"Ruthenium Benzylidene and Vinylidene Complexes in a Sulfur-rich Coordination Environment"
W.-H. Leung et al.

Supporting Information I

Experimental Details and Crystal Data for $Ru(=CHPh)[N(PPh_2S)_2]_2$ 1

Empirical formula	$C_{55}H_{46}N_2P_4RuS_4$
Formula weight	1088.19
Color; habit	red; block
Crystal dimensions, mm	0.12x0.13x0.22
Crystal system	triclinic
Lattice type	primitive
a, Å	10.066(1)
b, Å	11.213(1)
c, Å	13.687(1)
α, deg	69.54(2)
β, deg	69.98(2)
γ, deg	61.37(2)
V, Å^3	1241.4(4)
Space group	*P* 1 (No. 1)
Z	1
Dcald, g cm^{-3}	1.456
Diffractometer	MAR-Research Image Plate
Radiation	MoKα, graphite-monochromated (λ 0.71073 Å)
F(000)	558
μ(MoKα), cm^{-1}	6.53
Temperature, °C	25
scan type	ω
$2\theta_{max}$, deg	50.3
No. of reflections measured	4469
No. of unique reflections	2670 (R_{int} = 0.062)
Corrections	Lorentz-polarization (inter-image scaling)
Structure solution	Direct methods
Program used	TEXSAN
Refinement	Full-matrix least-squares
Function minimized	$\Sigma w (\|F_o\| - \|F_c\|)^2$
Weighing factor	$w^{-1} = \sigma^2(F_o) + 0.02xF_o^2/4$
No. of observation	1920 ($I > 1.50\ \sigma(I)$)
No. of variables	317
Reflection/Parameter ratio	6.06
R, Rw	0.069, 0.070
Goodness of fit	1.11
Max. peak in final diff map, e$^-$/ Å^3	0.84
Min. peak in final diff map, e$^-$/ Å^3	-0.68

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Ru(1)	0.9434	0.7519	0.4799	3.36(4)
S(1)	1.0280(8)	0.5406(8)	0.4271(6)	4.2(2)
S(2)	1.0356(7)	0.8859(7)	0.3147(6)	2.8(2)
S(3)	0.9169(6)	0.9431(7)	0.5364(6)	3.4(2)
S(4)	0.9167(8)	0.6003(7)	0.6505(6)	3.9(2)
P(1)	1.1889(6)	0.5188(7)	0.2891(6)	2.7(2)
P(2)	1.0590(7)	0.8116(8)	0.1907(6)	2.7(2)
P(3)	0.7572(7)	0.9700(7)	0.6744(6)	2.7(2)
P(4)	0.8849(7)	0.6783(8)	0.7727(6)	2.5(2)
N(1)	1.170(2)	0.652(2)	0.193(2)	3.3(6)
N(2)	0.768(2)	0.836(2)	0.772(2)	2.3(5)
C(1)	1.384(3)	0.453(3)	0.311(2)	3.8(5)
C(2)	1.474(2)	0.307(2)	0.337(2)	3.5(5)
C(3)	1.622(3)	0.268(3)	0.356(2)	4.6(5)
C(4)	1.677(3)	0.361(3)	0.344(2)	4.4(5)
C(5)	1.585(3)	0.492(3)	0.322(3)	5.6(6)
C(6)	1.445(3)	0.539(3)	0.303(2)	4.1(5)
C(7)	1.183(2)	0.387(2)	0.246(2)	2.9(5)
C(8)	1.133(2)	0.285(3)	0.320(2)	4.1(5)
C(9)	1.132(3)	0.188(3)	0.282(2)	5.5(6)
C(10)	1.177(3)	0.191(3)	0.174(3)	5.5(6)
C(11)	1.230(3)	0.285(3)	0.099(2)	5.0(6)
C(12)	1.227(2)	0.391(2)	0.138(2)	2.9(5)
C(13)	1.148(2)	0.917(2)	0.068(2)	2.6(5)

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C(14)	1.298(3)	0.874(3)	0.046(2)	4.0(5)
C(15)	1.366(3)	0.951(3)	-0.038(2)	3.8(5)
C(16)	1.280(2)	1.070(2)	-0.097(2)	3.0(5)
C(17)	1.126(3)	1.115(3)	-0.077(2)	5.0(6)
C(18)	1.055(3)	1.031(3)	0.014(2)	4.5(6)
C(19)	0.874(2)	0.852(3)	0.175(2)	3.2(5)
C(20)	0.746(3)	0.976(3)	0.188(2)	4.8(6)
C(21)	0.602(3)	1.014(3)	0.169(2)	4.8(5)
C(22)	0.591(3)	0.913(3)	0.139(3)	6.0(6)
C(23)	0.707(3)	0.796(4)	0.121(3)	6.9(7)
C(24)	0.853(3)	0.765(3)	0.138(2)	5.0(6)
C(25)	0.560(2)	1.053(2)	0.651(2)	2.7(4)
C(26)	0.490(3)	1.194(3)	0.621(2)	4.1(5)
C(27)	0.334(3)	1.252(3)	0.602(2)	5.0(6)
C(28)	0.272(3)	1.164(3)	0.617(2)	5.8(6)
C(29)	0.338(4)	1.024(4)	0.645(3)	7.0(7)
C(30)	0.495(3)	0.962(3)	0.662(2)	4.6(6)
C(31)	0.769(2)	1.098(2)	0.723(2)	2.7(5)
C(32)	0.828(3)	1.194(3)	0.652(2)	4.6(5)
C(33)	0.830(3)	1.292(3)	0.690(2)	4.2(5)
C(34)	0.776(3)	1.292(3)	0.796(2)	4.3(5)
C(35)	0.723(3)	1.197(3)	0.865(2)	5.1(6)
C(36)	0.717(3)	1.100(3)	0.829(2)	4.3(6)
C(37)	0.804(2)	0.581(2)	0.889(2)	2.8(5)

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C(38)	0.889(3)	0.475(3)	0.963(2)	4.8(6)
C(39)	0.821(4)	0.402(3)	1.050(3)	7.1(7)
C(40)	0.675(3)	0.423(3)	1.068(2)	4.9(6)
C(41)	0.582(3)	0.533(3)	1.003(3)	5.4(6)
C(42)	0.646(3)	0.615(3)	0.912(2)	4.2(5)
C(43)	1.072(2)	0.639(2)	0.789(2)	3.2(5)
C(44)	1.197(3)	0.511(3)	0.771(2)	4.7(6)
C(45)	1.337(4)	0.482(4)	0.793(3)	7.8(7)
C(46)	1.357(3)	0.560(3)	0.827(3)	6.6(7)
C(47)	1.244(4)	0.692(4)	0.841(3)	7.8(7)
C(48)	1.090(3)	0.727(3)	0.826(2)	4.8(6)
C(49)	0.739(2)	0.835(2)	0.460(2)	2.7(4)
C(50)	0.630(2)	0.779(2)	0.475(2)	3.8(5)
C(51)	0.639(2)	0.648(2)	0.529(2)	4.3(5)
C(52)	0.517(3)	0.608(3)	0.544(2)	5.9(6)
C(53)	0.380(3)	0.703(3)	0.512(2)	5.8(6)
C(54)	0.367(3)	0.830(3)	0.460(3)	7.1(7)
C(55)	0.490(3)	0.869(3)	0.443(2)	4.7(5)
H(1)	1.4384	0.2402	0.3423	4.2657
H(2)	1.6846	0.1721	0.3766	5.5555
H(3)	1.7788	0.3322	0.3525	5.2345
H(4)	1.6195	0.5586	0.3189	6.6658
H(5)	1.3867	0.6370	0.2833	4.9573
H(6)	1.1003	0.2837	0.3938	4.9195

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ru(1)	0.062(1)	0.0291(9)	0.032(1)	-0.0215(9)	-0.0009(9)	-0.0057(7)
S(1)	0.074(4)	0.032(4)	0.037(5)	-0.026(4)	0.021(3)	-0.013(4)
S(2)	0.040(3)	0.041(4)	0.036(5)	-0.022(3)	-0.005(3)	-0.014(4)
S(3)	0.036(4)	0.037(5)	0.057(6)	-0.017(3)	0.002(3)	-0.020(4)
S(4)	0.092(5)	0.031(4)	0.034(5)	-0.033(4)	-0.022(4)	0.003(4)
P(1)	0.034(4)	0.027(4)	0.037(5)	-0.013(3)	-0.002(3)	-0.009(4)
P(2)	0.030(3)	0.034(4)	0.038(5)	-0.013(3)	-0.008(3)	-0.006(4)
P(3)	0.034(3)	0.031(4)	0.035(5)	-0.012(3)	-0.006(3)	-0.007(4)
P(4)	0.038(3)	0.031(4)	0.028(5)	-0.016(3)	-0.006(3)	-0.008(3)
N(1)	0.03(1)	0.03(1)	0.05(2)	-0.01(1)	-0.02(1)	0.00(1)
N(2)	0.03(1)	0.02(1)	0.03(1)	-0.010(9)	0.002(9)	0.00(1)

