Supplementary Information

Experimental

Materials

All solvents were purchased from Nacalai Tesque for the reactions and from Sigma-Aldrich Japan or Merck for the measurements and used without further purification. All other reagents were used as received.

General procedure

^{1}H and ^{13}C NMR spectra were recorded on a JEOL Lambda300 FT-NMR spectrometer, and chemical shifts were referenced to tetramethylsilane. Electrospray ionization (ESI) mass spectrometry measurements were performed on an Applied Biosystem Mariner spectrometer using HPLC grade solvents. Elemental analyses were performed by the Analytical Research Service Centre at Osaka City University on Perkin Elmer 240C or FISONS Instrument EA108 elemental analysers.

Synthesis of $[Rh(Py_3S_3)_2](PF_6)_3$.

To a heated solution of Py_3S_3 (327 mg, 1.00 mmol) in ethanol (200 mL), an aqueous solution (50 mL) of $RhCl_3 \bullet 3H_2O$ (197 mg, 0.75 mmol) was slowly added dropwise with stirring. Stirring for further 30 min with heating give a red solution of the reaction mixture. After insoluble solids were filtered off, a solution of KPF_6 (430 mg, 2.34 mmol) in water (20 mL) was added to form a yellow microcrystalline solid, which was collected by filtration and washed with water and ethanol. Yield 415 mg, 70%, (Found: C, 30.16; H, 1.46; N, 7.27. $C_{30}H_{18}N_6F_{18}P_3RhS_6$ requires C, 30.21, H, 1.52; N, 7.05%); δ_H(300 MHz, CD_3CN, TMS) 8.19 (6H, dd, 4-pyridyl), 8.01 (12H, d, 3-pyridyl); δ_C(75 MHz, CD_3CN, TMS) 155.8 (s, 2-pyridyl), 143.8 (s, 4-pyridyl), 131.8 (s, 3-pyridyl); ESI-MS m/z = 252 (100%, $[M]^{3+}$), 451 (31%, $[M+PF_6]^{2+}$), 1047 (4%, $[M+2PF_6]^{+}$).

Synthesis of $[Rh(Py_3S_3)_2](BPh_4)_3$.

The BPh_4 salt of the Rh(III) complex was prepared by the similar method using $NaBPh_4$ (200 mg, 0.584 mmol) instead of KPF_6 with 1/4 amounts of the starting materials and solvents. Yield 109 mg, 51%, (Found: C, 68.80; H, 4.71; N, 6.40. $C_{102}H_{78}N_6B_3RhS_6$ requires C, 71.41, H, 4.58; N, 4.90%); δ_H(400 MHz, CD_3CN, TMS) 8.12 (6H, t, 4-pyridyl), 7.94 (12H, d, 3-pyridyl); 7.26 (24H, m, *o*-H-Ph); 6.98 (24H, t, *m*-H-Ph); 6.82 (12H, t, *p*-H-Ph); δ_C(100 MHz, CD_3CN, TMS) 164.0 (m,

Ph); 155.8 (s, 2-pyridyl), 144.0 (s, 4-pyridyl), 136.7 (s, Ph); 131.9 (s, 3-pyridyl); 126.6 (q, Ph); 122.8 (s, Ph). The result of the elemental analysis is not match to the calculated. This may be caused by difficulty of purification due to the low solubility of the BPh_4 salts and the sample still contained chloride. If 2/9 of counter anions are no replaced with BPh_4^- and some solvent acetonitrile molecules are remained, we can obtain closer value to the measured ones. $[Rh(Py_3S_3)_2]_3(BPh_4)_7Cl_2 \bullet 3CH_3CN$: C, 67.44; H, 4.35; N, 6.26.

Synthesis of $[Rh(Py_3S_3)_2](PF_6)_2$.

Zinc powder (126 mg, 1.93 mmol) was added to a solution of $[Rh(Py_3S_3)_2](PF_6)_3$ (150 mg, 0.126 mmol) in a mixture of 5 mL each of acetonitrile and methanol. The color of the reaction mixture changed from yellow to violet within 15 min. After stirring for 24 h, the solvent was removed under reduced pressure to afford a black residue, which was re-dissolved in dichloromethane to give a violet solution. After insoluble solids and unreacted Zn powder were filtered off, the solvent of the violet filtrate was removed under reduced pressure to result in the formation of black crystals of the Rh(II) complex. Yield 93mg, 71%, (Found: C, 34.41; H, 1.65; N, 8.05. $C_{30}H_{18}N_6F_{12}P_2RhS_6$ requires C, 34.39, H, 1.73; N, 8.02%); ESI-MS m/z = 378 (100%, $[M]^{2+}$), 902 (43%, $[M+PF_6]^{2+}$).

