Supporting Information for

Structural Analysis of the Mn(IV)/Fe(III) Cofactor of *Chlamydia trachomatis* Ribonucleotide Reductase by EXAFS Spectroscopy and Density Functional Theory Calculations

Jarod M. Younker, Courtney M. Krest, Wei Jiang, Carsten Krebs, J. Martin Bollinger, Jr., and Michael T. Green

Department of Chemistry and Department of Biochemistry and Molecular Biology, The Pennsylvania State University, University Park, Pennsylvania 16802

Results

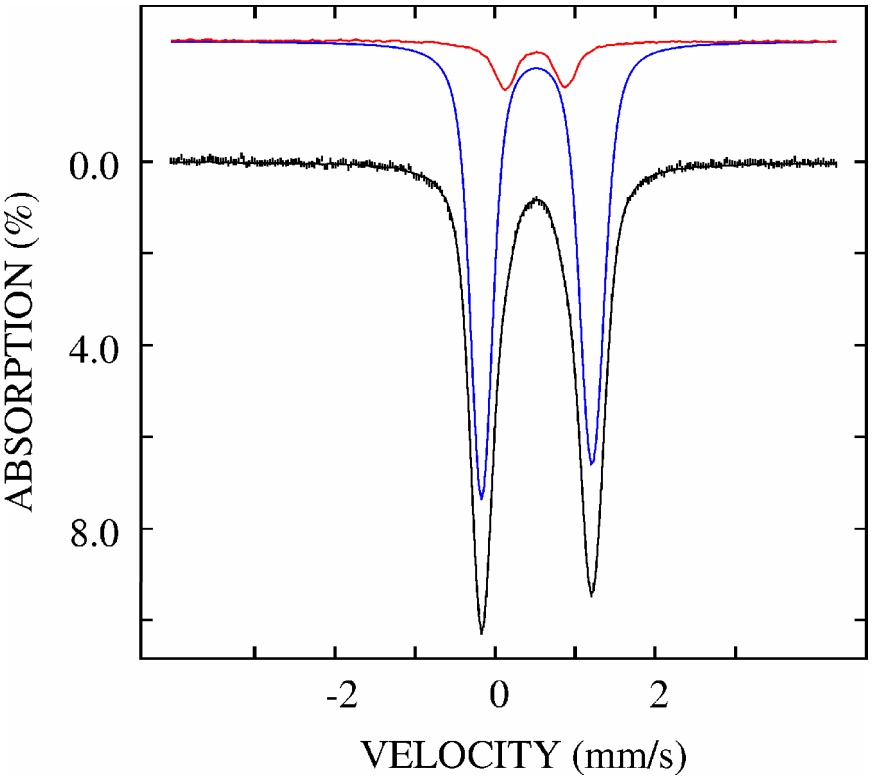

Figure S1. 4.2-K/zero-field Mössbauer spectrum of a sample of Mn^{IV}/Fe^{III} *C. trachomatis* R2, which was prepared according to the method described in the manuscript. The spectrum is analyzed as a superposition of 10% of the experimental spectrum of $Fe_2^{III/III}$-R2 (red line) and 90% of a quadrupole doublet assigned to Mn^{IV}/Fe^{III}-R2 (blue line). The parameters ($\delta = 0.52$ mm/s and $\Delta E_Q = 1.38$ mm/s) are slightly different from those previously reported for Mn^{IV}/Fe^{III}-R2 ($\delta = 0.52$ mm/s and $\Delta E_Q = 1.32$ mm/s, Jiang et al. *J. Am. Chem. Soc.* **2007**, ***129***, 7504-7505). We attribute the difference to the greater glycerol content (45% vs 10%) in the sample characterized here. A second batch of Mn^{IV}/Fe^{III}-R2 used for XAS-spectroscopic experiments had a similar composition (15% $Fe_2^{III/III}$-R2 and 85% Mn^{IV}/Fe^{III}-R2, data not shown).

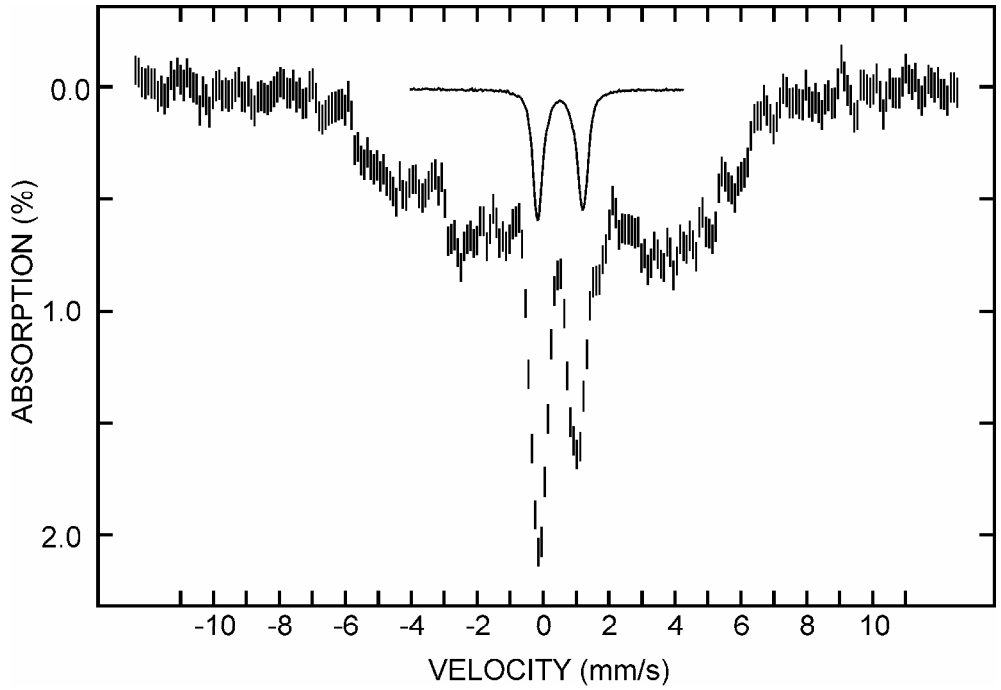

Figure S2. Mössbauer spectrum of a sample of Mn^{III}/Fe^{III} *Ct* R2 produced by treatment of the Mn^{IV}/Fe^{III} protein with excess dithionite for 2 min at room temperature. The spectrum was collected at 4.2 K without an applied magnetic field. The broad features are due to the hyperfine interaction of the ^{57}Fe nucleus with the $S = 1/2$ ground state of the cluster, which arises from antiferromagnetic coupling of its Mn^{III} ($S_{Mn} = 2$) and Fe^{III} ($S_{Fe} = 5/2$) constituents. The Mn^{IV}/Fe^{III} complex gives rise to a sharp quadrupole doublet under these conditions. We estimate an upper limit of 6% of the total Fe intensity for the Mn^{IV}/Fe^{III} complex (solid line).

Table S1. Results of fitting Mn *K*-edge EXAFS data for Mn^{IV}/Fe^{III}-R2. Scale factor S_0=0.8. Best fits for each coordination number are shown in bold. Fits with negative and unusually large Debye-Waller factors are shown in red and blue, respectively. Fits were performed over the region k = 1–11.6 $Å^{-1}$. Number of scatterers *N*, inter-atomic distance *R* (Å), mean-square deviation in *R*, σ^2 ($Å^2$), and the threshold energy shift E_0 (eV) are listed. The fit-error *F* is defined as $(\Sigma k^6(\chi_{exptl} - \chi_{calc})^2/\Sigma k^6\chi_{exptl}^2)^{1/2}$.

		Mn-O			*Mn-O/N*			*Mn-Fe*			
S_0	*N*	*R*	σ^2	*N*	*R*	σ^2	*N*	*R*	σ^2	E_0	*F*
0.8	**1.00**	**1.787(7)**	**0.0043**	**3.00**	**1.959(3)**	**0.0017**	**1.00**	**2.911(3)**	**0.0015**	**-2.893**	**0.2511**
	2.00	1.857(8)	0.0104	2.00	1.959(3)	0.0005	1.00	2.910(3)	0.0016	-3.234	0.2546
	3.00	1.908(8)	0.0118	1.00	1.971(3)	-0.0021	1.00	2.912(3)	0.0015	-2.972	0.2554
	0.00	-	-	4.00	1.961(3)	0.0057	1.00	2.921(3)	0.0015	0.102	0.3174
	1.00	**1.738(6)**	**0.0033**	**4.00**	**1.945(3)**	**0.0038**	**1.00**	**2.907(2)**	**0.0014**	**-3.829**	**0.2374**
	2.00	1.801(6)	0.0103	3.00	1.960(2)	0.0022	1.00	2.905(3)	0.0015	-4.405	0.2409
	3.00	1.853(7)	0.0154	2.00	1.964(3)	0.0007	1.00	2.905(3)	0.0015	-4.428	0.2410
	4.00	1.904(7)	0.0159	1.00	1.966(3)	-0.0022	1.00	2.909(3)	0.0015	-3.646	0.2411
	0.00	-	-	5.00	1.956(4)	0.0081	1.00	2.916(3)	0.0014	-0.702	0.3628
	1.00	**1.708(5)**	**0.0025**	**5.00**	**1.935(3)**	**0.0060**	**1.00**	**2.904(2)**	**0.0013**	**-4.485**	**0.2463**
	2.00	1.756(5)	0.0091	4.00	1.951(2)	0.0037	1.00	2.901(2)	0.0015	-5.173	0.2440
	3.00	1.800(3)	0.0152	3.00	1.957(2)	0.0025	1.00	2.899(3)	0.0015	-5.664	0.2437
	4.00	1.848(7)	0.0200	2.00	1.959(2)	0.0084	1.00	2.901(3)	0.0015	-5.232	0.2411
	5.00	1.899(7)	0.0197	1.00	1.962(2)	-0.0023	1.00	2.907(3)	0.0014	-4.366	0.2419
	0.00	-	-	6.00	1.951(4)	0.0106	1.00	2.911(4)	0.0014	-1.575	0.4163
	1.00	1.688(4)	0.0018	6.00	1.927(3)	0.0081	1.00	2.901(3)	0.0012	-5.123	0.2733
	2.00	**1.727(5)**	**0.0079**	**5.00**	**1.941(3)**	**0.0053**	**1.00**	**2.898(2)**	**0.0014**	**-5.919**	**0.2624**
	3.00	1.762(6)	0.0139	4.00	1.950(2)	0.0040	1.00	2.895(2)	0.0015	-6.440	0.2577
	4.00	1.797(6)	0.0197	3.00	1.954(2)	0.0028	1.00	2.895(3)	0.0015	-6.602	0.2539
	5.00	1.842(7)	0.0243	2.00	1.956(2)	0.0009	1.00	2.898(3)	0.0027	-5.969	0.2491
	6.00	1.891(7)	0.0231	1.00	1.959(2)	-0.0023	1.00	2.904(3)	0.0014	-5.110	0.2520
	0.00	-	-	7.00	1.951(4)	0.0106	1.00	2.912(4)	0.0014	-1.470	0.4164
range		1.71-1.79			1.94-1.96			2.90-2.91			
best	1.00	1.738(6)	0.0033	4.00	1.945(3)	0.0038	1.00	2.907(2)	0.0014	-3.829	0.2374

Table S2. Results of fitting Mn *K*-edge EXAFS data for Mn^{IV}/Fe^{III}-R2. Scale factor S_0=0.9. Best fits for each coordination number are shown in bold. Fits with negative and unusually large Debye-Waller factors are shown in red and blue, respectively. Fits were performed over the region k = 1–11.6 $Å^{-1}$. Number of scatterers *N*, inter-atomic distance *R* (Å), mean-square deviation in *R*, σ^2 ($Å^2$), and the threshold energy shift E_0 (eV) are listed. The fit-error *F* is defined as $(\Sigma k^6(\chi_{exptl} - \chi_{calc})^2/\Sigma k^6\chi_{exptl}^2)^{1/2}$.

	Mn-O			*Mn-O/N*			*Mn-Fe*				
S_0	*N*	*R*	σ^2	*N*	*R*	σ^2	*N*	*R*	σ^2	E_0	*F*
0.9	**1.00**	**1.698(4)**	**0.0028**	**5.00**	**1.931(3)**	**0.0071**	**1.00**	**2.902(2)**	**0.0019**	**-5.058**	**0.2635**
	2.00	1.745(5)	0.0097	4.00	1.947(3)	0.0045	1.00	2.898(2)	0.0021	-5.804	0.2551
	3.00	1.785(6)	0.0164	3.00	1.954(2)	0.0032	1.00	2.896(3)	0.0021	-6.284	0.2515
	4.00	1.832(7)	0.0224	2.00	1.957(2)	0.0015	1.00	2.898(3)	0.0021	-5.940	0.2470
	5.00	1.887(7)	0.0230	1.00	1.960(2)	-0.0018	1.00	2.904(3)	0.0020	-4.968	0.2470
	0.00	-	-	6.00	1.946(5)	0.0126	1.00	2.908(4)	0.0020	-2.190	0.4537
	1.00	**1.726(5)**	**0.0037**	**4.00**	**1.941(3)**	**0.0047**	**1.00**	**2.905(2)**	**0.0020**	**-4.337**	**0.2400**
	2.00	1.786(6)	0.0112	3.00	1.957(2)	0.0028	1.00	2.902(2)	0.0021	-4.956	0.2406
	3.00	1.837(7)	0.0173	2.00	1.961(2)	0.0013	1.00	2.902(3)	0.0021	-5.074	0.2396
	4.00	1.895(7)	0.0185	1.00	1.964(2)	-0.0017	1.00	2.907(3)	0.0021	-4.158	0.2391
	0.00	-	-	5.00	1.953(4)	0.0097	1.00	2.914(3)	0.0020	-1.198	0.3954
	1.00	**1.773(7)**	**0.0049**	**3.00**	**1.956(3)**	**0.0025**	**1.00**	**2.909(3)**	**0.0022**	**-3.347**	**0.2414**
	2.00	1.845(7)	0.0123	2.00	1.967(3)	0.0011	1.00	2.908(3)	0.0022	-3.619	0.2449
	3.00	1.899(7)	0.0140	1.00	1.968(3)	-0.0017	1.00	2.910(3)	0.0021	-3.459	0.2449
	0.00	-	-	4.00	1.959(3)	0.0069	1.00	2.919(3)	0.0021	-0.257	0.3371
	1.00	1.680(4)	0.0023	6.00	1.923(3)	0.0093	1.00	2.898(3)	0.0018	-5.745	0.3131
	2.00	**1.715(5)**	**0.0085**	**5.00**	**1.937(3)**	**0.0062**	**1.00**	**2.894(3)**	**0.0020**	**-6.555**	**0.2840**
	3.00	1.749(5)	0.0148	4.00	1.947(3)	0.0048	1.00	2.892(3)	0.0026	-7.055	0.2745
	4.00	1.781(6)	0.0213	3.00	1.951(2)	0.0035	1.00	2.892(3)	0.0021	-7.277	0.2677
	5.00	1.826(7)	0.0273	2.00	1.953(2)	0.0016	1.00	2.895(3)	0.0020	-6.606	0.2602
	6.00	1.880(7)	0.0265	1.00	1.956(2)	-0.0018	1.00	2.901(3)	0.0020	-5.679	0.2626
	0.00	-	-	7.00	1.936(7)	0.0161	1.00	2.903(5)	0.0020	-3.356	0.5035
range		1.70-1.77			1.93-1.96			2.89-2.91			
best	1.00	1.726(5)	0.0037	4.00	1.941(3)	0.0047	1.00	2.905(2)	0.0020	-4.337	0.2400

Table S3. Results of fitting Mn *K*-edge EXAFS data for Mn^{IV}/Fe^{III}-R2. Scale factor S_0=1.0. Best fits for each coordination number are shown in bold. Fits with negative and unusually large Debye-Waller factors are shown in red and blue, respectively. Fits were performed over the region k = 1–11.6 $Å^{-1}$. Number of scatterers *N*, inter-atomic distance *R* (Å), mean-square deviation in *R*, σ^2 ($Å^2$), and the threshold energy shift E_0 (eV) are listed. The fit-error *F* is defined as $(\Sigma k^6(\chi_{exptl} - \chi_{calc})^2/\Sigma k^6\chi_{exptl}^2)^{1/2}$.

	Mn-O			*Mn-O/N*			*Mn-Fe*				
S_0	*N*	*R*	σ^2	*N*	*R*	σ^2	*N*	*R*	σ^2	E_0	*F*
1.0	**1.00**	**1.690(4)**	**0.0032**	**5.00**	**1.928(3)**	**0.0081**	**1.00**	**2.899(3)**	**0.0025**	**-5.552**	**0.2874**
	2.00	1.733(5)	0.0100	4.00	1.943(3)	0.0053	1.00	2.895(3)	0.0026	-6.400	0.2720
	3.00	1.771(6)	0.0177	3.00	1.951(2)	0.0039	1.00	2.893(3)	0.0027	-6.865	0.2648
	4.00	1.817(7)	0.0245	2.00	1.954(2)	0.0020	1.00	2.895(3)	0.0026	-6.566	0.2577
	5.00	1.878(7)	0.0256	1.00	1.958(2)	-0.0013	1.00	2.901(3)	0.0026	-5.501	0.2568
	0.00	-	-	6.00	1.940(6)	0.0150	1.00	2.905(4)	0.0026	-2.931	0.4880
	1.00	**1.716(5)**	**0.0040**	**4.00**	**1.937(3)**	**0.0056**	**1.00**	**2.903(2)**	**0.0026**	**-4.824**	**0.2508**
	2.00	1.773(6)	0.0120	3.00	1.954(2)	0.0035	1.00	2.900(2)	0.0027	-5.450	0.2470
	3.00	1.823(6)	0.0189	2.00	1.959(2)	0.0019	1.00	2.899(3)	0.0027	-5.696	0.2442
	4.00	1.886(7)	0.0211	1.00	1.962(2)	-0.0013	1.00	2.904(3)	0.0027	-4.680	0.2426
	0.00	-	-	5.00	1.949(5)	0.0113	1.00	2.911(4)	0.0026	-1.739	0.4286
	1.00	**1.758(6)**	**0.0053**	**3.00**	**1.951(3)**	**0.0032**	**1.00**	**2.907(2)**	**0.0027**	**-3.892**	**0.2387**
	2.00	1.829(7)	0.0132	2.00	1.964(2)	0.0016	1.00	2.905(3)	0.0028	-4.250	0.2411
	3.00	1.893(7)	0.0161	1.00	1.967(3)	-0.0012	1.00	2.908(3)	0.0027	-3.793	0.2406
	0.00	-	-	4.00	1.957(4)	0.0081	1.00	2.917(3)	0.0026	-0.634	0.3623
	1.00	1.673(4)	0.0028	6.00	1.920(4)	0.0105	1.00	2.895(3)	0.0024	-6.316	0.3367
	2.00	**1.705(5)**	**0.0090**	**5.00**	**1.933(3)**	**0.0071**	**1.00**	**2.891(3)**	**0.0025**	**-7.159**	**0.3101**
	3.00	1.736(6)	0.0157	4.00	1.944(2)	0.0055	1.00	2.889(3)	0.0026	-7.676	0.2956
	4.00	1.767(6)	0.0228	3.00	1.948(2)	0.0042	1.00	2.889(3)	0.0026	-7.888	0.2852
	5.00	1.811(8)	0.0300	2.00	1.950(2)	0.0022	1.00	2.892(3)	0.0026	-7.229	0.2747
	6.00	1.870(8)	0.0299	1.00	1.954(2)	-0.0013	1.00	2.898(3)	0.0026	-6.197	0.2759
	0.00	-	-	7.00	1.927(8)	0.0189	1.00	2.899(5)	0.0025	-4.329	0.5358
range		1.69-1.76			1.93-1.95			2.89-2.91			
best	1.00	1.758(6)	0.0053	3.00	1.951(3)	0.0032	1.00	2.907(2)	0.0027	-3.892	0.2387

Table S4. Results of fitting Fe *K*-edge EXAFS data for Mn^{IV}/Fe^{III}-R2. Scale factor S_0=0.8. Best fits for each coordination number are shown in bold. Fits with negative and unusually large Debye-Waller factors are shown in red and blue, respectively. Fits were performed over the region k = 1–11.6 $Å^{-1}$. Number of scatterers *N*, inter-atomic distance *R* (Å), mean-square deviation in *R*, σ^2 ($Å^2$), and the threshold energy shift E_0 (eV) are listed. The fit-error *F* is defined as $(\Sigma k^6(\chi_{exptl} - \chi_{calc})^2/\Sigma k^6\chi_{exptl}^2)^{1/2}$.

		Fe-O			*Fe-O/N*			*Fe-Mn*			
S_0	*N*	*R*	σ^2	*N*	*R*	σ^2	*N*	*R*	σ^2	E_0	*F*
0.8	1.00	1.912(5)	-0.0039	3.00	2.059(5)	0.0005	1.00	2.930(5)	0.0034	-2.057	0.3526
	2.00	1.945(5)	-0.0018	2.00	2.093(5)	-0.0025	1.00	2.926(6)	0.0032	-2.792	0.3548
	3.00	1.976(5)	0.0010	1.00	2.124(5)	-0.0047	1.00	2.923(5)	0.0030	-3.410	0.3515
	0.00	**-**	**-**	**4.00**	**2.015(5)**	**0.0075**	**1.00**	**2.939(7)**	**0.0043**	**-1.520**	**0.4031**
	1.00	1.903(4)	-0.0024	4.00	2.051(4)	0.0033	1.00	2.931(4)	0.0035	-2.193	0.2952
	2.00	1.930(4)	-0.0007	3.00	2.080(4)	0.0004	1.00	2.927(4)	0.0033	-2.725	0.2963
	3.00	1.956(4)	0.0012	2.00	2.106(4)	-0.0015	1.00	2.924(4)	0.0032	-3.289	0.2952
	4.00	1.979(4)	0.0037	1.00	2.128(5)	-0.0035	1.00	2.921(4)	0.0031	-3.900	0.2915
	0.00	**-**	**-**	**5.00**	**2.012(4)**	**0.0092**	**1.00**	**2.936(5)**	**0.0042**	**-2.048**	**0.3401**
	1.00	1.894(5)	-0.0009	5.00	2.043(4)	0.0058	1.00	2.930(4)	0.0036	-2.621	0.2628
	2.00	1.917(4)	0.0007	4.00	2.067(4)	0.0031	1.00	2.927(4)	0.0035	-3.097	0.2612
	3.00	**1.941(4)**	**0.0020**	**3.00**	**2.091(4)**	**0.0012**	**1.00**	**2.925(4)**	**0.0034**	**-3.402**	**0.2596**
	4.00	1.962(4)	0.0038	2.00	2.112(4)	-0.0003	1.00	2.923(4)	0.0033	-3.861	0.2570
	5.00	1.979(3)	0.0060	1.00	2.129(4)	-0.0024	1.00	2.919(4)	0.0032	-4.456	0.2541
	0.00	-	-	6.00	2.009(4)	0.0108	1.00	2.933(5)	0.0041	-2.638	0.2990
	1.00	1.885(6)	0.0008	6.00	2.034(4)	0.0081	1.00	2.927(4)	0.0038	-3.227	0.2542
	2.00	1.906(4)	0.0024	5.00	2.055(4)	0.0058	1.00	2.925(4)	0.0037	-3.533	0.2494
	3.00	1.927(4)	0.0034	4.00	2.077(4)	0.0039	1.00	2.924(4)	0.0036	-3.741	0.2459
	4.00	1.947(4)	0.0046	3.00	2.097(4)	0.0024	1.00	2.923(4)	0.0035	-4.020	0.2432
	5.00	**1.964(3)**	**0.0062**	**2.00**	**2.114(4)**	**0.0011**	**1.00**	**2.921(4)**	**0.0034**	**-4.419**	**0.2406**
	6.00	1.979(3)	0.0082	1.00	2.129(4)	-0.0012	1.00	2.918(4)	0.0033	-4.936	0.2386
	0.00	-	-	7.00	2.005(4)	0.0124	1.00	2.929(4)	0.0040	-3.256	0.2800
range		1.94-1.96			2.01-2.11			2.92-2.94			
best	**5.00**	**1.964(3)**	**0.0062**	**2.00**	**2.114(4)**	**0.0011**	**1.00**	**2.921(4)**	**0.0034**	**-4.419**	**0.2406**

Table S5. Results of fitting Fe *K*-edge EXAFS data for Mn^{IV}/Fe^{III}-R2. Scale factor S_0=0.9. Best fits for each coordination number are shown in bold. Fits with negative and unusually large Debye-Waller factors are shown in red and blue, respectively. Fits were performed over the region k = 1–11.6 $Å^{-1}$. Number of scatterers *N*, inter-atomic distance *R* (Å), mean-square deviation in *R*, σ^2 ($Å^2$), and the threshold energy shift E_0 (eV) are listed. The fit-error *F* is defined as $(\Sigma k^6(\chi_{exptl} - \chi_{calc})^2/\Sigma k^6\chi_{exptl}^2)^{1/2}$.

	Fe-O			*Fe-O/N*			*Fe-Mn*				
S_0	*N*	*R*	σ^2	*N*	*R*	σ^2	*N*	*R*	σ^2	E_0	*F*
0.9	1.00	1.910(5)	-0.0028	3.00	2.058(4)	0.0015	1.00	2.930(5)	0.0041	-2.235	0.3179
	2.00	1.944(4)	-0.0007	2.00	2.093(4)	-0.0014	1.00	2.926(5)	0.0039	-2.933	0.3198
	3.00	1.975(4)	0.0021	1	2.123(5)	-0.0037	1.00	2.923(5)	0.0038	-3.570	0.3166
	0.00	**-**	**-**	**4.00**	**2.014(5)**	**0.0084**	**1.00**	**2.938(6)**	**0.0049**	**-1.747**	**0.3647**
	1.00	1.900(4)	-0.0011	4.00	2.049(4)	0.0049	1.00	2.930(4)	0.0042	-2.532	0.2675
	2.00	**1.928(4)**	**0.0005**	**3.00**	**2.078(4)**	**0.0016**	**1.00**	**2.927(4)**	**0.0041**	**-2.996**	**0.2672**
	3.00	1.954(4)	0.0024	2.00	2.104(4)	-0.0003	1.00	2.924(4)	0.0040	-3.533	0.2656
	4.00	1.978(4)	0.0049	1.00	2.127(4)	-0.0023	1.00	2.922(4)	0.0039	-4.097	0.2620
	0.00	-	-	5.00	2.012(4)	0.0102	1.00	2.936(5)	0.0049	-2.176	0.3065
	1.00	1.890(5)	0.0007	5.00	2.039(4)	0.0072	1.00	2.928(4)	0.0044	-3.097	0.2484
	2.00	1.915(4)	0.0021	4.00	2.064(4)	0.0045	1.00	2.926(4)	0.0042	-3.397	0.2442
	3.00	1.938(4)	0.0035	3.00	2.088(4)	0.0027	1.00	2.924(4)	0.0042	-3.739	0.2414
	4.00	**1.959(3)**	**0.0053**	**2.00**	**2.109(4)**	**0.0012**	**1.00**	**2.922(4)**	**0.0041**	**-4.198**	**0.2386**
	5.00	1.977(3)	0.0075	1.00	2.126(5)	-0.0009	1.00	2.919(4)	0.0040	-4.803	0.2361
	0.00	-	-	6.00	2.006(4)	0.0120	1.00	2.931(4)	0.0048	-3.015	0.2771
	1.00	1.877(6)	0.0025	6.00	2.029(4)	0.0094	1.00	2.925(4)	0.0045	-3.872	0.2554
	2.00	1.897(5)	0.0043	5.00	2.048(4)	0.0071	1.00	2.922(4)	0.0045	-4.295	0.2488
	3.00	1.924(4)	0.0050	4.00	2.073(4)	0.0053	1.00	2.923(4)	0.0043	-4.184	0.2426
	4.00	1.942(4)	0.0066	3.00	2.089(5)	0.0042	1.00	2.920(4)	0.0043	-4.678	0.2397
	5.00	**1.958(4)**	**0.0081**	**2.00**	**2.105(5)**	**0.0028**	**1.00**	**2.917(4)**	**0.0043**	**-5.165**	**0.2375**
	6.00	1.976(3)	0.0098	1.00	2.123(5)	0.0005	1.00	2.916(4)	0.0041	-5.359	0.2354
	0.00	-	-	7.00	2.001(4)	0.0137	1.00	2.927(4)	0.0046	-3.737	0.2738
range		1.93-1.96			2.01-2.11			2.92-2.94			
best	**5.00**	**1.958(4)**	**0.0081**	**2.00**	**2.105(5)**	**0.0028**	**1.00**	**2.917(4)**	**0.0043**	**-5.165**	**0.2375**

Table S6. Results of fitting Fe *K*-edge EXAFS data for Mn^{IV}/Fe^{III}-R2. Scale factor S_0=1.0. Best fits for each coordination number are shown in bold. Fits with negative and unusually large Debye-Waller factors are shown in red and blue, respectively. Fits were performed over the region k = 1–11.6 $Å^{-1}$. Number of scatterers *N*, inter-atomic distance *R* (Å), mean-square deviation in *R*, σ^2 ($Å^2$), and the threshold energy shift E_0 (eV) are listed. The fit-error *F* is defined as $(\Sigma k^6(\chi_{exptl} - \chi_{calc})^2/\Sigma k^6\chi_{exptl}^2)^{1/2}$.

