Supplementary Information for "Characterization of Monomeric MnII/III/IV-Hydroxo Complexes from X- and Q-band Dual Mode EPR Spectroscopy."

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Table S1: Covalency factors, γ_d, used in D-value calculation

d-orbital	Formal N_d	Mulliken N_d[a]	γ_d[b]	
z^2	0	1.019	$(2 - N_d)/2$	0.49
xy	1	1.088	$2 - N_d$	0.91
x^2-y^2	1	0.943	$2 - N_d$	1.06
xz	1	1.070	$2 - N_d$	0.93
yz	1	0.818	$2 - N_d$	1.18

a: Obtained from DFT calculation of the Mn^{III}-OH ground state
b: Calculated using the Mulliken spin population.

Table S2: Comparison of calculated values of selected bond distances (Å) of M^{n+}-OH complexes.

Complex	S	M-OH	M-N_{eq}1	M-N_{eq}2	M-N_{eq}3	Avg. M-N_{eq}	M-N_{ax}
Mn^{II}-OH	5/2	2.101	2.147	2.159	2.175	2.160	2.427
Mn^{III}-OH	2	1.872	2.033	2.066	2.072	2.057	2.058
Mn^{IV}-OH	3/2	1.838	1.927	1.929	1.946	1.934	2.048
Fe^{III}-OH	5/2	1.938	1.997	1.990	2.015	1.975	2.365

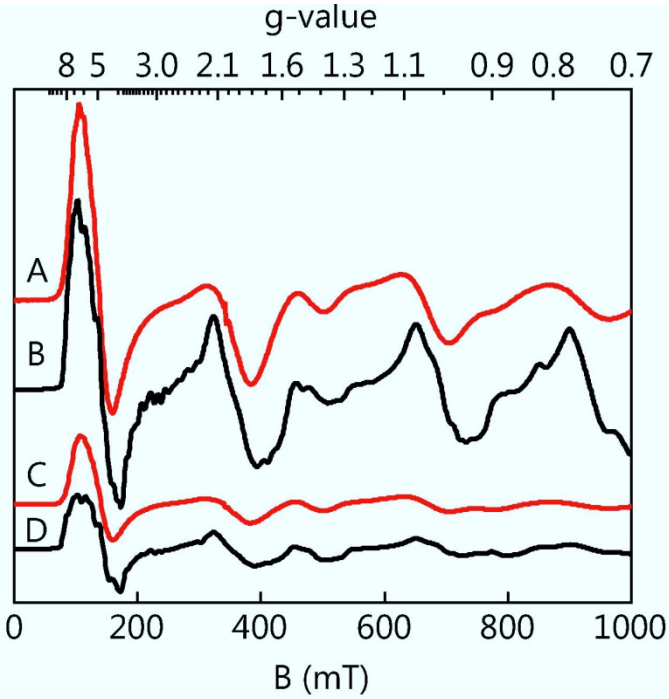

Figure S1. X-band EPR spectra (colored) and simulations (black) of the Mn^{II}-OH complex, 5mM in DMF/THF with $B_1 \perp B$, (A) 2K, (C) 10K . Experimental condition: temperature 10 K, power 0.02 mW (A), 0.2mW (C), frequency 9.634 GHz. The simulation parameters are in Table 1.

Full Reference 25: Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; J. A. Montgomery, J.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; N. Rega; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; K. Toyota; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; K. Raghavachari; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. Wallingford CT 2004; Vol. Gaussian 03, Revision E.01.