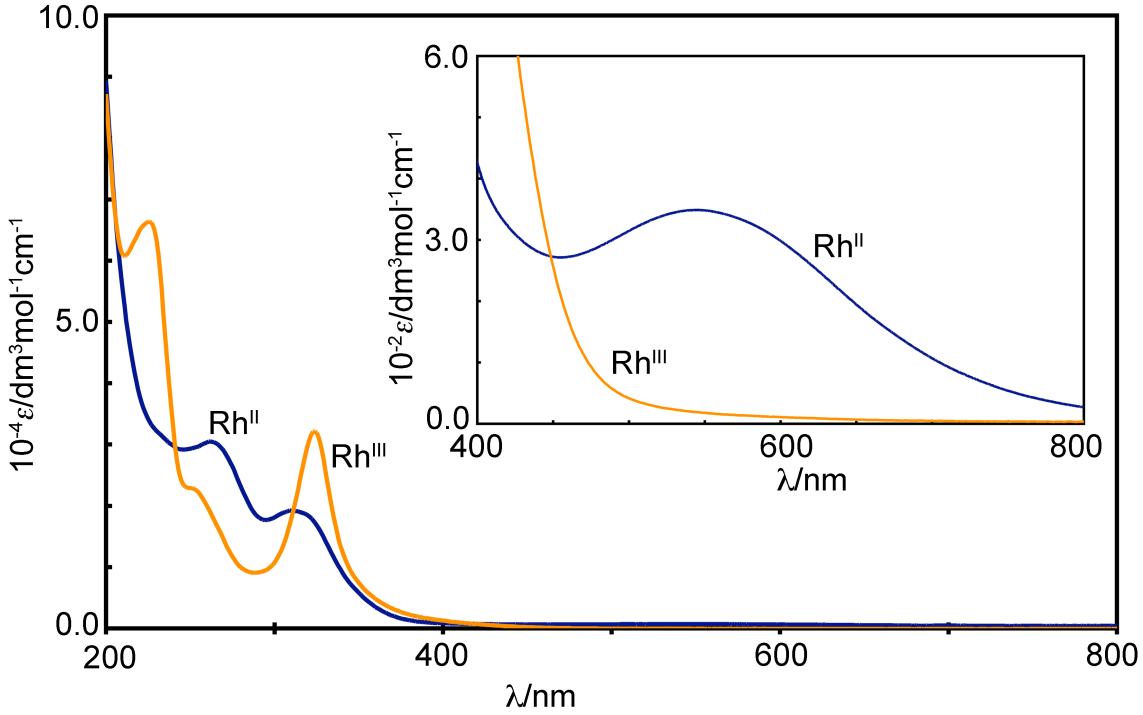
Synthesis of $[Rh(Py_3S_3)_2](BPh_4)_2$.

Black microcrystalline solid of the BPh_4 salt of the Rh(II) complex was obtained almost quantitatively by addition of a solution of $NaBPh_4$ in methanol into a solution of the PF_6 salt in acetonitrile. (Found: C, 66.41; H, 4.09; N, 6.04. $C_{78}H_{58}N_6B_2RhS_6$ requires C, 67.10, H, 4.19; N, 6.02%)

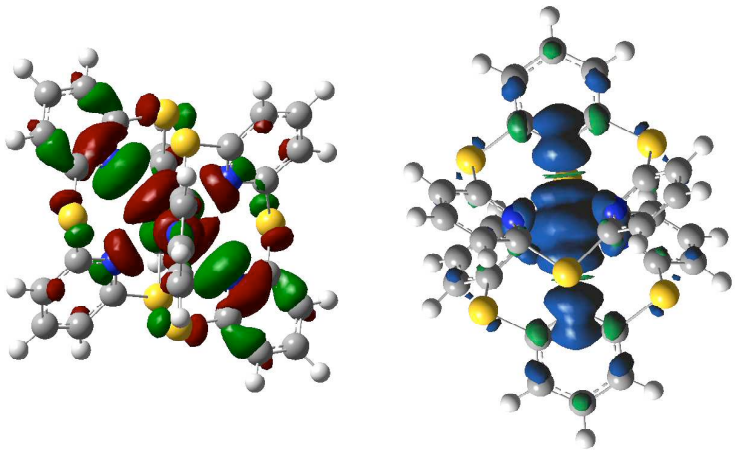
Crystal growth and X-ray crystallography

