.0
C(42)-C(43)-H(43)	119.8	C(87)-C(92)-C(91)	121.0(10)
C(44)-C(43)-H(43)	119.8	C(87)-C(92)-H(92)	119.5
C(43)-C(44)-C(45)	120.0(11)	C(91)-C(92)-H(92)	119.5
C(43)-C(44)-H(44)	120.0	C(21)-C(20)-H(20)	119.6
C(45)-C(44)-H(44)	120.0	C(19)-C(20)-H(20)	119.6
C(19)-C(18)-C(17)	120.3(12)	C(103)-C(104)-C(99)	120.6(13)
C(19)-C(18)-H(18)	119.8	C(103)-C(104)-H(104)	119.7
C(17)-C(18)-H(18)	119.8	C(99)-C(104)-H(104)	119.7
C(43)-C(42)-C(41)	121.1(11)	C(96)-C(97)-C(98)	120.5(14)
C(43)-C(42)-H(42)	119.4	C(96)-C(97)-H(97)	119.7
C(41)-C(42)-H(42)	119.4	C(98)-C(97)-H(97)	119.7
C(8)-C(10)-C(9)	118.2(11)	C(5)-C(9)-C(10)	118.3(13)
C(8)-C(10)-C(1)	121.4(10)	C(5)-C(9)-C(4)	123.8(12)
C(9)-C(10)-C(1)	120.4(10)	C(10)-C(9)-C(4)	117.8(11)
C(12)-C(13)-C(14)	120.7(12)	C(59)-C(60)-C(62)	123.3(12)
C(12)-C(13)-H(13)	119.6	C(59)-C(60)-H(60)	118.4
C(14)-C(13)-H(13)	119.6	C(62)-C(60)-H(60)	118.4
C(90)-C(91)-C(92)	119.1(11)	C(15)-C(16)-C(11)	118.8(13)
C(90)-C(91)-H(91)	120.4	C(15)-C(16)-H(16)	120.6
C(92)-C(91)-H(91)	120.4	C(11)-C(16)-H(16)	120.6
C(48)-C(47)-C(52)	119.5(11)	C(47)-C(52)-C(51)	119.2(14)
C(48)-C(47)-P(2)	120.6(8)	C(47)-C(52)-H(52)	120.4
C(52)-C(47)-P(2)	119.7(9)	C(51)-C(52)-H(52)	120.4
C(66)-C(65)-C(64)	121.0(12)	C(35)-C(40)-C(39)	118.9(13)
C(66)-C(65)-H(65)	119.5	C(35)-C(40)-H(40)	120.6
C(64)-C(65)-H(65)	119.5	C(39)-C(40)-H(40)	120.5
C(29)-C(34)-C(33)	122.6(13)	C(38)-C(39)-C(40)	121.7(14)
C(29)-C(34)-H(34)	118.7	C(38)-C(39)-H(39)	119.2
C(33)-C(34)-H(34)	118.7	C(40)-C(39)-H(39)	119.1
C(45)-C(46)-C(41)	120.8(11)	C(31)-C(32)-C(33)	118.7(13)
C(45)-C(46)-H(46)	119.6	C(31)-C(32)-H(32)	120.7
C(41)-C(46)-H(46)	119.6	C(33)-C(32)-H(32)	120.7
C(67)-C(68)-C(63)	119.8(13)	C(72)-C(73)-C(74)	120.6(12)
C(67)-C(68)-H(68)	120.1	C(72)-C(73)-H(73)	119.7
C(63)-C(68)-H(68)	120.1	C(74)-C(73)-H(73)	119.7
C(57)-C(61)-C(62)	117.5(12)	C(34)-C(33)-C(32)	118.4(12)
C(57)-C(61)-C(56)	123.2(12)	C(34)-C(33)-H(33)	120.8
C(62)-C(61)-C(56)	119.2(11)	C(32)-C(33)-H(33)	120.8
C(20)-C(19)-C(18)	120.2(13)	C(35)-C(36)-C(37)	120.7(13)
C(20)-C(19)-H(19)	119.9	C(35)-C(36)-H(36)	119.6
C(18)-C(19)-H(19)	119.9	C(37)-C(36)-H(36)	119.6
C(47)-C(48)-C(49)	119.4(14)	C(83)-C(84)-C(85)	119.5(13)
C(47)-C(48)-H(48)	120.3	C(83)-C(84)-H(84)	120.2
C(49)-C(48)-H(48)	120.3	C(85)-C(84)-H(84)	120.2
C(28)-C(23)-C(24)	120.4(12)	C(73)-C(74)-C(69)	119.6(12)
C(28)-C(23)-P(1)	123.1(10)	C(73)-C(74)-H(74)	120.2
C(24)-C(23)-P(1)	116.4(9)	C(69)-C(74)-H(74)	120.2
C(91)-C(90)-C(89)	120.7(11)	C(84)-C(83)-C(82)	120.4(13)
C(91)-C(90)-H(90)	119.7	C(84)-C(83)-H(83)	119.8
C(89)-C(90)-H(90)	119.7	C(82)-C(83)-H(83)	119.8
C(20)-C(21)-C(22)	120.0(12)	C(7)-C(8)-C(10)	122.7(11)
C(20)-C(21)-H(21)	120.0	C(7)-C(8)-H(8)	118.6
C(22)-C(21)-H(21)	120.0	C(10)-C(8)-H(8)	118.6
C(81)-C(86)-C(85)	122.3(13)	C(56)-C(55)-C(54)	119.0(11)
C(81)-C(86)-H(86)	118.9	C(56)-C(55)-H(80)	120.5
C(85)-C(86)-H(86)	118.9	C(54)-C(55)-H(80)	120.5
C(17)-C(22)-C(21)	120.3(11)	C(55)-C(56)-C(61)	121.9(11)
C(17)-C(22)-H(22)	119.9	C(55)-C(56)-H(56)	119.1
C(21)-C(22)-H(22)	119.9	C(61)-C(56)-H(56)	119.1
C(89)-C(88)-C(87)	120.5(11)	C(71)-C(72)-C(73)	120.7(13)
C(89)-C(88)-H(88)	119.7	C(71)-C(72)-H(72)	119.7
C(87)-C(88)-H(88)	119.7	C(73)-C(72)-H(72)	119.7
C(21)-C(20)-C(19)	120.9(12)	C(15)-C(14)-C(13)	120.0(13)

