Multi-site Effects on Intervalence Charge Transfer in a "Cluster-like" Trinuclear Assembly containing Ruthenium and Osmium

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SUPPLEMENTARY INFORMATION

Table S1. Crystal data and structure refinement parameters for ΛΔ/ΔΛ-[{Ru(bpy)$_2$}(HAT){Os(bpy)$_2$}](PF$_6$)$_3$Cl.

Crystal Colour	green / purple dichroic
Crystal Dimensions	0.5 x 0.1 x 0.1 mm
Crystal Habit	Plates
Crystal System	monoclinic
space group	$P2_1/n$
a (Å)	10.061(5)
b (Å)	17.521(5)
c (Å)	38.001(19)
α (°)	90
β (°)	90.431 (10)
γ (°)	90
V (Å^3)	6685(6)
Z	4
Mol.Wt.	1620.6
T (K)	293
λ (MoKα, Å)	0.71069
range h	12<h<12
range k	0<k<21
range l	0<l<47
range 2θ(°)	2.16<θ<53.1
No. reflections	14283
No. reflections > 4σ	3195
No. Parameters	820
S	0.818
R_{all}	0.3497
$R_{2\sigma}$	0.117
wR (all)	0.377
wR (2σ)	0.306

Table S2. Fractional Atomic Coordinates for ΛΔ/ΔΛ-[{Ru(bpy)$_2$}(HAT){Os(bpy)$_2$}](PF$_6$)$_3$Cl.

Atom	x	y	z	Uiso
C(1)	0.183(2)	0.595(1)	0.153(1)	0.076
C(10)	0.062(2)	0.401(1)	0.137(1)	0.066
C(11)	-0.071(2)	0.277(1)	0.144(1)	0.079
C(12)	-0.0783(19)	0.3304(10)	0.1691(5)	0.054
C(13)	0.270(2)	0.435(1)	0.215(1)	0.091
C(14)	0.362(2)	0.387(1)	0.235(1)	0.091
C(15)	0.325(3)	0.349(2)	0.263(1)	0.133
C(16)	0.195(3)	0.355(1)	0.273(1)	0.089
C(17)	0.106(2)	0.399(1)	0.254(1)	0.073
C(18)	-0.040(2)	0.407(1)	0.262(1)	0.068
C(19)	-0.100(2)	0.376(1)	0.292(1)	0.084
C(2)	0.261(3)	0.603(2)	0.120(1)	0.093
C(20)	-0.227(3)	0.388(1)	0.297(1)	0.090
C(21)	-0.302(2)	0.431(1)	0.275(1)	0.093
C(22)	-0.240(2)	0.455(1)	0.244(1)	0.073
C(23)	0.082(2)	0.607(1)	0.252(1)	0.088
C(24)	0.058(2)	0.667(1)	0.274(1)	0.083
C(25)	-0.042(3)	0.715(2)	0.270(1)	0.107
C(26)	-0.130(2)	0.696(1)	0.243(1)	0.100
C(27)	-0.109(2)	0.635(1)	0.221(1)	0.082
C(28)	-0.197(2)	0.617(1)	0.191(1)	0.073
C(29)	-0.304(3)	0.662(2)	0.177(1)	0.117
C(3)	0.219(2)	0.486(2)	0.102(1)	0.079
C(30)	-0.373(2)	0.637(2)	0.151(1)	0.130
C(31)	-0.341(3)	0.573(2)	0.134(1)	0.110
C(32)	-0.235(2)	0.528(1)	0.147(1)	0.091
C(33)	-0.194(3)	0.318(2)	0.046(1)	0.106
C(34)	-0.275(3)	0.354(2)	0.022(1)	0.124
C(35)	-0.280(4)	0.323(3)	-0.013(1)	0.168
C(36)	-0.195(3)	0.268(2)	-0.021(1)	0.131
C(37)	-0.095(3)	0.225(2)	0.005(1)	0.125
C(38)	-0.005(3)	0.160(2)	0.000(1)	0.107
C(39)	0.007(4)	0.124(2)	-0.030(1)	0.165
C(4)	0.136(2)	0.471(1)	0.131(1)	0.071
C(40)	0.092(5)	0.068(3)	-0.036(1)	0.187
C(41)	0.158(4)	0.054(2)	-0.009(1)	0.159
C(42)	0.144(3)	0.091(2)	0.023(1)	0.119
C(43)	-0.224(2)	0.119(2)	0.081(1)	0.095
C(44)	-0.305(3)	0.063(2)	0.097(1)	0.105
C(45)	-0.249(3)	0.011(2)	0.118(1)	0.100
C(46)	-0.122(3)	0.013(2)	0.129(1)	0.118
C(47)	-0.046(2)	0.073(1)	0.114(1)	0.069
C(48)	0.099(3)	0.088(1)	0.122(1)	0.093
C(49)	0.164(3)	0.038(1)	0.143(1)	0.102
C(5)	0.230(2)	0.423(1)	0.076(1)	0.078
C(50)	0.297(3)	0.053(2)	0.149(1)	0.118
C(51)	0.358(3)	0.113(2)	0.132(1)	0.107
C(52)	0.278(3)	0.159(2)	0.110(1)	0.097
C(6)	0.154(2)	0.357(2)	0.080(1)	0.075
C(7)	0.244(3)	0.304(2)	0.034(1)	0.115
C(8)	0.326(3)	0.367(2)	0.028(1)	0.100
C(9)	0.065(2)	0.349(1)	0.111(1)	0.076
CL(1)	0.522(3)	0.543(2)	0.038(1)	0.514
F(1)	-0.0489(16)	0.2206(9)	0.2409(6)	0.165
F(10)	-0.1585(15)	0.8697(10)	0.3855(4)	0.129
F(11)	-0.1034(15)	0.8626(9)	0.3287(4)	0.121

