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Supporting Information file

Reversible Complexation of Ammonia by Breaking a Manganese-Manganese Bond in a Manganese Carbonyl Ethylenedithiolate Complex: A Theoretical Study of an Unusual Type of Lewis Acid

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Complete Gaussian09 Reference (reference 17)

Gaussian 09, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

Table S1. The initial $H_2C_2S_2Mn_2(CO)_n$ (n = 4 – 8) structures were constructed by systematic placement of CO ligands as terminal CO and bridging CO ligands coordinating through only the carbon atom or through both the carbon and oxygen atoms. This led to 225 different starting structures for $H_2C_2S_2Mn_2(CO)_4$, 241 different starting structures for $H_2C_2S_2Mn_2(CO)_5$, 255 different structures for $H_2C_2S_2Mn_2(CO)_6$, 299 different structures for $H_2C_2S_2Mn_2(CO)_7$ and 263 different structures for $H_2C_2S_2Mn_2(CO)_8$. The following table shows some representative geometries:

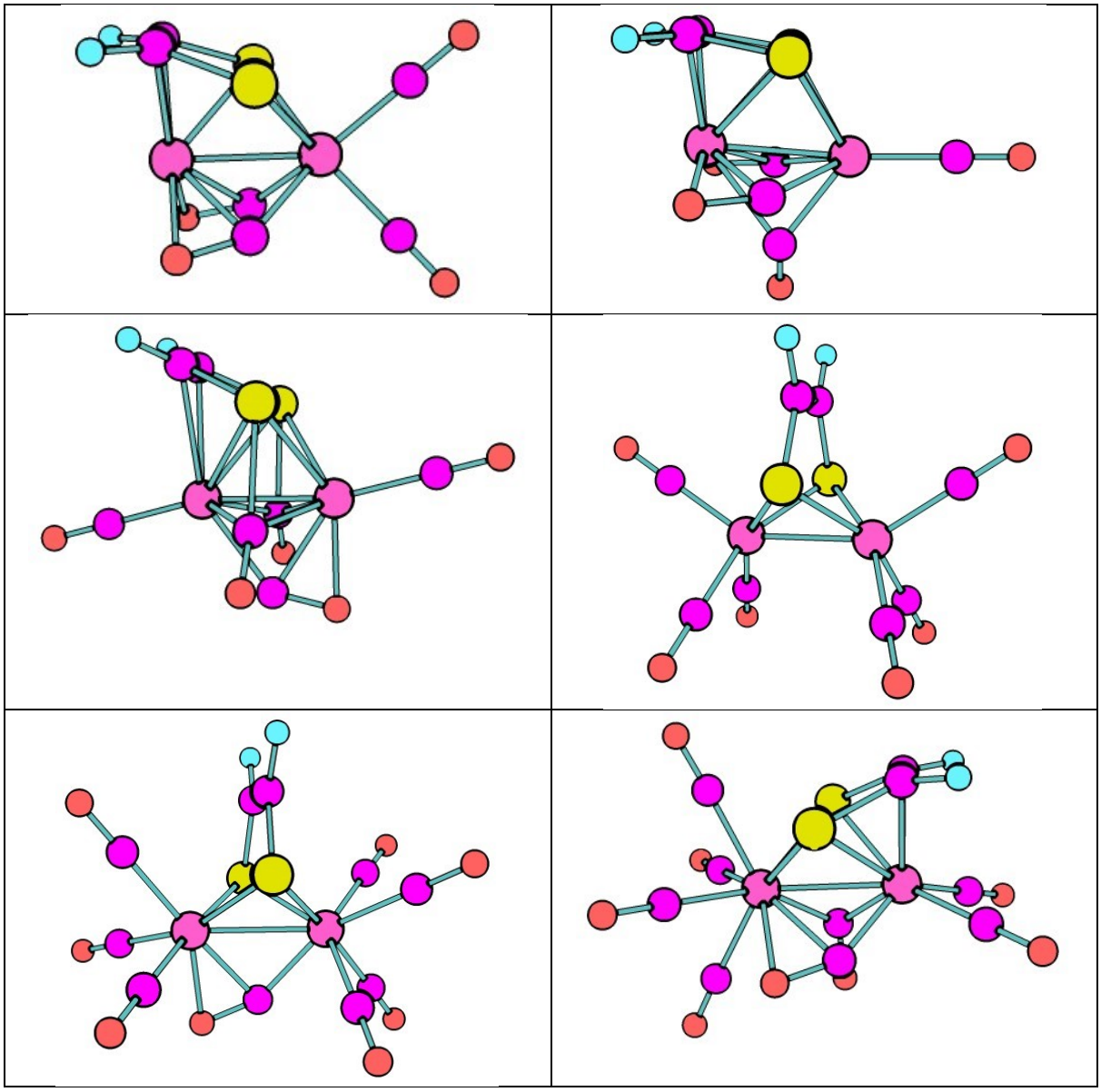
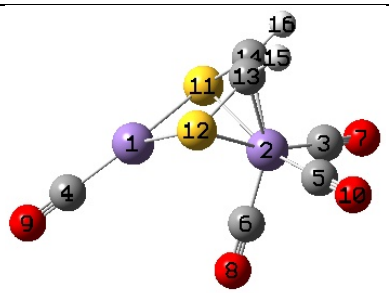


Table S2A. Distance table for the lowest-lying $H_2C_2S_2Mn_2(CO)_4$ structures after PBE0/6-311G(d,p) optimization followed by a single point CCSD(T) energy calculation. Provided are the absolute CCSD(T) energy (a.u.), relative energy (kcal/mol), symmetry and WBI.



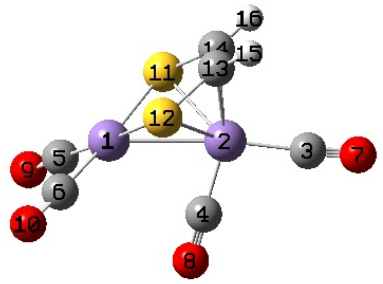
1Q. -3625.87664394157 0.00 C_s
WBI 0.02

		1	2	3	4	5
1	Mn	0.000000				
2	Mn	3.009678	0.000000			
3	C	4.433311	1.780897	0.000000		
4	C	1.877256	4.598254	5.899013	0.000000	
5	C	4.433096	1.780914	2.543010	5.898612	0.000000
6	C	3.137042	1.798832	2.601337	4.058878	2.601361
7	O	5.461528	2.922776	1.141987	6.855547	3.449002
8	O	3.691881	2.940850	3.526512	4.095956	3.526528
9	O	3.029331	5.660212	6.896635	1.152078	6.896091
10	O	5.461170	2.922798	3.449065	6.854825	1.141988
11	S	2.388375	2.428381	3.001838	3.955794	4.168830
12	S	2.388263	2.428337	4.168705	3.955543	3.001669
13	C	3.249590	2.105972	3.358307	5.097470	2.785671
14	C	3.249602	2.105987	2.785503	5.097527	3.358579
15	H	4.291102	2.857101	3.864449	6.111912	2.941085
16	H	4.291111	2.857131	2.940834	6.111989	3.864876

		6	7	8	9	10
6	C	0.000000				
7	O	3.526859	0.000000			
8	O	1.142052	4.279858	0.000000		
9	O	4.900554	7.810478	4.708892	0.000000	
10	O	3.526677	4.165024	4.279595	7.809499	0.000000
11	S	3.326794	3.787814	4.203565	5.023925	5.296551
12	S	3.327068	5.296346	4.203930	5.023505	3.787624
13	C	3.745877	4.351249	4.843736	6.240084	3.629392
14	C	3.745761	3.628992	4.843587	6.240201	4.351767
15	H	4.534396	4.743936	5.637480	7.243526	3.494991
16	H	4.534231	3.494350	5.637256	7.243697	4.744741

		11	12	13	14	15
11	S	0.000000				
12	S	3.290629	0.000000			
13	C	2.757194	1.745786	0.000000		
14	C	1.745758	2.757189	1.384047	0.000000	
15	H	3.749991	2.434780	1.084054	2.143953	0.000000
16	H	2.434711	3.750005	2.143968	1.084055	2.472020

		16
16	H	0.000000



2Q. -3625.82102440092 +34.90 C_s
WBI 0.05

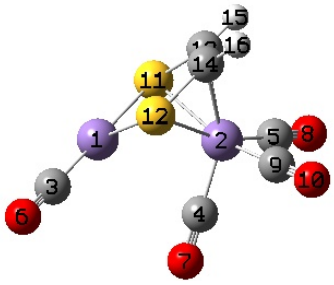
		1	2	3	4	5
1	Mn	0.000000				
2	Mn	2.630860	0.000000			
3	C	4.504030	1.881060	0.000000		
4	C	2.766642	1.811083	2.800133	0.000000	
5	C	1.825415	4.002526	5.754051	3.582885	0.000000
6	C	1.825427	4.002643	5.754387	3.582895	2.417965
7	O	5.639525	3.016530	1.135971	3.764532	6.852378
8	O	3.404652	2.956792	3.726519	1.145786	3.784947
9	O	2.967785	5.027509	6.693936	4.421314	1.143225
10	O	2.967796	5.027676	6.694421	4.421357	3.256869
11	S	2.297963	2.407714	3.886689	3.395201	3.028233

12 S	2.297992	2.407629	3.886967	3.394891	4.119674
13 C	3.194742	2.089705	3.091375	3.780241	4.872323
14 C	3.194722	2.089712	3.091191	3.780329	4.514940
15 H	4.236716	2.854540	3.282142	4.550691	5.947556
16 H	4.236691	2.854548	3.281824	4.550823	5.415479

	6	7	8	9	10
6 C	0.000000				
7 O	6.852775	0.000000			
8 O	3.784830	4.546103	0.000000		
9 O	3.256877	7.757708	4.409746	0.000000	
10 O	1.143225	7.758292	4.409622	3.846317	0.000000
11 S	4.119644	4.906302	4.312357	3.905103	5.259231
12 S	3.028322	4.906654	4.311923	5.259269	3.905216
13 C	4.515012	3.993746	4.896903	5.980653	5.516578
14 C	4.872336	3.993529	4.897037	5.516485	5.980676
15 H	5.415570	3.945053	5.660972	7.061033	6.343680
16 H	5.947566	3.944651	5.661182	6.343557	7.061055

	11	12	13	14	15
11 S	0.000000				
12 S	3.226318	0.000000			
13 C	2.744369	1.747983	0.000000		
14 C	1.747986	2.744352	1.387360	0.000000	
15 H	3.747126	2.444221	1.084203	2.155062	0.000000
16 H	2.444219	3.747109	2.155054	1.084203	2.500274

	16
16 H	0.000000



3T. -3625.81881231100 +36.29 C_1
WBI 0.03

	1	2	3	4	5
1 Mn	0.000000				
2 Mn	2.821008	0.000000			
3 C	1.770578	4.127411	0.000000		
4 C	2.921082	1.794983	3.720151	0.000000	
5 C	4.262119	1.778782	5.694270	2.597710	0.000000
6 O	2.926024	5.136440	1.155544	4.558379	6.722551
7 O	3.489496	2.937938	3.879736	1.143015	3.525933
8 O	5.298595	2.920852	6.760015	3.523532	1.142164
9 C	4.227141	1.780442	5.103384	2.594944	2.546742
10 O	5.253651	2.922323	5.937240	3.520648	3.454984
11 S	2.309554	2.421027	4.078216	3.318539	3.026727
12 S	2.225503	2.430130	2.928253	3.318903	4.168724
13 C	3.187686	2.109944	4.815095	3.748448	2.786555
14 C	3.162396	2.108440	4.442242	3.745966	3.355885
15 H	4.231283	2.859540	5.890076	4.530205	2.934678
16 H	4.198383	2.857699	5.332544	4.527431	3.869121

	6	7	8	9	10
6 O	0.000000				
7 O	4.520865	0.000000			
8 O	7.790079	4.280018	0.000000		
9 C	5.900589	3.519852	3.456913	0.000000	
10 O	6.609698	4.272511	4.177589	1.141991	0.000000
11 S	5.233366	4.196381	3.819797	4.160485	5.287989
12 S	3.780117	4.191138	5.296682	3.033454	3.827261
13 C	5.919607	4.847517	3.627500	3.359324	4.351067
14 C	5.424810	4.843928	4.347972	2.785629	3.627474
15 H	7.000172	5.633641	3.483037	3.875581	4.757854
16 H	6.230406	5.629237	4.751566	2.932994	3.482325

