

Two tetra-nuclear Mn-complexes as biomimetic models of the oxygen evolving complex in Photosystem II – A synthesis, characterisation and reactivity study

Gustav Berggren,^a Anders Thapper,^a Ping Huang,^a Philipp Kurz,^b Lars Eriksson,^c

Stenbjörn Styring,^a Magnus F. Anderlund^{*a}

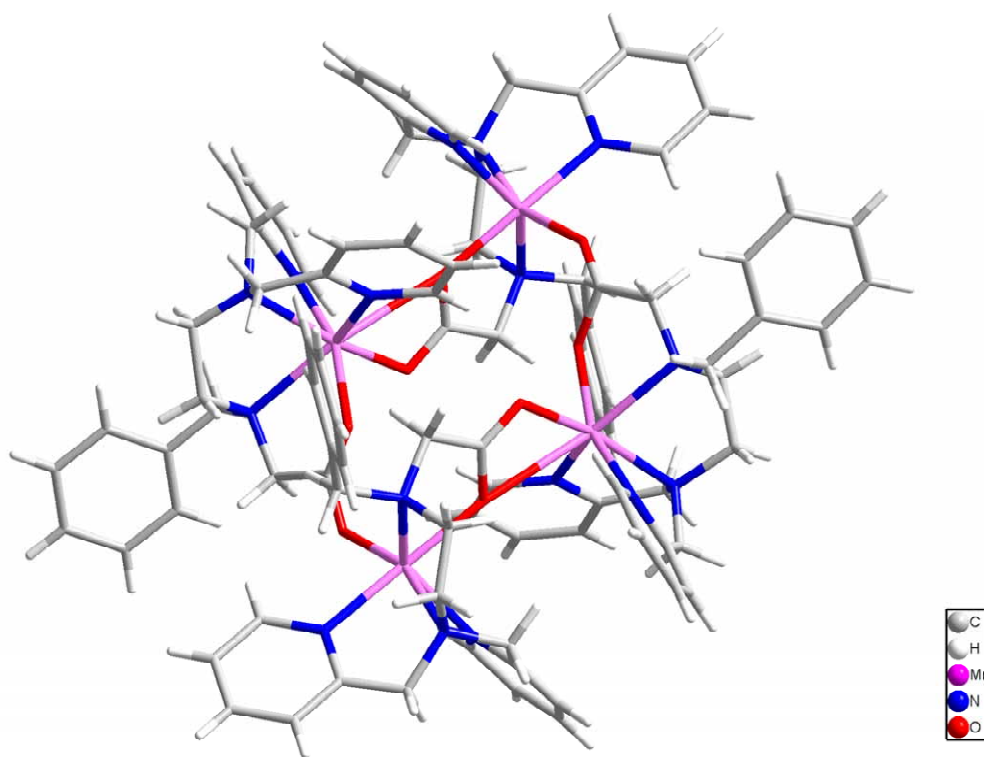


Fig. S1 Crystal structure of $2(\text{ClO}_4)_4$

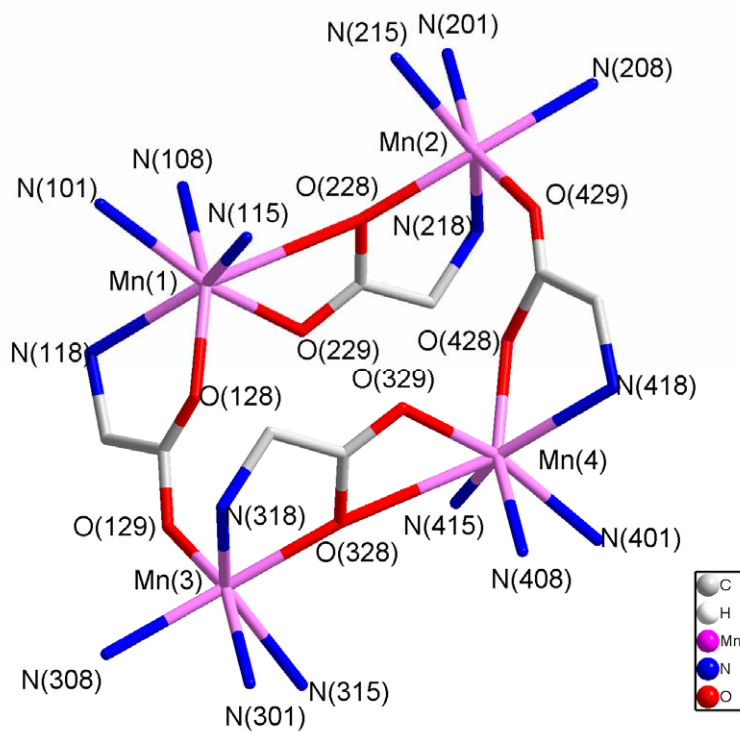


Fig. S2 Crystal structure of $2(\text{ClO}_4)_4$

