Supplementary Material (ESI) for PCCP

ELECTRONIC SUPPLEMENTARY INFORMATION

Structure of the oxygen evolving complex of Photosystem II: Information on the S_2 state through quantum chemical calculation of its magnetic properties

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1. Cartesian coordinates of all models discussed in the paper.

Model 1:

Mn	0.553290	3.153980	0.544680
Mn	0.324780	1.030490	-1.155970
Mn	-2.091340	0.015500	-1.824990
Mn	-1.111660	-1.487970	0.334900
Ca	2.261920	-1.544070	-0.082240
O	-0.740413	0.705024	-2.706642
O	-1.227159	0.378813	-0.220072
O	-0.231381	2.812505	-1.000302
O	-1.713107	-1.731631	-1.375317
O	1.129030	1.391763	0.480167
O	2.118430	3.933037	-0.365110
O	3.763409	3.247110	1.034406
O	-1.114228	3.030855	1.662317
O	-0.369148	4.926695	0.880189
O	1.571028	3.350048	2.360363
O	4.683300	-1.676227	-0.388166
O	5.199513	-3.835555	-0.721443
O	-0.593403	-1.072984	2.196876
O	1.627626	-1.409799	2.199080
O	3.717388	0.652640	-0.496961
O	0.952131	-0.728764	-1.611375
O	2.684329	-3.838251	-0.667689
O	-3.209451	1.755977	-1.920456
O	-4.080336	-0.083610	-1.110713
O	-2.859161	-0.508139	-3.717732
O	1.932999	1.731060	-2.208117
N	0.283456	-5.461164	0.966843
N	-0.293569	-3.433866	0.336174
N	-4.684947	-2.394556	2.591378
N	-3.014357	-2.106290	1.188095
C	4.327823	4.730736	-0.772429
C	3.361547	3.901476	0.038086
C	-0.184677	-5.578457	-0.330784
C	-0.546918	-4.312502	-0.711193
C	0.211184	-4.163968	1.336696
C	-2.415897	5.032196	2.173977
C	-1.262104	4.310434	1.558015
C	6.995512	-2.242661	-0.726949
C	5.534712	-2.624096	-0.606252
C	0.595492	-0.556456	4.196934
C	0.568790	-1.036120	2.762968
C	-5.431045	1.934459	-0.962219
C	-4.199274	1.173211	-1.351939
C	-5.073024	-2.982944	1.398525
C	-4.024716	-2.790322	0.535462
C	-3.440688	-1.876511	2.428237
H	4.507886	5.668924	-0.225153
H	5.288984	4.208652	-0.856058

H	3.927650	4.980713	-1.760872
H	0.680051	-6.209877	1.528727
H	-0.982123	-3.948448	-1.635528
H	0.545460	-3.786428	2.295408
H	-0.232357	-6.531199	-0.844940
H	-2.946004	4.390154	2.886280
H	-2.060746	5.945288	2.669189
H	-3.107144	5.336628	1.373855
H	1.351259	2.568632	2.898290
H	2.530667	3.213844	2.020077
H	7.316633	-1.707732	0.178193
H	7.621391	-3.128310	-0.876466
H	7.126274	-1.554259	-1.574903
H	-0.112618	0.268948	4.342375
H	0.282481	-1.378725	4.859010
H	1.610477	-0.259033	4.482007
H	4.492364	0.014294	-0.515133
H	3.863222	1.329237	0.199171
H	0.478862	-0.901310	-2.443859
H	2.303061	-4.497422	-1.266552
H	3.743126	-3.939335	-0.704055
H	-5.553401	2.822465	-1.593355
H	-6.317357	1.290598	-1.017826
H	-5.318422	2.267091	0.081001
H	-3.829035	-0.454474	-3.802025
H	-2.472344	0.151121	-4.327740
H	2.732039	1.351355	-1.728490
H	1.934949	2.697098	-2.013216
H	-5.238261	-2.350319	3.442268
H	-3.928842	-3.063528	-0.508255
H	-2.882608	-1.351702	3.194792
H	-6.036537	-3.463280	1.277186

Model 2:

Mn	3.187504	0.568033	-0.757484
Mn	1.153004	-1.197002	-0.372775
Mn	-1.472049	-1.102475	-1.000062
Mn	-1.314460	-1.280777	1.792852
Ca	-0.814671	1.860374	0.558610
O	-0.333303	-0.305027	0.351181
O	2.423170	-0.251018	0.678901
O	-2.301910	-1.867007	0.387196
O	1.679785	0.012666	-1.649699
O	-0.081365	-1.983534	-1.522400
O	-0.581700	4.933864	-1.846716
O	-1.167705	4.232733	0.218065
O	-4.625940	-1.703633	-1.800128
O	-2.452563	-1.692427	-2.472744
O	-2.333698	1.561084	2.307185
O	-2.976647	-0.536084	2.755902

O	4.229426	-0.997938	-1.321557
O	2.546079	-2.460320	-0.987362
O	4.777475	1.125819	0.273827
O	3.784838	2.589604	1.688019
O	-1.470902	-2.838349	3.143754
O	2.495229	2.308773	-0.567757
O	4.112420	1.384486	-2.485808
O	1.175695	1.439989	2.109159
O	0.270206	2.436074	-1.634561
O	-0.178508	-0.443779	3.277999
O	-0.057874	-4.510071	2.022920
O	0.585652	-2.602151	1.060629
N	-4.909752	1.256593	-0.986057
N	-2.781596	0.683370	-0.967695
C	-1.522778	6.543412	-0.371337
C	-1.085531	5.133767	-0.636114
C	-4.044733	-2.621574	-3.961539
C	-3.760006	-1.953949	-2.631627
C	-4.018445	1.226422	3.990662
C	-3.046987	0.733766	2.944935
C	4.627146	-3.304449	-1.788657
C	3.734611	-2.175280	-1.343114
C	6.058000	1.915012	2.118865
C	4.772188	1.898856	1.326167
C	-4.324014	1.928369	-2.047539
C	-3.006416	1.562681	-2.033988
C	-3.976740	0.497686	-0.381303
C	1.179970	-4.757008	0.018059
C	0.538953	-3.920709	1.090338
H	-1.838203	7.043403	-1.293988
H	-2.319831	6.555091	0.379586
H	-0.664432	7.100686	0.036069
H	-5.123952	-2.640879	-4.146689
H	-3.519962	-2.107338	-4.777194
H	-3.663891	-3.653071	-3.929706
H	-4.392207	2.223739	3.731038
H	-4.843915	0.519763	4.132329
H	-3.477136	1.309255	4.946052
H	5.416898	-2.932335	-2.450318
H	5.103627	-3.744668	-0.899202
H	4.039410	-4.083855	-2.286471
H	6.928075	1.828133	1.456746
H	6.119982	2.824040	2.726918
H	6.066783	1.041160	2.788598
H	-0.898853	-3.655177	2.755516
H	-2.374424	-3.115656	3.374932
H	2.856936	2.651195	0.311328
H	1.244151	2.497577	-1.185706
H	4.233580	2.333306	-2.287522
H	4.999977	0.991284	-2.592661
H	1.738697	0.766550	1.533909
H	1.861364	2.057365	2.443517