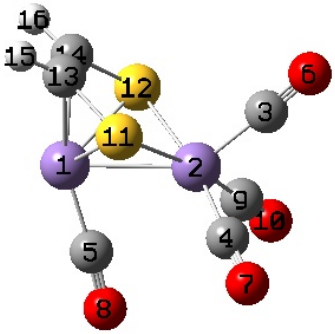
	11 12 13 14 15 11 S 0.000000 12 S 3.205080 0.000000 13 C 1.747370 2.742934 0.000000 14 C 2.731662 1.759177 1.378705 0.000000 15 H 2.439825 3.751168 1.083439 2.153256 0.000000 16 H 3.738810 2.453454 2.151475 1.084151 2.508199 16 16 H 0.000000
 4T. -3625.81391511592 +39.36 C_s WBI 0.07	1 2 3 4 5 1 Mn 0.000000 2 Mn 2.523694 0.000000 3 C 4.048798 1.768820 0.000000 4 C 3.631507 1.789241 2.583876 0.000000 5 C 1.784710 2.673599 4.442361 3.123566 0.000000 6 O 5.101053 2.911188 1.143110 3.518082 5.584745 7 O 4.569436 2.931853 3.507879 1.142616 3.840880 8 O 2.938711 3.373403 5.083823 3.365325 1.155253 9 C 3.631511 1.789236 2.583832 2.558420 3.123586 10 O 4.569468 2.931848 3.507780 3.467940 3.840970 11 S 2.322958 2.350678 3.122917 2.927387 3.332567 12 S 2.322957 2.350669 3.122873 4.122035 3.332581 13 C 2.109477 3.214409 3.952266 4.395637 3.793237 14 C 2.109475 3.214407 3.952254 4.781924 3.793241 15 H 2.898900 4.261835 4.931646 5.291180 4.577709 16 H 2.898896 4.261833 4.931630 5.856451 4.577713 6 7 8 9 10 6 O 0.000000 7 O 4.270892 0.000000 8 O 6.214619 3.822988 0.000000 9 C 3.518372 3.467909 3.365355 0.000000 10 O 4.271222 4.190450 3.823117 1.142616 0.000000 11 S 3.953727 3.723734 4.288614 4.122039 5.259272 12 S 3.954065 5.259260 4.288634 2.927382 3.723703 13 C 4.694094 5.330360 4.928434 4.781925 5.849726 14 C 4.694216 5.849730 4.928440 4.395637 5.330343 15 H 5.585705 6.134092 5.697601 5.856453 6.924458 16 H 5.585889 6.924459 5.697609 5.291180 6.134071 11 12 13 14 15 11 S 0.000000 12 S 3.291722 0.000000 13 C 1.744087 2.757381 0.000000 14 C 2.757381 1.744088 1.385691 0.000000 15 H 2.438078 3.748575 1.085883 2.142925 0.000000 16 H 3.748575 2.438081 2.142926 1.085883 2.463022 16 16 H 0.000000

Table S2B. Energy rank for all of the $H_2C_2S_2Mn_2(CO)_4$ optimized structures. PBE0/6-311G(d,p).

No	Initial structure	Final energy (a.u.)	ΔE (kcal/mol)
1	1_b_Mn_CO4_A1A2BB----40-Q-xqc	-3627.9173	0.00
2	1_b_Mn_CO4_A1D1BD1----52-Q	-3627.917295	0.00
3	4-5-mn-Q	-3627.917294	0.00
4	1_a_Mn_CO4_A1BD1B----16-Q-xqc	-3627.916463	0.53
5	2_a_Mn_CO4_A1A1A1pA2----61-Q	-3627.904035	8.32
6	1_b_Mn_CO4_A1BBD1----44-Q	-3627.904035	8.32
7	1_a_Mn_CO4_A1A1A2D1----4-Q-xqc	-3627.904033	8.33
8	4-3-mn-Q	-3627.896527	13.04
9	1_a_Mn_CO4_A1A1A1A2----1-Q	-3627.896217	13.23
10	1_a_Mn_CO4_A1A2BB----10-Q-xqc	-3627.889098	17.70
11	3_b_Mn_CO4_A1A1A2A2----198-Q	-3627.889098	17.70
12	1_a_Mn_CO4_A1D1BD2----23-Q-xqc	-3627.889098	17.70
13	4-4-3-mn-Q	-3627.889097	17.70
14	2_b_Mn_CO4_A1BpD2B----130-Q-ref	-3627.889088	17.70
15	1_a_Mn_CO4_A1BD1B----16-T	-3627.882375	21.92
16	4-5-mn-T	-3627.882363	21.92
17	1_b_Mn_CO4_A1D1BD1----52-T	-3627.88237	21.92
18	1_a_Mn_CO4_A1A1A1A2----1-T	-3627.882268	21.98
19	3_b_Mn_CO4_A1A1A2A2----198-T	-3627.876676	25.49
20	1_a_Mn_CO4_A1A1A2D1----4-T	-3627.874804	26.67
21	2_a_Mn_CO4_A1A1A1pA2----61-T	-3627.874803	26.67
22	1_b_Mn_CO4_A1BBD1----44-T	-3627.874801	26.67
23	1_b_Mn_CO4_A1A1A2A2----32-Q	-3627.871571	28.70
24	1_a_Mn_CO4_A1D1BD2----23-T	-3627.870477	29.38
25	1_b_Mn_CO4_A1A2BB----40-T	-3627.8691	30.25
26	1_a_Mn_CO4_A1A2BB----10-T	-3627.863724	33.62
27	3_b_Mn_CO4_A1A1D2D2----205-T-xqc	-3627.863723	33.62
28	4-3-mn-T	-3627.856428	38.20
29	2_b_Mn_CO4_pA1BBD2----146-T	-3627.849133	42.78
30	1_a_Mn_CO4_A1A1A2D1----4	-3627.848113	43.42
31	1_a_Mn_CO4_A1BD2D2----21	-3627.848113	43.42
32	1_a_Mn_CO4_A1D1D1D1----24	-3627.848113	43.42
33	1_b_Mn_CO4_A1BD2D2----51	-3627.848113	43.42
34	1_b_Mn_CO4_A1D1D1D1----54	-3627.848113	43.42
35	2_a_Mn_CO4_A1A1D1D1----64	-3627.848113	43.42
36	2_a_Mn_CO4_A1BBB----71	-3627.848113	43.42
37	2_a_Mn_CO4_A1BBD1----72	-3627.848113	43.42
38	2_a_Mn_CO4_A1D1BD1----80	-3627.848113	43.42
39	2_a_Mn_CO4_A1pA2D1D1----85	-3627.848113	43.42
40	2_a_Mn_CO4_pA1D2BD2----101	-3627.848113	43.42
41	2_a_Mn_CO4_pA1D2D2D2----102	-3627.848113	43.42

42	2_b_Mn_CO4_A1A1BB----116	-3627.848113	43.42
43	2_b_Mn_CO4_A1A1D1D1----117	-3627.848113	43.42
44	2_b_Mn_CO4_A1BBB----124	-3627.848113	43.42
45	2_b_Mn_CO4_A1BBD1----125	-3627.848113	43.42
46	2_b_Mn_CO4_A1D1BD1----133	-3627.848113	43.42
47	2_b_Mn_CO4_A1D1D1D1----134	-3627.848113	43.42
48	2_b_Mn_CO4_A1pA2D1D1----138	-3627.848113	43.42
49	2_b_Mn_CO4_pA1D2BD2----154	-3627.848113	43.42
50	3_b_Mn_CO4_A1A2BB----206	-3627.848113	43.42
51	1_b_Mn_CO4_A1A2D1D1----41	-3627.848112	43.42
52	2_b_Mn_CO4_pA1D2D2D2----155	-3627.848112	43.42
53	1_a_Mn_CO4_A1A2BB----10	-3627.847665	43.70
54	1_a_Mn_CO4_A1BBB----13	-3627.847664	43.70
55	1_a_Mn_CO4_A1D2BD2----28	-3627.847664	43.70
56	1_b_Mn_CO4_A1BBB----43	-3627.847664	43.70
57	2_a_Mn_CO4_A1A1D1pD2----65	-3627.847664	43.70
58	2_a_Mn_CO4_A1A1pD2pD2----69	-3627.847664	43.70
59	2_b_Mn_CO4_A1A1pD2pD2----122	-3627.847664	43.70
60	3_a_Mn_CO4_A1A1D2D2----175	-3627.847664	43.70
61	2_a_Mn_CO4_A1A1pA2pD2----68	-3627.847663	43.70
62	2_b_Mn_CO4_A1A1pA2pD2----121	-3627.847663	43.70
63	2_b_Mn_CO4_A1A1D1pD2----118	-3627.847662	43.70
64	1_a_Mn_CO4_A1A2D1D2----12	-3627.846951	44.14
65	1_b_Mn_CO4_A1A1D1D2----38	-3627.846951	44.14
66	2_a_Mn_CO4_A1A1A2A2----62	-3627.846951	44.14
67	1_a_Mn_CO4_A1A1D1D2----8	-3627.84695	44.15
68	2_a_Mn_CO4_A1A2BB----70	-3627.84695	44.15
69	4-4-mn-T	-3627.846517	44.42
70	2_b_Mn_CO4_pA1BBD2----146	-3627.845925	44.79
71	1_a_Mn_CO4_A1BD2B----19	-3627.845923	44.79
72	2_a_Mn_CO4_pA1BBD2----93	-3627.845923	44.79
73	2_a_Mn_CO4_pA1BD2D2----96	-3627.845923	44.79
74	2_a_Mn_CO4_pA1pA1A2D2----104	-3627.845923	44.79
75	2_b_Mn_CO4_A1A2BB----123	-3627.845923	44.79
76	2_b_Mn_CO4_pA1BD2D2----149	-3627.845923	44.79
77	2_b_Mn_CO4_pA1pA1A2D2----157	-3627.845923	44.79
78	1_a_Mn_CO4_A1A1A2D2----5	-3627.845922	44.79
79	1_b_Mn_CO4_A1A1A2D2----35	-3627.845922	44.79
80	2_a_Mn_CO4_pA1BD2B----95	-3627.845922	44.79
81	2_b_Mn_CO4_pA1pD1D2D2----163	-3627.845921	44.79
82	1_a_Mn_CO4_A1A1A1A2----1	-3627.845707	44.93
83	1_a_Mn_CO4_A1A1D1D1----7	-3627.845707	44.93
84	1_b_Mn_CO4_A1A1A1A2----31	-3627.845707	44.93
85	1_b_Mn_CO4_A1A1BB----36	-3627.845707	44.93
86	1_b_Mn_CO4_A1A1D1D1----37	-3627.845707	44.93

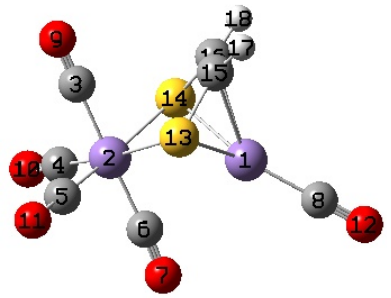
87	2_a_Mn_CO4_A1A1BB----63	-3627.845707	44.93
88	2_b_Mn_CO4_A1A1A1pA2----114	-3627.845707	44.93
89	1_a_Mn_CO4_A1A1BB----6	-3627.845706	44.93
90	1_a_Mn_CO4_A1BBD1----14	-3627.845706	44.93
91	2_a_Mn_CO4_A1BD1B----74-Q	-3627.845043	45.34
92	1_a_Mn_CO4_A1BBD2----15-Q	-3627.844975	45.38
93	1_b_Mn_CO4_A1A1A2A2----32	-3627.84477	45.51
94	2_b_Mn_CO4_A1A1A2A2----115	-3627.84477	45.51
95	1_a_Mn_CO4_A1A1A2A2----2	-3627.844769	45.51
96	4-4-mn-Q	-3627.844046	45.97
97	1_b_Mn_CO4_A1A2BB----40	-3627.842644	46.85
98	2_a_Mn_CO4_pA1pA1A2B----103	-3627.842644	46.85
99	2_b_Mn_CO4_pA1pA1A2B----156	-3627.842644	46.85
100	1_b_Mn_CO4_A1BBD1----44	-3627.839879	48.58
101	1_a_Mn_CO4_A1A2D1D1----11	-3627.839877	48.58
102	3_b_Mn_CO4_A1A1A2A2----198	-3627.838659	49.35
103	2_b_Mn_CO4_A1BpD2B----130	-3627.83702	50.38
104	1_b_Mn_CO4_A1D2D2D2----59	-3627.836997	50.39
105	2_b_Mn_CO4_A1pD2BpD2----142	-3627.836997	50.39
106	1_a_Mn_CO4_A1D2D2D2----29	-3627.836996	50.39
107	2_a_Mn_CO4_A1BpD2B----78	-3627.836996	50.39
108	2_a_Mn_CO4_A1BpD2pD2----79	-3627.836996	50.39
109	2_a_Mn_CO4_A1D1pD2pD2----84	-3627.836996	50.39
110	2_a_Mn_CO4_A1pA2pD2pD2----87	-3627.836996	50.39
111	2_a_Mn_CO4_A1pD2BD1----88	-3627.836996	50.39
112	2_a_Mn_CO4_A1pD2BpD2----89	-3627.836996	50.39
113	2_a_Mn_CO4_pA1pA1A2pD1----105	-3627.836996	50.39
114	2_b_Mn_CO4_A1BBpD2----126	-3627.836996	50.39
115	2_b_Mn_CO4_A1BpD2pD2----132	-3627.836996	50.39
116	2_b_Mn_CO4_A1D1pD2pD2----137	-3627.836996	50.39
117	2_b_Mn_CO4_A1pA2pD2pD2----140	-3627.836996	50.39
118	2_b_Mn_CO4_pA1pA1A2pD1----158	-3627.836996	50.39
119	1_a_Mn_CO4_A1BD1B----16	-3627.83471	51.83
120	2_a_Mn_CO4_BBBB----91	-3627.83471	51.83
121	3_a_Mn_CO4_A1A1A1A2----167	-3627.83471	51.83
122	2_b_Mn_CO4_pA1BpD1B----151	-3627.834708	51.83
123	2_a_Mn_CO4_pA1BpD1B----98	-3627.834707	51.83
124	4-4-3-mn-T	-3627.831057	54.12
125	1_b_Mn_CO4_A1A1A2A2----32-T	-3627.829426	55.14
126	1_b_Mn_CO4_A1D1BD1----52	-3627.829046	55.38
127	2_a_Mn_CO4_pA1pA1BB----106	-3627.829045	55.38
128	2_a_Mn_CO4_pA1pA1pA1A2----107	-3627.829045	55.38
129	2_b_Mn_CO4_pA1BBpD1----147	-3627.829045	55.38
130	2_b_Mn_CO4_pA1BpD1D2----152	-3627.829045	55.38
131	2_b_Mn_CO4_pA1pA1pA1A2----160	-3627.829045	55.38