Single crystals of **1a•2CH$_3$CN** were obtained by slow diffusion of diethyl ether into a solution of the complex in acetonitrile. Single crystals of **2a** were obtained from a solution in a mixture of dichloromethane and methanol by slow evaporation of the solvents. Upon crystallisation of **1b** in nitromethane by slow diffusion of methanol, reduction of the Rh(III) complex occurred and black single crystals of **2b** and **2b•2CH$_3$NO$_2$** were obtained. Each single crystal was mounted on a glass fibre. Diffraction data were collected on an AFC7/CCD Mercury diffractometer using a rotation method with 0.5 frame width with 10 and 5 s exposure times per frame for **2b•CH$_3$NO$_2$** and for the others, respectively. The data were integrated, scaled, sorted and averages using the CrystalClear software. Absorption corrections were applied using Coppens numerical method. The structures

were solved using SIR97 and refined with CRYSTALS using Crystal Structure as a graphical interface. All non-hydrogen atoms were refined anisotropically. All hydrogen atoms in **1a** and **2a** were found in difference Fourier maps and refined isotropically, while those in **2b** and **2b•2CH$_3$NO$_2$** were located on the calculated positions and refined as ridding models.



UV-vis spectra of [Rh^{III}(Py$_3$S$_3$)$_2$](PF$_6$)$_3$ **1a** and [Rh^{II}(Py$_3$S$_3$)$_2$](PF$_6$)$_2$ **2a** in acetonitrile.



SOMO of [Rh(Py$_3$S$_3$)$_2$]$^{2+}$ (left) and spin density of the complex (right).