C(95)-C(96)-H(96)	119.6	C(15)-C(14)-H(14)	120.0
C(79)-C(80)-C(75)	118.4(14)	C(13)-C(14)-H(14)	120.0
C(79)-C(80)-H(80A)	120.8	C(68)-C(67)-C(66)	120.4(13)
C(75)-C(80)-H(80A)	120.8	C(68)-C(67)-H(67)	119.8
C(32)-C(31)-C(30)	122.6(13)	C(66)-C(67)-H(67)	119.8
C(32)-C(31)-H(31)	118.7	C(76)-C(75)-C(80)	121.9(12)
C(30)-C(31)-H(31)	118.7	C(76)-C(75)-P(3)	121.8(11)
C(4)-C(3)-C(2)	119.2(10)	C(80)-C(75)-P(3)	116.2(9)
C(4)-C(3)-H(3)	120.4	C(97)-C(96)-C(95)	120.8(13)
C(2)-C(3)-H(3)	120.4	C(97)-C(96)-H(96)	119.6
C(88)-C(89)-C(90)	120.2(11)	C(78)-C(79)-C(80)	123.2(17)
C(88)-C(89)-H(89)	119.9	C(78)-C(79)-H(79)	118.4
C(90)-C(89)-H(89)	119.9	C(80)-C(79)-H(79)	118.4
C(46)-C(45)-C(44)	119.6(12)	C(96)-C(95)-C(94)	119.2(14)
C(46)-C(45)-H(45)	120.2	C(96)-C(95)-H(95)	120.4
C(44)-C(45)-H(45)	120.2	C(94)-C(95)-H(95)	120.4
C(102)-C(101)-C(100)	121.8(14)	C(51)-C(50)-C(49)	121.8(13)
C(102)-C(101)-H(101)	119.1	C(51)-C(50)-H(50)	119.1
C(100)-C(101)-H(101)	119.1	C(49)-C(50)-H(50)	119.1
C(65)-C(66)-C(67)	120.0(13)	C(60)-C(59)-C(58)	119.0(14)
C(65)-C(66)-H(66)	120.0	C(60)-C(59)-H(59)	120.5
C(67)-C(66)-H(66)	120.0	C(58)-C(59)-H(59)	120.5
C(72)-C(71)-C(70)	120.9(14)	C(50)-C(49)-C(48)	120.3(15)
C(72)-C(71)-H(71)	119.6	C(50)-C(49)-H(49)	119.9
C(70)-C(71)-H(71)	119.6	C(48)-C(49)-H(49)	119.9
C(3)-C(4)-C(9)	122.8(11)	C(7)-C(6)-C(5)	119.1(13)
C(3)-C(4)-H(4)	118.6	C(7)-C(6)-H(6)	120.5
C(9)-C(4)-H(4)	118.6	C(5)-C(6)-H(6)	120.5
C(50)-C(51)-C(52)	119.7(14)	C(9)-C(5)-C(6)	122.3(13)
C(50)-C(51)-H(51)	120.1	C(9)-C(5)-H(5)	118.9
C(52)-C(51)-H(51)	120.1	C(6)-C(5)-H(5)	118.9
C(84)-C(85)-C(86)	119.1(13)	C(102)-C(103)-C(104)	119.8(15)
C(84)-C(85)-H(85)	120.4	C(102)-C(103)-H(103)	120.1
C(86)-C(85)-H(85)	120.4	C(104)-C(103)-H(103)	120.1
C(25)-C(24)-C(23)	121.0(14)	C(25)-C(26)-C(27)	122.1(14)
C(25)-C(24)-H(24)	119.5	C(25)-C(26)-H(26)	118.9
C(23)-C(24)-H(24)	119.5	C(27)-C(26)-H(26)	118.9
C(23)-C(28)-C(27)	116.5(15)	C(101)-C(102)-C(103)	120.4(14)
C(23)-C(28)-H(28)	121.8	C(101)-C(102)-H(102)	119.8
C(27)-C(28)-H(28)	121.8	C(103)-C(102)-H(102)	119.8
C(8)-C(7)-C(6)	119.3(14)	C(58)-C(57)-C(61)	122.2(13)
C(8)-C(7)-H(7)	120.3	C(58)-C(57)-H(57)	118.9
C(6)-C(7)-H(7)	120.3	C(61)-C(57)-H(57)	118.9
C(93)-C(94)-C(95)	120.8(13)	C(57)-C(58)-C(59)	119.6(13)
C(93)-C(94)-H(94)	119.6	C(57)-C(58)-H(58)	120.2
C(95)-C(94)-H(94)	119.6	C(59)-C(58)-H(58)	120.2
C(37)-C(38)-C(39)	118.9(13)	C(16)-C(15)-H(15)	119.5
C(37)-C(38)-H(38)	120.6	C(14)-C(15)-H(15)	119.5
C(39)-C(38)-H(38)	120.6	C(79)-C(78)-C(77)	121.1(14)
C(26)-C(27)-C(28)	120.7(15)	C(79)-C(78)-H(78)	119.4
C(26)-C(27)-H(27)	119.6	C(77)-C(78)-H(78)	119.4
C(28)-C(27)-H(27)	119.7	C(75)-C(76)-C(77)	116.3(15)
C(78)-C(77)-C(76)	119.0(15)	C(75)-C(76)-H(76)	121.8
C(78)-C(77)-H(77)	120.5	C(77)-C(76)-H(76)	121.8
C(76)-C(77)-H(77)	120.5	C(38)-C(37)-C(36)	120.6(14)
C(26)-C(25)-C(24)	119.2(16)	C(38)-C(37)-H(37)	119.7
C(26)-C(25)-H(25)	120.4	C(36)-C(37)-H(37)	119.7
C(24)-C(25)-H(25)	120.4	C(16)-C(15)-C(14)	121.1(13)

Table 14.

Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$]
for $[\text{Rh}(\text{L}'')(\text{PPh}_3)_2]$ (**2-Rh**)