		Fe-O			*Fe-O/N*			*Fe-Mn*			
S_0	*N*	*R*	σ^2	*N*	*R*	σ^2	*N*	*R*	σ^2	E_0	*F*
1.0	1.00	1.909(4)	-0.0017	3.00	2.057(4)	0.0025	1.00	2.931(4)	0.0048	-2.405	0.2890
	2.00	1.942(4)	0.0003	2.00	2.091(4)	-0.0004	1.00	2.926(4)	0.0046	-3.103	0.2903
	3.00	1.973(4)	0.0031	1.00	2.122(4)	-0.0027	1.00	2.923(4)	0.0045	-3.741	0.2870
	0.00	**-**	**-**	**4.00**	**2.013(4)**	**0.0092**	**1.00**	**2.937(5)**	**0.0054**	**-1.987**	**0.3318**
	1.00	1.896(4)	0.0001	4.00	2.046(4)	0.0056	1.00	2.929(4)	0.0049	-2.931	0.2490
	2.00	1.926(4)	0.0018	3.00	2.075(4)	0.0029	1.00	2.926(4)	0.0048	-3.319	0.2468
	3.00	**1.953(3)**	**0.0036**	**2.00**	**2.102(4)**	**0.0009**	**1.00**	**2.924(4)**	**0.0047**	**-3.789**	**0.2445**
	4.00	1.976(3)	0.0061	1.00	2.124(4)	-0.0011	1.00	2.921(4)	0.0046	-4.376	0.2411
	0.00	-	-	5.00	2.008(4)	0.0112	1.00	2.933(4)	0.0053	-2.740	0.2826
	1.00	1.884(6)	0.0025	5.00	2.034(4)	0.0085	1.00	2.926(4)	0.0051	-3.665	0.2455
	2.00	1.910(4)	0.0038	4.00	2.059(4)	0.0059	1.00	2.923(4)	0.0050	-3.960	0.2388
	3.00	1.936(4)	0.0049	3.00	2.085(4)	0.0040	1.00	2.923(4)	0.0049	-4.130	0.2344
	4.00	**1.957(4)**	**0.0068**	**2.00**	**2.105(4)**	**0.0027**	**1.00**	**2.921(3)**	**0.0048**	**-4.530**	**0.2314**
	5.00	1.975(3)	0.0089	1.00	2.122(5)	0.0004	1.00	2.918(3)	0.0047	-5.106	0.2293
	0.00	-	-	6.00	2.003(3)	0.0132	1.00	2.928(4)	0.0052	-3.543	0.2681
	1.00	1.869(9)	0.0049	6.00	2.024(4)	0.0109	1.00	2.923(4)	0.0051	-4.314	0.2655
	2.00	1.892(6)	0.0064	5.00	2.042(4)	0.0087	1.00	2.920(4)	0.0051	-4.812	0.2573
	3.00	1.916(5)	0.0071	4.00	2.063(5)	0.0070	1.00	2.918(4)	0.0050	-5.068	0.2511
	4.00	**1.935(5)**	**0.0086**	**3.00**	**2.079(5)**	**0.0058**	**1.00**	**2.916(4)**	**0.0050**	**-5.497**	**0.2478**
	5.00	1.953(4)	0.0099	2.00	2.096(6)	0.0044	1.00	2.914(4)	0.0049	-5.772	0.2453
	6.00	1.972(4)	0.0116	1.00	2.115(7)	0.0022	1.00	2.914(4)	0.0049	-5.834	0.2433
	0.00	-	-	7.00	1.997(4)	0.0150	1.00	2.924(4)	0.0051	-4.373	0.2816
range		1.94-1.96			2.01-2.11			2.92-2.94			
best	**4.00**	**1.957(4)**	**0.0068**	**2.00**	**2.105(4)**	**0.0027**	**1.00**	**2.921(3)**	**0.0048**	**-4.530**	**0.2314**

Table S7. Results of fitting the Mn *K*-edge Fourier-filtered EXAFS data. Fits were performed over the region k = 1–11.6 Å^{-1}. Number of scatterers *N*, interatomic distance *R* (Å), mean-square deviation in *R*, σ^2 (Å^2), and the threshold energy shift E_0 (eV) are given. Metal coordination number was constrained to the value obtained from best fits of the raw data.

	Mn-O			*Mn-O/N*			
S_0	*N*	*R*	σ^2	*N*	*R*	σ^2	E_0
0.8	0.00	-	-	5.00	1.964(4)	0.0083	-0.006
	1.00	1.758(3)	0.0023	4.00	1.954(2)	0.0036	-3.626

Table S8. Results of fitting the Fe *K*-edge Fourier-filtered EXAFS data. Fits were performed over the region k = 1–11.6 Å^{-1}. Number of scatterers *N*, interatomic distance *R* (Å), mean-square deviation in *R*, σ^2 (Å^2), and the threshold energy shift E_0 (eV) are given. Metal coordination number was constrained to the value obtained from best fits of the raw data.

	Fe-O			*Fe-O/N*			
S_0	*N*	*R*	s^2	*N*	*R*	s^2	E_0
1.0	0.00	-	-	6.00	2.006(3)	0.0120	-3.608
	4.00	1.952(3)	0.0068	2.00	2.092(4)	0.0027	-5.176

Figure S3. Photoreduction of Mn(IV)/Fe(III) sample. **A)** Mn(IV)/Fe(III) second-scan data was fit to a linear combination of Mn(IV)/Fe(III) and Mn(III)/Fe(III) *Ct*-R2 first-scan data. Best fit indicates sample was 27% reduced after first-scan. **B)** Exposure time at second scan edge is 870 seconds. Assuming that reduction is linear with exposure time, photoreduction of the first-scan at k=8 (365.7 s) is 11%. **C)** Mn *K*-edge EXAFS data (left) and Fourier transform (right) for the Mn(IV)/Fe(III) complex of *Ct* R2 from k = 3.5–8 Å^{-1}. Arrow designates contributions resulting from metal backscattering. Values from the fit are given in Table S9.

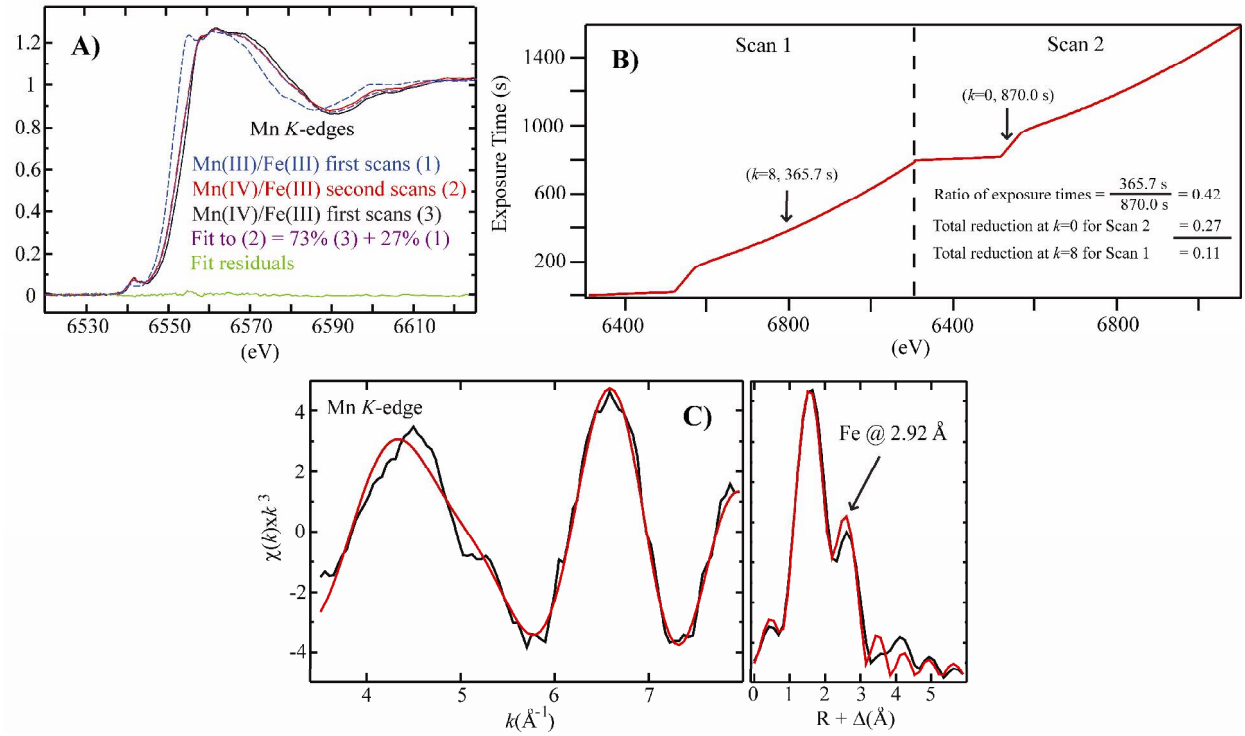

Table S9. Fit for Mn(IV)/Fe(III) *Ct* R2 data over the region k = 3.5–8 Å^{-1}. Number of scatterers N, inter-atomic distance R (Å), mean-square deviation in R, σ^2 (Å^2), and the threshold energy shift E_0 (eV) are listed. The fit-error F is defined as $(\Sigma k^6(\chi_{exptl} - \chi_{calc})^2/\Sigma k^6 \chi_{exptl}^2)^{1/2}$. N was constrained during fit.

		Fe-O/N			*Fe-Mn*			
S_0	N	R	σ^2	N	R	σ^2	E_0	F
0.9	4	1.948(5)	0.0091	1	2.919(6)	0.0005	-1.214	0.1933

Figure S4. Model for *Ct* R2 Mn(IV)/Fe(III) cofactor (with metals M1 and M2), [(2,2'-bipyridine)$_2$Mn(III)(μ-O)$_2$Mn(IV)(2,2'-bipyridine)$_2$]$^{3+}$ **(1)** (*J. Am. Chem. Soc.* **1972**, *94*, 2121-2222), [LFe(III)(μ-O)$_2$Fe(IV)L]$^{3+}$ **(2)** with L = *tris*-(5-ethyl-2-pyridylmethyl)amine (*J. Am. Chem. Soc.* **1999**, *121*, 5230-5237), [L'Fe(IV)(μ-O)$_2$Fe(IV)L']$^{4+}$ **(3)** with L' = *tris*-(3,5-methyl-4-methoxy-2-pyridylmethyl)amine (*Proc. Nat. Acad. Sci. USA* **2007**, *104*, 20713-20718), [L"Mn(III)μ-(OCH$_3$)μ-1,3-(CH$_3$COO)(OHCH$_3$)Mn(III)L"]$^{+}$ **(4)** with L" = 1,5-bis(salicylideneamino)-3-pentanol (*Z. Naturforsch* **1988**, *43b*, 472-474), and [L'"Mn(IV)(μ-O)$_2$μ-1,3-(CH$_3$COO)Mn(III)L'"]$^{2+}$ **(5)** with L'" = *N*,*N*-bis(2-pyridylmethyl)ethylamine (*Inorg. Chem.* **1995**, *34*, 4708-4715). Hydrogens have been omitted.

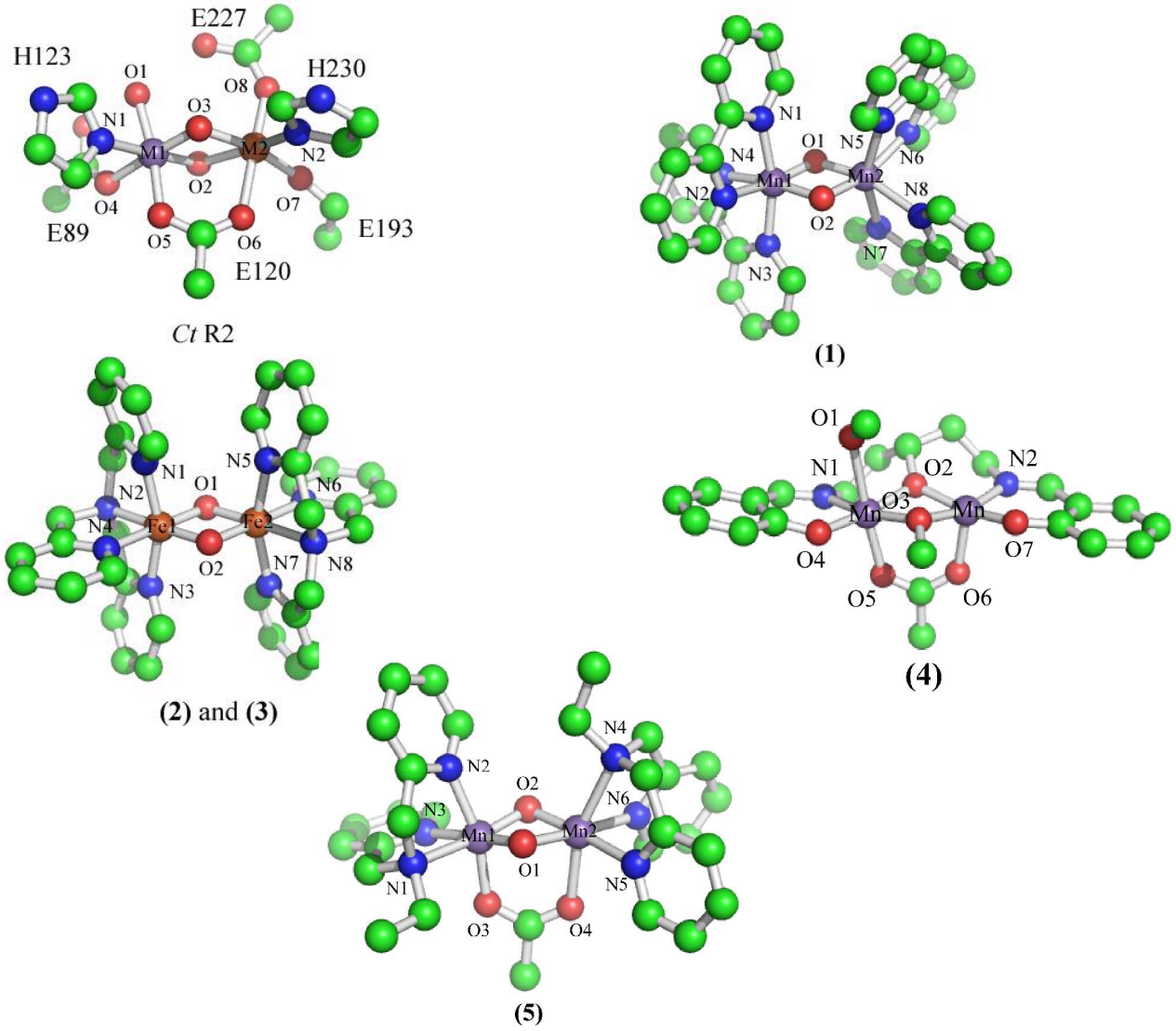

Figure S5. Selected experimental and theoretical bond distances for [(2,2'-bipyridine)$_2$Mn(III)(μ-O)$_2$Mn(IV)(2,2'-bipyridine)$_2$]$^{3+}$ **(1)** (*J. Am. Chem. Soc.* **1972**, *94*, 2121-2222), [LFe(III)(μ-O)$_2$Fe(IV)L]$^{3+}$ **(2)** with L = *tris*-(5-ethyl-2-pyridylmethyl)amine .(*J. Am. Chem. Soc.* **1999**, *121*, 5230-5237), [L'Fe(IV)(μ-O)$_2$Fe(IV)L']$^{4+}$ **(3)** with L' = *tris*-(3,5-methyl-4-methoxy-2-pyridylmethyl)amine (*Proc. Nat. Acad. Sci. USA* **2007**, *104*, 20713-20718), [L"Mn(III)μ-(OCH$_3$)μ-1,3-(CH$_3$COO)(OHCH$_3$)Mn(III)L"]$^{+}$ **(4)** with L" = 1,5-bis(salicylideneamino)-3-pentanol (*Z. Naturforsch* **1988**, *43b*, 472-474), and [L'"Mn(IV)(μ-O)$_2$μ-1,3-(CH$_3$COO)Mn(III)L'"]$^{2+}$ **(5)** with L'" = *N*,*N*-bis(2-pyridylmethyl)ethylamine (*Inorg. Chem.* **1995**, *34*, 4708-4715). Calculations with the BP86 functional employed the TZP basis set via ADF for **(1-3)** and 6-311G* via G03 for **(4-5)**. B3LYP calculations employed 6-311G* via G03. Experimental bond distances for **(1)**, **(2)**, **(4)**, and **(5)** are from crystal structures; distances for **(3)** are from EXAFS spectroscopy (average Fe-O distance shown). A second crystal structure for **(1)**, with all Mn-O bonds ~0.03 Å longer, has been reported (*Inorg. Chem*. **1995**, *34*, 4244-4252).

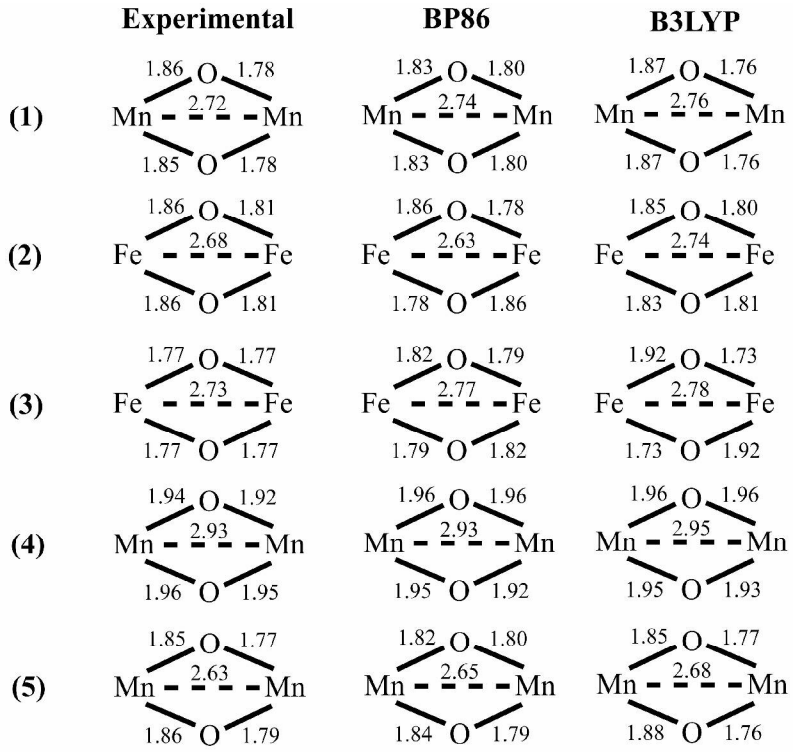

Figure S6. Selected core bond lengths for the BP86/TZP-optimized cofactor models (μ-1,3-carboxylate is omitted). Structures containing metal-metal and Mn-O distances consistent with EXAFS measurements are shown in blue (metal-metal and Mn-O distances are in red).

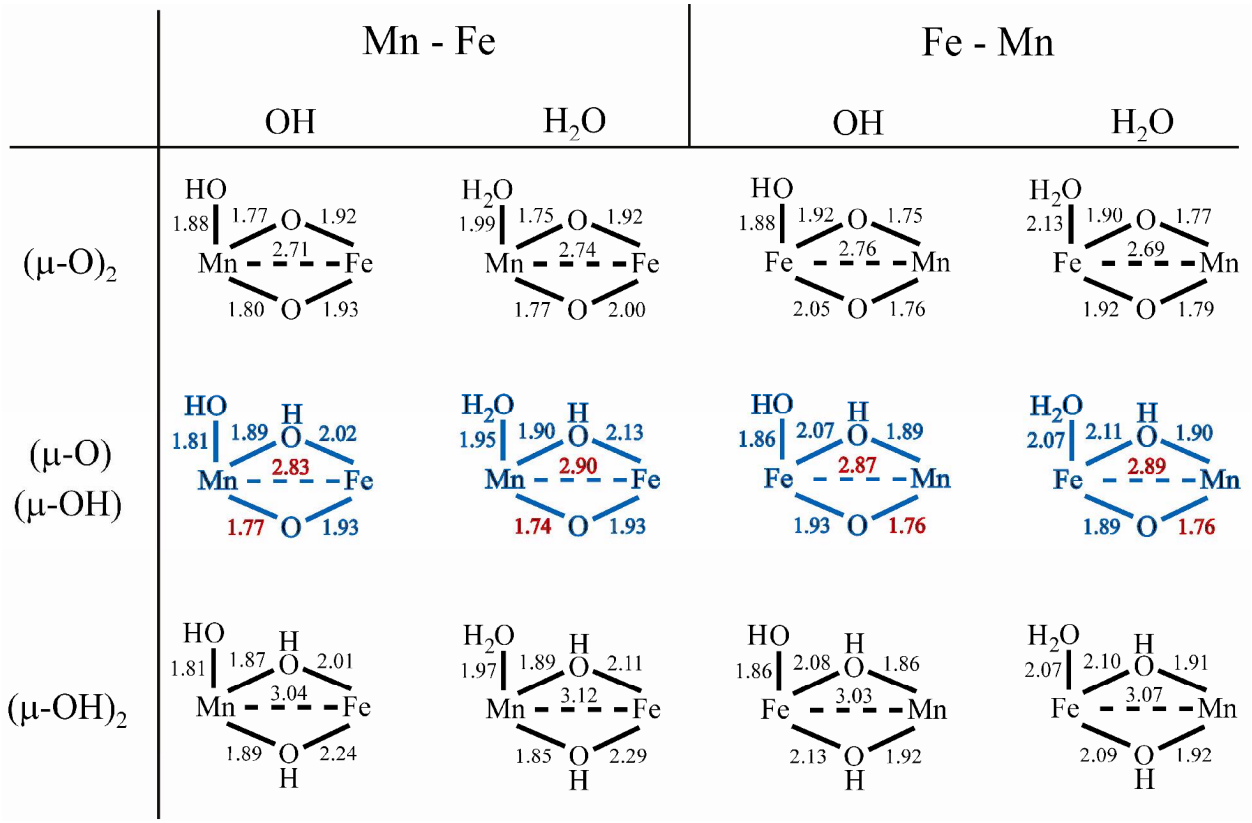

Table S10. Calculated ^{57}Fe Mössbauer and hyperfine coupling constants for the *Ct* R2 Mn(IV)/Fe(III) models with experimental Mössbauer parameters and ^{57}Fe hyperfine tensor (Jiang et al. *J. Am. Chem. Soc*. **2007** *129*, 7504-7505). Hyperfine tensors are given in MHz, where $\mathbf{A}=A_{iso}\mathbf{I}+\mathbf{T}$ and ΔT is the range of **T**. Quadrupole splittings, ΔE_Q, and isomer shifts, δ, are given in mm/s. The experimental values describing the electric field gradient tensor (ΔE_Q = 1.32 mm/s and asymmetry parameter, η, of -2.6) were rotated through the Euler angles ($0,{}^{\pi}/_{2},{}^{\pi}/_{2}$) to place them in the coordinate frame of the calculations. Isomer shifts determined with the B3LYP functional using Neese's core properties basis set and (6-311G* for Mn) (Neese, F. Inorg. Chim, Acta **2002**, *337*, 181-192).

		$^2M^1_0$				$^2M^0_0$				$^2M^1_1$			
	exp[a]	BP86		B3LYP		BP86		B3LYP		BP86		B3LYP	
	M	Mn	Fe	Mn	Fe	Mn	Fe	Mn	Fe	Mn	Fe	Mn	Fe
A_{iso}	-53.7	-22.3	-20.4	-36.1	-34.2	-25.5	-24.0	-38.7	-37.8	-22.3	-21.5	-35.5	-35.2
T1	-1.6	-2.5	-2.5	-3.0	-3.2	-1.0	-1.6	-2.0	-1.4	-1.1	-0.8	-1.9	-1.6
T2	0.2	0.8	-0.1	1.4	0.3	-0.1	0.2	0.7	-0.7	0.1	0.0	0.7	0.3
T3	1.4	1.8	2.6	1.7	2.8	1.0	1.4	1.3	2.2	1.0	0.8	1.2	1.3
Δ**T**	3.0	4.3	5.1	4.7	6.0	2.0	3.0	3.2	3.6	2.1	1.6	3.1	2.9
ΔE_q	-1.32	-1.23	-1.45	-1.20	-1.44	0.81	-0.59	1.23	1.06	-0.55	-0.59	-0.71	-0.82
η	0.11	0.24	0.71	0.10	0.29	0.99	0.96	0.85	0.89	0.50	0.14	0.32	0.50
δ	0.52	-	-	0.56	0.54	-	-	0.60	0.57	-	-	0.55	0.53

		$^1M^1_0$				$^1M^0_0$				$^1M^1_1$			
	exp[a]	BP86		B3LYP		BP86		B3LYP		BP86		B3LYP	
	M	Mn	Fe	Mn	Fe	Mn	Fe	Mn	Fe	Mn	Fe	Mn	Fe
A_{iso}	-53.7	-23.6	-20.0	-35.7	-35.0	-24.8	-21.2	-38.1	-38.2	-23.0	-19.9	-36.3	-33.1
T1	-1.6	-1.7	-1.0	-2.9	-1.2	-1.7	-1.6	-1.6	-1.1	-0.6	-1.0	-1.2	-1.3
T2	0.2	-0.6	0.0	0.6	0.5	0.3	0.3	-0.5	0.1	0.1	-0.4	0.3	0.1
T3	1.4	2.3	1.1	2.3	0.7	1.4	1.3	2.1	1.0	0.5	1.4	1.0	1.2
Δ**T**	3.0	4.0	2.1	5.2	1.9	3.1	2.9	3.7	2.1	1.1	2.4	2.2	2.5
ΔE_q	-1.32	-1.03	-1.02	-1.39	1.28	0.67	-1.11	1.10	-0.96	-0.45	-1.15	-0.38	-1.52
η	0.11	0.47	0.84	0.16	0.94	0.72	0.40	0.85	0.61	0.35	0.38	0.33	0.29
δ	0.52	-	-	0.58	0.51	-	-	0.61	0.53	-	-	0.56	0.52

Table S11. BP86/TZP-optimized coordinate for model $^{2}Mn^{1}_{0}$. The broken-symmetry structure is on the left, ferromagnetic on the right.

