Vinyl Ruthenium-Modified Biphenyl and 2,2'-Bipyridines

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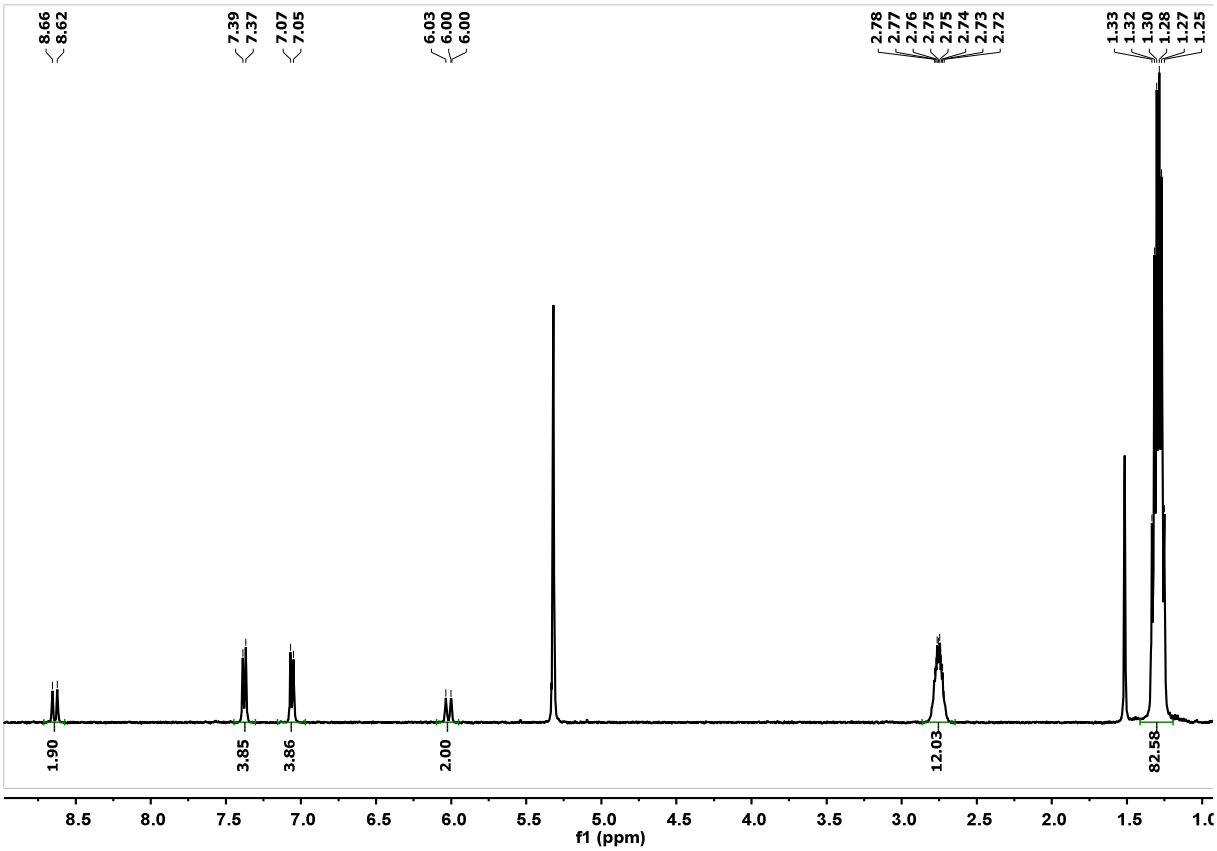

Figure 1. ^{1}H NMR spectrum of complex **1**.

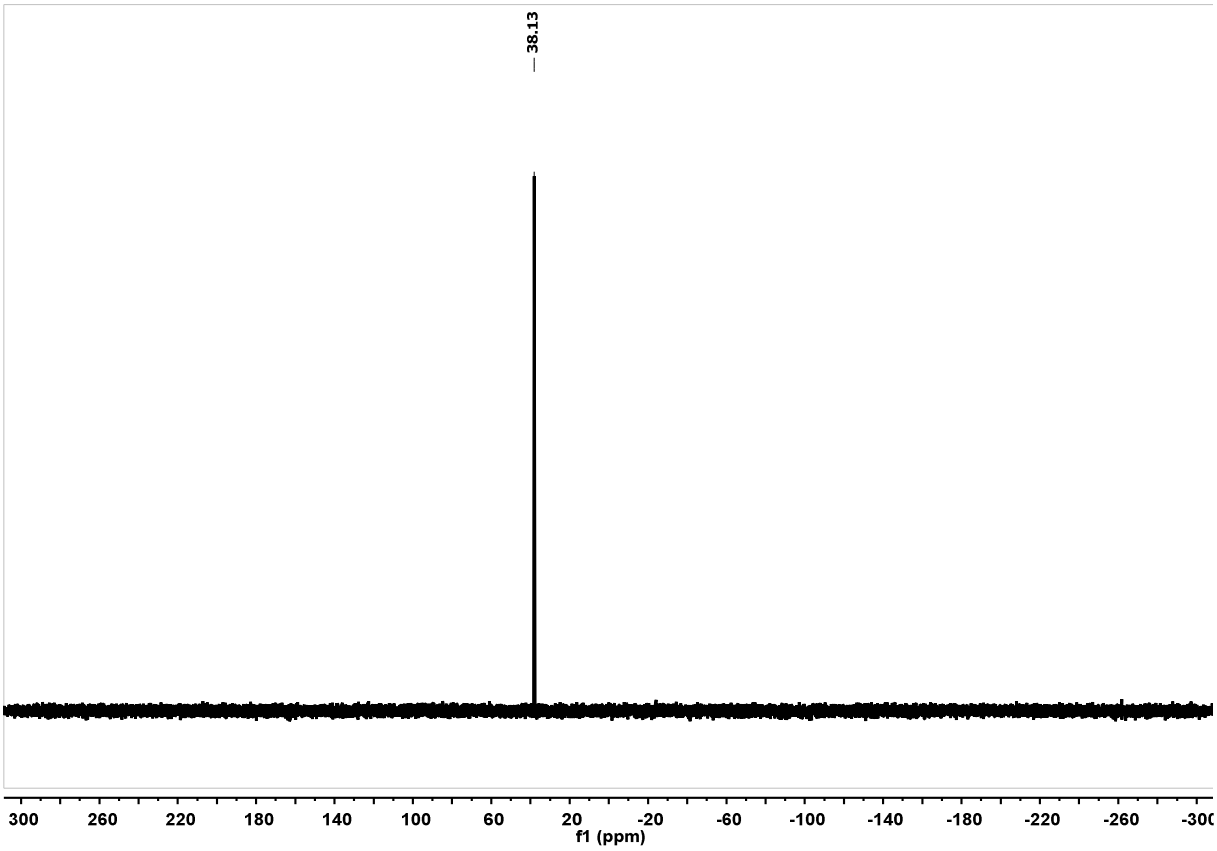

Figure 2. ^{31} P NMR spectrum of complex **1**.

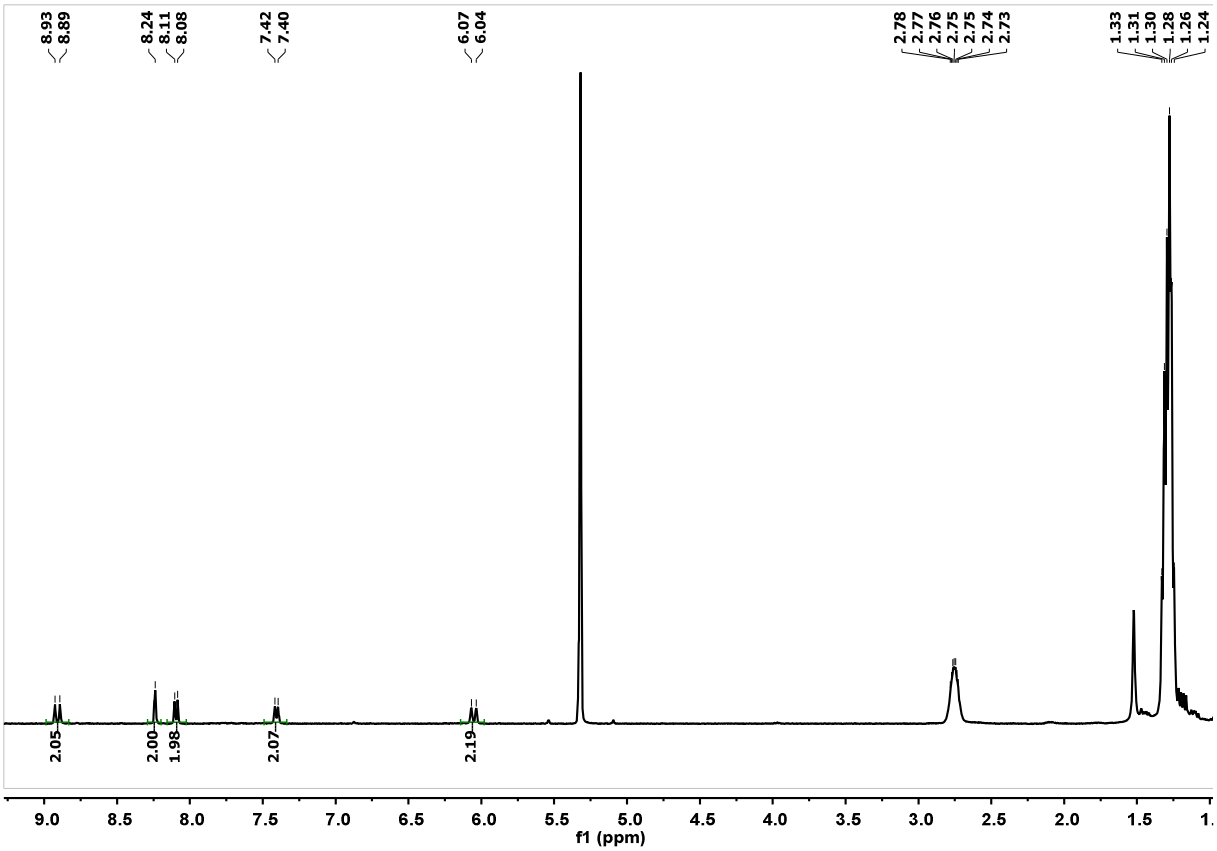

Figure 3. ^{1}H NMR spectrum of complex **2**.

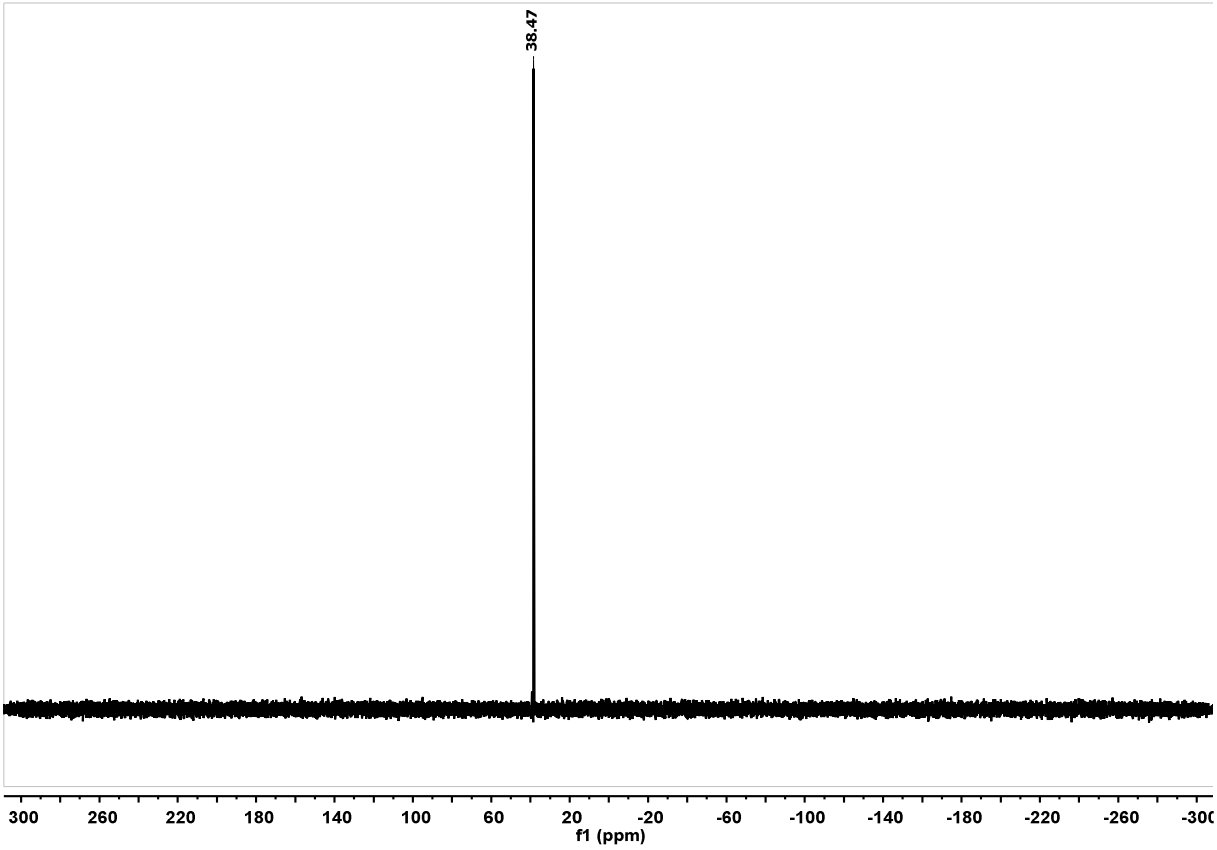

Figure 4. ^{31} P NMR spectrum of complex **2**.

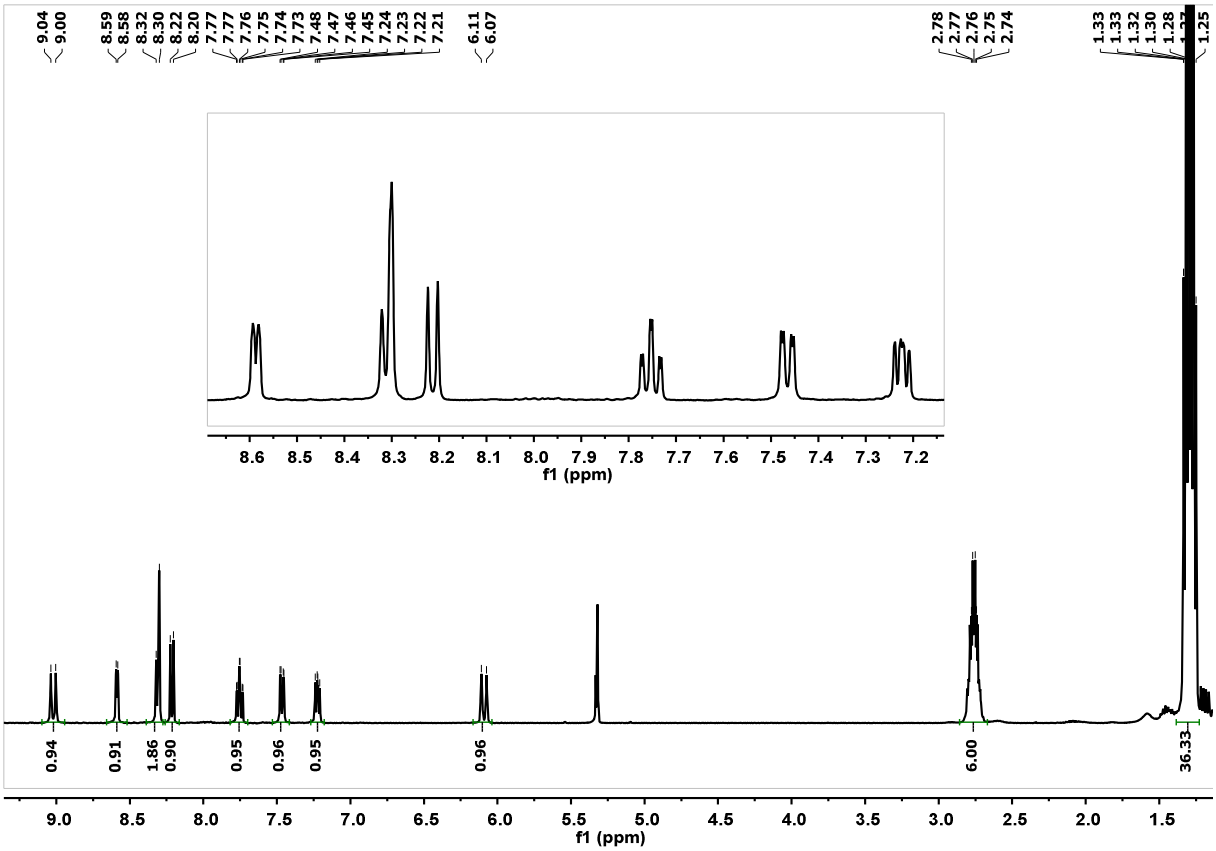

Figure 5. ^{1}H NMR spectrum of complex **3**.