	x	y	z	U(eq)
Rh(1)	4710(1)	9162(1)	2832(1)	23(1)
Rh(2)	292(1)	4162(1)	2168(1)	23(1)
P(2)	2732(3)	9138(1)	3133(2)	33(1)
P(4)	2268(3)	4138(1)	1866(2)	31(1)
P(1)	6671(3)	9316(1)	2576(1)	30(1)
P(3)	-1671(2)	4315(1)	2424(1)	29(1)
Cl(2)	423(2)	5485(1)	2279(1)	36(1)
Cl(1)	4577(2)	10485(1)	2721(1)	36(1)
N(3)	213(7)	3080(4)	2112(4)	31(2)
N(1)	4802(7)	8079(4)	2888(4)	28(2)
O(1)	4963(7)	9006(3)	3907(3)	32(2)
O(2)	37(7)	4009(3)	1097(3)	35(2)
N(2)	4684(8)	7652(5)	2371(5)	37(2)
N(4)	329(8)	2654(5)	2627(4)	37(2)
C(64)	466(10)	3888(6)	3113(5)	36(3)
C(12)	4538(9)	8900(6)	1888(5)	3(3)
C(53)	-64(9)	3293(6)	1012(5)	2(2)
C(81)	-2494(9)	3518(5)	2209(5)	29(2)
C(1)	5067(9)	8305(6)	4003(5)	33(2)
C(93)	2813(10)	4816(5)	1209(5)	30(2)
C(54)	33(9)	2767(5)	1508(5)	30(2)
C(35)	2180(9)	9824(5)	3789(5)	30(2)
C(17)	7261(10)	10080(5)	3009(5)	32(3)
C(87)	3117(9)	4345(5)	2545(5)	27(2)
C(2)	4937(9)	7760(5)	3493(5)	29(2)
C(99)	2780(10)	3241(6)	1510(6)	39(3)
C(41)	1895(9)	9345(5)	2456(5)	27(2)
C(30)	8181(11)	8560(6)	3309(6)	41(3)
C(69)	-2261(9)	5088(5)	1988(5)	30(2)
C(29)	7498(9)	8508(5)	2794(5)	31(2)
C(62)	-302(10)	3022(5)	357(5)	33(3)
C(11)	4519(11)	8107(6)	1814(6)	42(3)
C(63)	482(10)	3101(6)	3191(6)	39(3)
C(70)	-1697(11)	5359(7)	1382(6)	45(3)
C(100)	2824(10)	2633(6)	1926(7)	48(3)
C(92)	2882(10)	4984(6)	2914(6)	40(3)
C(98)	2199(11)	5010(7)	714(6)	48(3)
C(82)	3180(10)	3558(6)	1694(6)	41(3)
C(43)	342(12)	9104(8)	1847(6)	52(3)
C(44)	575(11)	9743(7)	1479(6)	47(3)
C(18)	6704(11)	10363(7)	3618(6)	46(3)
C(42)	970(11)	8913(6)	2336(6)	40(3)
C(10)	5291(9)	8023(6)	4647(5)	33(3)
C(13)	4458(10)	9327(7)	1321(6)	43(3)
C(91)	3536(11)	5194(7)	3405(6)	45(3)
C(47)	2225(10)	8249(6)	3494(6)	35(3)
C(65)	545(10)	4323(7)	3687(6)	41(3)
C(34)	7466(12)	7821(6)	2479(7)	53(4)
C(46)	2126(11)	9990(6)	2079(6)	45(3)
C(68)	649(12)	2776(8)	3792(7)	55(4)
C(61)	-463(12)	2251(7)	267(6)	52(3)
C(19)	7191(13)	10921(8)	3954(7)	62(4)
C(48)	1962(11)	8165(7)	4184(7)	53(3)
C(23)	7136(10)	9519(7)	1684(6)	40(3)
C(90)	4405(10)	4753(7)	3523(6)	45(3)
C(21)	8749(12)	10971(6)	3095(7)	52(4)
C(86)	-2451(12)	2827(6)	2522(7)	55(4)
C(22)	8281(10)	10389(6)	2750(6)	41(3)
C(88)	4041(11)	3914(6)	2665(6)	40(3)
C(20)	8203(13)	11224(7)	3683(7)	58(4)

C(104)	3053(12)	3151(7)	814(7)	52(3)
C(97)	2671(14)	5469(8)	191(7)	68(4)
C(9)	5469(12)	7247(7)	4740(7)	52(3)
C(60)	-398(13)	3497(7)	-179(6)	56(4)
C(16)	4368(12)	7773(8)	1210(7)	57(4)
C(52)	2168(11)	7630(6)	3075(7)	51(3)
C(40)	2800(11)	10015(7)	4287(6)	47(3)
C(39)	2316(14)	10467(9)	4807(7)	69(4)
C(32)	8818(12)	7297(7)	3142(8)	66(4)
C(73)	-3730(12)	5973(6)	1910(7)	52(4)
C(33)	8091(12)	7205(7)	2647(8)	58(4)
C(36)	1115(12)	10089(7)	3815(7)	53(3)
C(84)	-3812(12)	2298(8)	1870(9)	66(4)
C(74)	-3284(10)	5398(6)	2250(6)	40(3)
C(83)	-3825(12)	2962(7)	1532(7)	54(4)
C(8)	5381(13)	8501(6)	5183(6)	54(4)
C(55)	-70(12)	1979(6)	1402(6)	46(3)
C(56)	-303(13)	1738(6)	805(7)	56(4)
C(72)	-3185(12)	6229(7)	1319(7)	52(3)
C(14)	4315(13)	8986(9)	707(7)	64(4)
C(67)	757(14)	3218(10)	4337(7)	73(5)
C(75)	-2135(10)	4525(7)	3320(6)	42(3)
C(96)	3728(15)	5728(8)	174(7)	67(4)
C(80)	-1942(12)	5264(8)	3529(7)	56(4)
C(31)	8823(13)	7962(7)	3462(7)	60(4)
C(3)	5069(12)	6983(6)	3596(6)	45(3)
C(89)	4647(11)	4102(7)	3160(7)	52(3)
C(45)	1474(11)	10192(7)	1593(6)	49(3)
C(101)	3206(11)	1953(7)	1632(10)	64(4)
C(66)	689(12)	3995(8)	4288(7)	60(4)
C(71)	-2189(13)	5933(9)	1054(8)	65(4)
C(4)	5282(13)	6740(7)	4192(7)	59(4)
C(51)	1802(12)	6942(7)	3361(10)	69(5)
C(85)	-3089(12)	2210(7)	2356(8)	65(4)
C(24)	6947(12)	10258(8)	1462(7)	59(4)
C(28)	7612(13)	8975(9)	1224(7)	66(4)
C(7)	5644(16)	8256(8)	5786(7)	79(5)
C(94)	3889(12)	5090(7)	1186(7)	57(4)
C(38)	1257(15)	10732(8)	4828(7)	69(5)
C(27)	7907(15)	9214(11)	541(8)	80(5)
C(77)	-2918(14)	4211(11)	4470(7)	77(5)
C(25)	7199(15)	10453(10)	799(7)	73(5)
C(15)	4231(14)	8219(10)	670(7)	78(5)
C(78)	-2682(15)	4956(11)	4651(7)	77(5)
C(76)	-2606(12)	3974(9)	3774(8)	67(4)
C(37)	669(15)	10559(9)	4325(8)	76(5)
C(79)	-2210(15)	5436(10)	4198(7)	77(5)
C(95)	4342(14)	5559(9)	669(8)	73(5)
C(50)	1536(14)	6882(8)	4033(11)	78(5)
C(59)	-636(16)	3255(9)	-786(7)	79(5)
C(49)	1605(16)	7472(8)	4447(8)	78(5)
C(6)	5866(18)	7508(9)	5868(8)	90(6)
C(5)	5736(17)	7012(9)	5347(8)	87(6)
C(103)	3396(15)	2468(9)	48(8)	77(5)
C(26)	7666(15)	9931(13)	348(7)	86(6)
C(102)	3497(13)	1883(8)	960(10)	75(5)
C(57)	-731(16)	2016(9)	-361(8)	78(5)
C(58)	-851(18)	2510(10)	-868(9)	95(7)

Table 15.