C	3.324958	1.901613	1.139415	C	3.333108	1.898881	1.138221
N	2.808749	1.435735	0.008187	N	2.825559	1.42639	0.005841
C	3.377785	2.147578	-1.03056	C	3.388613	2.143133	-1.03271
C	4.255672	3.06566	-0.51197	C	4.25363	3.07226	-0.51291
N	4.206255	2.894946	0.861709	N	4.202212	2.902779	0.861171
Mn	1.472778	-0.14199	-0.09739	Mn	1.482989	-0.13582	-0.10231
O	1.195409	0.360983	-1.96318	O	1.197847	0.371224	-1.96161
C	0.026525	0.498113	-2.52349	C	0.02872	0.510297	-2.52254
C	0.08139	1.026123	-3.94688	C	0.084103	1.033564	-3.94737
Fe	-1.41389	-0.30835	0.111419	Fe	-1.42748	-0.32139	0.108419
O	-1.77756	-0.9435	1.953748	O	-1.76609	-0.93732	1.970649
C	-1.15512	-1.10602	3.073912	C	-1.14425	-1.10537	3.088467
O	0.087782	-1.05362	3.26516	O	0.100242	-1.05573	3.276698
O	2.935643	-1.31643	-0.8329	O	2.943297	-1.32454	-0.83338
C	3.683564	-2.16236	-0.18933	C	3.677321	-2.17728	-0.18417
C	4.630729	-2.96772	-1.0624	C	4.637249	-2.9812	-1.04428
O	2.016758	-0.58072	1.723635	O	2.004147	-0.58627	1.711746
O	0.253991	-1.59774	-0.16767	O	0.250371	-1.57708	-0.18787
O	0.129149	0.776169	0.517481	O	0.145082	0.841392	0.521072
N	-2.6337	1.4534	0.283703	N	-2.64783	1.444251	0.287412
C	-2.20177	2.60163	0.791072	C	-2.20718	2.591424	0.791016
N	-3.21541	3.504872	0.812417	N	-3.21483	3.501719	0.808879
C	-4.34788	2.896188	0.2888	C	-4.352	2.899671	0.2881
C	-3.97084	1.617455	-0.03703	C	-3.98361	1.61727	-0.03315
O	-2.78239	-1.4719	-0.59156	O	-2.78873	-1.48835	-0.59044
C	-3.7664	-1.69948	-1.43619	C	-3.77014	-1.70951	-1.44228
C	-3.63582	-3.0047	-2.20758	C	-3.63648	-3.01084	-2.21851
O	-1.08539	0.23862	-2.00921	O	-1.08288	0.255743	-2.00626
O	-4.74062	-0.95038	-1.59174	O	-4.74027	-0.95703	-1.59705
O	3.674182	-2.35178	1.05582	O	3.644594	-2.3745	1.059578
C	-2.06119	-1.41283	4.257893	C	-2.04874	-1.41219	4.273145
H	-0.87495	0.853919	-4.44962	H	-0.87247	0.859137	-4.44934
H	0.903032	0.554047	-4.49888	H	0.905553	0.560097	-4.49882
H	0.275416	2.107975	-3.91374	H	0.277271	2.115761	-3.91742
H	5.273813	-2.28693	-1.63643	H	5.282469	-2.30051	-1.61611
H	5.241635	-3.63512	-0.44706	H	5.245503	-3.64403	-0.42071
H	4.050746	-3.55514	-1.78757	H	4.065639	-3.57472	-1.77139
H	-2.55787	-2.37764	4.083541	H	-2.55121	-2.37378	4.096256
H	-2.85007	-0.65241	4.330366	H	-2.83393	-0.64784	4.347275
H	-1.48272	-1.45763	5.186015	H	-1.47116	-1.46211	5.201735
H	1.162477	-0.81985	2.288597	H	1.149131	-0.81788	2.288448
H	2.657258	-1.4	1.595636	H	2.643435	-1.40974	1.587854
H	-2.76179	-2.9466	-2.87178	H	-2.75984	-2.95012	-2.87939
H	-4.53809	-3.18585	-2.80107	H	-4.53622	-3.19036	-2.81639
H	-3.46347	-3.83591	-1.51074	H	-3.46589	-3.84472	-1.52419

H	-4.52683	0.800796	-0.49876	H	-4.54571	0.804644	-0.49313
H	-5.29087	3.419851	0.194972	H	-5.29186	3.429283	0.193488
H	-3.15075	4.457036	1.152322	H	-3.14293	4.455036	1.144847
H	-1.19037	2.790522	1.1295	H	-1.19217	2.77167	1.125093
H	3.092788	1.521975	2.125855	H	3.097943	1.522308	2.12545
H	4.747722	3.405528	1.549582	H	4.736604	3.420243	1.549722
H	4.895162	3.801469	-0.98231	H	4.886259	3.81425	-0.98331
H	3.113453	1.93921	-2.05909	H	3.127375	1.932078	-2.06159
H	0.411926	-2.12878	-0.97214	H	0.358432	-2.0658	-1.02664

Table S12. BP86/TZP-optimized coordinate for model $^{2}Fe^{1}_{0}$. The broken-symmetry structure is on the left, ferromagnetic on the right.

Fe	1.542086	-0.12669	-0.09017	Fe	1.545992	-0.12335	-0.09019
Mn	-1.34485	-0.19951	0.043668	Mn	-1.357	-0.20055	0.041777
O	-0.02119	-1.53815	-0.23573	O	-0.02607	-1.52803	-0.23531
O	0.025692	0.723557	0.643195	O	0.021782	0.78371	0.662174
O	2.120289	-0.72623	1.803652	O	2.129286	-0.72821	1.806332
H	1.241328	-0.93525	2.269939	H	1.248834	-0.9341	2.273161
H	2.633485	-1.59975	1.578029	H	2.638446	-1.60241	1.588691
N	3.019089	1.458387	0.073489	N	3.03259	1.450061	0.065857
C	3.725043	1.684438	1.1757	C	3.736152	1.6821	1.167981
H	3.612749	1.134877	2.102719	H	3.625263	1.134177	2.09618
N	4.60967	2.692054	0.960319	N	4.611914	2.697252	0.952914
H	5.270529	3.050451	1.640429	H	5.268282	3.062076	1.63395
C	4.462408	3.127925	-0.34689	C	4.460979	3.132483	-0.35389
H	5.06526	3.92609	-0.76167	H	5.055694	3.937108	-0.76802
C	3.468471	2.348491	-0.88421	C	3.474293	2.34446	-0.89163
H	3.047057	2.352572	-1.88189	H	3.050198	2.348738	-1.88807
O	2.809756	-1.46165	-0.91851	O	2.801031	-1.47755	-0.90372
C	3.476376	-2.41976	-0.34863	C	3.477751	-2.43384	-0.33952
O	3.489102	-2.66495	0.886368	O	3.497106	-2.6806	0.893843
C	4.289719	-3.28918	-1.2927	C	4.292257	-3.2935	-1.29091
H	3.603308	-3.85209	-1.94141	H	3.60753	-3.85832	-1.93955
H	4.90607	-2.65626	-1.94492	H	4.90221	-2.65308	-1.94182
H	4.918523	-3.98706	-0.73053	H	4.927625	-3.98902	-0.73329
O	1.130528	0.641363	-1.99878	O	1.125116	0.639595	-1.99475
C	-0.05674	0.822783	-2.41798	C	-0.062	0.821489	-2.41531
O	-1.14546	0.521304	-1.81256	O	-1.14857	0.518846	-1.80661
C	-0.22249	1.466401	-3.78301	C	-0.22796	1.468405	-3.77791
H	-1.23746	1.317262	-4.1643	H	-1.24278	1.322309	-4.16061
H	-0.03478	2.545695	-3.68402	H	-0.03875	2.547073	-3.6743
H	0.520874	1.057073	-4.47758	H	0.515683	1.061433	-4.47355
O	-2.60172	-1.46481	-0.7766	O	-2.61848	-1.47324	-0.76683
C	-3.68047	-1.54692	-1.52188	C	-3.67932	-1.54299	-1.53922
O	-4.48801	-0.63952	-1.76734	O	-4.46359	-0.62357	-1.815
C	-3.87817	-2.9465	-2.10267	C	-3.8884	-2.94445	-2.11025
H	-3.73959	-3.70725	-1.32312	H	-3.74199	-3.70329	-1.33056

H	-4.87349	-3.03321	-2.55086	H	-4.8883	-3.03022	-2.54845
H	-3.11584	-3.12508	-2.87561	H	-3.13557	-3.12548	-2.89208
N	-2.56444	1.42122	0.396064	N	-2.57657	1.415301	0.3966
C	-2.16915	2.427543	1.17031	C	-2.17724	2.420072	1.171041
H	-1.19495	2.505476	1.636614	H	-1.19813	2.491157	1.628561
N	-3.16965	3.335812	1.273375	N	-3.1768	3.328574	1.275891
H	-3.12487	4.195957	1.807019	H	-3.12863	4.189169	1.808568
C	-4.24963	2.883376	0.528423	C	-4.25869	2.879216	0.531624
H	-5.17307	3.443333	0.451892	H	-5.18081	3.441424	0.455653
C	-3.85923	1.68589	-0.01571	C	-3.87155	1.681468	-0.01388
H	-4.36891	0.982156	-0.67537	H	-4.3804	0.981716	-0.67796
C	-1.32784	-1.22184	2.832293	C	-1.31166	-1.22624	2.838584
O	-1.95001	-0.89196	1.730238	O	-1.93263	-0.8901	1.736531
O	-0.10949	-1.16323	3.081253	O	-0.09406	-1.17376	3.087532
C	-2.2869	-1.75893	3.88956	C	-2.27512	-1.76108	3.893132
H	-2.58958	-2.77542	3.599307	H	-2.57775	-2.77794	3.604028
H	-1.78594	-1.79615	4.862516	H	-1.77753	-1.79719	4.867835
H	-3.1952	-1.14575	3.938376	H	-3.18295	-1.14697	3.938249
H	-0.31858	-2.11881	-0.96456	H	-0.28117	-2.09005	-0.99337

Table S13. BP86/TZP-optimized coordinate for model $^{2}Mn^{0}_{0}$. The broken-symmetry structure is on the left, ferromagnetic on the right.

Mn	1.467852	-0.15279	-0.03066	Mn	1.467083	-0.15077	-0.04111
Fe	-1.25787	-0.35287	0.125836	Fe	-1.25769	-0.35019	0.123947
C	-2.35103	2.610968	0.405376	C	-2.34817	2.610524	0.405506
N	-2.66169	1.413809	-0.05684	N	-2.65543	1.411456	-0.05465
C	-3.9657	1.473016	-0.50928	C	-3.9605	1.464502	-0.50607
C	-4.4507	2.745294	-0.31562	C	-4.44976	2.734991	-0.31346
N	-3.41086	3.460596	0.268962	N	-3.41183	3.454929	0.26916
O	-2.7216	-1.63009	-0.32511	O	-2.72836	-1.62153	-0.31336
C	-3.59911	-2.03702	-1.18909	C	-3.59763	-2.02791	-1.18798
O	-4.57019	-1.38016	-1.62367	O	-4.56007	-1.36877	-1.63486
O	3.099069	-1.376	-0.37283	O	3.099136	-1.38089	-0.36971
C	3.605379	-2.22859	0.452743	C	3.608874	-2.22899	0.458969
O	3.455857	-2.24337	1.703295	O	3.466025	-2.23834	1.710022
N	2.865632	1.48808	-0.30949	N	2.864034	1.49536	-0.30389
C	4.209194	1.520082	-0.61489	C	4.20763	1.522486	-0.60975
C	4.630945	2.826877	-0.68112	C	4.63387	2.827795	-0.67589
N	3.504873	3.59123	-0.40795	N	3.510322	3.59587	-0.40072
C	2.46274	2.739553	-0.18927	C	2.464998	2.747801	-0.18203
O	1.979919	-0.11548	1.893904	O	1.973059	-0.11661	1.88195
O	0.314254	-1.4529	0.156996	O	0.309319	-1.48054	0.148379
O	0.182263	1.031755	0.262671	O	0.183631	1.06062	0.238964
O	1.283214	-0.0928	-1.99867	O	1.276061	-0.09931	-1.99858
C	0.13861	-0.12505	-2.59983	C	0.132764	-0.13258	-2.59903
O	-1.00424	-0.17057	-2.0839	O	-1.00917	-0.18292	-2.07692
O	-1.81645	-0.41985	2.097529	O	-1.82687	-0.41409	2.102423

C	-1.25278	-0.33435	3.24432	C	-1.25606	-0.3384	3.24827
C	-2.21499	-0.52878	4.42136	C	-2.20893	-0.52823	4.435015
C	0.233502	-0.13686	-4.12434	C	0.228156	-0.14235	-4.12282
C	4.446	-3.32489	-0.20109	C	4.450868	-3.32732	-0.19227
O	-0.03484	-0.12398	3.503974	O	-0.03654	-0.14177	3.501475
C	-3.38197	-3.48007	-1.65575	C	-3.38067	-3.47256	-1.65208
H	-0.66584	0.317474	-4.55622	H	-0.66836	0.312773	-4.55875
H	0.284197	-1.18399	-4.45839	H	0.281635	-1.18884	-4.45738
H	1.139548	0.377401	-4.46774	H	1.135652	0.372094	-4.46143
H	4.992025	-2.93209	-1.06892	H	5.000439	-2.93679	-1.05872
H	5.133578	-3.77657	0.524397	H	5.136047	-3.77714	0.536097
H	3.758463	-4.10245	-0.56679	H	3.765054	-4.10555	-0.55916
H	-2.54657	-1.5779	4.42947	H	-2.53832	-1.57757	4.452626
H	-3.11064	0.091113	4.276503	H	-3.10632	0.091015	4.30196
H	-1.72946	-0.29249	5.375572	H	-1.70828	-0.28889	5.38069
H	1.116358	-0.15376	2.463602	H	1.113191	-0.16463	2.450134
H	2.497309	-0.9927	1.993369	H	2.497744	-0.98774	1.988898
H	-2.40663	-3.55028	-2.15875	H	-2.40507	-3.54308	-2.15373
H	-4.18115	-3.79663	-2.3373	H	-4.1789	-3.78629	-2.33566
H	-3.33987	-4.14742	-0.78275	H	-3.34142	-4.14076	-0.78012
H	-4.43045	0.57967	-0.93571	H	-4.42209	0.569402	-0.93153
H	-5.40959	3.203123	-0.53157	H	-5.40971	3.188479	-0.53042
H	-3.43723	4.430562	0.560573	H	-3.44325	4.424871	0.558634
H	-1.39129	2.876486	0.834889	H	-1.38837	2.878089	0.832686
H	1.441115	3.018699	0.044806	H	1.444129	3.027504	0.052956
H	3.461314	4.602371	-0.36885	H	3.470909	4.606886	-0.36313
H	5.596962	3.273108	-0.88757	H	5.600157	3.271177	-0.88435
H	4.765523	0.602004	-0.76471	H	4.758883	0.601706	-0.76026

Table S14. BP86/TZP-optimized coordinate for model $^{2}Fe^{0}_{0}$. The broken-symmetry structure is on the left, ferromagnetic on the right.

C	1.57251	-0.12037	-0.07032	C	1.573566	-0.12875	-0.06033
N	0.191645	-0.15668	-0.00355	N	0.193307	-0.16822	0.003399
C	-0.185	-1.40966	-0.20484	C	-0.18227	-1.42118	-0.19631
N	0.908268	-2.19775	-0.39878	N	0.913414	-2.20778	-0.38361
C	2.037867	-1.38965	-0.31779	C	2.041443	-1.39804	-0.30269
Mn	-1.31396	1.365237	0.334131	Mn	-1.29613	1.366369	0.327431
O	-1.28255	0.761305	2.20138	O	-1.30377	0.763235	2.191148
C	-2.1663	0.31212	3.023848	C	-2.18911	0.309867	3.019383
C	-1.56995	0.008601	4.403923	C	-1.58613	0.008044	4.397928
Fe	-3.83624	1.497478	-0.59143	Fe	-3.83903	1.506219	-0.5909
O	-2.93191	2.077565	-2.45664	O	-2.93254	2.10702	-2.4288
C	-1.66371	2.201132	-2.46859	C	-1.66747	2.212671	-2.46262
C	-1.03014	2.637227	-3.78623	C	-1.04074	2.636667	-3.78715
O	-2.65367	2.509351	0.491145	O	-2.63968	2.546222	0.477404
O	-2.48832	0.164676	-0.26944	O	-2.47102	0.153213	-0.312
O	-5.07625	0.611623	0.899774	O	-5.08567	0.610132	0.904415

N	-5.07498	0.150044	-2.01041	N	-5.07361	0.141942	-2.00423
C	-5.94191	-0.74758	-1.55184	C	-5.93703	-0.74865	-1.55177
N	-6.55943	-1.37871	-2.59207	N	-6.55567	-1.38325	-2.59076
C	-6.0564	-0.85063	-3.77325	C	-6.05052	-0.85655	-3.77151
C	-5.13613	0.093815	-3.3815	C	-5.1309	0.088926	-3.38229
O	-5.31149	2.964588	-0.85151	O	-5.31388	2.965082	-0.83392
C	-6.24369	3.321076	-0.03782	C	-6.25296	3.317686	-0.03003
C	-6.94434	4.631026	-0.40879	C	-6.9573	4.624934	-0.3983
O	-0.84605	1.991669	-1.51361	O	-0.8378	1.989808	-1.51535
O	0.04385	2.730583	0.978763	O	0.053455	2.725293	0.979373
C	1.200287	3.276412	0.766507	C	1.199703	3.276501	0.759836
C	1.270908	4.724533	1.289528	C	1.273216	4.719733	1.284446
O	-6.61325	2.709816	1.001228	O	-6.62969	2.699884	1.007055
O	2.2074	2.780924	0.225987	O	2.20843	2.781294	0.20333
O	-3.39297	0.103024	2.845472	O	-3.40922	0.100634	2.845507
H	-4.40219	0.477718	1.64831	H	-4.41536	0.473508	1.654219
H	-5.67744	1.405416	1.114441	H	-5.69121	1.405443	1.118685
H	-6.1302	-0.92876	-0.50101	H	-6.12948	-0.93061	-0.49956
H	-7.2705	-2.09649	-2.51021	H	-7.26646	-2.10032	-2.50838
H	-6.39495	-1.18548	-4.74621	H	-6.38838	-1.19324	-4.74462
H	-4.51161	0.744396	-3.98567	H	-4.50659	0.738617	-3.98516
H	-6.22414	5.456571	-0.31566	H	-6.23695	5.451068	-0.31089
H	-7.26536	4.596571	-1.45906	H	-7.28474	4.588506	-1.44681
H	-7.80234	4.816693	0.247764	H	-7.81189	4.810459	0.26257
H	-0.00017	2.974915	-3.62843	H	-0.00945	2.974016	-3.6384
H	-1.02255	1.778075	-4.47334	H	-1.03732	1.771415	-4.46688
H	-1.6344	3.430924	-4.24317	H	-1.64663	3.427074	-4.24772
H	0.928176	4.767584	2.332489	H	0.931052	4.757356	2.328137
H	2.293275	5.114104	1.206769	H	2.293067	5.114506	1.200612
H	0.586303	5.352086	0.7005	H	0.583235	5.345205	0.69902
H	-1.21989	-1.73264	-0.23034	H	-1.21756	-1.74302	-0.22814
H	0.890652	-3.19466	-0.57241	H	0.897985	-3.20441	-0.56015
H	3.03802	-1.78507	-0.44884	H	3.042784	-1.79106	-0.43267
H	2.084397	0.840115	0.044326	H	2.083612	0.833277	0.048752
H	-1.19922	0.943056	4.848792	H	-1.21631	0.943629	4.840717
H	-2.32706	-0.43902	5.057383	H	-2.34319	-0.43848	5.052708
H	-0.70828	-0.66519	4.297734	H	-0.72466	-0.66579	4.293106

Table S15. BP86/TZP-optimized coordinate for model $^{2}Mn^{1}_{1}$. The broken-symmetry structure is on the left, ferromagnetic on the right.

C	2.852594	2.486229	0.787644	C	2.85284	2.486469	0.791024
N	3.062068	1.284947	0.249404	N	3.062215	1.285953	0.251067
C	4.411725	1.190122	-0.04398	C	4.411253	1.191895	-0.04523
C	5.023862	2.359157	0.326112	C	5.023423	2.360537	0.325614
N	4.023519	3.159967	0.846621	N	4.023795	3.160217	0.849246
Mn	1.618871	-0.13257	-0.02941	Mn	1.61956	-0.13187	-0.02998
O	1.455104	0.560635	-1.81612	O	1.455993	0.559019	-1.81677

C	0.3581	0.807516	-2.46872
C	0.555119	1.299887	-3.88241
Fe	-1.49742	-0.1767	-0.24134
O	-1.94615	-0.78223	1.604637
C	-1.37199	-0.66863	2.751385
O	-0.26502	-0.05956	2.92963
O	2.940556	-1.37428	-0.70969
C	3.345452	-2.50289	-0.16001
C	4.259737	-3.33797	-1.01992
O	2.017592	-0.769	1.788975
O	0.229494	-1.3908	-0.26127
O	0.282335	0.965886	0.627505
N	-2.74466	1.519416	-0.05699
C	-2.40527	2.807942	-0.05193
N	-3.51604	3.571721	0.074407
C	-4.61685	2.734745	0.155048
C	-4.12486	1.458388	0.071639
O	-2.61073	-1.39206	-1.12804
C	-3.75084	-2.08357	-0.932
C	-3.71575	-3.48326	-1.49762
O	-0.81075	0.650214	-2.02925
O	-4.72304	-1.59643	-0.36547
O	3.037675	-2.8732	0.996103
C	-2.06185	-1.31265	3.927006
H	-0.29493	1.920802	-4.1836
H	0.590342	0.422981	-4.54597
H	1.50131	1.841925	-3.98183
H	5.299985	-3.07843	-0.77195
H	4.117056	-4.39887	-0.78683
H	4.096881	-3.14036	-2.08464
H	-1.78847	-2.37855	3.946535
H	-3.15004	-1.2512	3.814719
H	-1.73178	-0.85073	4.862834
H	1.184898	-0.75402	2.345166
H	2.374524	-1.75989	1.60642
H	-3.44518	-3.44523	-2.56172
H	-4.6901	-3.96451	-1.37076
H	-2.94073	-4.06716	-0.98124
H	-4.63825	0.500308	0.072971
H	-5.62533	3.114922	0.257608
H	-3.53543	4.585793	0.106725
H	-1.40047	3.200577	-0.13789
H	1.896994	2.863694	1.12622
H	4.141779	4.097659	1.217176
H	6.056238	2.680899	0.270598
H	4.834571	0.303284	-0.4964
H	0.387727	-1.98815	-1.01964
H	0.074819	0.670628	1.598928

C	0.358891	0.808648	-2.46981
C	0.556788	1.301768	-3.8833
Fe	-1.49846	-0.17797	-0.24211
O	-1.94644	-0.78408	1.605903
C	-1.37295	-0.66904	2.752233
O	-0.26449	-0.06068	2.92753
O	2.939699	-1.3762	-0.71025
C	3.345471	-2.50448	-0.15934
C	4.262108	-3.33824	-1.01806
O	2.016721	-0.76765	1.787485
O	0.230426	-1.39177	-0.26442
O	0.283992	0.969398	0.627204
N	-2.74502	1.519035	-0.05631
C	-2.40522	2.807438	-0.05131
N	-3.5158	3.57173	0.0744
C	-4.61686	2.735111	0.154126
C	-4.12523	1.458494	0.072091
O	-2.61209	-1.39244	-1.129
C	-3.75188	-2.08319	-0.9305
C	-3.7171	-3.48294	-1.49627
O	-0.80963	0.65045	-2.03072
O	-4.7235	-1.59623	-0.36271
O	3.036028	-2.87534	0.996017
C	-2.0615	-1.31137	3.92937
H	-0.29389	1.922247	-4.18404
H	0.59156	0.424883	-4.54719
H	1.502744	1.844046	-3.98378
H	5.302281	-3.07806	-0.76986
H	4.119969	-4.39913	-0.78467
H	4.099522	-3.14089	-2.08287
H	-1.78727	-2.3772	3.94891
H	-3.14975	-1.25082	3.816761
H	-1.73185	-0.84957	4.865493
H	1.183695	-0.75101	2.343935
H	2.376146	-1.75878	1.605991
H	-3.44639	-3.44543	-2.56036
H	-4.69178	-3.96384	-1.37049
H	-2.94197	-4.06692	-0.97978
H	-4.63924	0.50059	0.073722
H	-5.62549	3.115507	0.255467
H	-3.53486	4.585794	0.106343
H	-1.40018	3.199861	-0.13706
H	1.897201	2.863139	1.13095
H	4.142416	4.097587	1.220894
H	6.055729	2.68239	0.268193
H	4.833452	0.305977	-0.5003
H	0.387608	-1.98987	-1.02196
H	0.07834	0.677	1.600615

Table S16. BP86/TZP-optimized coordinate for model $^{2}Fe^{1}_{1}$. The broken-symmetry structure is on the left, ferromagnetic on the right.

C	2.885516	2.587436	0.809773	C	2.887031	2.580934	0.816418
N	3.094438	1.405066	0.232817	N	3.09844	1.404143	0.228864
C	4.45301	1.319241	-0.02934	C	4.456029	1.324716	-0.03878
C	5.0656	2.469024	0.396196	C	5.066142	2.47303	0.394084
N	4.057272	3.256564	0.92186	N	4.057257	3.252534	0.930635
Fe	1.69639	-0.15247	-0.08636	Fe	1.695556	-0.15271	-0.08833
O	1.346647	0.515495	-1.97785	O	1.341605	0.513365	-1.97899
C	0.231548	0.80108	-2.51506	C	0.22796	0.802362	-2.51782
C	0.237501	1.341041	-3.92468	C	0.238077	1.341924	-3.92747
Mn	-1.37311	-0.1042	-0.21022	Mn	-1.37421	-0.10304	-0.21245
O	-2.03388	-0.76153	1.463105	O	-2.03019	-0.76279	1.462553
C	-1.50758	-0.66236	2.653373	C	-1.50533	-0.66533	2.655115
O	-0.44596	-0.0312	2.909651	O	-0.44358	-0.03772	2.914723
O	2.956379	-1.50781	-0.67654	O	2.962676	-1.50801	-0.67231
C	3.360766	-2.63736	-0.12109	C	3.36274	-2.6392	-0.11647
C	4.2707	-3.49021	-0.96825	C	4.273169	-3.49355	-0.96228
O	1.976713	-0.83897	1.849311	O	1.977712	-0.83791	1.852405
O	0.01835	-1.40458	-0.28341	O	0.018107	-1.40395	-0.29194
O	0.031803	0.928121	0.581783	O	0.033329	0.942999	0.58448
N	-2.68246	1.445882	-0.03984	N	-2.68289	1.447271	-0.03678
C	-2.33314	2.733202	-0.04986	C	-2.33327	2.734815	-0.05072
N	-3.44378	3.496363	0.05315	N	-3.44422	3.497514	0.048684
C	-4.54766	2.664246	0.134875	C	-4.54829	2.665302	0.132297
C	-4.06313	1.384272	0.077246	C	-4.06374	1.385143	0.079402
O	-2.49431	-1.28388	-1.1303	O	-2.4999	-1.28263	-1.13252
C	-3.59975	-1.9941	-0.80548	C	-3.59976	-1.99659	-0.80304
C	-3.641	-3.33625	-1.50612	C	-3.64619	-3.33355	-1.51333
O	-0.92605	0.651141	-1.97136	O	-0.92964	0.653434	-1.97418
O	-4.47799	-1.60339	-0.04764	O	-4.47081	-1.61351	-0.0336
O	3.047484	-2.97897	1.038712	O	3.046268	-2.98206	1.041751
C	-2.25837	-1.3901	3.738828	C	-2.26273	-1.39018	3.738477
H	-0.69039	1.879326	-4.14169	H	-0.68755	1.881857	-4.14954
H	0.315478	0.488769	-4.61609	H	0.317896	0.488496	-4.61731
H	1.114985	1.979289	-4.07786	H	1.117845	1.977873	-4.07741
H	5.310509	-3.19192	-0.76399	H	5.312906	-3.19393	-0.75982
H	4.163167	-4.54403	-0.68966	H	4.166189	-4.54624	-0.67994
H	4.074467	-3.33856	-2.03545	H	4.076907	-3.34616	-2.03005
H	-1.9365	-2.44253	3.731317	H	-1.93964	-2.44241	3.738432
H	-3.33704	-1.36957	3.547638	H	-3.34038	-1.37155	3.541958
H	-2.01615	-0.95546	4.714039	H	-2.02542	-0.95092	4.712895
H	1.163281	-0.85178	2.407663	H	1.160306	-0.84815	2.405516
H	2.33895	-1.80037	1.684711	H	2.338264	-1.79942	1.689638
H	-3.33807	-3.23918	-2.55603	H	-3.35038	-3.23183	-2.56492
H	-4.64705	-3.76016	-1.4303	H	-4.65241	-3.75623	-1.43301
H	-2.92748	-4.01266	-1.01184	H	-2.93075	-4.01493	-1.02865

H	-4.56907	0.423396	0.113126	H	-4.57032	0.424819	0.11686
H	-5.5562	3.04679	0.229091	H	-5.55709	3.048312	0.221769
H	-3.4583	4.510787	0.077715	H	-3.45905	4.512068	0.0696
H	-1.32377	3.114516	-0.1228	H	-1.32388	3.115437	-0.12422
H	1.930497	2.965348	1.15309	H	1.932012	2.953015	1.165473
H	4.174055	4.177642	1.332657	H	4.172023	4.170331	1.348893
H	6.100557	2.787207	0.376958	H	6.099856	2.794851	0.373201
H	4.885311	0.443643	-0.49793	H	4.890115	0.45494	-0.51564
H	-0.13593	-2.02242	-1.02605	H	-0.12622	-2.02179	-1.03609
H	-0.09329	0.685607	1.577078	H	-0.09245	0.702272	1.576479

Table S17. BP86/TZP-optimized coordinate for model $^{1}Mn^{1}_{0}$. The broken-symmetry structure is on the left, ferromagnetic on the right.