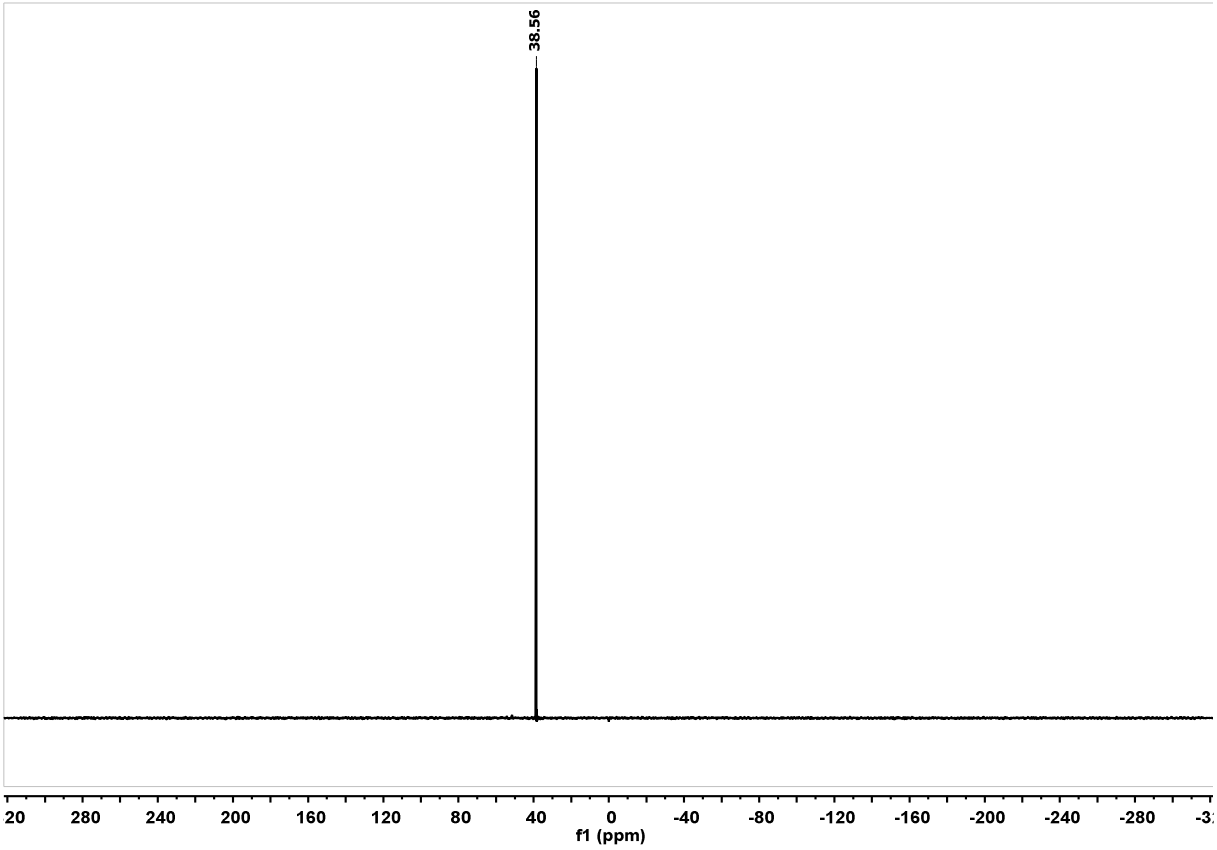

Figure 6. ^{31} P NMR spectrum of complex **3**.

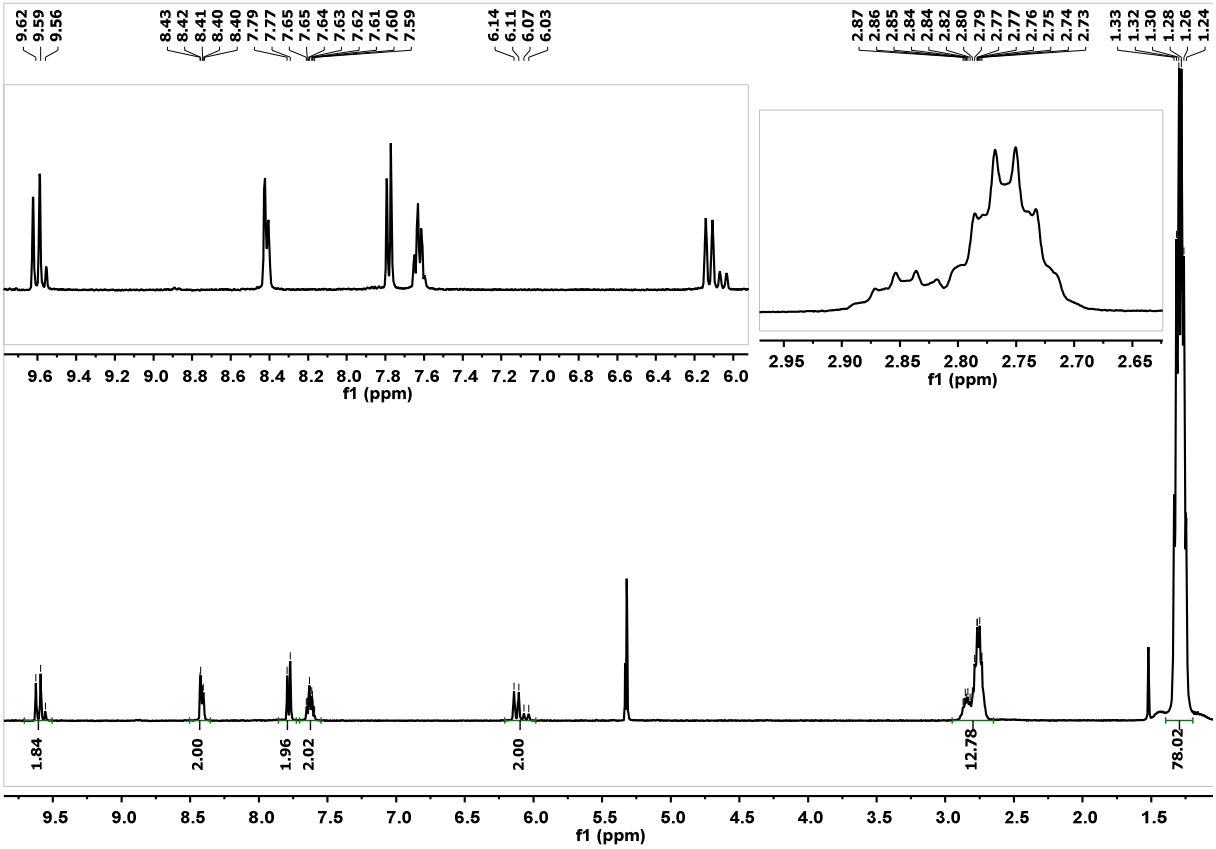

Figure 7. ^{1}H NMR spectrum of complex **4a**.

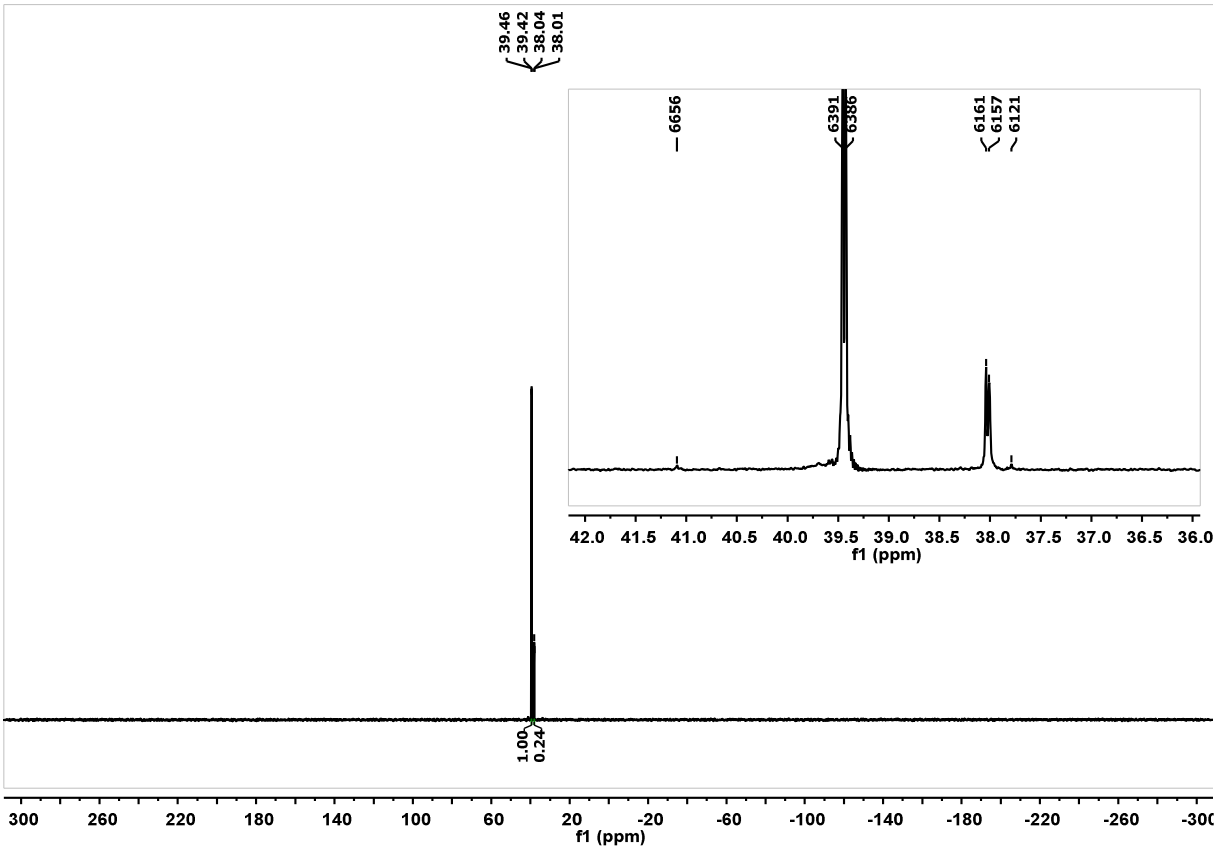

Figure 8. ^{31} P NMR spectrum of complex **4a**.

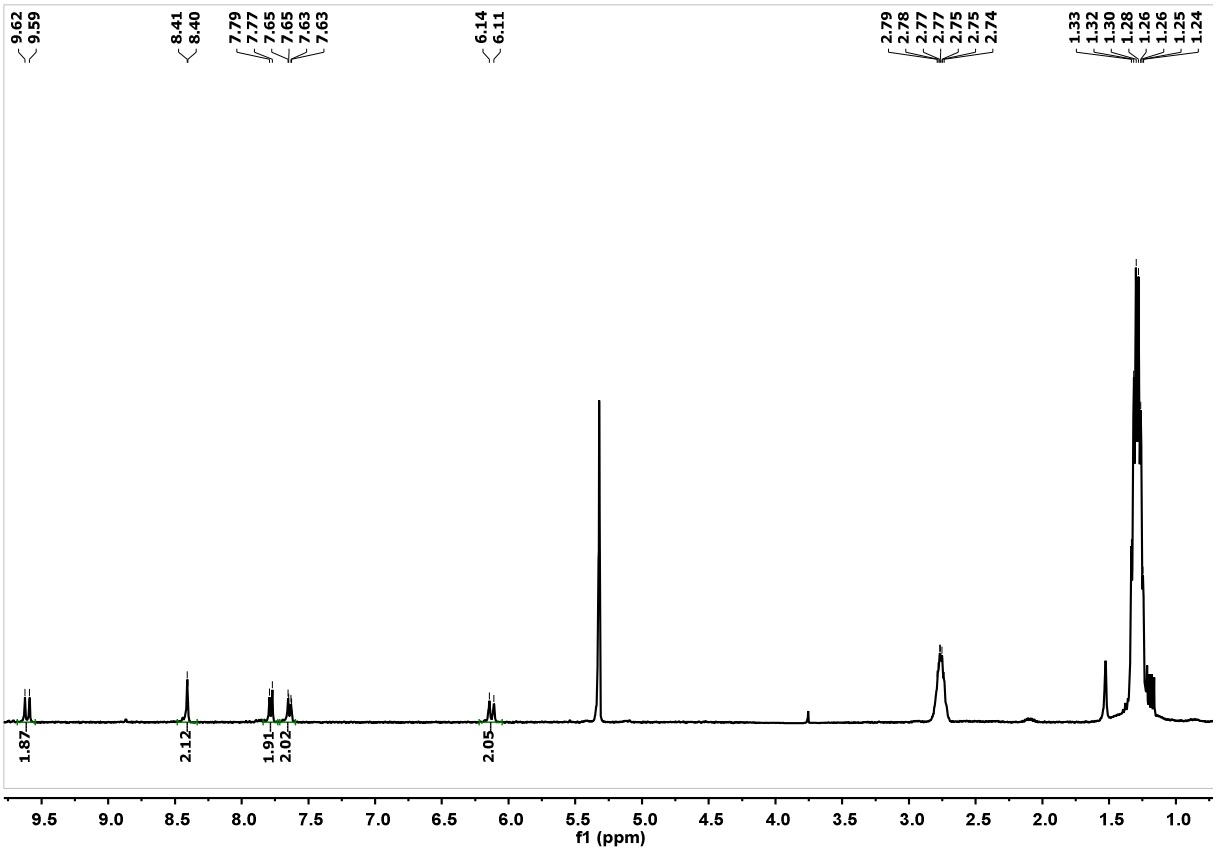

Figure 9. ^{1}H NMR spectrum of complex **4b**.

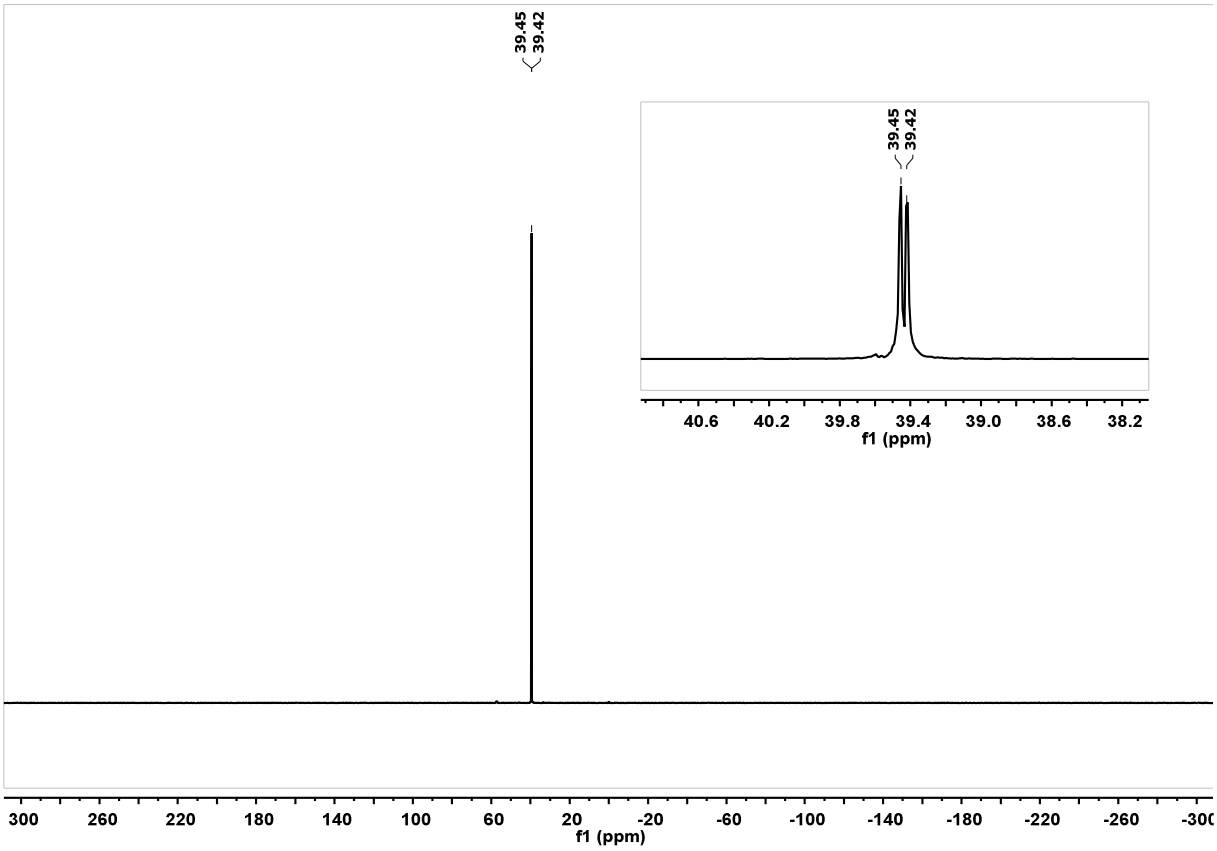

Figure 10. ^{31} P NMR spectrum of complex **4b**.

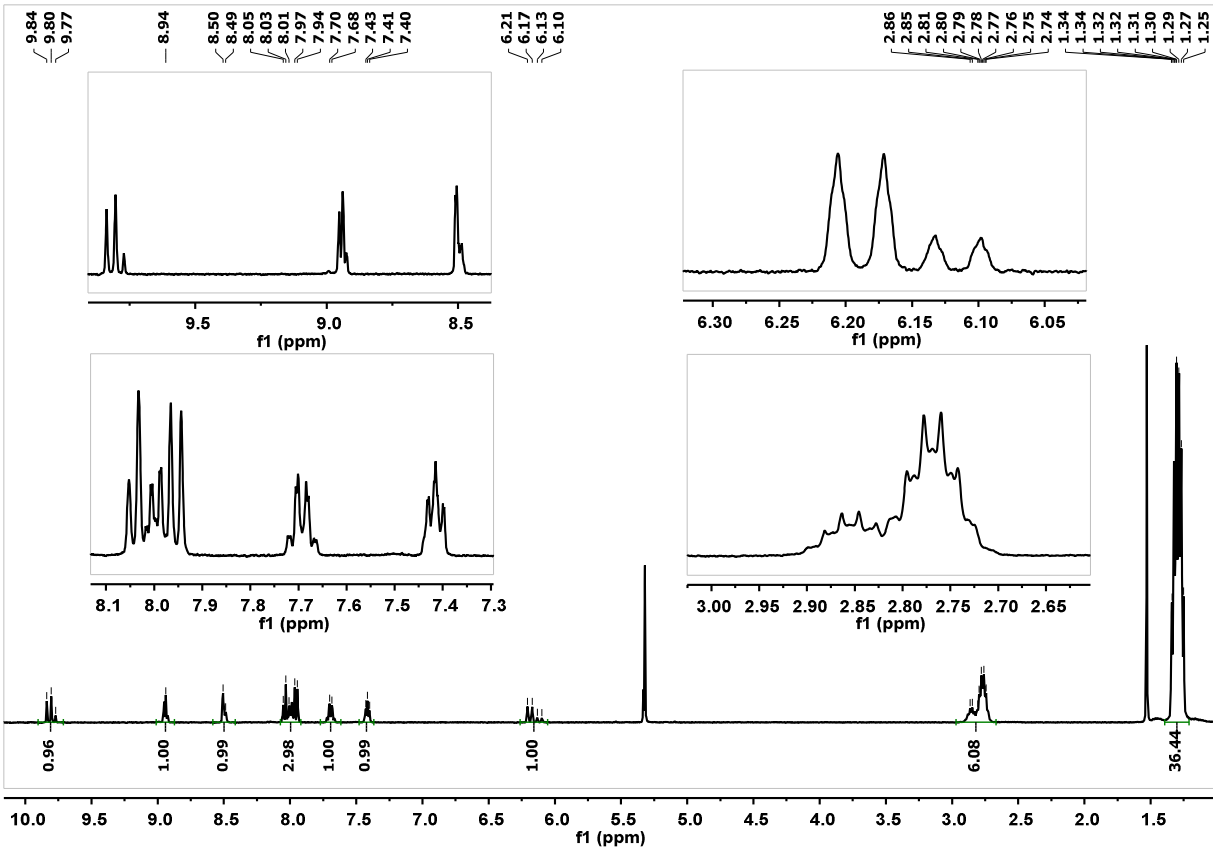

Figure 11. ^{1}H NMR spectrum of complex **5**.

