

Supplementary Information

Structures of Manganese Polysulfides: Mass-selected Photodissociation and Density Functional Calculations

Yu-Chao Zhao, Jinyun Yuan, Zeng-Guang Zhang, Hong-Guang Xu, and Weijun Zheng*

*Beijing National Laboratory for Molecular Sciences, State Key Laboratory of
Molecular Reaction Dynamics, Institute of Chemistry, Chinese Academy of sciences,
Beijing 100190, China*

* Corresponding author. E-mail: zhengwj@iccas.ac.cn

Tel: +86 10 62635054

Fax: +86 10 62563167

MnS⁺

1A:

Mn	0.000000	0.000000	0.841789
S	0.000000	0.000000	-1.315296

1B:

Mn	0.000000	0.000000	0.876229
S	0.000000	0.000000	-1.369107

MnS₂⁺

2A:

Mn	0.000000	0.000000	1.172882
S	0.000000	1.034096	-0.916314
S	0.000000	-1.034096	-0.916314

2B:

Mn	0.000000	0.000000	1.097751
S	0.000000	1.044649	-0.857618
S	0.000000	-1.044649	-0.857618

2C:

S	1.938213	0.678059	0.000000
S	0.000000	0.973215	0.000000
Mn	-1.240456	-1.056816	0.000000

2D:

S	1.929828	0.586585	0.000000
S	0.000000	1.010288	0.000000
Mn	-1.235090	-1.021999	0.000000

2E:

S	0.000000	0.000000	1.133738
S	0.000000	0.992871	-0.885733
Mn	0.000000	-0.992871	-0.885733

MnS₃⁺

3A:

Mn	0.000000	0.000000	1.371545
S	0.000000	1.667085	-0.305787
S	0.000000	-1.667085	-0.305787
S	0.000000	0.000000	-1.531465

3B:

S	0.000000	0.000000	2.598958
Mn	0.000000	0.000000	0.447958
S	0.000000	0.998613	-1.649446
S	0.000000	-0.998613	-1.649446

3C:

Mn	1.486245	-0.726875	-0.080663
S	0.764822	1.351732	-0.215225
S	-0.771062	0.099628	0.739372
S	-2.316018	-0.315618	-0.398111

MnS₄⁺

4A:

Mn	0.000000	0.000000	0.000000
S	0.000000	1.005134	2.092671
S	0.000000	-1.005134	2.092671
S	0.000000	1.005134	-2.092671
S	0.000000	-1.005134	-2.092671

4B:

S	0.096412	0.078705	-0.025622
S	0.096413	-0.078705	2.102641
S	1.962222	0.044590	2.942124
S	1.962221	-0.044590	-0.865105
Mn	3.281737	0.000000	1.038509

4C:

S	0.231790	-0.353729	1.867929
S	0.231790	-0.353729	-1.867929
S	0.231790	1.536929	1.073068
S	0.231790	1.536929	-1.073068
Mn	-0.593383	-1.514496	0.000000

4D:

Mn	0.000000	0.000000	1.052519
S	1.513874	0.999539	-0.411140
S	1.513874	-0.999539	-0.411140
S	-1.513874	0.999539	-0.411140
S	-1.513874	-0.999539	-0.411140

4E:

Mn	-0.454284	-1.230748	-0.366767
S	-0.727060	1.134316	-0.649544
S	-1.928135	0.264472	0.790807
S	1.900509	-0.703497	0.366510
S	1.464505	1.227752	0.065300

4F:

Mn	-0.003677	-0.258189	-0.054416
S	-2.160984	-0.641803	-0.567451
S	-1.788865	0.878610	0.710522
S	2.085406	-0.596103	0.711015
S	1.870188	0.762717	-0.769062

MnS₅⁺

5A:

S	0.000000	1.595474	-1.366438
S	0.000000	0.995633	2.435068
S	0.000000	-1.595474	-1.366438
S	0.000000	-0.995633	2.435068
Mn	0.000000	0.000000	0.338937
S	0.000000	0.000000	-2.666850

5B:

Mn	0.000000	0.000000	0.321001
S	0.000000	0.000000	-2.645924
S	0.000000	0.995802	2.436518
S	0.000000	-0.995802	2.436518
S	0.000000	-1.620917	-1.364337
S	0.000000	1.620917	-1.364337