The general temperature factor expression:

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

Table 3. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
Ru(1)	S(1)	2.388(7)	Ru(1)	S(2)	2.399(8)
Ru(1)	S(3)	2.395(7)	Ru(1)	S(4)	2.376(8)
Ru(1)	C(49)	1.88(2)	S(1)	P(1)	2.024(9)
S(2)	P(2)	2.039(9)	S(3)	P(3)	2.024(10)
S(4)	P(4)	2.012(10)	P(1)	N(1)	1.59(2)
P(1)	C(1)	1.83(2)	P(1)	C(7)	1.80(2)
P(2)	N(1)	1.59(2)	P(2)	C(13)	1.90(2)
P(2)	C(19)	1.77(2)	P(3)	N(2)	1.61(2)
P(3)	C(25)	1.83(2)	P(3)	C(31)	1.84(2)
P(4)	N(2)	1.59(2)	P(4)	C(37)	1.77(3)
P(4)	C(43)	1.79(2)	C(1)	C(2)	1.43(3)
C(1)	C(6)	1.32(3)	C(2)	C(3)	1.42(3)
C(3)	C(4)	1.34(3)	C(4)	C(5)	1.30(3)
C(5)	C(6)	1.33(3)	C(7)	C(8)	1.41(3)
C(7)	C(12)	1.38(3)	C(8)	C(9)	1.36(3)
C(9)	C(10)	1.38(3)	C(10)	C(11)	1.36(4)
C(11)	C(12)	1.44(3)	C(13)	C(14)	1.30(3)
C(13)	C(18)	1.32(3)	C(14)	C(15)	1.36(3)
C(15)	C(16)	1.34(3)	C(16)	C(17)	1.33(3)
C(17)	C(18)	1.47(3)	C(19)	C(20)	1.39(3)
C(19)	C(24)	1.37(3)	C(20)	C(21)	1.39(3)
C(21)	C(22)	1.40(4)	C(22)	C(23)	1.31(4)
C(23)	C(24)	1.42(4)	C(25)	C(26)	1.36(3)
C(25)	C(30)	1.39(3)	C(26)	C(27)	1.46(3)

Table 3. Bond Lengths(Å) (continued)

atom	atom	distance	atom	atom	distance
C(27)	C(28)	1.32(3)	C(28)	C(29)	1.34(4)
C(29)	C(30)	1.45(4)	C(31)	C(32)	1.39(3)
C(31)	C(36)	1.37(3)	C(32)	C(33)	1.39(3)
C(33)	C(34)	1.36(3)	C(34)	C(35)	1.35(3)
C(35)	C(36)	1.37(3)	C(37)	C(38)	1.40(3)
C(37)	C(42)	1.39(3)	C(38)	C(39)	1.36(4)
C(39)	C(40)	1.32(3)	C(40)	C(41)	1.38(4)
C(41)	C(42)	1.42(4)	C(43)	C(44)	1.42(3)
C(43)	C(48)	1.36(3)	C(44)	C(45)	1.41(4)
C(45)	C(46)	1.24(4)	C(46)	C(47)	1.40(4)
C(47)	C(48)	1.47(4)	C(49)	C(50)	1.44(3)
C(50)	C(51)	1.37(3)	C(50)	C(55)	1.40(3)
C(51)	C(52)	1.43(3)	C(52)	C(53)	1.38(3)
C(53)	C(54)	1.32(3)	C(54)	C(55)	1.43(4)

Table 5. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
S(1)	Ru(1)	S(2)	99.8(2)	S(1)	Ru(1)	S(3)	167.3(2)
S(1)	Ru(1)	S(4)	80.2(2)	S(1)	Ru(1)	C(49)	98.2(6)
S(2)	Ru(1)	S(3)	78.4(2)	S(2)	Ru(1)	S(4)	165.2(2)
S(2)	Ru(1)	C(49)	94.3(6)	S(3)	Ru(1)	S(4)	98.3(3)
S(3)	Ru(1)	C(49)	94.5(6)	S(4)	Ru(1)	C(49)	100.3(6)
Ru(1)	S(1)	P(1)	115.2(4)	Ru(1)	S(2)	P(2)	109.7(4)
Ru(1)	S(3)	P(3)	111.1(4)	Ru(1)	S(4)	P(4)	114.3(4)
S(1)	P(1)	N(1)	118.1(9)	S(1)	P(1)	C(1)	111.3(9)
S(1)	P(1)	C(7)	105.6(8)	N(1)	P(1)	C(1)	105(1)
N(1)	P(1)	C(7)	108(1)	C(1)	P(1)	C(7)	107(1)
S(2)	P(2)	N(1)	116.6(9)	S(2)	P(2)	C(13)	104.6(8)
S(2)	P(2)	C(19)	109.8(8)	N(1)	P(2)	C(13)	106(1)
N(1)	P(2)	C(19)	111(1)	C(13)	P(2)	C(19)	107(1)
S(3)	P(3)	N(2)	118.5(8)	S(3)	P(3)	C(25)	111.0(8)
S(3)	P(3)	C(31)	107.7(8)	N(2)	P(3)	C(25)	107.2(10)
N(2)	P(3)	C(31)	107(1)	C(25)	P(3)	C(31)	104.3(10)
S(4)	P(4)	N(2)	118.0(8)	S(4)	P(4)	C(37)	106.3(8)
S(4)	P(4)	C(43)	107.8(8)	N(2)	P(4)	C(37)	104.7(10)
N(2)	P(4)	C(43)	113(1)	C(37)	P(4)	C(43)	105(1)
P(1)	N(1)	P(2)	130(1)	P(3)	N(2)	P(4)	127(1)
P(1)	C(1)	C(2)	119(1)	P(1)	C(1)	C(6)	121(2)
C(2)	C(1)	C(6)	118(2)	C(1)	C(2)	C(3)	115(2)
C(2)	C(3)	C(4)	123(2)	C(3)	C(4)	C(5)	116(2)
C(4)	C(5)	C(6)	124(2)	C(1)	C(6)	C(5)	121(2)

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
P(1)	C(7)	C(8)	120(1)	P(1)	C(7)	C(12)	117(1)
C(8)	C(7)	C(12)	121(2)	C(7)	C(8)	C(9)	118(2)
C(8)	C(9)	C(10)	120(2)	C(9)	C(10)	C(11)	123(2)
C(10)	C(11)	C(12)	116(2)	C(7)	C(12)	C(11)	119(2)
P(2)	C(13)	C(14)	117(1)	P(2)	C(13)	C(18)	118(1)
C(14)	C(13)	C(18)	124(2)	C(13)	C(14)	C(15)	118(2)
C(14)	C(15)	C(16)	121(2)	C(15)	C(16)	C(17)	121(2)
C(16)	C(17)	C(18)	117(2)	C(13)	C(18)	C(17)	117(2)
P(2)	C(19)	C(20)	123(1)	P(2)	C(19)	C(24)	120(1)
C(20)	C(19)	C(24)	115(2)	C(19)	C(20)	C(21)	124(2)
C(20)	C(21)	C(22)	114(2)	C(21)	C(22)	C(23)	124(2)
C(22)	C(23)	C(24)	118(3)	C(19)	C(24)	C(23)	122(2)
P(3)	C(25)	C(26)	119(1)	P(3)	C(25)	C(30)	115(1)
C(26)	C(25)	C(30)	124(1)	C(25)	C(26)	C(27)	116(2)
C(26)	C(27)	C(28)	118(2)	C(27)	C(28)	C(29)	127(2)
C(28)	C(29)	C(30)	116(2)	C(25)	C(30)	C(29)	117(2)
P(3)	C(31)	C(32)	120(1)	P(3)	C(31)	C(36)	119(2)
C(32)	C(31)	C(36)	120(2)	C(31)	C(32)	C(33)	119(2)
C(32)	C(33)	C(34)	119(2)	C(33)	C(34)	C(35)	121(2)
C(34)	C(35)	C(36)	120(2)	C(31)	C(36)	C(35)	119(2)
P(4)	C(37)	C(38)	123(1)	P(4)	C(37)	C(42)	119(1)
C(38)	C(37)	C(42)	117(2)	C(37)	C(38)	C(39)	121(2)
C(38)	C(39)	C(40)	122(2)	C(39)	C(40)	C(41)	119(2)
C(40)	C(41)	C(42)	120(2)	C(37)	C(42)	C(41)	118(2)