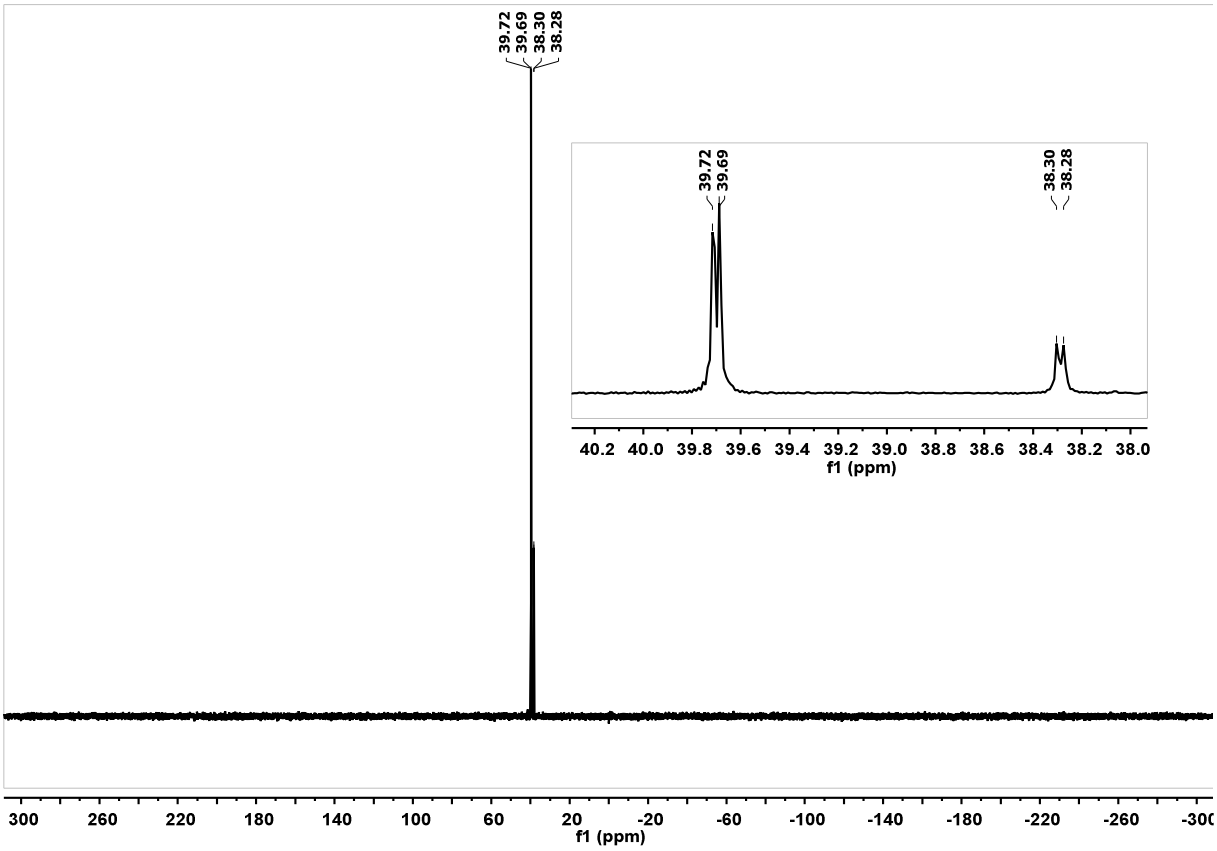

Figure 12. ^{31} P NMR spectrum of complex **5**.

Table 1. Characteristic NMR data for complexes **1-5.**

complex	δ(Ru-C*H*) [ppm], $^{3}J_{H\text{-}H}$ [Hz]	δ(Ru-CH=C*H*) [ppm]	δ (C*H*, bridge) [ppm]	δ (^{31}P) [ppm]
1	8.64, 13.3	6.02	7.38, 7.06	38.13
2	8.92, 13.6	6.06	8.24, 7.42, 8.11	38.49
3	9.02, 13.6	6.09	8.30, 7.47, 8.21 8.31, 7.75, 7.22, 8.59	38.56
4a	9.61, 13.8	6.12	8.44 - 8.39, 7.66 - 7.59, 7.80 - 7.76	39.46, 39.43
4b	9.61, 13.8	6.13	8.41, 7.64, 7.79	39.42, 39.45
5	9.82, 13.8	6.19	8.52 - 8.47, 7.73 - 7.65, 7.95 - 7.93 8.06 - 8.02, 8.02 - 7.97, 7.44 - 7.39, 8.96 - 8.91	39.71, 39.68

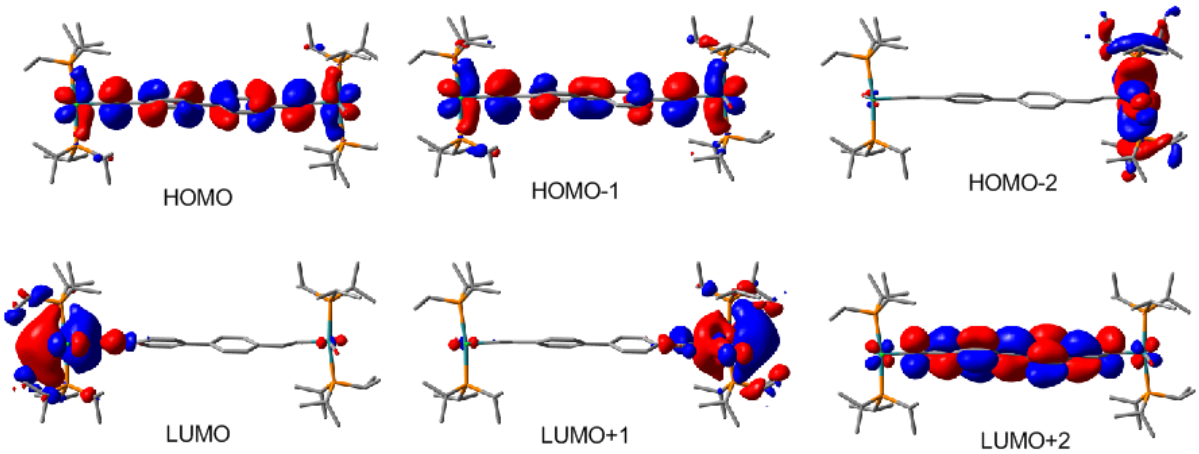

Figure 13. Isodensity plots of selected MOs of the full model complex **1**[c].

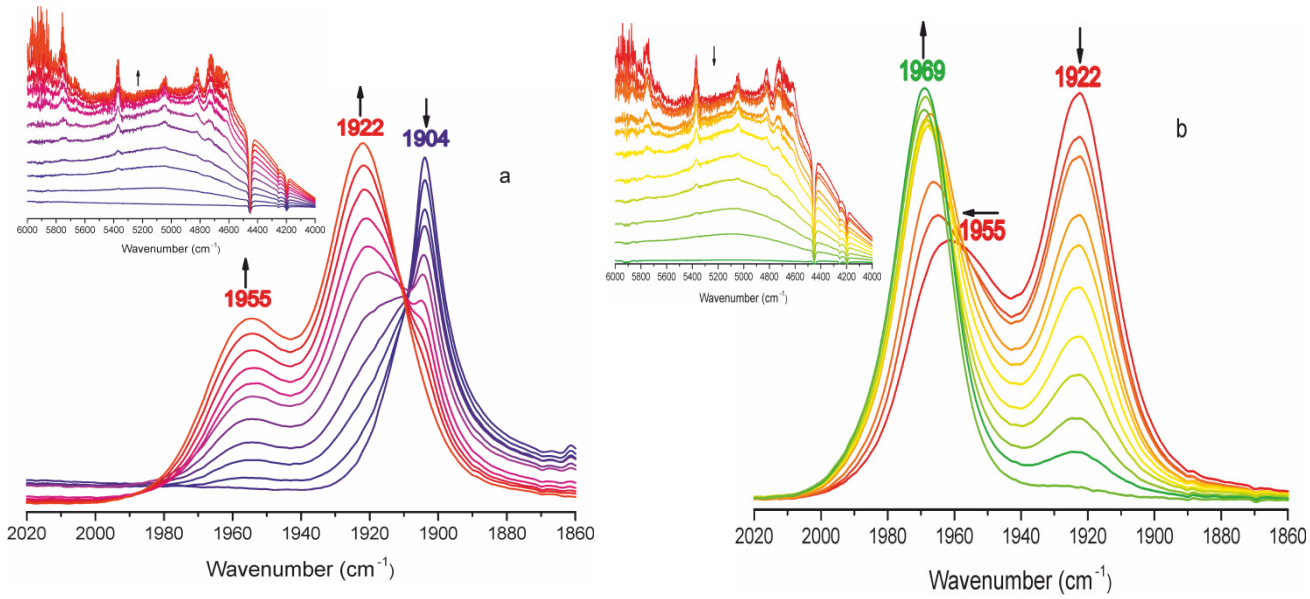

Figure 14. Spectroscopic changes during a) the first, and b) the second oxidation of complex **1** in the range of the Ru(CO) absorptions in the IR (1,2-$C_2H_4Cl_2$ / NBu_4^+ PF_6^- (0.2 M) at 293 K. The insert shows the growth and the collapse of the NIR band during the first/second oxidation.

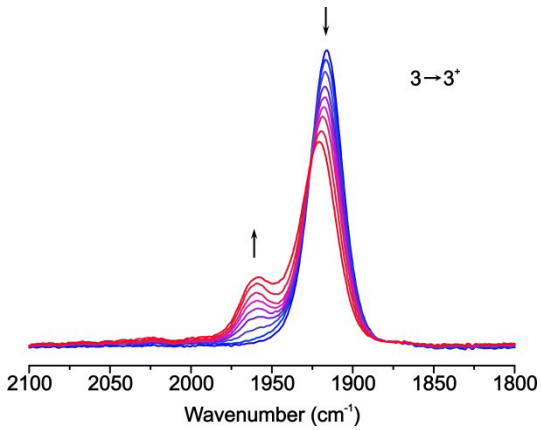

Figure 15. Spectroscopic changes during the oxidation of complex **3** in the range of the Ru(CO) absorptions in the IR (1,2-$C_2H_4Cl_2$ / NBu_4^+ PF_6^- (0.2 M) at 293 K.

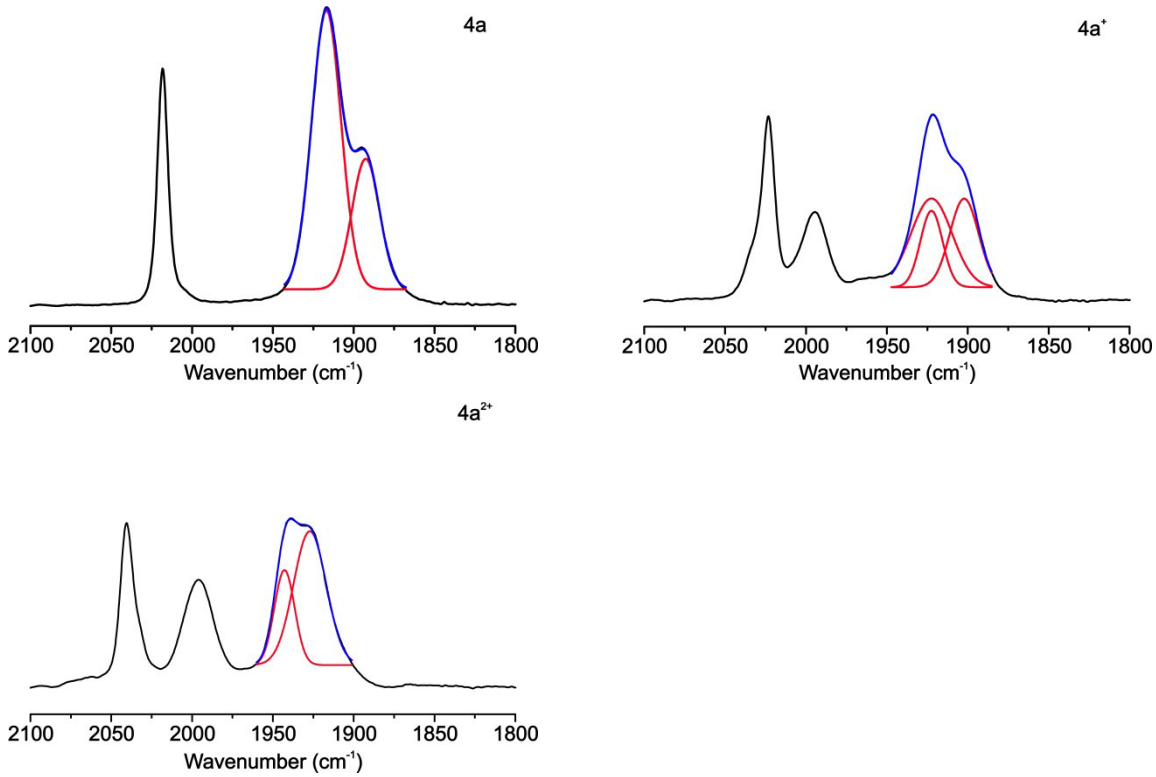

Figure 16. Deconvolution of the IR bands of complex a) **4a**, b) **4a**$^{+}$, and c) **4a**$^{2+}$.

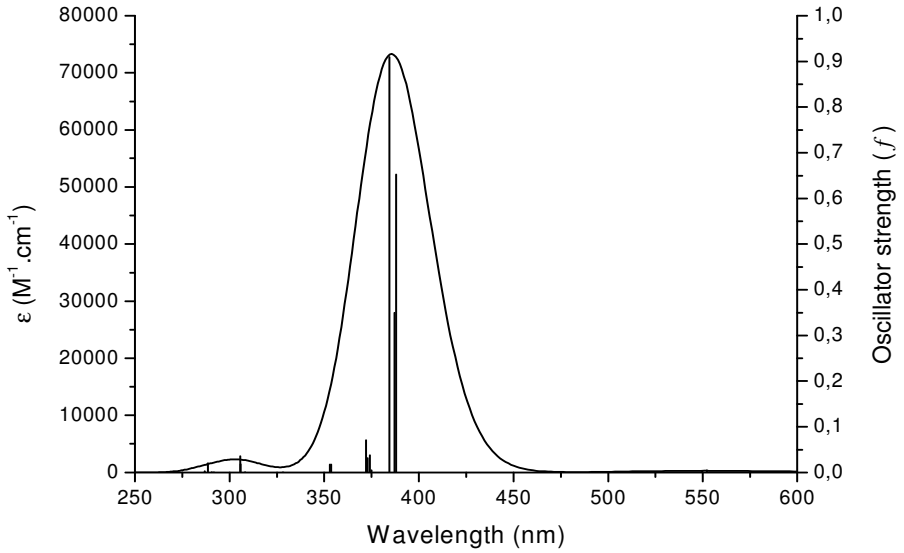

Figure 17. TD-DFT calculated electronic spectrum of complex **1**^{c}.

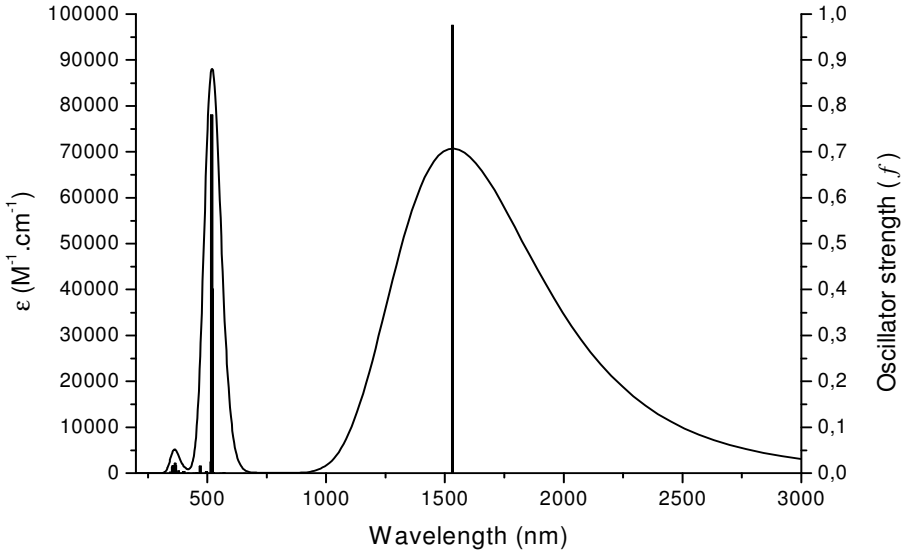

Figure 18. TD-DFT calculated electronic spectrum of complex $\mathbf{1}^{c+}$.

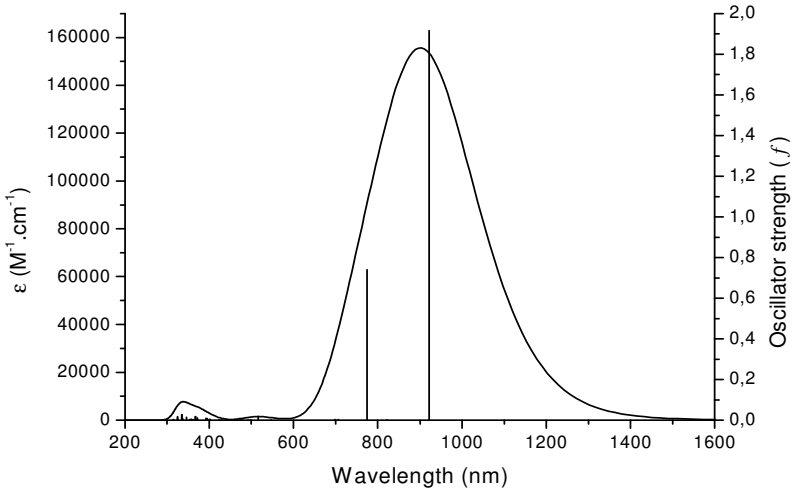

Figure 19. TD-DFT calculated electronic spectrum of complex $\mathbf{1}^{c\,2+}$.