C	-2.977	-2.52088	0.139479	C	-2.99056	-2.5243	0.124651
N	-3.22641	-1.16041	0.178516	N	-3.22583	-1.16316	0.19128
C	-4.5357	-0.99769	0.117706	C	-4.53286	-0.98349	0.132274
N	-5.15824	-2.20929	0.039565	N	-5.16797	-2.18646	0.027278
C	-4.1733	-3.19102	0.053086	C	-4.19393	-3.17938	0.022678
Fe	-1.70553	0.454641	0.354039	Fe	-1.70868	0.448614	0.36292
O	-2.10288	0.78292	-1.78133	O	-2.10724	0.782077	-1.77252
C	-2.39749	1.91896	-2.25213	C	-2.38741	1.918233	-2.24947
C	-2.72754	1.980693	-3.74537	C	-2.68365	1.983279	-3.749
O	-2.43708	3.043501	-1.63807	O	-2.43205	3.04153	-1.63296
Mn	-2.14494	3.245218	0.408791	Mn	-2.15289	3.251846	0.404702
O	-3.07424	1.768446	0.682009	O	-3.13209	1.762813	0.692265
N	-3.85415	4.456145	0.334663	N	-3.85801	4.466728	0.321363
C	-5.04835	4.029705	0.703662	C	-5.04739	4.030324	0.693
N	-5.92657	5.071636	0.722377	N	-5.93651	5.062961	0.696909
C	-5.23873	6.218081	0.348816	C	-5.2616	6.212887	0.309636
C	-3.9478	5.811805	0.110991	C	-3.96556	5.818296	0.079888
O	-1.0924	4.906969	-0.14047	O	-1.09366	4.913515	-0.14149
C	0.056443	4.891217	-0.73634	C	0.053255	4.890649	-0.73967
O	0.741741	3.881129	-1.03283	O	0.729733	3.874749	-1.03741
O	-1.97919	3.71628	2.147886	O	-2.00502	3.712335	2.144055
O	-0.60681	2.147527	0.35838	O	-0.62238	2.154912	0.377667
O	-1.31062	-0.09771	2.261896	O	-1.30537	-0.12552	2.271292
C	-1.60474	0.409605	3.418601	C	-1.54141	0.386983	3.43798
C	-1.03847	-0.38394	4.603737	C	-1.03786	-0.46923	4.608265
O	-0.32027	-0.83612	-0.29947	O	-0.32369	-0.81488	-0.30166
C	0.466532	-1.83656	-0.04534	C	0.45742	-1.8194	-0.04124
O	0.104485	-3.01313	0.172459	O	0.087544	-2.99529	0.1617
O	-2.24949	1.452888	3.663475	O	-2.0891	1.479384	3.703962
C	0.591171	6.279814	-1.09702	C	0.595982	6.276237	-1.10257
C	1.956556	-1.48394	-0.07271	C	1.946639	-1.46763	-0.04373
H	-3.23222	1.058381	-4.05846	H	-3.17259	1.058003	-4.07749
H	-1.78597	2.059161	-4.3078	H	-1.72864	2.071901	-4.28697
H	-3.34225	2.859896	-3.97324	H	-3.29927	2.858522	-3.98926

H	0.569043	6.929813	-0.21127	H	0.573077	6.92964	-0.21927
H	1.613007	6.207269	-1.48594	H	1.618799	6.199716	-1.48808
H	-0.05938	6.734335	-1.85899	H	-0.05012	6.730745	-1.86828
H	-0.03263	0.007602	4.819409	H	-0.0186	-0.1356	4.856174
H	-0.94492	-1.44994	4.363787	H	-0.99478	-1.53147	4.339721
H	-1.66216	-0.23154	5.493616	H	-1.66931	-0.30964	5.491449
H	-2.12197	2.873009	2.6739	H	-2.07115	2.859569	2.674703
H	2.216349	-1.06999	-1.05773	H	2.21839	-1.0446	-1.02165
H	2.568727	-2.36979	0.136257	H	2.556679	-2.35451	0.165546
H	2.159263	-0.69838	0.66829	H	2.137745	-0.68801	0.706601
H	-1.94745	-2.89173	0.165835	H	-1.9646	-2.90425	0.144761
H	-4.41413	-4.24658	0.002766	H	-4.44596	-4.23064	-0.05205
H	-6.15772	-2.36256	-0.02068	H	-6.16859	-2.32812	-0.03644
H	-5.04594	-0.04218	0.127106	H	-5.02705	-0.01967	0.161138
H	-5.27195	3.005911	0.978233	H	-5.25146	3.004375	0.977158
H	-6.90078	5.018495	0.993256	H	-6.91123	5.00178	0.96348
H	-5.71753	7.188161	0.296742	H	-5.75171	7.17652	0.242941
H	-3.07168	6.377998	-0.1827	H	-3.09682	6.391961	-0.22072
H	0.013981	2.630397	-0.28477	H	-0.00544	2.620322	-0.28286

Table S18. BP86/TZP-optimized coordinate for model $^{1}Fe^{1}_{0}$. The broken-symmetry structure is on the left, ferromagnetic on the right.

C	-3.03788	-2.68923	0.194695	C	-3.0441	-2.67812	0.212313
N	-3.22992	-1.38797	0.089851	N	-3.23755	-1.37671	0.105735
C	-4.58735	-1.19169	-0.03989	C	-4.59275	-1.18354	-0.04921
C	-5.23282	-2.4063	-0.01809	C	-5.23593	-2.39938	-0.03888
N	-4.22929	-3.35349	0.128116	N	-4.23287	-3.34451	0.124782
Fe	-1.61951	0.107211	0.566349	Fe	-1.62872	0.107629	0.586357
O	-1.63163	0.179512	-1.78008	O	-1.62571	0.167877	-1.79712
C	-0.5699	0.274338	-2.43455	C	-0.56207	0.271604	-2.44362
C	-0.6559	0.319013	-3.96097	C	-0.63552	0.328988	-3.97083
Mn	1.169735	0.183499	-0.08351	Mn	1.169593	0.178836	-0.08816
O	2.045527	0.120848	1.646833	O	2.039062	0.115842	1.644836
C	1.735441	-0.42054	2.796776	C	1.73875	-0.41763	2.801426
O	0.7319	-1.08388	3.107944	O	0.737356	-1.07634	3.125112
O	-2.98282	1.637228	0.273296	O	-2.97768	1.639319	0.287113
C	-2.7449	2.796688	-0.24673	C	-2.73668	2.790731	-0.25026
C	-3.98709	3.682901	-0.40825	C	-3.97528	3.679528	-0.41898
O	-1.83345	-0.23958	2.375709	O	-1.8392	-0.23459	2.406894
O	-0.06113	1.473681	0.528256	O	-0.05831	1.462417	0.515506
O	-0.07983	-1.0086	0.240169	O	-0.07822	-1.06639	0.200578
N	2.441817	-1.36286	-0.70095	N	2.451523	-1.35746	-0.70787
C	1.99162	-2.56449	-1.02331	C	1.993102	-2.55726	-1.02754
N	3.026873	-3.3514	-1.42398	N	3.024299	-3.34967	-1.42669
C	4.194325	-2.59993	-1.33664	C	4.196264	-2.60471	-1.3426
C	3.812601	-1.36032	-0.88474	C	3.821989	-1.36199	-0.89306
O	2.523574	1.592495	-0.57529	O	2.499254	1.619751	-0.54872

C	3.697823	2.025663	-0.23914	C	3.684695	2.038271	-0.23239
C	3.775446	3.556116	-0.1769	C	3.779876	3.56804	-0.17122
O	0.642089	0.370225	-1.98244	O	0.648785	0.369505	-1.98296
O	4.723175	1.348296	-0.00177	O	4.706405	1.350713	-0.01179
O	-1.63445	3.250026	-0.62065	O	-1.62444	3.230399	-0.63503
C	2.795839	-0.11757	3.862785	C	2.811284	-0.11055	3.854762
H	0.22288	-0.15088	-4.41946	H	0.248846	-0.1319	-4.4278
H	-0.6825	1.372049	-4.27587	H	-0.66615	1.38463	-4.27644
H	-1.57994	-0.16705	-4.2956	H	-1.55459	-0.15919	-4.31605
H	-4.5797	3.671365	0.516848	H	-4.57235	3.673094	0.503201
H	-3.69804	4.709179	-0.6632	H	-3.68415	4.704231	-0.67753
H	-4.61797	3.275641	-1.21268	H	-4.60315	3.269931	-1.22458
H	2.598055	0.890037	4.258543	H	2.608238	0.891767	4.261099
H	3.805095	-0.11659	3.432807	H	3.814496	-0.09631	3.411633
H	2.712853	-0.8395	4.684242	H	2.746449	-0.83902	4.671961
H	-0.95349	-0.59226	2.676362	H	-0.95579	-0.5782	2.707222
H	3.370982	3.988003	-1.10277	H	3.382174	4.004059	-1.09824
H	4.808229	3.889356	-0.01801	H	4.817073	3.887768	-0.01327
H	3.136928	3.908446	0.645998	H	3.146093	3.930425	0.650844
H	4.383626	-0.45631	-0.645	H	4.396291	-0.46051	-0.65413
H	5.163754	-3.01139	-1.59083	H	5.162747	-3.02182	-1.59891
H	2.954903	-4.31965	-1.71043	H	2.94594	-4.31758	-1.71251
H	0.953357	-2.86578	-0.95863	H	0.951178	-2.84476	-0.95312
H	-2.07679	-3.16869	0.340295	H	-2.08342	-3.15461	0.370691
H	-4.35731	-4.35515	0.206175	H	-4.36039	-4.34632	0.201133
H	-6.27873	-2.68065	-0.08366	H	-6.28017	-2.67524	-0.1229
H	-4.99327	-0.18984	-0.12612	H	-4.99968	-0.18311	-0.14473
H	-0.40577	2.196218	-0.08903	H	-0.41998	2.173221	-0.10868

Table S19. BP86/TZP-optimized coordinate for model $^{1}Mn^{0}_{0}$. The broken-symmetry structure is on the left, ferromagnetic on the right.

Mn	1.522619	-0.28389	-0.009	Mn	1.551804	-0.28405	-0.01792
Fe	-1.17855	-0.38785	0.086577	Fe	-1.17824	-0.39598	0.127235
C	2.423965	2.66349	-0.31044	C	2.425118	2.645844	-0.31742
N	2.855309	1.421173	-0.39042	N	2.876634	1.410685	-0.40178
C	4.202757	1.462264	-0.66539	C	4.223332	1.47351	-0.67521
C	4.605676	2.77531	-0.75401	C	4.605443	2.793398	-0.75982
N	3.458905	3.53225	-0.52436	N	3.446122	3.530284	-0.52852
O	1.252459	-0.16999	-2.07742	O	1.229173	-0.1699	-2.07081
C	0.098499	-0.15444	-2.62353	C	0.066527	-0.13656	-2.59998
C	0.100866	-0.11456	-4.15928	C	0.044412	-0.08258	-4.13515
O	-1.58288	-0.58563	2.164844	O	-1.64661	-0.52973	2.170344
C	-1.17234	-0.0011	3.22919	C	-1.19594	0.01866	3.242137
O	-1.03853	1.237914	3.4376	O	-1.05201	1.249667	3.47768
O	3.219091	-1.31716	-0.46772	O	3.228746	-1.32527	-0.47393
C	3.781889	-2.36008	0.074818	C	3.788678	-2.37228	0.066353
C	2.938129	-3.16235	1.060715	C	2.939488	-3.17419	1.047369

O	2.089538	-0.24332	1.77843	O	2.066424	-0.2318	1.779018
O	0.322337	-1.58048	0.071745	O	0.322338	-1.59861	0.093644
O	0.221355	0.928411	0.288884	O	0.231522	0.94173	0.271159
N	-2.6766	1.400296	0.090361	N	-2.65292	1.395504	0.082545
C	-2.53931	2.339531	1.009484	C	-2.5188	2.345219	0.990953
N	-3.46819	3.326086	0.809208	N	-3.45504	3.322177	0.785272
C	-4.23648	2.972768	-0.29995	C	-4.22651	2.95102	-0.31541
C	-3.72398	1.768378	-0.72877	C	-3.70738	1.746211	-0.73467
O	-2.80724	-1.64347	-0.24286	O	-2.80413	-1.64485	-0.27078
C	-3.78345	-1.88823	-1.04137	C	-3.77743	-1.89677	-1.07038
C	-4.20506	-3.3789	-1.03751	C	-4.21379	-3.3836	-1.03802
O	-1.04076	-0.19278	-2.07365	O	-1.0631	-0.16861	-2.033
O	-4.41495	-1.09273	-1.78185	O	-4.39519	-1.11336	-1.83378
O	4.959959	-2.71099	-0.18206	O	4.965483	-2.72348	-0.18948
C	-0.78042	-0.9729	4.361808	C	-0.78232	-0.98823	4.33243
H	-0.82197	0.354202	-4.52394	H	-0.88891	0.379724	-4.48062
H	0.131156	-1.1498	-4.53127	H	0.078852	-1.11413	-4.51697
H	0.987081	0.412219	-4.53673	H	0.918954	0.455828	-4.52288
H	1.970345	-3.41726	0.605492	H	1.967749	-3.41371	0.591932
H	3.480687	-4.05987	1.386175	H	3.473758	-4.07952	1.364981
H	2.696074	-2.51048	1.913806	H	2.704054	-2.52869	1.906994
H	0.19809	-1.40516	4.101131	H	0.190538	-1.41134	4.038593
H	-1.49946	-1.8019	4.422468	H	-1.50083	-1.81845	4.380096
H	-0.70017	-0.45388	5.327114	H	-0.68406	-0.49947	5.311506
H	1.365326	0.266138	2.197106	H	1.328124	0.28569	2.162649
H	-3.37169	-3.98893	-1.41739	H	-3.38443	-4.00895	-1.40162
H	-5.0967	-3.54147	-1.65868	H	-5.10373	-3.5498	-1.6607
H	-4.3972	-3.70614	-0.00461	H	-4.41475	-3.68831	0.000047
H	-4.05147	1.086918	-1.51278	H	-4.03157	1.055603	-1.51241
H	-5.0534	3.593018	-0.65387	H	-5.05208	3.559835	-0.66865
H	-3.5974	4.142364	1.39497	H	-3.59001	4.14077	1.366098
H	-1.84278	2.272231	1.854561	H	-1.82041	2.294711	1.833097
H	1.392079	2.922949	-0.09013	H	1.386563	2.880423	-0.09766
H	3.396609	4.542918	-0.51348	H	3.366056	4.539215	-0.51394
H	5.569333	3.234133	-0.94746	H	5.560908	3.268521	-0.95265
H	4.753788	0.531207	-0.77057	H	4.79138	0.554031	-0.78189

Table S20. BP86/TZP-optimized coordinate for model $^{1}Fe^{0}_{0}$. The broken-symmetry structure is on the left, ferromagnetic on the right.

C	-2.86439	-2.56631	0.071295	C	-2.81253	-2.5242	0.090383
N	-3.20153	-1.29696	-0.00257	N	-3.16381	-1.25793	0.033955
C	-4.57464	-1.25025	-0.05222	C	-4.53574	-1.22365	-0.04562
C	-5.09027	-2.52771	-0.01455	C	-5.03713	-2.50741	-0.04339
N	-3.98092	-3.36536	0.061217	N	-3.91943	-3.33376	0.039641
Fe	-1.54262	0.405647	0.488019	Fe	-1.56109	0.443611	0.498292
O	-1.5639	0.406385	-1.78314	O	-1.55979	0.408711	-1.81638
C	-0.48842	0.347584	-2.42182	C	-0.47852	0.343436	-2.44369

C	-0.57843	0.471766	-3.95004	C	-0.5481	0.461576	-3.97536
Mn	1.142737	0.04758	-0.0242	Mn	1.133035	0.045809	-0.03302
O	2.052889	-0.13177	1.72646	O	2.031547	-0.12742	1.731373
C	1.67526	-0.48888	2.913729	C	1.674083	-0.50962	2.915189
O	0.569475	-0.89753	3.317098	O	0.583891	-0.96187	3.317609
O	-3.24551	1.665021	0.207046	O	-3.25785	1.651713	0.233054
C	-3.51219	2.858817	-0.20354	C	-3.54391	2.840602	-0.18787
C	-5.00508	3.251088	0.020419	C	-5.04434	3.199691	0.025746
O	-1.93173	0.118428	2.302409	O	-1.88753	0.137233	2.331069
O	0.115276	1.373722	0.45702	O	0.110394	1.416136	0.407014
O	-0.17459	-1.09867	0.221903	O	-0.17754	-1.11208	0.192375
N	2.478618	-1.58585	-0.67364	N	2.462927	-1.60761	-0.66852
C	2.032925	-2.79572	-0.94274	C	2.021221	-2.8183	-0.93942
N	3.056169	-3.59045	-1.38252	N	3.048511	-3.61153	-1.37344
C	4.215459	-2.81653	-1.3805	C	4.205735	-2.83434	-1.36809
C	3.835617	-1.5713	-0.93582	C	3.820426	-1.58978	-0.92653
O	2.834336	1.210138	-0.58873	O	2.839011	1.183239	-0.58466
C	3.934538	1.819305	-0.37448	C	3.931312	1.804942	-0.36646
C	3.792948	3.324088	-0.06816	C	3.772105	3.308742	-0.0671
O	0.714363	0.212209	-1.9756	O	0.719189	0.207029	-1.98494
O	5.096965	1.320722	-0.43511	O	5.098146	1.316945	-0.42178
O	-2.77063	3.699826	-0.74743	O	-2.81399	3.68877	-0.73115
C	2.809646	-0.33417	3.95224	C	2.806064	-0.32357	3.951557
H	0.299435	0.033332	-4.44176	H	0.343467	0.034869	-4.45277
H	-0.62983	1.540848	-4.20277	H	-0.6112	1.529028	-4.23301
H	-1.50364	-0.00386	-4.30128	H	-1.46074	-0.02838	-4.34038
H	-5.36708	2.875268	0.988576	H	-5.39356	2.844689	1.006351
H	-5.12438	4.342057	-0.03685	H	-5.1943	4.284315	-0.06571
H	-5.61845	2.791469	-0.77225	H	-5.64587	2.696706	-0.74918
H	2.70362	0.656184	4.421538	H	2.681502	0.669562	4.410559
H	3.800293	-0.3892	3.48376	H	3.797012	-0.36168	3.48139
H	2.70099	-1.09501	4.737502	H	2.715193	-1.07889	4.744432
H	-1.08825	-0.24947	2.667375	H	-1.0448	-0.25464	2.673785
H	3.280133	3.813158	-0.90983	H	3.277205	3.790667	-0.92351
H	4.771028	3.796054	0.101963	H	4.742328	3.788809	0.123647
H	3.144044	3.452811	0.809556	H	3.100029	3.43737	0.79275
H	4.414405	-0.65176	-0.79225	H	4.395686	-0.66884	-0.78104
H	5.173907	-3.21915	-1.68981	H	5.166462	-3.2336	-1.67448
H	2.97954	-4.55912	-1.6661	H	2.976253	-4.5802	-1.65828
H	0.997619	-3.09679	-0.82582	H	0.986109	-3.12157	-0.82794
H	-1.84037	-2.91785	0.155569	H	-1.78289	-2.85876	0.183747
H	-3.9997	-4.3743	0.148166	H	-3.92758	-4.34473	0.103935
H	-6.10336	-2.91623	-0.02591	H	-6.04507	-2.90672	-0.08639
H	-5.08285	-0.29233	-0.09667	H	-5.05391	-0.27122	-0.08516

Table S21. BP86/TZP-optimized coordinate for model $^{1}Mn^{1}_{1}$. The broken-symmetry structure is on the left, ferromagnetic on the right.

C	-2.93817	-2.59831	0.179568
N	-3.147	-1.29023	0.193767
C	-4.5111	-1.08729	0.142874
C	-5.14049	-2.30603	0.094366
N	-4.12812	-3.2507	0.116948
Mn	-1.64475	0.14288	0.387268
O	-1.64979	0.10897	-1.644
C	-0.63147	0.169373	-2.41613
C	-0.91971	0.268765	-3.90308
Fe	1.344486	0.286988	-0.14399
O	2.05073	0.116383	1.740524
C	1.614001	-0.48721	2.791522
O	0.568568	-1.20294	2.838235
O	-3.03504	1.51669	0.223343
C	-2.83897	2.766991	-0.09598
C	-4.11208	3.587361	-0.19972
O	-1.8991	0.057069	2.179304
O	-0.24561	1.377466	0.422092
O	-0.28373	-1.16225	0.374295
N	2.54561	-1.44602	-0.70666
C	2.093223	-2.65432	-1.01376
N	3.132098	-3.47204	-1.33052
C	4.305018	-2.74049	-1.21715
C	3.924442	-1.48058	-0.82834
O	2.614163	1.614831	-0.63645
C	3.795509	2.115827	-0.2985
C	3.775872	3.61418	-0.05696
O	0.588953	0.170221	-2.06446
O	4.82759	1.444377	-0.21272
O	-1.72418	3.299627	-0.30911
C	2.435098	-0.28777	4.050939
H	-0.13367	-0.23567	-4.47607
H	-0.90928	1.333164	-4.17928
H	-1.90746	-0.14169	-4.1383
H	-4.67558	3.513645	0.740322
H	-3.87279	4.633232	-0.41483
H	-4.74603	3.178561	-0.99913
H	2.296335	0.74581	4.39986
H	3.501619	-0.41617	3.827138
H	2.114595	-0.98085	4.835091
H	-1.06398	-0.23351	2.620728
H	3.365796	4.125822	-0.93852
H	4.78725	3.975552	0.156075
H	3.108581	3.838376	0.786886
H	4.514436	-0.58569	-0.63336
H	5.276688	-3.17398	-1.41943
H	3.057345	-4.44582	-1.60101
H	1.052819	-2.95298	-1.00985
H	-1.96581	-3.07187	0.224877
H	-4.24747	-4.25692	0.1049

C	-2.93839	-2.60089	0.180219
N	-3.14632	-1.29235	0.193464
C	-4.51031	-1.08881	0.142579
C	-5.14055	-2.30699	0.094385
N	-4.12898	-3.25258	0.118972
Mn	-1.64439	0.142465	0.387152
O	-1.64974	0.110262	-1.64356
C	-0.63209	0.169767	-2.41738
C	-0.9218	0.268501	-3.90403
Fe	1.345041	0.287121	-0.14398
O	2.051576	0.116012	1.742021
C	1.614265	-0.48706	2.792938
O	0.567499	-1.20166	2.838187
O	-3.03331	1.51763	0.223553
C	-2.83827	2.767974	-0.09781
C	-4.112	3.587599	-0.19956
O	-1.89614	0.058694	2.179143
O	-0.24475	1.379998	0.422363
O	-0.28408	-1.16524	0.374006
N	2.54394	-1.44614	-0.70677
C	2.091722	-2.65453	-1.01364
N	3.130595	-3.47147	-1.33169
C	4.303497	-2.73986	-1.21799
C	3.922782	-1.48002	-0.829
O	2.614592	1.614445	-0.63536
C	3.795802	2.115726	-0.29685
C	3.77507	3.614002	-0.05547
O	0.588383	0.171902	-2.06593
O	4.828532	1.445264	-0.21154
O	-1.72463	3.301046	-0.31388
C	2.434946	-0.28913	4.053035
H	-0.13579	-0.23582	-4.4772
H	-0.91153	1.332986	-4.1803
H	-1.90956	-0.14191	-4.13934
H	-4.67439	3.513204	0.741039
H	-3.87301	4.633943	-0.41313
H	-4.74652	3.17924	-0.99883
H	2.296925	0.744655	4.401786
H	3.501489	-0.4179	3.82945
H	2.11401	-0.98183	4.837423
H	-1.06156	-0.23452	2.620073
H	3.365282	4.12506	-0.93754
H	4.786106	3.975942	0.158262
H	3.107025	3.837858	0.787859
H	4.512613	-0.58491	-0.63416
H	5.275068	-3.17307	-1.42096
H	3.056594	-4.44499	-1.60292
H	1.051174	-2.95336	-1.00879
H	-1.96632	-3.07481	0.225278
H	-4.24922	-4.25871	0.107862

H	-6.18718	-2.57879	0.048402	H	-6.18753	-2.57909	0.048321
H	-4.9247	-0.08684	0.151932	H	-4.92338	-0.08817	0.151414
H	-0.67463	2.251259	0.057624	H	-0.67233	2.254555	0.060794
H	0.009478	-1.29364	1.346913	H	0.008783	-1.2978	1.346265

Table S22. BP86/TZP-optimized coordinate for model $^{1}Fe^{1}_{1}$. The broken-symmetry structure is on the left, ferromagnetic on the right.

C	-3.00729	-2.67496	0.169173	C	-3.00878	-2.67661	0.170638
N	-3.19486	-1.36524	0.179391	N	-3.19764	-1.36676	0.180889
C	-4.55881	-1.15307	0.098213	C	-4.5605	-1.15497	0.098058
C	-5.20355	-2.36386	0.037944	C	-5.20472	-2.36568	0.035495
N	-4.20301	-3.32015	0.081842	N	-4.20402	-3.32199	0.080675
Fe	-1.7109	0.176369	0.569498	Fe	-1.7116	0.174861	0.572581
O	-1.62876	0.168822	-1.6752	O	-1.63021	0.160881	-1.67808
C	-0.60552	0.206435	-2.39337	C	-0.60708	0.202755	-2.39467
C	-0.7507	0.28109	-3.90201	C	-0.75004	0.280569	-3.9041
Mn	1.235777	0.202496	-0.14909	Mn	1.235032	0.203296	-0.14997
O	2.074849	0.167796	1.599985	O	2.07442	0.169127	1.599369
C	1.748257	-0.50707	2.661668	C	1.748466	-0.50608	2.662241
O	0.82802	-1.36356	2.727974	O	0.829131	-1.36347	2.728587
O	-3.02821	1.635094	0.257652	O	-3.0212	1.643173	0.265181
C	-2.7404	2.803004	-0.23288	C	-2.73283	2.809691	-0.23247
C	-3.93568	3.725657	-0.40524	C	-3.93003	3.730197	-0.40788
O	-1.81923	0.003049	2.413789	O	-1.82011	-0.00565	2.417118
O	-0.04572	1.410748	0.443211	O	-0.04955	1.410919	0.440899
O	-0.06115	-1.14041	0.315343	O	-0.0595	-1.14199	0.313199
N	2.508168	-1.35977	-0.70101	N	2.508114	-1.35963	-0.70006
C	2.058581	-2.56488	-1.03442	C	2.05932	-2.56471	-1.03501
N	3.101721	-3.36547	-1.36378	N	3.103209	-3.36344	-1.36605
C	4.2721	-2.63318	-1.22902	C	4.272859	-2.63035	-1.23065
C	3.888272	-1.38195	-0.81744	C	3.888434	-1.38076	-0.81556
O	2.457796	1.570643	-0.666	O	2.45433	1.572215	-0.66479
C	3.607748	2.040386	-0.198	C	3.605345	2.041429	-0.19517
C	3.643614	3.559327	-0.1545	C	3.642396	3.560453	-0.15598
O	0.631745	0.208829	-1.98536	O	0.630569	0.209438	-1.98561
O	4.577728	1.362362	0.152246	O	4.571985	1.35969	0.156278
O	-1.59091	3.199054	-0.55178	O	-1.58474	3.202872	-0.56078
C	2.577637	-0.17465	3.884035	C	2.579766	-0.17339	3.883763
H	0.088433	-0.21441	-4.40327	H	0.089384	-0.21294	-4.40662
H	-0.74238	1.341219	-4.19402	H	-0.74193	1.341439	-4.19313
H	-1.70749	-0.15564	-4.20744	H	-1.70652	-0.1557	-4.21076
H	-4.5176	3.745486	0.525682	H	-4.51437	3.751549	0.521862
H	-3.61389	4.735917	-0.6742	H	-3.61037	4.740778	-0.67985
H	-4.59091	3.325372	-1.1927	H	-4.58275	3.32583	-1.19543
H	2.376388	0.865547	4.175465	H	2.37904	0.866793	4.176464
H	3.645553	-0.24548	3.641406	H	3.647673	-0.24336	3.639998
H	2.319854	-0.8474	4.707614	H	2.323647	-0.84684	4.7075

H	-1.03366	-0.39718	2.842939	H	-1.03156	-0.39861	2.847501
H	3.269675	3.981908	-1.09543	H	3.269029	3.980573	-1.09861
H	4.662268	3.906227	0.04911	H	4.661636	3.905871	0.046355
H	2.969374	3.898505	0.644954	H	2.968037	3.90382	0.641791
H	4.466875	-0.49407	-0.56725	H	4.4664	-0.49302	-0.56401
H	5.246944	-3.06157	-1.4255	H	5.24794	-3.05692	-1.42991
H	3.030256	-4.33761	-1.64017	H	3.033101	-4.33499	-1.64499
H	1.018431	-2.86128	-1.0273	H	1.019291	-2.86163	-1.02886
H	-2.04792	-3.17411	0.22933	H	-2.04917	-3.17533	0.232173
H	-4.33457	-4.32487	0.066449	H	-4.33535	-4.32674	0.064564
H	-6.25225	-2.62537	-0.02656	H	-6.25316	-2.62747	-0.03095
H	-4.96635	-0.14892	0.094681	H	-4.96765	-0.15069	0.094638
H	-0.45726	2.184953	-0.11171	H	-0.45485	2.185673	-0.1124
H	0.225197	-1.36279	1.273477	H	0.227075	-1.36671	1.271487

Table S23. B3LYP/6-311G*-optimized coordinate for model $^{2}Mn^{1}_{0}$. The broken-symmetry structure is on the left, ferromagnetic on the right.