F(12)	0.0829(17)	0.7978(11)	0.3454(5)	0.167
F(13)	0.474(2)	0.364(1)	0.333(0)	0.192
F(14)	0.320(3)	0.268(2)	0.342(1)	0.284
F(15)	0.591(3)	0.323(2)	0.379(1)	0.295
F(16)	0.406(4)	0.249(1)	0.391(1)	0.284
F(17)	0.497(3)	0.245(2)	0.336(1)	0.262
F(18)	0.389(4)	0.367(2)	0.386(1)	0.379
F(2)	0.1053(17)	0.0709(10)	0.2235(5)	0.154
F(3)	0.1207(18)	0.1589(12)	0.2632(5)	0.160
F(4)	-0.0707(16)	0.1016(8)	0.2561(4)	0.122
F(5)	0.119(2)	0.192(1)	0.206(1)	0.180
F(6)	-0.063(2)	0.135(1)	0.201(1)	0.174
F(7)	-0.1077(18)	0.7571(10)	0.3648(6)	0.165
F(8)	0.0329(18)	0.9157(11)	0.3678(6)	0.171
F(9)	0.0312(17)	0.8084(10)	0.4025(4)	0.137
N(1)	0.1146(17)	0.5261(9)	0.1562(5)	0.065
N(10)	-0.1612(16)	0.5522(9)	0.1753(5)	0.070
N(11)	-0.1101(17)	0.2592(13)	0.0381(5)	0.082
N(12)	0.063(2)	0.144(1)	0.029(1)	0.109
N(13)	-0.1013(18)	0.1253(11)	0.0897(5)	0.078
N(14)	0.1557(18)	0.1432(10)	0.1047(5)	0.076
N(2)	0.2851(17)	0.5488(12)	0.0959(5)	0.072
N(3)	0.1628(18)	0.2926(12)	0.0602(5)	0.084
N(4)	0.3106(19)	0.4293(12)	0.0490(5)	0.085
N(5)	-0.0014(16)	0.2800(10)	0.1131(4)	0.065
N(6)	-0.0136(15)	0.3967(8)	0.1654(4)	0.050
N(7)	0.1400(16)	0.4380(9)	0.2233(5)	0.069
N(8)	-0.1094(16)	0.4492(9)	0.2380(4)	0.063
N(9)	-0.0067(15)	0.5922(7)	0.2243(4)	0.051
OS(1_)	0.0300(10)	0.2078(6)	0.0726(2)	0.087
OS(2_)	-0.0059(6)	0.4870(2)	0.1965(2)	0.067
P(1)	0.0258(8)	0.1460(5)	0.2318(3)	0.105
P(2)	-0.0351(7)	0.8353(5)	0.3662(2)	0.090
P(3)	0.4487(13)	0.3031(7)	0.3609(3)	0.144
RU(1_)	0.0292(15)	0.2082(8)	0.0730(4)	0.055(5)
RU(2_)	-0.0045(12)	0.5008(5)	0.1964(3)	0.044(2)

Table S3. Fractional Hydrogen Positions for ΛΔ/ΔΛ-[{Ru(bpy)$_2$}(HAT){Os(bpy)$_2$}](PF$_6$)$_3$Cl.

Atom	x	y	z	U_{iso}
H(1)	0.17987	0.63317	0.16995	0.092
H(11)	-0.11851	0.23222	0.14796	0.095
H(12)	-0.12852	0.32145	0.18918	0.065
H(13)	0.30059	0.46242	0.19551	0.109
H(14)	0.44995	0.38421	0.22808	0.109
H(15)	0.38506	0.31917	0.27596	0.160
H(16)	0.16542	0.32963	0.29284	0.107
H(19)	-0.05055	0.34734	0.30799	0.101
H(2)	0.29747	0.65133	0.11581	0.111
H(20)	-0.26723	0.36706	0.31714	0.107
H(21)	-0.38960	0.44304	0.27991	0.111
H(22)	-0.29327	0.47649	0.22621	0.088
H(23)	0.15625	0.57622	0.25602	0.105
H(24)	0.11467	0.67448	0.29354	0.100
H(25)	-0.05255	0.75837	0.28313	0.129
H(26)	-0.20734	0.72454	0.24021	0.119
H(29)	-0.32358	0.70881	0.18725	0.141
H(30)	-0.44860	0.66404	0.14417	0.156
H(31)	-0.38765	0.55871	0.11368	0.132
H(32)	-0.21542	0.48138	0.13675	0.110
H(33)	-0.19594	0.33530	0.06915	0.127
H(34)	-0.32459	0.39698	0.02795	0.148
H(35)	-0.34162	0.34155	-0.02917	0.202
H(36)	-0.19327	0.25298	-0.04474	0.157
H(39)	-0.04921	0.13932	-0.04808	0.198
H(40)	0.10058	0.04277	-0.05774	0.224
H(41)	0.22276	0.01608	-0.01057	0.190
H(42)	0.19737	0.07502	0.04133	0.143
H(43)	-0.26012	0.15179	0.06438	0.114
H(44)	-0.39664	0.06169	0.09207	0.125
H(45)	-0.30102	-0.02998	0.12522	0.120
H(46)	-0.08640	-0.02123	0.14533	0.142
H(49)	0.12235	-0.00433	0.15241	0.122
H(50)	0.34584	0.02243	0.16400	0.141
H(51)	0.44830	0.12289	0.13466	0.128
H(52)	0.31529	0.20206	0.10011	0.116
H(7)	0.24717	0.26552	0.01655	0.138
H(8)	0.39036	0.36693	0.01079	0.120

Table S4. Anistropic Thermal Parameters for ΛΔ/ΔΛ-[{Ru(bpy)$_2$}(HAT){Os(bpy)$_2$}](PF$_6$)$_3$Cl.