132	2_b_Mn_CO4_pA1pD1pD1D2----165	-3627.829045	55.38
133	1_a_Mn_CO4_A1D1BD1----22	-3627.829044	55.38
134	2_a_Mn_CO4_pA1pD1pD1D2----112	-3627.829044	55.38
135	2_b_Mn_CO4_pA1pD1BD2----161	-3627.829043	55.38
136	2_a_Mn_CO4_pA1BpD1pD1----100	-3627.829041	55.38
137	2_b_Mn_CO4_pA1pA1BB----159	-3627.82904	55.38
138	2_b_Mn_CO4_A1BpD2B----130-T	-3627.826763	56.81
139	2_a_Mn_CO4_A1BD1B----74-T	-3627.823532	58.84
140	1_a_Mn_CO4_A1D1BD2----23	-3627.814291	64.64
141	2_a_Mn_CO4_A1pA2D1pD2----86	-3627.814291	64.64
142	3_a_Mn_CO4_A1BD2D1----186	-3627.814291	64.64
143	3_a_Mn_CO4_A1D1D2D1----192	-3627.814291	64.64
144	3_a_Mn_CO4_A1D1D2D2----193	-3627.814291	64.64
145	3_b_Mn_CO4_A1BD2D1----215	-3627.814291	64.64
146	7-3_b_Mn_CO4_A1D1D2D2----225	-3627.814291	64.64
147	2_b_Mn_CO4_A1pA2D1pD2----139	-3627.81429	64.64
148	3_b_Mn_CO4_A1D1D2D1----221	-3627.81429	64.64
149	2_a_Mn_CO4_A1A1A1pA2----61	-3627.813304	65.26
150	2_a_Mn_CO4_A1A1pA2B----66	-3627.813304	65.26
151	2_a_Mn_CO4_A1A1pA2D1----67	-3627.813304	65.26
152	2_b_Mn_CO4_A1A1pA2B----119	-3627.813304	65.26
153	2_b_Mn_CO4_A1A1pA2D1----120	-3627.813303	65.26
154	1_a_Mn_CO4_A1BBD2----15	-3627.811939	66.12
155	1_b_Mn_CO4_A1BBD2----45	-3627.811937	66.12
156	1_b_Mn_CO4_A1BD1D1----47	-3627.811731	66.25
157	3_b_Mn_CO4_A1A1D2D2----205	-3627.806455	69.56
158	1_a_Mn_CO4_A1A1D2D2----9	-3627.806454	69.56
159	1_b_Mn_CO4_A1A1D2D2----39	-3627.806454	69.56
160	3_a_Mn_CO4_A1A1A2D2----171	-3627.806454	69.56
161	3_b_Mn_CO4_A1A1A2D2----201	-3627.806454	69.56
162	2_a_Mn_CO4_A1BD1B----74	-3627.803832	71.20
163	2_a_Mn_CO4_A1BD1pD2----76	-3627.803832	71.20
164	2_a_Mn_CO4_A1D1D1pD2----82	-3627.803832	71.20
165	2_b_Mn_CO4_A1D1D1pD2----135	-3627.803832	71.20
166	3_a_Mn_CO4_A1A2D1D1----177	-3627.798629	74.47
167	3_a_Mn_CO4_A1BD2B----185	-3627.798629	74.47
168	3_a_Mn_CO4_A1BD2D2----187	-3627.798629	74.47
169	3_a_Mn_CO4_A1D2BD2----194	-3627.798629	74.47
170	3_a_Mn_CO4_A1D2D2D2----195	-3627.798629	74.47
171	3_b_Mn_CO4_A1A2D1D1----207	-3627.798629	74.47
172	3_b_Mn_CO4_A1BD2B----214	-3627.798629	74.47
173	3_b_Mn_CO4_A1BD2D2----216	-3627.798629	74.47
174	3_b_Mn_CO4_A1A1A1A2----197	-3627.796604	75.74
175	2_a_Mn_CO4_A1BD2D1----77	-3627.79629	75.93
176	3_a_Mn_CO4_A1A2D1D2----178	-3627.79629	75.93

177	3_b_Mn_CO4_A1A2D1D2----208	-3627.79629	75.93
178	1_b_Mn_CO4_A1D1BD2----53	-3627.796126	76.04
179	2_a_Mn_CO4_pA1BBB----92	-3627.796125	76.04
180	2_b_Mn_CO4_pA1BBB----145	-3627.796123	76.04
181	2_a_Mn_CO4_A1BBpD2----73	-3627.79537	76.51
182	2_a_Mn_CO4_A1pD2pD2pD2----90	-3627.795369	76.51
183	3_a_Mn_CO4_A1A2BB-4----176	-3627.795049	76.71
184	3_a_Mn_CO4_A1A1BB----172	-3627.795044	76.72
185	3_a_Mn_CO4_BBBB----196	-3627.795044	76.72
186	2_b_Mn_CO4_A1pD2pD2pD2----143	-3627.794796	76.87
187	3_a_Mn_CO4_A1BBD1----180	-3627.794302	77.18
188	3_a_Mn_CO4_A1BD1B----182	-3627.794301	77.18
189	3_a_Mn_CO4_A1BD1D1----183	-3627.794301	77.18
190	3_b_Mn_CO4_A1BBD1----210	-3627.794301	77.18
191	3_b_Mn_CO4_A1D1D1D2----220	-3627.794301	77.18
192	3_a_Mn_CO4_A1D1BD2----189	-3627.7943	77.18
193	3_a_Mn_CO4_A1D1D1D1----190	-3627.7943	77.18
194	3_a_Mn_CO4_A1D1D1D2----191	-3627.7943	77.18
195	3_b_Mn_CO4_A1BD1D1----212	-3627.7943	77.18
196	3_b_Mn_CO4_A1D1D1D1----219	-3627.7943	77.18
197	3_a_Mn_CO4_A1A1A2D1----170	-3627.793927	77.42
198	3_b_Mn_CO4_A1A1A2D1----200	-3627.793927	77.42
199	2_b_Mn_CO4_BBBB----144	-3627.793641	77.60
200	1_a_Mn_CO4_A1A1A2B----3	-3627.792415	78.37
201	1_b_Mn_CO4_A1A2D1D2----42	-3627.792415	78.37
202	1_b_Mn_CO4_A1A1A2B----33	-3627.79241	78.37
203	3_a_Mn_CO4_A1A1A2A2----168	-3627.78992	79.93
204	3_a_Mn_CO4_A1A1A2B----169	-3627.78992	79.93
205	2_a_Mn_CO4_pA1pD1D2pD1----111	-3627.789557	80.16
206	2_a_Mn_CO4_A1BD1D1----75	-3627.785315	82.82
207	2_b_Mn_CO4_A1BD1D1----128	-3627.785314	82.82
208	1_b_Mn_CO4_A1D2BD2----58	-3627.784558	83.30
209	1_b_Mn_CO4_A1D1D2D1----56	-3627.783589	83.90
210	2_a_Mn_CO4_pA1pD1BD2----108	-3627.783314	84.08
211	2_a_Mn_CO4_pA1BBpD1----94	-3627.782415	84.64
212	2_b_Mn_CO4_pA1pD1pD1pD1----166	-3627.782415	84.64
213	1_a_Mn_CO4_A1BD2D1----20	-3627.782342	84.69
214	3_b_Mn_CO4_BBBB----223	-3627.780119	86.08
215	1_b_Mn_CO4_A1BD2B----49	-3627.774585	89.56
216	3_b_Mn_CO4_A1A1A2B----199	-3627.772529	90.85
217	2_b_Mn_CO4_A1BD1B----127	-3627.771393	91.56
218	1_b_Mn_CO4_A1A1A2D1----34	-3627.765001	95.57
219	1_a_Mn_CO4_A1BD1D1----17	-3627.760057	98.67
220	2_b_Mn_CO4_pA1BD2B----148	-3627.756799	100.72
221	1_a_Mn_CO4_A1D1D1D2----25	-3627.756064	101.18

222	2_a_Mn_CO4_pA1BD2pD1----97	-3627.75395	102.50
223	2_b_Mn_CO4_pA1pD1D2pD1----164	-3627.753949	102.50
224	2_a_Mn_CO4_pA1pD1D2D2----110	-3627.752855	103.19
225	2_b_Mn_CO4_A1pD2BD1----141	-3627.751358	104.13
226	1_a_Mn_CO4_A1BD1D2----18	-3627.74961	105.23
227	1_b_Mn_CO4_A1BD1D2----48	-3627.749609	105.23
228	1_b_Mn_CO4_A1BD1B----46	-3627.749606	105.23
229	2_b_Mn_CO4_A1BD1pD2----129	-3627.74536	107.89
230	3_b_Mn_CO4_A1BBD2----211	-3627.741668	110.21
231	3_a_Mn_CO4_A1BBB----179	-3627.741663	110.21
232	3_a_Mn_CO4_A1BD1D2----184	-3627.741663	110.21
233	3_b_Mn_CO4_A1BD1D2----213	-3627.741662	110.21
234	3_a_Mn_CO4_A1BBD2----181	-3627.74166	110.22
235	3_b_Mn_CO4_A1BBB----209	-3627.74166	110.22
236	3_b_Mn_CO4_A1D1BD2----218	-3627.74166	110.22
237	3_b_Mn_CO4_A1D2BD2----222	-3627.741656	110.22
238	3_b_Mn_CO4_A1A1BB----202	-3627.738551	112.17
239	5-3_b_Mn_CO4_A1D2D2D2----224	-3627.735018	114.38
240	1_b_Mn_CO4_BBBB----60	-3627.733319	115.45
241	1_a_Mn_CO4_BBBB----30	-3627.733317	115.45
242	3_a_Mn_CO4_A1A1D1D1----173	-3627.733014	115.64
243	3_b_Mn_CO4_A1A1D1D1----203	-3627.733014	115.64
244	2_a_Mn_CO4_pA1pD1pD1pD1----113	-3627.732278	116.10
245	2_b_Mn_CO4_pA1pD1BpD1----162	-3627.732277	116.10
246	2_a_Mn_CO4_pA1pD1BpD1----109	-3627.732276	116.10
247	2_b_Mn_CO4_pA1BpD1pD1----153	-3627.730263	117.37
248	2_a_Mn_CO4_A1D1D1D1----81	-3627.727736	118.95
249	3_a_Mn_CO4_A1D1BD1----188	-3627.727233	119.27
250	3_b_Mn_CO4_A1D1BD1----217	-3627.727233	119.27
251	2_a_Mn_CO4_pA1BpD1D2----99	-3627.723996	121.30
252	3_a_Mn_CO4_A1A1D1D2----174	-3627.720779	123.32
253	3_b_Mn_CO4_A1A1D1D2----204	-3627.720779	123.32
254	2_a_Mn_CO4_A1D1pD2D1----83	-3627.715563	126.59
255	1_a_Mn_CO4_A1D1D2D1----26	-3627.715562	126.59
256	1_b_Mn_CO4_A1BD2D1----50	-3627.704862	133.31
257	2_b_Mn_CO4_A1BpD2D1----131	-3627.696251	138.71
258	2_b_Mn_CO4_A1D1pD2D1----136	-3627.696251	138.71
259	1_b_Mn_CO4_A1D1D1D2----55	-3627.695383	139.26
260	1_a_Mn_CO4_A1D1D2D2----27	-3627.695335	139.29
261	1_b_Mn_CO4_A1D1D2D2----57	-3627.695335	139.29
262	2_b_Mn_CO4_pA1BD2pD1----150	-3627.677984	150.17

Table S3A. Distance table for the lowest-lying $H_2C_2S_2Mn_2(CO)_5$ structures after PBE0/6-311G(d,p) optimization followed by a single point CCSD(T) energy calculation. Provided are the absolute CCSD(T) energy (a.u.), relative energy (kcal/mol), symmetry and WBI.



