Dalton Transactions

Supplementary Information for

$[Ru(tmphen)_3]_2[Fe(CN)_6]$ and $[Ru(phen)_3][Fe(CN)_5(NO)]$ complexes; Heterostructured RuO_2–Fe_2O_3 nanocomposite: an efficient alkaline HER and OER electrocatalyst

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Table S4. The angles of selected bonds in complex (**2**). **6**

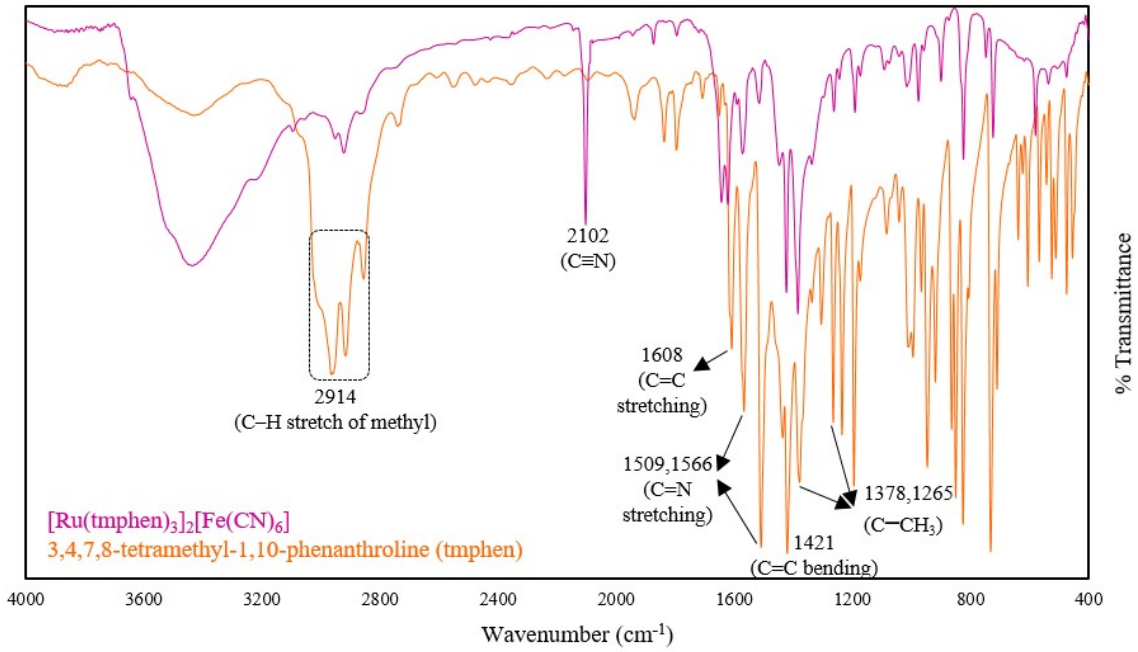

Figure S1. FT–IR spectra of 3,4,7,8-tetramethyl-1,10-phenanthroline (tmphen) and $[Ru(tmphen)_3]_2[Fe(CN)_6]$ (KBr pellet).