Atom	U11	U22	U33	U12	U13	U23
C(1)	0.06(1)	0.03(1)	0.13(2)	-0.02(1)	0.02(1)	0.00(1)
C(10)	0.08(2)	0.05(1)	0.07(1)	0.01(1)	0.03(1)	0.00(1)
C(11)	0.09(2)	0.09(2)	0.06(1)	-0.02(1)	0.03(1)	-0.02(1)
C(12)	0.06(1)	0.04(1)	0.06(1)	0.00(1)	0.02(1)	0.00(1)
C(13)	0.06(1)	0.13(2)	0.08(2)	0.01(1)	0.00(1)	0.02(1)
C(14)	0.06(1)	0.11(2)	0.10(2)	0.02(1)	-0.01(1)	0.00(1)
C(15)	0.12(2)	0.17(3)	0.10(2)	0.11(2)	0.03(2)	0.04(2)
C(16)	0.11(2)	0.08(2)	0.07(1)	0.04(1)	0.02(1)	0.00(1)
C(17)	0.07(1)	0.08(2)	0.07(1)	0.02(1)	0.00(1)	-0.01(1)
C(18)	0.08(1)	0.05(1)	0.08(1)	0.01(1)	0.01(1)	0.00(1)
C(19)	0.08(1)	0.10(2)	0.08(1)	-0.01(1)	-0.01(1)	0.03(1)
C(2)	0.08(2)	0.07(2)	0.13(2)	-0.02(2)	-0.03(2)	0.03(2)
C(20)	0.11(2)	0.08(2)	0.08(1)	0.02(1)	0.04(1)	0.00(1)
C(21)	0.06(1)	0.12(2)	0.09(2)	0.01(1)	0.02(1)	0.00(1)
C(22)	0.07(1)	0.04(1)	0.11(2)	0.02(1)	0.03(1)	0.01(1)
C(23)	0.07(1)	0.11(2)	0.08(2)	-0.02(1)	0.00(1)	-0.03(1)
C(24)	0.08(2)	0.09(2)	0.07(1)	-0.03(1)	-0.01(1)	-0.02(1)
C(25)	0.10(2)	0.10(2)	0.12(2)	-0.01(1)	0.00(2)	-0.01(2)
C(26)	0.07(2)	0.11(2)	0.13(2)	0.02(1)	0.01(1)	-0.04(1)
C(27)	0.05(1)	0.08(2)	0.11(2)	0.00(1)	0.04(1)	-0.01(1)
C(28)	0.06(1)	0.06(1)	0.10(2)	0.00(1)	0.01(1)	-0.01(1)
C(29)	0.06(2)	0.10(2)	0.19(3)	0.02(1)	-0.01(2)	-0.03(2)
C(3)	0.07(1)	0.12(2)	0.05(1)	-0.01(1)	0.03(1)	0.02(1)
C(30)	0.03(1)	0.13(2)	0.23(4)	0.03(1)	-0.03(2)	-0.02(2)
C(31)	0.11(2)	0.11(2)	0.12(2)	0.00(1)	-0.02(2)	0.02(1)
C(32)	0.08(2)	0.08(2)	0.11(2)	0.00(1)	-0.01(1)	-0.02(1)
C(33)	0.07(2)	0.15(2)	0.10(2)	0.01(1)	0.01(1)	0.01(2)
C(34)	0.12(2)	0.11(2)	0.14(2)	0.03(2)	0.00(2)	0.03(2)
C(35)	0.11(3)	0.28(5)	0.11(2)	0.04(2)	0.00(2)	0.03(2)
C(36)	0.12(3)	0.19(3)	0.08(2)	-0.03(2)	-0.01(2)	-0.01(2)
C(37)	0.10(2)	0.18(3)	0.09(2)	0.00(2)	0.02(2)	0.00(2)
C(38)	0.14(2)	0.12(2)	0.07(1)	-0.05(1)	0.03(1)	-0.04(1)
C(39)	0.18(4)	0.22(4)	0.09(2)	-0.01(2)	0.02(2)	-0.09(2)
C(4)	0.06(1)	0.10(2)	0.06(1)	0.01(1)	-0.01(1)	0.02(1)
C(40)	0.22(5)	0.21(4)	0.13(3)	0.00(3)	0.03(3)	-0.10(3)
C(41)	0.16(3)	0.19(3)	0.13(2)	-0.01(2)	0.06(2)	-0.08(3)
C(42)	0.11(2)	0.13(2)	0.12(2)	-0.02(1)	0.05(1)	-0.07(2)
C(43)	0.07(1)	0.12(2)	0.10(2)	0.00(1)	0.01(1)	-0.03(1)
C(44)	0.06(1)	0.13(2)	0.13(2)	-0.01(1)	0.02(1)	-0.03(2)
C(45)	0.09(1)	0.10(2)	0.12(2)	-0.02(1)	0.02(1)	-0.04(1)
C(46)	0.09(2)	0.15(2)	0.11(2)	-0.03(2)	0.00(2)	0.03(2)
C(47)	0.08(1)	0.09(1)	0.05(1)	-0.01(1)	0.01(1)	-0.04(1)
C(48)	0.08(2)	0.08(2)	0.11(2)	0.01(1)	0.03(1)	0.01(1)
C(49)	0.09(2)	0.06(2)	0.15(3)	0.00(1)	-0.01(2)	0.00(1)
C(5)	0.08(2)	0.09(2)	0.06(1)	0.01(1)	0.01(1)	0.04(1)
C(50)	0.09(2)	0.11(2)	0.16(3)	0.00(2)	0.00(2)	-0.01(2)
C(51)	0.07(2)	0.12(2)	0.14(3)	0.00(1)	0.02(1)	-0.03(2)
C(52)	0.08(1)	0.10(2)	0.11(2)	-0.02(1)	0.00(1)	-0.04(1)
C(6)	0.07(1)	0.11(2)	0.05(1)	-0.02(1)	0.03(1)	-0.02(1)
C(7)	0.10(2)	0.12(2)	0.13(2)	-0.04(2)	0.05(2)	0.02(2)
C(8)	0.09(2)	0.15(3)	0.06(2)	0.00(2)	0.02(1)	-0.01(2)
C(9)	0.08(2)	0.09(2)	0.06(2)	-0.02(1)	0.03(1)	0.01(1)
CL(1)	0.48(4)	0.59(5)	0.47(4)	-0.23(3)	0.03(3)	0.17(4)
F(1)	0.10(1)	0.11(1)	0.28(2)	0.02(1)	0.06(1)	-0.01(1)
F(10)	0.12(1)	0.17(2)	0.10(1)	0.06(1)	0.05(1)	0.00(1)

F(11)	0.11(1)	0.12(1)	0.13(1)	0.01(1)	0.00(1)	0.01(1)
F(12)	0.12(1)	0.20(2)	0.18(2)	0.08(1)	0.07(1)	0.01(1)
F(13)	0.23(2)	0.24(2)	0.11(1)	-0.10(2)	-0.01(1)	0.03(2)
F(14)	0.23(3)	0.31(4)	0.31(4)	-0.06(3)	-0.16(3)	0.02(3)
F(15)	0.23(3)	0.32(4)	0.33(4)	-0.08(3)	-0.09(3)	0.05(3)
F(16)	0.53(5)	0.17(2)	0.15(2)	-0.17(3)	-0.12(3)	0.04(2)
F(17)	0.29(4)	0.24(3)	0.26(3)	0.06(3)	0.08(3)	-0.13(3)
F(18)	0.40(5)	0.22(3)	0.53(6)	0.19(3)	0.28(5)	0.16(4)
F(2)	0.14(1)	0.13(1)	0.19(2)	0.07(1)	0.03(1)	0.03(1)
F(3)	0.13(1)	0.20(2)	0.15(2)	-0.01(1)	-0.04(1)	-0.03(1)
F(4)	0.14(1)	0.09(1)	0.13(1)	-0.02(1)	0.05(1)	0.00(1)
F(5)	0.16(2)	0.19(2)	0.19(2)	0.00(1)	0.09(1)	0.07(2)
F(6)	0.15(2)	0.19(2)	0.18(2)	0.00(2)	-0.05(2)	0.00(2)
F(7)	0.15(2)	0.11(1)	0.24(2)	-0.06(1)	-0.02(1)	0.01(1)
F(8)	0.14(2)	0.15(2)	0.23(2)	-0.05(1)	-0.07(1)	0.00(1)
F(9)	0.15(1)	0.16(1)	0.10(1)	0.03(1)	0.00(1)	-0.02(1)
N(1)	0.07(1)	0.04(1)	0.08(1)	0.01(1)	-0.01(1)	0.02(1)
N(10)	0.06(1)	0.06(1)	0.09(1)	-0.01(1)	0.01(1)	-0.02(1)
N(11)	0.05(1)	0.13(2)	0.07(1)	-0.01(1)	0.01(1)	0.03(1)
N(12)	0.11(2)	0.14(2)	0.08(1)	-0.01(1)	0.04(1)	-0.04(1)
N(13)	0.06(1)	0.09(1)	0.08(1)	0.00(1)	0.04(1)	-0.02(1)
N(14)	0.06(1)	0.06(1)	0.11(1)	0.00(1)	0.03(1)	-0.02(1)
N(2)	0.05(1)	0.07(1)	0.10(1)	-0.01(1)	0.00(1)	0.03(1)
N(3)	0.07(1)	0.12(2)	0.06(1)	-0.01(1)	0.04(1)	-0.01(1)
N(4)	0.08(1)	0.11(2)	0.06(1)	-0.04(1)	0.01(1)	0.01(1)
N(5)	0.07(1)	0.08(1)	0.05(1)	0.00(1)	0.02(1)	-0.01(1)
N(6)	0.05(1)	0.04(1)	0.05(1)	-0.01(1)	0.01(1)	0.00(1)
N(7)	0.057(9)	0.057(11)	0.094(12)	0.010(9)	0.003(9)	0.000(9)
N(8)	0.058(9)	0.063(11)	0.069(10)	0.016(9)	0.012(8)	0.014(8)
N(9)	0.050(9)	0.023(7)	0.080(10)	-0.024(6)	-0.005(8)	-0.007(7)
OS(1_)	0.082(4)	0.101(5)	0.077(4)	-0.021(1)	0.036(2)	-0.033(2)
OS(2_)	0.060(2)	0.056(2)	0.083(2)	-0.004(2)	0.014(1)	-0.007(2)
P(1)	0.081(5)	0.107(6)	0.128(7)	-0.003(5)	0.024(6)	-0.014(6)
P(2)	0.075(5)	0.110(6)	0.086(5)	0.013(5)	0.009(4)	-0.002(5)
P(3)	0.17(1)	0.16(1)	0.10(1)	-0.01(1)	0.04(1)	0.00(1)

Table S5. Bond Lengths (Å) for ΛΔ/ΔΛ-[{Ru(bpy)$_2$}(HAT){Os(bpy)$_2$}](PF$_6$)$_3$Cl.