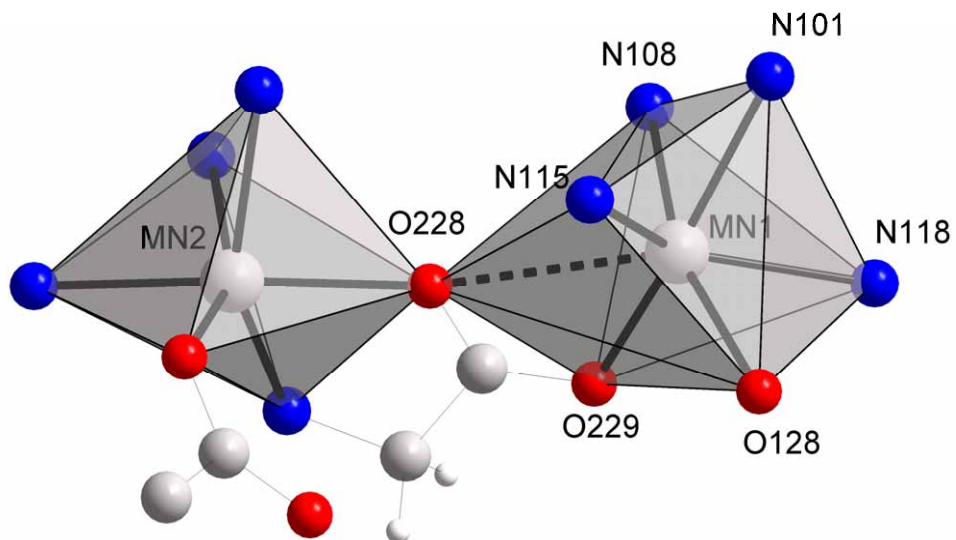


Fig. S3 Geometry of first coordination sphere around Mn atoms in $1(\text{ClO}_4)_4$

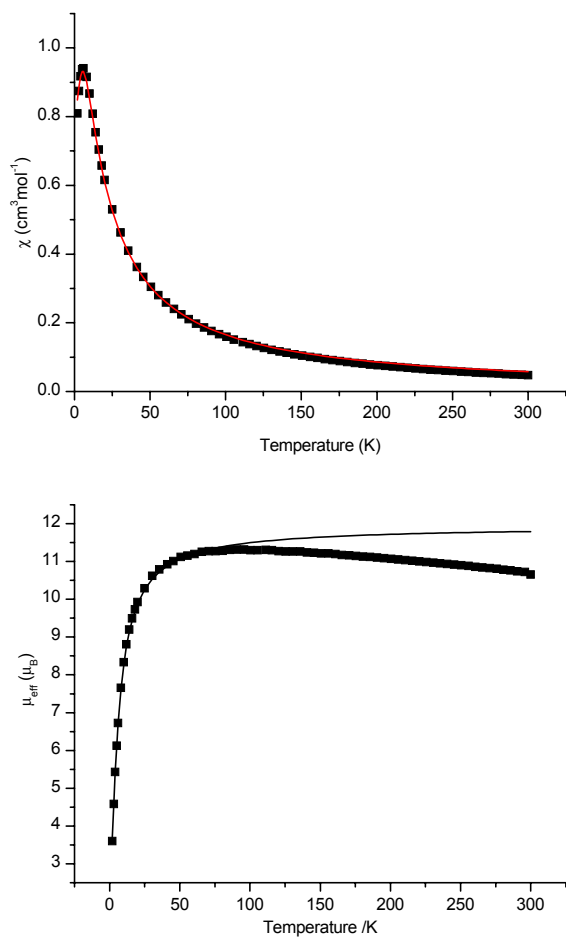


Fig. S4 (top) Temperature dependence of the molar susceptibility of $2(\text{ClO}_4)_4$ in the solid state. The red line represents fitted curve using eq. 1 (see text). **(bottom)** The effective magnetic moment (μ_{eff}) of $2(\text{ClO}_4)_4$ in solid state. The black line represents fitted curve using eq. 1 (see text).