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
P(4)	C(43)	C(44)	119(1)	P(4)	C(43)	C(48)	119(1)
C(44)	C(43)	C(48)	120(2)	C(43)	C(44)	C(45)	116(2)
C(44)	C(45)	C(46)	124(3)	C(45)	C(46)	C(47)	123(3)
C(46)	C(47)	C(48)	115(2)	C(43)	C(48)	C(47)	119(2)
Ru(1)	C(49)	C(50)	132(1)	C(49)	C(50)	C(51)	126(1)
C(49)	C(50)	C(55)	118(1)	C(51)	C(50)	C(55)	114(2)
C(50)	C(51)	C(52)	121(2)	C(51)	C(52)	C(53)	121(2)
C(52)	C(53)	C(54)	118(2)	C(53)	C(54)	C(55)	119(2)
C(50)	C(55)	C(54)	124(2)				

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Supporting Information II

Experimental Details and Crystal Data for $Ru(=CHPh)[Ph_2PNP(Se)Ph_2]_2$ 4

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Formula weight	1117.87
Color; habit	red; block
Crystal dimensions, mm	0.14x0.12x0.06
Crystal system	triclinic
Lattice type	primitive
a, Å	10.986(1)
b, Å	11.401(1)
c, Å	21.140(2)
α, deg	86.24(1)
β, deg	82.78(1)
γ, deg	69.49(1)
V, Å^3	2459.7(4)
Space group	*P* -1 (No. 2)
Z	2
Dcald, g cm^{-3}	1.509
Diffractometer	Bruker SMART CCD
Radiation	MoKα, graphite-monochromated (λ 0.71073 Å)
F(000)	1124
μ(MoKα), cm^{-1}	19.68
Temperature, °C	25
scan type	ω
$2\theta_{max}$, deg	55.1
No. of reflections measured	28673
No. of unique reflections	11080 (R_{int} = 0.051)
Corrections	Lorentz-polarization (inter-image scaling)
Structure solution	Direct methods (SIR 92)
Program used	TEXSAN
Refinement	Full-matrix least-squares
Function minimized	$\Sigma\, w\, (\|F_o\| - \|F_c\|)^2$
Weighing factor	$w^{-1} = \sigma^2(F_o) + 0.038xF_o^2/4$
No. of observation	5513 ($I > 1.50\ \sigma(I)$)
No. of variables	557
Reflection/Parameter ratio	9.55
R, Rw	0.062, 0.054
Goodness of fit	1.04
Max. peak in final diff map, e$^-$/ Å^3	1.44
Min. peak in final diff map, e$^-$/ Å^3	-0.62

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Ru(1)	0.27008(7)	-0.00270(6)	0.26220(3)	3.31(2)
Se(1)	0.09457(9)	0.19927(8)	0.24494(4)	4.58(2)
Se(2)	0.35076(9)	-0.23016(8)	0.26431(4)	4.22(2)
P(1)	0.1765(2)	-0.0045(2)	0.37003(10)	3.37(5)
P(2)	0.0514(2)	0.2472(2)	0.3470(1)	3.65(5)
P(3)	0.3385(2)	-0.0031(2)	0.15064(10)	3.35(5)
P(4)	0.4203(2)	-0.2647(2)	0.16127(10)	3.48(5)
N(1)	0.0669(6)	0.1307(5)	0.3931(3)	3.5(2)
N(2)	0.4146(6)	-0.1437(6)	0.1214(3)	3.6(2)
C(1)	0.3989(8)	0.0455(7)	0.2917(4)	4.1(2)
C(2)	0.5336(9)	0.0300(9)	0.2673(4)	4.7(3)
C(3)	0.615(1)	-0.066(1)	0.2291(5)	6.9(3)
C(4)	0.741(1)	-0.071(2)	0.2072(5)	10.2(5)
C(5)	0.784(1)	0.021(2)	0.2239(6)	11.6(6)
C(6)	0.710(1)	0.110(2)	0.2647(7)	10.3(6)
C(7)	0.582(1)	0.120(1)	0.2870(4)	6.6(3)
C(8)	0.0899(8)	-0.1161(8)	0.3853(4)	3.9(2)
C(9)	0.1162(9)	-0.2096(9)	0.4291(5)	5.9(3)
C(10)	0.047(1)	-0.2900(10)	0.4384(6)	7.4(4)
C(11)	-0.051(1)	-0.278(1)	0.4011(6)	7.2(4)
C(12)	-0.078(1)	-0.188(1)	0.3561(5)	7.7(4)
C(13)	-0.009(1)	-0.1027(10)	0.3475(4)	6.3(3)
C(14)	0.2901(8)	-0.0536(7)	0.4309(4)	3.7(2)
C(15)	0.4157(9)	-0.1315(8)	0.4182(4)	4.6(2)

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C(16)	0.5003(9)	-0.1699(8)	0.4653(5)	5.2(3)
C(17)	0.456(1)	-0.1303(9)	0.5262(5)	6.1(3)
C(18)	0.331(1)	-0.0516(9)	0.5406(4)	5.7(3)
C(19)	0.2452(8)	-0.0130(7)	0.4935(4)	4.3(2)
C(20)	-0.1146(8)	0.3571(7)	0.3596(4)	3.4(2)
C(21)	-0.1506(9)	0.4746(8)	0.3314(4)	5.3(3)
C(22)	-0.279(1)	0.5564(9)	0.3413(6)	6.6(3)
C(23)	-0.3695(10)	0.522(1)	0.3781(6)	7.2(3)
C(24)	-0.3353(10)	0.404(1)	0.4074(6)	7.8(4)
C(25)	-0.2064(9)	0.3217(8)	0.3977(5)	5.7(3)
C(26)	0.1558(8)	0.3343(7)	0.3624(5)	4.3(2)
C(27)	0.184(1)	0.3336(9)	0.4237(5)	6.3(3)
C(28)	0.259(1)	0.399(1)	0.4402(7)	8.8(4)
C(29)	0.308(1)	0.465(1)	0.394(1)	10.6(6)
C(30)	0.288(2)	0.462(1)	0.3328(9)	11.1(6)
C(31)	0.206(1)	0.3997(10)	0.3149(5)	7.2(3)
C(32)	0.4404(8)	0.0890(7)	0.1210(3)	3.5(2)
C(33)	0.4171(8)	0.2048(8)	0.1465(4)	4.5(2)
C(34)	0.497(1)	0.2736(8)	0.1250(5)	5.6(3)
C(35)	0.599(1)	0.229(1)	0.0797(5)	5.8(3)
C(36)	0.6228(9)	0.115(1)	0.0528(4)	6.0(3)
C(37)	0.5432(9)	0.0446(8)	0.0742(4)	4.7(2)
C(38)	0.1970(8)	0.0665(7)	0.1035(4)	3.8(2)
C(39)	0.1827(9)	0.1652(9)	0.0621(4)	5.1(3)

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C(40)	0.076(1)	0.2116(10)	0.0285(5)	6.8(3)
C(41)	-0.0207(10)	0.159(1)	0.0368(5)	6.2(3)
C(42)	-0.0070(9)	0.061(1)	0.0781(5)	6.3(3)
C(43)	0.1009(9)	0.0134(9)	0.1117(4)	5.7(3)
C(44)	0.3254(8)	-0.3472(7)	0.1307(4)	3.9(2)
C(45)	0.220(1)	-0.366(1)	0.1656(5)	7.1(3)
C(46)	0.151(1)	-0.430(1)	0.1384(6)	8.6(4)
C(47)	0.188(1)	-0.470(1)	0.0783(6)	6.7(4)
C(48)	0.289(1)	-0.4491(10)	0.0429(5)	6.1(3)
C(49)	0.3566(9)	-0.3874(9)	0.0700(4)	5.3(3)
C(50)	0.5851(8)	-0.3774(8)	0.1535(4)	3.9(2)
C(51)	0.6164(9)	-0.4879(8)	0.1849(4)	4.8(2)
C(52)	0.744(1)	-0.5729(8)	0.1785(5)	6.3(3)
C(53)	0.8402(10)	-0.546(1)	0.1415(6)	6.3(3)
C(54)	0.8088(10)	-0.436(1)	0.1087(5)	7.7(4)
C(55)	0.6814(9)	-0.3478(9)	0.1149(5)	6.0(3)
H(1)	0.3704	0.0893	0.3308	4.9087
H(2)	0.5844	-0.1293	0.2175	8.1948
H(3)	0.7963	-0.1374	0.1808	12.1084
H(4)	0.8682	0.0214	0.2063	13.8331
H(5)	0.7456	0.1681	0.2786	12.2562
H(6)	0.5287	0.1856	0.3148	7.8968
H(7)	0.1852	-0.2205	0.4547	6.9946
H(8)	0.0679	-0.3547	0.4704	8.7726