Bond	Length (Å)	Bond	Length (Å)
OS(2_)-RU(2_)	0.242(10)	OS(2_)-N(6)	1.976(16)
OS(2_)-N(7)	1.974(18)	OS(2_)-N(8)	2.009(17)
RU(1_)-OS(1_)	0.019(18)	RU(1_)-N(14)	2.08(3)
RU(1_)-N(5)	2.00(3)	RU(1_)-N(3)	2.06(3)
RU(1_)-N(13)	2.06(3)	RU(1_)-N(12)	2.06(3)
RU(2_)-N(9)	1.920(17)	RU(2_)-N(7)	2.08(2)
RU(2_)-N(10)	1.98(2)	RU(2_)-N(1)	2.00(3)
OS(1_)-N(5)	2.019(19)	OS(1_)-N(12)	2.04(3)
P(3)-F(13)	1.52(3)	P(3)-F(14)	1.61(4)
P(3)-F(16)	1.57(3)	P(3)-F(18)	1.59(4)
P(3)-F(15)	1.61(4)	P(3)-F(17)	1.48(4)
F(6)-P(1)	1.48(3)	C(36)-H(36)	0.93(4)
C(36)-C(35)	1.34(6)	C(41)-H(41)	0.93(5)
C(41)-C(40)	1.25(6)	C(41)-C(42)	1.38(5)
C(38)-C(37)	1.46(5)	C(38)-C(39)	1.30(5)
C(38)-N(12)	1.31(4)	C(37)-N(11)	1.40(4)
C(40)-H(40)	0.93(5)	C(40)-C(39)	1.33(7)
C(42)-H(42)	0.93(3)	C(42)-N(12)	1.25(4)
C(35)-H(35)	0.93(4)	C(35)-C(34)	1.42(6)
C(39)-H(39)	0.93(4)	C(33)-H(33)	0.93(3)
C(33)-C(34)	1.37(5)	C(33)-N(11)	1.37(4)
C(34)-H(34)	0.93(4)	P(2)-F(12)	1.57(2)
P(2)-F(10)	1.567(17)	P(2)-F(11)	1.646(17)
P(2)-F(9)	1.598(18)	P(2)-F(8)	1.57(3)
P(2)-F(7)	1.553(19)	N(14)-C(48)	1.31(4)
N(14)-C(52)	1.28(4)	N(9)-C(23)	1.41(3)
N(9)-C(27)	1.28(3)	N(6)-C(12)	1.34(3)
N(6)-C(10)	1.32(3)	N(7)-C(17)	1.41(3)
N(7)-C(13)	1.35(3)	C(22)-H(22)	0.93(3)
C(22)-N(8)	1.34(3)	C(22)-C(21)	1.41(4)
N(10)-C(28)	1.33(3)	N(10)-C(32)	1.36(4)
N(8)-C(18)	1.35(3)	N(5)-C(9)	1.39(3)
N(5)-C(11)	1.37(3)	N(1)-C(1)	1.40(3)
N(1)-C(4)	1.37(3)	C(3)-N(2)	1.30(4)
C(3)-C(5)	1.51(4)	C(3)-C(4)	1.42(4)
C(17)-C(18)	1.51(4)	C(17)-C(16)	1.36(4)
N(4)-C(5)	1.31(3)	N(4)-C(8)	1.35(4)
N(3)-C(6)	1.37(4)	N(3)-C(7)	1.32(4)
C(12)-H(12)	0.93(2)	C(12)-C(11)	1.34(3)
N(13)-C(47)	1.40(3)	N(13)-C(43)	1.28(4)
N(2)-C(2)	1.35(4)	C(5)-C(6)	1.39(4)
C(47)-C(48)	1.51(4)	C(47)-C(46)	1.42(4)
C(31)-H(31)	0.93(3)	C(31)-C(32)	1.42(4)
C(31)-C(30)	1.34(5)	C(21)-H(21)	0.93(3)
C(21)-C(20)	1.35(4)	C(23)-H(23)	0.93(3)
C(23)-C(24)	1.36(4)	C(18)-C(19)	1.41(4)
C(29)-H(29)	0.93(3)	C(29)-C(28)	1.42(4)
C(29)-C(30)	1.28(5)	C(28)-C(27)	1.47(4)
C(14)-H(14)	0.93(3)	C(14)-C(15)	1.32(4)
C(14)-C(13)	1.46(4)	C(15)-H(15)	0.93(4)
C(15)-C(16)	1.37(4)	C(6)-C(9)	1.47(4)
C(8)-H(8)	0.93(3)	C(8)-C(7)	1.40(5)
C(24)-H(24)	0.93(3)	C(24)-C(25)	1.32(4)
C(27)-C(26)	1.38(4)	C(9)-C(10)	1.36(4)
C(11)-H(11)	0.93(3)	C(10)-C(4)	1.44(4)
C(19)-H(19)	0.93(3)	C(19)-C(20)	1.31(4)

C(48)-C(49)	1.34(4)	C(50)-H(50)	0.93(4)
C(50)-C(49)	1.37(4)	C(50)-C(51)	1.38(5)
C(13)-H(13)	0.93(3)	C(49)-H(49)	0.93(3)
C(46)-H(46)	0.93(3)	C(46)-C(45)	1.34(5)
C(1)-H(1)	0.93(3)	C(1)-C(2)	1.48(4)
C(7)-H(7)	0.93(3)	C(44)-H(44)	0.93(3)
C(44)-C(45)	1.34(4)	C(44)-C(43)	1.41(4)
C(45)-H(45)	0.93(3)	C(20)-H(20)	0.93(3)
C(52)-H(52)	0.93(3)	C(52)-C(51)	1.39(4)
C(16)-H(16)	0.93(3)	C(2)-H(2)	0.93(3)
C(43)-H(43)	0.93(3)	C(51)-H(51)	0.93(3)
C(25)-H(25)	0.93(3)	C(25)-C(26)	1.38(4)
C(26)-H(26)	0.93(3)	C(32)-H(32)	0.93(3)
C(30)-H(30)	0.93(3)	P(1)-F(1)	1.547(19)
P(1)-F(4)	1.552(18)	P(1)-F(3)	1.54(3)
P(1)-F(2)	1.57(2)	P(1)-F(5)	1.59(3)

Table S6. Bond Angles (°) for ΛΔ/ΔΛ-[{Ru(bpy)$_2$}(HAT){Os(bpy)$_2$}](PF$_6$)$_3$Cl.