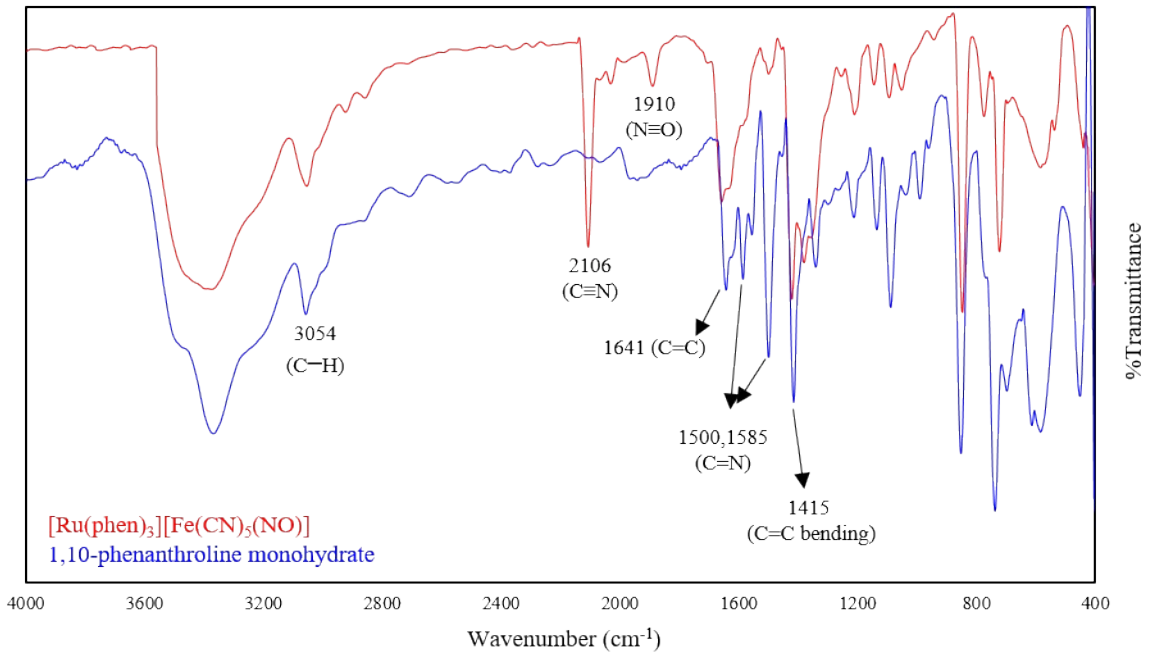

Figure S2. FT–IR spectra of 1,10-phenanthroline monohydrate (phen) and $[Ru(phen)_3][Fe(CN)_5(NO)]$ (KBr pellet).

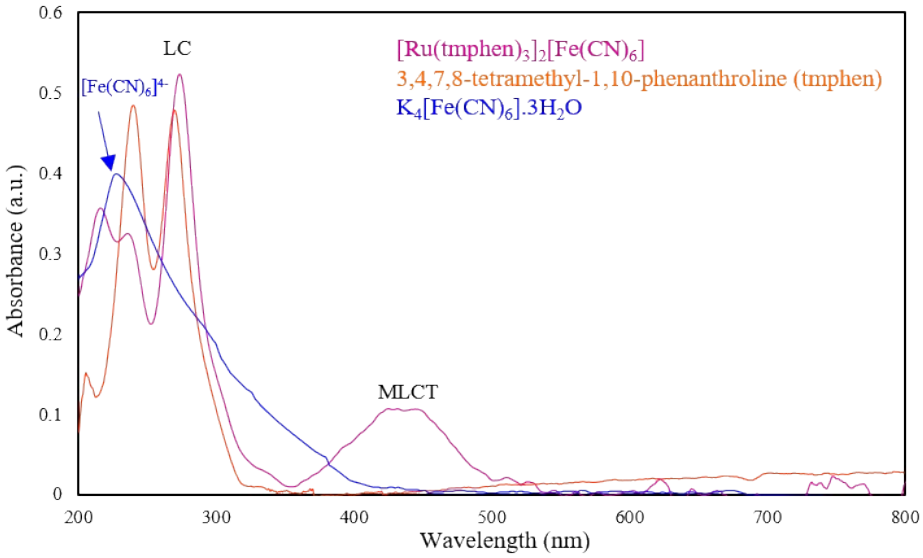

Figure S3. UV–Vis absorption spectra of 3,4,7,8-tetramethyl-1,10-phenanthroline (tmphen), $K_4[Fe(CN)_6].3H_2O$, and $[Ru(tmphen)_3]_2[Fe(CN)_6]$ (10^{-5} M) in acetonitrile.

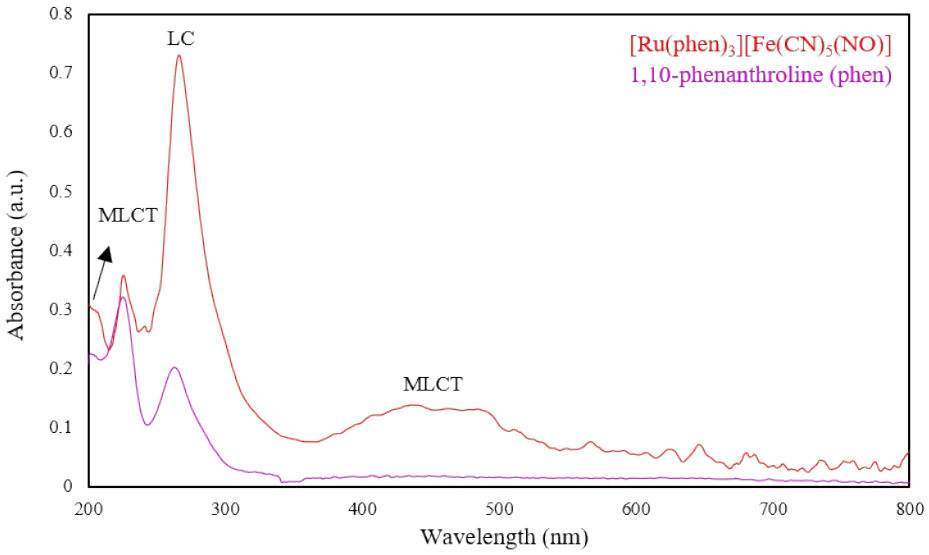

Figure S4. UV–Vis absorption spectra of 1,10-phenanthroline (phen) and $[Ru(phen)_3][Fe(CN)_5(NO)]$ (10^{-5} M) in acetonitrile.

Table S1. The lengths of selected bonds in complex (**1**).