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ru(1)	0.0388(4)	0.0405(4)	0.0438(4)	-0.0105(3)	-0.0034(3)	-0.0023(3)
Se(1)	0.0575(6)	0.0526(6)	0.0480(5)	0.0004(5)	-0.0056(5)	0.0012(4)
Se(2)	0.0640(7)	0.0436(5)	0.0480(5)	-0.0140(5)	-0.0019(5)	-0.0010(4)
P(1)	0.040(1)	0.041(1)	0.043(1)	-0.009(1)	-0.002(1)	-0.004(1)
P(2)	0.039(1)	0.041(1)	0.051(1)	-0.006(1)	-0.002(1)	-0.002(1)
P(3)	0.040(1)	0.042(1)	0.044(1)	-0.013(1)	-0.003(1)	-0.001(1)
P(4)	0.041(1)	0.044(1)	0.047(1)	-0.012(1)	-0.006(1)	-0.007(1)
N(1)	0.042(4)	0.041(4)	0.045(4)	-0.011(3)	0.004(3)	-0.008(3)
N(2)	0.047(4)	0.048(4)	0.041(4)	-0.018(4)	-0.002(3)	-0.001(3)
C(1)	0.052(6)	0.052(5)	0.058(6)	-0.024(5)	-0.010(5)	-0.001(4)
C(2)	0.055(6)	0.084(7)	0.046(6)	-0.032(6)	-0.020(5)	0.019(5)
C(3)	0.046(7)	0.16(1)	0.059(7)	-0.032(7)	-0.015(5)	-0.008(7)
C(4)	0.051(8)	0.26(2)	0.066(8)	-0.043(10)	-0.010(6)	-0.024(9)
C(5)	0.07(1)	0.33(3)	0.061(9)	-0.10(1)	-0.018(7)	0.04(1)
C(6)	0.11(1)	0.24(2)	0.09(1)	-0.13(1)	-0.054(9)	0.07(1)
C(7)	0.095(9)	0.118(9)	0.070(7)	-0.070(8)	-0.039(6)	0.029(6)
C(8)	0.046(6)	0.055(6)	0.046(5)	-0.016(5)	-0.001(4)	-0.002(4)
C(9)	0.067(7)	0.061(6)	0.099(8)	-0.031(6)	-0.013(6)	0.023(6)
C(10)	0.087(9)	0.064(7)	0.12(1)	-0.026(7)	0.005(8)	0.016(7)
C(11)	0.11(1)	0.082(9)	0.100(10)	-0.063(9)	0.017(8)	-0.012(7)
C(12)	0.097(9)	0.14(1)	0.089(9)	-0.079(9)	-0.011(7)	-0.020(8)
C(13)	0.094(9)	0.103(8)	0.065(7)	-0.060(7)	-0.025(6)	0.022(6)
C(14)	0.044(5)	0.049(5)	0.045(5)	-0.012(4)	-0.008(4)	-0.004(4)
C(15)	0.054(6)	0.061(6)	0.052(6)	-0.009(5)	-0.009(5)	-0.006(5)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(16)	0.051(6)	0.061(6)	0.077(7)	-0.003(5)	-0.021(5)	-0.005(5)
C(17)	0.081(8)	0.075(7)	0.065(7)	-0.007(6)	-0.027(6)	-0.007(6)
C(18)	0.085(8)	0.079(7)	0.044(6)	-0.016(6)	-0.007(6)	-0.011(5)
C(19)	0.046(6)	0.055(6)	0.054(6)	-0.007(5)	-0.009(5)	0.003(5)
C(20)	0.035(5)	0.045(5)	0.047(5)	-0.010(4)	-0.003(4)	-0.011(4)
C(21)	0.055(7)	0.053(6)	0.090(7)	-0.016(5)	-0.008(6)	0.005(5)
C(22)	0.063(8)	0.050(6)	0.13(1)	-0.004(6)	-0.025(7)	0.003(6)
C(23)	0.038(6)	0.075(8)	0.15(1)	-0.001(6)	-0.012(7)	-0.011(8)
C(24)	0.052(7)	0.085(9)	0.15(1)	-0.017(7)	0.001(7)	0.020(8)
C(25)	0.042(6)	0.063(7)	0.101(8)	-0.007(5)	0.000(6)	0.007(6)
C(26)	0.041(5)	0.040(5)	0.081(7)	-0.010(4)	-0.007(5)	-0.004(5)
C(27)	0.081(8)	0.064(7)	0.107(9)	-0.034(6)	-0.043(7)	0.017(6)
C(28)	0.10(1)	0.072(8)	0.19(1)	-0.028(7)	-0.091(10)	0.005(8)
C(29)	0.058(9)	0.09(1)	0.27(2)	-0.030(8)	-0.05(1)	0.00(1)
C(30)	0.11(1)	0.09(1)	0.23(2)	-0.07(1)	0.05(1)	-0.03(1)
C(31)	0.094(9)	0.071(7)	0.105(9)	-0.031(7)	0.014(7)	-0.001(7)
C(32)	0.047(5)	0.049(5)	0.037(5)	-0.017(5)	-0.010(4)	0.007(4)
C(33)	0.065(6)	0.054(6)	0.051(5)	-0.023(5)	0.000(5)	-0.001(4)
C(34)	0.093(8)	0.055(6)	0.080(7)	-0.042(6)	-0.018(6)	-0.002(5)
C(35)	0.081(8)	0.102(9)	0.064(7)	-0.062(7)	-0.012(6)	0.009(6)
C(36)	0.065(7)	0.106(9)	0.066(7)	-0.044(7)	0.005(5)	-0.006(6)
C(37)	0.060(6)	0.078(7)	0.046(5)	-0.029(6)	0.001(5)	-0.008(5)
C(38)	0.052(6)	0.052(5)	0.039(5)	-0.019(5)	-0.008(4)	0.000(4)
C(39)	0.058(6)	0.072(7)	0.067(6)	-0.027(5)	-0.019(5)	0.015(5)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(40)	0.085(9)	0.085(8)	0.083(8)	-0.017(7)	-0.033(7)	0.023(6)
C(41)	0.058(7)	0.107(9)	0.068(7)	-0.016(7)	-0.028(6)	0.003(6)
C(42)	0.053(7)	0.112(9)	0.083(8)	-0.034(7)	-0.021(6)	-0.003(7)
C(43)	0.057(7)	0.088(8)	0.077(7)	-0.033(6)	-0.022(6)	0.021(6)
C(44)	0.041(5)	0.050(5)	0.061(6)	-0.018(5)	-0.005(5)	-0.008(4)
C(45)	0.075(8)	0.13(1)	0.087(8)	-0.063(8)	0.005(6)	-0.024(7)
C(46)	0.079(9)	0.16(1)	0.13(1)	-0.093(9)	0.006(8)	-0.016(9)
C(47)	0.093(9)	0.088(8)	0.097(9)	-0.048(8)	-0.043(8)	-0.001(7)
C(48)	0.075(8)	0.087(8)	0.079(8)	-0.033(7)	-0.021(6)	-0.017(6)
C(49)	0.062(7)	0.074(7)	0.073(7)	-0.031(6)	-0.008(5)	-0.015(5)
C(50)	0.041(5)	0.052(6)	0.053(6)	-0.009(5)	-0.007(4)	-0.020(4)
C(51)	0.049(6)	0.043(6)	0.086(7)	-0.010(5)	-0.009(5)	0.000(5)
C(52)	0.070(8)	0.049(6)	0.120(10)	-0.016(6)	-0.030(7)	0.015(6)
C(53)	0.052(7)	0.073(8)	0.102(9)	0.001(6)	-0.024(6)	-0.007(7)
C(54)	0.044(7)	0.12(1)	0.112(10)	-0.019(7)	0.014(6)	0.014(8)
C(55)	0.050(7)	0.076(7)	0.085(8)	-0.008(6)	0.008(6)	0.012(6)