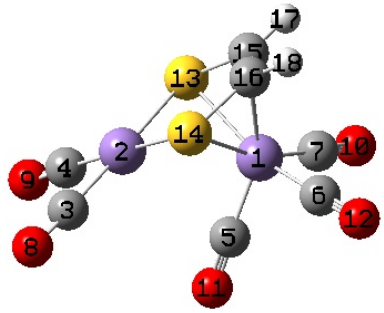
1Q. -3739.04042682617 0.00 C_1
WBI 0.02

		1	2	3	4	5
1	Mn	0.000000				
2	Mn	3.041793	0.000000			
3	C	4.180001	1.860204	0.000000		
4	C	4.362310	1.794528	2.618816	0.000000	
5	C	4.363168	1.794448	2.618176	2.647543	0.000000
6	C	2.761547	1.836014	3.695808	2.559795	2.558759
7	O	3.237588	2.975479	4.835682	3.435497	3.433847
8	C	1.887300	4.785569	6.062892	5.937006	5.939647
9	O	5.075954	2.992850	1.132739	3.536620	3.535888
10	O	5.342791	2.934446	3.511095	1.140006	3.580316
11	O	5.344244	2.934376	3.509944	3.580181	1.140017
12	O	3.040849	5.897205	7.215284	6.979152	6.982783
13	S	2.467239	2.417265	2.899954	4.206508	2.987253
14	S	2.466413	2.417443	2.900297	2.986867	4.206614
15	C	2.418678	3.231084	3.171932	4.772478	4.381935
16	C	2.418412	3.231148	3.172023	4.381705	4.772635
17	H	3.191505	4.265647	4.021958	5.833501	5.247393
18	H	3.191138	4.265720	4.022077	5.247141	5.833612

		6	7	8	9	10
6	C	0.000000				
7	O	1.141495	0.000000			
8	C	3.948540	3.887152	0.000000		
9	O	4.828129	5.968294	6.960045	0.000000	
10	O	3.456981	4.132206	6.811557	4.248913	0.000000
11	O	3.456109	4.130469	6.815775	4.247421	4.350658
12	O	4.900014	4.637031	1.153569	8.111991	7.801633
13	S	3.146451	4.013655	4.068506	3.646651	5.344086
14	S	3.148019	4.016024	4.064746	3.647013	3.760488
15	C	4.155688	5.041659	3.988804	3.620827	5.821108
16	C	4.156216	5.042482	3.987323	3.620919	5.292119
17	H	5.152918	5.982657	4.442086	4.265673	6.880769
18	H	5.153675	5.983900	4.439674	4.265807	6.055370

		11	12	13	14	15
11	O	0.000000				
12	O	7.807457	0.000000			
13	S	3.761193	5.143785	0.000000		
14	S	5.344190	5.138660	3.313497	0.000000	
15	C	5.292479	5.053884	1.770234	2.758689	0.000000
16	C	5.821289	5.051840	2.758714	1.770249	1.351043
17	H	6.055773	5.388330	2.444630	3.755906	1.085291
18	H	6.880864	5.384852	3.755935	2.444642	2.119695

		16	17	18
16	C	0.000000		
17	H	2.119671	0.000000	
18	H	1.085287	2.453810	0.000000



2T. -3739.03115019921 +5.82 C_1
WBI 0.04

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4	C	4.111836	1.825447	2.398511	0.000000	
5	C	1.800089	2.850303	3.648102	3.652410	0.000000
6	C	1.781242	4.190003	5.089532	5.658663	2.587735
7	C	1.781217	4.190367	5.656413	5.091688	2.587712
8	O	5.123304	2.968009	1.143588	3.231498	4.472818
9	O	5.125292	2.968076	3.232272	1.143558	4.478806
10	O	2.922666	5.222901	6.714127	5.925939	3.509793
11	O	2.941975	3.457121	3.821715	3.827393	1.142139
12	O	2.922685	5.222136	5.923170	6.716343	3.509666
13	S	2.423023	2.285631	4.109486	3.040420	3.350053
14	S	2.422348	2.285791	3.043086	4.109778	3.349631
15	C	2.113017	3.213874	4.894672	4.543356	3.768747
16	C	2.113158	3.213986	4.545488	4.893683	3.769089
17	H	2.863595	4.252613	5.967961	5.438499	4.542672
18	H	2.863644	4.252656	5.440847	5.967043	4.542979

		6	7	8	9	10
6	C	0.000000				
7	C	2.540514	0.000000			
8	O	5.905250	6.674040	0.000000		
9	O	6.677387	5.907778	3.809581	0.000000	
10	O	3.447856	1.141555	7.726666	6.623987	0.000000
11	O	3.494908	3.494915	4.432770	4.441268	4.236565
12	O	1.141547	3.448205	6.620768	7.730309	4.166785
13	S	4.160256	3.036445	5.249990	3.926703	3.831650
14	S	3.035082	4.159558	3.930759	5.250400	5.285606
15	C	3.352088	2.781686	6.005142	5.548868	3.619460
16	C	2.782054	3.351781	5.552235	6.003514	4.339868
17	H	3.866255	2.926994	7.084050	6.370599	3.469807
18	H	2.927367	3.865737	6.374544	7.082522	4.743072

		11	12	13	14	15
11	O	0.000000				
12	O	4.236351	0.000000			
13	S	4.252440	5.286322	0.000000		
14	S	4.252101	3.829790	3.183990	0.000000	
15	C	4.877758	4.340401	1.750599	2.729141	0.000000
16	C	4.878140	3.619813	2.728882	1.750935	1.376361
17	H	5.648229	4.744032	2.446554	3.738899	1.083983
18	H	5.648597	3.470298	3.738725	2.446639	2.151877

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16	C	0.000000		
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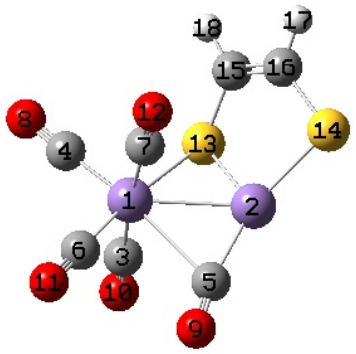

3Q. -3739.02933839033 +6.96 C_1
WBI 0.07

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4	C	1.790704	4.173345	2.637879	0.000000	
5	C	2.604774	1.967190	3.083133	4.384982	0.000000
6	C	1.791088	3.812191	2.596593	2.644224	2.806273
7	C	1.835552	2.841765	3.676153	2.607734	3.173952
8	O	2.929239	5.237943	3.544731	1.138865	5.522596
9	O	3.378752	3.097351	3.629898	5.064105	1.144436
10	O	2.982333	4.178551	1.137299	3.555307	3.822019
11	O	2.932716	4.777502	3.494855	3.574178	3.447721
12	O	2.972923	3.528967	4.813640	3.507647	3.953909
13	S	2.382143	2.333751	2.891873	2.989921	3.751586
14	S	4.467492	2.293130	5.497122	5.681799	4.004985
15	C	3.503219	3.001751	4.548885	3.856079	4.733431
16	C	4.224624	2.958022	5.391394	4.910626	4.794874
17	H	5.164935	3.995591	6.419702	5.674114	5.780265
18	H	4.073692	4.040537	5.098866	3.948756	5.672938

		6	7	8	9	10
6	C	0.000000				
7	C	2.588200	0.000000			
8	O	3.585672	3.506986	0.000000		
9	O	2.964563	3.958762	6.174389	0.000000	
10	O	3.509749	4.812585	4.286731	4.206462	0.000000
11	O	1.141638	3.488699	4.355113	3.228813	4.224028
12	O	3.492608	1.137666	4.220673	4.672226	5.949814
13	S	4.166786	3.057492	3.766421	4.833369	3.661554
14	S	5.758758	3.895671	6.574526	5.024926	6.321499
15	C	5.189150	3.187559	4.429587	5.857854	5.409824
16	C	5.758703	3.545982	5.583282	5.903968	6.275321
17	H	6.639479	4.251034	6.223510	6.861818	7.318881
18	H	5.725850	3.710268	4.246315	6.773921	5.930039

		11	12	13	14	15
11	O	0.000000				
12	O	4.206139	0.000000			
13	S	5.306282	3.883226	0.000000		
14	S	6.700479	3.978780	3.418582	0.000000	
15	C	6.294191	3.509556	1.775160	2.794839	0.000000
16	C	6.801584	3.583016	2.755606	1.756829	1.342020
17	H	7.649679	4.034077	3.738353	2.408435	2.086124
18	H	6.816603	3.928023	2.439466	3.777587	1.083841

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16	C	0.000000		
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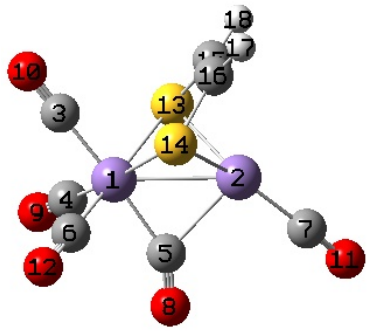
18	H	2.116965	2.413661	0.000000



4Q. -3739.02680958553 +8.54 C_1
WBI 0.06

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4	C	1.791311	3.898991	2.591076	0.000000	
5	C	1.953994	2.254729	3.782361	2.531805	0.000000
6	C	1.792150	3.850986	2.601194	2.615906	2.579863
7	C	4.225736	1.929317	5.805267	5.090447	2.991894
8	O	3.004900	3.159055	4.797796	3.156229	1.150238
9	O	2.932007	4.888959	3.485188	1.140762	3.385530
10	O	2.965978	4.985496	1.135336	3.504582	4.917381
11	O	5.264688	3.070040	6.895046	5.947995	3.819384
12	O	2.933148	4.823570	3.505288	3.536037	3.436415
13	S	2.400958	2.469139	2.933422	2.961388	3.219329
14	S	2.409216	2.395851	2.916103	4.197836	3.307182
15	C	3.232091	2.509524	3.402731	4.411980	4.162095
16	C	3.240768	2.482528	3.402890	4.804601	4.194510
17	H	4.283809	3.303148	4.303479	5.880818	5.166944
18	H	4.274907	3.338365	4.307434	5.298217	5.120807

		6	7	8	9	10
6	C	0.000000				
7	C	5.257410	0.000000			
8	O	3.195622	3.284658	0.000000		
9	O	3.538938	5.870292	3.740303	0.000000	
10	O	3.518327	6.842707	5.923034	4.214304	0.000000
11	O	6.213659	1.141711	3.818977	6.610774	7.945107
12	O	1.140998	6.100463	3.783062	4.286195	4.243315
13	S	4.191844	3.869207	4.243465	3.740810	3.698258
14	S	2.984710	4.182304	4.326749	5.337264	3.674879
15	C	4.809056	4.082013	5.257880	5.338753	3.944293
16	C	4.438458	4.204581	5.289706	5.865245	3.940909
17	H	5.328839	4.806419	6.223170	6.943761	4.678146
18	H	5.885948	4.608314	6.175639	6.130493	4.687828

		11	12	13	14	15
11	O	0.000000				
12	O	6.992206	0.000000			
13	S	4.847964	5.332479	0.000000		
14	S	5.297241	3.772447	3.348339	0.000000	
15	C	5.124506	5.877662	1.765482	2.763478	0.000000
16	C	5.300188	5.376064	2.764527	1.772657	1.346983
17	H	5.833082	6.175645	3.757579	2.442138	2.115400
18	H	5.538379	6.957936	2.434586	3.756152	1.085472

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17	H	1.085072	0.000000	
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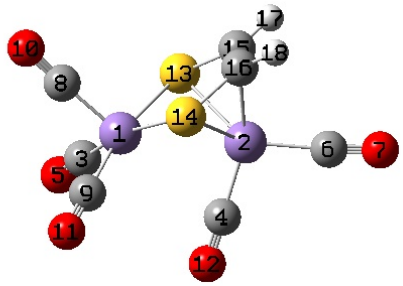

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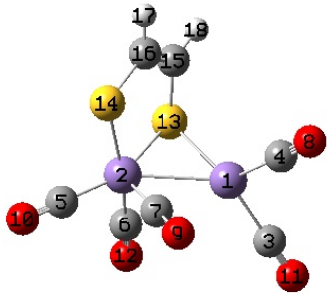
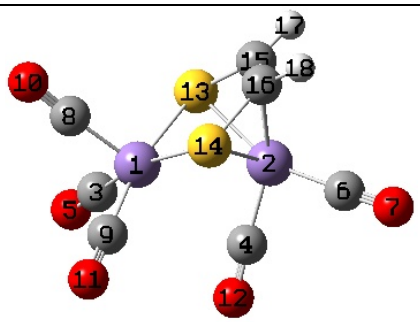
4	C	3.017548	1.814621	3.440836	0.000000	
5	O	2.934145	4.750612	1.142391	4.108402	0.000000
6	C	4.650005	1.864330	5.593638	2.836893	6.382379
7	O	5.785190	3.000003	6.702288	3.826347	7.449121
8	C	1.756501	4.315285	2.567886	4.773634	3.495012