Mn	1.470934	-0.12802	-0.10419	Mn	1.479464	-0.12387	-0.10717
Fe	-1.44537	-0.30793	0.072986	Fe	-1.44697	-0.29325	0.03343
C	3.319788	1.821605	1.246168	C	3.333612	1.751319	1.324357
N	2.865348	1.370623	0.092121	N	2.895558	1.337271	0.150234
C	3.508542	2.06688	-0.90772	C	3.56494	2.052109	-0.81885
C	4.368432	2.960203	-0.3392	C	4.425052	2.918539	-0.21071
N	4.233952	2.790795	1.026933	N	4.263205	2.71414	1.147869
O	1.203028	0.463891	-1.91798	O	1.229453	0.535703	-1.89886
C	0.051007	0.655471	-2.46935	C	0.083482	0.763343	-2.44825
C	0.112573	1.248432	-3.86112	C	0.158634	1.410715	-3.8147
O	-1.79587	-0.92144	1.892491	O	-1.80543	-0.94919	1.83912
C	-1.22822	-1.23957	2.99958	C	-1.25302	-1.3205	2.936885
O	-0.01069	-1.23368	3.233763	O	-0.03761	-1.33922	3.181844
O	2.884995	-1.32093	-0.85839	O	2.876914	-1.31749	-0.90008
C	3.680366	-2.16351	-0.28642	C	3.654775	-2.19062	-0.35102
C	4.594273	-2.91293	-1.23861	C	4.564325	-2.92262	-1.32111
O	1.976303	-0.66937	1.699481	O	1.960333	-0.73922	1.677324
O	0.209872	-1.51388	-0.25287	O	0.198286	-1.48099	-0.3174
O	0.157539	0.780338	0.516287	O	0.17463	0.803252	0.539525
N	-2.62415	1.455398	0.333038	N	-2.61963	1.466607	0.347945
C	-2.16942	2.542155	0.927866	C	-2.14534	2.539703	0.95293
N	-3.14621	3.473455	0.994997	N	-3.11441	3.475677	1.056657
C	-4.28368	2.945025	0.406995	C	-4.26745	2.965225	0.483238
C	-3.94422	1.687776	-0.00068	C	-3.94478	1.713485	0.046181
O	-2.7377	-1.43651	-0.73857	O	-2.71797	-1.40986	-0.82091
C	-3.77466	-1.63293	-1.50989	C	-3.81371	-1.6032	-1.50755
C	-3.74161	-2.96292	-2.24715	C	-3.84211	-2.9373	-2.2377
O	-1.04831	0.399941	-1.95978	O	-1.02214	0.501688	-1.95438
O	-4.70511	-0.85237	-1.63951	O	-4.7467	-0.8182	-1.57207
O	3.73895	-2.38594	0.931924	O	3.701791	-2.45405	0.859857

C	-2.1902	-1.6684	4.094404	C	-2.23015	-1.7825	4.004583
H	-0.85527	1.159953	-4.35105	H	-0.80169	1.333626	-4.3212
H	0.886253	0.756171	-4.45225	H	0.944929	0.949626	-4.41401
H	0.376954	2.307424	-3.7873	H	0.410735	2.468593	-3.695
H	5.182474	-2.20318	-1.82514	H	5.17179	-2.20326	-1.87552
H	5.256345	-3.57948	-0.68824	H	5.20845	-3.62085	-0.78902
H	3.995348	-3.49209	-1.94606	H	3.962192	-3.46411	-2.0551
H	-2.7011	-2.58432	3.786238	H	-2.7497	-2.67813	3.654148
H	-2.9606	-0.90675	4.234381	H	-2.99208	-1.01738	4.169772
H	-1.65983	-1.84365	5.029248	H	-1.71045	-2.00333	4.935724
H	1.168979	-0.89361	2.267709	H	1.147179	-0.97299	2.234037
H	2.628378	-1.42701	1.631201	H	2.603402	-1.50241	1.586379
H	-2.8747	-2.99199	-2.9134	H	-3.02476	-2.9774	-2.9632
H	-4.65216	-3.10075	-2.82888	H	-4.79271	-3.07117	-2.75235
H	-3.62792	-3.78367	-1.53466	H	-3.68454	-3.75477	-1.52982
H	-4.51398	0.929428	-0.52082	H	-4.53078	0.967158	-0.4728
H	-5.20248	3.502468	0.333919	H	-5.18396	3.529482	0.439753
H	-3.05804	4.389722	1.402927	H	-3.01159	4.383723	1.479228
H	-1.16265	2.66369	1.293131	H	-1.12993	2.645753	1.2989
H	3.019584	1.447802	2.210125	H	3.00994	1.356337	2.272081
H	4.741713	3.286506	1.741701	H	4.763463	3.184199	1.884914
H	5.048409	3.677932	-0.76613	H	5.121652	3.638668	-0.60555
H	3.295807	1.863486	-1.94283	H	3.368024	1.880317	-1.86278
H	0.370156	-2.16727	-0.94022	H	0.340045	-2.11209	-1.02896

Table S24. B3LYP/6-311G*-optimized coordinate for model $^{2}Fe^{1}_{0}$. The broken-symmetry structure is on the left, ferromagnetic on the right.

Fe	1.536825	-0.13848	-0.10395	Fe	1.535383	-0.13248	-0.10164
Mn	-1.3553	-0.1929	0.046924	Mn	-1.36055	-0.19339	0.049426
O	-0.01196	-1.48236	-0.24492	O	-0.01076	-1.46834	-0.25375
O	0.007587	0.744242	0.613791	O	0.006399	0.773381	0.632286
O	2.085251	-0.72413	1.788266	O	2.087455	-0.7317	1.787441
H	1.265052	-0.92089	2.30983	H	1.267404	-0.93578	2.307498
H	2.666497	-1.52543	1.693415	H	2.669174	-1.53071	1.686007
N	2.986653	1.444115	0.082251	N	2.998306	1.437014	0.086147
C	3.653599	1.69507	1.193907	C	3.663779	1.684264	1.199391
H	3.523959	1.153436	2.116617	H	3.530522	1.141929	2.121163
N	4.522266	2.710821	0.993233	N	4.535475	2.698104	1.002016
H	5.154645	3.086104	1.681565	H	5.167062	3.071007	1.692342
C	4.402932	3.127148	-0.32036	C	4.41931	3.117261	-0.31093
H	4.998953	3.927405	-0.72603	H	5.017683	3.91706	-0.71402
C	3.443596	2.328616	-0.8717	C	3.458845	2.32221	-0.86533
H	3.047305	2.309434	-1.87283	H	3.063128	2.307105	-1.86675
O	2.827777	-1.44317	-0.85396	O	2.818176	-1.43064	-0.86754
C	3.573472	-2.36174	-0.33228	C	3.571452	-2.35017	-0.35644
O	3.670029	-2.59884	0.87949	O	3.676099	-2.59546	0.852332
C	4.368488	-3.17826	-1.3342	C	4.363662	-3.15455	-1.37021

H	3.682104	-3.7191	-1.99109	H	3.676024	-3.68858	-2.03128
H	4.960048	-2.51458	-1.96918	H	4.952728	-2.48295	-1.99919
H	5.019809	-3.88652	-0.82436	H	5.017401	-3.86753	-0.87021
O	1.100324	0.614938	-1.98185	O	1.088	0.63906	-1.96749
C	-0.07089	0.799453	-2.40898	C	-0.08376	0.824324	-2.3926
O	-1.14221	0.515562	-1.79444	O	-1.15249	0.531301	-1.77757
C	-0.23238	1.42545	-3.7769	C	-0.25033	1.46098	-3.75446
H	-1.23951	1.269176	-4.15873	H	-1.26066	1.312468	-4.13088
H	-0.05113	2.501542	-3.69608	H	-0.06224	2.535353	-3.66714
H	0.508192	1.015039	-4.46436	H	0.483587	1.05145	-4.44964
O	-2.57384	-1.48013	-0.76565	O	-2.58075	-1.48181	-0.76015
C	-3.62669	-1.55858	-1.53025	C	-3.60528	-1.54356	-1.56424
O	-4.41188	-0.65654	-1.78867	O	-4.35569	-0.62484	-1.86412
C	-3.82604	-2.9553	-2.11077	C	-3.82044	-2.94312	-2.1322
H	-3.82066	-3.70092	-1.31242	H	-3.87223	-3.67506	-1.32288
H	-4.76468	-3.00636	-2.66113	H	-4.73538	-2.97606	-2.72243
H	-2.99887	-3.19766	-2.78442	H	-2.97222	-3.22126	-2.76455
N	-2.58586	1.415946	0.394193	N	-2.59978	1.401287	0.410578
C	-2.1891	2.408753	1.170761	C	-2.21799	2.378963	1.21355
H	-1.21581	2.471924	1.627793	H	-1.25069	2.434913	1.683968
N	-3.17856	3.31814	1.283173	N	-3.21188	3.283203	1.327379
H	-3.13145	4.168667	1.819876	H	-3.17543	4.123354	1.880961
C	-4.25849	2.878029	0.535601	C	-4.27793	2.856331	0.552541
H	-5.17446	3.439966	0.463823	H	-5.19373	3.417909	0.476078
C	-3.87655	1.689605	-0.01444	C	-3.88379	1.680305	-0.0151
H	-4.38755	1.004559	-0.67676	H	-4.38029	1.009892	-0.70261
C	-1.34799	-1.26462	2.815433	C	-1.33684	-1.29394	2.812169
O	-1.92991	-0.85812	1.728129	O	-1.91761	-0.86589	1.732924
O	-0.14831	-1.26756	3.077958	O	-0.13653	-1.31061	3.071781
C	-2.35019	-1.7985	3.82879	C	-2.34047	-1.83507	3.82015
H	-2.79168	-2.7216	3.444606	H	-2.79445	-2.74578	3.421275
H	-1.85382	-2.00094	4.776673	H	-1.8426	-2.0601	4.762145
H	-3.16597	-1.08712	3.970667	H	-3.14736	-1.11701	3.978586
H	-0.283	-2.18824	-0.84067	H	-0.25828	-2.18063	-0.85123

Table S25. B3LYP/6-311G*-optimized coordinate for model $^{2}Mn^{0}_{0}$. The broken-symmetry structure is on the left, ferromagnetic on the right.

Mn	1.408602	-0.1774	-0.00891	Mn	1.4547	-0.14696	-0.02372
Fe	-1.32425	-0.37079	0.231716	Fe	-1.27498	-0.34811	0.172782
C	-2.2992	2.569104	-0.25062	C	-2.3292	2.599635	0.093664
N	-2.70156	1.319378	-0.24714	N	-2.66033	1.36147	-0.19007
C	-4.05314	1.320925	-0.51661	C	-3.97976	1.369354	-0.58873
C	-4.47117	2.611548	-0.68485	C	-4.44937	2.652515	-0.54447
N	-3.34196	3.39927	-0.51104	N	-3.38577	3.428826	-0.10633

O	-2.78256	-1.64356	-0.04966
C	-3.61095	-2.18084	-0.88089
O	-4.70773	-1.72025	-1.19757
O	3.042243	-1.39864	-0.23298
C	3.659521	-2.10359	0.63888
O	3.605846	-1.97128	1.873827
N	2.815965	1.435232	-0.43263
C	4.005404	1.465267	-1.1174
C	4.548449	2.716622	-1.02811
N	3.654331	3.451646	-0.26585
C	2.625687	2.631505	0.069794
O	1.936724	0.064138	1.884395
O	0.263266	-1.43945	0.33476
O	0.11657	0.996243	0.169507
O	1.189723	-0.31089	-1.94288
C	0.055218	-0.44595	-2.51818
O	-1.0606	-0.47437	-1.97387
O	-1.81452	-0.15853	2.171408
C	-1.27569	0.03436	3.307905
C	-2.26943	0.063505	4.47102
C	0.134756	-0.61625	-4.02886
C	4.530327	-3.21483	0.055843
O	-0.06899	0.190157	3.564651
C	-3.13106	-3.50645	-1.47278
H	-0.83612	-0.42103	-4.48363
H	0.427715	-1.64643	-4.25273
H	0.896409	0.042111	-4.45096
H	5.111765	-2.84333	-0.79141
H	5.192376	-3.62818	0.817543
H	3.880383	-4.00958	-0.32226
H	-2.73825	-0.91984	4.567694
H	-3.06947	0.777654	4.259544
H	-1.77065	0.322853	5.405508
H	1.135053	0.095797	2.482514
H	2.530337	-0.69615	2.121102
H	-2.22645	-3.32117	-2.05815
H	-3.89839	-3.95354	-2.10704
H	-2.85561	-4.1979	-0.67203
H	-4.58966	0.383828	-0.59865
H	-5.43511	3.037363	-0.91201
H	-3.30016	4.40281	-0.56741
H	-1.27731	2.869291	-0.08144
H	1.7723	2.904454	0.668823
H	3.75769	4.413065	0.01202
H	5.456596	3.145306	-1.41933
H	4.373212	0.580156	-1.60952

O	-2.73181	-1.61656	-0.14097
C	-3.53584	-2.14353	-1.00155
O	-4.5559	-1.62048	-1.45073
O	3.08714	-1.37284	-0.18695
C	3.59675	-2.15035	0.695974
O	3.489686	-2.04088	1.928354
N	2.851977	1.462661	-0.48083
C	4.197531	1.466115	-0.75406
C	4.618017	2.752782	-0.9441
N	3.487682	3.53708	-0.78055
C	2.447301	2.710164	-0.50198
O	1.952105	0.103154	1.872083
O	0.313103	-1.42961	0.308589
O	0.164883	1.041664	0.105948
O	1.245894	-0.30878	-1.95982
C	0.114729	-0.42459	-2.54115
O	-1.00567	-0.43425	-2.00064
O	-1.76922	-0.18364	2.124836
C	-1.25518	0.028341	3.269478
C	-2.25145	-0.05859	4.427675
C	0.190893	-0.59961	-4.05079
C	4.397114	-3.31937	0.126739
O	-0.0681	0.285346	3.535973
C	-3.13573	-3.55202	-1.44297
H	-0.75677	-0.32121	-4.51166
H	0.388412	-1.6528	-4.27279
H	1.011069	-0.01294	-4.46795
H	4.9906	-3.00112	-0.73325
H	5.037636	-3.75996	0.891872
H	3.69501	-4.08047	-0.22715
H	-2.6103	-1.08821	4.514163
H	-3.12385	0.56581	4.218932
H	-1.7867	0.243549	5.366857
H	1.146014	0.19623	2.456048
H	2.483739	-0.69135	2.137698
H	-2.15602	-3.50638	-1.9261
H	-3.87119	-3.97149	-2.13141
H	-3.0283	-4.20079	-0.56937
H	-4.46204	0.442652	-0.87746
H	-5.41059	3.080893	-0.77821
H	-3.39739	4.422197	0.052371
H	-1.35299	2.898768	0.440133
H	1.425878	3.004695	-0.32279
H	3.44423	4.540147	-0.84446
H	5.582492	3.176203	-1.17253
H	4.746341	0.540027	-0.79355

Table S26. B3LYP/6-311G*-optimized coordinate for model $^{2}Fe^{0}_{0}$. The broken-symmetry structure is on the left, ferromagnetic on the right.

Fe	1.392586	-0.15515	-0.08174	Fe	1.389706	-0.16683	-0.08099
Mn	-1.31568	-0.27903	0.097149	Mn	-1.31382	-0.27222	0.092553
C	-4.09611	1.350538	0.036257	C	-4.09363	1.34508	0.010428
N	-2.76068	1.312269	0.363191	N	-2.75425	1.321642	0.322437
C	-2.44781	2.465624	0.904592	C	-2.43949	2.491822	0.825481
N	-3.54055	3.270348	0.947422	N	-3.53503	3.293051	0.857565
C	-4.60276	2.568762	0.393915	C	-4.60081	2.571632	0.337408
O	-1.81401	-0.86107	1.871605	O	-1.79946	-0.79589	1.889899
C	-1.2453	-1.22824	2.959491	C	-1.24244	-1.13391	2.991927
C	-2.25485	-1.70392	4.006497	C	-2.26136	-1.57029	4.046865
O	1.022293	0.590304	-2.02811	O	1.025755	0.507503	-2.04682
C	-0.16269	0.686768	-2.43455	C	-0.15761	0.600488	-2.46118
C	-0.37118	1.210789	-3.84704	C	-0.35778	1.081997	-3.88931
O	-0.02111	-1.42414	-0.21174	O	-0.02637	-1.44921	-0.18616
O	-0.05712	0.877859	0.610757	O	-0.0576	0.915125	0.563564
O	2.091451	-0.59627	1.842817	O	2.082703	-0.54425	1.861161
N	2.861126	1.571225	0.034495	N	2.847594	1.566974	-0.00867
C	3.480495	1.883734	1.150232	C	3.449604	1.925375	1.102656
N	4.29441	2.954215	0.956223	N	4.256732	2.995402	0.87988
C	4.178574	3.337336	-0.36972	C	4.154806	3.328941	-0.46049
C	3.282832	2.464174	-0.92144	C	3.273839	2.428174	-0.99119
O	2.928526	-1.32613	-0.78865	O	2.94137	-1.33963	-0.74032
C	3.709106	-2.17655	-0.24415	C	3.72862	-2.16632	-0.16871
C	4.539282	-3.00244	-1.22536	C	4.57271	-3.00876	-1.12342
O	-1.21402	0.403021	-1.79092	O	-1.2109	0.343005	-1.81063
O	-2.89125	-1.28711	-0.51614	O	-2.88764	-1.30255	-0.47679
C	-3.26437	-1.83804	-1.63032	C	-3.26761	-1.89086	-1.56958
C	-2.25537	-2.77404	-2.29744	C	-2.26162	-2.84591	-2.21339
O	3.842546	-2.38513	0.976981	O	3.85713	-2.34057	1.057986
O	-4.38298	-1.68929	-2.11762	O	-4.39027	-1.75996	-2.0526
O	-0.04324	-1.25155	3.244973	O	-0.04191	-1.15745	3.286652
H	1.297762	-0.84411	2.38377	H	1.290575	-0.77799	2.412175
H	2.721552	-1.35459	1.748093	H	2.72009	-1.29916	1.795255
H	3.355793	1.345895	2.076964	H	3.317462	1.420181	2.046547
H	4.883484	3.381159	1.651423	H	4.83279	3.452859	1.566506
H	4.731964	4.167759	-0.77727	H	4.706134	4.148984	-0.89118
H	2.904871	2.398945	-1.92867	H	2.909176	2.323295	-1.99996
H	3.87147	-3.64474	-1.80657	H	3.915467	-3.67951	-1.68426
H	5.046007	-2.34278	-1.93449	H	5.069608	-2.36383	-1.85265
H	5.267931	-3.61984	-0.69884	H	5.310079	-3.59823	-0.5774
H	-1.41173	1.11034	-4.15161	H	-1.39944	0.98566	-4.19152
H	-0.0827	2.265727	-3.88594	H	-0.05557	2.131326	-3.96167
H	0.277917	0.667748	-4.53726	H	0.284205	0.508767	-4.56152
H	-2.50797	-3.80383	-2.01949	H	-2.51388	-3.86719	-1.90534
H	-2.33941	-2.69861	-3.38433	H	-2.3503	-2.80156	-3.30167

H	-1.23661	-2.57477	-1.96655	H	-1.24168	-2.63753	-1.89192
H	-1.45434	2.712445	1.245536	H	-1.4428	2.751368	1.146996
H	-3.57102	4.205496	1.317005	H	-3.56481	4.238637	1.1996
H	-5.5884	2.996761	0.308788	H	-5.58905	2.993304	0.25104
H	-4.55662	0.49495	-0.43524	H	-4.55623	0.474107	-0.42973
H	-2.7105	-2.63742	3.665035	H	-2.71863	-2.51268	3.732994
H	-1.76181	-1.86946	4.964848	H	-1.77629	-1.70638	5.013926
H	-3.06093	-0.97466	4.114517	H	-3.06507	-0.83461	4.12469

Table S27. B3LYP/6-311G*-optimized coordinate for model $^{2}Mn^{1}_{1}$. The broken-symmetry structure is on the left, ferromagnetic on the right.

Mn	1.577312	-0.15875	-0.07293	C	2.835695	2.490587	0.733592
Fe	-1.55774	-0.19351	-0.2171	N	3.055178	1.272434	0.260603
C	3.563501	1.506225	1.478356	C	4.40794	1.163654	0.004101
N	3.078373	1.172507	0.289341	C	5.009411	2.339127	0.339845
C	3.797023	1.872659	-0.66183	N	3.999884	3.161874	0.798048
C	4.725585	2.641052	-0.02699	Mn	1.631606	-0.1401	-0.03766
N	4.55933	2.396005	1.321963	O	1.464971	0.513474	-1.80236
O	1.40044	0.630768	-1.77735	C	0.376369	0.753462	-2.46025
C	0.301454	0.917365	-2.4099	C	0.588101	1.224905	-3.87474
C	0.506781	1.555542	-3.75853	Fe	-1.50727	-0.20612	-0.23148
O	-1.95744	-0.83654	1.587287	O	-1.90532	-0.692	1.623755
C	-1.4195	-0.83542	2.749625	C	-1.37997	-0.57878	2.786194
O	-0.29187	-0.33906	2.993328	O	-0.27854	-0.01178	2.996285
O	2.818325	-1.39056	-0.80742	O	2.922566	-1.38644	-0.64693
C	3.490604	-2.38312	-0.26221	C	3.348169	-2.52295	-0.11998
C	4.382361	-3.11949	-1.22637	C	4.268245	-3.30576	-1.02009
O	1.927291	-0.82669	1.726427	O	1.95334	-0.74829	1.793873
O	0.176949	-1.35137	-0.36442	O	0.22739	-1.34817	-0.27185
O	0.217942	0.895943	0.617392	O	0.28364	0.977872	0.568027
N	-2.72051	1.532018	0.068782	N	-2.74258	1.489846	-0.09539
C	-2.28486	2.775126	0.213633	C	-2.39945	2.762526	-0.22296
N	-3.32854	3.606004	0.399343	N	-3.48127	3.547958	-0.058
C	-4.49094	2.85786	0.371622	C	-4.57385	2.736636	0.18603
C	-4.10167	1.567868	0.166646	C	-4.10347	1.457873	0.162017
O	-2.64017	-1.36103	-1.15059	O	-2.55011	-1.47631	-1.07608
C	-3.85411	-1.91965	-1.09752	C	-3.73642	-2.07293	-0.9072
C	-3.93117	-3.24808	-1.81134	C	-3.84174	-3.39727	-1.62523
O	-0.83874	0.706574	-1.97821	O	-0.77336	0.603671	-2.01532
O	-4.79419	-1.3973	-0.5413	O	-4.63203	-1.58654	-0.2538
O	3.415347	-2.69664	0.925743	O	3.045356	-2.9119	1.003796
C	-2.21844	-1.4846	3.849875	C	-2.15147	-1.18579	3.928463
H	-0.4459	1.655806	-4.27356	H	-0.32078	1.685649	-4.25671
H	1.197663	0.957642	-4.35534	H	0.830419	0.360003	-4.49893
H	0.957288	2.543173	-3.6298	H	1.429359	1.915434	-3.93196
H	5.127547	-2.43361	-1.63589	H	5.231051	-2.79197	-1.09118
H	4.878794	-3.94433	-0.71976	H	4.428903	-4.30104	-0.61076

H	3.796714	-3.49572	-2.06778	H	3.860726	-3.36749	-2.03008
H	-2.23027	-2.56669	3.690888	H	-2.03908	-2.27357	3.892763
H	-3.25531	-1.14773	3.810668	H	-3.21553	-0.97203	3.823424
H	-1.78222	-1.27026	4.82336	H	-1.77647	-0.82326	4.883554
H	1.131557	-0.87697	2.317374	H	1.192051	-0.64453	2.414948
H	2.474791	-1.67618	1.655916	H	2.316969	-1.6825	1.757442
H	-3.616	-3.13315	-2.85103	H	-3.63098	-3.26425	-2.68882
H	-4.94715	-3.63612	-1.77417	H	-4.83743	-3.81661	-1.49507
H	-3.24961	-3.96272	-1.34265	H	-3.09747	-4.09469	-1.23208
H	-4.68175	0.662411	0.069214	H	-4.6167	0.515718	0.279401
H	-5.46371	3.303269	0.494653	H	-5.56149	3.135615	0.34456
H	-3.26895	4.603164	0.535671	H	-3.49137	4.554789	-0.10952
H	-1.25192	3.08089	0.199335	H	-1.40674	3.126914	-0.42616
H	3.228886	1.112339	2.422061	H	1.875778	2.879713	1.025824
H	5.098942	2.803311	2.070911	H	4.112613	4.105303	1.136946
H	5.473321	3.319048	-0.40244	H	6.037338	2.656862	0.294157
H	3.58866	1.762603	-1.71115	H	4.829721	0.264917	-0.40916
H	0.320813	-2.06638	-0.9944	H	0.357315	-2.14094	-0.80292
H	0.103054	0.75831	1.585518	H	0.123584	0.868114	1.539699

Table S28. B3LYP/6-311G*-optimized coordinate for model $^{2}Fe^{1}_{1}$. The broken-symmetry structure is on the left, ferromagnetic on the right.

Fe	-1.65493	-0.17111	0.148022	Fe	-1.6565	-0.17083	0.147175
Mn	1.42296	-0.0768	0.21707	Mn	1.422746	-0.07897	0.221159
C	-3.74149	1.340696	-1.54358	C	-3.74467	1.338281	-1.54302
N	-3.12156	1.266193	-0.37333	N	-3.12361	1.264528	-0.37339
C	-3.68107	2.236243	0.438735	C	-3.68251	2.234661	0.438928
C	-4.64634	2.89917	-0.25867	C	-4.64896	2.896763	-0.25766
N	-4.66734	2.317915	-1.51137	N	-4.67104	2.315001	-1.51008
O	-1.28298	0.903649	1.81301	O	-1.28347	0.897005	1.816788
C	-0.17434	1.269334	2.293522	C	-0.17516	1.260289	2.300282
C	-0.18615	2.076497	3.565239	C	-0.18791	2.060411	3.576374
O	2.028298	-1.05008	-1.26773	O	2.02179	-1.04618	-1.26807
C	1.538711	-1.23344	-2.4623	C	1.537981	-1.21605	-2.46757
O	0.512983	-0.69053	-2.89128	O	0.515661	-0.66748	-2.89634
O	-2.83997	-1.47014	0.879521	O	-2.84119	-1.47077	0.87454
C	-3.48009	-2.52161	0.420813	C	-3.47151	-2.52823	0.415041
C	-4.31194	-3.25243	1.44089	C	-4.30542	-3.2601	1.432791
O	-1.93821	-1.0126	-1.71968	O	-1.93388	-1.01012	-1.72396
O	0.012925	-1.27848	0.578947	O	0.010106	-1.27778	0.581887
O	-0.00231	0.790257	-0.7101	O	-0.00759	0.80022	-0.70122
N	2.683161	1.411147	-0.31456	N	2.678604	1.413511	-0.30736
C	2.297512	2.668737	-0.49176	C	2.295609	2.674576	-0.46504
N	3.360077	3.415968	-0.835	N	3.356191	3.421423	-0.81497

C	4.47619	2.60095	-0.88234	C	4.468242	2.602624	-0.88751
C	4.045167	1.350283	-0.55803	C	4.036814	1.350091	-0.57124
O	2.535549	-1.0221	1.339202	O	2.537531	-1.02897	1.33734
C	3.693958	-1.69228	1.217935	C	3.697144	-1.69538	1.207175
C	3.861705	-2.71423	2.321324	C	3.875981	-2.71718	2.309003
O	0.961582	1.01645	1.782676	O	0.96126	1.005734	1.791243
O	4.512032	-1.49996	0.350516	O	4.508468	-1.50033	0.334008
O	-3.4161	-2.88826	-0.75304	O	-3.39708	-2.89919	-0.75656
C	2.334702	-2.20336	-3.29725	C	2.337065	-2.17918	-3.30755
H	0.82287	2.245272	3.933754	H	0.822199	2.270634	3.919728
H	-0.7794	1.555075	4.318795	H	-0.7341	1.505937	4.342354
H	-0.67371	3.036918	3.378576	H	-0.72561	2.997522	3.412473
H	-5.04685	-2.57082	1.875314	H	-5.04298	-2.57989	1.8648
H	-4.81715	-4.09981	0.98236	H	-4.80716	-4.10883	0.972952
H	-3.67574	-3.59831	2.259071	H	-3.67105	-3.60462	2.253017
H	1.987163	-3.21782	-3.07877	H	1.984847	-3.19493	-3.10293
H	3.393646	-2.15675	-3.04731	H	3.394386	-2.13875	-3.04985
H	2.171363	-2.00447	-4.35534	H	2.181541	-1.96818	-4.36448
H	-1.18083	-1.128	-2.32132	H	-1.17506	-1.1148	-2.32584
H	-2.47582	-1.84872	-1.59285	H	-2.46229	-1.85171	-1.60008
H	3.69637	-2.25391	3.297128	H	3.716685	-2.2575	3.286102
H	4.860253	-3.14442	2.274765	H	4.875311	-3.14466	2.254861
H	3.120404	-3.50944	2.204628	H	3.13587	-3.51425	2.197712
H	4.57708	0.41696	-0.4687	H	4.566692	0.414293	-0.49748
H	5.453046	2.976288	-1.13614	H	5.443099	2.977243	-1.14991
H	3.339022	4.404878	-1.03154	H	3.33637	4.412627	-0.99977
H	1.288979	3.031615	-0.39671	H	1.290075	3.040432	-0.35193
H	-3.541	0.70607	-2.39023	H	-3.54476	0.703228	-2.3895
H	-5.27798	2.571205	-2.27319	H	-5.28264	2.567676	-2.27134
H	-5.30631	3.705738	0.013046	H	-5.30904	3.703095	0.014476
H	-3.35171	2.368812	1.454794	H	-3.35203	2.367846	1.454541
H	0.170038	-1.91456	1.285023	H	0.160869	-1.92851	1.275718
H	0.090568	0.58539	-1.66417	H	0.088988	0.61395	-1.65784

Table S29. B3LYP/6-311G*-optimized coordinate for model $^{1}Mn^{1}_{0}$. The broken-symmetry structure is on the left, ferromagnetic on the right.