The general temperature factor expression:

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

Table 3. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
Ru(1)	Se(1)	2.471(1)	Ru(1)	Se(2)	2.428(1)
Ru(1)	P(1)	2.382(2)	Ru(1)	P(3)	2.383(2)
Ru(1)	C(1)	1.873(8)	Se(1)	P(2)	2.213(2)
Se(2)	P(4)	2.228(2)	P(1)	N(1)	1.647(6)
P(1)	C(8)	1.828(8)	P(1)	C(14)	1.829(8)
P(2)	N(1)	1.568(6)	P(2)	C(20)	1.812(8)
P(2)	C(26)	1.828(9)	P(3)	N(2)	1.647(6)
P(3)	C(32)	1.820(8)	P(3)	C(38)	1.860(8)
P(4)	N(2)	1.555(6)	P(4)	C(44)	1.824(8)
P(4)	C(50)	1.812(8)	C(1)	C(2)	1.46(1)
C(2)	C(3)	1.38(1)	C(2)	C(7)	1.42(1)
C(3)	C(4)	1.38(1)	C(4)	C(5)	1.38(2)
C(5)	C(6)	1.34(2)	C(6)	C(7)	1.40(1)
C(8)	C(9)	1.34(1)	C(8)	C(13)	1.39(1)
C(9)	C(10)	1.37(1)	C(10)	C(11)	1.38(1)
C(11)	C(12)	1.33(1)	C(12)	C(13)	1.42(1)
C(14)	C(15)	1.36(1)	C(14)	C(19)	1.40(1)
C(15)	C(16)	1.39(1)	C(16)	C(17)	1.36(1)
C(17)	C(18)	1.36(1)	C(18)	C(19)	1.40(1)
C(20)	C(21)	1.37(1)	C(20)	C(25)	1.37(1)
C(21)	C(22)	1.39(1)	C(22)	C(23)	1.34(1)
C(23)	C(24)	1.38(1)	C(24)	C(25)	1.40(1)
C(26)	C(27)	1.37(1)	C(26)	C(31)	1.39(1)
C(27)	C(28)	1.38(1)	C(28)	C(29)	1.36(2)

Table 3. Bond Lengths($\AA$) (continued)

atom	atom	distance	atom	atom	distance
C(29)	C(30)	1.34(2)	C(30)	C(31)	1.42(2)
C(32)	C(33)	1.39(1)	C(32)	C(37)	1.38(1)
C(33)	C(34)	1.39(1)	C(34)	C(35)	1.35(1)
C(35)	C(36)	1.38(1)	C(36)	C(37)	1.40(1)
C(38)	C(39)	1.36(1)	C(38)	C(43)	1.38(1)
C(39)	C(40)	1.38(1)	C(40)	C(41)	1.37(1)
C(41)	C(42)	1.36(1)	C(42)	C(43)	1.38(1)
C(44)	C(45)	1.37(1)	C(44)	C(49)	1.35(1)
C(45)	C(46)	1.40(1)	C(46)	C(47)	1.34(1)
C(47)	C(48)	1.35(1)	C(48)	C(49)	1.38(1)
C(50)	C(51)	1.34(1)	C(50)	C(55)	1.38(1)
C(51)	C(52)	1.39(1)	C(52)	C(53)	1.35(1)
C(53)	C(54)	1.35(1)	C(54)	C(55)	1.40(1)

Table 5. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
Se(1)	Ru(1)	Se(2)	150.28(4)	Se(1)	Ru(1)	P(1)	88.76(6)
Se(1)	Ru(1)	P(3)	88.14(6)	Se(1)	Ru(1)	C(1)	103.2(2)
Se(2)	Ru(1)	P(1)	89.68(6)	Se(2)	Ru(1)	P(3)	89.69(6)
Se(2)	Ru(1)	C(1)	106.4(2)	P(1)	Ru(1)	P(3)	172.61(8)
P(1)	Ru(1)	C(1)	88.0(3)	P(3)	Ru(1)	C(1)	99.2(3)
Ru(1)	Se(1)	P(2)	94.68(6)	Ru(1)	Se(2)	P(4)	99.73(6)
Ru(1)	P(1)	N(1)	114.0(2)	Ru(1)	P(1)	C(8)	113.0(3)
Ru(1)	P(1)	C(14)	116.7(3)	N(1)	P(1)	C(8)	104.4(3)
N(1)	P(1)	C(14)	106.0(3)	C(8)	P(1)	C(14)	101.3(4)
Se(1)	P(2)	N(1)	113.5(2)	Se(1)	P(2)	C(20)	108.1(3)
Se(1)	P(2)	C(26)	107.3(3)	N(1)	P(2)	C(20)	109.6(4)
N(1)	P(2)	C(26)	112.5(4)	C(20)	P(2)	C(26)	105.5(4)
Ru(1)	P(3)	N(2)	114.3(2)	Ru(1)	P(3)	C(32)	118.0(3)
Ru(1)	P(3)	C(38)	111.6(3)	N(2)	P(3)	C(32)	105.7(3)
N(2)	P(3)	C(38)	104.4(3)	C(32)	P(3)	C(38)	101.3(4)
Se(2)	P(4)	N(2)	113.6(3)	Se(2)	P(4)	C(44)	107.9(3)
Se(2)	P(4)	C(50)	109.2(3)	N(2)	P(4)	C(44)	112.0(4)
N(2)	P(4)	C(50)	110.3(4)	C(44)	P(4)	C(50)	103.3(4)
P(1)	N(1)	P(2)	117.8(4)	P(3)	N(2)	P(4)	121.9(4)
Ru(1)	C(1)	C(2)	133.3(7)	C(1)	C(2)	C(3)	124.9(9)
C(1)	C(2)	C(7)	115.6(10)	C(3)	C(2)	C(7)	119.5(9)
C(2)	C(3)	C(4)	120(1)	C(3)	C(4)	C(5)	119(1)
C(4)	C(5)	C(6)	120(1)	C(5)	C(6)	C(7)	121(1)
C(2)	C(7)	C(6)	117(1)	P(1)	C(8)	C(9)	125.0(7)

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
P(1)	C(8)	C(13)	116.6(7)	C(9)	C(8)	C(13)	118.4(8)
C(8)	C(9)	C(10)	122.2(10)	C(9)	C(10)	C(11)	120(1)
C(10)	C(11)	C(12)	119(1)	C(11)	C(12)	C(13)	120(1)
C(8)	C(13)	C(12)	119.2(9)	P(1)	C(14)	C(15)	122.4(6)
P(1)	C(14)	C(19)	119.1(6)	C(15)	C(14)	C(19)	118.5(7)
C(14)	C(15)	C(16)	121.7(8)	C(15)	C(16)	C(17)	119.5(8)
C(16)	C(17)	C(18)	120.4(9)	C(17)	C(18)	C(19)	120.4(8)
C(14)	C(19)	C(18)	119.4(8)	P(2)	C(20)	C(21)	121.7(7)
P(2)	C(20)	C(25)	119.1(7)	C(21)	C(20)	C(25)	119.2(8)
C(20)	C(21)	C(22)	120.4(9)	C(21)	C(22)	C(23)	120.5(9)
C(22)	C(23)	C(24)	120.1(10)	C(23)	C(24)	C(25)	119.6(10)
C(20)	C(25)	C(24)	120.1(9)	P(2)	C(26)	C(27)	117.4(7)
P(2)	C(26)	C(31)	122.7(8)	C(27)	C(26)	C(31)	119.8(9)
C(26)	C(27)	C(28)	121(1)	C(27)	C(28)	C(29)	118(1)
C(28)	C(29)	C(30)	120(1)	C(29)	C(30)	C(31)	121(1)
C(26)	C(31)	C(30)	117(1)	P(3)	C(32)	C(33)	120.1(6)
P(3)	C(32)	C(37)	121.1(7)	C(33)	C(32)	C(37)	118.8(8)
C(32)	C(33)	C(34)	120.0(8)	C(33)	C(34)	C(35)	121.3(9)
C(34)	C(35)	C(36)	119.6(9)	C(35)	C(36)	C(37)	119.7(9)
C(32)	C(37)	C(36)	120.5(8)	P(3)	C(38)	C(39)	124.4(7)
P(3)	C(38)	C(43)	117.2(6)	C(39)	C(38)	C(43)	118.4(8)
C(38)	C(39)	C(40)	121.3(9)	C(39)	C(40)	C(41)	120.4(9)
C(40)	C(41)	C(42)	118.6(9)	C(41)	C(42)	C(43)	121.1(10)
C(38)	C(43)	C(42)	120.2(9)	P(4)	C(44)	C(45)	123.0(7)