5C:

Mn	0.000000	0.000000	0.326830
S	0.000000	0.000000	-2.645683
S	0.000000	0.993455	2.434126
S	0.000000	-0.993455	2.434126
S	0.000000	-1.622006	-1.366621
S	0.000000	1.622006	-1.366621

5D:

Mn	0.524088	-1.373692	0.000000
S	0.854004	1.452293	0.000000
S	-0.418223	0.848201	2.046298
S	-0.418223	-0.848201	-2.046298
S	-0.418223	1.195251	1.683630
S	-0.418223	1.195251	-1.683630

5E:

Mn	-0.982766	-1.304545	-0.217762
S	-1.998963	0.435393	0.856091
S	-0.903882	1.265785	-0.716941
S	1.033544	1.823598	-0.170672
S	2.065580	0.161392	0.560873
S	1.339292	-1.647816	-0.189098

5F:

Mn	0.865079	-1.399197	0.020887
S	2.243400	0.303265	-0.600612
S	0.901720	1.148092	0.820521
S	-0.755827	1.912606	-0.098547
S	-2.190276	0.320554	-0.415914
S	-1.550704	-1.498271	0.261915

MnS_6^+

6A:

S	0.000000	0.998236	2.389506
S	1.441228	-0.984899	-1.313400
S	1.441228	0.984899	-1.313400
S	-1.441228	0.984899	-1.313400
S	-1.441228	-0.984899	-1.313400
Mn	0.000000	0.000000	0.303738
S	0.000000	-0.998236	2.389506

6B:

Mn	-0.370581	-1.396190	0.110494
S	1.902969	-1.485624	-0.418725
S	-1.695462	0.365443	-0.975661
S	-2.427957	-0.590889	0.718049
S	0.847180	1.352162	0.986833
S	-0.510490	2.084746	-0.438523
S	2.462793	0.455708	-0.044620

6C:

S	0.000000	2.123663	0.989968
S	-1.839146	-1.061831	-0.989968
S	-1.839146	-1.061831	0.989968
S	1.839146	-1.061831	0.989968
S	1.839146	-1.061831	-0.989968
Mn	0.000000	0.000000	0.000000
S	0.000000	2.123663	-0.989968

6D:

S	-1.530254	1.012309	0.983743
S	-2.623071	-0.848333	0.224904
S	-0.716846	1.928447	-0.647578
Mn	0.563910	0.168311	0.014428
S	-1.221182	-1.684952	-0.893103
S	2.794275	0.317518	-0.581466
S	2.415968	-0.987974	0.890957

6E:				6F:			
S	0.751914	2.826168	1.007982	Mn	-0.440981	-1.057112	-0.447727
S	0.751914	2.826168	-1.007982	S	-2.487036	-0.529388	0.388581
Mn	-0.280928	1.001823	0.000000	S	1.256678	-1.753426	0.892923
S	0.751914	-2.810826	-0.951211	S	-1.607258	1.001915	-0.651592
S	-1.284353	-0.798016	-1.015244	S	1.872849	-0.563974	-0.658333
S	-1.284353	-0.798016	1.015244	S	-0.020240	1.787422	0.883685
S	0.751914	-2.810826	0.951211	S	1.674041	1.709188	-0.155690

MnS₇⁺

7A:				7B:			
S	-0.615406	0.291959	2.070586	S	2.911029	-0.486001	0.493263
S	-0.615406	-1.779149	1.997745	S	0.136659	-1.935287	-0.912812
S	1.206830	2.216502	0.000000	S	-3.144217	-0.342870	-0.461173
S	-0.615406	-1.779149	-1.997745	S	-2.706373	0.967274	0.979071
S	1.429972	1.030630	-1.696088	S	0.558095	1.870646	-0.457444
S	-0.615406	0.291959	-2.070586	S	2.505365	1.462313	-0.368296
Mn	-1.027295	-0.834164	0.000000	S	1.092837	-1.439068	0.866052
S	1.429972	1.030630	1.696088	Mn	-0.866172	-0.062085	-0.088743