Bonds	Bond Angle (°)	Bonds	Bond Angle (°)
RU(2_)-OS(2_)-N(6)	142.7(29)	RU(2_)-OS(2_)-N(7)	113.5(31)
RU(2_)-OS(2_)-N(8)	111.4(30)	N(6)-OS(2_)-N(7)	89.2(7)
N(6)-OS(2_)-N(8)	100.9(7)	N(7)-OS(2_)-N(8)	80.6(8)
OS(1_)-RU(1_)-N(14)	89.5(520)	OS(1_)-RU(1_)-N(5)	157.5(533)
OS(1_)-RU(1_)-N(3)	77.5(525)	OS(1_)-RU(1_)-N(13)	105.9(526)
OS(1_)-RU(1_)-N(12)	18.7(531)	N(14)-RU(1_)-N(5)	90.0(9)
N(14)-RU(1_)-N(3)	97.7(10)	N(14)-RU(1_)-N(13)	79.8(9)
N(14)-RU(1_)-N(12)	94.2(11)	N(5)-RU(1_)-N(3)	80.3(9)
N(5)-RU(1_)-N(13)	96.1(10)	N(5)-RU(1_)-N(12)	174.0(12)
N(3)-RU(1_)-N(13)	175.6(11)	N(3)-RU(1_)-N(12)	94.8(11)
N(13)-RU(1_)-N(12)	88.9(11)	OS(2_)-RU(2_)-N(9)	145.7(31)
OS(2_)-RU(2_)-N(7)	60.4(29)	OS(2_)-RU(2_)-N(10)	114.5(32)
OS(2_)-RU(2_)-N(1)	105.2(30)	N(9)-RU(2_)-N(7)	100.4(8)
N(9)-RU(2_)-N(10)	80.3(8)	N(9)-RU(2_)-N(1)	104.2(8)
N(7)-RU(2_)-N(10)	171.4(9)	N(7)-RU(2_)-N(1)	94.2(9)
N(10)-RU(2_)-N(1)	93.9(9)	RU(1_)-OS(1_)-N(5)	22.3(528)
RU(1_)-OS(1_)-N(12)	161.1(535)	N(5)-OS(1_)-N(12)	174.2(10)
F(13)-P(3)-F(14)	95.3(16)	F(13)-P(3)-F(16)	171.1(17)
F(13)-P(3)-F(18)	88.8(18)	F(13)-P(3)-F(15)	89.3(17)
F(13)-P(3)-F(17)	88.9(16)	F(14)-P(3)-F(16)	83.0(18)
F(14)-P(3)-F(18)	103.5(20)	F(14)-P(3)-F(15)	169.3(20)
F(14)-P(3)-F(17)	73.2(19)	F(16)-P(3)-F(18)	83.1(18)
F(16)-P(3)-F(15)	93.8(19)	F(16)-P(3)-F(17)	98.9(17)
F(18)-P(3)-F(15)	86.1(20)	F(18)-P(3)-F(17)	175.8(22)
F(15)-P(3)-F(17)	97.4(19)	H(36)-C(36)-C(35)	116.9(34)
H(41)-C(41)-C(40)	117.5(41)	H(41)-C(41)-C(42)	117.5(35)
C(40)-C(41)-C(42)	125.0(40)	C(37)-C(38)-C(39)	123.6(31)
C(37)-C(38)-N(12)	112.1(26)	C(39)-C(38)-N(12)	124.3(32)
C(38)-C(37)-N(11)	121.4(26)	C(41)-C(40)-H(40)	125.4(50)
C(41)-C(40)-C(39)	109.2(40)	H(40)-C(40)-C(39)	125.4(45)
C(41)-C(42)-H(42)	117.4(31)	C(41)-C(42)-N(12)	125.1(30)
H(42)-C(42)-N(12)	117.4(29)	C(36)-C(35)-H(35)	120.7(38)
C(36)-C(35)-C(34)	118.7(33)	H(35)-C(35)-C(34)	120.7(40)
C(38)-C(39)-C(40)	126.0(36)	C(38)-C(39)-H(39)	117.0(39)
C(40)-C(39)-H(39)	117.0(36)	H(33)-C(33)-C(34)	117.8(29)
H(33)-C(33)-N(11)	117.9(26)	C(34)-C(33)-N(11)	124.3(27)
C(35)-C(34)-C(33)	117.4(30)	C(35)-C(34)-H(34)	121.3(33)
C(33)-C(34)-H(34)	121.3(32)	F(12)-P(2)-F(10)	176.6(11)
F(12)-P(2)-F(11)	89.9(10)	F(12)-P(2)-F(9)	90.0(10)
F(12)-P(2)-F(8)	93.8(11)	F(12)-P(2)-F(7)	88.3(11)
F(10)-P(2)-F(11)	88.1(9)	F(10)-P(2)-F(9)	91.9(9)
F(10)-P(2)-F(8)	88.9(11)	F(10)-P(2)-F(7)	89.0(10)
F(11)-P(2)-F(9)	179.8(10)	F(11)-P(2)-F(8)	87.2(10)
F(11)-P(2)-F(7)	92.0(10)	F(9)-P(2)-F(8)	93.0(11)
F(9)-P(2)-F(7)	87.9(11)	F(8)-P(2)-F(7)	177.7(11)
RU(1_)-N(14)-C(48)	115.7(17)	RU(1_)-N(14)-C(52)	124.3(18)
C(48)-N(14)-C(52)	119.6(23)	RU(2_)-N(9)-C(23)	124.2(14)
RU(2_)-N(9)-C(27)	116.3(16)	C(23)-N(9)-C(27)	118.4(19)
OS(2_)-N(6)-C(12)	130.4(13)	OS(2_)-N(6)-C(10)	114.6(13)
C(12)-N(6)-C(10)	114.9(17)	OS(2_)-N(7)-RU(2_)	6.1(3)
OS(2_)-N(7)-C(17)	117.5(14)	OS(2_)-N(7)-C(13)	127.4(16)
RU(2_)-N(7)-C(17)	119.8(14)	RU(2_)-N(7)-C(13)	125.0(16)
C(17)-N(7)-C(13)	115.1(19)	H(22)-C(22)-N(8)	118.2(22)
H(22)-C(22)-C(21)	118.3(22)	N(8)-C(22)-C(21)	123.5(21)
RU(2_)-N(10)-C(28)	115.5(15)	RU(2_)-N(10)-C(32)	127.0(16)