H	-0.247794	3.972625	-1.915349
H	0.431785	1.704383	-2.267482
H	0.475940	0.288491	3.026658
H	0.240861	-1.112856	3.847985
H	-5.902500	1.237176	-0.767227
H	-2.212184	1.864959	-2.706751
H	-4.166445	-0.185343	0.438918
H	-4.884241	2.591379	-2.696034
H	0.863838	-5.796353	0.152153
H	0.902238	-4.387626	-0.976264
H	2.272644	-4.692673	0.094912

Model 3:

Mn	2.920430	-0.726648	-0.715975
Mn	0.444266	-1.136324	0.335703
Mn	-2.035122	-0.783200	-0.672328
Mn	-1.811062	0.926975	1.538019
Ca	1.025421	2.208353	0.183397
O	0.260542	2.940652	-1.916057
O	-1.219727	1.765020	-3.153687
O	-3.220997	1.844075	2.488088
O	-3.901238	2.445820	0.430724
O	3.342025	-2.398678	0.131843
O	1.295715	-2.764293	1.024027
O	4.821648	-0.219171	-0.189523
O	4.800128	2.010383	-0.484745
O	3.804663	-1.517063	-2.492609
O	2.962365	3.554937	0.833680
O	2.776972	1.153779	-1.537741
O	-1.097813	-0.792967	-2.549436
O	-3.068154	0.785896	-1.515695
O	-0.617476	2.402706	1.839758
O	-0.619523	0.381799	-0.094572
O	2.075807	-0.051742	0.676145
O	-2.861132	-0.447721	0.887912
O	1.338819	-1.299635	-1.338354
O	-0.985649	-2.133310	-0.155566
O	1.384144	-1.375772	3.513501
O	-0.271611	-0.629388	2.142924
N	-5.240797	-3.344067	-1.207558
N	-3.502442	-2.019807	-1.287885
C	-4.856939	-3.284188	-2.537501
C	-3.766314	-2.453485	-2.574450
C	-4.403283	-2.570457	-0.476448
C	-0.629631	3.952174	-3.904099
C	-0.509863	2.806307	-2.916147
C	-5.259621	3.090482	2.314036
C	-4.064573	2.431548	1.668227
C	3.048010	-4.265592	1.596212
C	2.512696	-3.064027	0.868839

C	6.589949	1.042641	0.802274
C	5.329960	0.935978	-0.008740
C	-0.618201	-0.453538	4.502331
C	0.285541	-0.876033	3.355644
H	-6.021252	-3.879688	-0.838509
H	-3.159139	-2.131043	-3.411406
H	-4.456904	-2.412929	0.594743
H	-5.384083	-3.819404	-3.317736
H	0.108876	4.734653	-3.699423
H	-0.520674	3.578925	-4.931159
H	-1.640900	4.379100	-3.828873
H	-4.989079	3.574725	3.260391
H	-5.707232	3.811094	1.621668
H	-6.006152	2.315017	2.544113
H	4.058226	-4.522089	1.262539
H	3.063550	-4.018856	2.668376
H	2.367626	-5.116085	1.462012
H	7.144666	0.098649	0.778228
H	7.209289	1.876515	0.452337
H	6.311608	1.238369	1.850112
H	4.681848	-1.905028	-2.309937
H	3.232390	-2.247563	-2.798020
H	3.139914	4.398584	1.279224
H	3.827986	3.221887	0.484702
H	3.739215	1.619929	-1.204839
H	2.647326	1.213716	-2.501920
H	-1.007138	0.186955	-2.826297
H	-0.175078	-1.103855	-2.363931
H	-2.477682	1.326354	-2.125075
H	-3.439626	1.400191	-0.816441
H	-1.006536	3.044572	2.454579
H	-0.124355	-0.675874	5.453950
H	-0.830691	0.624867	4.449628
H	-1.578608	-0.985534	4.451872

Model 4:

Mn	-2.955320	0.244430	-0.320880
Mn	-0.631280	-1.118850	0.060010
Mn	1.602880	-0.539000	1.498190
Mn	2.340160	-0.733030	-1.200130
Ca	0.936240	2.244350	-0.338300
O	0.719284	4.551655	0.666513
O	-0.765076	3.025977	1.263514
O	3.510136	-1.075058	2.205278
O	2.261998	0.543298	2.981827
O	3.699639	0.306292	-2.310532
O	4.469212	-1.640306	-1.618073
O	-3.236821	-1.107096	-1.737606
O	-1.300882	-2.274634	-1.439420
O	0.983522	-1.973857	2.685364

O	-0.661725	-2.706088	1.313911
O	-4.776083	0.303147	0.058644
O	-6.948025	-0.120697	0.191822
O	-2.862712	1.842745	0.855124
O	1.198850	-1.649114	-0.088515
O	-1.149035	0.368390	-0.952596
O	2.452173	0.481248	0.180798
O	-2.361675	-0.960919	0.773091
O	-0.003780	0.130784	1.286557
O	-3.509049	1.780876	-1.854936
O	0.868851	0.555744	-2.375708
O	-0.812869	3.160833	-1.966545
O	2.020917	-2.286212	-2.620320
O	2.866149	2.871007	-1.737293
C	-1.119398	5.296307	2.050418
C	-0.342600	4.262744	1.275343
C	4.383202	0.174473	4.104840
C	3.373115	-0.140323	3.052564
C	6.045716	-0.158488	-2.713697
C	4.692488	-0.541193	-2.190400
C	-2.839075	-3.019013	-3.102991
C	-2.421402	-2.062249	-2.014945
C	-0.209225	-3.937985	3.308553
C	0.053994	-2.795165	2.363214
C	-5.465401	-1.944236	0.751743
C	-5.813675	-0.540030	0.320025
H	-0.771104	6.305346	1.807639
H	-2.196332	5.204485	1.853122
H	-0.970766	5.117485	3.126162
H	5.331848	-0.326217	3.882928
H	4.525521	1.260236	4.183657
H	4.005746	-0.181503	5.075502
H	6.548457	0.467819	-1.960097
H	6.657762	-1.052032	-2.877530
H	5.960114	0.428109	-3.636881
H	-3.730462	-2.658379	-3.625871
H	-2.013268	-3.167732	-3.811041
H	-3.058314	-3.995010	-2.645121
H	-0.684297	-3.538484	4.216904
H	-0.874141	-4.675683	2.848435
H	0.739596	-4.401853	3.606631
H	-4.557489	-1.971834	1.366718
H	-6.316230	-2.379288	1.287557
H	-5.275959	-2.550526	-0.147073
H	-1.962959	2.381323	1.140730
H	-3.438430	1.713504	1.630556
H	-3.848148	1.299362	-2.634815
H	-4.308934	2.115401	-1.394454
H	0.986851	0.751493	-3.320780
H	-0.116263	0.419378	-2.138894
H	-0.911176	4.097858	-2.205508
H	-1.721111	2.789241	-1.938011