Atomic coordinates and B_{iso}/B_{eq} for 1a•CH_3CN

atom	x	y	z	B_{eq}/B_{iso}
Rh(1)	0.79466(3)	0.08643(3)	0.85609(2)	1.331(7)
S(1)	0.64121(11)	0.13660(10)	0.73660(6)	2.16(3)
S(2)	0.65410(11)	-0.03914(10)	0.95092(6)	2.09(3)
S(3)	0.97885(11)	-0.04652(10)	0.80028(6)	2.18(3)
S(4)	0.95581(11)	0.03472(10)	0.97068(6)	2.25(3)
S(5)	0.92727(11)	0.22130(10)	0.76141(6)	2.28(3)
S(6)	0.60820(11)	0.21406(9)	0.91721(6)	1.97(3)
P(1)	0.63753(12)	-0.18891(10)	0.74379(6)	2.23(3)
P(2)	0.89071(13)	0.38888(11)	0.96482(8)	2.93(4)
P(3)	0.71236(16)	0.67186(12)	1.08402(8)	3.88(4)
F(1)	0.5303(2)	-0.2239(2)	0.76317(18)	5.31(11)
F(2)	0.7460(2)	-0.1557(2)	0.72304(18)	4.81(10)
F(3)	0.6140(3)	-0.2242(3)	0.67831(16)	6.40(13)
F(4)	0.5921(3)	-0.0976(2)	0.7236(2)	8.17(15)
F(5)	0.6577(3)	-0.1524(3)	0.80833(18)	7.35(14)
F(6)	0.6844(3)	-0.2802(2)	0.7601(2)	7.41(14)
F(7)	1.0003(2)	0.4139(3)	0.9854(2)	6.80(12)
F(8)	0.7790(3)	0.3619(3)	0.9489(2)	8.73(16)
F(9)	0.9106(5)	0.4027(5)	0.8998(2)	14.5(2)
F(10)	0.9173(4)	0.2899(2)	0.9609(2)	9.91(18)
F(11)	0.8671(5)	0.3727(4)	1.0329(2)	12.5(2)
F(12)	0.8620(4)	0.4854(3)	0.9734(3)	12.9(2)
F(13)	0.7780(4)	0.6589(3)	1.0284(2)	8.96(16)
F(14)	0.6503(3)	0.6979(5)	1.1415(2)	13.0(2)
F(15)	0.6442(4)	0.7399(4)	1.0537(2)	11.1(2)
F(16)	0.7849(5)	0.7432(6)	1.1005(5)	23.1(4)
F(17)	0.7752(5)	0.6049(7)	1.1129(3)	20.3(3)
F(18)	0.6362(5)	0.6064(4)	1.0673(5)	21.7(3)
N(1)	0.8133(3)	0.0480(2)	0.76574(18)	1.65(9)
N(2)	0.6433(2)	0.0508(2)	0.84467(18)	1.59(9)
N(3)	0.8188(3)	-0.0455(2)	0.87679(17)	1.68(9)
N(4)	0.7807(3)	0.1241(2)	0.94597(17)	1.51(9)
N(5)	0.9471(2)	0.1255(2)	0.86532(19)	1.56(9)
N(6)	0.7637(2)	0.2178(2)	0.83618(18)	1.66(9)
N(7)	0.8629(6)	-0.4267(6)	0.7937(4)	12.4(3)
N(8)	0.9535(6)	0.9157(6)	1.0871(3)	10.7(2)
C(1)	0.8947(4)	0.0007(3)	0.7483(2)	1.85(11)
C(2)	0.9202(4)	-0.0119(3)	0.6884(2)	2.32(13)
C(3)	0.8617(4)	0.0257(3)	0.6453(2)	2.90(13)
C(4)	0.7741(4)	0.0664(3)	0.6613(2)	2.33(13)
C(5)	0.7513(3)	0.0776(3)	0.7216(2)	1.92(11)
C(6)	0.5887(3)	0.0804(3)	0.7971(2)	2.03(12)
C(7)	0.4834(4)	0.0704(3)	0.7952(2)	2.19(12)
C(8)	0.4341(4)	0.0289(3)	0.8410(2)	2.55(13)
C(9)	0.4885(4)	-0.0067(3)	0.8874(2)	2.35(13)
C(10)	0.5923(4)	0.0032(3)	0.8879(2)	1.73(11)
C(11)	0.7614(3)	-0.0877(3)	0.9186(2)	1.79(11)
C(12)	0.7847(4)	-0.1706(3)	0.9418(2)	2.41(13)

C(13)	0.8676(4)	-0.2148(4)	0.9193(2)	3.06(15)
C(14)	0.9224(4)	-0.1766(3)	0.8728(2)	2.45(13)
C(15)	0.8968(3)	-0.0917(3)	0.8534(2)	1.92(10)
C(16)	0.7019(4)	0.1724(3)	0.9651(2)	1.85(11)
C(17)	0.6833(4)	0.1879(3)	1.0264(2)	2.36(13)
C(18)	0.7490(4)	0.1538(4)	1.0691(2)	2.84(14)
C(19)	0.8308(4)	0.1088(3)	1.0499(2)	2.42(13)
C(20)	0.8477(3)	0.0964(3)	0.9888(2)	1.79(11)
C(21)	1.0058(3)	0.0950(3)	0.9110(2)	1.82(11)
C(22)	1.1095(3)	0.1054(3)	0.9111(2)	2.12(12)
C(23)	1.1559(4)	0.1504(3)	0.8655(2)	2.66(13)
C(24)	1.0959(4)	0.1876(3)	0.8214(2)	2.22(13)
C(25)	0.9928(4)	0.1741(3)	0.8226(2)	1.91(12)
C(26)	0.8163(3)	0.2640(3)	0.7937(2)	1.86(12)
C(27)	0.7823(4)	0.3418(3)	0.7685(2)	2.28(12)
C(28)	0.6903(4)	0.3749(3)	0.7860(2)	2.93(14)
C(29)	0.6407(4)	0.3339(3)	0.8331(2)	2.60(13)
C(30)	0.6800(3)	0.2582(3)	0.8576(2)	1.87(11)
C(31)	0.7262(6)	-0.4169(5)	0.8743(3)	6.3(2)
C(32)	0.8045(7)	-0.4191(6)	0.8305(4)	6.9(2)
C(33)	1.0157(5)	0.7594(5)	1.0796(3)	5.5(2)
C(34)	0.9782(5)	0.8453(5)	1.0828(3)	5.3(2)
H(1)	0.9797	-0.0435	0.6779	2.78
H(2)	0.8811	0.0241	0.6041	3.48
H(3)	0.7274	0.0853	0.6314	2.80
H(4)	0.4473	0.0938	0.7618	2.63
H(5)	0.3623	0.0267	0.8407	3.07
H(6)	0.4558	-0.0409	0.9175	2.81
H(7)	0.7462	-0.1943	0.9740	2.89
H(8)	0.8895	-0.2691	0.9361	3.67
H(9)	0.9737	-0.2090	0.8526	2.94
H(10)	0.6270	0.2228	1.0382	2.82
H(11)	0.7362	0.1601	1.1109	3.40
H(12)	0.8781	0.0855	1.0779	2.90
H(13)	1.1487	0.0819	0.9432	2.54
H(14)	1.2276	0.1522	0.8628	3.20
H(15)	1.1262	0.2242	0.7917	2.65
H(16)	0.8199	0.3722	0.7386	2.73
H(17)	0.6616	0.4251	0.7669	3.52
H(18)	0.5799	0.3592	0.8479	3.12
H(19)	0.6667	-0.3876	0.8572	7.63
H(20)	0.7489	-0.3846	0.9101	7.63
H(21)	0.7086	-0.4774	0.8856	7.62
H(22)	1.0492	0.7533	1.0404	6.56
H(23)	0.9617	0.7155	1.0830	6.57
H(24)	1.0653	0.7501	1.1118	6.56