Mn	1.56188	-0.16707	0.410958	Mn	1.565751	-0.1681	0.41152
Fe	-1.25549	-0.26955	-0.1062	Fe	-1.25223	-0.26562	-0.11441
C	-3.64568	1.642135	-1.24239	C	-3.65297	1.632844	-1.25574
N	-2.3505	1.503768	-0.79114	N	-2.36074	1.499721	-0.79503
C	-1.79571	2.69556	-0.80469	C	-1.81254	2.694745	-0.7978
N	-2.68409	3.617565	-1.25217	N	-2.70298	3.613743	-1.24751
C	-3.87217	2.957826	-1.53437	C	-3.88504	2.948687	-1.54262
O	-0.49168	-0.42136	-2.12031	O	-0.47689	-0.39408	-2.12631
C	0.716368	-0.37973	-2.43578	C	0.732343	-0.35076	-2.43568
C	1.065888	-0.52916	-3.91194	C	1.090265	-0.48181	-3.91124
O	1.709731	-0.25345	-1.65233	O	1.72129	-0.23689	-1.64431

O	0.205825	0.927132	0.259069	O	0.205544	0.954704	0.264217
N	3.002382	1.349253	0.264618	N	3.006415	1.343861	0.283469
C	3.390352	2.029848	1.319472	C	3.361861	2.040926	1.339066
N	4.32546	2.942751	0.959894	N	4.294371	2.960285	0.990315
C	4.539676	2.821697	-0.40432	C	4.540953	2.826696	-0.36742
C	3.705385	1.821778	-0.81702	C	3.727752	1.812766	-0.78758
O	3.087419	-1.4788	0.332252	O	3.079186	-1.49367	0.334264
C	3.048851	-2.70228	-0.05061	C	3.03532	-2.70989	-0.07071
O	2.044006	-3.35479	-0.36771	O	2.028705	-3.34911	-0.40872
O	1.712802	-0.01534	2.195308	O	1.700985	-0.01955	2.196275
O	0.250593	-1.51292	0.415398	O	0.254179	-1.50628	0.402621
O	-2.16222	-0.16291	1.6704	O	-2.16411	-0.16915	1.66391
C	-1.88953	0.236552	2.861862	C	-1.89933	0.215645	2.86167
C	-3.12697	0.341196	3.759242	C	-3.14397	0.323709	3.748881
O	-2.6655	-1.48148	-0.71498	O	-2.64351	-1.48636	-0.72941
C	-3.87813	-1.85186	-0.46436	C	-3.85229	-1.86518	-0.46631
O	-4.895	-1.22736	-0.76436	O	-4.87542	-1.25716	-0.77605
O	-0.78383	0.513085	3.33303	O	-0.79542	0.476697	3.34577
C	4.420663	-3.37805	-0.09193	C	4.402434	-3.39504	-0.11098
C	-3.98031	-3.19626	0.254385	C	-3.93657	-3.19544	0.279479
H	0.172878	-0.44071	-4.52993	H	0.201587	-0.38021	-4.53346
H	1.512757	-1.51522	-4.0678	H	1.532634	-1.46813	-4.07809
H	1.80749	0.216488	-4.20954	H	1.837516	0.263898	-4.19408
H	4.857781	-3.38136	0.910613	H	4.831036	-3.41684	0.894967
H	4.33439	-4.40176	-0.4573	H	4.311915	-4.41232	-0.49289
H	5.096345	-2.80894	-0.73646	H	5.087594	-2.82103	-0.74101
H	-3.53586	-0.65913	3.930101	H	-3.56631	-0.67357	3.904127
H	-3.90619	0.921886	3.259369	H	-3.91165	0.919445	3.248767
H	-2.87271	0.794922	4.718116	H	-2.89362	0.763337	4.715311
H	0.826405	0.168999	2.577373	H	0.81121	0.151162	2.577362
H	-3.42975	-3.96188	-0.29881	H	-3.38177	-3.96647	-0.26184
H	-5.022	-3.49768	0.374799	H	-4.9744	-3.50468	0.412486
H	-3.50457	-3.10559	1.234777	H	-3.45542	-3.07982	1.254501
H	-4.29386	0.775494	-1.29529	H	-4.29553	0.762979	-1.31838
H	-4.74051	3.477973	-1.90485	H	-4.75346	3.465772	-1.9172
H	-2.51023	4.60347	-1.35132	H	-2.53422	4.601163	-1.34006
H	-0.78031	2.886663	-0.49339	H	-0.79992	2.887339	-0.47747
H	3.009117	1.842863	2.310974	H	2.959083	1.861262	2.323319
H	4.790029	3.58103	1.583439	H	4.73667	3.611349	1.616823
H	5.248981	3.438056	-0.93193	H	5.25473	3.44565	-0.88585
H	3.547759	1.39287	-1.79205	H	3.595141	1.37322	-1.76154
H	0.645592	-2.34675	0.076477	H	0.636474	-2.33887	0.045871

Table S30. B3LYP/6-311G*-optimized coordinate for model $^{1}Fe^{1}_{0}$. The broken-symmetry structure is on the left, ferromagnetic on the right.

Fe	-1.60726	0.126909	0.632037	Fe	-1.60453	0.125915	0.628001
Mn	1.184393	0.145611	-0.15246	Mn	1.182832	0.143353	-0.1589

C	-3.67648	-2.06248	1.171069	C	-3.68085	-2.05189	1.1791
N	-3.22542	-1.31397	0.187773	N	-3.23109	-1.30503	0.194043
C	-3.9595	-1.62716	-0.93146	C	-3.96786	-1.61833	-0.92333
C	-4.87528	-2.59203	-0.61803	C	-4.88436	-2.5815	-0.60685
N	-4.68141	-2.85996	0.728584	N	-4.68794	-2.84829	0.739628
O	-1.71694	0.320168	-1.63762	O	-1.71249	0.309088	-1.64584
C	-0.71115	0.519661	-2.33952	C	-0.70672	0.498644	-2.35046
C	-0.90613	0.873233	-3.80728	C	-0.90143	0.832393	-3.82293
O	2.192618	-0.10655	1.470464	O	2.183447	-0.09578	1.470292
C	1.975344	-0.64574	2.631274	C	1.972431	-0.63342	2.632686
O	0.93126	-1.09322	3.087708	O	0.931699	-1.08512	3.092705
O	-2.83889	1.726176	0.517726	O	-2.83812	1.721139	0.517577
C	-2.6451	2.880984	-0.00641	C	-2.64611	2.87484	-0.00977
C	-3.9128	3.731207	-0.11888	C	-3.91346	3.725408	-0.11843
O	-1.74582	-0.39218	2.398979	O	-1.74034	-0.38924	2.397675
O	0.019764	1.400607	0.596194	O	0.015066	1.396224	0.573755
O	-0.06548	-1.00395	0.172236	O	-0.06387	-1.03649	0.152166
N	2.338092	-1.38658	-0.96705	N	2.34791	-1.38544	-0.9574
C	1.886953	-2.61601	-1.084	C	1.903359	-2.61772	-1.07156
N	2.846571	-3.40537	-1.62229	N	2.872035	-3.40485	-1.59642
C	3.967591	-2.61878	-1.84953	C	3.991393	-2.61411	-1.81792
C	3.633759	-1.36047	-1.43595	C	3.647774	-1.35524	-1.41436
O	2.61572	1.388592	-0.6929	O	2.612352	-1.38853	0.69978
C	3.688585	1.849553	-0.12781	C	3.67537	1.863178	-0.12699
C	3.450833	2.93248	0.920043	C	3.417838	2.949543	0.912525
O	0.509547	0.505459	-1.96127	O	0.513868	0.489276	-1.97132
O	4.830474	1.495677	-0.41938	O	4.823014	1.518254	-0.40607
O	-1.56977	3.347595	-0.40901	O	-1.57199	3.339795	-0.41776
C	3.243382	-0.65183	3.491392	C	3.242614	-0.63084	3.489516
H	-0.02348	0.621846	-4.39551	H	-0.01447	0.58376	-4.40576
H	-1.06784	1.953174	-3.87391	H	-1.07627	1.909303	-3.90408
H	-1.7912	0.374382	-4.20612	H	-1.77942	0.317989	-4.21786
H	-4.37	3.845637	0.867844	H	-4.36571	3.842709	0.870199
H	-3.68659	4.712128	-0.53816	H	-3.68843	4.705011	-0.5413
H	-4.64195	3.218505	-0.75313	H	-4.64595	3.21153	-0.74779
H	3.393837	0.349242	3.907246	H	3.391668	0.373011	3.899108
H	4.12316	-0.88972	2.891244	H	4.121414	-0.86963	2.888266
H	3.133682	-1.35858	4.315109	H	3.137229	-1.3333	4.317444
H	-0.88527	-0.68797	2.744348	H	-0.8807	-0.68249	2.747502
H	2.951482	3.788695	0.456838	H	2.90839	3.795664	0.441895
H	4.391414	3.254888	1.369854	H	4.351938	3.287692	1.364238
H	2.774999	2.546294	1.685338	H	2.744443	2.558918	1.677725
H	4.207951	-0.44346	-1.40208	H	4.217008	-0.43522	-1.38109
H	4.874301	-3.02221	-2.26949	H	4.903848	-3.01521	-2.22752
H	2.75828	-4.38932	-1.81187	H	2.790127	-4.39021	-1.78137
H	0.899864	-2.91949	-0.77333	H	0.914523	-2.92134	-0.76642
H	-3.28244	-2.00233	2.175274	H	-3.28361	-1.99198	2.182062
H	-5.19947	-3.51751	1.286791	H	-5.20502	-3.50522	1.299435
H	-5.62621	-3.09981	-1.20142	H	-5.63703	-3.08906	-1.18819
H	-3.76053	-1.12748	-1.86491	H	-3.76939	-1.12061	-1.85793

H	-0.19998	2.231543	0.124684	H	-0.21498	2.225089	0.102437

Table S31. B3LYP/6-311G*-optimized coordinate for model $^{1}Mn^{0}_{0}$. The broken-symmetry structure is on the left, ferromagnetic on the right.

Mn	1.533988	-0.25462	0.061255	Mn	1.526988	-0.25356	0.047414
Fe	-1.21192	-0.42135	0.175933	Fe	-1.20961	-0.42324	0.16414
C	2.29461	2.685143	-0.49052	C	2.304937	2.682329	-0.47865
N	2.799104	1.478587	-0.45469	N	2.800467	1.471854	-0.44687
C	4.134301	1.573112	-0.7521	C	4.138576	1.558346	-0.73365
C	4.451547	2.886217	-0.97383	C	4.467005	2.870468	-0.94431
N	3.264404	3.589082	-0.80398	N	3.283745	3.580926	-0.77878
O	1.235034	-0.26745	-1.99448	O	1.228688	-0.25619	-2.00388
C	0.096075	-0.29753	-2.53795	C	0.089801	-0.28241	-2.54664
C	0.102757	-0.36356	-4.06887	C	0.090552	-0.32967	-4.07795
O	-1.70836	-0.37263	2.158195	O	-1.68208	-0.39337	2.15459
C	-1.21895	0.159189	3.2125	C	-1.18735	0.128199	3.211491
O	-1.29956	1.354755	3.543051	O	-1.24154	1.325657	3.540986
O	3.2318	-1.2504	-0.33141	O	3.219137	-1.25599	-0.33915
C	3.907303	-2.17355	0.267281	C	3.879629	-2.19485	0.25226
C	3.139211	-3.00052	1.298048	C	3.097886	-3.0209	1.272964
O	2.061987	-0.05598	1.823901	O	2.03772	-0.07069	1.815763
O	0.333476	-1.53638	0.247944	O	0.329821	-1.55379	0.223498
O	0.184416	0.9126	0.266085	O	0.186085	0.925808	0.251468
N	-2.72536	1.298262	-0.00786	N	-2.70417	1.307836	0.011186
C	-2.74283	2.244997	0.902994	C	-2.69409	2.253783	0.922891
N	-3.66559	3.191639	0.574756	N	-3.61553	3.208286	0.614899
C	-4.27145	2.798999	-0.61364	C	-4.24978	2.821865	-0.56075
C	-3.66861	1.61887	-0.95499	C	-3.66451	1.636954	-0.91571
O	-2.70795	-1.74972	-0.21928	O	-2.7292	-1.72393	-0.22553
C	-3.63739	-2.07897	-1.02879	C	-3.6636	-2.04425	-1.03301
C	-3.90742	-3.60016	-1.04868	C	-3.94968	-3.56225	-1.05038
O	-1.02539	-0.30909	-1.98208	O	-1.03073	-0.30419	-1.9876
O	-4.32089	-1.3516	-1.75923	O	-4.34072	-1.31049	-1.76307
O	5.104439	-2.39582	0.054956	O	5.074295	-2.4309	0.040547
C	-0.4563	-0.81397	4.118953	C	-0.45019	-0.86049	4.122045
H	-0.82187	0.052811	-4.4728	H	-0.81568	0.133138	-4.47344
H	0.16561	-1.41354	-4.37351	H	0.101487	-1.37759	-4.3958
H	0.972836	0.156818	-4.47502	H	0.9818	0.155729	-4.48101
H	2.172011	-3.31229	0.898576	H	2.122845	-3.30577	0.872662
H	3.734237	-3.8603	1.618379	H	3.677056	-3.89653	1.579258
H	2.913156	-2.35318	2.149067	H	2.887618	-2.38157	2.134053
H	0.46391	-1.09226	3.597134	H	0.477885	-1.13706	3.613416
H	-1.0359	-1.72923	4.268322	H	-1.03772	-1.77374	4.25041
H	-0.21152	-0.35494	5.080464	H	-0.21994	-0.41285	5.092535
H	1.396742	0.529558	2.206593	H	1.374819	0.519655	2.195447
H	-3.01169	-4.12038	-1.40198	H	-3.06071	-4.09203	-1.40642
H	-4.75283	-3.84256	-1.69794	H	-4.79992	-3.79631	-1.69636

H	-4.1021	-3.9583	-0.03307	H	-4.14431	-3.91728	-0.0337
H	-3.87325	0.923448	-1.7552	H	-3.89139	0.943511	-1.71195
H	-5.05596	3.378647	-1.07545	H	-5.03823	3.409059	-1.00599
H	-3.896	3.99898	1.128447	H	-3.82785	4.016502	1.174494
H	-2.15666	2.233034	1.817885	H	-2.08951	2.234682	1.825355
H	1.252495	2.88658	-0.28684	H	1.26273	2.889484	-0.28133
H	3.140319	4.583404	-0.88908	H	3.167637	4.576694	-0.85793
H	5.376106	3.379874	-1.23003	H	5.397063	3.358922	-1.19034
H	4.733453	0.675245	-0.78078	H	4.73092	0.656041	-0.76389

Table S32. B3LYP/6-311G*-optimized coordinate for model $^{1}Fe^{0}_{0}$. The broken-symmetry structure is on the left, ferromagnetic on the right.

Fe	-1.47273	-0.19442	-0.74212	Fe	-1.46986	-0.20408	-0.73588
Mn	1.198152	-0.30413	0.03636	Mn	1.186426	-0.30887	0.054881
C	3.760955	0.91819	1.70645	C	3.762049	0.920476	1.690023
N	2.48671	1.071194	1.219664	N	2.480882	1.071956	1.220664
C	2.056603	2.24814	1.593545	C	2.057205	2.251382	1.594319
N	3.013841	2.891369	2.319028	N	3.025203	2.89755	2.302491
C	4.114547	2.045673	2.397429	C	4.126297	2.051399	2.369608
O	0.619419	-0.95401	1.816938	O	0.612705	-0.95934	1.835611
C	-0.59569	-1.16448	2.140625	C	-0.60242	-1.17323	2.157529
C	-0.76494	-1.73337	3.554638	C	-0.77344	-1.73612	3.573835
O	-0.02594	0.954414	0.04425	O	-0.03464	0.954711	0.079754
N	-2.89494	1.421539	0.032091	N	-2.88425	1.413334	0.021245
C	-2.4629	2.653723	-0.04859	C	-2.44589	2.644649	-0.0378
N	-3.48443	3.531412	0.157907	N	-3.46765	3.523601	0.160959
C	-4.63749	2.782176	0.366744	C	-4.62687	2.776731	0.342069
C	-4.24514	1.472496	0.284021	C	-4.23835	1.46656	0.2509
O	-1.61185	-0.9918	1.453716	O	-1.61748	-1.00865	1.466649
O	-3.13147	-1.35755	-0.90082	O	-3.13388	-1.34791	-0.91391
C	-3.95875	-2.05117	-0.2168	C	-3.9607	-2.05239	-0.23924
O	-5.05972	-1.67569	0.213163	O	-5.07238	-1.68944	0.172651
O	-1.52456	0.597912	-2.41251	O	-1.49556	0.586969	-2.40993
O	0.118513	-1.35241	-0.81997	O	0.118454	-1.38221	-0.79594
O	2.235725	0.358533	-1.51728	O	2.208619	0.350335	-1.51418
C	2.090074	1.196947	-2.47509	C	2.076101	1.218875	-2.44587
C	3.395898	1.379482	-3.27884	C	3.36656	1.366702	-3.28079
O	2.82666	-1.51345	0.34793	O	2.817312	-1.51228	0.354971
C	3.516469	-2.3545	-0.3359	C	3.513184	-2.34397	-0.33438
O	4.668059	-2.70773	-0.0465	O	4.670137	-2.68422	-0.05061
O	1.092901	1.823883	-2.83422	O	1.097499	1.897911	-2.76134
C	-3.50135	-3.49195	0.059939	C	-3.48685	-3.48501	0.048528
C	2.845407	-2.9181	-1.59311	C	2.842379	-2.91264	-1.58892
H	-0.55336	-2.80745	3.531886	H	-0.57707	-2.81319	3.552894
H	-1.78885	-1.58575	3.901739	H	-1.79431	-1.57477	3.924141
H	-1.05357	.2728634	0.244495	H	-0.05392	-1.28342	4.260303
H	-2.59706	-3.44728	0.671228	H	-2.58939	-3.42477	0.668242

H	-4.27594	-4.06477	0.577284	H	-4.25898	-4.06591	0.560455
H	-3.23015	-3.98757	-0.87719	H	-3.19963	-3.98086	-0.88369
H	3.533491	0.51374	-3.93535	H	3.444495	0.517175	-3.96763
H	4.260508	1.420962	-2.61223	H	4.250263	1.346783	-2.63876
H	3.341647	2.280246	-3.89503	H	3.337723	2.288154	-3.86746
H	-0.68214	1.029725	-2.62637	H	-0.6649	1.050737	-2.60138
H	1.774863	-3.05878	-1.43873	H	1.775837	-3.07243	-1.42581
H	3.33888	-3.84357	-1.90388	H	3.349516	-3.82761	-1.90868
H	2.939221	-2.17645	-2.39225	H	2.915418	-2.16446	-2.38397
H	4.286907	-0.00536	1.513724	H	4.284725	-0.00434	1.494203
H	5.01302	2.325843	2.925097	H	5.032573	2.333686	2.882561
H	2.936656	3.810744	2.719293	H	2.955109	3.819955	2.697044
H	1.072282	2.617339	1.347717	H	1.070362	2.620893	1.359905
H	-1.44167	2.912419	-0.28351	H	-1.41902	2.900314	-0.25082
H	-3.42464	4.533816	0.101863	H	-3.40287	4.526317	0.117949
H	-5.594	3.247736	0.548464	H	-5.58441	3.243779	0.514158
H	-4.81237	0.550864	0.346652	H	-4.81053	0.547093	0.296059

Table S33. B3LYP/6-311G*-optimized coordinate for model $^{1}Mn^{1}_{1}$. The broken-symmetry structure is on the left, ferromagnetic on the right.

C	-2.93358	-2.57419	0.150231	C	-2.92486	-2.57823	0.154305
N	-3.13515	-1.27269	0.170972	N	-3.1291	-1.27703	0.173277
C	-4.49461	-1.06273	0.137723	C	-4.48918	-1.06994	0.14417
C	-5.12594	-2.27147	0.092927	C	-5.11805	-2.28007	0.10357
N	-4.1201	-3.21989	0.100976	N	-4.11023	-3.22635	0.110064
Mn	-1.65377	0.160631	0.372743	Mn	-1.65353	0.162006	0.368296
O	-1.62265	0.139952	-1.64489	O	-1.62435	0.141407	-1.64695
C	-0.61279	0.175757	-2.40929	C	-0.61584	0.174323	-2.41404
C	-0.88801	0.284351	-3.89364	C	-0.89529	0.274076	-3.89824
Fe	1.367268	0.249525	-0.14159	Fe	1.366242	0.254061	-0.14581
O	2.040741	0.050766	1.716306	O	2.039779	0.06321	1.716753
C	1.631156	-0.49878	2.799011	C	1.63477	-0.49608	2.795875
O	0.598192	-1.19203	2.90139	O	0.604845	-1.19488	2.895391
O	-3.0082	1.506518	0.197441	O	-3.00831	1.505546	0.197367
C	-2.8688	2.774718	-0.07784	C	-2.8759	2.776856	-0.06939
C	-4.18808	3.51491	-0.18385	C	-4.20058	3.50787	-0.17458
O	-1.86862	0.075466	2.136364	O	-1.85973	0.083103	2.133001
O	-0.22706	1.351411	0.39445	O	-0.2259	1.358681	0.38431
O	-0.27995	-1.13691	0.362966	O	-0.27516	-1.13551	0.3579
N	2.548399	-1.46091	-0.70144	N	2.542844	-1.45985	-0.69795
C	2.088957	-2.6597	-1.00152	C	2.08282	-2.65844	-0.9981
N	3.113767	-3.48527	-1.31141	N	3.107443	-3.48509	-1.30545
C	4.290645	-2.76477	-1.20105	C	4.284835	-2.76569	-1.1932
C	3.924108	-1.50649	-0.82089	C	3.918816	-1.5068	-0.81472
O	2.582489	1.602951	-0.58098	O	2.586258	1.600109	-0.58915
C	3.762445	2.116706	-0.29822	C	3.765	2.11406	-0.30051
C	3.728631	3.617498	-0.08172	C	3.730042	3.615035	-0.0857

O	0.589813	0.150051	-2.04144	O	0.587168	0.153405	-2.04825
O	4.791097	1.468205	-0.23134	O	4.793098	1.465566	-0.22763
O	-1.79913	3.358239	-0.24119	O	-1.8103	3.368627	-0.22537
C	2.491071	-0.24142	4.019659	C	2.496205	-0.24491	4.016844
H	-0.11209	-0.22749	-4.46278	H	-0.11723	-0.23508	-4.46684
H	-0.86337	1.342037	-4.17222	H	-0.87889	1.330572	-4.18192
H	-1.87375	-0.11033	-4.13719	H	-1.87887	-0.12848	-4.13775
H	-4.74258	3.418773	0.75258	H	-4.75667	3.402373	0.759909
H	-4.01139	4.566854	-0.40125	H	-4.03098	4.562303	-0.38541
H	-4.80031	3.07346	-0.9743	H	-4.80755	3.066514	-0.96911
H	2.343676	0.792331	4.345558	H	2.357068	0.789961	4.342642
H	3.547068	-0.35195	3.768383	H	3.551353	-0.36327	3.76517
H	2.217355	-0.91203	4.832946	H	2.218177	-0.91395	4.829946
H	-1.06964	-0.18044	2.628936	H	-1.06185	-0.1825	2.622258
H	3.296034	4.111429	-0.95508	H	3.299849	4.107999	-0.96078
H	4.732134	3.99859	0.102682	H	4.732822	3.99665	0.101503
H	3.082813	3.849421	0.76922	H	3.081636	3.847362	0.763167
H	4.516855	-0.62239	-0.62931	H	4.512192	-0.62319	-0.62277
H	5.252983	-3.2052	-1.40126	H	5.247147	-3.20715	-1.39122
H	3.032139	-4.45381	-1.57424	H	3.02539	-4.45374	-1.56775
H	1.049175	-2.94116	-0.99495	H	1.042742	-2.93862	-0.99318
H	-1.96717	-3.04767	0.178396	H	-1.95744	-3.04967	0.180021
H	-4.24452	-4.21902	0.084662	H	-4.23263	-4.22577	0.095961
H	-6.16855	-2.53897	0.059018	H	-6.16021	-2.54978	0.073448
H	-4.89263	-0.06318	0.15727	H	-4.88926	-0.0712	0.163234
H	-0.53561	2.255566	0.142118	H	-0.53284	2.265736	0.144726
H	-0.04683	-1.39038	1.288178	H	-0.04052	-1.39113	1.282109

Table S34. B3LYP/6-311G*-optimized coordinate for model $^{1}Fe^{1}_{1}$. The broken-symmetry structure is on the left, ferromagnetic on the right.

Fe	3.914386	-0.26761	2.298918	Fe	3.90748	-0.27797	2.301792
Mn	1.064541	-1.08869	1.472782	Mn	1.064077	-1.10049	1.463303
C	-1.61391	-0.47467	-0.0214	C	-1.6086	-0.46534	-0.02566
N	-0.26355	-0.23336	0.142294	N	-0.25676	-0.23084	0.136372
C	0.093288	0.67554	-0.74774	C	0.103012	0.678968	-0.75168
N	-0.97747	1.030067	-1.48702	N	-0.96742	1.04077	-1.48781
C	-2.07177	0.309982	-1.03842	C	-2.06439	0.324624	-1.03944
O	1.977823	-1.82176	-0.06888	O	1.97465	-1.83334	-0.07725
C	3.238636	-1.81614	-0.31132	C	3.236236	-1.82464	-0.3217
C	3.650682	-2.6168	-1.52794	C	3.64588	-2.62169	-1.54172
O	2.12225	0.466048	1.330157	O	2.128297	0.457411	1.323498
N	5.396539	1.053722	1.447417	N	5.383946	1.04912	1.455517
C	5.715265	2.186202	2.046312	C	5.707036	2.174945	2.064508
N	6.736106	2.785296	1.393303	N	6.725725	2.779164	1.412902
C	7.090132	1.984513	0.321437	C	7.073726	1.988754	0.33142
C	6.247449	0.912416	0.372571	C	6.229793	0.917317	0.375485
O	4.110813	-1.24691	0.366937	O	4.107935	-1.25671	0.356971

O	5.201067	-1.5876	2.970937	O	5.203729	-1.58914	2.966286
C	5.134579	-2.87781	3.044161	C	5.147201	-2.88011	3.041841
O	4.121887	-3.55944	2.839555	O	4.1404	-3.57031	2.839554
O	3.671447	0.938969	3.661601	O	3.661854	0.919723	3.675254
O	2.396681	-1.6072	2.629953	O	2.403142	-1.63064	2.614244
O	-0.01878	-0.40875	2.876236	O	-0.01101	-0.42134	2.873447
C	0.021005	0.702684	3.546843	C	0.018314	0.697796	3.532826
C	-0.97167	0.743027	4.688664	C	-0.96952	0.736217	4.679062
O	0.170575	-2.72473	1.577854	O	0.160304	-2.72814	1.567923
C	-0.92981	-3.17989	2.155155	C	-0.93735	-3.1747	2.159235
O	-2.01449	-2.62996	2.132272	O	-2.02315	-2.6283	2.125074
O	0.782598	1.649538	3.324829	O	0.766319	1.651816	3.297765
C	6.441058	-3.5496	3.427766	C	6.460101	-3.53973	3.425117
C	-0.70746	-4.51718	2.836679	C	-0.70941	-4.49526	2.869917
H	2.836679	-2.68782	-2.24808	H	2.831177	-2.68923	-2.26145
H	3.902235	-3.62851	-1.1966	H	3.896574	-3.63497	-1.21453
H	4.53791	-2.18191	-1.98835	H	4.533181	-2.18623	-2.00147
H	6.754614	-3.20059	4.414952	H	6.774087	-3.1833	4.409481
H	6.327432	-4.6326	3.440468	H	6.354932	-4.6235	3.443392
H	7.225875	-3.2643	2.722964	H	7.240402	-3.252	2.716275
H	-0.55128	0.19337	5.535967	H	-0.54514	0.187092	5.524671
H	-1.90184	0.249722	4.406724	H	-1.89982	0.240959	4.400654
H	-1.15181	1.773053	4.993916	H	-1.15099	1.765898	4.984558
H	2.810674	1.292152	3.916208	H	2.802374	1.283972	3.917827
H	-0.23416	-5.2186	2.146434	H	-0.23307	-5.20984	2.19546
H	-1.65325	-4.92131	3.195194	H	-1.6533	-4.89535	3.237787
H	-0.02033	-4.3839	3.67656	H	-0.02274	-4.33996	3.706437
H	-2.1189	-1.18389	0.617934	H	-2.11587	-1.17493	0.6115
H	-3.0506	0.422491	-1.47315	H	-3.04335	0.442858	-1.47232
H	-0.9756	1.710895	-2.22902	H	-0.96363	1.72381	-2.22778
H	1.08552	1.081388	-0.84835	H	1.097122	1.079841	-0.85313
H	5.2296	2.549136	2.937733	H	5.225803	2.529349	2.961768
H	7.170347	3.655327	1.655368	H	7.162511	3.645795	1.681889
H	7.887901	2.247473	-0.35304	H	7.868746	2.257421	-0.34405
H	6.181323	0.049711	-0.26784	H	6.159481	0.060945	-0.27292
H	2.744912	-2.5348	2.674229	H	2.749137	-2.55753	2.664099
H	1.733028	1.150091	1.918671	H	1.730996	1.147453	1.898597

Table S35. BP86/TZP-optimized coordinate for model **(1)**. The broken-symmetry structure is on the left, ferromagnetic on the right.