Bond lengths (Å) and bond angles (°) for [Ir(L'')(PPh₃)₂] (**2-Ir**)

Bond lengths	(Å)	Bond lengths	(Å)
Ir(1)-N(1)	1.986(10)	C(18)-H(18)	0.9300
Ir(1)-C(12)	2.046(13)	C(3)-C(4)	1.32(2)
Ir(1)-O(1)	2.282(9)	C(3)-H(3)	0.9300
Ir(1)-P(2)	2.352(3)	C(48)-H(48)	0.9300
Ir(1)-P(1)	2.363(3)	C(21)-C(20)	1.29(2)
Ir(1)-C(1)	2.406(3)	C(21)-H(21)	0.9300
P(1)-C(41)	1.830(14)	C(43)-C(44)	1.40(3)
P(1)-C(47)	1.834(11)	C(43)-H(43)	0.9300
P(1)-C(35)	1.851(13)	C(33)-C(32)	1.34(3)
P(2)-C(23)	1.825(12)	C(33)-H(33)	0.9300
P(2)-C(17)	1.826(14)	C(30)-C(31)	1.39(2)
P(2)-C(29)	1.831(15)	C(30)-H(30)	0.9300
O(1)-C(1)	1.345(16)	C(4)-H(4)	0.9300
N(2)-N(1)	1.323(14)	C(8)-C(7)	1.36(2)
N(2)-C(11)	1.39(2)	C(8)-H(8)	0.9300
C(35)-C(40)	1.353(17)	C(39)-C(38)	1.38(3)
C(35)-C(36)	1.365(19)	C(39)-H(39)	0.9300
C(2)-N(1)	1.374(17)	C(31)-C(32)	1.38(3)
C(2)-C(3)	1.387(18)	C(31)-H(31)	0.9300
C(2)-C(1)	1.430(18)	C(38)-C(37)	1.39(3)
C(51)-C(50)	1.31(2)	C(38)-H(38)	0.9300
C(51)-C(52)	1.38(2)	C(36)-C(37)	1.43(2)
C(51)-H(51)	0.9300	C(36)-H(36)	0.9300
C(41)-C(42)	1.373(19)	C(20)-C(19)	1.42(2)
C(41)-C(46)	1.44(2)	C(20)-H(20)	0.9300
C(47)-C(48)	1.353(17)	C(45)-C(44)	1.34(3)
C(47)-C(52)	1.386(16)	C(45)-H(45)	0.9300
C(1)-C(10)	1.43(2)	C(19)-H(19)	0.9300
C(52)-H(52)	0.9300	C(32)-H(32)	0.9300
C(27)-C(26)	1.36(2)	C(6)-C(7)	1.36(3)
C(27)-C(28)	1.468(19)	C(6)-C(5)	1.39(3)
C(27)-H(27)	0.9300	C(6)-H(6)	0.9300
C(10)-C(8)	1.39(2)	C(44)-H(44)	0.9300
C(10)-C(9)	1.42(2)	C(37)-H(37)	0.9300
C(24)-C(25)	1.33(2)	C(5)-H(5)	0.9300
C(24)-C(23)	1.372(17)	C(7)-H(7)	0.9300
C(24)-H(24)	0.9300	C(12)-C(13)	1.39(2)
C(23)-C(28)	1.342(16)	C(12)-C(11)	1.49(2)
C(50)-C(49)	1.40(2)	C(11)-C(16)	1.476(13)
C(50)-H(50)	0.9300	C(13)-C(14)	1.447(18)
C(29)-C(30)	1.38(2)	C(13)-H(13)	0.9300
C(29)-C(34)	1.41(2)	C(16)-C(15)	1.20(3)
C(42)-C(43)	1.35(2)	C(16)-H(16)	0.9300
C(42)-H(42)	0.9300	C(14)-C(15)	1.49(3)
C(17)-C(18)	1.385(19)	C(14)-H(14)	0.9300
C(17)-C(22)	1.423(18)	C(15)-H(15)	0.9300
C(26)-C(25)	1.38(2)	C(25)-H(25)	0.9300
C(26)-H(26)	0.9300	C(40)-C(39)	1.38(2)
C(22)-C(21)	1.393(19)	C(40)-H(40)	0.9300
C(22)-H(22)	0.9300	C(9)-C(5)	1.42(2)
C(34)-C(33)	1.42(3)	C(9)-C(4)	1.43(2)
C(34)-H(34)	0.9300	C(28)-H(28)	0.9300
C(49)-C(48)	1.372(19)	C(46)-C(45)	1.36(2)
C(49)-H(49)	0.9300	C(46)-H(46)	0.9300
C(18)-C(19)	1.41(2)		
Bond angles	(°)	Bond lengths	(°)
N(1)-Ir(1)-C(12)	81.1(6)	C(44)-C(45)-C(46)	119(2)
N(1)-Ir(1)-O(1)	79.8(4)	C(44)-C(45)-H(45)	120.4
C(12)-Ir(1)-O(1)	160.9(6)	C(46)-C(45)-H(45)	120.4
N(1)-Ir(1)-P(2)	94.6(3)	C(18)-C(19)-C(20)	119.0(18)