H	2.866391	-2.782836	-2.610367
H	1.328056	-2.889240	-2.283475
H	3.401038	2.089505	-2.028852
H	3.417404	3.662490	-1.840050

Model 5:

Mn	-3.176510	-0.009460	-0.582890
Mn	-0.840060	-1.143550	0.229310
Mn	1.302590	-0.135660	1.566980
Mn	2.180330	-0.975120	-0.960280
Ca	0.657620	2.067830	-0.941580
O	0.399341	4.688162	-0.595034
O	0.852564	3.367611	1.132450
O	3.107076	-1.002519	2.030941
O	3.943038	0.647296	3.333109
O	3.634742	-0.250699	-2.148990
O	4.544250	-2.167168	-2.931668
O	-3.427133	-1.662117	-1.582846
O	-1.507530	-2.683701	-0.877757
O	0.634507	-1.220623	3.063617
O	-0.905028	-2.342491	1.847801
O	-5.003279	0.194928	-0.307130
O	-7.105522	0.387736	0.356526
O	-2.783181	1.733747	0.419318
O	0.979450	-1.633463	0.247645
O	-1.345574	-0.034465	-1.197217
O	2.176123	0.547030	0.040548
O	-2.616303	-0.869920	0.806795
O	-0.320915	0.437690	1.063839
O	-3.807726	1.166302	-2.321500
O	0.713598	0.004216	-2.510913
O	-1.539394	3.267954	-1.476517
O	2.390796	-2.728156	-1.889119
O	2.648978	2.369736	-2.371413
O	1.663561	1.302861	2.669743
C	0.865587	5.747322	1.534743
C	0.690483	4.542284	0.645932
C	5.273332	-1.299860	3.012995
C	4.022638	-0.511319	2.759725
C	5.634397	-0.095952	-3.461828
C	4.548486	-0.918714	-2.817900
C	-3.017311	-3.902077	-2.264220
C	-2.605674	-2.657531	-1.521005
C	-0.519237	-3.025585	4.103550
C	-0.246083	-2.137668	2.917364
C	-5.542946	-0.504260	1.974119
C	-5.972969	0.050753	0.640843
H	0.580530	6.667223	1.014592
H	0.272280	5.625379	2.451266
H	1.919022	5.815966	1.844670

H	5.348859	-2.143428	2.319940
H	6.153101	-0.648552	2.933625
H	5.243076	-1.684389	4.043734
H	6.166367	0.484342	-2.694450
H	6.339472	-0.744603	-3.990579
H	5.192387	0.619476	-4.170700
H	-3.718611	-3.664288	-3.071321
H	-2.135043	-4.426678	-2.648616
H	-3.525499	-4.570511	-1.552115
H	-0.884979	-2.407163	4.935448
H	-1.261338	-3.789787	3.853154
H	0.417312	-3.496782	4.431339
H	-4.923587	0.240218	2.496103
H	-6.429446	-0.723249	2.578422
H	-4.927598	-1.404652	1.849606
H	-2.412861	2.416346	-0.210945
H	-2.031115	1.470453	1.009961
H	-3.783204	0.630402	-3.136340
H	-4.750251	1.150018	-2.018633
H	0.868923	-0.226449	-3.442713
H	-0.266697	-0.201243	-2.230253
H	-1.066357	4.125868	-1.236160
H	-2.179965	3.421696	-2.192792
H	3.360098	-2.687884	-2.356927
H	2.220902	-3.552422	-1.401193
H	3.215323	1.555514	-2.330337
H	3.236855	3.126929	-2.523870
H	1.402871	2.185000	2.279180
H	2.973547	1.077731	3.094917

Model 6:

Mn	-3.299856	-0.470814	-0.244379
Mn	-0.798889	-1.271638	0.468567
Mn	1.449497	0.124923	1.093226
Mn	1.991489	-1.404169	-1.193637
Ca	0.292738	1.480527	-1.803066
O	-0.304114	4.969606	-2.861540
O	-0.030390	3.710101	-1.013091
O	3.307509	-0.342909	1.649791
O	4.524092	0.813716	0.135988
O	3.467529	-1.458951	-2.578566
O	3.713051	-2.334871	-0.594589
O	-3.520873	-2.373120	-0.755715
O	-1.404651	-3.059017	-0.225961
O	1.048664	-0.567001	2.901315
O	-0.504457	-2.089356	2.298901
O	-5.134425	-0.384278	0.434487
O	-5.024515	1.505435	1.669027
O	-3.026992	1.428915	0.256175
O	1.062886	-1.568812	0.355733

O	-1.632674	-0.547106	-1.024508
O	2.149264	0.732015	-0.554498
O	-2.484503	-0.987207	1.226513
O	-0.255212	0.532181	0.745143
O	-4.023449	0.188055	-2.110853
O	0.730831	-0.755100	-2.433831
O	-1.840484	1.186358	-3.470464
O	0.963317	-3.553120	-1.722064
O	0.215098	2.795371	-3.901570
N	1.722076	4.023110	2.650752
N	1.764767	1.919261	2.050974
C	2.387134	3.347239	3.659963
C	2.405575	2.033140	3.275405
C	1.353881	3.138216	1.693376
C	-0.529139	6.051082	-0.745207
C	-0.277267	4.825276	-1.599292
C	5.675039	-0.389685	1.874156
C	4.433231	0.074916	1.154897
C	5.638689	-2.435196	-2.086504
C	4.232177	-2.073803	-1.745965
C	-2.948803	-4.654867	-1.101563
C	-2.604416	-3.252606	-0.668381
C	0.324188	-2.135346	4.539898
C	0.275335	-1.561095	3.147029
C	-6.949386	0.089585	1.908339
C	-5.616678	0.449243	1.310018
H	1.535950	5.021361	2.622757
H	2.809165	1.164117	3.778530
H	0.806712	3.412466	0.786482
H	2.775481	3.848128	4.538423
H	-1.070372	6.815878	-1.312546
H	-1.085318	5.784394	0.162406
H	0.441056	6.477743	-0.444990
H	5.739895	-1.484766	1.802905
H	6.567070	0.068423	1.434442
H	5.610167	-0.138828	2.941632
H	6.271454	-1.546898	-1.934439
H	6.000980	-3.240695	-1.437550
H	5.713564	-2.720563	-3.143233
H	-3.927403	-4.678868	-1.590759
H	-2.175332	-5.042038	-1.778583
H	-2.968081	-5.303065	-0.213079
H	0.300640	-1.324698	5.279349
H	-0.511119	-2.824232	4.700100
H	1.274331	-2.675032	4.665800
H	-6.783070	-0.654901	2.702185
H	-7.423475	0.973505	2.347954
H	-7.599827	-0.373036	1.156118
H	-2.174455	1.421808	0.750488
H	-3.870057	1.583010	0.970777
H	-3.350662	0.757591	-2.573747
H	-4.865933	0.674965	-2.085141

