Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information

Synthesis of Ruthenium (II) Complexes of Tetradentate Bis(N-pyridylimidazolylidenyl)methane and Their Reactivities towards N-Donors

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Table S1. Half Potential of Oxidation Peaks of Various Ru^{2+} Complexes

Half Potential	**1**	**5a**	**10**
Ru^{2+}/Ru^{3+} ($E_{1/2}$/V (ΔE/mV)[a])	0.90 (74)	0.82 (80)	0.75 (73)

[a] $\Delta E = E_{pa} - E_{pc}$.

The molecular Structures of Compounds 4, 6, and 8

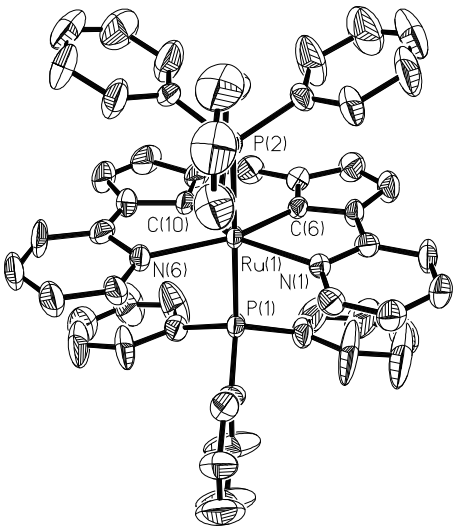

Figure S1. ORTEP drawing of the cationic section of $[RuL(PPh_3)_2](PF_6)_2$ (**4**). Thermal ellipsoids are shown at the 30% probability level with hydrogen atoms omitted for clarity. Selected bond distances (Å) and angles (°): Ru(1)-C(6) 1.901(5), Ru(1)-C(10) 1.909(6), Ru(1)-N(6) 2.266(4), Ru(1)-N(1) 2.278(4), Ru(1)-P(1) 2.4071(15), Ru(1)-P(2) 2.4153(14), C(6)-Ru(1)-C(10) 86.8(2), C(6)-Ru(1)-N(6) 162.0(2), C(10)-Ru(1)-N(6) 75.3(2), C(6)-Ru(1)-N(1) 75.24(18), C(10)-Ru(1)-N(1) 162.0(2), N(6)-Ru(1)-N(1) 122.64(17), C(6)-Ru(1)-P(1) 90.44(14), C(10)-Ru(1)-P(1) 90.28(16), N(6)-Ru(1)-P(1) 90.72(12), N(1)-Ru(1)-P(1) 90.98(11), C(6)-Ru(1)-P(2) 89.84(14), C(10)-Ru(1)-P(2) 89.81(16), N(6)-Ru(1)-P(2) 89.03(12), N(1)-Ru(1)-P(2) 89.03(11), P(1)-Ru(1)-P(2) 179.71(5).

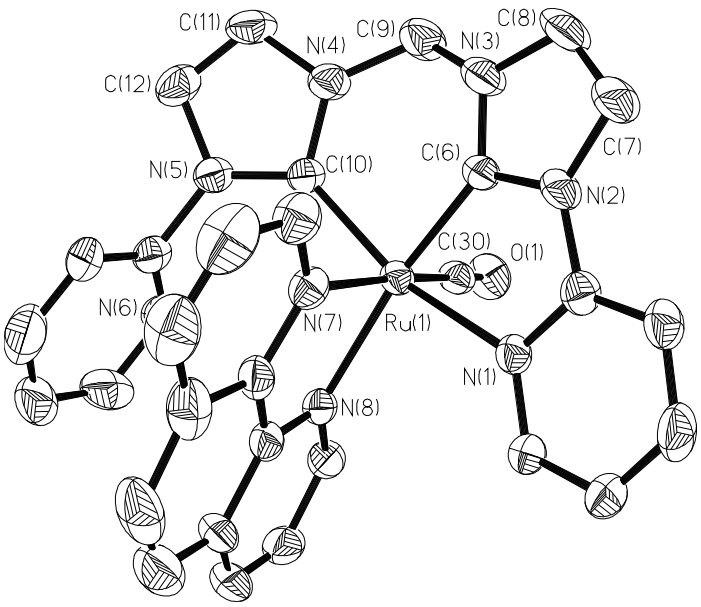

Figure S2. ORTEP drawing of the cationic section of [Ru(L)(phen)(CO)]$(PF_6)_2$ (**6**). Thermal ellipsoids are shown at the 30% probability level with hydrogen atoms omitted for clarity. Selected bond distances (Å) and angles (°): Ru(1)-C(6) 1.937(5), Ru(1)-C(10) 2.038(5), Ru(1)-C(30) 1.868(6), Ru(1)-N(1) 2.181(4), Ru(1)-N(7) 2.127(5), Ru(1)-N(8) 2.139(4), C(30)-O(1) 1.132(7), C(30)-Ru(1)-C(6) 90.5(2), C(30)-Ru(1)-C(10) 92.1(2), C(6)-Ru(1)-C(10) 86.7(2), C(30)-Ru(1)-N(7) 173.84(19), C(6)-Ru(1)-N(7) 95.5(2), C(10)-Ru(1)-N(7) 86.80(19), C(30)-Ru(1)-N(8) 96.8(2), C(6)-Ru(1)-N(8) 166.9(2), C(10)-Ru(1)-N(8) 103.92(19), N(7)-Ru(1)-N(8) 77.65(18), C(30)-Ru(1)-N(1) 97.2(2), C(6)-Ru(1)-N(1) 75.9(2), C(10)-Ru(1)-N(1) 160.34(19), N(7)-Ru(1)-N(1) 85.76(16), N(8)-Ru(1)-N(1) 92.22(16).