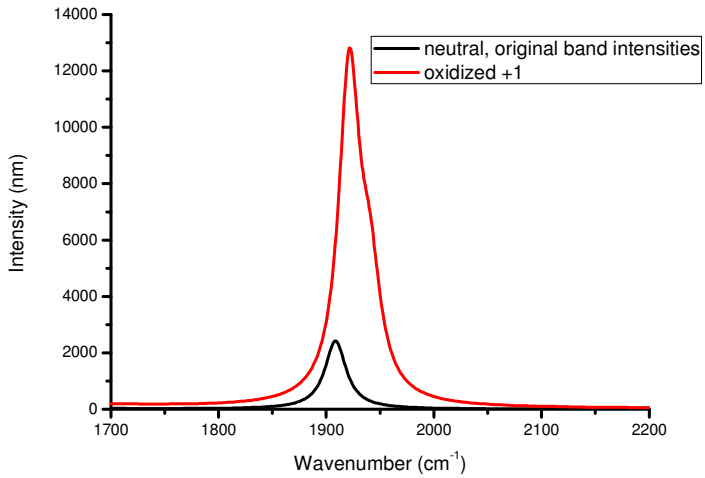

Figure 20. Simulated IR spectra of $\mathbf{1}^{c}$ and $\mathbf{1}^{c+}$ from DFT calculations.

Table 2. TD-DFT (PBE0/PCM-CH_2Cl_2) calculated lowest lying transitions of $\mathbf{2}^{c}$ with oscillator strength larger than 0.005. MOs involved in calculated transitions are depicted in Figure 17.

Major Contribution (%)	Wavelength (nm)	Oscillator Strength
HOMO → LUMO+1 (56) HOMO–1 → LUMO+1 (32)	486	0.0076
HOMO → LUMO+2 (62) HOMO–1 → LUMO+2 (28)	477	0.0076
HOMO → LUMO (95)	407	2.0485
HOMO–5 → LUMO+1 (90)	367	0.0085
HOMO–4 → LUMO+2 (72) HOMO–3 → LUMO+1 (16)	362	0.0087
HOMO–3 → LUMO+1 (64) HOMO–4 → LUMO+2 (17)	362	0.0019
HOMO–2 → LUMO+2 (80)	356	0.0001
HOMO–1 → LUMO (94)	337	0.0019
HOMO–1 → LUMO+1 (52) HOMO → LUMO+1 (33)	333	0.0023
HOMO–1 → LUMO+2 (30) HOMO → LUMO+2 (22) HOMO → LUMO+5 (21) HOMO–1 → LUMO+5 (10)	324	0.0001

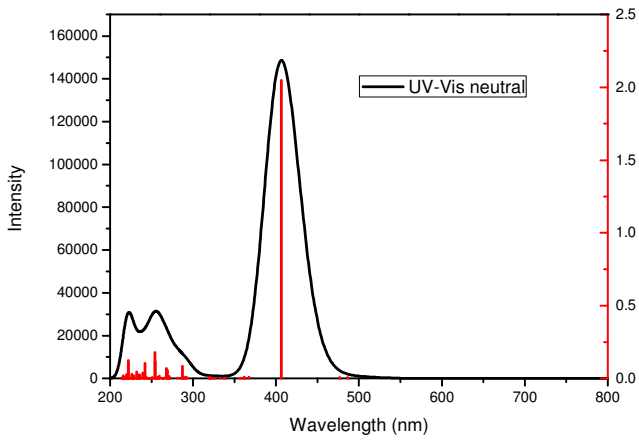

Figure 21. Simulated UV-VIS spectra of **2**[c] from TD-DFT calculations. Red vertical lines indicate the calculated transitions.

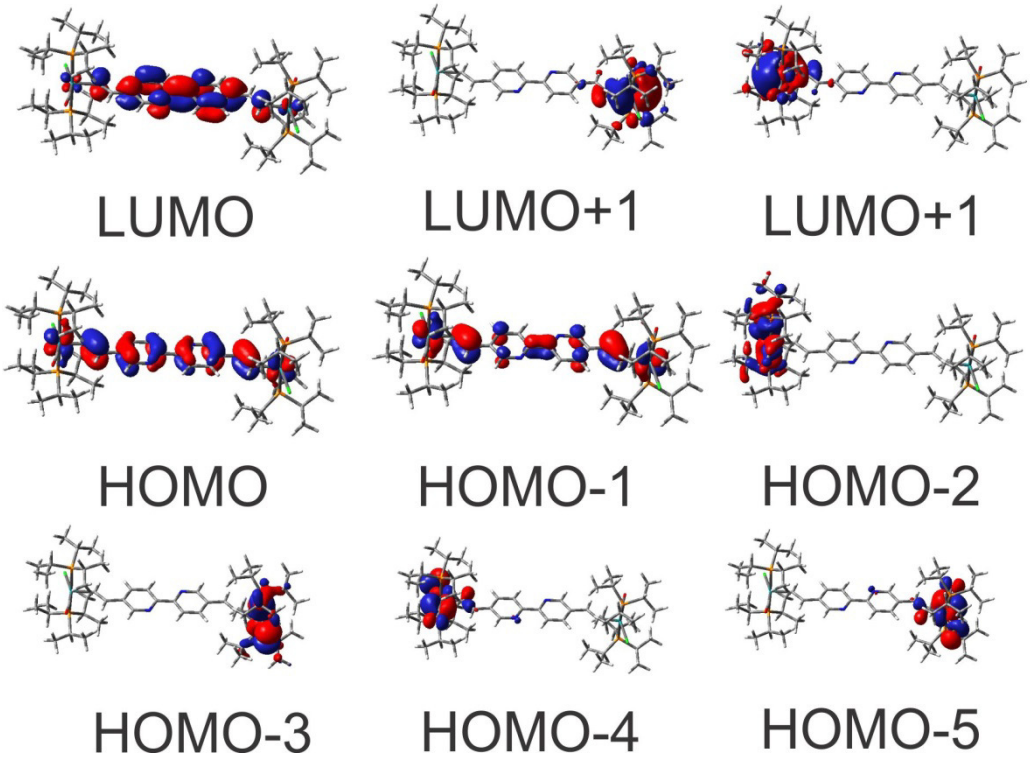

Figure 22. Shapes of FMOs of **2**[c] involved in the lowest excitations.

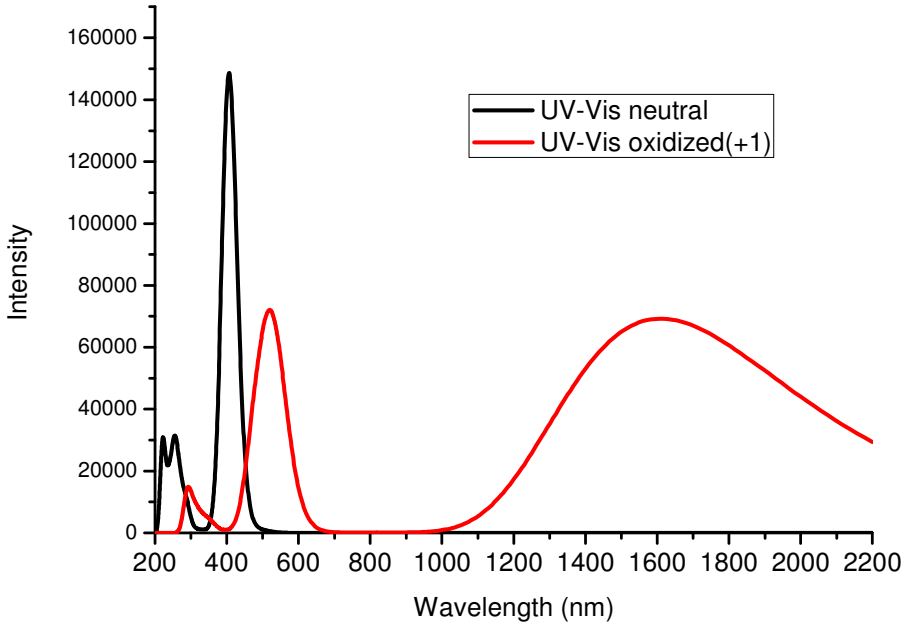

Figure 23. Simulated UV-VIS spectra of $\mathbf{2^c}$ and $\mathbf{2^{c+}}$ from TD-DFT calculations.

Table 3. The comparison of experimental and calculated CO stretching frequencies of $\mathbf{3^c}$**.**

	Neutral	Oxidized (+1)
Experimental	1917	1960
Calculated	1909	1962

scaling factor = 0.9575

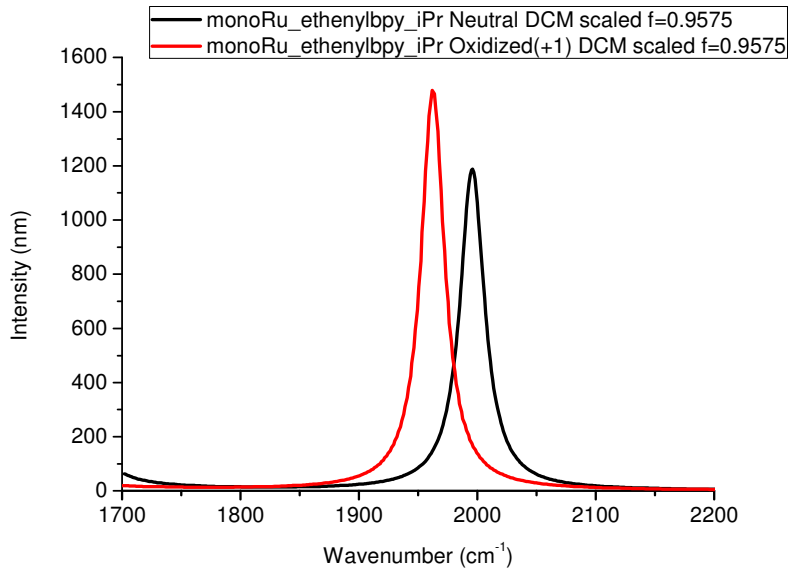

Figure 24. Simulated IR spectra of $\mathbf{3^c}$ and $\mathbf{3^{c+}}$ from DFT calculations.

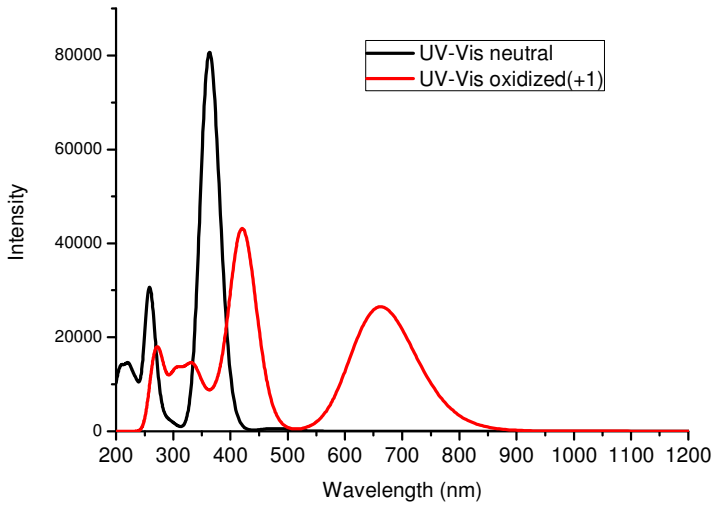

Figure 25. Simulated UV-VIS spectra of **3**^{c} and **3**$^{c+}$ from TD-DFT calculations.

Table 4. TD-DFT (PBE0/PCM-CH_2Cl_2) calculated lowest lying transitions of **4a**^{c} with oscillator strength larger than 0.005. MOs involved in calculated transitions are depicted in Figure 21.

Major Contribution (%)	Wavelength (nm)	Oscillator Strength
HOMO → LUMO (94)	470	1.4527
HOMO → LUMO+1 (58) HOMO–1 → LUMO+1 (29)	461	0.0217
HOMO → LUMO+2 (56) HOMO–1 → LUMO+2 (30)	459	0.0423
HOMO–2 → LUMO (97)	401	0.0715
HOMO–1 → LUMO (55) HOMO–3 → LUMO (43)	393	0.0094
HOMO–3 → LUMO (55) HOMO–1 → LUMO (43)	381	0.0319
HOMO–6 → LUMO+2 (86)	367	0.0298
HOMO–7 → LUMO+1 (85)	367	0.0130
HOMO–5 → LUMO+1 (80)	363	0.0015
HOMO–4 → LUMO+2 (81)	363	0.0007
HOMO → LUMO+3 (92)	354 (state 11)	0.3025
HOMO–11 → LUMO (50) HOMO–13 → LUMO (21)	271 (state 45)	0.2271

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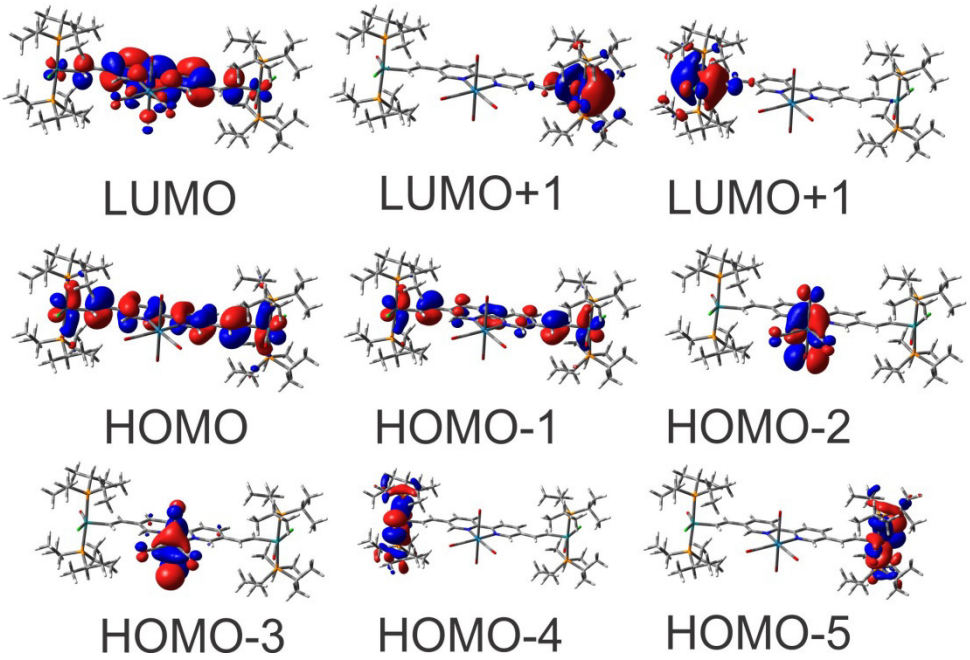

Figure 26. Shapes of FMOs of **4a**^{c} involved in the lowest excitations.

Table 5. Comparison of experimental and calculated CO stretching frequencies of **5.**

	Neutral				Oxidized (+1)			
	Re	Re	Ru	Re	Re	Re	Ru	Re
Exp	2020	1918	1918	1897	2038	1939	1986	1922
Calc	2021 sym in phase	1918 equator + weakly coupled Ru	1915 + weakly coupled Re equat	1900 sym out of phase	2026 sym in phase	1928 equat, Ru is almost not coupled	1971 equat Re is almost not coupled	1909 sym out of phase

frequency scaling f = 0.9575

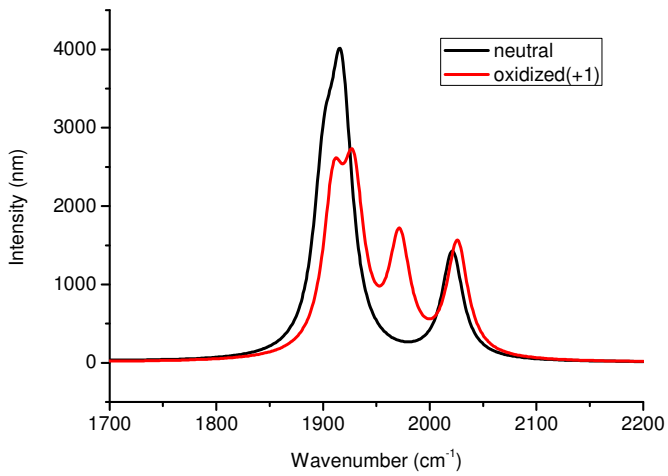

Figure 27. Simulated IR spectra of **5**^{c} and **5**$^{c+}$ from DFT calculations.

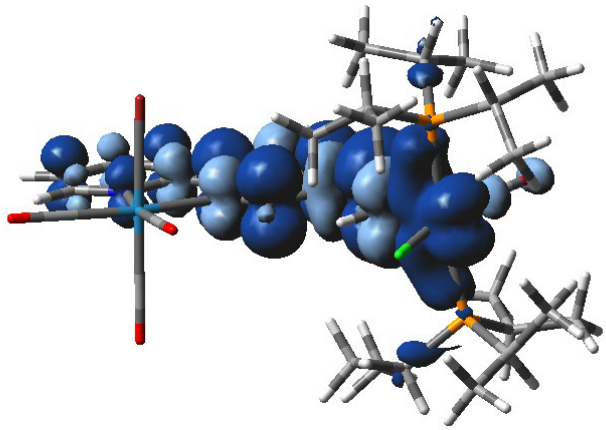

Figure 28. Spin density in the optimized complex **5**$^{c+}$.

Table 6. The comparison of TD DFT calculated transitions with experimental spectra of **5**^{c} and **5a**$^{c+}$**.**

	Neutral	Oxidized(+1)
Experimental λ (ε)	292 (24000), 361 (11000), 453 (24000)	300 (23000), 375 (6000)
Calculated λ (f)^{a}	275 (0.316), 345 (0.173), 432 (0.607)	417 (0.263), 595 (0.236)

^{a}Oscillator strength.