5T. -3739.02471071291 +9.86 C_1 WBI 0.03	9 C 1.791471 3.856208 2.559647 3.476426 3.468769 10 O 2.899051 5.364674 3.502604 5.914995 4.258698 11 O 2.933833 4.765959 3.469215 4.157670 4.191540 12 O 3.640587 2.958056 3.642051 1.143496 4.069321 13 S 2.283014 2.382335 2.872098 3.375562 3.678328 14 S 2.278674 2.393116 4.041152 3.405341 5.174384 15 C 3.209479 2.088831 4.381482 3.783676 5.311021 16 C 3.206993 2.090135 4.767503 3.791502 5.830869 17 H 4.249756 2.854415 5.266805 4.547454 6.102785 18 H 4.246663 2.855970 5.843188 4.559285 6.909731 6 7 8 9 10 6 C 0.000000 7 O 1.137484 0.000000 8 C 6.140099 7.249111 0.000000 9 C 5.586637 6.688115 2.568685 0.000000 10 O 7.148979 8.234887 1.143623 3.503105 0.000000 11 O 6.372478 7.428380 3.495616 1.142382 4.258884 12 O 3.790222 4.654547 5.354185 3.691430 6.490276 13 S 3.848257 4.860114 3.128331 4.046754 3.984288 14 S 3.824531 4.825600 3.134160 2.866783 3.992943 15 C 3.024836 3.893257 4.009746 4.770756 4.770949 16 C 3.007659 3.870868 4.012449 4.378334 4.775624 17 H 3.214569 3.829312 4.954721 5.847025 5.619757 18 H 3.184693 3.787310 4.959083 5.261743 5.627366 11 12 13 14 15 11 O 0.000000 12 O 4.142265 0.000000 13 S 5.180501 4.280317 0.000000 14 S 3.672665 4.317256 3.172299 0.000000 15 C 5.834261 4.893324 1.738975 2.727749 0.000000 16 C 5.307362 4.903779 2.726364 1.738603 1.391253 17 H 6.913781 5.652087 2.440988 3.736030 1.083992 18 H 6.096531 5.668584 3.734733 2.439883 2.163541 16 17 18 16 C 0.000000 17 H 2.164228 0.000000 18 H 1.083992 2.521006 0.000000
 6Q. -3739.01627562394 +15.16 C_1 WBI 0.05	1 2 3 4 5 1 Mn 0.000000 2 Mn 2.677774 0.000000 3 C 1.993087 4.183416 0.000000 4 C 2.004931 4.158206 3.027364 0.000000 5 C 4.324135 1.793190 5.573697 5.652524 0.000000 6 C 2.989151 1.796731 3.656320 4.892248 2.571247 7 C 2.467941 1.742827 3.703312 3.416945 2.467670 8 O 3.138725 5.147961 3.970672 1.134038 6.552416 9 O 2.976746 2.898554 3.857935 3.369185 3.358576 10 O 5.424181 2.933270 6.566684 6.686936 1.140186 11 O 3.128680 5.182416 1.135741 3.967431 6.445377 12 O 3.684795 2.940685 3.786955 5.638069 3.476398 13 S 2.384759 2.280856 3.945053 3.868506 3.957528 14 S 3.925684 2.237126 5.826190 4.567359 2.812757 15 C 3.332132 3.202120 5.169042 3.993231 4.695844 16 C 3.912336 3.158988 5.885397 4.328016 4.291296 17 H 4.849182 4.190973 6.824112 4.940457 5.159651

	18 H 3.955627 4.237590 5.632211 4.393838 5.763080 6 7 8 9 10 6 C 0.000000 7 C 2.654776 0.000000 8 O 5.997607 4.288576 0.000000 9 O 3.620482 1.156447 4.045046 0.000000 10 O 3.478888 3.382738 7.540010 4.070477 0.000000 11 O 4.395358 4.646037 4.778239 4.677701 7.370920 12 O 1.144319 3.616831 6.758863 4.434037 4.196156 13 S 2.817580 3.480171 4.863584 4.484404 5.061028 14 S 4.007260 2.976772 5.227393 3.813846 3.617751 15 C 4.354804 4.209079 4.695476 5.091821 5.730841 16 C 4.706008 4.032230 4.899596 4.854050 5.203815 17 H 5.782668 4.934992 5.310305 5.647701 5.972691 18 H 5.224342 5.194770 4.970862 6.020241 6.796021 11 12 13 14 15 11 O 0.000000 12 O 4.262577 0.000000 13 S 4.967166 3.609960 0.000000 14 S 6.929252 5.140334 3.137057 0.000000 15 C 6.256197 5.277118 1.751245 2.703316 0.000000 16 C 7.013234 5.763469 2.675721 1.730661 1.340898 17 H 7.953607 6.845272 3.693623 2.412281 2.118370 18 H 6.664659 6.047574 2.439850 3.721172 1.083666 16 17 18 16 C 0.000000 17 H 1.085882 0.000000 18 H 2.141761 2.506432 0.000000
 7S. -3739.01154592022 +18.12 C_1 WBI 0.13	1 2 3 4 5 1 Mn 0.000000 2 Mn 2.704824 0.000000 3 C 1.794106 3.770644 0.000000 4 C 2.853455 1.787426 3.322849 0.000000 5 O 2.936427 4.688540 1.142327 4.030609 0.000000 6 C 4.275629 1.783604 5.407201 2.564072 6.291609 7 O 5.363707 2.926667 6.508044 3.494125 7.373949 8 C 1.758841 4.237914 2.579368 4.611815 3.502990 9 C 1.791021 3.791329 2.552323 3.275167 3.457694 10 O 2.901438 5.289986 3.514040 5.753892 4.266232 11 O 2.933057 4.711218 3.458368 3.960304 4.174004 12 O 3.484285 2.931971 3.552509 1.145247 4.034460 13 S 2.298012 2.324031 2.886708 3.336476 3.695249 14 S 2.277139 2.337112 4.039700 3.239952 5.173345 15 C 3.212849 2.096715 4.394275 3.782932 5.330580 16 C 3.202525 2.101420 4.768220 3.744127 5.835670 17 H 4.256221 2.862509 5.283526 4.566078 6.127789 18 H 4.241759 2.869146 5.841710 4.508150 6.911853 6 7 8 9 10 6 C 0.000000 7 O 1.143555 0.000000 8 C 5.787120 6.848573 0.000000 9 C 4.925811 5.849220 2.561811 0.000000 10 O 6.811739 7.852060 1.143604 3.495397 0.000000 11 O 5.602088 6.401530 3.485648 1.142049 4.246345 12 O 3.456247 4.200113 5.188503 3.430185 6.321481

13 S	4.036019	5.151640	3.152889	4.060893	4.009916
14 S	3.147363	4.022216	3.137780	2.868256	4.000122
15 C	3.267655	4.232499	4.002998	4.777798	4.760599
16 C	2.813116	3.665029	3.994142	4.383217	4.753632
17 H	3.709542	4.522000	4.963957	5.853520	5.630394
18 H	2.958788	3.511372	4.950300	5.263733	5.618850

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11 O	0.000000				
12 O	3.850892	0.000000			
13 S	5.194307	4.285858	0.000000		
14 S	3.676173	4.122006	3.183577	0.000000	
15 C	5.843123	4.908907	1.745141	2.727097	0.000000
16 C	5.316692	4.845296	2.724936	1.741764	1.379441
17 H	6.920849	5.693323	2.447289	3.733051	1.084704
18 H	6.102745	5.594103	3.732120	2.439231	2.150734

	16	17	18
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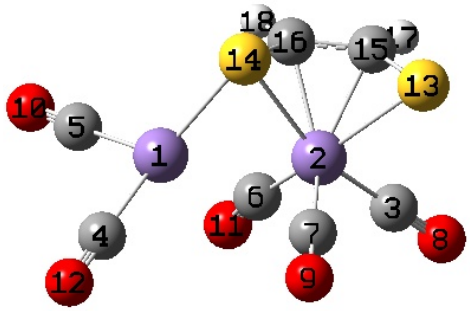
17 H	2.151084	0.000000	
18 H	1.084333	2.501180	0.000000



8Q. -3739.01099689395 +18.47 C_1
WBI 0.05

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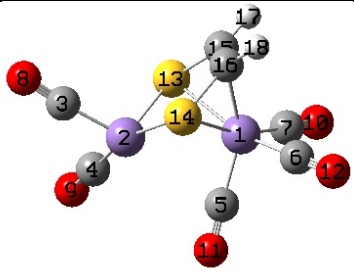
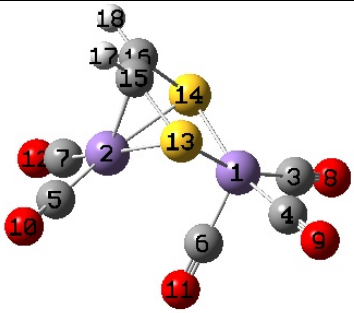
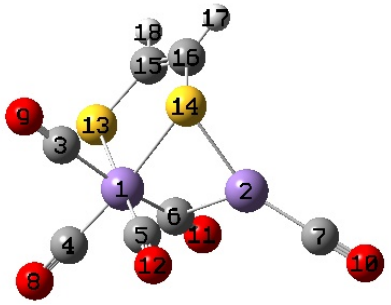
4 C	1.985308	4.166538	5.496362	0.000000	
5 C	1.999955	4.295544	5.598975	3.014094	0.000000
6 C	2.373450	1.770575	2.378418	3.752481	3.309286
7 C	3.080475	1.802390	2.610422	3.615854	4.974051
8 O	5.337042	2.931647	1.139542	6.464462	6.548014
9 O	3.761640	2.941922	3.545188	3.714286	5.674555
10 O	3.134227	5.319192	6.522138	3.954111	1.135287
11 O	2.975122	2.915524	3.130854	4.098030	3.284353
12 O	3.121577	5.147469	6.362969	1.136347	3.950492
13 S	4.700515	2.357475	2.819647	6.099441	6.271876
14 S	2.352027	2.412254	4.160026	3.899821	3.777872
15 C	4.120479	2.116582	2.784124	5.893510	5.250227
16 C	3.045205	2.085130	3.391790	4.948656	3.991057
17 H	4.897762	2.862600	2.969637	6.726117	5.774195
18 H	3.231359	2.851224	3.974745	5.215806	3.589571

	6	7	8	9	10
6 C	0.000000				
7 C	2.755236	0.000000			
8 O	3.255819	3.531816	0.000000		
9 O	3.734693	1.140543	4.298984	0.000000	
10 O	4.207603	6.088349	7.409906	6.793359	0.000000
11 O	1.157969	3.729101	3.737445	4.581992	3.964492
12 O	4.736007	4.309402	7.267939	4.125502	4.754933
13 S	4.049843	3.181111	3.576373	4.016875	7.250319
14 S	3.373704	3.201832	5.285257	4.023790	4.751918
15 C	3.302782	3.718020	3.621712	4.790136	6.084260
16 C	2.853710	3.687112	4.398100	4.761174	4.808070
17 H	3.692172	4.532999	3.532498	5.623643	6.490836
18 H	3.007955	4.506013	4.893208	5.593315	4.205660