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
P(4)	C(44)	C(49)	119.0(7)	C(45)	C(44)	C(49)	117.9(8)
C(44)	C(45)	C(46)	119.5(9)	C(45)	C(46)	C(47)	120.3(10)
C(46)	C(47)	C(48)	120(1)	C(47)	C(48)	C(49)	118.7(10)
C(44)	C(49)	C(48)	122.7(9)	P(4)	C(50)	C(51)	121.9(7)
P(4)	C(50)	C(55)	119.1(7)	C(51)	C(50)	C(55)	119.1(8)
C(50)	C(51)	C(52)	120.9(9)	C(51)	C(52)	C(53)	121.2(9)
C(52)	C(53)	C(54)	118.1(10)	C(53)	C(54)	C(55)	121.8(10)
C(50)	C(55)	C(54)	118.8(9)				

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Supporting Information III

Experimental Details and Crystal Data for Ru(=C=CHPh)(PCy$_3$)[N(PPh$_2$S)$_2$]$_2$ 9

Empirical formula	$C_{74}H_{79}N_2P_5RuS_4$
Formula weight	1380.66
Color; habit	red; block
Crystal dimensions, mm	0.23x0.25x0.20
Crystal system	monoclinic
Lattice type	primitive
a, Å	21.573(3)
b, Å	14.281(3)
c, Å	23.245(3)
β, deg	107.110(9)
V, Å^3	6844(1)
Space group	*P* 2$_1$/n (No. 14)
Z	4
Dcald, g cm^{-3}	1.133
Diffractometer	Rigaku AFC7R
Radiation	MoKα, graphite-monochromated (λ 0.71073 Å)
F(000)	2324
μ(MoKα), cm^{-1}	4.13
Temperature, °C	25
scan type	ω
2θ$_{max}$, deg	50.0
No. of reflections measured	10584
No. of unique reflections	10231 (R_{int} = 0.098)
Corrections	Lorentz-polarization
	Absorption (trans factor: 0.9284-1.0000)
Structure solution	Direct methods (SIR 92)
Program used	TEXSAN
Refinement	Full-matrix least-squares
Function minimized	$\Sigma w (\|F_o\| - \|F_c\|)^2$
Weighing factor	$w^{-1} = \sigma^2(F_o) + 0.0090xF_o^2/4$
No. of observation	4662 (I > 1.50 σ(I))
No. of variables	405
Reflection/Parameter ratio	11.51
R, Rw	0.084, 0.067
Goodness of fit	1.63
Max. peak in final diff map, e$^-$/ Å^3	0.77
Min. peak in final diff map, e$^-$/ Å^3	-0.68

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Ru(1)	0.78537(5)	-0.21398(7)	1.01319(4)	2.22(2)
S(1)	0.8746(1)	-0.0978(2)	1.0041(2)	3.34(8)
S(2)	0.7049(1)	-0.1054(2)	0.9548(1)	2.76(7)
S(3)	0.7859(2)	-0.1316(2)	1.1061(1)	3.09(8)
S(4)	0.8785(1)	-0.3068(2)	1.0693(1)	3.22(8)
P(1)	0.8572(2)	0.0333(2)	1.0258(1)	2.89(8)
P(2)	0.7158(2)	0.0224(2)	0.9948(1)	2.79(8)
P(3)	0.7883(1)	-0.2203(2)	1.1742(1)	2.77(7)
P(4)	0.8571(2)	-0.3734(2)	1.1383(1)	2.87(8)
P(5)	0.7876(1)	-0.2848(3)	0.9192(1)	3.03(8)
N(1)	0.7866(4)	0.0599(6)	1.0291(4)	2.8(2)
N(2)	0.8119(4)	-0.3246(7)	1.1722(4)	2.9(2)
C(1)	0.8792(5)	0.1126(8)	0.9748(5)	3.0(2)
C(2)	0.9338(7)	0.101(1)	0.9572(6)	5.1(3)
C(3)	0.9514(7)	0.166(1)	0.9194(7)	5.8(4)
C(4)	0.9124(7)	0.242(1)	0.8985(6)	5.3(3)
C(5)	0.8587(7)	0.255(1)	0.9160(7)	5.8(4)
C(6)	0.8413(6)	0.1917(9)	0.9538(6)	4.0(3)
C(7)	0.9141(5)	0.0615(8)	1.0994(5)	2.9(2)
C(8)	0.9386(7)	0.150(1)	1.1131(6)	4.9(3)
C(9)	0.9837(7)	0.169(1)	1.1690(6)	5.2(3)
C(10)	1.0023(7)	0.098(1)	1.2105(6)	5.4(3)
C(11)	0.9781(7)	0.013(1)	1.1980(7)	5.5(4)
C(12)	0.9345(7)	-0.008(1)	1.1424(6)	5.0(3)

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C(13)	0.6750(6)	0.0974(9)	0.9307(5)	3.3(3)
C(14)	0.6953(6)	0.0927(10)	0.8798(6)	4.4(3)
C(15)	0.6647(7)	0.150(1)	0.8288(7)	5.6(4)
C(16)	0.6184(7)	0.212(1)	0.8343(6)	5.5(3)
C(17)	0.5986(7)	0.219(1)	0.8839(7)	5.9(4)
C(18)	0.6281(6)	0.162(1)	0.9334(6)	4.7(3)
C(19)	0.6681(5)	0.0342(8)	1.0470(5)	2.7(2)
C(20)	0.6938(6)	0.0785(10)	1.1020(6)	4.5(3)
C(21)	0.6561(7)	0.087(1)	1.1409(7)	6.2(4)
C(22)	0.5953(7)	0.050(1)	1.1254(6)	5.0(3)
C(23)	0.5685(6)	0.0066(9)	1.0714(6)	4.1(3)
C(24)	0.6059(6)	-0.0012(8)	1.0323(5)	3.4(3)
C(25)	0.7102(5)	-0.2267(8)	1.1886(5)	2.9(2)
C(26)	0.6557(7)	-0.1880(10)	1.1517(6)	4.9(3)
C(27)	0.5972(8)	-0.195(1)	1.1652(8)	7.1(4)
C(28)	0.5927(7)	-0.239(1)	1.2142(7)	6.2(4)
C(29)	0.6449(8)	-0.278(1)	1.2512(7)	7.3(4)
C(30)	0.7049(7)	-0.272(1)	1.2373(7)	6.8(4)
C(31)	0.8401(6)	-0.1643(9)	1.2411(5)	3.3(3)
C(32)	0.8330(6)	-0.0700(10)	1.2518(6)	4.5(3)
C(33)	0.8755(7)	-0.026(1)	1.3037(7)	6.1(4)
C(34)	0.9223(7)	-0.079(1)	1.3431(7)	6.2(4)
C(35)	0.9276(7)	-0.169(1)	1.3326(7)	5.5(4)
C(36)	0.8875(6)	-0.213(1)	1.2817(6)	4.5(3)