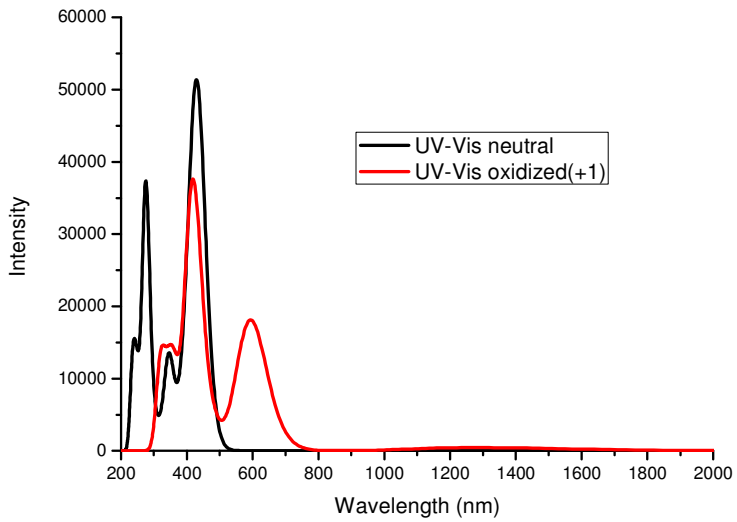

Figure 29. Calculated UV-Vis-NIR absorption spectra of complex **5**^{c} and **5**$^{c+}$.

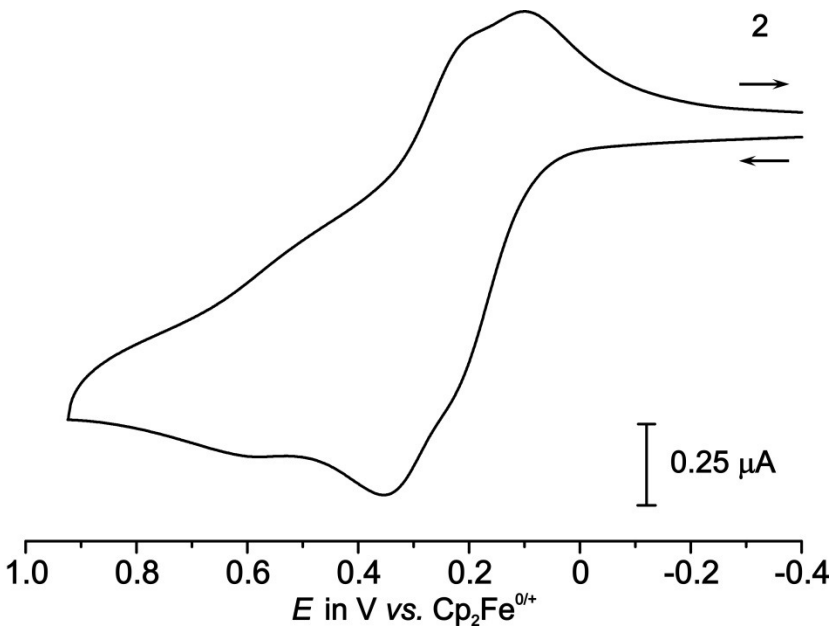

Figure 30. Representative voltammogram of complex 2 in CH_2Cl_2/NBu_4^+ $B\{C_6H_3(CF_3)_2\text{-}3,5]^-$ without added oxidant at v = 0.1 V/s and at r. t.

Table 7. Selected bond parameters for the two independent molecules in the unit cell of complex **5**.

bond lengths *d*[Å]; angles ∡[deg]	molecule 1	molecule 2
d [Re-N_{Ru}]	2.185(11)	2.166(14)
d [Re-N]	2.178(12)	2.140(17)
d [Re-Br]	2.584(3)	2.600(3)
d [Re-$C_{CO,eq,Ru}$]	1.928(18)	1.942(18)
d [Re-$C_{CO,ap}$]	2.140(15)	1.961(18)
d [Re-$C_{CO,eq}$]	1.928(16)	1.930(2)
d [C_{bipy}-$C_{vinyl,\beta}$]	1.46(2)	1.43(2)
d [$C_{vinyl,\alpha}$-$C_{vinyl,\beta}$]	1.36(2)	1.36(2)
d [Ru-$C_{vinyl,\alpha}$]	1.935(13)	1.944(18)
d [Ru-P_{syn-Br}]	2.423(5)	2.441(4)
d [Ru-$P_{anti-Br}$]	2.455(5)	2.429(4)
d [Ru-Cl]	2.495(3)	2.503(4)
d [Ru-C_{CO}]	1.85(2)	1.87(2)
d [Ru-(P,P,Cl,CO)]	0.189	0.199
∡[(py);(py_{Ru})]	4.6	3.3
∡[(Ru, Vinyl);(bipy)]	15.2	17.8
∡[(Re, N, N);(bipy)]	4.6	4.9
∡[(CO, Ru, Cl);(bipy)]	25.7	25.5

Table 8. Crystal data and structure refinement for complex **5**.

Empirical formula	C40 H57 Br Cl N2 O4 P2 Re Ru
Formula weight	1094.45
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	triclinic, P-1
Unit cell dimensions	a = 15.517(3) A α = 81.96(3) deg.
	b = 16.217(3) A β = 69.36(3) deg.
	c = 20.349(4) A γ = 68.36(3) deg.
Volume	4453.6(15) $Å^3$
Z, Calculated density ρ	1.632 Mg/m^3
Absorption coefficient μ	4.123 mm^-1
F(000)	2176
Crystal size, color, habit	0.5 x 0.4 x 0.3 mm, red block
Theta range for data collection	1.71 to 28.39 deg.
Limiting indices	$-20 \leq h \leq 20$, $-21 \leq k \leq 21$, $-26 \leq l \leq 26$
Reflections collected / unique	75201 / 21355 [R(int) = 0.2076]
Completeness to theta = 28.39	95.5 %
Absorption correction	Integration
Max. and min. transmission	0.7230 and 0.5587
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	21355 / 0 / 929
Goodness-of-fit on F^2	1.052
Final R indices [I>2sigma(I)]	$R1$ = 0.1231, w$R2$ = 0.2615
R indices (all data)	$R1$ = 0.1750, w$R2$ = 0.2987
Largest diff. peak and hole	4.871 and -3.944 eA^{-3}

Table 9. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **5**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Re(1)	2458(1)	10595(1)	9501(1)	30(1)
Ru(1)	1730(1)	6177(1)	8195(1)	31(1)
Cl(1)	2823(2)	5466(2)	7041(2)	18(1)
Br(1)	2204(2)	11335(2)	8341(1)	64(1)
P(1)	767(3)	7313(3)	7574(2)	32(1)
N(1)	3066(10)	9348(7)	8937(6)	27(3)
O(1)	274(11)	10813(9)	10150(9)	53(4)
C(1)	4008(11)	9082(9)	8540(8)	25(3)
Re(2)	2439(1)	10647(1)	4491(1)	33(1)
Ru(2)	1800(1)	6138(1)	3249(1)	25(1)
Br(2)	2173(2)	11363(2)	3320(1)	56(1)
Cl(2)	2900(3)	5428(2)	2091(2)	26(1)
P(2)	2580(4)	4882(3)	8798(2)	39(1)
O(2)	2791(11)	9608(8)	10845(7)	50(3)
N(2)	4005(8)	10384(8)	8947(7)	24(2)
C(2)	4455(11)	8268(10)	8170(8)	28(3)
P(3)	788(3)	7220(3)	2617(2)	31(1)
C(3)	3927(12)	7759(9)	8203(9)	30(3)
O(3)	2009(11)	12348(8)	10180(8)	49(4)
N(3)	3026(11)	9403(10)	3944(7)	36(3)
P(4)	2689(3)	4871(3)	3830(2)	31(1)
O(4)	216(11)	6883(10)	9554(9)	57(4)
N(4)	3958(12)	10439(11)	3941(9)	44(4)
C(4)	2930(13)	8020(8)	8635(8)	30(3)
O(5)	283(9)	10841(10)	5137(8)	48(3)
C(5)	2519(10)	8843(9)	8985(7)	22(3)
C(6)	4547(12)	9650(10)	8549(9)	29(3)
O(6)	2877(10)	9755(9)	5728(13)	79(7)
O(7)	1952(10)	12421(8)	5151(7)	41(3)
C(7)	5520(14)	9482(10)	8155(8)	34(4)
O(8)	285(9)	6841(8)	4611(6)	36(3)
C(8)	5964(13)	10047(10)	8198(9)	32(3)
C(9)	5398(14)	10825(11)	8611(9)	35(4)
C(10)	4411(13)	10964(12)	8971(9)	36(4)
C(11)	1092(13)	10715(10)	9895(9)	34(4)
C(12)	2843(11)	9919(9)	10393(8)	24(3)
C(13)	2145(14)	11706(10)	9924(10)	42(4)
C(14)	2263(13)	7548(11)	8695(9)	35(4)
C(15)	2455(12)	6892(10)	8262(9)	30(3)
C(16)	783(14)	6617(12)	9041(11)	45(5)
C(21)	-163(14)	6929(12)	7472(10)	39(4)
C(22)	-767(15)	6647(14)	8186(12)	53(5)
C(23)	303(16)	6149(13)	6953(12)	52(5)
C(24)	1419(15)	7554(12)	6643(10)	47(5)
C(25)	762(14)	8178(14)	6228(10)	52(6)
C(26)	2389(19)	7787(13)	6581(12)	56(6)
C(27)	-962(16)	8943(13)	7904(13)	57(6)
C(28)	-8(15)	8378(11)	8060(10)	42(4)
C(29)	611(19)	8975(12)	7950(11)	53(5)
C(30)	2160(18)	3974(14)	8775(10)	51(5)
C(31)	1045(18)	4280(12)	9051(13)	54(6)
C(32)	2490(20)	3612(17)	8018(12)	79(9)

C(33)	2520(20)	4922(14)	9744(11)	59(6)
C(34)	1780(30)	4620(20)	10280(12)	83(10)
C(35)	2500(20)	5777(15)	9927(13)	73(8)
C(36)	3919(16)	4374(12)	8388(11)	46(5)
C(37)	4398(18)	3415(13)	8628(11)	55(6)
C(38)	4461(18)	4962(16)	8475(15)	62(6)
C(41)	3983(14)	9138(11)	3527(8)	34(4)
C(42)	4440(13)	8321(12)	3166(10)	38(4)
C(43)	3896(13)	7809(11)	3193(10)	36(4)
C(44)	2924(13)	8059(10)	3626(8)	30(3)
C(45)	2556(13)	8863(12)	3984(9)	36(4)
C(46)	4504(13)	9725(11)	3515(9)	37(4)
C(47)	5487(14)	9549(12)	3145(10)	39(4)
C(48)	5938(15)	10106(13)	3180(9)	43(4)
C(49)	5376(14)	10863(13)	3590(10)	41(4)
C(50)	4392(15)	11019(14)	3960(11)	46(4)
C(51)	1065(13)	10762(10)	4891(10)	34(4)
C(52)	2663(13)	10055(11)	5354(9)	32(3)
C(53)	2091(12)	11768(14)	4910(9)	41(4)
C(54)	2295(12)	7557(11)	3726(9)	34(4)
C(55)	2483(12)	6917(11)	3278(9)	33(3)
C(56)	849(15)	6589(10)	4102(11)	39(4)
C(61)	-54(15)	6770(13)	2496(10)	45(4)
C(62)	-665(14)	6523(15)	3218(11)	47(5)
C(63)	444(17)	5961(16)	2033(12)	59(6)
C(64)	1432(15)	7450(13)	1667(9)	39(4)
C(65)	765(19)	8074(15)	1252(13)	60(6)
C(66)	2326(16)	7734(13)	1576(10)	53(6)
C(67)	-31(14)	8287(12)	3086(10)	47(5)
C(68)	-1007(19)	8750(20)	2929(13)	82(10)
C(69)	490(20)	8920(13)	2987(15)	77(9)
C(70)	4033(12)	4400(14)	3414(11)	49(5)
C(71)	4526(17)	4979(19)	3446(15)	70(7)
C(72)	4493(18)	3470(20)	3695(16)	112(16)
C(73)	2285(14)	3944(10)	3802(9)	35(4)
C(74)	2720(30)	3522(16)	3079(14)	102(13)
C(75)	1170(20)	4269(15)	4020(20)	84(10)
C(76)	2556(12)	4936(12)	4781(8)	34(3)
C(77)	2612(15)	5797(12)	4963(9)	39(4)
C(78)	1681(14)	4758(12)	5333(10)	46(5)
C(101)	4618(16)	2065(13)	401(10)	43(4)
C(102)	5419(18)	2335(14)	78(11)	53(5)
C(103)	5340(17)	3154(13)	229(12)	50(5)
C(104)	4497(19)	3698(13)	744(13)	56(6)
C(105)	3740(17)	3388(15)	1062(14)	57(6)
C(106)	3802(18)	2588(18)	872(13)	66(7)
C(108)	4610(20)	1981(18)	5395(14)	68(7)
C(109)	5385(16)	2266(15)	5132(11)	50(5)
C(110)	5311(16)	3061(15)	5288(12)	52(5)
C(111)	4445(19)	3597(15)	5766(13)	62(6)
C(112)	3673(18)	3340(20)	6034(12)	64(7)
C(113)	3750(20)	2510(30)	5859(17)	86(10)

Table 10. Bond lengths [A] and angles [deg] for **5**.

Re(1)-C(13)	1.928(16)
Re(1)-C(11)	1.928(18)
Re(1)-C(12)	2.140(15)
Re(1)-N(2)	2.178(12)
Re(1)-N(1)	2.185(11)
Re(1)-Br(1)	2.584(3)
Ru(1)-C(16)	1.850(19)
Ru(1)-C(15)	1.935(13)
Ru(1)-P(1)	2.423(5)
Ru(1)-P(2)	2.455(5)
Ru(1)-Cl(1)	2.495(3)
P(1)-C(21)	1.85(2)
P(1)-C(24)	1.870(18)
P(1)-C(28)	1.874(18)
N(1)-C(1)	1.33(2)
N(1)-C(5)	1.354(18)
O(1)-C(11)	1.15(2)
C(1)-C(2)	1.423(19)
C(1)-C(6)	1.46(2)
Re(2)-C(53)	1.93(2)
Re(2)-C(51)	1.942(18)
Re(2)-C(52)	1.961(18)
Re(2)-N(4)	2.140(17)
Re(2)-N(3)	2.166(14)
Re(2)-Br(2)	2.600(3)
Ru(2)-C(56)	1.87(2)
Ru(2)-C(55)	1.944(18)
Ru(2)-P(4)	2.429(4)
Ru(2)-P(3)	2.441(4)
Ru(2)-Cl(2)	2.503(4)
P(2)-C(30)	1.828(19)
P(2)-C(36)	1.84(2)
P(2)-C(33)	1.91(2)
O(2)-C(12)	0.977(19)
N(2)-C(10)	1.32(2)
N(2)-C(6)	1.354(19)
C(2)-C(3)	1.34(2)
C(2)-H(2A)	0.9500
P(3)-C(61)	1.81(2)
P(3)-C(67)	1.872(17)
P(3)-C(64)	1.894(18)
C(3)-C(4)	1.42(2)
C(3)-H(3A)	0.9500
O(3)-C(13)	1.146(19)
N(3)-C(45)	1.31(2)
N(3)-C(41)	1.36(2)
P(4)-C(73)	1.844(16)
P(4)-C(70)	1.847(17)
P(4)-C(76)	1.887(17)
O(4)-C(16)	1.12(2)
N(4)-C(50)	1.35(3)
N(4)-C(46)	1.36(2)
C(4)-C(5)	1.418(17)
C(4)-C(14)	1.46(2)
O(5)-C(51)	1.10(2)
C(5)-H(5A)	0.9500
C(6)-C(7)	1.38(2)
O(6)-C(52)	0.94(2)

O(7)-C(53)	1.14(2)
C(7)-C(8)	1.36(2)
C(7)-H(7A)	0.9500
O(8)-C(56)	1.10(2)
C(8)-C(9)	1.42(2)
C(8)-H(8A)	0.9500
C(9)-C(10)	1.39(2)
C(9)-H(9A)	0.9500
C(10)-H(10A)	0.9500
C(14)-C(15)	1.36(2)
C(14)-H(14A)	0.9500
C(15)-H(15A)	0.9500
C(21)-C(22)	1.54(3)
C(21)-C(23)	1.55(2)
C(21)-H(21A)	1.0000
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-C(25)	1.54(3)
C(24)-C(26)	1.64(3)
C(24)-H(24A)	1.0000
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-C(28)	1.54(3)
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-C(29)	1.54(3)
C(28)-H(28A)	1.0000
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(30)-C(31)	1.52(3)
C(30)-C(32)	1.57(3)
C(30)-H(30A)	1.0000
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-C(34)	1.46(3)
C(33)-C(35)	1.47(3)
C(33)-H(33A)	1.0000
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
C(36)-C(38)	1.55(3)
C(36)-C(37)	1.55(3)
C(36)-H(36A)	1.0000
C(37)-H(37A)	0.9800

C(37)-H(37B)	0.9800
C(37)-H(37C)	0.9800
C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800
C(38)-H(38C)	0.9800
C(41)-C(42)	1.42(2)
C(41)-C(46)	1.45(2)
C(42)-C(43)	1.37(2)
C(42)-H(42A)	0.9500
C(43)-C(44)	1.39(2)
C(43)-H(43A)	0.9500
C(44)-C(45)	1.41(2)
C(44)-C(54)	1.43(2)
C(45)-H(45A)	0.9500
C(46)-C(47)	1.38(3)
C(47)-C(48)	1.35(3)
C(47)-H(47A)	0.9500
C(48)-C(49)	1.40(3)
C(48)-H(48A)	0.9500
C(49)-C(50)	1.39(3)
C(49)-H(49A)	0.9500
C(50)-H(50A)	0.9500
C(54)-C(55)	1.36(2)
C(54)-H(54A)	0.9500
C(55)-H(55A)	0.9500
C(61)-C(63)	1.51(3)
C(61)-C(62)	1.53(3)
C(61)-H(61A)	1.0000
C(62)-H(62A)	0.9800
C(62)-H(62B)	0.9800
C(62)-H(62C)	0.9800
C(63)-H(63A)	0.9800
C(63)-H(63B)	0.9800
C(63)-H(63C)	0.9800
C(64)-C(65)	1.55(3)
C(64)-C(66)	1.56(3)
C(64)-H(64A)	1.0000
C(65)-H(65A)	0.9800
C(65)-H(65B)	0.9800
C(65)-H(65C)	0.9800
C(66)-H(66A)	0.9800
C(66)-H(66B)	0.9800
C(66)-H(66C)	0.9800
C(67)-C(69)	1.48(4)
C(67)-C(68)	1.55(3)
C(67)-H(67A)	1.0000
C(68)-H(68A)	0.9800
C(68)-H(68B)	0.9800
C(68)-H(68C)	0.9800
C(69)-H(69A)	0.9800
C(69)-H(69B)	0.9800
C(69)-H(69C)	0.9800
C(70)-C(71)	1.43(3)
C(70)-C(72)	1.54(3)
C(70)-H(70A)	1.0000
C(71)-H(71A)	0.9800
C(71)-H(71B)	0.9800
C(71)-H(71C)	0.9800
C(72)-H(72A)	0.9800
C(72)-H(72B)	0.9800
C(72)-H(72C)	0.9800