	11	12	13	14	15
11 O	0.000000				
12 O	4.987522	0.000000			

	13 S 5.142557 7.019423 0.000000 14 S 4.386412 4.925247 3.106361 0.000000 15 C 4.265271 6.954711 1.722308 2.707827 0.000000 16 C 3.776236 6.058948 2.714441 1.759150 1.393649 17 H 4.461541 7.802414 2.456937 3.713478 1.087005 18 H 3.655414 6.351666 3.722047 2.490640 2.166904 16 17 18 16 C 0.000000 17 H 2.139437 0.000000 18 H 1.084271 2.481711 0.000000
 9S. -3739.01049087647 +18.79 C_1 WBI 0.10	1 2 3 4 5 1 Mn 0.000000 2 Mn 2.775989 0.000000 3 C 4.366845 1.749168 0.000000 4 C 3.849476 1.785561 2.520993 0.000000 5 C 1.794010 2.883051 4.625222 3.303560 0.000000 6 C 1.784473 4.231093 5.769302 5.404336 2.588835 7 C 1.785105 4.182184 5.748648 4.756016 2.598466 8 O 5.441864 2.895175 1.147814 3.446048 5.773018 9 O 4.774721 2.931087 3.434316 1.145566 3.998654 10 O 2.926466 5.208561 6.734656 5.572306 3.524429 11 O 2.937177 3.493898 5.145189 3.465841 1.143518 12 O 2.925981 5.273260 6.764061 6.467954 3.512847 13 S 2.396853 2.187520 3.154967 2.869601 3.308411 14 S 2.394905 2.265155 3.170824 4.012687 3.278610 15 C 2.118696 3.144153 4.068117 4.389369 3.763332 16 C 2.110396 3.165177 4.073939 4.762421 3.743964 17 H 2.866698 4.179717 5.021267 5.274262 4.544754 18 H 2.867265 4.206471 5.021157 5.835082 4.526264 6 7 8 9 10 6 C 0.000000 7 C 2.548847 0.000000 8 O 6.817206 6.796534 0.000000 9 O 6.315648 5.419260 4.173804 0.000000 10 O 3.454720 1.141469 7.755964 6.086976 0.000000 11 O 3.488900 3.517577 6.273248 3.909925 4.268879 12 O 1.141615 3.454358 7.786204 7.366759 4.170796 13 S 4.140017 3.014813 4.041821 3.721537 3.816649 14 S 3.027615 4.142318 4.059081 5.148244 5.270598 15 C 3.363265 2.805857 4.873145 5.357271 3.649108 16 C 2.788285 3.372095 4.881383 5.848345 4.366182 17 H 3.872923 2.955265 5.740029 6.155787 3.509199 18 H 2.940505 3.903646 5.741161 6.924353 4.791481 11 12 13 14 15 11 O 0.000000 12 O 4.230174 0.000000 13 S 4.217352 5.267276 0.000000 14 S 4.162074 3.834675 3.147369 0.000000 15 C 4.874911 4.352677 1.747983 2.718094 0.000000 16 C 4.846034 3.630609 2.718845 1.742520 1.380283 17 H 5.658108 4.750792 2.451932 3.729695 1.083951 18 H 5.623136 3.489127 3.732711 2.439781 2.158891 16 17 18 16 C 0.000000 17 H 2.156707 0.000000

	18 H 1.083294 2.522650 0.000000
 10T. -3739.00845486550 +20.06 C_s WBI 0.04	1 2 3 4 5 1 Mn 0.000000 2 Mn 2.799180 0.000000 3 C 1.790927 4.208514 0.000000 4 C 1.790978 4.208290 2.589152 0.000000 5 C 4.049381 1.829799 5.624695 4.937332 0.000000 6 C 1.751561 2.831974 2.525128 2.525177 3.635453 7 C 4.049428 1.829796 4.937805 5.624537 2.802743 8 O 2.932470 5.231555 1.141804 3.508223 6.691589 9 O 2.932558 5.231164 3.508354 1.141835 5.732194 10 O 5.005126 2.967601 6.611856 5.638130 1.138713 11 O 2.899852 3.379614 3.435949 3.436169 3.794731 12 O 5.005182 2.967604 5.638684 6.611719 3.768877 13 S 2.264497 2.426834 4.013653 2.821776 3.027559 14 S 2.264515 2.426843 2.821832 4.013835 4.240937 15 C 3.219495 2.122352 4.744271 4.353260 3.070312 16 C 3.219505 2.122354 4.353209 4.744408 3.643942 17 H 4.251701 2.883957 5.812931 5.215481 3.338775 18 H 4.251718 2.883973 5.215458 5.813093 4.275616 6 7 8 9 10 6 C 0.000000 7 C 3.635251 0.000000 8 O 3.455135 5.733037 0.000000 9 O 3.455025 6.691238 4.250170 0.000000 10 O 4.466553 3.768882 7.686176 6.284465 0.000000 11 O 1.148313 3.794202 4.182428 4.182478 4.457270 12 O 4.466256 1.138718 6.285491 7.685841 4.605409 13 S 3.215017 4.240917 5.139736 3.611612 3.789403 14 S 3.214555 3.027445 3.611683 5.140042 5.371360 15 C 4.187212 3.643805 5.787458 5.258886 3.952667 16 C 4.187057 3.070104 5.258780 5.787700 4.685327 17 H 5.147551 4.275454 6.857568 6.017553 3.995268 18 H 5.147328 3.338522 6.017488 6.857856 5.261533 11 12 13 14 15 11 O 0.000000 12 O 4.456491 0.000000 13 S 4.129609 5.371341 0.000000 14 S 4.128825 3.789270 3.146807 0.000000 15 C 5.050554 4.685178 1.756688 2.722203 0.000000 16 C 5.050274 3.952436 2.722211 1.756686 1.374237 17 H 5.939591 5.261351 2.446726 3.741098 1.083452 18 H 5.939161 3.994962 3.741105 2.446735 2.161392 16 17 18 16 C 0.000000 17 H 2.161394 0.000000 18 H 1.083454 2.545230 0.000000



11Q. -3739.00741159938 +20.72 C_1
WBI 0.04

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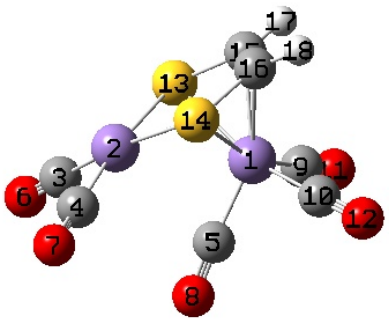
2	Mn	2.737147	0.000000			
3	C	1.857127	4.198804	0.000000		
4	C	1.793625	4.166673	2.624714	0.000000	
5	C	1.787758	2.690702	2.691915	2.557513	0.000000
6	C	1.839415	2.351542	3.650008	2.514135	2.838920
7	C	4.457324	1.887159	6.009878	5.574574	4.016934
8	O	2.932937	5.196618	3.518399	1.139339	3.464363
9	O	2.989052	5.216837	1.132827	3.544838	3.646046
10	O	5.561161	3.033277	7.134270	6.559337	5.013489
11	O	2.981446	2.898661	4.769170	3.350575	3.844110
12	O	2.934364	3.259221	3.599826	3.456569	1.146932
13	S	2.378130	4.205383	2.858818	2.977955	4.165592
14	S	2.417328	2.317082	2.851955	4.205897	3.026193
15	C	3.194827	4.001436	3.594016	4.420230	4.788949
16	C	3.243115	3.332136	3.645995	4.837142	4.469094
17	H	4.285598	3.931800	4.591021	5.915302	5.364777
18	H	4.234690	4.941123	4.543887	5.304202	5.866163

		6	7	8	9	10
6	C	0.000000				
7	C	3.620758	0.000000			
8	O	3.400814	6.449728	0.000000		
9	O	4.764358	7.035994	4.260898	0.000000	
10	O	4.607754	1.146314	7.357393	8.160595	0.000000
11	O	1.147749	3.651490	4.014060	5.870597	4.453490
12	O	3.808881	4.169200	4.171362	4.394754	5.011994
13	S	2.683121	5.896047	3.775804	3.581884	6.971696
14	S	3.215802	4.100687	5.343346	3.582268	5.215961
15	C	3.354491	5.656860	5.368171	4.195452	6.715283
16	C	3.545135	4.972030	5.909957	4.252799	6.030080
17	H	4.492475	5.358823	6.992890	5.076101	6.331265
18	H	4.215049	6.474941	6.162101	5.020939	7.476622

		11	12	13	14	15
11	O	0.000000				
12	O	4.695528	0.000000			
13	S	3.343854	5.312078	0.000000		
14	S	4.133482	3.841468	3.332316	0.000000	
15	C	3.909916	5.878174	1.741437	2.731324	0.000000
16	C	4.195558	5.435099	2.757379	1.772834	1.334800
17	H	5.027539	6.246440	3.752593	2.437831	2.121575
18	H	4.576530	6.960975	2.398204	3.727645	1.087184

		16	17	18
16	C	0.000000		
17	H	1.084001	0.000000	
18	H	2.092593	2.443881	0.000000



12S. -3739.00377483534 +23.00 C_s
WBI 0.12

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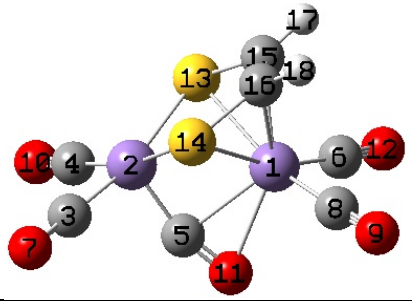
2	Mn	2.726529	0.000000			
3	C	3.874500	1.788216	0.000000		
4	C	3.874954	1.788207	2.548969	0.000000	
5	C	1.799079	2.762249	3.318942	3.319879	0.000000
6	O	4.816234	2.932609	1.144425	3.455672	4.060716
7	O	4.816896	2.932602	3.455700	1.144427	4.062088
8	O	2.940383	3.396763	3.513221	3.514395	1.143111
9	C	1.784549	4.143384	4.773497	5.414071	2.577683
10	C	1.784550	4.143277	5.413421	4.773862	2.577726
11	O	2.925738	5.175081	5.586311	6.471597	3.497508
12	O	2.925739	5.174940	6.470879	5.586617	3.497557
13	S	2.390861	2.289038	2.910238	4.067965	3.305050
14	S	2.390866	2.288954	4.067820	2.910079	3.305179
15	C	2.116458	3.224202	4.425684	4.806539	3.766166
16	C	2.116461	3.224183	4.806497	4.425639	3.766215
17	H	2.871674	4.262561	5.307936	5.880653	4.548145
18	H	2.871672	4.262534	5.880589	5.307864	4.548213

		6	7	8	9	10
6	O	0.000000				
7	O	4.171119	0.000000			
8	O	4.018315	4.020144	0.000000		
9	C	5.450979	6.355555	3.462772	0.000000	
10	C	6.354605	5.451632	3.462853	2.558142	0.000000
11	O	6.112937	7.405216	4.193159	1.141298	3.465441
12	O	7.404155	6.113552	4.193264	3.465443	1.141298
13	S	3.730480	5.209288	4.226243	3.002634	4.138054
14	S	5.209109	3.730289	4.226433	4.138043	3.002581
15	C	5.371100	5.882391	4.882262	2.803732	3.374902
16	C	5.882333	5.371041	4.882333	3.374846	2.803760
17	H	6.161713	6.960789	5.655510	2.962657	3.899849
18	H	6.960699	6.161614	5.655615	3.899750	2.962705

		11	12	13	14	15
11	O	0.000000				
12	O	4.185353	0.000000			
13	S	3.803766	5.266266	0.000000		
14	S	5.266248	3.803695	3.169409	0.000000	
15	C	3.647475	4.367831	1.744936	2.723369	0.000000
16	C	4.367756	3.647512	2.723385	1.744932	1.379433
17	H	3.516998	4.784540	2.443637	3.733491	1.084015
18	H	4.784403	3.517069	3.733505	2.443640	2.154734

		16	17	18
16	C	0.000000		
17	H	2.154731	0.000000	
18	H	1.084014	2.513920	0.000000



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2	Mn	2.683841	0.000000			
3	C	4.066870	1.800229	0.000000		
4	C	4.067083	1.800234	2.589997	0.000000	
5	C	2.224378	1.720729	2.631090	2.631189	0.000000
6	C	1.780062	4.107164	5.650115	5.035035	3.376004
7	O	5.078704	2.940642	1.140444	3.505429	3.578431
8	C	1.780071	4.106821	5.034191	5.650062	3.375823

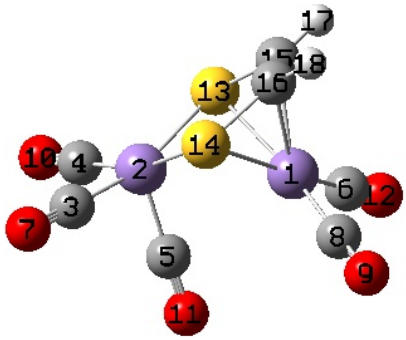
13S. -3739.00278558389 +23.62 C_s
WBI 0.12

9 O	2.921994	5.141808	5.866442	6.725373	4.360075
10 O	5.079020	2.940643	3.505405	1.140440	3.578605
11 O	2.314401	2.862896	3.663136	3.663278	1.168934
12 O	2.921993	5.142315	6.725575	5.867621	4.360349
13 S	2.464746	2.273982	4.046132	2.853907	3.008894
14 S	2.464841	2.273907	2.853769	4.045984	3.009162
15 C	2.071975	3.190385	4.772337	4.381569	3.728862
16 C	2.071990	3.190362	4.381499	4.772316	3.728936
17 H	2.828859	4.227843	5.848945	5.260075	4.658502
18 H	2.828892	4.227814	5.259970	5.848916	4.658620

	6	7	8	9	10
6 C	0.000000				
7 O	6.694305	0.000000			
8 C	2.539067	5.834098	0.000000		
9 O	3.450021	6.540717	1.142393	0.000000	
10 O	5.835194	4.242221	6.694404	7.777963	0.000000
11 O	3.029002	4.484173	3.029005	3.892464	4.484438
12 O	1.142401	7.777997	3.449963	4.173728	6.542263
13 S	3.090931	5.178084	4.197299	5.319335	3.652160
14 S	4.197342	3.652007	3.090676	3.877809	5.177899
15 C	2.735117	5.836969	3.314858	4.297355	5.311424
16 C	3.314708	5.311338	2.735119	3.563933	5.836942
17 H	2.875735	6.918597	3.832072	4.701466	6.095246
18 H	3.831784	6.095106	2.875844	3.399943	6.918558

