

**UV-vis-NIR and EPR characterisation of the redox series  $[\text{MQ}_3]^{2+,+,0,-,2-}$ , M  
= Ru or Os, and Q = *o*-quinone derivative**

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**Supporting Information**

**Table S1** Comparison of selected symmetry-averaged<sup>a</sup> bond lengths (Å) and angles (deg) of *cis-1*, *trans-1*, and *trans-2* with G03/PBEO calculation results.

	<i>cis-1</i>		<i>trans-1</i>		<i>trans-2</i>	
	exp.	calc.	exp.	calc.	exp.	calc.
M-O1	1.973	1.983	1.978	1.983	1.966	1.974
M-O2	1.972	1.981	1.959	1.981	1.950	1.971
O1-C1	1.326	1.300	1.290	1.300	1.323	1.319
O2-C2	1.313	1.300	1.316	1.300	1.336	1.320
C1-C2	1.417	1.433	1.453	1.433	1.406	1.416
C2-C3	1.426	1.418	1.410	1.418	1.413	1.409
C3-C4	1.382	1.379	1.360	1.379	1.373	1.385
C4-C5	1.426	1.425	1.456	1.425	1.423	1.417
C5-C6	1.382	1.380	1.373	1.380	1.370	1.386
C1-C6	1.405	1.408	1.393	1.408	1.396	1.400
O1-M-O2	80.9	80.1	81.3	80.0	80.2	79.3
O1-M-O3	89.0	92.4	98.9	96.2	98.7	100.9
O1-M-O4	170.0	168.9	99.3	92.4	99.2	91.2
O1-M-O5	96.2	92.3	92.5	92.4	92.9	90.7
O1-M-O6	105.4	96.2	172.5	168.9	171.9	164.0
O2-M-O4	99.6	92.3	176.5	168.8	174.6	164.9
O2-M-O5	170.5	168.8	96.2	96.3	96.8	91.3
O3-M-O5	91.9	92.4	164.9	168.8	165.1	164.4

<sup>a</sup> Experimental data from ref. 5.

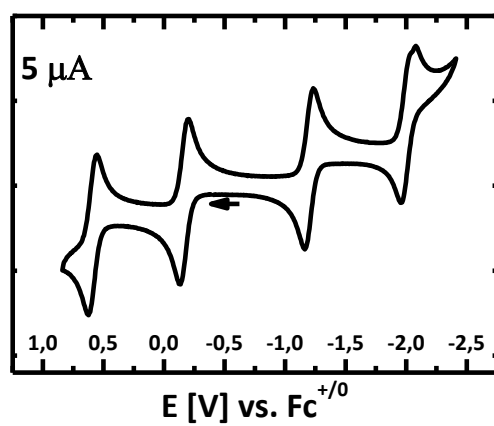
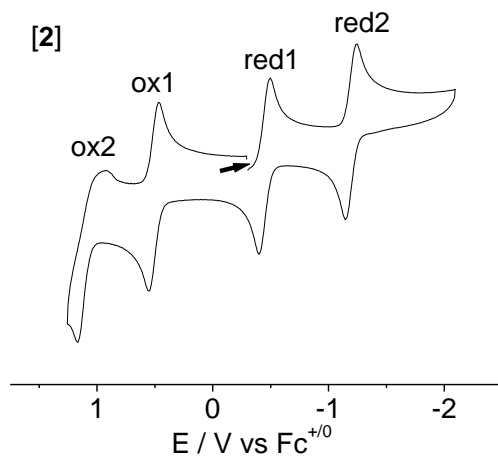
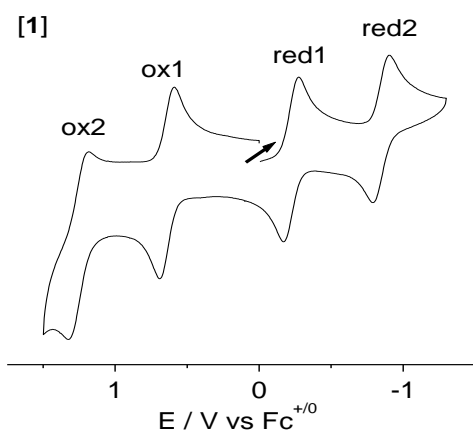
**Table S2** Bond angles (in deg) in compound **4** (see Figure 1)