H	0.313072	-1.496363	-2.902670
H	-1.368116	1.914227	-3.966854
H	-1.732638	0.388680	-4.018266
H	1.518489	-4.333209	-1.548070
H	0.185452	-3.634153	-1.118900
H	0.728348	2.887419	-4.720486
H	0.004851	3.814587	-3.509187
H	3.192858	0.900279	-0.358256

Model 7:

Mn	-2.889440	-1.495880	-0.044720
Mn	-0.418660	-1.020740	-1.081130
Mn	2.053190	-0.984960	0.052350
Mn	1.525140	1.581160	-0.946810
Ca	-1.420970	1.665020	0.779860
O	-0.577502	1.711168	4.377007
O	-1.646125	0.439136	2.868019
O	3.727165	-0.436262	-0.694872
O	5.014107	0.373337	1.000671
O	2.345165	3.409323	-0.684823
O	2.122981	2.558137	-2.695110
O	-3.565759	-1.285350	-1.903152
O	-1.548357	-0.739055	-2.841067
O	2.324591	-2.715310	-0.830419
O	0.486564	-2.523894	-2.133434
O	-4.472988	-0.527090	0.664469
O	-3.830096	1.632112	0.836202
O	-2.154580	-1.774346	1.784531
O	1.124571	-0.100887	-1.563615
O	-1.824099	-0.102529	-0.393058
O	1.698720	0.801708	0.677467
O	-1.611558	-2.496474	-0.698876
O	0.337575	-1.416877	0.509544
O	-4.208695	-3.090229	0.212017
O	0.183119	2.940005	2.262591
O	-0.632607	1.704810	-3.721041
O	-0.508017	2.526312	-1.324908
O	-1.425160	4.252065	0.662668
N	3.683853	-1.630795	3.755742
N	2.796576	-1.653685	1.761633
C	3.593350	-2.964724	3.383897
C	3.033858	-2.967563	2.134146
C	3.203005	-0.861688	2.756437
C	-1.752819	-0.218660	5.184328
C	-1.277403	0.710306	4.087955
C	5.946856	0.214678	-1.220344
C	4.851413	0.071673	-0.177427
C	3.237981	4.716829	-2.526519
C	2.537398	3.525878	-1.957489
C	-3.483082	-0.840250	-4.236982

C	-2.809960	-0.961123	-2.890946
C	2.014616	-4.304274	-2.578775
C	1.562039	-3.099299	-1.793786
C	-6.146181	1.081875	1.183742
C	-4.704274	0.738714	0.877776
H	4.083754	-1.276373	4.619895
H	2.793828	-3.793213	1.476558
H	3.180266	0.219514	2.743236
H	3.927298	-3.770361	4.026141
H	-2.834958	-0.078780	5.327066
H	-1.598450	-1.269270	4.901675
H	-1.239868	-0.000288	6.126409
H	6.728470	0.887488	-0.850691
H	6.389175	-0.775728	-1.405444
H	5.540591	0.573982	-2.174436
H	4.323594	4.568842	-2.416270
H	3.009479	4.830143	-3.592144
H	2.971158	5.623024	-1.968651
H	-4.567964	-0.952855	-4.146165
H	-3.243949	0.132638	-4.688351
H	-3.084237	-1.619154	-4.903045
H	2.390599	-5.079051	-1.898732
H	1.196276	-4.694126	-3.192299
H	2.847606	-4.003453	-3.231440
H	-6.537081	0.420767	1.968831
H	-6.235104	2.128246	1.492695
H	-6.757021	0.915756	0.283932
H	-2.049656	-0.888012	2.348850
H	-1.218541	-2.024597	1.573127
H	-5.069001	-2.653188	0.383129
H	-4.305150	-3.639059	-0.588409
H	1.136920	2.791357	2.132350
H	-0.065259	2.509710	3.181843
H	0.288105	1.740869	-4.044444
H	-0.867549	0.743902	-3.632963
H	-0.634859	2.269460	-2.334986
H	-0.593678	3.496075	-1.207657
H	-0.763400	4.296862	1.399272
H	-2.070293	4.966580	0.791202

Model 8:

Mn	-3.290565	-0.083883	-0.621311
Mn	-1.013148	-1.152086	0.416510
Mn	1.214810	-0.006951	1.475298
Mn	1.987044	-1.457451	-0.796678
Ca	0.657254	1.601797	-1.468397
O	0.496286	3.926738	-2.508790
O	0.634854	3.765990	-0.281065
O	2.769056	-0.850047	2.207502
O	4.572893	0.430709	1.660297

O	3.535672	-1.168722	-2.018027
O	4.310965	-3.280291	-2.243653
O	-3.738231	-1.886709	-1.159459
O	-1.859713	-2.864856	-0.282398
O	0.374080	-0.535168	3.194509
O	-1.123344	-1.948557	2.270649
O	-5.016424	0.540781	-0.291670
O	-7.041383	1.033116	0.479745
O	-2.586225	1.808160	-0.130441
O	0.758803	-1.725129	0.538629
O	-1.516903	-0.425481	-1.223845
O	2.089746	0.262459	-0.137812
O	-2.769306	-0.636891	0.932460
O	-0.405610	0.560922	0.817585
O	-3.830162	0.708432	-2.603305
O	0.595022	-0.826030	-2.478212
O	-1.130520	1.897745	-3.196809
O	2.091376	-3.396201	-1.217018
O	2.725448	1.395382	-2.802445
N	2.501897	3.754092	2.554329
N	1.588254	1.801901	2.215499
C	1.338604	3.733858	3.305510
C	0.773030	2.507383	3.086666
C	2.626359	2.582902	1.898351
C	0.444672	5.976766	-1.247801
C	0.526388	4.466101	-1.347035
C	4.898408	-1.604000	2.919040
C	4.072502	-0.561989	2.182876
C	5.621264	-1.484788	-3.150082
C	4.423954	-2.043841	-2.429485
C	-3.506255	-4.249186	-1.306515
C	-2.976903	-2.902802	-0.882524
C	-0.798229	-2.032339	4.634406
C	-0.503782	-1.463405	3.270736
C	-5.995935	-0.958826	1.371063
C	-6.088801	0.280602	0.515657
H	3.149634	4.532613	2.477891
H	-0.133762	2.075301	3.489010
H	3.461099	2.274972	1.277718
H	1.025354	4.573058	3.914167
H	-0.428048	6.340690	-1.807523
H	0.385212	6.307668	-0.205196
H	1.331182	6.419818	-1.725049
H	4.597079	-2.619875	2.631132
H	5.963318	-1.447324	2.716399
H	4.718339	-1.505399	3.999658
H	6.169598	-0.808139	-2.478754
H	6.279947	-2.294602	-3.478539
H	5.296721	-0.896448	-4.020441
H	-4.276919	-4.147207	-2.077830
H	-2.683241	-4.883914	-1.656053
H	-3.952205	-4.735640	-0.425460