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Atomic coordinates and B_{iso}/B_{eq} for 2a

atom	x	y	z	B_{eq}/B_{iso}	occ
Rh(1)	0.0000	0.0000	0.5000	1.797(11)	1/4
S(1)	-0.07321(9)	0.13060(5)	0.22079(14)	2.98(2)	
S(2)	0.30660(12)	0.0000	0.6259(2)	3.30(3)	1/2
P(1)	0.0000	0.33857(8)	0.0000	3.50(3)	1/2
F(1)	-0.1362(2)	0.33821(18)	-0.1105(4)	5.21(7)	
F(2)	0.0291(4)	0.3882(3)	-0.1268(8)	14.22(19)	
F(3)	-0.0276(4)	0.2864(4)	0.1177(13)	17.8(2)	
N(1)	-0.0793(4)	0.0000	0.2139(6)	2.74(9)	1/2
N(2)	0.1205(2)	0.06935(16)	0.4280(4)	2.64(6)	
C(1)	-0.2650(5)	0.0000	-0.0935(7)	3.00(12)	1/2
C(2)	-0.2143(3)	0.0566(2)	-0.0211(5)	2.82(8)	
C(3)	-0.1214(3)	0.05497(19)	0.1315(5)	2.50(7)	
C(4)	0.0801(3)	0.1208(2)	0.3274(5)	2.64(7)	
C(5)	0.1515(4)	0.1734(2)	0.3108(6)	3.27(9)	
C(6)	0.2715(4)	0.1718(2)	0.3956(6)	3.63(10)	
C(7)	0.3172(4)	0.1170(2)	0.4890(6)	3.43(9)	
C(8)	0.2403(3)	0.0664(2)	0.4985(5)	2.79(7)	
H(1)	-0.337(5)	0.0000	-0.207(8)	2.8(12)	1/2
H(2)	-0.239(4)	0.087(2)	-0.058(6)	2.7(10)	
H(3)	0.113(3)	0.211(2)	0.250(6)	2.5(8)	
H(4)	0.324(3)	0.201(2)	0.374(5)	2.2(8)	
H(5)	0.400(4)	0.109(2)	0.562(6)	3.1(9)	

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Atomic coordinates and B_{iso}/B_{eq} for 2b