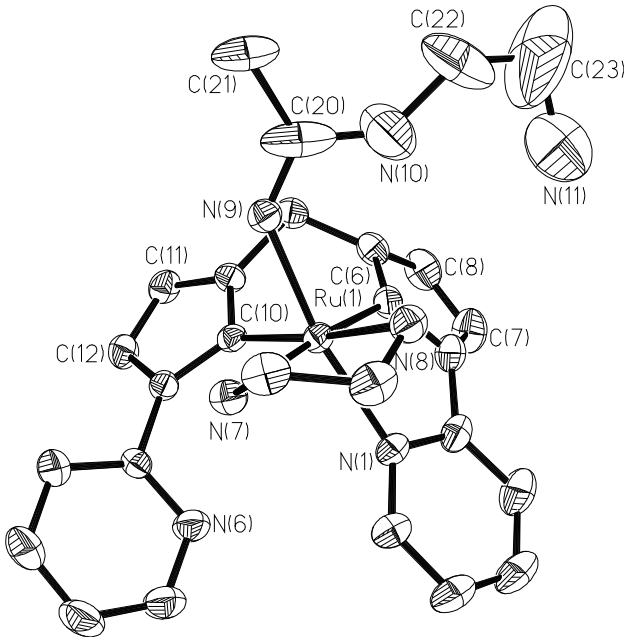

Figure S3. ORTEP drawing of the cationic section of [RuL(ethane-1,2-diamine)(N-(2-aminoethyl)acetimidamide)]$(PF_6)_2$ (**8**). Thermal ellipsoids are shown at the 30 % probability level with hydrogen atoms omitted for clarity. Selected bond distances (Å) and angles (°): Ru(1)-C(6) 1.922(5), Ru(1)-C(10) 2.015(4), Ru(1)-N(9) 2.069(4), Ru(1)-N(1) 2.105(4), Ru(1)-N(8) 2.190(4), Ru(1)-N(7) 2.223(4), C(20)-N(9) 1.246(8), C(20)-N(10) 1.381(8), C(6)-Ru(1)-C(10) 80.09(18), C(6)-Ru(1)-N(9) 100.38(18), C(10)-Ru(1)-N(9) 87.43(16), C(6)-Ru(1)-N(1) 76.82(17), C(10)-Ru(1)-N(1) 102.45(15), N(9)-Ru(1)-N(1) 168.95(15), C(6)-Ru(1)-N(8) 104.12(18), C(10)-Ru(1)-N(8) 172.18(15), N(9)-Ru(1)-N(8) 85.33(15), N(1)-Ru(1)-N(8) 85.02(15), C(6)-Ru(1)-N(7) 174.06(17), C(10)-Ru(1)-N(7) 97.71(16), N(9)-Ru(1)-N(7) 84.97(15), N(1)-Ru(1)-N(7) 98.40(15), N(8)-Ru(1)-N(7) 78.73(16).

Table S2. Summary of X-ray crystallographic data for complexes 4, 6, and 8.

	4	**6**	**8**
Formula	$C_{53}H_{44}F_{12}N_6P_4Ru$	$C_{33}H_{26.5}F_{12}N_{9.5}OP_2Ru$	$C_{25}H_{36}F_{12}N_{12}P_2Ru$
Fw	1217.89	963.15	895.67
Crystal system	Monoclinic	Triclinic	Triclinic
Space group	*C2/c*	*P*-1	*P*-1
a, Å	21.5296(7)	11.7158(7)	12.0111(5)
b, Å	21.6088(6)	11.7418(9)	12.4027(4)
c, Å	24.4791(9)	14.8628(11)	13.1637(4)
α, deg.	90	107.818(7)	90.600(3)
β, deg.	108.963(4)	90.493(6)	93.233(3)
γ, deg.	90	96.708(6)	113.242(4)
V, Å3	10770.3(6)	1931.1(2)	1797.84(11)
Z	8	2	2
D_{calcd}, Mg/m^3	1.502	1.656	1.655
Reflections collected	21011	13018	12177
Reflections independent, R_{int}	9484, 0.0347	6793, 0.0312	6342, 0.0252
Goodness-of-fit on F^2	1.087	1.053	1.055
*R*1, *wR*2 ($I>2\sigma(I)$)	0.0602, 0.1276	0.0627, 0.1702	0.0505, 0.1342
*R*1, *wR*2 (all data)	0.0951, 0.1562	0.0817, 0.1911	0.0612, 0.1434