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C(37)	0.8215(6)	-0.4871(9)	1.1153(5)	3.3(3)
C(38)	0.8399(7)	-0.537(1)	1.0728(7)	6.0(4)
C(39)	0.8133(9)	-0.628(1)	1.0567(8)	7.9(5)
C(40)	0.7680(9)	-0.660(1)	1.0818(8)	8.0(5)
C(41)	0.7494(8)	-0.613(1)	1.1242(8)	7.9(5)
C(42)	0.7778(7)	-0.525(1)	1.1421(6)	5.0(3)
C(43)	0.9372(6)	-0.3965(9)	1.1915(5)	3.5(3)
C(44)	0.9505(7)	-0.483(1)	1.2219(6)	5.1(3)
C(45)	1.0100(8)	-0.494(1)	1.2671(7)	6.9(4)
C(46)	1.0508(8)	-0.426(1)	1.2810(7)	6.6(4)
C(47)	1.0420(8)	-0.344(1)	1.2527(7)	6.6(4)
C(48)	0.9821(7)	-0.326(1)	1.2064(6)	5.0(3)
C(49)	0.7244(5)	-0.2912(8)	1.0249(5)	2.6(2)
C(50)	0.6812(5)	-0.3429(8)	1.0406(5)	2.9(2)
C(51)	0.6103(5)	-0.3300(8)	1.0254(5)	2.7(2)
C(52)	0.5794(6)	-0.2520(9)	0.9949(6)	4.2(3)
C(53)	0.5130(7)	-0.242(1)	0.9826(6)	5.3(3)
C(54)	0.4768(7)	-0.311(1)	0.9996(6)	4.9(3)
C(55)	0.5071(7)	-0.385(1)	1.0289(6)	5.6(4)
C(56)	0.5746(7)	-0.398(1)	1.0429(6)	5.1(3)
C(57)	0.7236(6)	-0.3759(10)	0.8897(6)	4.4(3)
C(58)	0.6557(7)	-0.332(1)	0.8795(7)	5.7(4)
C(59)	0.6041(8)	-0.408(1)	0.8505(8)	7.7(5)
C(60)	0.6136(9)	-0.491(1)	0.8853(8)	8.1(5)

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C(61)	0.6798(9)	-0.538(1)	0.9009(8)	8.1(5)
C(62)	0.7324(7)	-0.461(1)	0.9276(7)	6.2(4)
C(63)	0.8622(5)	-0.3538(8)	0.9229(5)	2.7(2)
C(64)	0.8602(6)	-0.4122(9)	0.8651(6)	4.3(3)
C(65)	0.9167(7)	-0.480(1)	0.8802(7)	5.8(4)
C(66)	0.9805(7)	-0.434(1)	0.9053(7)	5.7(4)
C(67)	0.9822(6)	-0.373(1)	0.9585(6)	4.9(3)
C(68)	0.9273(6)	-0.3017(9)	0.9436(5)	3.5(3)
C(69)	0.7742(7)	-0.198(1)	0.8546(6)	5.2(3)
C(70)	0.7424(8)	-0.240(1)	0.7905(8)	8.0(5)
C(71)	0.725(1)	-0.154(2)	0.747(1)	11.7(7)
C(72)	0.8323(8)	-0.145(1)	0.8527(8)	7.4(4)
C(73)	0.815(1)	-0.059(2)	0.805(1)	11.8(7)
C(74)	0.7776(10)	-0.095(1)	0.7471(9)	9.5(6)
H(1)	0.9604	0.0484	0.9712	6.0561
H(2)	0.9900	0.1571	0.9084	7.0221
H(3)	0.9231	0.2856	0.8720	6.2655
H(4)	0.8325	0.3082	0.9023	6.9608
H(5)	0.8031	0.2022	0.9655	4.7130
H(6)	0.9252	0.1986	1.0840	5.8272
H(7)	1.0007	0.2298	1.1779	6.3969
H(8)	1.0329	0.1113	1.2485	6.4637
H(9)	0.9905	-0.0347	1.2278	6.5286
H(10)	0.9190	-0.0705	1.1338	5.8948

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ru(1)	0.0285(5)	0.0314(6)	0.0245(5)	0.0019(6)	0.0080(4)	0.0009(6)
S(1)	0.036(2)	0.038(2)	0.057(2)	-0.001(2)	0.020(2)	-0.006(2)
S(2)	0.038(2)	0.032(2)	0.033(2)	0.002(2)	0.007(1)	-0.002(2)
S(3)	0.049(2)	0.038(2)	0.030(2)	0.006(2)	0.011(2)	-0.001(2)
S(4)	0.035(2)	0.052(2)	0.038(2)	0.013(2)	0.013(2)	0.010(2)
P(1)	0.034(2)	0.037(2)	0.040(2)	-0.003(2)	0.012(2)	0.003(2)
P(2)	0.033(2)	0.034(2)	0.038(2)	0.005(2)	0.009(2)	0.001(2)
P(3)	0.032(2)	0.043(2)	0.028(2)	0.003(2)	0.007(1)	0.000(2)
P(4)	0.034(2)	0.043(2)	0.031(2)	0.005(2)	0.008(2)	0.007(2)
P(5)	0.035(2)	0.047(2)	0.032(2)	0.001(2)	0.009(2)	-0.003(2)
N(1)	0.030(6)	0.038(6)	0.040(7)	-0.006(5)	0.013(5)	-0.008(5)
N(2)	0.034(6)	0.041(6)	0.040(6)	0.013(5)	0.019(5)	0.002(5)

The general temperature factor expression:

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

Table 3. Bond Lengths($\AA$)

atom	atom	distance	atom	atom	distance
Ru(1)	S(1)	2.595(3)	Ru(1)	S(2)	2.424(3)
Ru(1)	S(3)	2.456(3)	Ru(1)	S(4)	2.439(3)
Ru(1)	P(5)	2.420(3)	Ru(1)	C(49)	1.80(1)
S(1)	P(1)	2.003(5)	S(2)	P(2)	2.031(4)
S(3)	P(3)	2.017(4)	S(4)	P(4)	2.032(4)
P(1)	N(1)	1.595(9)	P(1)	C(1)	1.80(1)
P(1)	C(7)	1.83(1)	P(2)	N(1)	1.594(9)
P(2)	C(13)	1.84(1)	P(2)	C(19)	1.81(1)
P(3)	N(2)	1.579(10)	P(3)	C(25)	1.81(1)
P(3)	C(31)	1.81(1)	P(4)	N(2)	1.583(9)
P(4)	C(37)	1.81(1)	P(4)	C(43)	1.84(1)
P(5)	C(57)	1.87(1)	P(5)	C(63)	1.87(1)
P(5)	C(69)	1.91(1)	C(1)	C(2)	1.37(2)
C(1)	C(6)	1.39(2)	C(2)	C(3)	1.40(2)
C(3)	C(4)	1.37(2)	C(4)	C(5)	1.35(2)
C(5)	C(6)	1.39(2)	C(7)	C(8)	1.37(2)
C(7)	C(12)	1.39(2)	C(8)	C(9)	1.40(2)
C(9)	C(10)	1.37(2)	C(10)	C(11)	1.33(2)
C(11)	C(12)	1.39(2)	C(13)	C(14)	1.38(2)
C(13)	C(18)	1.39(2)	C(14)	C(15)	1.43(2)
C(15)	C(16)	1.36(2)	C(16)	C(17)	1.35(2)
C(17)	C(18)	1.40(2)	C(19)	C(20)	1.39(2)
C(19)	C(24)	1.38(1)	C(20)	C(21)	1.39(2)
C(21)	C(22)	1.36(2)	C(22)	C(23)	1.37(2)

Table 3. Bond Lengths(Å) (continued)

atom	atom	distance	atom	atom	distance
C(23)	C(24)	1.38(2)	C(25)	C(26)	1.35(2)
C(25)	C(30)	1.34(2)	C(26)	C(27)	1.39(2)
C(27)	C(28)	1.33(2)	C(28)	C(29)	1.32(2)
C(29)	C(30)	1.43(2)	C(31)	C(32)	1.39(2)
C(31)	C(36)	1.36(2)	C(32)	C(33)	1.43(2)
C(33)	C(34)	1.37(2)	C(34)	C(35)	1.33(2)
C(35)	C(36)	1.39(2)	C(37)	C(38)	1.37(2)
C(37)	C(42)	1.38(2)	C(38)	C(39)	1.43(2)
C(39)	C(40)	1.36(2)	C(40)	C(41)	1.34(2)
C(41)	C(42)	1.41(2)	C(43)	C(44)	1.41(2)
C(43)	C(48)	1.37(2)	C(44)	C(45)	1.41(2)
C(45)	C(46)	1.28(2)	C(46)	C(47)	1.34(2)
C(47)	C(48)	1.44(2)	C(49)	C(50)	1.32(1)
C(50)	C(51)	1.48(1)	C(51)	C(52)	1.38(2)
C(51)	C(56)	1.37(2)	C(52)	C(53)	1.38(2)
C(53)	C(54)	1.38(2)	C(54)	C(55)	1.33(2)
C(55)	C(56)	1.41(2)	C(57)	C(58)	1.55(2)
C(57)	C(62)	1.48(2)	C(58)	C(59)	1.56(2)
C(59)	C(60)	1.41(2)	C(60)	C(61)	1.52(2)
C(61)	C(62)	1.57(2)	C(63)	C(64)	1.57(2)
C(63)	C(68)	1.54(1)	C(64)	C(65)	1.51(2)
C(65)	C(66)	1.48(2)	C(66)	C(67)	1.50(2)
C(67)	C(68)	1.52(2)	C(69)	C(70)	1.56(2)
C(69)	C(72)	1.47(2)	C(70)	C(71)	1.58(3)