120.5	(118)-C(19)-H(19)	92.8(4)	(12)-H(1)-P(2)
120.5	(120)-C(19)-H(19)	88.0(2)	O(1)-H(1)-P(2)
120.5	(120)-C(19)-H(19)	91.4(3)	N(1)-H(1)-P(1)
118.6	(120)-C(19)-H(19)	91.1(4)	(12)-H(1)-P(1)
118.6	(120)-C(19)-H(19)	90.1(2)	O(1)-H(1)-P(1)
118.6	(120)-C(19)-H(19)	173.34(12)	P(2)-H(1)-P(1)
119.3	(120)-C(19)-H(19)	178.3(3)	N(1)-H(1)-C(11)
119.3	(120)-C(19)-H(19)	97.4(5)	(12)-H(1)-C(11)
119.3	(120)-C(19)-H(19)	101.7(2)	O(1)-H(1)-C(11)
118.4	(120)-C(19)-H(19)	86.38(11)	P(2)-H(1)-C(11)
118.4	(120)-C(19)-H(19)	87.77(12)	P(1)-H(1)-C(11)
118.0(18)	(120)-C(19)-H(19)	105.3(6)	(41)-P(1)-C(35)
118.0(18)	(120)-C(19)-H(19)	106.0(6)	(41)-P(1)-C(35)
121.0	(120)-C(19)-H(19)	101.4(5)	(47)-P(1)-C(35)
122(2)	(120)-C(19)-H(19)	112.3(4)	(41)-P(1)-H(1)
118.8	(120)-C(19)-H(19)	115.9(4)	(47)-P(1)-H(1)
118.8	(120)-C(19)-H(19)	114.5(4)	(35)-P(1)-H(1)
108.2(7)	(120)-C(19)-H(19)	102.0(6)	(23)-P(2)-C(17)
120.8	(120)-C(19)-H(19)	101.7(6)	(23)-P(2)-C(29)
120.8	(120)-C(19)-H(19)	108.2(7)	(17)-P(2)-C(29)
118.6(15)	(120)-C(19)-H(19)	116.0(4)	(23)-P(2)-H(1)
133.7(15)	(120)-C(19)-H(19)	114.2(4)	(17)-P(2)-H(1)
107.7(9)	(120)-C(19)-H(19)	113.4(4)	(29)-P(2)-H(1)
119.8(15)	(120)-C(19)-H(19)	102.8(8)	N(1)-N(2)-C(11)
118.9(11)	(120)-C(19)-H(19)	112.5(12)	(40)-C(35)-C(36)
121.4(14)	(120)-C(19)-H(19)	120.8(14)	(40)-C(35)-P(1)
117.1(16)	(120)-C(19)-H(19)	117.9(11)	(36)-C(35)-P(1)
121.4	(120)-C(19)-H(19)	125.1(3)	N(1)-C(2)-C(3)
121.4	(120)-C(19)-H(19)	111.8(12)	N(1)-C(2)-C(1)
116.5(14)	(120)-C(19)-H(19)	123.1(5)	(3)-C(2)-C(1)
121.8	(120)-C(19)-H(19)	120.7(13)	(50)-C(31)-C(52)
121.8	(120)-C(19)-H(19)	119.7	(50)-C(31)-H(51)
118.4(12)	(120)-C(19)-H(19)	119.7	(52)-C(31)-H(51)
120.8	(120)-C(19)-H(19)	120.0(14)	(42)-C(41)-C(46)
120.8	(120)-C(19)-H(19)	122.4(2)	(42)-C(41)-P(1)
126.7(18)	(120)-C(19)-H(19)	117.3(11)	(46)-C(41)-P(1)
116.7	(120)-C(19)-H(19)	121.4(11)	N(2)-N(1)-C(2)
116.7	(120)-C(19)-H(19)	119.3(10)	N(2)-N(1)-H(1)
112.4(10)	(120)-C(19)-H(19)	119.0(8)	(2)-N(1)-H(1)
117.8(14)	(120)-C(19)-H(19)	117.5(11)	(48)-C(47)-C(52)
121.1	(120)-C(19)-H(19)	118.8(9)	(48)-C(47)-P(1)
121.1	(120)-C(19)-H(19)	123.6(9)	(52)-C(47)-P(1)
120.9(13)	(120)-C(19)-H(19)	117.9(11)	O(1)-C(1)-C(10)
119.5	(120)-C(19)-H(19)	126.6(13)	O(1)-C(1)-C(2)
119.5	(120)-C(19)-H(19)	115.6(14)	(10)-C(1)-C(2)
119(2)	(120)-C(19)-H(19)	121.1(13)	(51)-C(52)-C(47)
120.7	(120)-C(19)-H(19)	119.5	(51)-C(52)-H(52)
120.7	(120)-C(19)-H(19)	119.5	(47)-C(52)-H(52)
122.6(16)	(120)-C(19)-H(19)	119.3(14)	(26)-C(27)-H(27)
118.7	(120)-C(19)-H(19)	120.4	(28)-C(27)-H(27)
120.3(15)	(120)-C(19)-H(19)	120.4	(8)-C(10)-C(9)
119.9	(120)-C(19)-H(19)	120.9(16)	(8)-C(10)-C(9)
119.9	(120)-C(19)-H(19)	119.3(14)	(8)-C(10)-C(1)
119.9	(120)-C(19)-H(19)	121.0(14)	(25)-C(47)-C(23)
124.9(18)	(120)-C(19)-H(19)	121.0(14)	(25)-C(47)-H(24)
120.5(17)	(120)-C(19)-H(19)	119.5	(23)-C(47)-H(24)
119.4(13)	(120)-C(19)-H(19)	119.5	(23)-C(47)-H(24)
120.4	(120)-C(19)-H(19)	119.9(13)	(28)-C(23)-C(24)
120.4	(120)-C(19)-H(19)	119.2(11)	(28)-C(23)-P(2)
120.9(10)	(120)-C(19)-H(19)	120.9(10)	(24)-C(23)-P(2)
120.6	(120)-C(19)-H(19)	120.0(14)	(51)-C(50)-H(50)
120.6	(120)-C(19)-H(19)	120.0	(51)-C(50)-H(50)
118.9(15)	(120)-C(19)-H(19)	120.0	(49)-C(50)-H(50)
120.6	(120)-C(19)-H(19)	118.2(16)	(30)-C(29)-C(34)
120.6	(120)-C(19)-H(19)	118.6(12)	(30)-C(29)-P(2)
120.6	(120)-C(19)-H(19)	122.4(15)	(34)-C(29)-P(2)
120.0	(120)-C(19)-H(19)	120.1(17)	(43)-C(42)-C(41)
119.9	(120)-C(19)-H(19)	119.9	(43)-C(42)-H(42)
120.0	(120)-C(19)-H(19)	119.9	(43)-C(42)-H(42)
121.3(15)	(120)-C(19)-H(19)	119.9	(43)-C(42)-H(42)