C(28)-N(10)-C(32)	117.5(19)	OS(2_)-N(8)-C(22)	128.1(15)
OS(2_)-N(8)-C(18)	116.0(14)	C(22)-N(8)-C(18)	115.7(18)
RU(1_)-N(5)-OS(1_)	0.2(6)	RU(1_)-N(5)-C(9)	115.1(14)
RU(1_)-N(5)-C(11)	135.1(16)	OS(1_)-N(5)-C(9)	114.9(14)
OS(1_)-N(5)-C(11)	135.3(15)	C(9)-N(5)-C(11)	109.7(18)
RU(2_)-N(1)-C(1)	124.0(15)	RU(2_)-N(1)-C(4)	117.8(14)
C(1)-N(1)-C(4)	118.0(19)	N(2)-C(3)-C(5)	117.1(20)
N(2)-C(3)-C(4)	127.6(24)	C(5)-C(3)-C(4)	115.3(23)
N(7)-C(17)-C(18)	110.7(18)	N(7)-C(17)-C(16)	123.2(21)
C(18)-C(17)-C(16)	126.0(21)	C(5)-N(4)-C(8)	117.3(23)
C(37)-N(11)-C(33)	126.1(23)	RU(1_)-N(3)-C(6)	114.7(15)
RU(1_)-N(3)-C(7)	134.0(19)	C(6)-N(3)-C(7)	110.5(22)
N(6)-C(12)-H(12)	120.0(18)	N(6)-C(12)-C(11)	120.1(19)
H(12)-C(12)-C(11)	120.0(19)	RU(1_)-N(13)-C(47)	114.2(15)
RU(1_)-N(13)-C(43)	126.7(18)	C(47)-N(13)-C(43)	119.0(21)
C(3)-N(2)-C(2)	112.0(21)	C(3)-C(5)-N(4)	120.4(22)
C(3)-C(5)-C(6)	118.7(21)	N(4)-C(5)-C(6)	120.8(23)
N(13)-C(47)-C(48)	113.9(20)	N(13)-C(47)-C(46)	122.5(22)
C(48)-C(47)-C(46)	123.6(22)	H(31)-C(31)-C(32)	120.9(28)
H(31)-C(31)-C(30)	120.9(29)	C(32)-C(31)-C(30)	118.2(27)
C(22)-C(21)-H(21)	121.5(24)	C(22)-C(21)-C(20)	117.0(22)
H(21)-C(21)-C(20)	121.5(25)	N(9)-C(23)-H(23)	120.2(22)
N(9)-C(23)-C(24)	119.5(21)	H(23)-C(23)-C(24)	120.2(23)
N(8)-C(18)-C(17)	115.0(19)	N(8)-C(18)-C(19)	122.2(20)
C(17)-C(18)-C(19)	122.8(20)	H(29)-C(29)-C(28)	120.1(29)
H(29)-C(29)-C(30)	120.1(29)	C(28)-C(29)-C(30)	119.8(27)
N(10)-C(28)-C(29)	121.3(23)	N(10)-C(28)-C(27)	110.8(19)
C(29)-C(28)-C(27)	127.8(22)	H(14)-C(14)-C(15)	118.6(27)
H(14)-C(14)-C(13)	118.6(24)	C(15)-C(14)-C(13)	122.9(24)
C(14)-C(15)-H(15)	121.6(30)	C(14)-C(15)-C(16)	116.8(27)
H(15)-C(15)-C(16)	121.6(29)	N(3)-C(6)-C(5)	125.0(20)
N(3)-C(6)-C(9)	113.5(22)	C(5)-C(6)-C(9)	121.3(22)
N(4)-C(8)-H(8)	120.4(29)	N(4)-C(8)-C(7)	119.2(23)
H(8)-C(8)-C(7)	120.4(30)	C(23)-C(24)-H(24)	118.6(24)
C(23)-C(24)-C(25)	122.7(24)	H(24)-C(24)-C(25)	118.6(25)
N(9)-C(27)-C(28)	116.0(21)	N(9)-C(27)-C(26)	120.9(23)
C(28)-C(27)-C(26)	123.0(21)	N(5)-C(9)-C(6)	115.5(21)
N(5)-C(9)-C(10)	121.8(20)	C(6)-C(9)-C(10)	122.1(22)
N(5)-C(11)-C(12)	127.9(21)	N(5)-C(11)-H(11)	116.1(21)
C(12)-C(11)-H(11)	116.1(21)	N(6)-C(10)-C(9)	125.2(20)
N(6)-C(10)-C(4)	118.3(19)	C(9)-C(10)-C(4)	116.2(21)
C(18)-C(19)-H(19)	120.4(24)	C(18)-C(19)-C(20)	119.1(23)
H(19)-C(19)-C(20)	120.4(25)	N(14)-C(48)-C(47)	116.0(22)
N(14)-C(48)-C(49)	124.4(25)	C(47)-C(48)-C(49)	118.9(23)
H(50)-C(50)-C(49)	119.9(30)	H(50)-C(50)-C(51)	119.9(29)
C(49)-C(50)-C(51)	120.2(28)	N(7)-C(13)-C(14)	120.1(21)
N(7)-C(13)-H(13)	119.9(23)	C(14)-C(13)-H(13)	119.9(23)
C(48)-C(49)-C(50)	116.2(26)	C(48)-C(49)-H(49)	121.9(28)
C(50)-C(49)-H(49)	121.9(28)	RU(1_)-N(12)-OS(1_)	0.2
RU(1_)-N(12)-C(38)	118.3(21)	RU(1_)-N(12)-C(42)	131.4(21)
OS(1_)-N(12)-C(38)	118.3(21)	OS(1_)-N(12)-C(42)	131.3(21)
C(38)-N(12)-C(42)	110.4(26)	C(47)-C(46)-H(46)	123.2(28)
C(47)-C(46)-C(45)	113.7(26)	H(46)-C(46)-C(45)	123.2(30)
N(1)-C(1)-H(1)	122.4(23)	N(1)-C(1)-C(2)	115.1(20)
H(1)-C(1)-C(2)	122.5(21)	N(3)-C(7)-C(8)	126.4(26)
N(3)-C(7)-H(7)	116.8(27)	C(8)-C(7)-H(7)	116.8(27)
H(44)-C(44)-C(45)	120.7(29)	H(44)-C(44)-C(43)	120.7(28)
C(45)-C(44)-C(43)	118.6(25)	C(46)-C(45)-C(44)	124.6(27)
C(46)-C(45)-H(45)	117.7(28)	C(44)-C(45)-H(45)	117.7(28)
C(21)-C(20)-C(19)	121.7(24)	C(21)-C(20)-H(20)	119.2(27)