Atom	Atom	Length (Å)
C1	N1	1.325(4)
C2	C3	1.393(5)
C5	C6	1.425(5)
C5	N1	1.380(4)
C6	N2	1.360(4)
C10	N2	1.329(4)
C17	Fe1	1.948(4)
C17	N3	1.152(5)
N1	Ru1	2.065(3)
N2	Ru1	2.063(3)

Table S2. The angles of selected bonds in complex (**1**).

Atom	Atom	Atom	Angle (°)	Atom	Atom	Atom	Angle (°)
N1	C1	C2	124.3(3)	$C17^{3}$	Fe1	C17	89.97(16)
N1	C5	C4	122.1(3)	$C17^{1}$	Fe1	C17	180.0
N1	C5	C6	116.2(3)	C17	Fe1	$C17^{2}$	90.03(16)
N3	C17	Fe1	179.8(4)	C10	N2	Ru1	128.3(2)
C1	N1	C5	117.6(3)	$N2^{7}$	Ru1	N1	174.08(9)
C1	N1	Ru1	128.8(2)	N2	Ru1	N1	79.74(11)
C5	N1	Ru1	113.4(2)	N2	Ru1	$N1^{7}$	88.26(10)
$N1^{6}$	Ru1	N1	97.18(10)				

Table S3. The lengths of selected bonds in complex (**2**).

Atom	Atom	Length (Å)	Atom	Atom	Length (Å)
C1	C2	1.396(3)	C37	Fe1	1.943(2)
C1	N1	1.337(2)	C37	N7	1.141(3)
C5	N1	1.369(2)	C38	Fe1	1.9500(19)
C6	N2	1.366(2)	C38	N8	1.146(3)
C10	N2	1.337(2)	C39	Fe1	1.9432(18)
C13	N3	1.332(2)	C39	N9	1.150(2)
C17	C18	1.424(2)	C40	Fe1	1.932(2)
C17	N3	1.371(2)	C40	N10	1.145(3)
C18	C19	1.405(2)	C41	Fe1	1.942(2)
C18	N4	1.370(2)	C41	N11	1.148(3)
C21	C22	1.404(2)	Fe1	N12A	1.66(3)
C22	N4	1.334(2)	N1	Ru1	2.0638(14)
C25	C26	1.406(3)	N2	Ru1	2.0625(14)
C25	N5	1.334(2)	N3	Ru1	2.0802(14)
C29	N5	1.370(2)	N4	Ru1	2.0672(14)
C30	C31	1.403(3)	N5	Ru1	2.0666(15)
C30	N6	1.368(2)	N6	Ru1	2.0697(14)
C34	N6	1.336(2)	N12A	O1A	1.13(3)

Table S4. The angles of selected bonds in complex (**2**).

Atom	Atom	Atom	Angle (°)	Atom	Atom	Atom	Angle (°)
N1	C1	C2	122.29(17)	C40	Fe1	C38	88.69(8)
N1	C5	C4	123.42(15)	C40	Fe1	C39	84.73(8)
N1	C5	C6	116.40(15)	C40	Fe1	C41	89.18(9)
C7	C6	C5	120.27(16)	C41	Fe1	C37	92.57(9)
N2	C6	C5	116.47(15)	C41	Fe1	C38	171.27(8)
N2	C6	C7	123.22(15)	C41	Fe1	C39	82.01(8)
N2	C10	C9	122.51(17)	N12A	Fe1	C37	101.5(10)
N3	C13	C14	122.86(17)	N12A	Fe1	C38	89.5(10)
N3	C17	C16	123.13(16)	N12A	Fe1	C39	174.2(9)
N3	C17	C18	116.43(15)	N12A	Fe1	C40	89.5(9)
C19	C18	C17	120.22(16)	N12A	Fe1	C41	98.9(10)
N4	C18	C17	116.73(15)	C1	N1	C5	117.60(15)
N4	C18	C19	123.05(16)	C1	N1	Ru1	128.92(12)
N4	C22	C21	122.53(16)	C5	N1	Ru1	113.38(11)
C24	C23	C16	121.44(17)	C6	N2	Ru1	113.41(11)
N5	C25	C26	122.0(2)	C10	N2	C6	117.89(14)
C27	C26	C25	120.3(2)	C10	N2	Ru1	128.58(12)
N7	C37	Fe1	177.73(19)	C13	N3	C17	117.34(15)
N8	C38	Fe1	177.29(18)	C13	N3	Ru1	128.97(12)
N9	C39	Fe1	175.07(16)	C17	N3	Ru1	113.48(11)
N10	C40	Fe1	178.32(18)	C18	N4	Ru1	113.81(11)
N11	C41	Fe1	177.0(2)	C22	N4	C18	117.56(14)
N37	Fe1	C38	87.87(8)	C22	N4	Ru1	128.61(12)
C37	Fe1	C39	84.22(8)	C25	N5	C29	117.70(16)
C39	Fe1	C38	89.36(8)	C25	N5	Ru1	128.75(14)
C40	Fe1	C37	168.46(8)	C29	N5	Ru1	113.24(12)
O1A	N12A	Fe1	178.8(16)	O1B	N12B	Fe1	176(2)