Solid-State ^{55}Mn NMR Spectroscopy of bis(μ-oxo)dimanganese(IV) [$Mn_2O_2(salpn)_2$], a Model for the Oxygen Evolving Complex in Photosystem II

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Electric Supporting Information:

- Evaluation of Heisenberg exchange constant of **1** using various methods:

1.) Approach proposed by L. Noodleman:[1]

$$J_{AB} = \frac{E_{BS} - E_{HS}}{S^2_{\max}} \qquad (1)$$

J_{AB} = -171 cm^{-1}

2.) Approach proposed by E. Ruiz and co-workers:[2]

$$J_{AB} = \frac{E_{BS} - E_{HS}}{S_{\max}(S_{\max}+1)} \qquad (2)$$

J_{AB} = -128 cm^{-1}

3.) Approach proposed by M. Nishino and co-workers: [3]

$$J_{AB} = \frac{E_{BS} - E_{HS}}{\langle S^2\rangle_{HS} - \langle S^2\rangle_{BS}} \qquad (3)$$

J_{AB} = -166 cm^{-1}

(1) Noodleman, L. *J Chem Phys* **1981**, *74*, 5737
(2) Ruiz, E.; Cano, J.; Alvarez, S.; Alemany, P. *Journal of Comp Chem* **1999**, *20*, 1391.
(3) Nishino, M.; Yamanaka, S.; Yoshioka, Y.; Yamaguchi, K. *J Phys Chem A* **1997**, *101*, 705.

- Coordinates of optimized structure of **1**

Mn	-1.574053	1.236837	8.057116
O	-2.921100	2.542783	7.608347
O	-0.427448	-0.080288	8.574925
O	-1.671887	0.634171	6.255139
N	-1.407015	2.201306	9.817668
N	0.030896	2.403550	7.485799
C	-3.885747	2.883243	8.440295
C	-5.153649	3.224720	7.925937
C	-6.172705	3.625142	8.766515
C	-5.964711	3.753196	10.143888
C	-4.732803	3.444241	10.672054
C	-3.686939	2.987922	9.843558
C	-2.380319	2.792792	10.409697
C	-0.070477	2.246023	10.407971
C	0.808095	3.272486	9.672681
C	0.332021	3.613963	8.265965
C	0.829147	2.075285	6.536482
C	0.630073	0.968534	5.632041
C	1.694269	0.587421	4.786286
C	1.537551	-0.420748	3.862859
C	0.290338	-1.023414	3.707516
C	-0.781013	-0.646367	4.499764
C	-0.627629	0.330298	5.509493
H	-5.304981	3.190166	7.002510
H	-7.007208	3.832467	8.398870
H	-6.622252	4.087559	10.615095
H	-4.549521	3.518431	11.631727
H	-2.260815	3.161709	11.284795
H	0.312235	1.373021	10.240546
H	-0.162003	2.466560	11.379727
H	1.758267	2.921863	9.603640
H	0.892481	4.108901	10.093833
H	-0.490940	4.178009	8.340185
H	0.963689	4.152602	7.812019
H	1.641925	2.616973	6.419112
H	2.536578	1.055936	4.838067
H	2.225072	-0.633155	3.364036
H	0.282374	-1.799867	3.063706
H	-1.693157	-1.043740	4.384120
Mn	-1.677958	-1.236837	9.203201
O	-0.330912	-2.542783	9.651969
C	0.633735	-2.883243	8.820022
C	1.901638	-3.224720	9.334379
C	2.920694	-3.625142	8.493802
C	2.712699	-3.753196	7.116428
C	1.480792	-3.444241	6.588263
C	0.434928	-2.987922	7.416758
C	-0.871693	-2.792792	6.850620
N	-1.844997	-2.201306	7.442648
O	-2.824564	0.080288	8.685391
O	-1.580125	-0.634171	11.005178

C	-2.624383	-0.330297	11.750823
C	-3.882084	-0.968534	11.628275
C	-4.081158	-2.075285	10.723835
N	-3.282908	-2.403549	9.774517
C	-3.584032	-3.613963	8.994351
C	-4.060107	-3.272486	7.587635
C	-3.181535	-2.246023	6.852346
H	-3.564246	-1.373021	7.019771
H	-3.090008	-2.466560	5.880590
H	-5.010279	-2.921863	7.656676
H	-4.144492	-4.108901	7.166483
H	-2.761071	-4.178009	8.920131
H	-4.215700	-4.152602	9.448297
H	-4.893937	-2.616972	10.841205
C	-4.946281	-0.587421	12.474031
C	-4.789563	0.420748	13.397457
C	-3.542349	1.023414	13.552800
C	-2.470998	0.646367	12.760552
H	-1.558855	1.043740	12.876196
H	-3.534385	1.799867	14.196610
H	-5.477083	0.633155	13.896281
H	-5.788590	-1.055936	12.422250
H	-0.991196	-3.161709	5.975521
H	1.297510	-3.518431	5.628589
H	3.370241	-4.087559	6.645222
H	3.755197	-3.832467	8.861446
H	2.052970	-3.190166	10.257806
N	2.467543	0.333346	11.567864
O	2.249248	1.624047	13.435430
C	2.744440	1.384201	12.339400
C	3.134397	0.060978	10.235368
C	1.522755	-0.674823	12.002824
H	3.404786	1.928937	11.956221
H	3.721776	0.828285	10.159422
H	3.532758	-0.839464	10.316491
H	2.341724	0.156510	9.565667
H	1.125671	-0.313020	12.755374
H	0.872597	-0.830317	11.331398
H	2.051131	-1.528515	12.085673