C(73)-C(75)	1.52(3)
C(73)-C(74)	1.53(3)
C(73)-H(73A)	1.0000
C(74)-H(74A)	0.9800
C(74)-H(74B)	0.9800
C(74)-H(74C)	0.9800
C(75)-H(75A)	0.9800
C(75)-H(75B)	0.9800
C(75)-H(75C)	0.9800
C(76)-C(78)	1.52(2)
C(76)-C(77)	1.53(2)
C(76)-H(76A)	1.0000
C(77)-H(77A)	0.9800
C(77)-H(77B)	0.9800
C(77)-H(77C)	0.9800
C(78)-H(78A)	0.9800
C(78)-H(78B)	0.9800
C(78)-H(78C)	0.9800
C(101)-C(106)	1.35(3)
C(101)-C(102)	1.38(3)
C(101)-H(10B)	0.9500
C(102)-C(103)	1.36(3)
C(102)-H(10C)	0.9500
C(103)-C(104)	1.42(3)
C(103)-H(10D)	0.9500
C(104)-C(105)	1.36(3)
C(104)-H(10E)	0.9500
C(105)-C(106)	1.37(4)
C(105)-H(10F)	0.9500
C(106)-H(10G)	0.9500
C(108)-C(109)	1.36(4)
C(108)-C(113)	1.38(4)
C(108)-H(10H)	0.9500
C(109)-C(110)	1.32(3)
C(109)-H(10I)	0.9500
C(110)-C(111)	1.40(3)
C(110)-H(11A)	0.9500
C(111)-C(112)	1.32(4)
C(111)-H(11B)	0.9500
C(112)-C(113)	1.40(4)
C(112)-H(11C)	0.9500
C(113)-H(11D)	0.9500

C(13)-Re(1)-C(11)	88.9(7)
C(13)-Re(1)-C(12)	88.8(7)
C(11)-Re(1)-C(12)	95.3(7)
C(13)-Re(1)-N(2)	96.9(7)
C(11)-Re(1)-N(2)	173.0(6)
C(12)-Re(1)-N(2)	88.7(5)
C(13)-Re(1)-N(1)	170.2(7)
C(11)-Re(1)-N(1)	100.9(6)
C(12)-Re(1)-N(1)	91.2(5)
N(2)-Re(1)-N(1)	73.3(5)
C(13)-Re(1)-Br(1)	93.7(6)
C(11)-Re(1)-Br(1)	90.8(5)
C(12)-Re(1)-Br(1)	173.5(4)
N(2)-Re(1)-Br(1)	85.0(3)
N(1)-Re(1)-Br(1)	85.2(3)
C(16)-Ru(1)-C(15)	90.3(9)
C(16)-Ru(1)-P(1)	89.9(7)
C(15)-Ru(1)-P(1)	94.1(5)

C(16)-Ru(1)-P(2)	90.7(6)
C(15)-Ru(1)-P(2)	94.6(5)
P(1)-Ru(1)-P(2)	171.31(16)
C(16)-Ru(1)-Cl(1)	170.7(7)
C(15)-Ru(1)-Cl(1)	99.0(6)
P(1)-Ru(1)-Cl(1)	88.32(13)
P(2)-Ru(1)-Cl(1)	89.67(13)
C(21)-P(1)-C(24)	101.7(10)
C(21)-P(1)-C(28)	102.3(8)
C(24)-P(1)-C(28)	109.9(9)
C(21)-P(1)-Ru(1)	108.7(6)
C(24)-P(1)-Ru(1)	117.1(7)
C(28)-P(1)-Ru(1)	115.1(6)
C(1)-N(1)-C(5)	119.7(12)
C(1)-N(1)-Re(1)	118.2(10)
C(5)-N(1)-Re(1)	122.1(10)
N(1)-C(1)-C(2)	121.1(13)
N(1)-C(1)-C(6)	115.6(13)
C(2)-C(1)-C(6)	123.2(14)
C(53)-Re(2)-C(51)	87.7(6)
C(53)-Re(2)-C(52)	88.6(7)
C(51)-Re(2)-C(52)	89.9(8)
C(53)-Re(2)-N(4)	98.3(7)
C(51)-Re(2)-N(4)	172.8(6)
C(52)-Re(2)-N(4)	94.2(7)
C(53)-Re(2)-N(3)	172.2(6)
C(51)-Re(2)-N(3)	100.1(6)
C(52)-Re(2)-N(3)	92.7(6)
N(4)-Re(2)-N(3)	73.9(6)
C(53)-Re(2)-Br(2)	94.0(5)
C(51)-Re(2)-Br(2)	90.5(5)
C(52)-Re(2)-Br(2)	177.4(5)
N(4)-Re(2)-Br(2)	85.1(5)
N(3)-Re(2)-Br(2)	84.8(4)
C(56)-Ru(2)-C(55)	90.1(7)
C(56)-Ru(2)-P(4)	91.8(5)
C(55)-Ru(2)-P(4)	96.8(5)
C(56)-Ru(2)-P(3)	90.1(5)
C(55)-Ru(2)-P(3)	93.5(5)
P(4)-Ru(2)-P(3)	169.46(16)
C(56)-Ru(2)-Cl(2)	171.3(5)
C(55)-Ru(2)-Cl(2)	98.4(5)
P(4)-Ru(2)-Cl(2)	89.01(14)
P(3)-Ru(2)-Cl(2)	87.56(14)
C(30)-P(2)-C(36)	101.9(10)
C(30)-P(2)-C(33)	105.5(9)
C(36)-P(2)-C(33)	99.2(11)
C(30)-P(2)-Ru(1)	108.5(8)
C(36)-P(2)-Ru(1)	116.9(6)
C(33)-P(2)-Ru(1)	122.5(8)
C(10)-N(2)-C(6)	119.9(14)
C(10)-N(2)-Re(1)	122.0(11)
C(6)-N(2)-Re(1)	118.0(10)
C(3)-C(2)-C(1)	120.4(14)
C(3)-C(2)-H(2A)	119.8
C(1)-C(2)-H(2A)	119.8
C(61)-P(3)-C(67)	103.9(10)
C(61)-P(3)-C(64)	99.4(8)
C(67)-P(3)-C(64)	110.2(9)
C(61)-P(3)-Ru(2)	109.3(7)
C(67)-P(3)-Ru(2)	115.3(6)

C(64)-P(3)-Ru(2)	116.7(6)
C(2)-C(3)-C(4)	119.4(13)
C(2)-C(3)-H(3A)	120.3
C(4)-C(3)-H(3A)	120.3
C(45)-N(3)-C(41)	115.9(15)
C(45)-N(3)-Re(2)	126.5(12)
C(41)-N(3)-Re(2)	117.6(12)
C(73)-P(4)-C(70)	102.9(10)
C(73)-P(4)-C(76)	104.6(7)
C(70)-P(4)-C(76)	102.4(9)
C(73)-P(4)-Ru(2)	107.5(6)
C(70)-P(4)-Ru(2)	117.2(6)
C(76)-P(4)-Ru(2)	120.4(6)
C(50)-N(4)-C(46)	117.8(17)
C(50)-N(4)-Re(2)	123.0(13)
C(46)-N(4)-Re(2)	119.0(13)
C(3)-C(4)-C(5)	117.8(14)
C(3)-C(4)-C(14)	124.9(12)
C(5)-C(4)-C(14)	117.0(15)
N(1)-C(5)-C(4)	121.6(14)
N(1)-C(5)-H(5A)	119.2
C(4)-C(5)-H(5A)	119.2
N(2)-C(6)-C(7)	122.1(14)
N(2)-C(6)-C(1)	114.8(14)
C(7)-C(6)-C(1)	123.0(14)
C(8)-C(7)-C(6)	118.9(15)
C(8)-C(7)-H(7A)	120.6
C(6)-C(7)-H(7A)	120.6
C(7)-C(8)-C(9)	119.3(16)
C(7)-C(8)-H(8A)	120.3
C(9)-C(8)-H(8A)	120.3
C(10)-C(9)-C(8)	118.1(15)
C(10)-C(9)-H(9A)	120.9
C(8)-C(9)-H(9A)	120.9
N(2)-C(10)-C(9)	121.5(15)
N(2)-C(10)-H(10A)	119.2
C(9)-C(10)-H(10A)	119.2
O(1)-C(11)-Re(1)	176.9(15)
O(2)-C(12)-Re(1)	160.4(16)
O(3)-C(13)-Re(1)	176.2(19)
C(15)-C(14)-C(4)	124.7(16)
C(15)-C(14)-H(14A)	117.6
C(4)-C(14)-H(14A)	117.6
C(14)-C(15)-Ru(1)	134.3(14)
C(14)-C(15)-H(15A)	112.9
Ru(1)-C(15)-H(15A)	112.9
O(4)-C(16)-Ru(1)	179(2)
C(22)-C(21)-C(23)	109.3(17)
C(22)-C(21)-P(1)	110.8(14)
C(23)-C(21)-P(1)	112.2(13)
C(22)-C(21)-H(21A)	108.2
C(23)-C(21)-H(21A)	108.2
P(1)-C(21)-H(21A)	108.2
C(21)-C(22)-H(22A)	109.5
C(21)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(21)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(21)-C(23)-H(23A)	109.5
C(21)-C(23)-H(23B)	109.5

H(23A)-C(23)-H(23B)	109.5
C(21)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(25)-C(24)-C(26)	115.4(16)
C(25)-C(24)-P(1)	115.9(13)
C(26)-C(24)-P(1)	111.2(14)
C(25)-C(24)-H(24A)	104.2
C(26)-C(24)-H(24A)	104.2
P(1)-C(24)-H(24A)	104.2
C(24)-C(25)-H(25A)	109.5
C(24)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(24)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(24)-C(26)-H(26A)	109.5
C(24)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(24)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(28)-C(27)-H(27A)	109.5
C(28)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(28)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(27)-C(28)-C(29)	107.8(16)
C(27)-C(28)-P(1)	118.3(13)
C(29)-C(28)-P(1)	109.9(14)
C(27)-C(28)-H(28A)	106.7
C(29)-C(28)-H(28A)	106.7
P(1)-C(28)-H(28A)	106.7
C(28)-C(29)-H(29A)	109.5
C(28)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(28)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(31)-C(30)-C(32)	107(2)
C(31)-C(30)-P(2)	110.4(14)
C(32)-C(30)-P(2)	113.1(13)
C(31)-C(30)-H(30A)	108.8
C(32)-C(30)-H(30A)	108.8
P(2)-C(30)-H(30A)	108.8
C(30)-C(31)-H(31A)	109.5
C(30)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(30)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(30)-C(32)-H(32A)	109.5
C(30)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(30)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(34)-C(33)-C(35)	112(2)
C(34)-C(33)-P(2)	116.0(17)
C(35)-C(33)-P(2)	113.2(16)

C(34)-C(33)-H(33A)	104.8
C(35)-C(33)-H(33A)	104.8
P(2)-C(33)-H(33A)	104.8
C(33)-C(34)-H(34A)	109.5
C(33)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(33)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(33)-C(35)-H(35A)	109.5
C(33)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(33)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(38)-C(36)-C(37)	108.8(19)
C(38)-C(36)-P(2)	111.4(15)
C(37)-C(36)-P(2)	116.2(15)
C(38)-C(36)-H(36A)	106.6
C(37)-C(36)-H(36A)	106.6
P(2)-C(36)-H(36A)	106.6
C(36)-C(37)-H(37A)	109.5
C(36)-C(37)-H(37B)	109.5
H(37A)-C(37)-H(37B)	109.5
C(36)-C(37)-H(37C)	109.5
H(37A)-C(37)-H(37C)	109.5
H(37B)-C(37)-H(37C)	109.5
C(36)-C(38)-H(38A)	109.5
C(36)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(36)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
N(3)-C(41)-C(42)	121.7(16)
N(3)-C(41)-C(46)	115.1(15)
C(42)-C(41)-C(46)	123.1(16)
C(43)-C(42)-C(41)	119.7(17)
C(43)-C(42)-H(42A)	120.1
C(41)-C(42)-H(42A)	120.1
C(42)-C(43)-C(44)	119.3(16)
C(42)-C(43)-H(43A)	120.3
C(44)-C(43)-H(43A)	120.3
C(43)-C(44)-C(45)	116.0(15)
C(43)-C(44)-C(54)	124.6(14)
C(45)-C(44)-C(54)	119.4(15)
N(3)-C(45)-C(44)	127.0(17)
N(3)-C(45)-H(45A)	116.5
C(44)-C(45)-H(45A)	116.5
N(4)-C(46)-C(47)	122.2(17)
N(4)-C(46)-C(41)	114.2(16)
C(47)-C(46)-C(41)	123.4(15)
C(48)-C(47)-C(46)	120.4(17)
C(48)-C(47)-H(47A)	119.8
C(46)-C(47)-H(47A)	119.8
C(47)-C(48)-C(49)	118.0(19)
C(47)-C(48)-H(48A)	121.0
C(49)-C(48)-H(48A)	121.0
C(50)-C(49)-C(48)	120.3(19)
C(50)-C(49)-H(49A)	119.8
C(48)-C(49)-H(49A)	119.8
N(4)-C(50)-C(49)	121.1(19)

N(4)-C(50)-H(50A)	119.5
C(49)-C(50)-H(50A)	119.5
O(5)-C(51)-Re(2)	177.6(15)
O(6)-C(52)-Re(2)	171(2)
O(7)-C(53)-Re(2)	175.2(15)
C(55)-C(54)-C(44)	123.2(15)
C(55)-C(54)-H(54A)	118.4
C(44)-C(54)-H(54A)	118.4
C(54)-C(55)-Ru(2)	133.8(13)
C(54)-C(55)-H(55A)	113.1
Ru(2)-C(55)-H(55A)	113.1
O(8)-C(56)-Ru(2)	178.7(15)
C(63)-C(61)-C(62)	108.8(16)
C(63)-C(61)-P(3)	113.9(15)
C(62)-C(61)-P(3)	108.6(14)
C(63)-C(61)-H(61A)	108.5
C(62)-C(61)-H(61A)	108.5
P(3)-C(61)-H(61A)	108.5
C(61)-C(62)-H(62A)	109.5
C(61)-C(62)-H(62B)	109.5
H(62A)-C(62)-H(62B)	109.5
C(61)-C(62)-H(62C)	109.5
H(62A)-C(62)-H(62C)	109.5
H(62B)-C(62)-H(62C)	109.5
C(61)-C(63)-H(63A)	109.5
C(61)-C(63)-H(63B)	109.5
H(63A)-C(63)-H(63B)	109.5
C(61)-C(63)-H(63C)	109.5
H(63A)-C(63)-H(63C)	109.5
H(63B)-C(63)-H(63C)	109.5
C(65)-C(64)-C(66)	111.7(17)
C(65)-C(64)-P(3)	116.2(15)
C(66)-C(64)-P(3)	112.5(12)
C(65)-C(64)-H(64A)	105.1
C(66)-C(64)-H(64A)	105.1
P(3)-C(64)-H(64A)	105.1
C(64)-C(65)-H(65A)	109.5
C(64)-C(65)-H(65B)	109.5
H(65A)-C(65)-H(65B)	109.5
C(64)-C(65)-H(65C)	109.5
H(65A)-C(65)-H(65C)	109.5
H(65B)-C(65)-H(65C)	109.5
C(64)-C(66)-H(66A)	109.5
C(64)-C(66)-H(66B)	109.5
H(66A)-C(66)-H(66B)	109.5
C(64)-C(66)-H(66C)	109.5
H(66A)-C(66)-H(66C)	109.5
H(66B)-C(66)-H(66C)	109.5
C(69)-C(67)-C(68)	110(2)
C(69)-C(67)-P(3)	112.1(16)
C(68)-C(67)-P(3)	115.8(17)
C(69)-C(67)-H(67A)	106.0
C(68)-C(67)-H(67A)	106.0
P(3)-C(67)-H(67A)	106.0
C(67)-C(68)-H(68A)	109.5
C(67)-C(68)-H(68B)	109.5
H(68A)-C(68)-H(68B)	109.5
C(67)-C(68)-H(68C)	109.5
H(68A)-C(68)-H(68C)	109.5
H(68B)-C(68)-H(68C)	109.5
C(67)-C(69)-H(69A)	109.5