C(18)-C(17)-C(22)	117.5(13)	C(4)-C(3)-H(3)	119.3
C(18)-C(17)-P(2)	120.0(12)	C(2)-C(3)-H(3)	119.3
C(47)-C(48)-C(49)	121.7(13)	C(10)-C(8)-H(8)	118.8
C(47)-C(48)-H(48)	119.1	C(38)-C(39)-C(40)	120.5(16)
C(49)-C(48)-H(48)	119.1	C(38)-C(39)-H(39)	119.8
C(20)-C(21)-C(22)	120.8(15)	C(40)-C(39)-H(39)	119.8
C(20)-C(21)-H(21)	119.6	C(32)-C(31)-C(30)	118(2)
C(22)-C(21)-H(21)	119.6	C(32)-C(31)-H(31)	121.1
C(42)-C(43)-C(44)	118.4(18)	C(30)-C(31)-H(31)	121.1
C(42)-C(43)-H(43)	120.8	C(39)-C(38)-C(37)	120.0(17)
C(44)-C(43)-H(43)	120.8	C(39)-C(38)-H(38)	120.0
C(32)-C(33)-C(34)	120(2)	C(37)-C(38)-H(38)	120.0
C(32)-C(33)-H(33)	120.2	C(35)-C(36)-C(37)	120.1(16)
C(34)-C(33)-H(33)	120.2	C(35)-C(36)-H(36)	119.9
C(29)-C(30)-C(31)	122.0(18)	C(37)-C(36)-H(36)	119.9
C(29)-C(30)-H(30)	119.0	C(21)-C(20)-C(19)	121.7(18)
C(31)-C(30)-H(30)	119.0	C(21)-C(20)-H(20)	119.1
C(3)-C(4)-C(9)	119.5(16)	C(19)-C(20)-H(20)	119.1
C(3)-C(4)-H(4)	120.2	C(7)-C(8)-C(10)	122.5(17)
C(9)-C(4)-H(4)	120.2	C(7)-C(8)-H(8)	118.8

Table 16.

Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$]
for $[\text{Ir}(\text{L}^*)(\text{PPh}_3)_2]$ (**2-Ir**)

		X	Y	Z
Ir(1)	279(1)	9173(1)	2839(1)	51(1)
P(1)	2244(3)	9156(2)	3147(2)	54(1)
Cl(1)	402(3)	10498(2)	2760(2)	66(1)
P(2)	-1673(3)	9327(2)	2589(2)	52(1)
O(1)	46(6)	9018(4)	3941(5)	55(2)
N(2)	331(9)	7679(6)	2344(6)	73(4)
C(35)	2785(11)	9849(7)	3791(6)	57(3)
C(2)	48(11)	7746(7)	3479(8)	63(4)
C(51)	4609(11)	9151(10)	1844(9)	79(5)
C(41)	2759(10)	8258(8)	3482(7)	64(4)
N(1)	207(8)	8076(6)	2883(6)	62(3)
C(47)	3076(9)	9367(6)	2472(6)	45(3)
C(1)	-51(10)	8280(9)	3994(7)	65(4)
C(52)	3991(11)	8952(7)	2345(7)	60(3)
C(27)	-3759(13)	10963(7)	3122(9)	79(5)
C(10)	-252(11)	7986(8)	4627(8)	70(4)
C(24)	-1732(12)	10350(8)	3627(6)	67(4)
C(23)	-2274(9)	10081(7)	3028(6)	53(3)
C(50)	4353(12)	9745(10)	1480(8)	76(4)
C(29)	-2140(10)	9565(10)	1705(7)	71(4)
C(42)	2802(11)	7647(8)	3079(9)	74(4)
C(17)	-2486(10)	8532(7)	2806(7)	62(4)
C(26)	-3187(13)	11225(9)	3710(8)	78(4)
C(22)	-3216(11)	8569(7)	3306(7)	62(3)
C(34)	-2609(14)	9038(12)	1229(9)	101(6)
C(25)	-2190(14)	10880(11)	3962(8)	94(5)
C(40)	2149(13)	10068(9)	4260(7)	80(4)

C(9)	-368(15)	7207(10)	4705(11)	101(6)
C(28)	-3277(11)	10356(8)	2769(7)	67(4)
C(46)	3015(13)	8189(10)	4204(9)	89(5)
C(49)	3454(13)	10193(9)	1606(7)	77(4)
C(18)	-2402(12)	7861(8)	2484(9)	82(5)
C(3)	-65(13)	6991(8)	3574(8)	73(4)
C(48)	2827(11)	9981(8)	2094(8)	74(4)
C(21)	-3851(13)	7959(9)	3444(9)	85(5)
C(43)	3169(13)	6992(9)	3354(13)	99(6)
C(33)	-2936(17)	9269(17)	553(10)	120(8)
C(30)	-1928(13)	10265(11)	1486(8)	85(5)
C(4)	-257(15)	6717(10)	4160(10)	94(5)
C(8)	-356(16)	8467(9)	5158(9)	95(5)
C(39)	2607(17)	10503(11)	4798(9)	101(6)
C(31)	-2222(18)	10479(14)	820(10)	119(7)
C(38)	3700(20)	10742(12)	4848(10)	126(8)
C(36)	3896(14)	10027(11)	3853(9)	103(6)
C(20)	-3775(14)	7341(12)	3135(10)	101(6)
C(45)	3367(17)	7524(11)	4471(12)	117(7)
C(19)	-3044(15)	7252(12)	2645(10)	112(7)
C(32)	-2700(19)	9956(18)	370(10)	128(9)
C(6)	-750(20)	7491(14)	5851(11)	154(11)
C(44)	3446(16)	6947(12)	4057(14)	117(8)
C(37)	4380(18)	10502(14)	4386(10)	135(9)
C(5)	-657(19)	6987(12)	5337(11)	121(7)
C(7)	-600(20)	8228(12)	5764(11)	132(9)
C(12)	443(10)	8938(11)	1859(6)	76(5)
C(11)	464(12)	8117(12)	1787(7)	85(5)
C(13)	515(13)	9370(11)	1295(8)	92(5)
C(16)	616	7763	1142	210(20)
C(14)	631	8987	674	112(8)
C(15)	780(20)	8168(15)	695(13)	185(11)

Table 17.

Bond lengths (Å) and bond angles (°) for [Ru(L¹)₂] (II)