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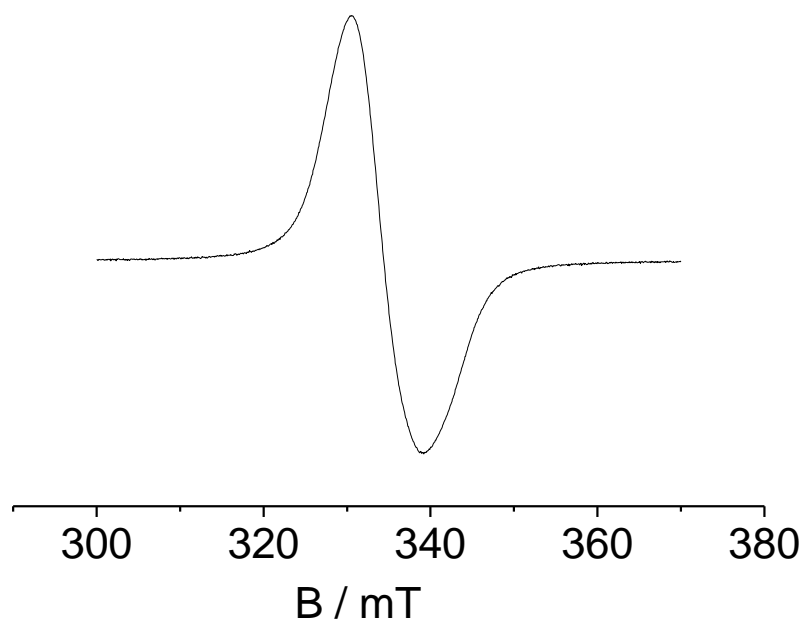
N1 – Os – N2	156.45(10)
O1 – Os – O3	174.11(8)
O2 – Os – N3	175.27(10)
N1 – Os – O1	79.75(10)
N2 – Os – O2	76.89(10)
N3 – Os – O3	78.75(9)
O3 – Os – N2	93.19(9)
O2 – Os – N1	81.64(10)
N1 – Os – N3	102.90(11)
O1 – Os – N3	95.59(9)
O1 – Os – N2	79.75(10)
O1 – Os – O2	86.44(9)
O2 – Os – N1	81.63(10)
O3 – Os – N1	95.53(8)
N2 – Os – N3	98.83(11)

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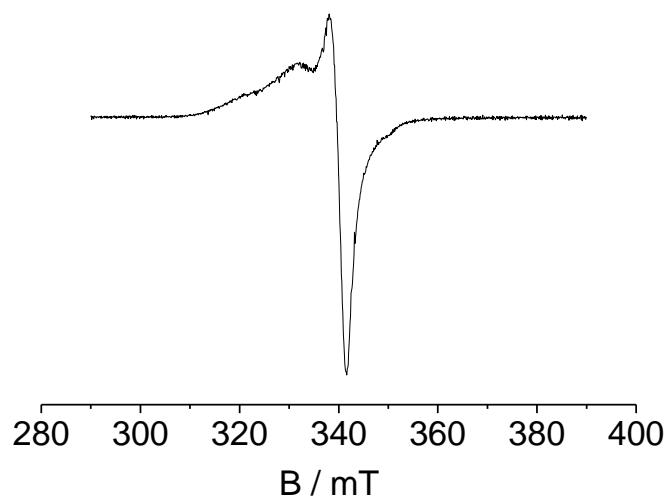
**Figure S1.** Cyclic voltammograms of **1**, **2** and **4** in CH<sub>2</sub>Cl<sub>2</sub>/0.1 M Bu<sub>4</sub>NPF<sub>6</sub>.