	11	12	13	14	15
11 O	0.000000				
12 O	3.892486	0.000000			
13 S	3.723232	3.878264	0.000000		
14 S	3.723602	5.319371	3.176140	0.000000	
15 C	4.201097	3.563967	1.749855	2.729253	0.000000
16 C	4.201210	4.297160	2.729256	1.749859	1.381183
17 H	4.992303	3.399835	2.443384	3.740701	1.084027
18 H	4.992490	4.701041	3.740702	2.443392	2.159602

	16	17	18
16 C	0.000000		
17 H	2.159604	0.000000	
18 H	1.084027	2.525929	0.000000



14T. -3738.99928078827 +25.82 C_1
WBI 0.04

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2 Mn	2.788360	0.000000			
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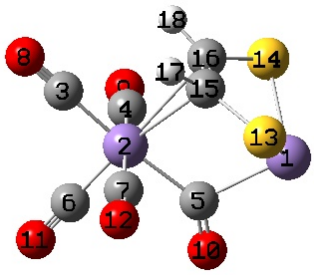
4 C	4.196475	1.791104	2.587291	0.000000	
5 C	2.813545	1.752528	2.525484	2.525163	0.000000
6 C	1.830224	4.037675	5.612411	4.920739	3.614646
7 O	5.222241	2.932726	1.141949	3.505779	3.455438
8 C	1.830008	4.039843	4.927129	5.612055	3.614179
9 O	2.967804	4.996571	5.628643	6.599419	4.445904
10 O	5.220179	2.932808	3.505145	1.141945	3.454641
11 O	3.367511	2.900980	3.433250	3.432837	1.148452
12 O	2.968017	4.993288	6.598615	5.619875	4.445899
13 S	2.425651	2.264170	4.013157	2.824126	3.216991
14 S	2.425086	2.264542	2.823092	4.015080	3.211496
15 C	2.122080	3.219213	4.745594	4.357127	4.181811
16 C	2.122034	3.219391	4.355153	4.747897	4.180074
17 H	2.884087	4.251591	5.814759	5.220374	5.141008

	18 H 2.884220 4.251887 5.218505 5.817236 5.138559 6 7 8 9 10 6 C 0.000000 7 O 6.679559 0.000000 8 C 2.802952 5.722904 0.000000 9 O 3.768848 6.275785 1.138702 0.000000 10 O 5.715353 4.245452 6.678313 7.672499 0.000000 11 O 3.778354 4.178503 3.776096 4.437377 4.177374 12 O 1.138682 7.672767 3.768931 4.605113 6.265118 13 S 3.026518 5.139284 4.240183 5.370656 3.616108 14 S 4.239710 3.613775 3.025982 3.788259 5.141813 15 C 3.070099 5.789647 3.641768 4.682610 5.265478 16 C 3.643805 5.261913 3.067608 3.949431 5.793251 17 H 3.338888 6.860462 4.272821 5.257703 6.026023 18 H 4.275710 6.022267 3.335629 3.990976 6.864367 11 12 13 14 15 11 O 0.000000 12 O 4.439790 0.000000 13 S 4.135587 3.788588 0.000000 14 S 4.128378 5.370157 3.146316 0.000000 15 C 5.048541 3.952859 1.756503 2.721785 0.000000 16 C 5.046084 4.685472 2.722069 1.756316 1.374278 17 H 5.935995 3.995998 2.446832 3.740633 1.083496 18 H 5.932344 5.261906 3.740795 2.446917 2.161117 16 17 18 16 C 0.000000 17 H 2.161275 0.000000 18 H 1.083477 2.544482 0.000000
 15Q. -3738.99380918072 +29.25 WBI 0.004	1 2 3 4 5 1 Mn 0.000000 2 Mn 3.429149 0.000000 3 C 4.965026 1.832271 0.000000 4 C 3.896095 1.853882 2.648737 0.000000 5 C 2.146802 2.014394 3.843210 2.697146 0.000000 6 C 4.715455 1.789086 2.654572 2.526415 2.707880 7 C 3.896171 1.853874 2.648744 3.703365 2.697142 8 O 6.004338 2.971467 1.139196 3.553307 4.981535 9 O 4.590589 2.986983 3.549856 1.134997 3.562565 10 O 2.792150 2.999592 4.813472 3.464902 1.179730 11 O 5.668773 2.929181 3.579682 3.405468 3.560127 12 O 4.590671 2.986975 3.549878 4.832946 3.562546 13 S 2.311525 3.643598 4.620405 4.850287 3.342877 14 S 2.311536 3.643554 4.620304 3.219708 3.342920 15 C 2.716766 2.521802 3.106636 3.562227 3.108204 16 C 2.716780 2.521788 3.106582 2.748890 3.108234 17 H 3.782712 2.833234 2.785046 4.032375 3.904675 18 H 3.782726 2.833186 2.784920 2.746748 3.904696 6 7 8 9 10 6 C 0.000000 7 C 2.526446 0.000000 8 O 3.580947 3.553338 0.000000 9 O 3.379337 4.832946 4.274822 0.000000 10 O 3.081573 3.464874 5.946924 4.146846 0.000000 11 O 1.140213 3.405527 4.339581 4.043273 3.609931 12 O 3.379381 1.134997 4.274880 5.959215 4.146794

13	S	5.149244	3.219807	5.454529	5.802243	4.219226
14	S	5.149184	4.850282	5.454396	3.534403	4.219305
15	C	4.268110	2.748886	3.883635	4.509754	4.250327
16	C	4.268091	3.562203	3.883565	3.475361	4.250369
17	H	4.470241	2.746725	3.312557	5.004174	5.042077
18	H	4.470180	4.032289	3.312398	3.319282	5.042117

		11	12	13	14	15
11	O	0.000000				
12	O	4.043363	0.000000			
13	S	6.182834	3.534497	0.000000		
14	S	6.182760	5.802242	3.553099	0.000000	
15	C	5.394921	3.475338	1.763730	2.834679	0.000000
16	C	5.394897	4.509720	2.834694	1.763724	1.386034
17	H	5.565529	3.319223	2.413247	3.766328	1.086749
18	H	5.565458	5.004077	3.766347	2.413255	2.107794

		16	17	18
16	C	0.000000		
17	H	2.107788	0.000000	
18	H	1.086751	2.353303	0.000000

Table S3B. Energy rank for all of the $H_2C_2S_2Mn_2(CO)_5$ optimized structures. PBE0/6-311G(d,p).

No	Initial structure	Final energy (a.u.)	ΔE(kcal/mol)
1	186-2_b_Mn_CO5_A1A1BD1D1-Q-xqc.log	-3741.158562	0.00
2	20-2_a_Mn_CO5_A1A1BD1D1-Q-xqc-1.log	-3741.158562	0.00
3	27-2_b_Mn_CO5_A1A1BD1B-Q-xqc-1.log	-3741.158562	0.00
4	30-1_a_Mn_CO5_A1A1BD1B-Q-xqc-1.log	-3741.158562	0.00
5	106-2_a_Mn_CO5_pA1pA1pA1A2A2-Q.log	-3741.157249	0.82
6	100-2_a_Mn_CO5_A1A1pA2pD2pD2-Q-xqc.log	-3741.157248	0.82
7	103-2_a_Mn_CO5_pA1pA1A2A2pD1-Q-xqc-1.log	-3741.157248	0.82
8	104-2_a_Mn_CO5_pA1pA1A2BB-Q-xqc.log	-3741.157248	0.82
9	107-2_a_Mn_CO5_pA1pA1pA1A2B-Q-xqc.log	-3741.157248	0.82
10	111-2_b_Mn_CO5_A1A1pA2pD2pD2-Q-xqc.log	-3741.157248	0.82
11	113-2_b_Mn_CO5_pA1pA1A2BB-Q-xqc.log	-3741.157248	0.82
12	116-2_b_Mn_CO5_pA1pA1pA1A2D2-Q-xqc.log	-3741.157248	0.82
13	125-2_a_Mn_CO5_pA1pA1A2BD2-Q-xqc.log	-3741.157248	0.82
14	134-2_a_Mn_CO5_A1A2BBB-Q-xqc.log	-3741.157248	0.82
15	138-2_a_Mn_CO5_pA1pA1pA1A2D2-Q-xqc.log	-3741.157248	0.82
16	139-2_b_Mn_CO5_pA1pA1A2A2B-Q-xqc.log	-3741.157248	0.82
17	141-2_b_Mn_CO5_pA1pA1pA1A2B-Q-xqc.log	-3741.157248	0.82
18	143-1_b_Mn_CO5_A1A2BBB-Q-xqc.log	-3741.157248	0.82
19	148-2_a_Mn_CO5_pA1pA1BBD2-Q-xqc.log	-3741.157248	0.82
20	150-2_b_Mn_CO5_pA1pA1BBB-Q-xqc.log	-3741.157248	0.82
21	151-2_b_Mn_CO5_pA1pA1BBD2-Q-xqc.log	-3741.157248	0.82
22	175-3_a_Mn_CO5_A1A1A1A2A2-Q-xqc.log	-3741.157248	0.82
23	220-2_b_Mn_CO5_A1A2D1BD2-Q.log	-3741.157248	0.82
24	68-1_a_Mn_CO5_A1A2BBD1-Q-xqc.log	-3741.157248	0.82
25	85-3_b_Mn_CO5_A1A1A2BD2-Q-xqc.log	-3741.157248	0.82
26	87-2_a_Mn_CO5_A1A2BD1D2-Q-xqc.log	-3741.157248	0.82
27	102-2_a_Mn_CO5_pA1pA1A2A2B-Q.log	-3741.157247	0.83
28	105-2_a_Mn_CO5_pA1pA1A2BpD1-Q.log	-3741.157247	0.83
29	114--2_b_Mn_CO5_pA1pA1A2BpD1-Q.log	-3741.157247	0.83
30	62-2_b_Mn_CO5_A1A2BD1D2-o-Q-xqc-1.log	-3741.157247	0.83
31	100-2_a_Mn_CO5_A1A1pA2pD2pD2-T-xqc.log	-3741.156962	1.00
32	102-2_a_Mn_CO5_pA1pA1A2A2B-T.log	-3741.156962	1.00
33	103-2_a_Mn_CO5_pA1pA1A2A2pD1-T-xqc.log	-3741.156962	1.00
34	105-2_a_Mn_CO5_pA1pA1A2BpD1-T-xqc.log	-3741.156962	1.00
35	110-2_b_Mn_CO5_A1A1pA2BpD2-T-xqc.log	-3741.156962	1.00
36	111-2_b_Mn_CO5_A1A1pA2pD2pD2-T-xqc.log	-3741.156962	1.00
37	112-2_b_Mn_CO5_pA1pA1A2A2pD1-T-xqc.log	-3741.156962	1.00
38	113-2_b_Mn_CO5_pA1pA1A2BB-T-xqc.log	-3741.156962	1.00
39	124-2_a_Mn_CO5_A1pA2BD1B-T-xqc.log	-3741.156962	1.00
40	125-2_a_Mn_CO5_pA1pA1A2BD2-T-xqc.log	-3741.156962	1.00
41	134-2_a_Mn_CO5_A1A2BBB-T-xqc.log	-3741.156962	1.00