Mn	1.288562	0.000008	-0.00024	Mn	1.288911	-0.00064	-0.00057
Mn	-1.45266	0.000084	-0.00025	Mn	-1.46488	-0.00055	0.000339
O	-0.10054	-0.12849	-1.18775	O	-0.15606	-0.13246	-1.22262
O	-0.1006	0.128967	1.187238	O	-0.15603	0.131347	1.222943
N	1.736444	-2.13232	-0.31317	N	1.783921	-2.20215	-0.35802
C	2.751524	-2.65329	0.421188	C	2.778539	-2.71195	0.405791
C	3.223037	-3.95195	0.181279	C	3.252597	-4.01653	0.204609

C	2.631696	-4.72094	-0.8202	C	2.683306	-4.80266	-0.79586
C	1.578394	-4.17894	-1.56276	C	1.649323	-4.27319	-1.57309
C	1.164975	-2.87924	-1.27824	C	1.233252	-2.96788	-1.31901
H	0.366221	-2.38798	-1.83478	H	0.444313	-2.4905	-1.90189
H	1.091763	-4.7459	-2.35557	H	1.180791	-4.85361	-2.367
H	2.993339	-5.72937	-1.02212	H	3.046092	-5.81587	-0.96822
H	4.049748	-4.35929	0.75884	H	4.0608	-4.41985	0.810356
C	3.289989	-1.76145	1.467999	C	3.296829	-1.8023	1.450729
C	4.259964	-2.16939	2.391169	C	4.274928	-2.1945	2.372539
H	4.670755	-3.17557	2.348708	H	4.701106	-3.19378	2.328102
N	2.76151	-0.50509	1.506235	N	2.75273	-0.55106	1.492796
C	3.178049	0.336981	2.473477	C	3.162338	0.295415	2.460354
H	2.723232	1.324047	2.486084	H	2.694801	1.27579	2.473177
C	4.137413	-0.00672	3.423015	C	4.131558	-0.03419	3.404115
H	4.43296	0.718799	4.179899	H	4.425142	0.696062	4.157016
C	4.69621	-1.28333	3.375571	C	4.705682	-1.30356	3.353723
H	5.454095	-1.58923	4.096813	H	5.47207	-1.59976	4.070124
N	2.760981	0.505221	-1.50709	N	2.753829	0.552876	-1.49548
C	3.177383	-0.33648	-2.47471	C	3.165867	-0.29293	-2.46264
C	4.137429	0.007403	-3.42365	C	4.134904	0.038059	-3.40565
C	4.69666	1.283964	-3.37533	C	4.707176	1.308021	-3.35615
C	4.261117	2.169192	-2.38987	C	4.276044	2.197823	-2.37385
C	3.290081	1.761223	-1.46781	C	3.296986	1.804676	-1.45303
H	4.671703	3.175488	-2.34748	H	4.702239	3.196939	-2.32799
H	5.454993	1.589747	-4.09614	H	5.473789	1.605358	-4.07173
H	4.435149	-0.71862	-4.1792	H	4.429058	-0.69234	-4.15826
H	2.72234	-1.32339	-2.48723	H	2.699784	-1.27417	-2.47585
C	2.751646	2.652531	-0.42045	C	2.779447	2.712421	-0.40627
C	3.223511	3.950938	-0.17992	C	3.255956	4.015717	-0.20142
H	4.050932	4.357966	-0.75683	H	4.0653	4.419157	-0.80563
C	2.631198	4.720184	0.820671	C	2.687686	4.800307	0.801004
H	2.992471	5.728824	1.022563	H	3.053725	5.811875	0.976326
C	1.57763	4.178462	1.562792	C	1.652041	4.271042	1.57581
H	1.091123	4.745803	2.355375	H	1.184199	4.850408	2.370995
C	1.164413	2.878807	1.278395	C	1.23345	2.967463	1.318331
H	0.365768	2.387724	1.835222	H	0.443457	2.48967	1.899219
N	1.735888	2.132016	0.313182	N	1.78366	2.202584	0.356178
N	-1.70736	1.971266	-0.4248	N	-1.72794	1.981479	-0.42391
C	-1.07556	2.596728	-1.44335	C	-1.09177	2.60149	-1.44084
C	-1.32551	3.927797	-1.76281	C	-1.33867	3.932976	-1.76302
C	-2.25866	4.639593	-1.00378	C	-2.26991	4.647793	-1.00549
C	-2.91321	3.994586	0.043909	C	-2.92766	4.006453	0.042945
C	-2.62662	2.651863	0.319928	C	-2.64594	2.663807	0.319732
H	-0.37302	1.98093	-2.00179	H	-0.39052	1.979661	-1.99473
H	-0.80055	4.39047	-2.59774	H	-0.81022	4.392526	-2.59721
H	-2.48059	5.682329	-1.2315	H	-2.49019	5.690775	-1.2332
H	-3.65441	4.528795	0.634315	H	-3.66656	4.544145	0.632855
C	-3.27954	1.862272	1.37206	C	-3.30334	1.879805	1.376078
N	-2.92011	0.546236	1.402897	N	-2.95326	0.562858	1.414597
C	-3.48124	-0.24955	2.335879	C	-3.50514	-0.22527	2.35712

C	-4.41291	0.210898	3.264015	C	-4.42725	0.245488	3.290062
H	-4.83569	-0.48265	3.990093	H	-4.84602	-0.43797	4.027456
H	-5.50954	1.950707	3.947019	H	-5.51222	1.993079	3.966195
C	-4.78336	1.55577	3.236583	C	-4.79326	1.590685	3.25247
C	-4.20623	2.388833	2.278934	C	-4.22173	2.416195	2.284449
H	-4.47803	3.44162	2.240898	H	-4.48935	3.469595	2.242697
H	-3.17538	-1.29262	2.338795	H	-3.19849	-1.26848	2.363873
N	-2.91989	-0.54648	-1.40355	N	-2.95415	-0.56307	-1.41246
C	-3.48161	0.249508	-2.33614	C	-3.50587	0.22556	-2.35478
C	-4.41379	-0.21068	-3.2638	C	-4.42716	-0.24504	-3.28887
C	-4.78472	-1.55556	-3.23564	C	-4.79099	-1.59098	-3.25465
C	-4.20595	-2.38938	-2.27949	C	-4.21807	-2.4172	-2.28807
C	-3.27857	-1.86272	-1.37311	C	-3.30327	-1.88022	-1.37604
H	-3.17588	1.292628	-2.33882	H	-3.1993	1.268546	-2.3619
H	-4.8365	0.482996	-3.98978	H	-4.84396	0.438937	-4.02699
H	-5.51188	-1.9502	-3.94526	H	-5.50613	-1.99439	-3.97161
H	-4.47792	-3.44212	-2.24149	H	-4.48137	-3.47206	-2.25043
N	-1.7071	-1.97106	0.424519	N	-1.72898	-1.98278	0.423808
C	-1.07566	-2.59618	1.443539	C	-1.09112	-2.60304	1.439527
H	-0.80114	-4.38946	2.598942	H	-0.80943	-4.39367	2.596571
C	-2.25864	-4.63928	1.004516	C	-2.27278	-4.64808	1.008161
C	-1.32605	-3.92697	1.763875	C	-1.33873	-3.93416	1.762833
C	-2.91333	-3.9945	-0.04337	C	-2.93181	-4.00669	-0.0397
C	-2.62621	-2.65193	-0.32019	C	-2.64818	-2.66474	-0.31896
H	-0.37277	-1.98041	2.001543	H	-0.38907	-1.98151	1.992839
H	-2.48067	-5.68187	1.232327	H	-2.49453	-5.69034	1.237849
H	-3.65475	-4.52885	-0.63326	H	-3.67283	-4.54428	-0.62696

Table S36. B3LYP/6-311G*-optimized coordinate for model **(1)**. The broken-symmetry structure is on the left, ferromagnetic on the right.

Mn	1.280626	0.000001	-1E-06	Mn	1.271955	0.000002	-1E-06
Mn	-1.47554	0	0	Mn	-1.48154	-1E-06	-1E-06
O	-0.16822	0.148983	1.173514	O	-0.17867	0.166479	1.189226
O	-0.16822	-0.14898	-1.17352	O	-0.17867	-0.16648	-1.18923
N	1.774636	2.213667	0.272513	N	1.776676	2.229539	0.263966
C	2.812767	2.668606	-0.45849	C	2.824679	2.665241	-0.46363
C	3.352342	3.938376	-0.23427	C	3.379453	3.929853	-0.24737
C	2.797121	4.749282	0.749658	C	2.826809	4.756748	0.724792
C	1.713464	4.278415	1.487197	C	1.731294	4.306665	1.457756
C	1.239153	3.001061	1.216679	C	1.243497	3.032285	1.195953
H	0.416431	2.565458	1.773049	H	0.411766	2.611351	1.750276
H	1.256315	4.879932	2.263566	H	1.275403	4.921679	2.22425
H	3.209726	5.733849	0.938987	H	3.2503	5.737787	0.908278
H	4.199749	4.296694	-0.80322	H	4.235433	4.272646	-0.81312
C	3.307794	1.739967	-1.50414	C	3.310481	1.722162	-1.50054
C	4.263515	2.116157	-2.44771	C	4.271723	2.080508	-2.44542
H	4.699667	3.105528	-2.42628	H	4.721403	3.06383	-2.42702

N	2.751752	0.500112	-1.52578
C	3.11969	-0.34974	-2.49847
H	2.640748	-1.31808	-2.49503
C	4.059924	-0.03647	-3.47048
H	4.316118	-0.76486	-4.22982
C	4.651029	1.220336	-3.43806
H	5.393437	1.506374	-4.17429
N	2.751751	-0.50011	1.525782
C	3.119688	0.349742	2.498476
C	4.059919	0.036472	3.470486
C	4.651021	-1.22034	3.438062
C	4.263509	-2.11616	2.44771
C	3.307791	-1.73997	1.50414
H	4.699659	-3.10553	2.42629
H	5.393426	-1.50638	4.174301
H	4.316112	0.764855	4.229829
H	2.640748	1.318079	2.495031
C	2.812767	-2.6686	0.458486
C	3.352344	-3.93837	0.234272
H	4.199752	-4.29669	0.803221
C	2.797124	-4.74928	-0.74966
H	3.209732	-5.73384	-0.93899
C	1.713467	-4.27841	-1.4872
H	1.256319	-4.87993	-2.26357
C	1.239154	-3.00106	-1.21668
H	0.416431	-2.56546	-1.77305
N	1.774635	-2.21367	-0.27251
N	-1.73856	-1.97831	0.436231
C	-1.10744	-2.58769	1.455844
C	-1.34405	-3.91523	1.781308
C	-2.2649	-4.63513	1.02522
C	-2.92113	-4.00279	-0.02559
C	-2.6472	-2.66436	-0.30493
H	-0.41766	-1.96575	2.010253
H	-0.82267	-4.36603	2.616658
H	-2.48002	-5.6727	1.254553
H	-3.6515	-4.5481	-0.60816
C	-3.30942	-1.88831	-1.36931
N	-2.98141	-0.57205	-1.40673
C	-3.53872	0.204298	-2.34741
C	-4.44594	-0.2772	-3.28322
H	-4.86888	0.394652	-4.01986
H	-5.49017	-2.03751	-3.96224
C	-4.78753	-1.62361	-3.24818
C	-4.20944	-2.43824	-2.27966
H	-4.46143	-3.48981	-2.2452
H	-3.24858	1.245645	-2.35301
N	-2.98141	0.572047	1.406734
C	-3.53872	-0.2043	2.347412
C	-4.44594	0.277197	3.283218

N	2.737904	0.489007	-1.51791
C	3.091361	-0.36793	-2.49036
H	2.596613	-1.32795	-2.48557
C	4.035293	-0.0707	-3.46345
H	4.278831	-0.80413	-4.22208
C	4.646229	1.176645	-3.43328
H	5.3929	1.449814	-4.1701
N	2.737907	-0.489	1.517914
C	3.091365	0.367931	2.490357
C	4.035299	0.070704	3.463449
C	4.646235	-1.17664	3.433275
C	4.271728	-2.08051	2.445419
C	3.310485	-1.72216	1.500537
H	4.721409	-3.06383	2.427019
H	5.392906	-1.44981	4.170092
H	4.278837	0.804133	4.222081
H	2.596616	1.327953	2.485575
C	2.824683	-2.66524	0.463624
C	3.379458	-3.92985	0.247363
H	4.235439	-4.27264	0.813121
C	2.826815	-4.75674	-0.72479
H	3.250308	-5.73778	-0.90828
C	1.7313	-4.30666	-1.45776
H	1.275409	-4.92168	-2.22425
C	1.243501	-3.03228	-1.19595
H	0.41177	-2.61135	-1.75028
N	1.776679	-2.22954	-0.26397
N	-1.7406	-1.97638	0.457057
C	-1.10762	-2.57045	1.484272
C	-1.33722	-3.89606	1.822502
C	-2.25211	-4.62886	1.071555
C	-2.91031	-4.01134	0.013
C	-2.64401	-2.67428	-0.27938
H	-0.42413	-1.93635	2.033089
H	-0.81507	-4.33549	2.6634
H	-2.46154	-5.66533	1.31095
H	-3.63642	-4.56694	-0.56518
C	-3.30958	-1.91219	-1.35204
N	-2.99053	-0.59442	-1.40081
C	-3.55087	0.1709	-2.34841
C	-4.4539	-0.32429	-3.28115
H	-4.88044	0.338364	-4.02401
H	-5.4858	-2.09706	-3.9462
C	-4.78672	-1.67262	-3.23482
C	-4.20476	-2.47566	-2.2588
H	-4.4502	-3.52848	-2.21589
H	-3.26653	1.213895	-2.36202
N	-2.99052	0.594412	1.400808
C	-3.55087	-0.1709	2.348415
C	-4.45389	0.324285	3.281154

C	-4.78754	1.623603	3.248176	C	-4.78672	1.672615	3.234826
C	-4.20945	2.438239	2.279657	C	-4.20476	2.475651	2.258803
C	-3.30942	1.888303	1.369306	C	-3.30957	1.912187	1.352042
H	-3.24858	-1.24565	2.353014	H	-3.26652	-1.2139	2.362027
H	-4.86888	-0.39466	4.01986	H	-4.88043	-0.33837	4.024018
H	-5.49017	2.037506	3.962242	H	-5.48579	2.097052	3.946208
H	-4.46144	3.489804	2.245194	H	-4.4502	3.528473	2.215893
N	-1.73857	1.978309	-0.43623	N	-1.7406	1.976375	-0.45706
C	-1.10745	2.587688	-1.45584	C	-1.10762	2.570446	-1.48427
H	-0.82268	4.366034	-2.61666	H	-0.81508	4.335487	-2.6634
C	-2.2649	4.635128	-1.02522	C	-2.25212	4.628855	-1.07155
C	-1.34405	3.915227	-1.78131	C	-1.33723	3.896055	-1.8225
C	-2.92113	4.002792	0.025585	C	-2.91032	4.011333	-0.013
C	-2.6472	2.664358	0.304926	C	-2.64401	2.67428	0.279385
H	-0.41767	1.965752	-2.01025	H	-0.42413	1.936351	-2.03309
H	-2.48003	5.672694	-1.25455	H	-2.46155	5.665324	-1.31095
H	-3.6515	4.548098	0.608155	H	-3.63642	4.56694	0.565186

Table S37. BP86/TZP-optimized coordinate for model **(2)**.

Fe	-1.25728	0.068135	-0.23999
Fe	1.32912	0.075146	0.224694
O	0.311148	0.075934	-1.24454
O	-0.23941	0.067953	1.229446
N	1.609832	-1.90013	0.393709
C	2.073629	-2.29134	1.612459
C	1.574813	-2.79161	-0.61745
C	2.475356	-3.60445	1.850701
C	1.966143	-4.11787	-0.4471
H	1.22531	-2.40997	-1.57462
C	2.415533	-4.53511	0.807504
H	2.849823	-3.89102	2.833572
H	1.928726	-4.80333	-1.29268
H	2.739202	-5.56324	0.968593
N	1.596101	2.053076	0.403833
C	1.55434	2.949948	-0.60235
C	2.057531	2.440999	1.624529
C	1.935912	4.278124	-0.4251
H	1.20731	2.570957	-1.56145
C	2.449357	3.755815	1.869856
C	2.38252	4.691783	0.831823
H	1.893041	4.967878	-1.26684
H	2.821797	4.039641	2.854312
H	2.698417	5.721393	0.998774
N	3.094393	0.08475	-0.72429
C	3.224558	0.088897	-2.07072
C	4.20195	0.085977	0.051519
C	4.468691	0.094155	-2.68927
H	2.292322	0.087716	-2.63232

C	5.48248	0.090631	-0.50561
C	5.618959	0.09497	-1.89369
H	4.533072	0.097032	-3.77639
H	6.360264	0.092808	0.14095
H	6.609243	0.100633	-2.34835
N	2.512394	0.075912	1.907842
C	2.126029	-1.17926	2.629863
C	3.978574	0.081408	1.545141
C	2.117246	1.323996	2.636066
N	-1.53792	2.044299	-0.40851
C	-1.50276	2.935892	0.602571
C	-2.00248	2.435324	-1.62701
C	-1.89422	4.262132	0.432144
H	-1.15305	2.554464	1.559747
C	-2.40444	3.748346	-1.86529
C	-2.34425	4.679147	-0.82225
H	-1.85674	4.947665	1.277665
H	-2.77929	4.034541	-2.84801
H	-2.6676	5.707402	-0.9833
N	-3.02229	0.060006	0.709567
C	-3.15246	0.056155	2.056012
C	-4.13002	0.058794	-0.06599
C	-4.39658	0.051195	2.674667
H	-2.22027	0.057227	2.61771
C	-5.41047	0.054036	0.491222
C	-5.54697	0.050118	1.879277
H	-4.4608	0.048445	3.7618
H	-6.28819	0.051568	-0.15543
H	-6.53724	0.044217	2.333968
N	-1.52476	-1.90883	-0.41932
C	-1.98645	-2.29701	-1.63983
C	-1.48291	-2.80563	0.586837
C	-2.3783	-3.61185	-1.88507
C	-1.86449	-4.13383	0.409303
H	-1.13594	-2.42673	1.546041
C	-2.3112	-4.54797	-0.84725
H	-2.7507	-3.89552	-2.86954
H	-1.82144	-4.8233	1.251336
H	-2.62684	-5.57764	-1.01389
C	-3.90702	0.06281	-1.55958
C	-2.05468	1.323236	-2.64437
C	-2.04679	-1.18013	-2.65142
N	-2.44103	0.068267	-1.92249
H	-4.38473	-0.81922	-2.00871
H	-4.38969	0.944604	-2.0039
H	4.456105	0.963329	1.994717
H	4.461414	-0.80052	1.989093
H	1.124737	-1.01224	3.048882
H	2.816962	-1.40333	3.453616
H	2.806072	1.547914	3.461583

H	1.117083	1.148612	3.054565
H	-1.04731	-1.00575	-3.07183
H	-2.73661	-1.40384	-3.47611
H	-2.7455	1.547305	-3.46819
H	-1.05327	1.156462	-3.0632

Table S38. B3LYP/6-311G*-optimized coordinate for model **(2)**.

Fe	-1.30476	0.067988	-0.26718
Fe	1.385909	0.075847	0.252158
O	0.255486	0.075417	-1.18973
O	-0.21916	0.068292	1.166646
N	1.69806	-1.90776	0.426468
C	2.138178	-2.28953	1.647985
C	1.637303	-2.80738	-0.56794
C	2.507474	-3.6025	1.906933
C	1.991728	-4.13583	-0.37908
H	1.300594	-2.43113	-1.52532
C	2.43043	-4.54145	0.878921
H	2.866731	-3.88393	2.890178
H	1.940293	-4.83167	-1.20749
H	2.727297	-5.5693	1.054892
N	1.684716	2.061883	0.436034
C	1.617532	2.96625	-0.55368
C	2.123581	2.440103	1.659135
C	1.963625	4.295909	-0.35823
H	1.282589	2.592726	-1.51275
C	2.48481	3.75403	1.924559
C	2.400876	4.697748	0.901518
H	1.907008	4.995759	-1.18291
H	2.843123	4.032668	2.908948
H	2.691432	5.726518	1.082583
N	3.134967	0.083993	-0.75351
C	3.265366	0.088761	-2.09278
C	4.232355	0.086602	0.025068
C	4.506134	0.095927	-2.70918
H	2.336849	0.08663	-2.65107
C	5.51038	0.093927	-0.52615
C	5.649401	0.098583	-1.91028
H	4.576125	0.099432	-3.78997
H	6.383823	0.095953	0.116599
H	6.635974	0.104328	-2.35965
N	2.568612	0.075758	1.9296
C	2.199948	-1.1712	2.657665
C	4.02185	0.080306	1.526879
C	2.193002	1.317262	2.663387
N	-1.62105	2.048797	-0.44238
C	-1.55522	2.9458	0.554122
C	-2.06664	2.431672	-1.66205

C	-1.91047	4.274441	0.368685
H	-1.21449	2.566978	1.508817
C	-2.43608	3.745451	-1.91601
C	-2.35432	4.682465	-0.8866
H	-1.85496	4.96855	1.198263
H	-2.79897	4.028824	-2.89735
H	-2.65137	5.71077	-1.05952
N	-3.06875	0.059533	0.735703
C	-3.19959	0.054962	2.074876
C	-4.1652	0.057458	-0.04351
C	-4.44071	0.048307	2.69061
H	-2.27082	0.056846	2.632688
C	-5.44361	0.050775	0.506777
C	-5.58343	0.046174	1.89092
H	-4.51139	0.044828	3.771363
H	-6.31668	0.049207	-0.13649
H	-6.57032	0.040939	2.339617
N	-1.60812	-1.9145	-0.45271
C	-2.05166	-2.29371	-1.67428
C	-1.53587	-2.81643	0.538887
C	-2.4126	-3.60849	-1.93518
C	-1.88233	-4.14638	0.346371
H	-1.19721	-2.44047	1.49546
C	-2.32414	-4.55048	-0.91091
H	-2.77404	-3.88895	-2.91789
H	-1.82178	-4.84464	1.17211
H	-2.61452	-5.57976	-1.08927
C	-3.95396	0.063172	-1.54507
C	-2.13181	1.316057	-2.67393
C	-2.12421	-1.17324	-2.68028
N	-2.50157	0.068414	-1.94752
H	-4.4445	-0.8083	-1.98475
H	-4.44876	0.935438	-1.9784
H	4.512921	0.951218	1.967059
H	4.515888	-0.79272	1.959529
H	1.209886	-1.01747	3.090708
H	2.898382	-1.38861	3.470331
H	2.890572	1.535256	3.476636
H	1.204188	1.155543	3.096426
H	-1.13573	-1.01053	-3.11336
H	-2.82224	-1.39378	-3.49235
H	-2.83109	1.536356	-3.48499
H	-1.14226	1.161805	-3.10763

Table S39. Broken-symmetry BP86/TZP-optimized coordinate for model **(3)**.

Fe	-1.32292	0.067251	-0.28132
Fe	1.394878	0.076792	0.266284
O	0.282439	0.075085	-1.14223

O	-0.21058	0.068847	1.127129
N	1.712701	-1.91157	0.459546
C	2.174455	-2.2929	1.684455
C	1.662682	-2.80595	-0.55164
C	2.564369	-3.60811	1.927815
C	2.049243	-4.13137	-0.36998
H	1.318053	-2.43307	-1.51374
C	2.50138	-4.5419	0.886944
H	2.936158	-3.89344	2.912569
H	2.009531	-4.82135	-1.21225
H	2.824859	-5.57016	1.051653
N	1.697733	2.066454	0.469868
C	1.642053	2.965697	-0.53672
C	2.155464	2.444707	1.697248
C	2.018506	4.292992	-0.34767
H	1.301164	2.595392	-1.50117
C	2.535132	3.761562	1.948011
C	2.466314	4.700257	0.911885
H	1.974288	4.987198	-1.1862
H	2.90453	4.044412	2.934386
H	2.78188	5.73009	1.082244
N	3.141084	0.085937	-0.71932
C	3.253416	0.089099	-2.06969
C	4.256169	0.089648	0.05098
C	4.490898	0.095752	-2.69949
H	2.318702	0.086246	-2.62744
C	5.529141	0.096572	-0.52103
C	5.64913	0.099861	-1.91231
H	4.547039	0.098357	-3.78724
H	6.415941	0.097658	0.113684
H	6.635372	0.103422	-2.37714
N	2.592336	0.07698	1.946733
C	2.229483	-1.17466	2.689887
C	4.056087	0.085883	1.547877
C	2.218789	1.321362	2.696621
N	-1.64063	2.055592	-0.47652
C	-1.59154	2.950788	0.533994
C	-2.10115	2.436043	-1.70226
C	-1.97744	4.276199	0.350886
H	-1.2479	2.5787	1.496764
C	-2.49079	3.751208	-1.94695
C	-2.42805	4.685876	-0.90685
H	-1.93829	4.966846	1.192608
H	-2.8625	4.036204	-2.93177
H	-2.75086	5.714225	-1.07276
N	-3.06859	0.058525	0.705526
C	-3.18094	0.052135	2.056345
C	-4.18359	0.057209	-0.06519
C	-4.41908	0.048427	2.685051
H	-2.24687	0.048279	2.616733

C	-5.45673	0.049618	0.506266
C	-5.57706	0.045561	1.897439
H	-4.47613	0.048031	3.772741
H	-6.34334	0.048615	-0.1288
H	-6.56352	0.041436	2.361837
N	-1.62676	-1.92228	-0.48349
C	-2.08581	-2.30149	-1.71011
C	-1.57104	-2.82038	0.524099
C	-2.46661	-3.61835	-1.95903
C	-1.94807	-4.14771	0.336684
H	-1.22985	-2.44896	1.488043
C	-2.39684	-4.55605	-0.92216
H	-2.83685	-3.9022	-2.94474
H	-1.9038	-4.84111	1.175898
H	-2.7127	-5.58597	-1.0914
C	-3.98394	0.062889	-1.56227
C	-2.15634	1.316767	-2.70665
C	-2.14961	-1.17952	-2.71082
N	-2.52039	0.066386	-1.9619
H	-4.47274	-0.81678	-2.00439
H	-4.47306	0.945382	-1.99805
H	4.53901	0.969308	1.988498
H	4.550695	-0.79298	1.985194
H	1.237508	-1.01835	3.136756
H	2.938871	-1.37723	3.50274
H	2.926553	1.525891	3.510494
H	1.22774	1.154154	3.141029
H	-1.15968	-1.01526	-3.1592
H	-2.8587	-1.38363	-3.52358
H	-2.86573	1.519649	-3.51951
H	-1.16428	1.158837	-3.15224

Table S40. Broken-symmetry B3LYP/6-311G*-optimized coordinate for model **(3)**.