H	-0.770308	-1.237980	5.390120
H	-1.766046	-2.544190	4.641046
H	-0.008751	-2.757225	4.884309
H	-5.025765	-1.014630	1.882855
H	-6.818508	-0.967332	2.093771
H	-6.075537	-1.845977	0.724775
H	-1.793874	1.570959	0.446570
H	-3.234605	2.275854	0.431583
H	-4.005678	0.004590	-3.256512
H	-4.711188	1.058555	-2.336849
H	0.731768	-1.070702	-3.409606
H	-0.398289	-0.865521	-2.234953
H	-0.939262	2.857062	-3.319994
H	-2.093697	1.789452	-3.078535
H	3.085869	-3.538208	-1.637136
H	1.860405	-4.036692	-0.521923
H	3.309422	0.630029	-2.586190
H	3.236194	2.042693	-3.313130

Model 9:

Mn	-3.067566	0.249831	0.218459
Mn	-0.877063	-1.362645	0.298460
Mn	1.686802	-0.910277	1.084680
Mn	1.725061	-1.582593	-1.637219
Ca	0.892381	1.654892	-1.001731
O	-1.174370	2.806967	-1.878240
O	-0.165271	4.407978	-3.103713
O	3.241725	-1.702545	-3.037674
O	3.128856	-2.982709	-1.272882
O	-3.714521	-1.342554	-0.970181
O	-1.785079	-2.587457	-0.967294
O	1.385668	-2.152901	2.549225
O	-0.639283	-2.821992	1.794662
O	-4.670551	0.624939	1.066516
O	-6.200327	0.776506	2.688438
O	-2.107167	1.560155	1.215852
O	0.802566	-2.074642	-0.156167
O	-1.414013	-0.020705	-0.752217
O	2.434511	-0.270081	-0.548098
O	-2.406635	-1.076646	1.250516
O	0.036589	0.121296	1.268598
O	-3.476755	1.656850	-1.221239
O	0.788147	-0.262823	-2.517095
O	0.456953	-2.987217	-2.603436
O	1.951634	3.169071	-2.541280
N	1.647445	5.524742	1.412772
N	1.426234	3.422475	0.759168
N	4.739541	1.347652	2.843148
N	3.043446	0.103673	2.223105
C	1.182105	4.828208	2.513504

C	1.051011	3.527709	2.090500
C	1.782294	4.649874	0.380365
C	-2.545686	4.509307	-2.908152
C	-1.199362	3.869140	-2.620580
C	5.118819	-3.208474	-2.654733
C	3.789051	-2.614925	-2.325954
C	-3.628637	-3.340432	-2.271247
C	-3.018865	-2.325594	-1.335570
C	0.328094	-3.994859	3.638984
C	0.336576	-2.922030	2.581139
C	-5.508512	-1.447354	2.043093
C	-5.501474	0.063994	1.990868
C	4.089695	0.969689	4.006740
C	3.032732	0.193959	3.606333
C	4.086533	0.810852	1.786205
H	1.838284	6.522069	1.374555
H	0.700918	2.669515	2.653528
H	2.111637	4.929593	-0.616469
H	0.978811	5.311432	3.461837
H	-2.988118	4.873977	-1.968676
H	-2.430302	5.354604	-3.593764
H	-3.239334	3.774528	-3.340792
H	5.314385	-3.142544	-3.731249
H	5.898376	-2.638549	-2.125797
H	5.174956	-4.247977	-2.309645
H	-4.633709	-3.030384	-2.572465
H	-2.994307	-3.458047	-3.161246
H	-3.672091	-4.315624	-1.765643
H	0.552439	-3.554438	4.619505
H	-0.642938	-4.498966	3.661263
H	1.117279	-4.727741	3.416676
H	-4.483605	-1.831449	2.142259
H	-6.127943	-1.783318	2.881299
H	-5.918504	-1.843718	1.102578
H	-0.771634	0.749733	1.445899
H	-2.648548	1.790481	1.995746
H	-2.598530	2.145925	-1.459920
H	-4.095314	2.308776	-0.842623
H	0.166818	-0.603520	-3.185073
H	0.816051	-3.893537	-2.560537
H	-0.386638	-3.001133	-2.059070
H	2.553090	3.084147	-3.296616
H	1.115678	3.730828	-2.859510
H	5.573185	1.925916	2.784149
H	2.280917	-0.319476	4.193051
H	4.376618	0.926342	0.747720
H	4.427955	1.278362	4.988495

Model 10:

Mn	-3.094127	-0.056092	0.026120

Mn	-0.633581	-0.807130	0.912877
Mn	1.709442	0.553687	1.145827
Mn	2.108449	-1.546484	-0.668612
Ca	0.579971	1.187311	-1.998536
Cl	-3.947248	0.142664	-2.123553
O	0.852434	3.677277	-2.154669
O	-1.114640	2.919266	-1.454431
O	3.556707	-0.018762	1.757176
O	3.763481	-1.793806	0.365657
O	3.327981	-2.157034	-2.269622
O	2.267074	-3.559392	-0.967707
O	-3.395545	-2.105894	0.115830
O	-1.286914	-2.637199	0.771024
O	1.316324	0.519320	3.072495
O	-0.288501	-1.063384	2.903865
O	-5.101865	0.215263	1.001980
O	-7.226691	0.593459	1.451435
O	-2.859709	1.992896	0.177978
O	1.208522	-1.309193	0.877110
O	-1.187959	-0.461586	-0.871198
O	2.310190	0.309236	-0.611447
O	-2.183810	-0.173760	1.557299
O	0.043375	0.964874	0.766799
O	0.787013	-1.448755	-2.002029
O	-1.175548	0.655179	-3.689672
O	2.346383	0.634982	-3.704782
N	3.265516	4.392101	0.798833
N	2.317639	2.476022	1.268118
C	2.573719	4.579318	1.982912
C	1.982421	3.375063	2.266302
C	3.092320	3.115177	0.390131
C	-0.915873	5.298578	-1.801892
C	-0.347529	3.897338	-1.794855
C	5.482476	-1.415668	1.961641
C	4.175197	-1.033067	1.314154
C	3.774178	-4.529054	-2.603424
C	3.098325	-3.378766	-1.928708
C	-2.904933	-4.377594	0.689536
C	-2.517467	-2.932354	0.504594
C	0.407647	-0.388450	5.084790
C	0.479053	-0.316782	3.581057
C	-6.701663	-1.147300	-0.197469
C	-6.270435	-0.085527	0.780719
H	3.783990	5.103884	0.291767
H	1.368566	3.074905	3.105870
H	3.517503	2.685284	-0.508882
H	2.567029	5.528533	2.504797
H	-1.700826	5.351717	-2.570694
H	-1.399042	5.520030	-0.840349
H	-0.143903	6.043098	-2.021789
H	5.938811	-0.541796	2.438962
H	5.271749	-2.168681	2.736166