atom	x	y	z	B_{eq}/B_{iso}	occ
Rh(1)	0.5000	0.5000	0.5000	1.438(8)	1/2
Rh(2)	0.0000	1.0000	1.0000	1.210(8)	1/2
S(1)	0.53455(9)	0.74687(6)	0.49306(5)	2.64(2)	
S(2)	0.67723(8)	0.46805(6)	0.62583(5)	2.40(2)	
S(3)	0.21324(8)	0.48272(6)	0.54518(5)	2.58(2)	
S(4)	0.01574(9)	0.75996(6)	1.00880(5)	2.92(2)	
S(5)	-0.28284(8)	1.00779(6)	0.92899(5)	2.81(2)	
S(6)	0.17826(8)	1.04570(6)	0.88552(5)	2.20(2)	
N(1)	0.3656(2)	0.62496(19)	0.52349(12)	1.93(6)	
N(2)	0.6167(2)	0.60952(19)	0.55928(12)	1.79(6)	
N(3)	0.4433(2)	0.46684(18)	0.58648(12)	1.68(6)	
N(4)	0.1078(2)	0.90150(18)	0.94871(12)	1.63(6)	
N(5)	-0.1424(2)	0.8768(2)	0.96795(12)	2.14(6)	
N(6)	-0.0550(2)	1.03054(18)	0.90241(13)	2.09(6)	
C(1)	0.2586(2)	0.6049(2)	0.54225(16)	2.07(7)	
C(2)	0.1782(3)	0.6757(2)	0.55569(17)	2.75(9)	
C(3)	0.2089(3)	0.7702(3)	0.55022(19)	3.34(10)	
C(4)	0.3196(3)	0.7926(2)	0.53324(18)	2.73(9)	

C(5)	0.3953(2)	0.7180(2)	0.51999(16)	2.10(8)
C(6)	0.6306(2)	0.7026(2)	0.54965(16)	2.23(8)
C(7)	0.7223(3)	0.7680(2)	0.5814(2)	3.38(10)
C(8)	0.8022(3)	0.7392(3)	0.6257(2)	3.79(11)
C(9)	0.7831(3)	0.6479(2)	0.64039(19)	2.75(9)
C(10)	0.6894(2)	0.5854(2)	0.60675(16)	2.00(7)
C(11)	0.5241(2)	0.4468(2)	0.63195(16)	1.83(7)
C(12)	0.4957(3)	0.4018(2)	0.68274(18)	2.44(9)
C(13)	0.3789(3)	0.3803(2)	0.68975(19)	3.00(9)
C(14)	0.2932(3)	0.4089(2)	0.64858(18)	2.58(9)
C(15)	0.3293(2)	0.4521(2)	0.59836(17)	1.93(7)
C(16)	0.1784(2)	0.9294(2)	0.90610(16)	1.82(7)
C(17)	0.2626(3)	0.8703(2)	0.87708(19)	2.56(8)
C(18)	0.2716(3)	0.7794(2)	0.8917(2)	3.15(9)
C(19)	0.1941(3)	0.7467(2)	0.9319(2)	2.80(9)
C(20)	0.1126(2)	0.8090(2)	0.95856(16)	2.09(8)
C(21)	-0.1227(3)	0.7853(2)	0.97577(17)	2.46(8)
C(22)	-0.2124(4)	0.7095(2)	0.9610(2)	3.59(11)
C(23)	-0.3211(4)	0.7255(3)	0.9361(2)	3.63(11)
C(24)	-0.3403(3)	0.8174(3)	0.92401(19)	3.04(10)
C(25)	-0.2490(2)	0.8898(2)	0.94010(16)	2.22(8)
C(26)	-0.1682(3)	1.0417(2)	0.88309(19)	2.43(8)
C(27)	-0.2018(3)	1.0839(2)	0.8305(2)	2.98(9)
C(28)	-0.1143(3)	1.1159(2)	0.7955(2)	3.29(10)
C(29)	0.0026(3)	1.0997(2)	0.8121(2)	2.87(10)
C(30)	0.0275(2)	1.0559(2)	0.86562(18)	2.23(8)
C(31)	0.2955(2)	1.0110(2)	0.66459(16)	1.58(7)
C(32)	0.1890(2)	0.9813(2)	0.68742(17)	2.00(8)
C(33)	0.0808(3)	0.9764(2)	0.65161(19)	2.24(8)
C(34)	0.0721(3)	1.0024(2)	0.59083(18)	2.32(8)
C(35)	0.1750(3)	1.0325(2)	0.56701(18)	2.54(9)
C(36)	0.2833(3)	1.0368(2)	0.60347(17)	2.05(8)
C(37)	0.5306(2)	1.0652(2)	0.67708(16)	1.75(7)
C(38)	0.5906(3)	1.1565(2)	0.70222(18)	2.32(8)
C(39)	0.6848(3)	1.1922(2)	0.6727(2)	3.16(10)
C(40)	0.7221(3)	1.1402(3)	0.6170(2)	3.60(11)
C(41)	0.6639(3)	1.0506(3)	0.5899(2)	3.72(11)
C(42)	0.5703(3)	1.0141(2)	0.61943(19)	3.03(9)
C(43)	0.4582(2)	0.9062(2)	0.71990(14)	1.75(7)
C(44)	0.5728(3)	0.8891(2)	0.74032(19)	2.57(9)
C(45)	0.6073(3)	0.8001(3)	0.7504(2)	3.26(10)
C(46)	0.5255(4)	0.7209(2)	0.7412(2)	3.39(11)
C(47)	0.4115(4)	0.7328(2)	0.7206(2)	3.65(11)
C(48)	0.3791(3)	0.8240(2)	0.71061(18)	2.65(9)
C(49)	0.4080(2)	1.0870(2)	0.78199(16)	1.76(7)
C(50)	0.4633(2)	1.0748(2)	0.84093(17)	1.97(8)
C(51)	0.4619(3)	1.1427(2)	0.89960(17)	2.50(8)
C(52)	0.4022(3)	1.2262(2)	0.90030(19)	2.64(9)
C(53)	0.3429(3)	1.2388(2)	0.84285(19)	2.54(9)
C(54)	0.3455(2)	1.1711(2)	0.78525(18)	2.15(8)