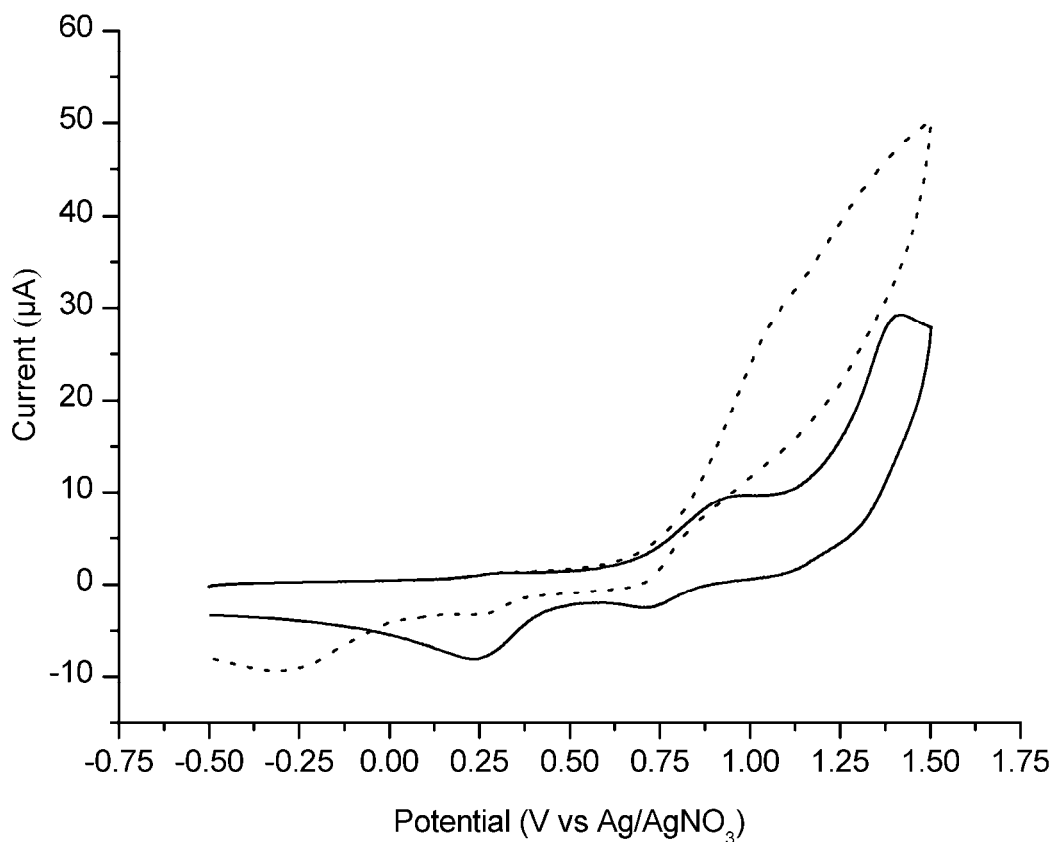


Fig. S5 Cyclic voltammograms of 2^{4+} [0.5 mM] in MeCN (solid line), in the presence of 6 mM lutidine (dotted line). Electrolyte 0.1 M TBAPF₆, scan rate 0.1 V s⁻¹ at 20 °C.

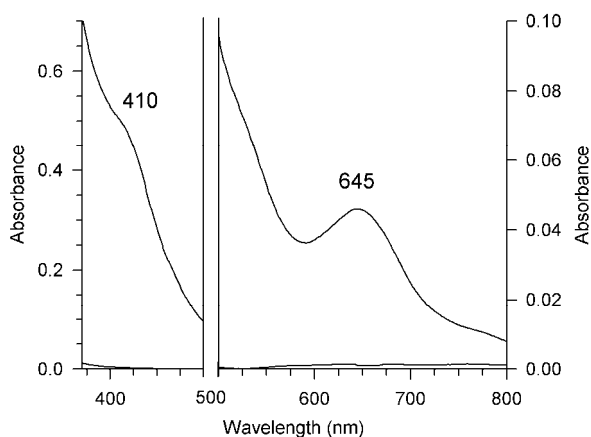


Fig. S6 Absorption spectra of 1^{4+} in MeCN + 2% H₂O in a spectroelectrochemical cell (0.1 M TBAPF₆). Spectra are collected at 0 V (bottom trace), and after exhaustive bulk electrolysis at 0.8 V (top trace).