H	6.165166	-1.863803	1.230864
H	4.632904	-4.841284	-1.989907
H	3.092239	-5.384872	-2.679732
H	4.139124	-4.235055	-3.594070
H	-3.701463	-4.652144	-0.011124
H	-2.033768	-5.030804	0.569549
H	-3.285095	-4.499009	1.715536
H	1.316431	0.025947	5.533620
H	-0.459319	0.199906	5.420947
H	0.253132	-1.425407	5.406061
H	-6.561044	-0.754268	-1.215974
H	-6.034381	-2.011998	-0.097478
H	-7.745331	-1.463215	-0.070476
H	-2.297870	2.459022	-0.539350
H	-2.335577	2.088957	0.997734
H	0.967416	-2.083086	-2.717874
H	-1.001876	-1.247725	-1.433285
H	-1.327880	0.811788	-4.634871
H	-2.076462	0.549627	-3.285042
H	2.847774	-0.181800	-3.512348
H	2.834400	1.105125	-4.400048
H	-8.110951	0.273620	1.188575

Model 11:

Mn	2.574713	-1.727777	4.350962
Mn	5.199996	-1.591969	5.188051
Mn	6.440897	0.045100	7.060256
Mn	4.599554	-1.613468	8.274022
O	3.546287	-1.631771	5.972714
O	5.467910	0.203625	5.528925
O	4.893671	0.188482	8.031021
O	6.036064	-1.751171	6.997744
Ca	3.288034	0.801232	6.406619
C	0.000000	-0.000000	0.000000
H	0.515033	-0.078705	-0.946016
H	-0.603411	0.895689	0.005971
H	-0.680607	-0.850950	0.097492
C	1.062959	-0.018798	1.108291
H	1.103794	0.939649	1.641744
H	2.063441	-0.154858	0.687566
C	0.862524	-1.080174	2.182162
O	-0.243555	-1.328916	2.667862
O	1.985260	-1.653141	2.544141
C	0.000000	-0.000000	12.184766
H	-0.800655	-0.717138	12.289955
H	-0.193658	0.973045	12.611474
H	0.877561	-0.416657	12.696044
C	0.328265	0.272405	10.710217
H	1.162449	0.983309	10.672933
H	-0.513234	0.782879	10.227691

C	0.700483	-0.991258	9.907142
H	-0.152286	-1.337154	9.309958
H	0.991219	-1.804822	10.578034
C	1.856863	-0.710549	8.967060
O	2.882671	-1.473119	9.146590
O	1.775680	0.219013	8.136308
C	2.463848	-7.781184	8.095388
H	2.056401	-8.742434	8.429860
H	1.674294	-7.256206	7.546801
C	3.672000	-8.032012	7.231017
O	4.715275	-8.505880	7.694672
C	2.885838	-6.953148	9.341254
H	3.486978	-7.597551	9.992010
H	1.992657	-6.667424	9.905198
C	3.666294	-5.716680	9.003231
N	4.997751	-5.769131	8.603970
H	5.503620	-6.636882	8.453366
C	3.337174	-4.387302	8.954956
H	2.410262	-3.895231	9.198668
C	5.409811	-4.519394	8.305579
H	6.389630	-4.257024	7.937542
N	4.426366	-3.658879	8.518803
N	3.544355	-7.625453	5.948904
H	2.678550	-7.198526	5.651921
C	4.641783	-7.738479	5.020863
H	5.370810	-8.393746	5.501875
H	4.289514	-8.252366	4.115993
C	5.306722	-6.414468	4.633638
H	6.236072	-6.651919	4.103327
H	5.601268	-5.872619	5.536767
C	4.407598	-5.521756	3.753570
H	3.419724	-5.963301	3.586514
H	4.849842	-5.396396	2.756418
C	4.197079	-4.113187	4.278018
O	3.061273	-3.607308	4.042478
O	5.171808	-3.556859	4.866597
C	9.218040	0.000000	11.089296
H	9.643271	-0.428291	11.984925
H	9.126860	1.056559	11.293664
H	9.857679	-0.178932	10.223541
C	7.875340	-0.739173	11.031242
H	7.193451	-0.340549	11.794071
H	8.027615	-1.787652	11.318439
C	7.072074	-0.808822	9.750508
O	7.485729	-0.155186	8.734107
O	6.046517	-1.542174	9.812527
C	6.504313	4.211999	7.913408
H	7.129559	3.787910	8.685173
H	6.898245	5.157832	7.533373
H	5.497842	4.389198	8.309780
C	6.432703	3.154301	6.805859
O	5.998536	3.474585	5.665830

O	6.837595	1.993230	7.160176
C	11.409360	-0.458576	3.018499
H	12.195362	-1.085542	3.412851
H	11.779082	0.540388	2.840252
H	11.086785	-0.885390	2.060859
C	10.216728	-0.256763	3.969511
H	9.530958	0.455541	3.489258
H	10.551531	0.231786	4.891659
C	9.423270	-1.517181	4.334883
H	9.993589	-2.134181	5.042594
H	9.217089	-2.127645	3.450339
C	8.086165	-1.171567	4.980291
O	7.059051	-1.691461	4.441609
O	8.102457	-0.386342	5.980374
C	11.347338	4.369563	-1.173663
H	12.033719	3.674646	-0.712818
H	11.578002	5.395727	-0.928317
H	11.506718	4.285057	-2.256431
C	9.874372	4.036446	-0.860770
H	9.556826	3.182937	-1.476499
H	9.249195	4.881910	-1.182490
C	9.559776	3.702698	0.609914
H	10.025650	4.437481	1.280979
H	9.989711	2.726933	0.872154
C	8.038562	3.676022	0.858185
H	7.534502	3.124794	0.058365
H	7.642578	4.698775	0.811699
N	7.628063	3.080861	2.132044
H	7.726659	3.647156	2.965526
C	6.859014	1.968186	2.281040
N	6.738082	1.089887	1.276762
H	7.404683	1.102338	0.521140
H	6.047372	0.304559	1.291476
N	6.225097	1.772025	3.427987
H	6.227571	2.449114	4.208769
H	5.885668	0.853113	3.712120
O	1.927575	0.104947	4.612910
H	1.033569	-0.155960	4.904423
O	3.249190	3.099929	5.739706
H	4.153333	3.462033	5.599519
H	2.751812	3.172516	4.886250
O	0.985113	-2.244989	5.042468
H	0.350803	-2.248545	4.287228
O	4.327004	-1.255214	3.698900
O	1.753999	2.584069	3.524172
H	0.811599	2.815456	3.593104
H	1.793027	1.616771	3.753201
O	5.065211	-1.092348	1.177058
H	4.200254	-1.002805	0.754407
H	4.823520	-1.272060	2.129113