C(55)	0.0059(2)	0.5985(2)	0.78194(16)	1.74(7)
C(56)	-0.0469(3)	0.6736(2)	0.82060(17)	2.20(8)
C(57)	-0.0434(3)	0.7689(2)	0.81090(18)	2.29(8)
C(58)	0.0199(3)	0.7948(2)	0.76221(18)	2.42(8)
C(59)	0.0761(3)	0.7241(2)	0.72405(18)	2.46(8)
C(60)	0.0694(2)	0.6287(2)	0.73307(18)	2.23(8)
C(61)	-0.1261(2)	0.4537(2)	0.82165(14)	1.92(7)
C(62)	-0.1391(3)	0.3717(2)	0.85117(18)	2.45(8)
C(63)	-0.2458(3)	0.3394(3)	0.8695(2)	3.04(10)
C(64)	-0.3463(3)	0.3866(3)	0.85996(19)	3.31(10)
C(65)	-0.3386(3)	0.4663(3)	0.83079(19)	3.14(9)
C(66)	-0.2305(3)	0.4976(2)	0.81157(18)	2.44(8)
C(67)	0.0176(2)	0.4046(2)	0.73225(16)	1.71(7)
C(68)	0.0702(3)	0.3182(2)	0.73399(18)	2.23(8)
C(69)	0.0749(3)	0.2446(2)	0.67869(18)	2.38(8)
C(70)	0.0251(3)	0.2557(2)	0.61903(19)	2.56(8)
C(71)	-0.0300(3)	0.3401(2)	0.61498(18)	2.43(8)
C(72)	-0.0328(2)	0.4124(2)	0.67062(18)	2.14(8)
C(73)	0.1118(2)	0.4908(2)	0.85410(16)	1.93(7)
C(74)	0.0993(3)	0.4951(2)	0.92083(18)	2.22(8)
C(75)	0.1956(3)	0.5077(2)	0.9678(2)	2.76(9)
C(76)	0.3083(3)	0.5157(2)	0.9504(2)	3.26(10)
C(77)	0.3262(3)	0.5117(2)	0.8855(2)	2.97(9)
C(78)	0.2287(3)	0.5007(2)	0.8388(2)	2.32(8)
B(1)	0.4216(3)	1.0165(2)	0.71037(18)	1.70(8)
B(2)	0.0022(3)	0.4876(2)	0.79796(19)	1.85(8)
H(1)	0.108(2)	0.656(2)	0.5713(15)	2.7(8)
H(2)	0.160(2)	0.820(2)	0.5561(16)	3.3(8)
H(3)	0.353(2)	0.850(2)	0.5277(14)	2.2(7)
H(4)	0.731(2)	0.831(2)	0.5692(15)	2.8(8)
H(5)	0.867(3)	0.778(3)	0.642(2)	6.7(12)
H(6)	0.830(2)	0.627(2)	0.6721(15)	2.4(7)
H(7)	0.559(2)	0.388(2)	0.7099(15)	2.6(8)
H(8)	0.354(2)	0.353(2)	0.7229(16)	3.4(8)
H(9)	0.213(3)	0.402(2)	0.6542(17)	4.3(9)
H(10)	0.310(2)	0.897(2)	0.8492(15)	3.2(8)
H(11)	0.331(2)	0.734(2)	0.8755(14)	2.7(7)
H(12)	0.191(3)	0.681(2)	0.9375(17)	4.3(9)
H(13)	-0.187(2)	0.656(2)	0.9711(13)	0.9(6)
H(14)	-0.381(3)	0.673(2)	0.9254(17)	5.2(10)
H(15)	-0.406(2)	0.831(2)	0.9029(16)	3.2(9)
H(16)	-0.281(2)	1.099(2)	0.8244(15)	2.7(7)
H(17)	-0.132(2)	1.143(2)	0.7609(17)	3.8(9)
H(18)	0.056(2)	1.113(2)	0.7868(15)	2.3(8)
H(19)	0.190(2)	0.9651(19)	0.7323(13)	1.5(6)
H(20)	0.013(2)	0.953(2)	0.6681(14)	2.3(7)
H(21)	0.001(2)	1.001(2)	0.5632(14)	2.2(7)
H(22)	0.170(2)	1.046(2)	0.5247(15)	2.4(7)
H(23)	0.344(2)	1.065(2)	0.5871(16)	3.8(9)
H(24)	0.565(2)	1.1952(19)	0.7410(13)	1.1(6)