C(19)-C(20)-H(20)	119.2(26)	N(14)-C(52)-H(52)	119.2(26)
N(14)-C(52)-C(51)	121.6(25)	H(52)-C(52)-C(51)	119.2(27)
C(17)-C(16)-C(15)	121.8(24)	C(17)-C(16)-H(16)	119.1(26)
C(15)-C(16)-H(16)	119.1(26)	N(2)-C(2)-C(1)	126.9(23)
N(2)-C(2)-H(2)	116.6(27)	C(1)-C(2)-H(2)	116.5(26)
N(13)-C(43)-C(44)	121.1(24)	N(13)-C(43)-H(43)	119.4(26)
C(44)-C(43)-H(43)	119.5(25)	N(1)-C(4)-C(3)	119.8(22)
N(1)-C(4)-C(10)	114.1(19)	C(3)-C(4)-C(10)	126.0(22)
C(50)-C(51)-C(52)	117.3(26)	C(50)-C(51)-H(51)	121.3(29)
C(52)-C(51)-H(51)	121.4(29)	C(24)-C(25)-H(25)	122.2(29)
C(24)-C(25)-C(26)	115.7(26)	H(25)-C(25)-C(26)	122.2(29)
C(27)-C(26)-C(25)	122.4(24)	C(27)-C(26)-H(26)	118.8(26)
C(25)-C(26)-H(26)	118.8(27)	N(10)-C(32)-C(31)	120.6(23)
N(10)-C(32)-H(32)	119.7(24)	C(31)-C(32)-H(32)	119.7(26)
C(31)-C(30)-C(29)	122.1(28)	C(31)-C(30)-H(30)	118.9(33)
C(29)-C(30)-H(30)	118.9(33)	F(6)-P(1)-F(1)	90.0(13)
F(6)-P(1)-F(4)	91.8(11)	F(6)-P(1)-F(3)	178.3(13)
F(6)-P(1)-F(2)	91.7(12)	F(6)-P(1)-F(5)	85.6(12)
F(1)-P(1)-F(4)	89.2(10)	F(1)-P(1)-F(3)	90.2(12)
F(1)-P(1)-F(2)	178.3(12)	F(1)-P(1)-F(5)	90.1(12)
F(4)-P(1)-F(3)	89.9(11)	F(4)-P(1)-F(2)	91.2(10)
F(4)-P(1)-F(5)	177.3(12)	F(3)-P(1)-F(2)	88.1(11)
F(3)-P(1)-F(5)	92.7(12)	F(2)-P(1)-F(5)	89.6(11)

Table S7. Redox potentials for the reductions based on the HAT bridging ligand for the di- and trinuclear complexes in 0.1 M $[(n\text{-}C_4H_9)_4N]PF_6/CH_3CN$ at +25°C.

Complex	E_{red1}	E_{red2}	E_{red3}
$[Os(bpy)_2(HAT)]^{2+}$	-1101	-1276	
meso-$[\{Os(bpy)_2\}_2(\mu\text{-HAT})]^{4+}$	-844	-1320	
rac-$[\{Os(bpy)_2\}_2(\mu\text{-HAT})]^{4+}$	-840	-1325	
ΔΛ/ΛΔ-$[\{Ru(bpy)_2\}(\mu\text{-HAT})\{Os(bpy)_2\}]^{n+}$	-804	-1316	
ΔΔ/ΛΛ-$[\{Ru(bpy)_2\}(\mu\text{-HAT})\{Os(bpy)_2\}]^{n+}$	-805	-1320	
$\Delta_2\Lambda'/\Lambda_2\Delta'$-$[\{Ru(bpy)_2\}_2\{Os(bpy)_2\}(\mu\text{-HAT})]^{n+}$	-624	-956	-1384

[a] All potentials are quoted ±3 mV *vs.* Fc^+/Fc^0.

Table S8. Deconvoluted NIR spectral data of the reduced absorption spectra (ε/ν *vs.* ν) for the di- and trinuclear complexes at -35 and -15°C, respectively.[a]

Complex	ν_{max} ± 10 /cm^{-1}	$(\varepsilon/\nu)_{max}$ ± 0.0001 /M^{-1}	$\Delta\nu_{1/2}$ ± 10 /cm^{-1}
meso-[{Os(bpy)$_2$}$_2$(μ-HAT)]$^{5+}$	4980	0.06612	444
	5420	0.02008	422
	5770	0.02298	1150
	8200	0.2782	663
	8780	0.07748	540
	9325	0.04413	695
	11110	0.3878	1445
	12470	0.1234	1482
	14285	0.1241	1398
rac-[{Os(bpy)$_2$}$_2$(μ-HAT)]$^{5+}$	5090	0.05752	932
	5935	0.02305	974
	8260	0.2726	920
	9130	0.06784	848
	11130	0.4123	1654
	12715	0.1266	2030
ΔΛ/ΛΔ-[{Ru(bpy)$_2$}(μ-HAT){Os(bpy)$_2$}]$^{5+}$	4080	0.4747	578
	4880	0.1107	596
	8610	0.1735	2055
	10405	0.02198	2160
	13950	0.1145	1970
ΔΔ/ΛΛ-[{Ru(bpy)$_2$}(μ-HAT){Os(bpy)$_2$}]$^{5+}$	4060	0.5990	577
	4880	0.1388	591
	8695	0.2125	2060
	14060	0.1906	2857
Δ$_2$Λ'/Λ$_2$Δ'-[{Ru(bpy)$_2$}$_2$}{Os(bpy)$_2$}(μ-HAT)]$^{7+}$	3975	0.5008	844
	4620	0.1754	632.8
	7670	0.2193	2597
	9480	0.0595	1695
	13080	0.07075	1345
	14650	0.2518	2197
Δ$_2$Λ'/Λ$_2$Δ'-[{Ru(bpy)$_2$}$_2$}{Os(bpy)$_2$}(μ-HAT)]$^{8+}$	3530	1.01798	414
	4040	0.20802	412
	4470	0.3064	881
	5530	0.1096	1088
	7765	0.1750	2854
	10550	0.4488	2235
	13110	0.5473	2562
	14890	0.2410	1854

[a] Due to the convoluted nature of the NIR spectra, unambiguous determination of the band characteristics for the IC transitions in the +9 species was not possible.

Table S9. Deconvoluted NIR spectral data (ε/ν *vs.* ν) of the fully-oxidized forms of the mono- and dinuclear complexes at -35°C. The parameters for the IC bands are indicated in bold type.[a]

Complex	ν_{max} ± 10 /cm^{-1}	$(\varepsilon/\nu)_{max}$ ± 0.0001 /M^{-1}	$\Delta\nu_{1/2}$ ± 10 /cm^{-1}
$[Os(bpy)_2(HAT)]^{3+}$	**4435**	0.06315	485
	5090	0.05405	645
	5735	0.004250	330
	6060	0.003798	1280
	10460	0.02746	1820
	12120	0.004165	908
meso-$[\{Os(bpy)_2\}_2(\mu\text{-HAT})]^{6+}$	**4320**	0.2144	514
	5060	0.1500	746
	5790	0.02133	560
	6645	0.03988	1210
rac-$[\{Os(bpy)_2\}_2(\mu\text{-HAT})]^{6+}$	**4280**	0.2788	396
	4600	0.06351	302
	5030	0.1457	600
	5607	0.01473	503
	6695	0.03058	990
$\Delta\Lambda/\Lambda\Delta$-$[\{Ru(bpy)_2\}(\mu\text{-HAT})\{Os(bpy)_2\}]^{6+}$	**4430**	0.2642	697
	5035	0.04626	405
	5335	0.06867	600
	6075	0.01228	1117
	9090	0.04851	1736
$\Delta\Delta/\Lambda\Lambda$-$[\{Ru(bpy)_2\}(\mu\text{-HAT})\{Os(bpy)_2\}]^{6+}$	**3920**	0.3529	578
	4720	0.1477	942
	8300	0.1677	2100
	10778	0.2550	2226

[a] Due to the convoluted nature of the NIR spectra, unambiguous determination of the band characteristics for the IC transitions in the +9 species was not possible.