Model 12:

Mn	3.263797	-1.235696	3.492543
Mn	5.484009	-1.516293	5.033518
Mn	6.530748	0.143505	7.024842
Mn	4.542281	-1.414616	8.135708
O	3.767527	-1.158665	5.349444
O	5.930568	0.265586	5.328646
O	4.860223	0.375522	7.739619
O	6.015129	-1.659146	6.992479
Ca	3.618600	1.368095	5.634056
C	-0.000000	-0.000001	0.000000
H	0.515033	-0.078705	-0.946016
H	-0.603411	0.895689	0.005971
H	-0.672198	-0.861985	0.065981
C	1.068433	-0.071322	1.084588
H	0.656660	-0.158913	2.094078
H	1.678730	0.844385	1.078029
C	2.002229	-1.268901	0.853961
O	1.833788	-2.057796	-0.060926
O	3.063410	-1.366072	1.653852
C	0.000000	0.000000	12.184766
H	-0.800655	-0.717138	12.289955
H	-0.193658	0.973045	12.611474
H	0.868311	-0.415925	12.712956
C	0.350453	0.231180	10.719959
H	1.201792	0.922619	10.678580
H	-0.469333	0.734716	10.195702
C	0.714764	-1.070877	9.981011
H	-0.171947	-1.502698	9.501285
H	1.126272	-1.809154	10.675358
C	1.752957	-0.743587	8.933062
O	2.895515	-1.309521	9.111617
O	1.488027	0.087793	8.042507
C	2.463848	-7.781184	8.095388
H	2.102841	-8.724067	8.524088
H	1.652372	-7.366597	7.487001
C	3.694344	-8.053783	7.257988
O	4.782637	-8.344789	7.768059
C	2.794087	-6.811870	9.267694
H	3.417160	-7.354865	9.987110
H	1.865400	-6.547808	9.782423
C	3.505409	-5.555818	8.853909
N	4.798826	-5.608084	8.354394
H	5.322337	-6.471876	8.227507
C	3.172843	-4.224189	8.821585
H	2.270636	-3.735807	9.149818
C	5.183442	-4.369819	8.011464
H	6.127680	-4.145441	7.554879
N	4.228934	-3.493701	8.292853
N	3.519856	-7.872056	5.929607
H	2.606881	-7.587116	5.606203

C	4.641783	-7.738479	5.020863
H	5.473302	-8.293339	5.459589
H	4.379805	-8.229089	4.075213
C	5.050256	-6.278368	4.769935
H	5.901965	-6.261101	4.078191
H	5.403598	-5.841739	5.706580
C	3.908257	-5.426514	4.209439
H	2.971358	-5.606464	4.760298
H	3.691727	-5.674613	3.160752
C	4.113417	-3.918667	4.275822
O	3.216572	-3.237944	3.695288
O	5.117611	-3.473640	4.915134
C	9.218040	0.000000	11.089295
H	9.643271	-0.428291	11.984925
H	9.126860	1.056559	11.293664
H	9.843723	-0.189063	10.216687
C	7.846106	-0.707057	11.041681
H	7.213597	-0.347946	11.864434
H	7.991531	-1.774400	11.248362
C	6.982705	-0.666352	9.791502
O	7.420166	-0.007303	8.790885
O	5.900852	-1.321671	9.826931
C	6.504313	4.211999	7.913408
H	7.129559	3.787910	8.685173
H	7.016309	5.040867	7.412896
H	5.556138	4.582079	8.312967
C	6.246760	3.065154	6.946011
O	5.371531	3.166719	6.054432
O	6.987755	2.032330	7.152676
C	11.409360	-0.458576	3.018499
H	12.195362	-1.085542	3.412851
H	11.779082	0.540388	2.840252
H	11.038623	-0.901610	2.088978
C	10.296265	-0.250481	4.054185
H	9.442054	0.216816	3.551669
H	10.624053	0.470484	4.811348
C	9.837276	-1.524752	4.782336
H	10.533974	-1.766460	5.591928
H	9.788699	-2.378223	4.098176
C	8.451774	-1.280086	5.346075
O	7.499727	-1.905280	4.770724
O	8.336966	-0.432481	6.282101
C	11.347338	4.369563	-1.173663
H	12.033719	3.674646	-0.712818
H	11.578002	5.395727	-0.928317
H	11.504553	4.273042	-2.255650
C	9.871065	4.089237	-0.862048
H	9.591145	3.093523	-1.234913
H	9.260045	4.802379	-1.434231
C	9.490519	4.189328	0.623386
H	9.918650	5.095317	1.070359
H	9.919027	3.345773	1.179334

C	7.957490	4.211776	0.801326
H	7.479283	3.541900	0.074823
H	7.569677	5.210719	0.582168
N	7.478350	3.850264	2.134972
H	7.225024	4.584601	2.779425
C	7.335876	2.572286	2.566123
N	7.753373	1.569727	1.789027
H	8.220876	1.761196	0.918202
H	7.607429	0.569415	2.038587
N	6.796210	2.325751	3.752234
H	6.337028	3.038169	4.316898
H	6.655942	1.377314	4.140119
C	3.588235	7.261292	3.508000
H	2.965123	8.112622	3.276985
H	4.499803	7.127463	2.944500
H	3.876296	7.325195	4.565541
C	2.725741	5.997694	3.245149
H	3.358102	5.119353	3.082585
H	2.174661	6.149670	2.310071
C	1.732903	5.637436	4.368491
H	1.419777	6.529051	4.926243
H	0.825079	5.197551	3.936658
C	2.291193	4.565742	5.299280
O	2.840143	3.562515	4.824114
N	2.139241	4.746221	6.626578
H	2.447456	4.012557	7.267972
H	1.646131	5.546835	6.988740
C	6.944516	-4.063363	-2.002868
H	6.174717	-4.564383	-2.571013
H	7.968061	-4.068328	-2.347441
H	6.641058	-3.013509	-1.948214
C	6.895900	-4.662889	-0.585415
H	7.343760	-5.662283	-0.545526
H	5.850393	-4.791254	-0.272460
C	7.529498	-3.818943	0.501011
O	7.790179	-2.573568	0.082183
O	7.728019	-4.205415	1.640480
C	11.863227	-5.771898	6.904426
H	11.411057	-6.388822	6.141964
H	12.851768	-6.137923	7.139397
H	11.970975	-4.752531	6.516344
C	11.060193	-5.790668	8.216192
H	11.714206	-5.481520	9.043000
H	10.771293	-6.824090	8.454447
C	9.851076	-4.906501	8.256536
N	9.140550	-4.752917	9.434190
C	9.313523	-4.103895	7.275736
H	9.562538	-3.961795	6.235788
C	8.203653	-3.868279	9.165327
H	7.450790	-3.508793	9.852916
N	8.258894	-3.438190	7.871735
H	7.649235	-2.732165	7.457633