Bond lengths	(Å)	Bond lengths	(Å)
C(17)-S(1)	1.784(12)	C(8)-H(8)	0.9300
C(17)-H(17A)	0.9600	C(9)-C(10)	1.399(11)
C(17)-H(17B)	0.9600	C(11)-C(16)	1.387(11)
C(17)-H(17C)	0.9600	C(11)-C(12)	1.410(11)
C(18)-N(3)	1.370(10)	C(11)-N(2)	1.422(9)
C(18)-C(19)	1.429(11)	C(12)-C(13)	1.377(11)
C(18)-C(27)	1.456(11)	C(12)-S(1)	1.748(9)
C(19)-O(2)	1.294(10)	C(13)-C(14)	1.365(14)
C(19)-C(20)	1.437(12)	C(13)-H(13)	0.9300
C(20)-C(21)	1.327(13)	C(14)-C(15)	1.360(14)
C(20)-H(20)	0.9300	C(14)-H(14)	0.9300
C(21)-C(26)	1.402(13)	C(15)-C(16)	1.389(12)
C(21)-H(21)	0.9300	C(15)-H(15)	0.9300
C(34)-S(2)	1.818(9)	C(16)-H(16)	0.9300
C(34)-H(34A)	0.9600	C(22)-C(23)	1.391(15)
C(34)-H(34B)	0.9600	C(22)-C(26)	1.431(12)
C(34)-H(34C)	0.9600	C(22)-H(22)	0.9300
O(10)-H(02)	1.24(5)	C(23)-C(24)	1.347(14)
O(10)-H(03)	1.29(5)	C(23)-H(23)	0.9300
O(51)-H(002)	1.20(5)	C(24)-C(25)	1.394(11)
O(51)-H(005)	1.11(5)	C(24)-H(24)	0.9300
C(1)-N(1)	1.377(9)	C(25)-C(27)	1.417(12)
C(1)-C(2)	1.414(10)	C(25)-H(25)	0.9300
C(1)-C(10)	1.462(11)	C(26)-C(27)	1.424(12)
C(2)-O(1)	1.296(9)	C(28)-C(33)	1.375(11)
C(2)-C(3)	1.418(11)	C(28)-C(29)	1.394(11)
C(3)-C(4)	1.327(12)	C(28)-N(4)	1.426(9)
C(3)-H(3)	0.9300	C(29)-C(30)	1.375(11)
C(4)-C(9)	1.415(13)	C(29)-S(2)	1.785(8)
C(4)-H(4)	0.9300	C(30)-C(31)	1.344(13)
C(5)-C(6)	1.337(15)	C(30)-H(30)	0.9300
C(5)-C(9)	1.379(13)	C(31)-C(32)	1.357(13)
C(5)-H(5)	0.9300	C(31)-H(31)	0.9300
C(6)-C(7)	1.398(16)	C(32)-C(33)	1.369(12)
C(6)-H(6)	0.9300	C(32)-H(32)	0.9300
C(7)-C(8)	1.379(13)	C(33)-H(33)	0.9300
C(7)-H(7)	0.9300	Ru(1)-N(2)	2.004(6)
C(8)-C(10)	1.408(12)	Ru(1)-N(4)	2.018(6)
Ru(1)-S(2)	2.294(2)	Ru(1)-O(2)	2.022(6)
N(1)-N(2)	1.270(8)	Ru(1)-O(1)	2.029(5)
N(3)-N(4)	1.286(8)	Ru(1)-S(1)	2.291(2)

Bond angles	(°)	Bond lengths	(°)
S(1)-C(17)-H(17A)	109.5	C(15)-C(14)-C(13)	118.5(8)
S(1)-C(17)-H(17B)	109.5	C(15)-C(14)-H(14)	120.8
H(17A)-C(17)-H(17B)	109.5	C(13)-C(14)-H(14)	120.8
S(1)-C(17)-H(17C)	109.5	C(14)-C(15)-C(16)	122.1(9)
H(17A)-C(17)-H(17C)	109.5	C(14)-C(15)-H(15)	118.9
H(17B)-C(17)-H(17C)	109.5	C(16)-C(15)-H(15)	118.9
N(3)-C(18)-C(19)	129.0(7)	C(11)-C(16)-C(15)	119.8(9)
N(3)-C(18)-C(27)	112.1(7)	C(11)-C(16)-H(16)	120.1
C(19)-C(18)-C(27)	118.9(7)	C(15)-C(16)-H(16)	120.1
O(2)-C(19)-C(18)	125.9(7)	C(23)-C(22)-C(26)	119.5(9)
O(2)-C(19)-C(20)	116.3(8)	C(23)-C(22)-H(22)	120.2
C(18)-C(19)-C(20)	117.8(8)	C(26)-C(22)-H(22)	120.2
C(21)-C(20)-C(19)	122.3(9)	C(24)-C(23)-C(22)	122.7(9)
C(21)-C(20)-H(20)	118.8	C(24)-C(23)-H(23)	118.7
C(19)-C(20)-H(20)	118.8	C(22)-C(23)-H(23)	118.7
C(20)-C(21)-C(26)	122.4(9)	C(23)-C(24)-C(25)	119.0(10)
C(20)-C(21)-H(21)	118.8	C(23)-C(24)-H(24)	120.5
C(26)-C(21)-H(21)	118.8	C(25)-C(24)-H(24)	120.5