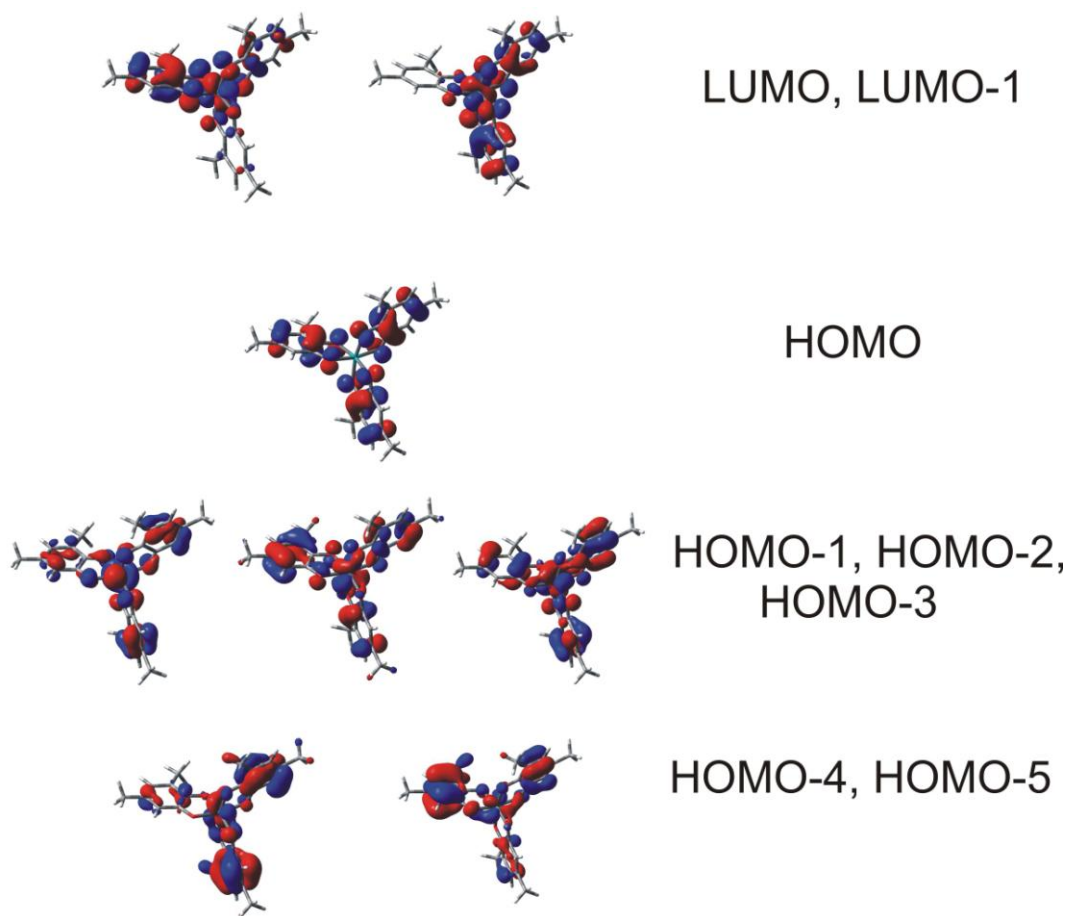
**Figure S2.** X band EPR spectrum of electrochemically generated  $2^+$  at 110 K in  $\text{CH}_2\text{Cl}_2/0.1$   
M  $\text{Bu}_4\text{NPF}_6$ .



**Figure S3.** X-band EPR spectrum of electrochemically generated  $\mathbf{1}^-$  at 110 K in  $\text{CH}_2\text{Cl}_2/0.1$   
M  $\text{Bu}_4\text{NPF}_6$ .



**Figure S4.** Representations of the frontier orbitals of complex **1**.



**Figure S5.** UV-vis-NIR spectroelectrochemical response of **4** in  $\text{CH}_2\text{Cl}_2/0.1 \text{ M Bu}_4\text{NPF}_6$ .