H(25)	0.728(2)	1.2510(19)	0.6934(12)	0.6(5)
H(26)	0.787(2)	1.167(2)	0.5927(15)	3.5(8)
H(27)	0.684(3)	1.009(2)	0.5517(19)	5.4(11)
H(28)	0.532(2)	0.954(2)	0.6013(16)	3.5(9)
H(29)	0.623(2)	0.934(2)	0.7423(13)	1.1(7)
H(30)	0.681(2)	0.790(2)	0.7621(16)	3.5(9)
H(31)	0.548(2)	0.660(2)	0.7447(16)	3.5(8)
H(32)	0.352(3)	0.681(2)	0.7128(19)	6.5(12)
H(33)	0.297(2)	0.831(2)	0.6975(14)	2.0(7)
H(34)	0.502(2)	1.0204(18)	0.8433(12)	0.6(6)
H(35)	0.499(2)	1.131(2)	0.9444(16)	3.5(8)
H(36)	0.401(2)	1.270(2)	0.9377(15)	2.6(8)
H(37)	0.304(2)	1.2967(19)	0.8440(12)	1.0(6)
H(38)	0.305(2)	1.1846(19)	0.7476(13)	1.3(6)
H(39)	-0.088(2)	0.659(2)	0.8506(13)	1.3(7)
H(40)	-0.082(2)	0.819(2)	0.8366(15)	2.9(7)
H(41)	0.025(2)	0.864(2)	0.7568(14)	2.5(7)
H(42)	0.124(2)	0.7419(19)	0.6930(13)	1.2(6)
H(43)	0.107(2)	0.577(2)	0.7066(15)	2.7(7)
H(44)	-0.065(2)	0.335(2)	0.8583(14)	2.5(7)
H(45)	-0.244(2)	0.289(2)	0.8888(16)	3.5(9)
H(46)	-0.417(2)	0.361(2)	0.8739(15)	3.3(8)
H(47)	-0.410(2)	0.500(2)	0.8210(16)	3.7(9)
H(48)	-0.230(2)	0.549(2)	0.7917(16)	3.2(9)
H(49)	0.104(2)	0.3088(18)	0.7713(12)	0.4(6)
H(50)	0.117(2)	0.186(2)	0.6854(13)	1.4(6)
H(51)	0.026(2)	0.210(2)	0.5795(14)	2.1(7)
H(52)	-0.067(2)	0.350(2)	0.5747(15)	2.6(7)
H(53)	-0.082(2)	0.467(2)	0.6617(15)	3.2(8)
H(54)	0.021(2)	0.4933(18)	0.9373(12)	0.8(6)
H(55)	0.177(3)	0.510(2)	1.0111(18)	4.7(10)
H(56)	0.374(2)	0.523(2)	0.9839(14)	1.7(6)
H(57)	0.407(2)	0.522(2)	0.8673(16)	3.8(8)
H(58)	0.248(2)	0.507(2)	0.7933(16)	3.5(8)

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$