

Supplementary Information

Two-Dimensional ^{14}N HYSCORE Spectroscopy of the Coordination Geometry of Ligands in Dimanganese Di- μ -oxo Mimics of the Oxygen Evolving Complex of Photosystem II[†]

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One-sentence summary: A Two-Dimensional ^{14}N HYSCORE Study of Dimanganese Di- μ -oxo Mimics of the Oxygen-Evolving Complex of Photosystem II.

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Key Words: Photosystem II, biomimetic models, mixed-valence coordination complexes, EPR spectroscopy, HYSCORE spectroscopy, $[(\text{bpy})_2\text{Mn}^{\text{III}}(\mu\text{-O})_2\text{Mn}^{\text{IV}}(\text{bpy})_2](\text{ClO}_4)_3$ (bpy, 2,2'-bipyridine) and $[\text{H}_2\text{O}(\text{terpy})\text{Mn}^{\text{III}}(\mu\text{-O})_2\text{Mn}^{\text{IV}}(\text{terpy})\text{OH}_2](\text{NO}_3)_3$ (terpy = 2,2':6',2''-terpyridine).

Tables

Table S1. The experimentally determined ^{14}N isotropic and anisotropic hyperfine interaction parameters of 2 in aqueous buffer.

Table S1.

Complex	Nitrogen	Assignment	A_{iso} (MHz)	T (MHz)	$K^2(3 + \eta^2)$ (MHz ²)
2 (Aqueous buffer)	N _I	Mn(III), axial	13.1 ± 1.0	~ 0.9	1.8 ± 0.5
	N _{II}	Mn(IV), axial	3.6 ± 0.3	~ 0.2	0.9 ± 0.3
	N _{III}	Mn(IV), equatorial	2.3 ± 0.6	~ 0.5	0.6 ± 0.2
	N _{IV}	Mn(III), equatorial	< 2.0	$\sim 0.6-1.3$	~ 1.9

Figure Legends.

Figure S1. The 2D ^{14}N HYSCORE spectrum of 2 in aqueous buffer at pH 4.3.

Figure S1