7C:				7D:			
Mn	0.219280	0.713284	0.000000	S	-1.057683	-0.647288	2.010943
S	-1.804065	0.187808	1.005852	S	-1.057683	-0.647288	-2.010943
S	-1.804065	0.187808	-1.005852	S	0.884702	-1.319759	-2.075250
S	3.119507	1.526300	0.000000	S	0.066200	1.798250	0.000000
S	1.877063	1.158880	1.598440	S	-1.057683	1.450389	1.758945
S	1.877063	1.158880	-1.598440	S	0.884702	-1.319759	2.075250
S	-1.804065	-2.667091	0.951297	S	-1.057683	1.450389	-1.758945
S	-1.804065	-2.667091	-0.951297	Mn	1.532883	-0.489558	0.000000

7E:				7F:			
S	-0.137564	3.490087	0.252816	S	2.910316	0.497244	0.520432
S	-1.308253	-1.213205	-1.250138	S	-3.174449	-0.364572	-0.421097
S	1.111976	2.546266	-1.055087	S	1.075031	-1.428081	0.874555
S	-1.175619	-2.909571	-0.228733	S	0.134490	-1.949406	-0.907644
S	1.771221	-1.380385	0.462687	S	2.534188	1.417271	-0.415854
S	0.734360	-3.041008	0.741848	S	0.606097	1.914677	-0.414438
S	-1.129267	2.028530	1.263446	Mn	-0.887149	-0.076092	-0.106608
Mn	0.133145	0.479287	-0.186839	S	-2.699503	1.026248	0.930620

MnS₈⁺

8A:

S	0.000000	1.811874	1.641422
S	0.000000	-1.057592	3.490578
S	-1.811874	0.000000	-1.641422
Mn	0.000000	0.000000	0.000000
S	0.000000	1.057592	3.490578
S	1.811874	0.000000	-1.641422
S	0.000000	-1.811874	1.641422
S	1.057592	0.000000	-3.490578
S	-1.057592	0.000000	-3.490578

8B:

S	1.649280	-2.194795	0.307746
S	0.883834	1.438174	1.225368
S	2.160385	-0.683752	-0.976888
Mn	-0.146392	-0.938647	-0.264702
S	-1.531610	0.946423	-1.097725
S	-0.522006	2.487422	0.041323
S	-1.979384	-1.666578	0.811521
S	2.631115	1.150561	0.126292
S	-3.062876	-0.010818	-0.024040

8C:

Mn	-0.749190	0.014138	0.106265
S	0.708934	-1.931887	-0.061007
S	-2.391488	-0.460956	-1.511611
S	-3.038924	-0.255046	0.356857
S	-0.473017	2.194976	0.798394
S	2.630638	0.791580	0.129257
S	0.744843	1.738652	-0.753354
S	2.653881	-0.916928	-0.887806
S	0.335743	-1.182481	1.763231

8D:

S	-1.863891	-1.325590	1.152824
S	-3.266593	0.932098	-0.958583
S	1.863035	1.325421	1.152786
Mn	-0.000195	-0.000551	0.337821
S	-3.445878	-0.978379	-0.027946
S	1.550246	-1.805448	-0.430854
S	-1.549387	1.805340	-0.430397
S	3.267277	-0.931566	-0.958246
S	3.445495	0.978985	-0.027429

8E:

S	-3.111836	0.628483	0.750762
S	-3.061936	-0.051348	-1.135048
S	1.918731	2.097890	0.369468
S	0.130841	1.927056	-0.447128
Mn	-1.053886	-0.211099	0.074985
S	2.239484	-0.915095	-1.243383
S	0.347116	-2.064988	-0.301505
S	0.228262	-1.378140	1.599421
S	2.956035	0.085985	0.290247

8F:

S	1.682313	-1.627652	1.343554
S	-2.024782	-1.513913	-1.134097
Mn	0.142518	-1.148041	-0.290011
S	-3.103773	-0.237785	0.062328
S	2.680056	-0.756115	-0.262756
S	0.554434	1.577761	-1.040244
S	-0.863457	2.326421	0.345976
S	-1.654559	0.655069	1.339106
S	2.507084	1.370027	-0.200725