C(67)-C(69)-H(69B)	109.5
H(69A)-C(69)-H(69B)	109.5
C(67)-C(69)-H(69C)	109.5
H(69A)-C(69)-H(69C)	109.5
H(69B)-C(69)-H(69C)	109.5
C(71)-C(70)-C(72)	111(2)
C(71)-C(70)-P(4)	112.9(16)
C(72)-C(70)-P(4)	113.2(15)
C(71)-C(70)-H(70A)	106.5
C(72)-C(70)-H(70A)	106.5
P(4)-C(70)-H(70A)	106.5
C(70)-C(71)-H(71A)	109.5
C(70)-C(71)-H(71B)	109.5
H(71A)-C(71)-H(71B)	109.5
C(70)-C(71)-H(71C)	109.5
H(71A)-C(71)-H(71C)	109.5
H(71B)-C(71)-H(71C)	109.5
C(70)-C(72)-H(72A)	109.5
C(70)-C(72)-H(72B)	109.5
H(72A)-C(72)-H(72B)	109.5
C(70)-C(72)-H(72C)	109.5
H(72A)-C(72)-H(72C)	109.5
H(72B)-C(72)-H(72C)	109.5
C(75)-C(73)-C(74)	109(2)
C(75)-C(73)-P(4)	109.5(12)
C(74)-C(73)-P(4)	113.1(15)
C(75)-C(73)-H(73A)	108.3
C(74)-C(73)-H(73A)	108.3
P(4)-C(73)-H(73A)	108.3
C(73)-C(74)-H(74A)	109.5
C(73)-C(74)-H(74B)	109.5
H(74A)-C(74)-H(74B)	109.5
C(73)-C(74)-H(74C)	109.5
H(74A)-C(74)-H(74C)	109.5
H(74B)-C(74)-H(74C)	109.5
C(73)-C(75)-H(75A)	109.5
C(73)-C(75)-H(75B)	109.5
H(75A)-C(75)-H(75B)	109.5
C(73)-C(75)-H(75C)	109.5
H(75A)-C(75)-H(75C)	109.5
H(75B)-C(75)-H(75C)	109.5
C(78)-C(76)-C(77)	108.9(14)
C(78)-C(76)-P(4)	117.5(13)
C(77)-C(76)-P(4)	113.6(11)
C(78)-C(76)-H(76A)	105.3
C(77)-C(76)-H(76A)	105.3
P(4)-C(76)-H(76A)	105.3
C(76)-C(77)-H(77A)	109.5
C(76)-C(77)-H(77B)	109.5
H(77A)-C(77)-H(77B)	109.5
C(76)-C(77)-H(77C)	109.5
H(77A)-C(77)-H(77C)	109.5
H(77B)-C(77)-H(77C)	109.5
C(76)-C(78)-H(78A)	109.5
C(76)-C(78)-H(78B)	109.5
H(78A)-C(78)-H(78B)	109.5
C(76)-C(78)-H(78C)	109.5
H(78A)-C(78)-H(78C)	109.5
H(78B)-C(78)-H(78C)	109.5
C(106)-C(101)-C(102)	121(2)
C(106)-C(101)-H(10B)	119.6

C(102)-C(101)-H(10B)	119.6
C(103)-C(102)-C(101)	118(2)
C(103)-C(102)-H(10C)	121.1
C(101)-C(102)-H(10C)	121.1
C(102)-C(103)-C(104)	122(2)
C(102)-C(103)-H(10D)	119.1
C(104)-C(103)-H(10D)	119.1
C(105)-C(104)-C(103)	118(2)
C(105)-C(104)-H(10E)	121.1
C(103)-C(104)-H(10E)	121.1
C(104)-C(105)-C(106)	120(2)
C(104)-C(105)-H(10F)	120.1
C(106)-C(105)-H(10F)	120.1
C(101)-C(106)-C(105)	122(2)
C(101)-C(106)-H(10G)	119.1
C(105)-C(106)-H(10G)	119.1
C(109)-C(108)-C(113)	119(3)
C(109)-C(108)-H(10H)	120.3
C(113)-C(108)-H(10H)	120.3
C(110)-C(109)-C(108)	121(2)
C(110)-C(109)-H(10I)	119.6
C(108)-C(109)-H(10I)	119.6
C(109)-C(110)-C(111)	120(2)
C(109)-C(110)-H(11A)	119.9
C(111)-C(110)-H(11A)	119.9
C(112)-C(111)-C(110)	121(2)
C(112)-C(111)-H(11B)	119.7
C(110)-C(111)-H(11B)	119.7
C(111)-C(112)-C(113)	119(2)
C(111)-C(112)-H(11C)	120.6
C(113)-C(112)-H(11C)	120.6
C(108)-C(113)-C(112)	120(3)
C(108)-C(113)-H(11D)	120.0
C(112)-C(113)-H(11D)	120.0

Table 11. Anisotropic displacement parameters ($Å^2$ x 10^3) for complex **5**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U11 + ... + 2 h k a^* b^* U12]$

	U11	U22	U33	U23	U13	U12
Re(1)	33(1)	22(1)	32(1)	-10(1)	-3(1)	-11(1)
Ru(1)	37(1)	31(1)	25(1)	-8(1)	0(1)	-19(1)
Cl(1)	19(1)	20(1)	14(1)	-4(1)	-3(1)	-6(1)
Br(1)	68(2)	51(1)	58(1)	0(1)	-9(1)	-17(1)
P(1)	35(2)	29(2)	28(2)	-9(2)	-2(2)	-14(2)
N(1)	47(8)	16(5)	16(5)	-5(4)	-6(5)	-13(5)
O(1)	41(8)	48(8)	62(9)	-14(7)	-1(7)	-16(6)
C(1)	28(7)	25(6)	24(7)	-3(5)	-6(6)	-12(6)
Re(2)	32(1)	35(1)	31(1)	-9(1)	-6(1)	-11(1)
Ru(2)	28(1)	22(1)	24(1)	-3(1)	-5(1)	-9(1)
Br(2)	58(1)	61(1)	49(1)	-4(1)	-15(1)	-23(1)
Cl(2)	21(2)	19(1)	27(2)	-4(1)	3(1)	-2(1)
P(2)	65(3)	32(2)	21(2)	-5(2)	2(2)	-31(2)
O(2)	60(9)	34(6)	33(7)	-8(5)	3(6)	-7(6)
N(2)	16(5)	33(6)	26(6)	-3(5)	-6(5)	-10(5)
C(2)	24(7)	28(7)	30(8)	-8(6)	-7(6)	-8(6)
P(3)	34(2)	30(2)	26(2)	-4(2)	-8(2)	-10(2)
C(3)	34(8)	20(6)	37(8)	-13(6)	-9(7)	-10(6)

O(3)	58(8)	26(6)	57(8)	-20(6)	3(7)	-24(6)
N(3)	39(8)	41(7)	24(7)	-14(6)	-7(6)	-6(6)
P(4)	30(2)	27(2)	29(2)	0(2)	-7(2)	-6(2)
O(4)	46(8)	64(9)	64(10)	-9(8)	3(8)	-39(7)
N(4)	41(9)	46(9)	43(9)	-6(7)	-9(7)	-15(7)
C(4)	57(10)	10(5)	19(6)	-6(5)	-10(7)	-8(6)
O(5)	30(7)	59(8)	47(8)	-17(6)	6(6)	-17(6)
C(5)	23(7)	24(6)	22(7)	-11(5)	-4(6)	-9(5)
C(6)	40(9)	23(7)	30(8)	3(6)	-16(7)	-15(6)
O(6)	34(7)	34(7)	170(20)	-65(10)	-49(10)	20(6)
O(7)	46(7)	41(6)	36(7)	-16(5)	-6(6)	-16(5)
C(7)	50(10)	26(7)	23(7)	-7(6)	3(7)	-20(7)
O(8)	33(6)	34(6)	27(6)	-2(5)	0(5)	-4(5)
C(8)	46(10)	27(7)	31(8)	1(6)	-10(7)	-23(7)
C(9)	47(10)	38(8)	31(8)	-2(7)	-15(8)	-25(7)
C(10)	39(9)	42(9)	35(9)	-9(7)	-7(8)	-23(7)
C(11)	36(9)	22(7)	39(9)	-12(6)	-3(7)	-10(6)
C(13)	49(10)	21(7)	50(11)	-13(7)	3(9)	-19(7)
C(14)	38(9)	34(8)	28(8)	-6(6)	-5(7)	-9(7)
C(15)	37(9)	25(7)	47(9)	-3(6)	-21(8)	-22(6)
C(16)	40(10)	37(9)	44(11)	-9(8)	4(9)	-9(8)
C(21)	37(9)	37(8)	39(9)	-14(7)	-13(8)	-4(7)
C(22)	40(10)	48(11)	61(13)	-10(10)	7(10)	-22(9)
C(23)	57(12)	47(10)	55(12)	-36(9)	-10(10)	-16(9)
C(24)	57(12)	33(8)	28(8)	4(7)	6(8)	-13(8)
C(25)	42(10)	56(11)	29(9)	24(8)	-3(8)	-2(9)
C(26)	89(17)	34(9)	50(12)	3(8)	-29(12)	-20(10)
C(27)	54(12)	35(9)	64(14)	-29(9)	0(11)	-2(8)
C(28)	57(12)	32(8)	40(10)	-8(7)	-20(9)	-14(8)
C(29)	95(17)	30(8)	48(11)	-8(8)	-32(12)	-27(10)
C(30)	80(15)	49(11)	36(10)	10(8)	-10(10)	-45(11)
C(31)	84(16)	38(9)	70(14)	0(9)	-31(12)	-48(10)
C(32)	120(20)	75(15)	47(12)	-43(11)	30(13)	-77(16)
C(33)	100(19)	47(11)	41(11)	-8(9)	-6(12)	-51(12)
C(34)	150(30)	110(20)	32(10)	11(12)	-21(15)	-110(20)
C(35)	120(20)	45(12)	43(12)	-8(9)	-3(14)	-33(13)
C(36)	65(13)	36(9)	39(10)	5(8)	-18(10)	-21(9)
C(37)	71(15)	45(11)	35(10)	3(8)	2(10)	-24(10)
C(38)	57(13)	67(14)	79(17)	14(13)	-23(13)	-45(12)
C(41)	44(10)	39(8)	22(7)	2(6)	-13(7)	-15(7)
C(42)	32(9)	41(9)	38(9)	3(7)	-7(8)	-16(7)
C(43)	34(9)	34(8)	40(9)	-6(7)	-9(8)	-10(7)
C(44)	42(9)	22(6)	26(7)	-3(6)	-9(7)	-13(6)
C(45)	38(9)	40(9)	28(8)	-7(7)	-8(7)	-12(7)
C(46)	37(9)	36(8)	31(8)	-12(7)	2(7)	-14(7)
C(47)	36(9)	39(9)	42(10)	-10(7)	-11(8)	-11(7)
C(48)	49(11)	48(10)	28(8)	1(7)	-14(8)	-13(8)
C(49)	38(10)	55(11)	41(10)	-3(8)	-16(8)	-23(8)
C(50)	41(10)	55(11)	41(10)	1(9)	-15(9)	-15(9)
C(51)	43(10)	23(7)	49(10)	-14(7)	-16(8)	-21(6)
C(53)	18(7)	75(13)	24(8)	3(8)	-1(6)	-17(8)
C(54)	26(8)	32(8)	31(8)	-3(6)	1(7)	-5(6)
C(55)	28(8)	33(8)	31(8)	-1(6)	-5(7)	-9(6)
C(56)	55(11)	21(7)	55(12)	9(7)	-32(10)	-19(7)
C(61)	49(11)	47(10)	35(9)	-8(8)	3(8)	-23(8)
C(62)	34(9)	70(13)	44(10)	0(9)	-18(8)	-22(9)
C(63)	54(12)	75(15)	45(11)	-9(10)	12(10)	-41(11)
C(64)	53(11)	49(10)	21(7)	-2(7)	-10(8)	-24(8)
C(65)	75(16)	51(12)	52(13)	1(10)	-30(12)	-9(11)
C(66)	68(13)	41(9)	40(10)	0(8)	17(9)	-43(9)
C(67)	45(10)	37(9)	32(9)	-12(7)	-1(8)	8(8)

C(68)	60(15)	100(20)	38(12)	0(13)	-11(11)	19(14)
C(69)	130(20)	25(9)	84(18)	-11(10)	-68(19)	1(12)
C(70)	18(7)	60(12)	38(10)	4(9)	6(7)	3(7)
C(71)	34(11)	93(19)	76(17)	-2(15)	-12(11)	-20(12)
C(72)	42(13)	120(30)	74(19)	41(18)	14(13)	34(15)
C(73)	58(11)	26(7)	30(8)	-3(6)	-16(8)	-24(7)
C(74)	200(40)	42(12)	59(15)	2(11)	-20(20)	-68(18)
C(75)	83(18)	45(12)	160(30)	41(16)	-70(20)	-53(13)
C(76)	31(8)	51(9)	22(7)	7(7)	-3(6)	-26(7)
C(77)	61(12)	44(9)	20(7)	-3(7)	-14(8)	-25(8)
C(78)	48(10)	39(9)	33(9)	-11(7)	19(8)	-20(8)
C(101)	60(12)	44(10)	40(10)	7(8)	-33(10)	-21(9)
C(102)	69(14)	50(11)	33(10)	4(8)	-12(10)	-18(10)
C(103)	53(12)	43(10)	54(12)	-1(9)	-14(10)	-18(9)
C(104)	82(16)	39(10)	68(14)	-10(9)	-50(14)	-16(10)
C(105)	46(12)	56(13)	67(15)	-9(11)	-17(11)	-13(10)
C(106)	53(13)	86(17)	50(13)	22(12)	-9(11)	-30(12)
C(108)	86(19)	68(15)	62(15)	-17(12)	-25(15)	-34(14)
C(109)	43(11)	57(12)	36(10)	-2(9)	-2(9)	-11(9)
C(110)	49(12)	57(12)	52(12)	-13(10)	-16(10)	-18(9)
C(111)	73(16)	41(11)	57(14)	-18(10)	-21(12)	3(10)
C(112)	45(12)	97(19)	38(11)	-7(12)	-15(10)	-8(12)
C(113)	70(19)	130(30)	73(19)	14(19)	-41(17)	-46(19)

Table 12. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for complex **5**.

	x	y	z	U(eq)
H(2A)	5131	8084	7898	33
H(3A)	4219	7229	7940	35
H(5A)	1844	9044	9261	27
H(7A)	5875	8980	7858	41
H(8A)	6644	9923	7956	39
H(9A)	5687	11238	8640	42
H(10A)	4018	11487	9239	44
H(14A)	1652	7713	9065	42
H(15A)	3086	6752	7915	36
H(21A)	-620	7435	7282	47
H(22A)	-1256	6449	8120	80
H(22B)	-1099	7152	8505	80
H(22C)	-329	6160	8386	80
H(23A)	-214	5971	6911	78
H(23B)	756	5645	7128	78
H(23C)	663	6335	6491	78
H(24A)	1695	6970	6403	56
H(25A)	1172	8259	5749	78
H(25B)	406	8754	6460	78
H(25C)	293	7918	6211	78
H(26A)	2718	7907	6088	84
H(26B)	2842	7283	6755	84
H(26C)	2187	8312	6861	84
H(27A)	-1295	9474	8196	86
H(27B)	-1394	8594	8008	86
H(27C)	-803	9121	7407	86
H(28A)	-203	8220	8571	50
H(29A)	201	9529	8207	79

H(29B)	862	9108	7448	79
H(29C)	1163	8666	8126	79
H(30A)	2425	3477	9081	61
H(31A)	831	3786	9039	82
H(31B)	778	4769	8757	82
H(31C)	808	4482	9536	82
H(32A)	2250	3128	8038	119
H(32B)	3212	3391	7826	119
H(32C)	2228	4091	7715	119
H(33A)	3164	4485	9767	71
H(34A)	1816	4661	10745	125
H(34B)	1902	3999	10192	125
H(34C)	1127	4989	10263	125
H(35A)	2476	5756	10417	109
H(35B)	1921	6252	9866	109
H(35C)	3095	5892	9619	109
H(36A)	4047	4349	7872	55
H(37A)	5106	3210	8379	82
H(37B)	4111	3022	8524	82
H(37C)	4279	3405	9135	82
H(38A)	5169	4676	8251	93
H(38B)	4320	5039	8976	93
H(38C)	4238	5543	8254	93
H(42A)	5121	8130	2907	45
H(43A)	4180	7289	2919	44
H(45A)	1894	9033	4286	43
H(47A)	5849	9033	2864	47
H(48A)	6617	9985	2933	51
H(49A)	5670	11273	3616	50
H(50A)	4015	11542	4231	55
H(54A)	1718	7678	4125	41
H(55A)	3077	6833	2896	39
H(61A)	-507	7241	2279	54
H(62A)	-1127	6282	3160	70
H(62B)	-1029	7054	3510	70
H(62C)	-229	6077	3444	70
H(63A)	-53	5757	1988	89
H(63B)	880	5488	2244	89
H(63C)	829	6114	1568	89
H(64A)	1722	6863	1430	47
H(65A)	1169	8144	768	91
H(65B)	420	8655	1478	91
H(65C)	285	7817	1248	91
H(66A)	2637	7841	1077	79
H(66B)	2803	7261	1755	79
H(66C)	2100	8278	1839	79
H(67A)	-217	8133	3598	56
H(68A)	-1382	9299	3201	124
H(68B)	-1390	8356	3060	124
H(68C)	-866	8897	2426	124
H(69A)	38	9466	3241	116
H(69B)	738	9057	2486	116
H(69C)	1042	8655	3169	116
H(70A)	4155	4330	2905	59
H(71A)	5234	4698	3217	105
H(71B)	4396	5093	3939	105
H(71C)	4285	5540	3206	105
H(72A)	5204	3255	3455	169
H(72B)	4209	3063	3609	169
H(72C)	4359	3499	4201	169
H(73A)	2498	3479	4146	42

H(74A)	2481	3034	3097	153
H(74B)	3435	3294	2942	153
H(74C)	2513	3969	2735	153
H(75A)	958	3775	4010	126
H(75B)	948	4740	3701	126
H(75C)	891	4501	4501	126
H(76A)	3146	4454	4849	41
H(77A)	2540	5788	5462	59
H(77B)	2085	6305	4865	59
H(77C)	3248	5848	4679	59
H(78A)	1698	4809	5802	70
H(78B)	1709	4158	5274	70
H(78C)	1073	5191	5278	70
H(10B)	4644	1505	290	52
H(10C)	6006	1960	-239	63
H(10D)	5861	3371	-16	60
H(10E)	4463	4258	862	68
H(10F)	3171	3728	1415	69
H(10G)	3255	2394	1076	79
H(10H)	4656	1424	5260	81
H(10I)	5990	1890	4832	60
H(11A)	5846	3268	5075	62
H(11B)	4414	4148	5900	75
H(11C)	3075	3720	6340	77
H(11D)	3209	2306	6060	103

Table 13. Torsion angles [deg] for complex **5**.