S(2)-C(34)-H(34A)	109.5	C(24)-C(25)-C(27)	122.2(9)
S(2)-C(34)-H(34B)	109.5	C(24)-C(25)-H(25)	118.9
H(34A)-C(34)-H(34B)	109.5	C(27)-C(25)-H(25)	118.9
S(2)-C(34)-H(34C)	109.5	C(21)-C(26)-C(27)	118.9(8)
H(34A)-C(34)-H(34C)	109.5	C(21)-C(26)-C(22)	122.2(9)
H(34B)-C(34)-H(34C)	109.5	C(27)-C(26)-C(22)	118.7(9)
H(02)-O(10)-H(03)	157(4)	C(25)-C(27)-C(26)	117.8(8)
H(002)-O(51)-H(005)	84(4)	C(25)-C(27)-C(18)	122.7(8)
N(1)-C(1)-C(2)	128.3(7)	C(26)-C(27)-C(18)	119.4(8)
N(1)-C(1)-C(10)	113.2(6)	C(33)-C(28)-C(29)	118.1(7)
C(2)-C(1)-C(10)	118.6(7)	C(33)-C(28)-N(4)	124.1(7)
O(1)-C(2)-C(1)	126.8(7)	C(29)-C(28)-N(4)	117.7(7)
O(1)-C(2)-C(3)	115.5(7)	C(30)-C(29)-C(28)	120.2(8)
C(1)-C(2)-C(3)	117.7(8)	C(30)-C(29)-S(2)	120.9(7)
C(4)-C(3)-C(2)	123.5(9)	C(28)-C(29)-S(2)	118.9(6)
C(4)-C(3)-H(3)	118.3	C(31)-C(30)-C(29)	120.6(9)
C(2)-C(3)-H(3)	118.3	C(31)-C(30)-H(30)	119.7
C(3)-C(4)-C(9)	121.4(8)	C(29)-C(30)-H(30)	119.7
C(3)-C(4)-H(4)	119.3	C(30)-C(31)-C(32)	119.8(9)
C(9)-C(4)-H(4)	119.3	C(30)-C(31)-H(31)	120.1
C(6)-C(5)-C(9)	120.8(10)	C(32)-C(31)-H(31)	120.1
C(6)-C(5)-H(5)	119.6	C(31)-C(32)-C(33)	121.1(9)
C(9)-C(5)-H(5)	119.6	C(31)-C(32)-H(32)	119.4
C(5)-C(6)-C(7)	120.8(10)	C(33)-C(32)-H(32)	119.4
C(5)-C(6)-H(6)	119.6	C(32)-C(33)-C(28)	120.1(9)
C(7)-C(6)-H(6)	119.6	C(32)-C(33)-H(33)	119.9
C(8)-C(7)-C(6)	119.9(11)	C(28)-C(33)-H(33)	119.9
C(8)-C(7)-H(7)	120.0	N(2)-Ru(1)-N(4)	178.1(2)
C(6)-C(7)-H(7)	120.0	N(2)-Ru(1)-O(2)	86.6(2)
C(7)-C(8)-C(10)	119.5(9)	N(4)-Ru(1)-O(2)	91.5(2)
C(7)-C(8)-H(8)	120.2	N(2)-Ru(1)-O(1)	92.2(2)
C(10)-C(8)-H(8)	120.2	N(4)-Ru(1)-O(1)	87.2(2)
C(5)-C(9)-C(10)	120.4(9)	O(2)-Ru(1)-O(1)	86.7(2)
C(5)-C(9)-C(4)	121.4(9)	N(2)-Ru(1)-S(1)	85.37(19)
C(10)-C(9)-C(4)	118.3(8)	N(4)-Ru(1)-S(1)	95.27(18)
C(9)-C(10)-C(8)	118.6(8)	O(2)-Ru(1)-S(1)	92.99(18)
C(9)-C(10)-C(1)	120.5(8)	O(1)-Ru(1)-S(1)	177.53(16)
C(8)-C(10)-C(1)	120.9(8)	N(2)-Ru(1)-S(2)	96.28(19)
C(16)-C(11)-C(12)	117.8(7)	N(4)-Ru(1)-S(2)	85.57(19)
C(16)-C(11)-N(2)	124.2(8)	O(2)-Ru(1)-S(2)	177.03(16)
C(12)-C(11)-N(2)	118.0(7)	O(1)-Ru(1)-S(2)	92.68(16)
C(13)-C(12)-C(11)	120.2(8)	S(1)-Ru(1)-S(2)	87.77(10)
C(13)-C(12)-S(1)	121.6(8)	N(2)-N(1)-C(1)	122.5(6)
C(11)-C(12)-S(1)	118.2(6)	N(1)-N(2)-C(1)	112.9(6)
C(14)-C(13)-C(12)	121.6(10)	N(1)-N(2)-Ru(1)	128.2(5)
C(14)-C(13)-H(13)	119.2	C(11)-N(2)-Ru(1)	118.9(5)
C(12)-C(13)-H(13)	119.2	N(4)-N(3)-C(18)	121.3(6)
C(12)-S(1)-Ru(1)	99.2(3)	N(3)-N(4)-C(28)	112.7(6)
C(17)-S(1)-Ru(1)	110.7(4)	N(3)-N(4)-Ru(1)	128.4(5)
C(29)-S(2)-C(34)	100.7(4)	C(28)-N(4)-Ru(1)	118.9(5)
C(29)-S(2)-Ru(1)	98.1(3)	C(2)-O(1)-Ru(1)	122.0(5)
C(34)-S(2)-Ru(1)	111.8(3)	C(19)-O(2)-Ru(1)	123.1(5)
		C(12)-S(1)-C(17)	99.4(5)

Table 18.

Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for $[\text{Ru}(\text{L}^1)_2]$ (11)

	x	y	z	U(eq)
C(17)	837(10)	2079(4)	3656(16)	112(5)
C(18)	466(6)	919(2)	8208(9)	44(2)
C(19)	1001(7)	1237(3)	6276(10)	51(2)
C(20)	447(9)	1353(3)	7470(12)	70(3)

C(21)	-494(9)	1159(3)	7656(12)	73(3)
C(34)	4948(8)	763(3)	3540(12)	78(3)
O(10)	8354(19)	2277(6)	5590(30)	285(9)
O(51)	6743(11)	1791(5)	4633(18)	201(6)
C(1)	5080(6)	1230(2)	7646(9)	40(2)
C(2)	4453(7)	855(3)	7136(9)	44(2)
C(3)	4852(7)	472(3)	7909(10)	51(2)
C(4)	5741(8)	451(3)	9125(11)	61(3)
C(5)	7322(9)	793(4)	10956(12)	76(3)
C(6)	7961(10)	1137(5)	11448(13)	96(4)
C(7)	7681(10)	1530(4)	10734(13)	90(4)
C(8)	6732(8)	1566(3)	9512(11)	68(3)
C(9)	6391(7)	816(3)	9704(10)	55(2)
C(10)	6074(7)	1204(3)	8962(9)	49(2)
C(11)	3980(7)	2160(2)	5549(9)	45(2)
C(12)	3082(8)	2296(3)	4316(10)	52(2)
C(13)	2965(9)	2720(3)	3932(11)	63(3)
C(14)	3703(9)	3018(3)	4720(13)	66(3)
C(15)	4560(9)	2890(3)	5927(13)	68(3)
C(16)	4723(8)	2466(3)	6349(11)	55(2)
C(22)	-2010(8)	608(4)	6935(13)	79(3)
C(23)	-2448(9)	264(3)	6005(14)	76(3)
C(24)	-1996(7)	132(3)	4848(12)	65(3)
C(25)	-1055(7)	350(3)	4559(10)	55(2)
C(26)	-1027(7)	830(3)	6688(10)	58(2)
C(27)	-546(7)	700(3)	5458(10)	52(2)
C(28)	1759(7)	768(2)	2070(9)	44(2)
C(29)	2768(7)	862(2)	1619(9)	45(2)
C(30)	2906(8)	725(3)	220(10)	60(2)
C(31)	2075(10)	500(3)	-729(11)	72(3)
C(32)	1090(9)	405(3)	-302(11)	68(3)
C(33)	917(8)	540(3)	1074(9)	54(2)
Ruf(1)	2868(1)	1325(1)	4694(1)	41(1)
N(1)	4879(5)	1634(2)	7060(7)	43(2)
N(2)	4049(5)	1721(2)	5921(7)	42(2)
N(3)	752(5)	784(2)	3897(7)	42(2)
N(4)	1653(5)	926(2)	3518(7)	41(2)
O(1)	3541(5)	822(2)	6018(6)	46(1)
O(2)	1936(5)	1440(2)	6254(6)	52(1)
S(1)	2163(2)	1913(1)	3269(3)	68(1)
S(2)	3858(2)	1168(1)	2873(3)	52(1)