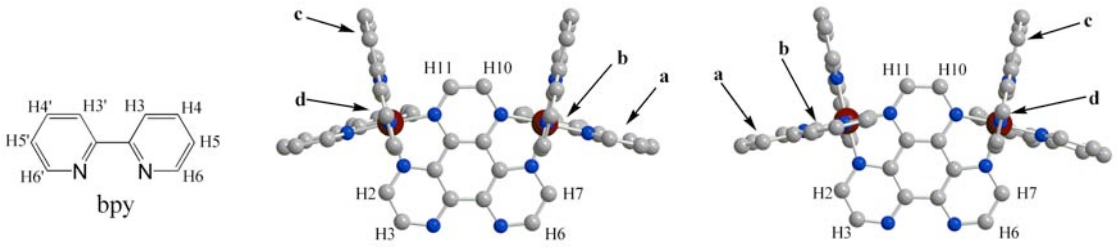

Figure S1. Proton numbering schemes for **(a)** ΛΔ- and **(b)** ΔΔ-[{Ru(bpy)$_2$}(μ-HAT){Os(bpy)$_2$}]$^{4+}$ {M,M' = Os,Os or Ru,Os} (Hydrogen atoms are omitted for clarity). *Left*: proton numbering scheme for bpy.

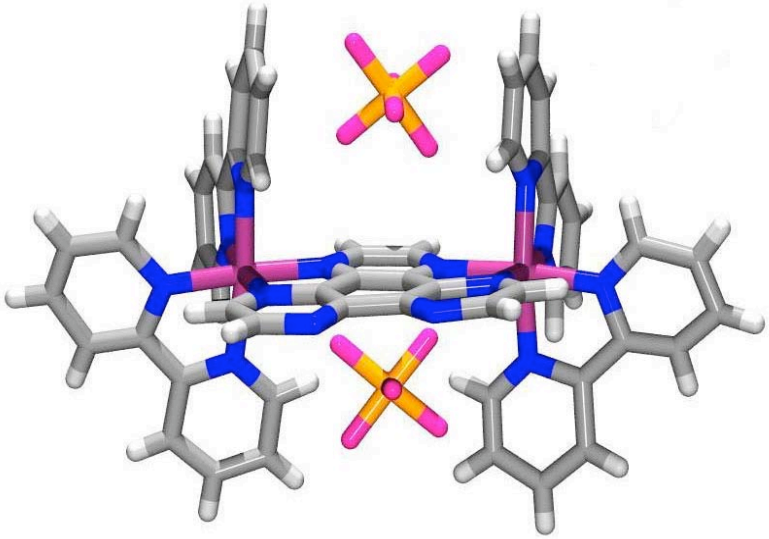

Figure S2. The ΛΔ-[{Ru(bpy)$_2$}(μ-HAT){Os(bpy)$_2$}]$^{4+}$ cation showing the association of two PF_6^- anions within the clefts between the bpy ligands.

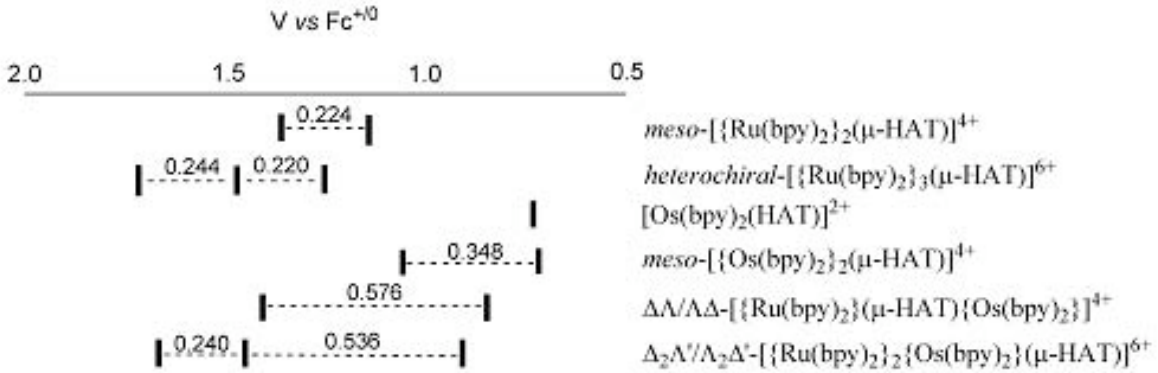

Figure S3. Schematic illustration of the relative potentials of the metal-based oxidation processes in selected mono-, di- and trinuclear ruthenium and osmium complexes in this study.

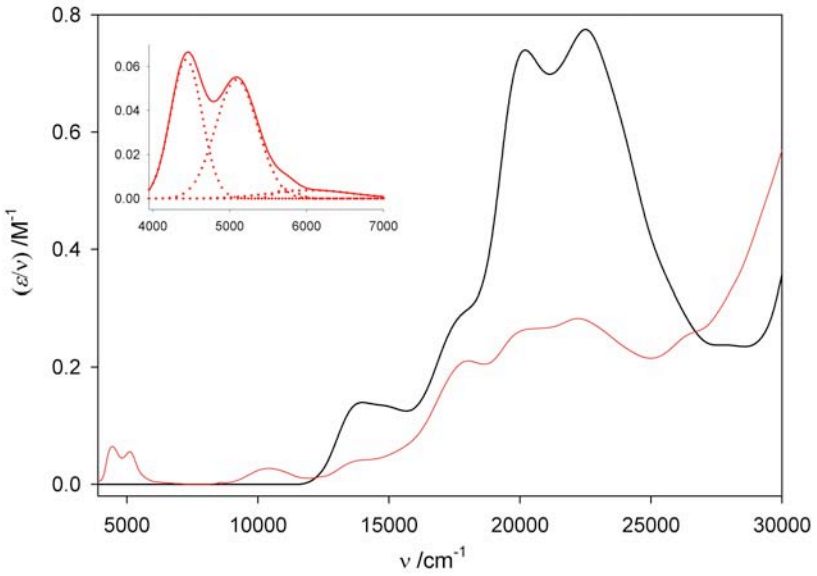

Figure S4. UV/Vis/NIR spectra of $[Os(bpy)_2(HAT)]^{n+}$ {n = 2 (──), 3 (──)} at -35°C. The inset shows the interconfigurational (IC) bands for the n = 3 species and the components of the Gaussian deconvolution of the bands (· · · · · · · · ·).

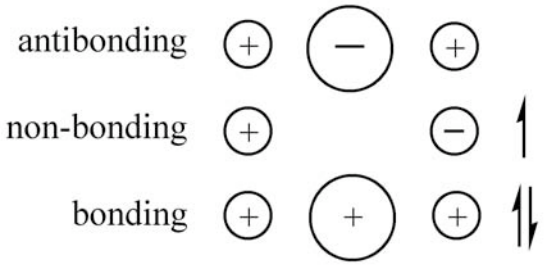

Figure S5. Qualitative molecular orbital diagram for the dinuclear $[\{Ru(bpy)_2\}_2(\mu\text{-BL})]^{5+}$ systems showing the bonding, non-bonding and antibonding molecular orbitals. The IVCT corresponds to a bonding → non-bonding transition.