Fe	-1.31419	0.067575	-0.3438
Fe	1.385104	0.076572	0.329058
O	0.202822	0.074607	-1.18018
O	-0.13206	0.069482	1.165407
N	1.696457	-1.90259	0.453587
C	2.154822	-2.29035	1.67219
C	1.641047	-2.79113	-0.55364
C	2.542362	-3.60047	1.912108
C	2.019424	-4.11503	-0.37914
H	1.29658	-2.4146	-1.50781
C	2.472449	-4.52894	0.872022
H	2.912359	-3.88997	2.889414
H	1.976091	-4.80194	-1.21586
H	2.787853	-5.55404	1.033494
N	1.681665	2.057495	0.46273

C	1.619317	2.950464	-0.54017
C	2.13687	2.44297	1.683251
C	1.987189	4.276466	-0.35919
H	1.277869	2.575947	-1.49622
C	2.514223	3.754886	1.929501
C	2.437027	4.687825	0.893957
H	1.938371	4.967064	-1.19256
H	2.881918	4.042519	2.908229
H	2.744421	5.714558	1.060419
N	3.127637	0.085419	-0.70821
C	3.232443	0.089024	-2.05335
C	4.238009	0.087618	0.055355
C	4.46477	0.094901	-2.68493
H	2.300632	0.086982	-2.60566
C	5.505328	0.093415	-0.51559
C	5.62139	0.097108	-1.90332
H	4.518126	0.097701	-3.76694
H	6.3893	0.095062	0.113039
H	6.600813	0.101674	-2.36898
N	2.570599	0.077257	1.954852
C	2.213121	-1.18169	2.689816
C	4.036217	0.083658	1.552092
C	2.203676	1.330036	2.695673
N	-1.62451	2.046782	-0.46933
C	-1.56796	2.935579	0.537604
C	-2.08329	2.434345	-1.68769
C	-1.94549	4.259726	0.3629
H	-1.22327	2.559185	1.491769
C	-2.47012	3.744712	-1.92789
C	-2.39897	4.673475	-0.88818
H	-1.90123	4.946844	1.199402
H	-2.84043	4.034068	-2.90511
H	-2.71378	5.698706	-1.04999
N	-3.0563	0.058913	0.693691
C	-3.16099	0.055378	2.039008
C	-4.16689	0.056555	-0.06968
C	-4.39332	0.049443	2.670692
H	-2.22907	0.057516	2.591124
C	-5.43417	0.05065	0.50145
C	-5.55001	0.047056	1.889281
H	-4.4464	0.046731	3.752729
H	-6.31825	0.048857	-0.127
H	-6.52945	0.042416	2.354889
N	-1.61004	-1.91339	-0.47783
C	-2.06591	-2.29897	-1.69791
C	-1.54674	-2.80626	0.52508
C	-2.44297	-3.6111	-1.94395
C	-1.91427	-4.13242	0.344432
H	-1.20497	-2.43161	1.480979
C	-2.3648	-4.54395	-0.90844

H	-2.8112	-3.89881	-2.92244
H	-1.86477	-4.82293	1.177836
H	-2.672	-5.57075	-1.07481
C	-3.96549	0.0606	-1.5664
C	-2.14269	1.325423	-2.70503
C	-2.13358	-1.18613	-2.71045
N	-2.49996	0.066747	-1.96966
H	-4.44507	-0.81401	-2.00979
H	-4.45125	0.933756	-2.00594
H	4.51555	0.958439	1.995443
H	4.522136	-0.78934	1.991806
H	1.2324	-1.03319	3.145549
H	2.92975	-1.38267	3.489086
H	2.918806	1.532763	3.495846
H	1.224159	1.171988	3.150793
H	-1.15451	-1.02823	-3.16645
H	-2.84936	-1.38911	-3.50997
H	-2.85988	1.526544	-3.50376
H	-1.16243	1.176643	-3.16153

Table S41. B3LYP/6-311G*-optimized coordinate for model **(4)**. The broken-symmetry structure is on the left, ferromagnetic on the right.

Mn	-3.59291	-2.80627	2.273314	Mn	-3.59759	-2.80972	2.27157
Mn	-1.20763	-1.34395	1.35386	Mn	-1.20371	-1.34462	1.347621
C	2.623689	1.065886	-0.00471	C	2.622755	1.073564	0.000003
C	1.505189	0.280135	0.365985	C	1.506112	0.283337	0.366559
C	0.347338	0.269933	-0.46532	C	0.351194	0.269209	-0.46886
C	0.355655	1.045361	-1.63795	C	0.360278	1.045384	-1.64085
C	1.462709	1.806961	-1.96769	C	1.465535	1.811463	-1.96645
C	2.608272	1.824768	-1.15318	C	2.608215	1.833124	-1.14809
C	1.581456	-0.49924	1.558396	C	1.581535	-0.49624	1.559091
N	0.644492	-1.23792	2.076589	N	0.645613	-1.23799	2.074696
C	0.92443	-1.97059	3.326606	C	0.924024	-1.97019	3.325543
C	0.53614	-3.45185	3.22179	C	0.534859	-3.45133	3.221698
C	-0.97396	-3.70512	3.351441	C	-0.97552	-3.70339	3.351196
C	-1.44976	-3.79653	4.816672	C	-1.45149	-3.7959	4.816346
C	-2.91143	-3.37951	5.070762	C	-2.91322	-3.37853	5.069433
N	-3.86123	-3.75414	4.009304	N	-3.86323	-3.75486	4.008454
C	-4.88766	-4.5	4.276607	C	-4.89	-4.49994	4.276891
C	-5.98021	-4.78759	3.396297	C	-5.98317	-4.78825	3.397514
C	-6.17265	-4.07392	2.171369	C	-6.1771	-4.07511	2.172437
C	-7.32091	-4.36236	1.407199	C	-7.32596	-4.36413	1.409483
C	-8.23175	-5.31327	1.82884	C	-8.23609	-5.31517	1.832373
C	-8.04922	-6.01742	3.032305	C	-8.05218	-6.01879	3.035924
C	-6.94299	-5.74398	3.804375	C	-6.94533	-5.7447	3.806875
O	-5.34323	-3.1426	1.748498	O	-5.34847	-3.14336	1.748807
O	-3.87327	-0.87898	3.149439	O	-3.87202	-0.87799	3.14098

C	-3.15182	0.153934	3.055202	C	-3.14803	0.153075	3.049315
C	-3.59181	1.405021	3.777805	C	-3.5813	1.402631	3.778689
O	-0.71229	-0.46633	-0.18881	O	-0.70595	-0.47248	-0.19656
O	-1.68929	-2.67164	2.667294	O	-1.69034	-2.66937	2.668358
O	-2.91823	-1.97032	0.633614	O	-2.917	-1.97535	0.63041
C	-3.71909	-1.21992	-0.28448	C	-3.71822	-1.22179	-0.28492
O	-2.05974	0.206918	2.407278	O	-2.0579	0.205487	2.397502
H	-1.21684	-4.64307	2.84608	H	-1.21833	-4.64166	2.84604
H	-0.52592	1.030642	-2.26759	H	-0.51903	1.027467	-2.27356
H	1.442798	2.401983	-2.87488	H	1.44639	2.406919	-2.87335
H	3.465151	2.428197	-1.42716	H	3.463701	2.43999	-1.41882
H	3.500292	1.065199	0.636134	H	3.497247	1.075912	0.643706
H	-7.47167	-3.80588	0.489615	H	-7.47777	-3.808	0.49186
H	-9.10823	-5.5118	1.220666	H	-9.11308	-5.51422	1.225109
H	-8.77628	-6.75433	3.351402	H	-8.77869	-6.75582	3.355993
H	-6.7954	-6.26514	4.745667	H	-6.79672	-6.26548	4.748214
H	-4.94337	-4.94118	5.274699	H	-4.94545	-4.93976	5.275581
H	2.537184	-0.46806	2.085591	H	2.535758	-0.46225	2.088803
H	-4.58562	-1.82049	-0.56345	H	-4.5833	-1.8224	-0.56841
H	-4.05969	-0.2875	0.17139	H	-4.06172	-0.29242	0.175161
H	-3.1187	-0.99341	-1.16549	H	-3.11741	-0.98921	-1.16409
H	-4.66498	1.391123	3.960561	H	-4.65269	1.388537	3.971503
H	-3.08015	1.453904	4.744177	H	-3.06007	1.450127	4.739999
H	-3.30791	2.293026	3.213592	H	-3.30287	2.291685	3.21332
H	-1.28902	-4.82687	5.14978	H	-1.29112	-4.82628	5.149543
H	-0.83057	-3.16545	5.462826	H	-0.83288	-3.16488	5.463191
H	0.899781	-3.84023	2.265315	H	0.898379	-3.84041	2.26543
H	1.05752	-4.01641	4.000514	H	1.056369	-4.01554	4.000601
H	-3.24808	-3.79491	6.02516	H	-3.25039	-3.79233	6.02435
H	-2.97397	-2.29331	5.153309	H	-2.97573	-2.29221	5.150125
H	1.989983	-1.88453	3.554846	H	1.989468	-1.88429	3.554321
H	0.375012	-1.47922	4.135137	H	0.374164	-1.47786	4.13316
O	-3.11706	-4.97149	1.29672	O	-3.12159	-4.97384	1.295798
C	-3.09753	-5.14085	-0.13435	C	-3.09951	-5.14524	-0.13504
H	-3.60129	-5.70657	1.689801	H	-3.60132	-5.71137	1.689779
H	-4.11215	-5.15975	-0.53886	H	-4.1136	-5.17227	-0.54045
H	-2.56965	-4.28072	-0.5357	H	-2.57758	-4.28174	-0.53688
H	-2.56985	-6.05841	-0.4033	H	-2.56481	-6.0593	-0.40212

Table S42. BP86/6-311G*-optimized coordinate for model **(4)**. The broken-symmetry structure is on the left, ferromagnetic on the right.

Mn	-3.59574	-2.7654	2.311158	Mn	-3.60558	-2.77281	2.307748
Mn	-1.20973	-1.33402	1.384324	Mn	-1.20058	-1.33988	1.369308
C	2.656708	1.01816	-0.04423	C	2.648985	1.047845	-0.02547
C	1.519726	0.261003	0.354843	C	1.518583	0.274464	0.360678
C	0.34054	0.271382	-0.46455	C	0.3487	0.26874	-0.47237
C	0.351035	1.03488	-1.65436	C	0.361723	1.032548	-1.66171

C	1.478582	1.76931	-2.01106
C	2.641521	1.768018	-1.20904
C	1.592875	-0.51138	1.554247
N	0.634725	-1.23597	2.086358
C	0.920957	-1.97355	3.33653
C	0.526495	-3.45714	3.225367
C	-0.98825	-3.69631	3.369348
C	-1.45439	-3.79698	4.840586
C	-2.91641	-3.36424	5.09506
N	-3.86242	-3.73061	4.023416
C	-4.86983	-4.52847	4.274259
C	-5.94884	-4.8295	3.378475
C	-6.15624	-4.08221	2.162812
C	-7.30163	-4.37782	1.382914
C	-8.1935	-5.37062	1.775828
C	-7.99423	-6.10807	2.964788
C	-6.89229	-5.82702	3.755742
O	-5.34625	-3.11195	1.771307
O	-3.89979	-0.83941	3.159113
C	-3.16366	0.197793	3.053814
C	-3.60536	1.459721	3.766358
O	-0.74051	-0.4317	-0.15815
O	-1.69821	-2.62618	2.717799
O	-2.92347	-1.9524	0.661287
C	-3.7351	-1.16274	-0.22354
O	-2.06088	0.245538	2.403321
H	-1.26209	-4.6248	2.840469
H	-0.54735	1.036073	-2.27613
H	1.459232	2.358888	-2.93264
H	3.516184	2.351471	-1.50515
H	3.549814	1.002071	0.589342
H	-7.46623	-3.79359	0.474138
H	-9.06982	-5.57573	1.153483
H	-8.70818	-6.87968	3.261574
H	-6.73298	-6.37509	4.690517
H	-4.91059	-4.99802	5.270653
H	2.559881	-0.49691	2.081393
H	-4.59358	-1.77035	-0.54514
H	-4.10078	-0.25672	0.284906
H	-3.1237	-0.875	-1.09048
H	-4.69409	1.469866	3.905577
H	-3.13464	1.490602	4.76369
H	-3.27432	2.35203	3.218454
H	-1.30307	-4.84055	5.166845
H	-0.82016	-3.1714	5.493352
H	0.882348	-3.84462	2.255448
H	1.054476	-4.03459	4.003261
H	-3.26496	-3.78073	6.055722
H	-2.96966	-2.26787	5.178169
H	1.996943	-1.88871	3.562508

C	1.482637	1.783385	-2.00526
C	2.636064	1.798422	-1.18994
C	1.590934	-0.49925	1.559658
N	0.637557	-1.23605	2.083281
C	0.921333	-1.974	3.334214
C	0.524147	-3.45685	3.223094
C	-0.99162	-3.69278	3.366753
C	-1.4576	-3.80465	4.837281
C	-2.91787	-3.36641	5.092139
N	-3.86692	-3.73231	4.022398
C	-4.876	-4.52746	4.276278
C	-5.95762	-4.82865	3.383809
C	-6.16719	-4.08431	2.166585
C	-7.31476	-4.3803	1.390215
C	-8.207	-5.37084	1.788014
C	-8.00588	-6.10535	2.978486
C	-6.90165	-5.82378	3.766032
O	-5.35697	-3.11562	1.771636
O	-3.89717	-0.83128	3.13275
C	-3.15267	0.199762	3.0344
C	-3.57533	1.458514	3.764311
O	-0.72419	-0.45259	-0.1789
O	-1.70062	-2.61456	2.728863
O	-2.91683	-1.97183	0.650303
C	-3.72729	-1.17799	-0.23221
O	-2.05457	0.244119	2.374415
H	-1.26675	-4.61767	2.83176
H	-0.52916	1.020544	-2.29405
H	1.465394	2.372957	-2.92686
H	3.505557	2.394614	-1.47571
H	3.535189	1.044075	0.617873
H	-7.48077	-3.79819	0.48035
H	-9.08513	-5.57639	1.168374
H	-8.7202	-6.87514	3.279073
H	-6.74086	-6.36967	4.701817
H	-4.91561	-4.99461	5.273815
H	2.553745	-0.475	2.09403
H	-4.57866	-1.78797	-0.56825
H	-4.10486	-0.28078	0.283435
H	-3.11179	-0.87516	-1.09113
H	-4.66133	1.473466	3.922748
H	-3.0861	1.480351	4.752941
H	-3.24961	2.353145	3.216866
H	-1.31133	-4.85101	5.15695
H	-0.82228	-3.18577	5.495541
H	0.879555	-3.8447	2.253069
H	1.052247	-4.03503	4.000378
H	-3.26763	-3.77915	6.053979
H	-2.96647	-2.26964	5.172322
H	1.997339	-1.89029	3.560355

H	0.369969	-1.48004	4.155674	H	0.370115	-1.47943	4.152506
O	-3.11761	-4.94616	1.332011	O	-3.1251	-4.95447	1.329229
C	-3.15176	-5.10641	-0.1082	C	-3.15958	-5.12065	-0.11028
H	-3.64921	-5.66034	1.729031	H	-3.64547	-5.67452	1.730344
H	-4.18539	-5.06588	-0.48756	H	-4.19444	-5.09681	-0.48785
H	-2.58546	-4.26434	-0.52027	H	-2.60659	-4.27149	-0.52582
H	-2.67755	-6.05566	-0.40384	H	-2.6721	-6.0639	-0.40366

Table S41. B3LYP/6-311G*-optimized coordinate for model **(5)**. The broken-symmetry structure is on the left, ferromagnetic on the right.

Mn	-1.37087	-0.20927	0.20965	Mn	-1.35396	-0.27466	0.194054
Mn	1.30549	-0.29509	0.07935	Mn	1.332397	-0.26015	0.052369
C	5.302448	0.393563	2.738323	C	5.272146	-0.23108	2.869202
C	4.078765	0.835282	3.238608	C	4.03364	0.076896	3.43131
C	2.938038	0.624661	2.480842	C	2.921658	0.104909	2.607145
N	2.983708	0.002531	1.290429	N	3.009805	-0.14629	1.288388
C	4.15317	-0.44673	0.807897	C	4.194757	-0.44654	0.735792
C	5.341042	-0.25482	1.508351	C	5.353472	-0.49813	1.507711
N	1.943577	1.457624	-0.79511	N	1.878957	1.627385	-0.56872
C	2.791334	1.324888	-1.83317	C	2.58499	1.680883	-1.71529
C	3.397404	2.433109	-2.41447	C	3.080397	2.886356	-2.19828
C	3.118091	3.699895	-1.90992	C	2.839982	4.053167	-1.47665
C	2.244615	3.823687	-0.83196	C	2.116039	3.981953	-0.28871
C	1.678912	2.67663	-0.29572	C	1.650163	2.746312	0.136764
C	2.972985	-0.07877	-2.34252	C	2.753324	0.358721	-2.41309
N	2.842031	-1.08902	-1.2538	N	2.88879	-0.73827	-1.4135
C	4.106494	-1.25459	-0.47044	C	4.235131	-0.72519	-0.75296
N	-2.84289	-1.26436	-0.92929	N	-2.80386	-1.14631	-1.10172
C	-3.19853	-2.53972	-0.68962	C	-3.11368	-2.45624	-1.08344
C	-4.07052	-3.23293	-1.51653	C	-3.96696	-3.02831	-2.01516
C	-4.59482	-2.5841	-2.63025	C	-4.52066	-2.21799	-3.00171
C	-4.23645	-1.26069	-2.87041	C	-4.20873	-0.86193	-3.01322
C	-3.35494	-0.6276	-2.00164	C	-3.34377	-0.35432	-2.05018
C	-2.91035	0.802898	-2.20925	C	-2.95061	1.105999	-2.02036
N	-2.63205	1.450035	-0.91195	N	-2.6588	1.538458	-0.64168
C	-1.84002	2.70308	-1.05135	C	-1.87843	2.804263	-0.58644
C	-2.43716	3.79942	-1.93535	C	-2.49679	4.020571	-1.27837
O	0.117654	0.508275	1.103598	O	0.128808	0.333605	1.202634
O	-0.04382	-0.5841	-1.02905	O	-0.01581	-0.41583	-1.09764
O	-1.00565	-2.09751	1.315938	O	-0.9315	-2.30697	0.959725
C	0.137976	-2.58555	1.396188	C	0.226863	-2.76621	0.972873
C	0.347911	-3.93326	2.036969	C	0.488403	-4.18692	1.401688
N	-2.69154	0.476884	1.689119	N	-2.68502	0.127169	1.756201
C	-3.64897	1.366821	1.361568	C	-3.64614	1.059696	1.59641
C	-4.45412	1.950301	2.33494	C	-4.44399	1.459846	2.663486
C	-4.27861	1.594737	3.66797	C	-4.26041	0.873841	3.911425
C	-3.29181	0.668915	3.99696	C	-3.27351	-0.09614	4.064565

C	-2.51322	0.139991	2.980543	C	-2.50068	-0.43513	2.965924
C	-3.8626	1.643927	-0.11033	C	-3.87637	1.587342	0.197363
O	1.202024	-2.01671	0.936068	O	1.272795	-2.09397	0.624833
C	2.396235	-2.41025	-1.83229	C	2.596678	-2.07192	-2.05383
C	3.334452	-3.02677	-2.86646	C	3.477217	-2.44422	-3.24449
H	0.297932	-4.70543	1.262791	H	0.778562	-4.78289	0.532082
H	-0.4385	-4.13505	2.762594	H	-0.40241	-4.62342	1.848633
H	1.327296	-3.99827	2.508882	H	1.318588	-4.22487	2.108492
H	1.003721	2.693937	0.550218	H	1.081435	2.613379	1.048549
H	4.078925	2.304071	-3.24722	H	3.650136	2.909207	-3.11996
H	2.013282	4.790779	-0.40275	H	1.922066	4.865832	0.306394
H	3.583742	4.576553	-2.34588	H	3.223141	5.003181	-1.83178
H	2.177461	-0.28038	-3.06488	H	1.850519	0.152393	-2.99367
H	3.9242	-0.18292	-2.87033	H	3.599866	0.383099	-3.10339
H	2.263666	-3.07789	-0.98251	H	2.68013	-2.81112	-1.25829
H	1.405446	-2.23356	-2.25181	H	1.546381	-2.03801	-2.34585
H	4.335225	-3.21759	-2.47182	H	4.542506	-2.46792	-3.002
H	2.927159	-3.99156	-3.17656	H	3.206908	-3.44889	-3.57668
H	3.432014	-2.42022	-3.76927	H	3.336606	-1.77946	-4.09909
H	-1.72689	-0.57677	3.175098	H	-1.71388	-1.17473	3.025977
H	-5.21302	2.669705	2.048932	H	-5.20518	2.217021	2.513947
H	-3.12271	0.364062	5.022224	H	-3.09962	-0.57948	5.017866
H	-4.90071	2.036153	4.438461	H	-4.87735	1.17171	4.751764
H	-2.75984	-2.99103	0.190343	H	-2.65356	-3.03574	-0.29443
H	-4.33444	-4.25724	-1.28395	H	-4.19397	-4.08581	-1.96002
H	-4.64035	-0.72132	-3.7196	H	-4.63587	-0.20033	-3.75827
H	-5.28141	-3.09515	-3.29578	H	-5.1937	-2.63175	-3.74424
H	-1.97983	0.806756	-2.78533	H	-2.03889	1.240928	-2.6103
H	-3.66043	1.343799	-2.79631	H	-3.73461	1.708177	-2.49298
H	-4.27826	2.645915	-0.24543	H	-4.29348	2.597164	0.243606
H	-4.6288	0.950996	-0.46873	H	-4.64776	0.965162	-0.26555
H	-1.6771	3.081497	-0.03865	H	-1.70732	3.018036	0.471952
H	-0.8621	2.409161	-1.43756	H	-0.90225	2.584926	-1.02261
H	-3.42092	4.132546	-1.59781	H	-3.47584	4.288128	-0.87506
H	-1.78372	4.674681	-1.91399	H	-1.84807	4.887452	-1.13303
H	-2.52404	3.490642	-2.97899	H	-2.60266	3.876797	-2.35568
H	1.953889	0.944936	2.802279	H	1.925118	0.323424	2.972522
H	4.009231	1.335696	4.196471	H	3.930889	0.285026	4.489063
H	6.278534	-0.61757	1.102179	H	6.303427	-0.74717	1.047926
H	6.215683	0.54913	3.301543	H	6.162988	-0.2674	3.486042
H	4.179897	-2.30705	-0.18738	H	4.719745	-1.68977	-0.91185
H	4.980084	-1.03811	-1.09125	H	4.878207	0.015428	-1.23682

Table S42. BP86/6-311G*-optimized coordinate for model **(5)**. The broken-symmetry structure is on the left, ferromagnetic on the right.

Mn	-1.35434	-0.2298	0.222505	Mn	-1.37153	-0.19897	0.20271
Mn	1.295959	-0.26056	0.047519	Mn	1.312324	-0.30624	0.07761

C	5.28337	0.397722	2.711754
C	4.056478	0.850266	3.214696
C	2.904877	0.642551	2.457143
N	2.941875	0.010264	1.262169
C	4.118687	-0.45081	0.776771
C	5.315333	-0.26055	1.47766
N	1.921108	1.494209	-0.76907
C	2.801394	1.389232	-1.79795
C	3.439605	2.515835	-2.32539
C	3.165628	3.774628	-1.77791
C	2.264158	3.870727	-0.7105
C	1.664645	2.707694	-0.22707
C	2.971838	-0.00217	-2.34915
N	2.7937	-1.04522	-1.28846
C	4.048361	-1.27262	-0.49309
N	-2.8387	-1.31511	-0.86295
C	-3.24336	-2.57367	-0.57328
C	-4.12805	-3.27802	-1.39112
C	-4.61614	-2.65985	-2.54785
C	-4.21293	-1.35128	-2.83816
C	-3.32135	-0.70571	-1.97607
C	-2.83023	0.706296	-2.21541
N	-2.56161	1.371715	-0.91597
C	-1.75106	2.619549	-1.0671
C	-2.32341	3.701631	-1.9894
O	0.077496	0.531978	1.090571
O	-0.09398	-0.54392	-1.05478
O	-1.02133	-2.05385	1.329647
C	0.131531	-2.56895	1.372402
C	0.316842	-3.92744	2.006462
N	-2.67908	0.460345	1.690047
C	-3.62805	1.363718	1.337968
C	-4.43827	1.980356	2.297704
C	-4.27789	1.645162	3.646079
C	-3.30131	0.706809	4.001495
C	-2.51526	0.145099	2.996869
C	-3.81547	1.604133	-0.14505
O	1.196904	-2.01813	0.884034
C	2.324417	-2.33974	-1.91893
C	3.271617	-2.9502	-2.95292
H	0.1064	-4.70675	1.254501
H	-0.39383	-4.06523	2.832212
H	1.345747	-4.06636	2.361385
H	0.965259	2.70062	0.611858
H	4.145023	2.405547	-3.15302
H	2.035328	4.832219	-0.24559
H	3.65869	4.666863	-2.17256
H	2.183133	-0.17265	-3.10185
H	3.941218	-0.11136	-2.86311
H	2.153509	-3.03168	-1.08259

C	5.315561	0.411022	2.728985
C	4.085608	0.857285	3.230555
C	2.935365	0.636846	2.474785
N	2.977886	-0.00357	1.284624
C	4.15648	-0.45899	0.800178
C	5.352295	-0.25435	1.498957
N	1.938253	1.449119	-0.78206
C	2.806878	1.32851	-1.81703
C	3.422915	2.450904	-2.38006
C	3.133268	3.718679	-1.86296
C	2.239023	3.829733	-0.79059
C	1.664274	2.670312	-0.26994
C	2.988662	-0.07325	-2.33942
N	2.832614	-1.09605	-1.25697
C	4.095158	-1.28926	-0.46532
N	-2.82794	-1.25337	-0.92189
C	-3.18842	-2.53295	-0.66315
C	-4.06131	-3.24209	-1.48892
C	-4.58264	-2.60925	-2.62275
C	-4.22214	-1.28217	-2.88225
C	-3.34101	-0.62978	-2.01444
C	-2.89885	0.802533	-2.23239
N	-2.64311	1.453772	-0.92874
C	-1.85592	2.715701	-1.04932
C	-2.45169	3.813121	-1.93895
O	0.124426	0.509804	1.126572
O	-0.04869	-0.59189	-1.05279
O	-1.01548	-2.09522	1.319723
C	0.135117	-2.59639	1.397043
C	0.338077	-3.94829	2.041527
N	-2.67334	0.491327	1.665359
C	-3.65848	1.368365	1.340723
C	-4.46831	1.945499	2.32519
C	-4.27205	1.600964	3.666162
C	-3.25782	0.692308	3.991847
C	-2.47417	0.167277	2.966512
C	-3.88461	1.630235	-0.13431
O	1.211853	-2.03071	0.929908
C	2.372359	-2.4093	-1.85481
C	3.314029	-3.02707	-2.88947
H	0.140737	-4.73595	1.294718
H	-0.37742	-4.08788	2.862989
H	1.365436	-4.07375	2.405796
H	0.972538	2.670499	0.575868
H	4.12172	2.330402	-3.21186
H	1.99817	4.799928	-0.35056
H	3.608517	4.607847	-2.28556
H	2.194386	-0.26724	-3.08035
H	3.95447	-0.18223	-2.86016
H	2.222777	-3.08652	-1.00246

H	1.337885	-2.11822	-2.35293	H	1.376701	-2.20904	-2.27837
H	4.26153	-3.19352	-2.53582	H	4.315546	-3.24066	-2.48382
H	2.838438	-3.89586	-3.3139	H	2.893289	-3.9897	-3.21889
H	3.415718	-2.31013	-3.83696	H	3.43029	-2.40706	-3.7917
H	-1.73337	-0.58551	3.210191	H	-1.6639	-0.53775	3.156612
H	-5.19116	2.710536	1.98864	H	-5.24962	2.654609	2.03847
H	-3.14411	0.416112	5.042386	H	-3.06982	0.395648	5.025885
H	-4.90507	2.113142	4.409472	H	-4.89972	2.039285	4.446567
H	-2.82802	-3.00017	0.34167	H	-2.74789	-2.97083	0.234472
H	-4.43126	-4.29086	-1.11703	H	-4.32914	-4.27075	-1.23795
H	-4.59097	-0.83071	-3.72221	H	-4.6254	-0.75026	-3.7482
H	-5.31257	-3.18297	-3.20854	H	-5.27098	-3.13572	-3.28922
H	-1.87569	0.67247	-2.76841	H	-1.94824	0.807549	-2.79453
H	-3.5571	1.264529	-2.83221	H	-3.64743	1.340318	-2.84299
H	-4.21734	2.615258	-0.32457	H	-4.32956	2.629607	-0.28094
H	-4.58505	0.90119	-0.50713	H	-4.63853	0.90812	-0.49266
H	-1.6062	3.016425	-0.04881	H	-1.71171	3.089712	-0.02174
H	-0.76174	2.297652	-1.42674	H	-0.86069	2.424454	-1.42216
H	-3.31807	4.05619	-1.67728	H	-3.45142	4.13742	-1.61035
H	-1.65778	4.578672	-1.97343	H	-1.80412	4.703089	-1.90523
H	-2.39102	3.369964	-3.03661	H	-2.52162	3.506021	-2.99365
H	1.914183	0.97154	2.781408	H	1.941256	0.961149	2.793719
H	3.991046	1.359345	4.17866	H	4.017215	1.372084	4.191246
H	6.25756	-0.63351	1.067163	H	6.297334	-0.62221	1.09031
H	6.206416	0.552781	3.276493	H	6.237859	0.576856	3.291936
H	4.053006	-2.33426	-0.19572	H	4.128489	-2.3489	-0.16254
H	4.945996	-1.1144	-1.11422	H	4.985299	-1.11308	-1.09245

Citation 1. Full citation for Gaussian 03 Revision E.01

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Jr., J. A. M.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; 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.; 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.; M. C. Strain; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; 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. *Gaussian 03, Revision E.01*, Gaussian, Inc.: Pittsburgh PA, 2003.