O	3.304009	0.613118	3.429482
H	3.200388	0.876874	2.505452
O	1.186000	0.901085	5.510778
H	0.912885	0.514099	6.361587
H	1.150190	0.142781	4.867969
O	1.445167	-1.254021	3.895517
H	1.260629	-2.143590	4.249501
O	5.137875	-1.360268	3.318408
O	7.427892	-1.079490	2.187714
H	7.760549	-1.564740	2.973608
H	7.859034	-1.997273	0.893849
O	3.009484	2.314487	7.986890
H	3.818096	1.859933	8.313015
H	2.306747	1.643203	8.151970
H	6.440153	-1.184844	2.355181

2. Evaluation of TPSSh-specific scaling factor for the isotropic hyperfine coupling constant.

Redox State	Complex	A_{iso} (exp)	A_{iso} (calc)	f
Mn^{II}	$[Mn(H_2O)^6]^{2+}$	−264	−201	1.31
Mn^{II}	$[Mn(porph)(NH_3)_2]$	−204	−123	1.66
Mn^{IV}	$[Mn(porph)(OCH_3)_2]$	−202	−139	1.45
Mn^{IV}	$[Mn(salahe)_2]$	−216	−128	1.68
Mn^{III}	$[Mn_2\mathbf{(\mu\text{-}O)}(bpmsed)_2]^{3+}$	−381	−239	1.59
Mn^{IV}	$[Mn_2\mathbf{(\mu\text{-}O)}(bpmsed)_2]^{3+}$	183	122	1.50
Mn^{III}	$[Mn_2\mathbf{(\mu\text{-}O)_2}(bpy)_4]^{3+}$	−454	−316	1.44
Mn^{IV}	$[Mn_2\mathbf{(\mu\text{-}O)_2}(bpy)_4]^{3+}$	218	143	1.53
Mn^{III}	$[Mn_2\mathbf{(\mu\text{-}O)_2}(phen)_4]^{3+}$	−451	−312	1.44
Mn^{IV}	$[Mn_2\mathbf{(\mu\text{-}O)_2}(phen)_4]^{3+}$	221	142	1.55
Mn^{III}	$[Mn_2\mathbf{(\mu\text{-}O)_2}(bispiMe_2en)_2]^{3}$	−408	−291	1.40
Mn^{IV}	$[Mn_2\mathbf{(\mu\text{-}O)_2}(bispiMe_2en)_2]^{3}$	230	143	1.60
Mn^{III}	$[Mn_2\mathbf{(\mu\text{-}O)_2}(bisimMe_2en)_2]^{3+}$	−456	−280	1.63
Mn^{IV}	$[Mn_2\mathbf{(\mu\text{-}O)_2}(bisimMe_2en)_2]^{3+}$	215	145	1.48
Mn^{III}	$[Mn_2\mathbf{(\mu\text{-}O)_2}(bispicen)_2]^{3+}$	−437	−270	1.62
Mn^{IV}	$[Mn_2\mathbf{(\mu\text{-}O)_2}(bispicen)_2]^{3+}$	218	143	1.53
Mn^{III}	$[Mn_2\mathbf{(\mu\text{-}O)_2}(tren)_2]^{3+}$	−428	−283	1.51
Mn^{IV}	$[Mn_2\mathbf{(\mu\text{-}O)_2}(tren)_2]^{3+}$	207	138	1.50
Mn^{III}	$[Mn_2\mathbf{(\mu\text{-}O)_2}(bpg)_2]^{+}$	−430	−273	1.58
Mn^{IV}	$[Mn_2\mathbf{(\mu\text{-}O)_2}(bpg)_2]^{+}$	210	144	1.46
Mn^{III}	$[Mn_2\mathbf{(\mu\text{-}O)_2(\mu\text{-}OAc)}(dtne)]^{2+}$	−389	−278	1.40
Mn^{IV}	$[Mn_2\mathbf{(\mu\text{-}O)_2(\mu\text{-}OAc)}(dtne)]^{2+}$	207	141	1.46
Mn^{III}	$[[Mn_2\mathbf{(\mu\text{-}O)_2(\mu\text{-}OAc)}(Me_4dtne)]^{2+}$	−403	−276	1.46

Mn^{IV}	$[Mn_2(\mu\text{-}O)_2(\mu\text{-}OAc)(Me_4dtne)]^{2+}$	210	142	1.48
Mn^{III}	$[Mn_2(\mu\text{-}O)_2(\mu\text{-}OAc)(tacn)_2]^{2+}$	−386	−261	1.48
Mn^{IV}	$[Mn_2(\mu\text{-}O)_2(\mu\text{-}OAc)(tacn)_2]^{2+}$	213	143	1.49
Mn^{III}	$[Mn_2(\mu\text{-}O)_2(\mu\text{-}OAc)(tpen)]^{2+}$	−448	−280	1.60
Mn^{IV}	$[Mn_2(\mu\text{-}O)_2(\mu\text{-}OAc)(tpen)]^{2+}$	224	143	1.56
Mn^{III}	$[Mn_2(\mu\text{-}O)_2(\mu\text{-}OAc)(bpea)_2]^{2+}$	−482	−273	1.77
Mn^{IV}	$[Mn_2(\mu\text{-}O)_2(\mu\text{-}OAc)(bpea)_2]^{2+}$	241	144	1.67
			average value	**1.53**

Ligand abbreviations:

porph = porphyrine; salahe = salicylaldehydeimine-1-hydroxyethane; bpmsed = *N,N*-bis(2-pyridylmethyl)-*N´*-salicylidene-1,2-diaminoethane; bpy = 2,2´-bipyridyl; phen = 1,10-phenanthroline; bispiMe_2en = *N,N´*-dimethyl-*N,N´*-bis(2-pyridylmethyl)-1,2-diaminoethane; bisimMe_2en = *N,N´*-dimethyl-*N,N´*-bis(imidazol-4-ylmethyl))-1,2-diaminoethane; bispicen = *N,N*-bis(2-pyridylmethyl)-1,2-diaminoethane; tren = tris(2-aminoethyl)amine; bpg = *N,N*-bis(2-pyridylmethyl)glycinate; dtne = 1,2-bis(1,4,7-triazacyclonon-1-yl)ethane; Me_4dtne = 1,2-bis(4,7-dimethyl-1,4,7-triazacyclonon-1-yl)ethane; tacn = 1,4,7-triazacyclononane; tpen = *N,N,N´,N´*-tetrakis(2-pyridylmethyl)-1,2-diaminoethane; bpea = *N,N*-bis(2-pyridylmethyl)ethylamine; hCl_2salpn = *N,N´*-bis(3,5-dichlorosalicylidene)-1,3-di-amino-2-hydroxypropane.