Table 3. Bond Lengths($\AA$) (continued)

atom	atom	distance	atom	atom	distance
C(71)	C(74)	1.41(3)	C(72)	C(73)	1.62(3)
C(73)	C(74)	1.45(2)			

Table 5. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
S(1)	Ru(1)	S(2)	88.4(1)	S(1)	Ru(1)	S(3)	87.3(1)
S(1)	Ru(1)	S(4)	83.0(1)	S(1)	Ru(1)	P(5)	88.9(1)
S(1)	Ru(1)	C(49)	175.8(3)	S(2)	Ru(1)	S(3)	90.2(1)
S(2)	Ru(1)	S(4)	171.3(1)	S(2)	Ru(1)	P(5)	87.9(1)
S(2)	Ru(1)	C(49)	92.4(4)	S(3)	Ru(1)	S(4)	90.0(1)
S(3)	Ru(1)	P(5)	175.9(1)	S(3)	Ru(1)	C(49)	88.6(3)
S(4)	Ru(1)	P(5)	91.3(1)	S(4)	Ru(1)	C(49)	96.3(4)
P(5)	Ru(1)	C(49)	95.2(3)	Ru(1)	S(1)	P(1)	112.3(2)
Ru(1)	S(2)	P(2)	110.5(2)	Ru(1)	S(3)	P(3)	112.4(2)
Ru(1)	S(4)	P(4)	109.5(2)	S(1)	P(1)	N(1)	119.1(4)
S(1)	P(1)	C(1)	108.5(4)	S(1)	P(1)	C(7)	108.5(4)
N(1)	P(1)	C(1)	108.7(5)	N(1)	P(1)	C(7)	106.9(5)
C(1)	P(1)	C(7)	104.1(5)	S(2)	P(2)	N(1)	119.8(4)
S(2)	P(2)	C(13)	100.9(4)	S(2)	P(2)	C(19)	112.2(4)
N(1)	P(2)	C(13)	111.7(5)	N(1)	P(2)	C(19)	106.3(5)
C(13)	P(2)	C(19)	105.0(5)	S(3)	P(3)	N(2)	120.2(4)
S(3)	P(3)	C(25)	111.5(4)	S(3)	P(3)	C(31)	105.3(4)
N(2)	P(3)	C(25)	106.5(5)	N(2)	P(3)	C(31)	108.6(5)
C(25)	P(3)	C(31)	103.6(5)	S(4)	P(4)	N(2)	120.2(4)
S(4)	P(4)	C(37)	111.2(4)	S(4)	P(4)	C(43)	103.2(4)
N(2)	P(4)	C(37)	105.8(5)	N(2)	P(4)	C(43)	109.9(5)
C(37)	P(4)	C(43)	105.8(6)	Ru(1)	P(5)	C(57)	114.4(4)
Ru(1)	P(5)	C(63)	115.2(4)	Ru(1)	P(5)	C(69)	113.6(5)
C(57)	P(5)	C(63)	100.4(6)	C(57)	P(5)	C(69)	103.9(6)

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(63)	P(5)	C(69)	108.0(6)	P(1)	N(1)	P(2)	133.2(6)
P(3)	N(2)	P(4)	132.9(6)	P(1)	C(1)	C(2)	122(1)
P(1)	C(1)	C(6)	119.9(9)	C(2)	C(1)	C(6)	117(1)
C(1)	C(2)	C(3)	121(1)	C(2)	C(3)	C(4)	119(1)
C(3)	C(4)	C(5)	119(1)	C(4)	C(5)	C(6)	121(1)
C(1)	C(6)	C(5)	120(1)	P(1)	C(7)	C(8)	121(1)
P(1)	C(7)	C(12)	119.9(10)	C(8)	C(7)	C(12)	118(1)
C(7)	C(8)	C(9)	120(1)	C(8)	C(9)	C(10)	119(1)
C(9)	C(10)	C(11)	120(1)	C(10)	C(11)	C(12)	121(1)
C(7)	C(12)	C(11)	119(1)	P(2)	C(13)	C(14)	118.1(10)
P(2)	C(13)	C(18)	122.3(10)	C(14)	C(13)	C(18)	119(1)
C(13)	C(14)	C(15)	119(1)	C(14)	C(15)	C(16)	117(1)
C(15)	C(16)	C(17)	124(1)	C(16)	C(17)	C(18)	118(1)
C(13)	C(18)	C(17)	120(1)	P(2)	C(19)	C(20)	120.5(9)
P(2)	C(19)	C(24)	120.1(9)	C(20)	C(19)	C(24)	119(1)
C(19)	C(20)	C(21)	119(1)	C(20)	C(21)	C(22)	120(1)
C(21)	C(22)	C(23)	122(1)	C(22)	C(23)	C(24)	117(1)
C(19)	C(24)	C(23)	121(1)	P(3)	C(25)	C(26)	122.8(10)
P(3)	C(25)	C(30)	119(1)	C(26)	C(25)	C(30)	117(1)
C(25)	C(26)	C(27)	120(1)	C(26)	C(27)	C(28)	121(1)
C(27)	C(28)	C(29)	119(1)	C(28)	C(29)	C(30)	118(1)
C(25)	C(30)	C(29)	122(1)	P(3)	C(31)	C(32)	120.6(10)
P(3)	C(31)	C(36)	120(1)	C(32)	C(31)	C(36)	118(1)
C(31)	C(32)	C(33)	120(1)	C(32)	C(33)	C(34)	118(1)

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(33)	C(34)	C(35)	120(1)	C(34)	C(35)	C(36)	122(1)
C(31)	C(36)	C(35)	120(1)	P(4)	C(37)	C(38)	119(1)
P(4)	C(37)	C(42)	120(1)	C(38)	C(37)	C(42)	120(1)
C(37)	C(38)	C(39)	118(1)	C(38)	C(39)	C(40)	118(1)
C(39)	C(40)	C(41)	123(1)	C(40)	C(41)	C(42)	117(1)
C(37)	C(42)	C(41)	120(1)	P(4)	C(43)	C(44)	120(1)
P(4)	C(43)	C(48)	119(1)	C(44)	C(43)	C(48)	119(1)
C(43)	C(44)	C(45)	118(1)	C(44)	C(45)	C(46)	120(1)
C(45)	C(46)	C(47)	123(1)	C(46)	C(47)	C(48)	119(1)
C(43)	C(48)	C(47)	118(1)	Ru(1)	C(49)	C(50)	172.4(9)
C(49)	C(50)	C(51)	128(1)	C(50)	C(51)	C(52)	122(1)
C(50)	C(51)	C(56)	118(1)	C(52)	C(51)	C(56)	119(1)
C(51)	C(52)	C(53)	120(1)	C(52)	C(53)	C(54)	120(1)
C(53)	C(54)	C(55)	118(1)	C(54)	C(55)	C(56)	122(1)
C(51)	C(56)	C(55)	118(1)	P(5)	C(57)	C(58)	109.8(10)
P(5)	C(57)	C(62)	113(1)	C(58)	C(57)	C(62)	111(1)
C(57)	C(58)	C(59)	108(1)	C(58)	C(59)	C(60)	111(1)
C(59)	C(60)	C(61)	118(1)	C(60)	C(61)	C(62)	107(1)
C(57)	C(62)	C(61)	112(1)	P(5)	C(63)	C(64)	115.8(8)
P(5)	C(63)	C(68)	117.0(8)	C(64)	C(63)	C(68)	108.6(9)
C(63)	C(64)	C(65)	108(1)	C(64)	C(65)	C(66)	113(1)
C(65)	C(66)	C(67)	112(1)	C(66)	C(67)	C(68)	111(1)
C(63)	C(68)	C(67)	109(1)	P(5)	C(69)	C(70)	114(1)
P(5)	C(69)	C(72)	115(1)	C(70)	C(69)	C(72)	107(1)

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(69)	C(70)	C(71)	105(1)	C(70)	C(71)	C(74)	114(1)
C(69)	C(72)	C(73)	112(1)	C(72)	C(73)	C(74)	108(1)
C(71)	C(74)	C(73)	116(2)				