C(16)-Ru(1)-P(1)-C(21)	-84.1(9)
C(15)-Ru(1)-P(1)-C(21)	-174.3(8)
P(2)-Ru(1)-P(1)-C(21)	10.1(13)
Cl(1)-Ru(1)-P(1)-C(21)	86.8(6)
C(16)-Ru(1)-P(1)-C(24)	161.4(10)
C(15)-Ru(1)-P(1)-C(24)	71.1(10)
P(2)-Ru(1)-P(1)-C(24)	-104.5(13)
Cl(1)-Ru(1)-P(1)-C(24)	-27.8(8)
C(16)-Ru(1)-P(1)-C(28)	29.9(10)
C(15)-Ru(1)-P(1)-C(28)	-60.3(9)
P(2)-Ru(1)-P(1)-C(28)	124.0(12)
Cl(1)-Ru(1)-P(1)-C(28)	-159.2(7)
C(13)-Re(1)-N(1)-C(1)	0(5)
C(11)-Re(1)-N(1)-C(1)	174.4(11)
C(12)-Re(1)-N(1)-C(1)	-89.9(11)
N(2)-Re(1)-N(1)-C(1)	-1.6(10)
Br(1)-Re(1)-N(1)-C(1)	84.6(10)
C(13)-Re(1)-N(1)-C(5)	180(52)
C(11)-Re(1)-N(1)-C(5)	-6.2(13)
C(12)-Re(1)-N(1)-C(5)	89.5(12)
N(2)-Re(1)-N(1)-C(5)	177.8(12)
Br(1)-Re(1)-N(1)-C(5)	-96.0(11)
C(5)-N(1)-C(1)-C(2)	-1(2)
Re(1)-N(1)-C(1)-C(2)	178.8(11)
C(5)-N(1)-C(1)-C(6)	-177.2(13)
Re(1)-N(1)-C(1)-C(6)	2.2(17)
C(16)-Ru(1)-P(2)-C(30)	94.7(10)
C(15)-Ru(1)-P(2)-C(30)	-174.9(9)
P(1)-Ru(1)-P(2)-C(30)	0.7(14)
Cl(1)-Ru(1)-P(2)-C(30)	-75.9(7)

C(16)-Ru(1)-P(2)-C(36)	-150.8(10)
C(15)-Ru(1)-P(2)-C(36)	-60.5(9)
P(1)-Ru(1)-P(2)-C(36)	115.2(12)
Cl(1)-Ru(1)-P(2)-C(36)	38.5(7)
C(16)-Ru(1)-P(2)-C(33)	-28.4(11)
C(15)-Ru(1)-P(2)-C(33)	62.0(11)
P(1)-Ru(1)-P(2)-C(33)	-122.4(13)
Cl(1)-Ru(1)-P(2)-C(33)	161.0(9)
C(13)-Re(1)-N(2)-C(10)	-1.5(14)
C(11)-Re(1)-N(2)-C(10)	144(5)
C(12)-Re(1)-N(2)-C(10)	-90.2(13)
N(1)-Re(1)-N(2)-C(10)	178.1(14)
Br(1)-Re(1)-N(2)-C(10)	91.6(13)
C(13)-Re(1)-N(2)-C(6)	-178.9(12)
C(11)-Re(1)-N(2)-C(6)	-33(5)
C(12)-Re(1)-N(2)-C(6)	92.4(11)
N(1)-Re(1)-N(2)-C(6)	0.7(10)
Br(1)-Re(1)-N(2)-C(6)	-85.8(11)
N(1)-C(1)-C(2)-C(3)	1(2)
C(6)-C(1)-C(2)-C(3)	177.6(15)
C(56)-Ru(2)-P(3)-C(61)	-87.5(8)
C(55)-Ru(2)-P(3)-C(61)	-177.6(8)
P(4)-Ru(2)-P(3)-C(61)	13.0(11)
Cl(2)-Ru(2)-P(3)-C(61)	84.1(6)
C(56)-Ru(2)-P(3)-C(67)	29.1(10)
C(55)-Ru(2)-P(3)-C(67)	-61.0(9)
P(4)-Ru(2)-P(3)-C(67)	129.6(11)
Cl(2)-Ru(2)-P(3)-C(67)	-159.3(8)
C(56)-Ru(2)-P(3)-C(64)	160.8(8)
C(55)-Ru(2)-P(3)-C(64)	70.6(8)
P(4)-Ru(2)-P(3)-C(64)	-98.7(10)
Cl(2)-Ru(2)-P(3)-C(64)	-27.6(7)
C(1)-C(2)-C(3)-C(4)	-3(2)
C(53)-Re(2)-N(3)-C(45)	-179(54)
C(51)-Re(2)-N(3)-C(45)	-8.1(16)
C(52)-Re(2)-N(3)-C(45)	82.3(15)
N(4)-Re(2)-N(3)-C(45)	175.9(16)
Br(2)-Re(2)-N(3)-C(45)	-97.6(14)
C(53)-Re(2)-N(3)-C(41)	3(5)
C(51)-Re(2)-N(3)-C(41)	173.3(12)
C(52)-Re(2)-N(3)-C(41)	-96.3(13)
N(4)-Re(2)-N(3)-C(41)	-2.7(12)
Br(2)-Re(2)-N(3)-C(41)	83.7(12)
C(56)-Ru(2)-P(4)-C(73)	95.6(8)
C(55)-Ru(2)-P(4)-C(73)	-174.1(8)
P(3)-Ru(2)-P(4)-C(73)	-4.9(11)
Cl(2)-Ru(2)-P(4)-C(73)	-75.8(6)
C(56)-Ru(2)-P(4)-C(70)	-149.3(10)
C(55)-Ru(2)-P(4)-C(70)	-59.0(10)
P(3)-Ru(2)-P(4)-C(70)	110.3(12)
Cl(2)-Ru(2)-P(4)-C(70)	39.3(9)
C(56)-Ru(2)-P(4)-C(76)	-23.8(8)
C(55)-Ru(2)-P(4)-C(76)	66.5(8)
P(3)-Ru(2)-P(4)-C(76)	-124.2(10)
Cl(2)-Ru(2)-P(4)-C(76)	164.8(6)
C(53)-Re(2)-N(4)-C(50)	0.1(17)
C(51)-Re(2)-N(4)-C(50)	146(5)
C(52)-Re(2)-N(4)-C(50)	-89.1(16)
N(3)-Re(2)-N(4)-C(50)	179.3(17)
Br(2)-Re(2)-N(4)-C(50)	93.4(15)
C(53)-Re(2)-N(4)-C(46)	-175.4(14)

C(51)-Re(2)-N(4)-C(46)	-29(6)
C(52)-Re(2)-N(4)-C(46)	95.4(15)
N(3)-Re(2)-N(4)-C(46)	3.8(14)
Br(2)-Re(2)-N(4)-C(46)	-82.1(14)
C(2)-C(3)-C(4)-C(5)	3(2)
C(2)-C(3)-C(4)-C(14)	177.3(15)
C(1)-N(1)-C(5)-C(4)	1(2)
Re(1)-N(1)-C(5)-C(4)	-178.0(10)
C(3)-C(4)-C(5)-N(1)	-3(2)
C(14)-C(4)-C(5)-N(1)	-177.2(14)
C(10)-N(2)-C(6)-C(7)	0(2)
Re(1)-N(2)-C(6)-C(7)	177.0(12)
C(10)-N(2)-C(6)-C(1)	-177.3(14)
Re(1)-N(2)-C(6)-C(1)	0.1(17)
N(1)-C(1)-C(6)-N(2)	-2(2)
C(2)-C(1)-C(6)-N(2)	-178.0(14)
N(1)-C(1)-C(6)-C(7)	-178.4(15)
C(2)-C(1)-C(6)-C(7)	5(2)
N(2)-C(6)-C(7)-C(8)	4(2)
C(1)-C(6)-C(7)-C(8)	-179.7(15)
C(6)-C(7)-C(8)-C(9)	-4(2)
C(7)-C(8)-C(9)-C(10)	2(2)
C(6)-N(2)-C(10)-C(9)	-2(2)
Re(1)-N(2)-C(10)-C(9)	-179.5(13)
C(8)-C(9)-C(10)-N(2)	2(3)
C(13)-Re(1)-C(11)-O(1)	-18(32)
C(12)-Re(1)-C(11)-O(1)	71(32)
N(2)-Re(1)-C(11)-O(1)	-164(29)
N(1)-Re(1)-C(11)-O(1)	163(32)
Br(1)-Re(1)-C(11)-O(1)	-112(32)
C(13)-Re(1)-C(12)-O(2)	98(4)
C(11)-Re(1)-C(12)-O(2)	9(4)
N(2)-Re(1)-C(12)-O(2)	-165(4)
N(1)-Re(1)-C(12)-O(2)	-92(4)
Br(1)-Re(1)-C(12)-O(2)	-149(3)
C(11)-Re(1)-C(13)-O(3)	148(26)
C(12)-Re(1)-C(13)-O(3)	53(26)
N(2)-Re(1)-C(13)-O(3)	-36(26)
N(1)-Re(1)-C(13)-O(3)	-38(29)
Br(1)-Re(1)-C(13)-O(3)	-121(26)
C(3)-C(4)-C(14)-C(15)	-12(3)
C(5)-C(4)-C(14)-C(15)	162.0(16)
C(4)-C(14)-C(15)-Ru(1)	-178.4(13)
C(16)-Ru(1)-C(15)-C(14)	-9.1(19)
P(1)-Ru(1)-C(15)-C(14)	80.8(17)
P(2)-Ru(1)-C(15)-C(14)	-99.8(17)
Cl(1)-Ru(1)-C(15)-C(14)	169.8(17)
C(15)-Ru(1)-C(16)-O(4)	-29(100)
P(1)-Ru(1)-C(16)-O(4)	-123(100)
P(2)-Ru(1)-C(16)-O(4)	66(100)
Cl(1)-Ru(1)-C(16)-O(4)	158(100)
C(24)-P(1)-C(21)-C(22)	177.3(13)
C(28)-P(1)-C(21)-C(22)	-69.1(14)
Ru(1)-P(1)-C(21)-C(22)	53.1(13)
C(24)-P(1)-C(21)-C(23)	54.9(16)
C(28)-P(1)-C(21)-C(23)	168.5(15)
Ru(1)-P(1)-C(21)-C(23)	-69.3(15)
C(21)-P(1)-C(24)-C(25)	53.0(18)
C(28)-P(1)-C(24)-C(25)	-54.8(19)
Ru(1)-P(1)-C(24)-C(25)	171.4(14)
C(21)-P(1)-C(24)-C(26)	-172.6(12)

C(28)-P(1)-C(24)-C(26)	79.6(14)
Ru(1)-P(1)-C(24)-C(26)	-54.2(14)
C(21)-P(1)-C(28)-C(27)	-33.8(19)
C(24)-P(1)-C(28)-C(27)	73.6(19)
Ru(1)-P(1)-C(28)-C(27)	-151.5(15)
C(21)-P(1)-C(28)-C(29)	-158.2(13)
C(24)-P(1)-C(28)-C(29)	-50.7(16)
Ru(1)-P(1)-C(28)-C(29)	84.1(14)
C(36)-P(2)-C(30)-C(31)	-176.2(15)
C(33)-P(2)-C(30)-C(31)	80.6(17)
Ru(1)-P(2)-C(30)-C(31)	-52.3(15)
C(36)-P(2)-C(30)-C(32)	-56(2)
C(33)-P(2)-C(30)-C(32)	-160(2)
Ru(1)-P(2)-C(30)-C(32)	68(2)
C(30)-P(2)-C(33)-C(34)	-29(3)
C(36)-P(2)-C(33)-C(34)	-134(2)
Ru(1)-P(2)-C(33)-C(34)	96(2)
C(30)-P(2)-C(33)-C(35)	-160(2)
C(36)-P(2)-C(33)-C(35)	95(2)
Ru(1)-P(2)-C(33)-C(35)	-36(2)
C(30)-P(2)-C(36)-C(38)	-169.1(15)
C(33)-P(2)-C(36)-C(38)	-61.0(16)
Ru(1)-P(2)-C(36)-C(38)	72.8(16)
C(30)-P(2)-C(36)-C(37)	-43.7(18)
C(33)-P(2)-C(36)-C(37)	64.4(17)
Ru(1)-P(2)-C(36)-C(37)	-161.8(13)
C(45)-N(3)-C(41)-C(42)	-1(2)
Re(2)-N(3)-C(41)-C(42)	178.1(12)
C(45)-N(3)-C(41)-C(46)	-177.4(15)
Re(2)-N(3)-C(41)-C(46)	1.4(19)
N(3)-C(41)-C(42)-C(43)	5(3)
C(46)-C(41)-C(42)-C(43)	-178.9(17)
C(41)-C(42)-C(43)-C(44)	-6(3)
C(42)-C(43)-C(44)-C(45)	3(2)
C(42)-C(43)-C(44)-C(54)	-176.8(17)
C(41)-N(3)-C(45)-C(44)	-2(3)
Re(2)-N(3)-C(45)-C(44)	179.2(13)
C(43)-C(44)-C(45)-N(3)	1(3)
C(54)-C(44)-C(45)-N(3)	-179.1(17)
C(50)-N(4)-C(46)-C(47)	4(3)
Re(2)-N(4)-C(46)-C(47)	-179.9(14)
C(50)-N(4)-C(46)-C(41)	179.9(16)
Re(2)-N(4)-C(46)-C(41)	-4(2)
N(3)-C(41)-C(46)-N(4)	2(2)
C(42)-C(41)-C(46)-N(4)	-174.8(16)
N(3)-C(41)-C(46)-C(47)	177.3(17)
C(42)-C(41)-C(46)-C(47)	1(3)
N(4)-C(46)-C(47)-C(48)	-2(3)
C(41)-C(46)-C(47)-C(48)	-177.1(17)
C(46)-C(47)-C(48)-C(49)	-1(3)
C(47)-C(48)-C(49)-C(50)	1(3)
C(46)-N(4)-C(50)-C(49)	-4(3)
Re(2)-N(4)-C(50)-C(49)	-179.3(14)
C(48)-C(49)-C(50)-N(4)	1(3)
C(53)-Re(2)-C(51)-O(5)	-35(43)
C(52)-Re(2)-C(51)-O(5)	54(43)
N(4)-Re(2)-C(51)-O(5)	179(100)
N(3)-Re(2)-C(51)-O(5)	147(43)
Br(2)-Re(2)-C(51)-O(5)	-129(43)
C(53)-Re(2)-C(52)-O(6)	-99(11)
C(51)-Re(2)-C(52)-O(6)	173(11)

N(4)-Re(2)-C(52)-O(6)	-1(11)
N(3)-Re(2)-C(52)-O(6)	73(11)
Br(2)-Re(2)-C(52)-O(6)	74(18)
C(51)-Re(2)-C(53)-O(7)	166(19)
C(52)-Re(2)-C(53)-O(7)	76(19)
N(4)-Re(2)-C(53)-O(7)	-18(19)
N(3)-Re(2)-C(53)-O(7)	-24(22)
Br(2)-Re(2)-C(53)-O(7)	-104(19)
C(43)-C(44)-C(54)-C(55)	-18(3)
C(45)-C(44)-C(54)-C(55)	161.8(16)
C(44)-C(54)-C(55)-Ru(2)	-179.3(13)
C(56)-Ru(2)-C(55)-C(54)	-3.1(18)
P(4)-Ru(2)-C(55)-C(54)	-94.9(17)
P(3)-Ru(2)-C(55)-C(54)	87.0(17)
Cl(2)-Ru(2)-C(55)-C(54)	175.1(17)
C(55)-Ru(2)-C(56)-O(8)	-143(75)
P(4)-Ru(2)-C(56)-O(8)	-46(75)
P(3)-Ru(2)-C(56)-O(8)	123(75)
Cl(2)-Ru(2)-C(56)-O(8)	49(77)
C(67)-P(3)-C(61)-C(63)	171.8(16)
C(64)-P(3)-C(61)-C(63)	58.1(17)
Ru(2)-P(3)-C(61)-C(63)	-64.6(16)
C(67)-P(3)-C(61)-C(62)	-66.7(16)
C(64)-P(3)-C(61)-C(62)	179.6(14)
Ru(2)-P(3)-C(61)-C(62)	56.8(15)
C(61)-P(3)-C(64)-C(65)	57.4(17)
C(67)-P(3)-C(64)-C(65)	-51.3(17)
Ru(2)-P(3)-C(64)-C(65)	174.7(13)
C(61)-P(3)-C(64)-C(66)	-172.2(14)
C(67)-P(3)-C(64)-C(66)	79.1(16)
Ru(2)-P(3)-C(64)-C(66)	-54.9(15)
C(61)-P(3)-C(67)-C(69)	-157.1(16)
C(64)-P(3)-C(67)-C(69)	-51.4(17)
Ru(2)-P(3)-C(67)-C(69)	83.3(16)
C(61)-P(3)-C(67)-C(68)	-30(2)
C(64)-P(3)-C(67)-C(68)	76(2)
Ru(2)-P(3)-C(67)-C(68)	-149.2(16)
C(73)-P(4)-C(70)-C(71)	-173.5(17)
C(76)-P(4)-C(70)-C(71)	-65.1(18)
Ru(2)-P(4)-C(70)-C(71)	68.9(19)
C(73)-P(4)-C(70)-C(72)	-47(2)
C(76)-P(4)-C(70)-C(72)	62(2)
Ru(2)-P(4)-C(70)-C(72)	-164(2)
C(70)-P(4)-C(73)-C(75)	-171.2(17)
C(76)-P(4)-C(73)-C(75)	82.2(18)
Ru(2)-P(4)-C(73)-C(75)	-46.9(17)
C(70)-P(4)-C(73)-C(74)	-49(2)
C(76)-P(4)-C(73)-C(74)	-156(2)
Ru(2)-P(4)-C(73)-C(74)	75(2)
C(73)-P(4)-C(76)-C(78)	-37.3(16)
C(70)-P(4)-C(76)-C(78)	-144.4(15)
Ru(2)-P(4)-C(76)-C(78)	83.5(14)
C(73)-P(4)-C(76)-C(77)	-166.0(13)
C(70)-P(4)-C(76)-C(77)	87.0(15)
Ru(2)-P(4)-C(76)-C(77)	-45.2(14)
C(106)-C(101)-C(102)-C(103)	-3(3)
C(101)-C(102)-C(103)-C(104)	5(3)
C(102)-C(103)-C(104)-C(105)	-3(3)
C(103)-C(104)-C(105)-C(106)	-1(3)
C(102)-C(101)-C(106)-C(105)	-2(3)
C(104)-C(105)-C(106)-C(101)	4(4)

C(113)-C(108)-C(109)-C(110)	-3(4)
C(108)-C(109)-C(110)-C(111)	4(4)
C(109)-C(110)-C(111)-C(112)	-4(4)
C(110)-C(111)-C(112)-C(113)	3(4)
C(109)-C(108)-C(113)-C(112)	2(4)
C(111)-C(112)-C(113)-C(108)	-2(4)