42	138-2_a_Mn_CO5_pA1pA1pA1A2D2-T-xqc.log	-3741.156962	1.00
43	143-1_b_Mn_CO5_A1A2BBB-T-xqc.log	-3741.156962	1.00
44	147-2_a_Mn_CO5_pA1A2BBpD1-T-xqc.log	-3741.156962	1.00
45	148-2_a_Mn_CO5_pA1pA1BBD2-T-xqc.log	-3741.156962	1.00
46	149-2_b_Mn_CO5_A1A2BBB-T-xqc.log	-3741.156962	1.00
47	150-2_b_Mn_CO5_pA1pA1BBB-T-xqc.log	-3741.156962	1.00
48	151-2_b_Mn_CO5_pA1pA1BBD2-T-xqc.log	-3741.156962	1.00
49	211-3_a_Mn_CO5_A1A1BD2D2-T-xqc.log	-3741.156962	1.00
50	221-2_b_Mn_CO5_pA1A2BBpD1-T.log	-3741.156962	1.00
51	4-2_a_Mn_CO5_A1A1BD1D2-T-xqc-1.log	-3741.156962	1.00
52	61-2_a_Mn_CO5_A1A2BD1D2-o-T-xqc-1.log	-3741.156962	1.00
53	7-2_b_Mn_CO5_pA1pA1pA1A2A2-T-xqc-1.log	-3741.156962	1.00
54	8-1_a_Mn_CO5_A1A2BBB-T-xqc-1.log	-3741.156962	1.00
55	114--2_b_Mn_CO5_pA1pA1A2BpD1-T-xqc.log	-3741.156961	1.00
56	3-2_b_Mn_CO5_A1A2BD1D2-T-xqc-1.log	-3741.156961	1.00
57	83-2_a_Mn_CO5_A1A1pA2BpD2-T-xqc.log	-3741.156961	1.00
58	73-2_b_Mn_CO5_A1A1A1pA2pA2-T.log	-3741.148913	6.05
59	10-1_a_Mn_CO5_A1A1A2A2D1-T-xqc-1.log	-3741.148911	6.06
60	108-2_b_Mn_CO5_A1A1BBD2-T-xqc.log	-3741.148911	6.06
61	121-1_a_Mn_CO5_A1A1A2D2D2-T-xqc.log	-3741.148911	6.06
62	126-2_b_Mn_CO5_A1A1BBD1-T-xqc.log	-3741.148911	6.06
63	132-2_b_Mn_CO5_pA1pA1A2D2D2-T-xqc.log	-3741.148911	6.06
64	139-2_b_Mn_CO5_pA1pA1A2A2B-T-xqc.log	-3741.148911	6.06
65	144-1_b_Mn_CO5_A1A1A2D2D2-T-xqc.log	-3741.148911	6.06
66	154-2_a_Mn_CO5_A1A1pA2BD1-T-xqc.log	-3741.148911	6.06
67	156-1_a_Mn_CO5_A1A1A1A2D1-T-xqc.log	-3741.148911	6.06
68	16-1_a_Mn_CO5_A1A1A1A2A2-T-xqc.log	-3741.148911	6.06
69	164-2_b_Mn_CO5_A1A1pA2BD1-T-xqc.log	-3741.148911	6.06
70	166-2_a_Mn_CO5_A1A1pA2D1D1-T-xqc.log	-3741.148911	6.06
71	167-2_b_Mn_CO5_A1A1pA2D1D1-T-xqc.log	-3741.148911	6.06
72	178-1_a_Mn_CO5_A1A1A2BD1-T-xqc.log	-3741.148911	6.06
73	180-1_b_Mn_CO5_A1A1A2BD1-T-xqc.log	-3741.148911	6.06
74	181-1_a_Mn_CO5_A1A1A1A2B-T-xqc.log	-3741.148911	6.06
75	184-1_b_Mn_CO5_A1A1A1A2B-T-xqc.log	-3741.148911	6.06
76	22-1_a_Mn_CO5_A1A1BBD2-T-xqc-2.log	-3741.148911	6.06
77	31-2_a_Mn_CO5_A1A2D1BD2-T-xqc-1.log	-3741.148911	6.06
78	68-1_a_Mn_CO5_A1A2BBD1-T-xqc.log	-3741.148911	6.06
79	69-1_b_Mn_CO5_A1A1A1A2D2-T.log	-3741.148911	6.06
80	71-1_b_Mn_CO5_A1A2BBD1-T-xqc.log	-3741.148911	6.06
81	76-2_b_Mn_CO5_A1pA2BBD1-T-xqc.log	-3741.148911	6.06
82	77-2_b_Mn_CO5_A1A1pA2BB-T-xqc.log	-3741.148911	6.06
83	78-2_b_Mn_CO5_A1A1BBB-T-xqc.log	-3741.148911	6.06
84	79-2_b_Mn_CO5_A1A1A1pA2pD2-T-xqc.log	-3741.148911	6.06
85	81-2_a_Mn_CO5_A1A1BBB-T-xqc.log	-3741.148911	6.06
86	82-2_a_Mn_CO5_A1A1A1pA2pA2-T.log	-3741.148911	6.06

87	89-2_a_Mn_CO5_A1A1A1pA2B-T-xqc.log	-3741.148911	6.06
88	91-1_b_Mn_CO5_A1A1A2A2D1-T-xqc.log	-3741.148911	6.06
89	94-2_b_Mn_CO5_A1A1D1BD2-T-xqc.log	-3741.148911	6.06
90	67-2_a_Mn_CO5_A1A1A1pA2pD2-T.log	-3741.148910	6.06
91	182-1_b_Mn_CO5_A1A1A1A2A2-T.log	-3741.148909	6.06
92	6-2_b_Mn_CO5_A1A1A1pA2B-T.log	-3741.148778	6.14
93	156-1_a_Mn_CO5_A1A1A1A2D1-Q-xqc.log	-3741.145866	7.97
94	156-1_a_Mn_CO5_A1A1A1A2D1-Q-xqc.log	-3741.145865	7.97
95	159-2_a_Mn_CO5_A1A1A1pA2D1-Q-xqc.log	-3741.145865	7.97
96	167-2_b_Mn_CO5_A1A1pA2D1D1-Q-xqc.log	-3741.145865	7.97
97	181-1_a_Mn_CO5_A1A1A1A2B-Q-xqc.log	-3741.145865	7.97
98	184-1_b_Mn_CO5_A1A1A1A2B-Q-xqc.log	-3741.145865	7.97
99	230-1_b_Mn_CO5_A1A1BD1D2-Q-xqc.log	-3741.145865	7.97
100	36-1_b_Mn_CO5_A1A1A1A2D1-Q-xqc.log	-3741.145865	7.97
101	17-2_a_Mn_CO5_pA1pA1pA1A2pD1-Q-xqc-1.log	-3741.145863	7.97
102	166-2_a_Mn_CO5_A1A1pA2D1D1-Q-xqc.log	-3741.145862	7.97
103	163-2_b_Mn_CO5_A1A1A1pA2D1-Q.log	-3741.145842	7.98
104	157-1_a_Mn_CO5_A1A2BD1D1-Q-xqc.log	-3741.145645	8.11
105	146-2_a_Mn_CO5_pA1pA1A2D2D2-Q-xqc-freq.log	-3741.145644	8.11
106	231-1_b_Mn_CO5_A1A1D1BD2-Q-xqc-freq.log	-3741.145644	8.11
107	72-1_b_Mn_CO5_A1A2D1BD2-Q-xqc-freq.log	-3741.145644	8.11
108	177-1_a_Mn_CO5_A1A1A2BB-Q-xqc.log	-3741.145643	8.11
109	182-1_b_Mn_CO5_A1A1A1A2A2-Q-xqc-freq.log	-3741.145643	8.11
110	154-2_a_Mn_CO5_A1A1pA2BD1-Q-xqc.log	-3741.145640	8.11
111	158-1_b_Mn_CO5_A1A2BD1D1-Q-xqc.log	-3741.145640	8.11
112	178-1_a_Mn_CO5_A1A1A2BD1-Q-xqc.log	-3741.145640	8.11
113	77-2_b_Mn_CO5_A1A1pA2BB-Q-xqc.log	-3741.145640	8.11
114	78-2_b_Mn_CO5_A1A1BBB-Q-xqc.log	-3741.145640	8.11
115	89-2_a_Mn_CO5_A1A1A1pA2B-Q.log	-3741.145640	8.11
116	164-2_b_Mn_CO5_A1A1pA2BD1-Q-xqc.log	-3741.145639	8.11
117	67-2_a_Mn_CO5_A1A1A1pA2pD2-Q-xqc-freq.log	-3741.145639	8.11
118	69-1_b_Mn_CO5_A1A1A1A2D2-Q.log	-3741.145639	8.11
119	79-2_b_Mn_CO5_A1A1A1pA2pD2-Q.log	-3741.145639	8.11
120	144-1_b_Mn_CO5_A1A1A2D2D2-Q-xqc.log	-3741.145638	8.11
121	16-1_a_Mn_CO5_A1A1A1A2A2-Q-xqc.log	-3741.145638	8.11
122	180-1_b_Mn_CO5_A1A1A2BD1-Q-xqc-1.log	-3741.145638	8.11
123	180-1_b_Mn_CO5_A1A1A2BD1-Q-xqc.log	-3741.145638	8.11
124	6-2_b_Mn_CO5_A1A1A1pA2B-Q.log	-3741.145638	8.11
125	93-1_b_Mn_CO5_A1A1A2BB-Q.log	-3741.145638	8.11
126	147-2_a_Mn_CO5_pA1A2BBpD1-Q-xqc.log	-3741.145636	8.11
127	37-3_a_Mn_CO5_A1A1A2BD1-Q-xqc.log	-3741.144323	8.94
128	80-2_a_Mn_CO5_A1A1pA2BB-Q.log	-3741.144061	9.10
129	233-3_b_Mn_CO5_A1A1BD1D1-Q-xqc.log	-3741.143601	9.39
130	1-1_a_Mn_CO5_A1A1BBB-Q-xqc-1.log	-3741.143600	9.39
131	119-3_a_Mn_CO5_A1A2BD1D1-Q-xqc.log	-3741.143600	9.39

132	140-3_b_Mn_CO5_A1A2BD1D1-Q-xqc.log	-3741.143600	9.39
133	153-3_b_Mn_CO5_A1A1D2BD2-Q-xqc.log	-3741.143600	9.39
134	169-3_b_Mn_CO5_A1A2BD1B-Q-xqc.log	-3741.143600	9.39
135	213-3_b_Mn_CO5_A1A1BBD1-Q.log	-3741.143600	9.39
136	232-3_b_Mn_CO5_A1A1BD1D2-Q-xqc.log	-3741.143600	9.39
137	235-3_a_Mn_CO5_A1A1BBB-Q-xqc.log	-3741.143600	9.39
138	238-3_a_Mn_CO5_A1A1BD1D2-Q-xqc.log	-3741.143600	9.39
139	239-3_b_Mn_CO5_A1A1BD1B-Q-xqc-freq.log	-3741.143600	9.39
140	240-3_a_Mn_CO5_A1A1BD1D1-Q-xqc.log	-3741.143600	9.39
141	26-2_b_Mn_CO5_pA1pA1A2pD1pD1-Q-xqc-1.log	-3741.143600	9.39
142	38-3_a_Mn_CO5_A1A2BBD1-Q-xqc-1.log	-3741.143600	9.39
143	52-3_a_Mn_CO5_A1A1BD1B-Q-xqc.log	-3741.143600	9.39
144	81-2_a_Mn_CO5_A1A1BBB-Q-xqc.log	-3741.143600	9.39
145	90-3_b_Mn_CO5_A1A1A2BB-Q-xqc.log	-3741.143600	9.39
146	122-2_a_Mn_CO5_A1A1BBD1-Q-xqc-freq.log	-3741.143599	9.39
147	124-2_a_Mn_CO5_A1pA2BD1B-Q-xqc.log	-3741.143599	9.39
148	126-2_b_Mn_CO5_A1A1BBD1-Q-xqc.log	-3741.143599	9.39
149	131-3_b_Mn_CO5_A1A1A2BD1-Q-xqc.log	-3741.143599	9.39
150	135-3_a_Mn_CO5_A1A2D1BD2-Q-xqc.log	-3741.143599	9.39
151	152-3_b_Mn_CO5_A1A1BBD2-Q-xqc.log	-3741.143599	9.39
152	179-1_a_Mn_CO5_A1A1A2D1D1-Q-xqc.log	-3741.143599	9.39
153	183-1_b_Mn_CO5_A1A1A2D1D1-Q-xqc.log	-3741.143599	9.39
154	187-1_a_Mn_CO5_A1A1BBD1-Q-xqc.log	-3741.143599	9.39
155	19-1_b_Mn_CO5_A1A1BBD1-Q-xqc-1.log	-3741.143599	9.39
156	194-3_b_Mn_CO5_A1A1BD2D2-Q-xqc-1.log	-3741.143599	9.39
157	21-3_a_Mn_CO5_A1A1A2BB-Q-xqc-1.log	-3741.143599	9.39
158	217-1_a_Mn_CO5_A1A2D1BD1-Q.log	-3741.143599	9.39
159	234-3_b_Mn_CO5_A1A1D1BD2-Q-xqc.log	-3741.143599	9.39
160	237-2_b_Mn_CO5_A1A1D1BD1-Q-xqc.log	-3741.143599	9.39
161	34-1_b_Mn_CO5_A1A1BD2B-Q-xqc-1.log	-3741.143599	9.39
162	35-3_b_Mn_CO5_A1A1A1A2D1-Q-xqc-1.log	-3741.143599	9.39
163	43-3_b_Mn_CO5_A1A2BBD1-Q-xqc-1-freq.log	-3741.143599	9.39
164	5-3_a_Mn_CO5_A1A1BBD2-Q-xqc-1.log	-3741.143599	9.39
165	50-2_a_Mn_CO5_A1A1D1BD1-Q-xqc-1.log	-3741.143599	9.39
166	56-3_a_Mn_CO5_A1A1BBD1-Q-xqc-1.log	-3741.143599	9.39
167	70-1_b_Mn_CO5_A1A1BBB-Q-xqc.log	-3741.143599	9.39
168	75-3_a_Mn_CO5_A1A1A1A2D1-Q-xqc-freq.log	-3741.143599	9.39
169	95-3_a_Mn_CO5_A1A2BBB-Q-xqc.log	-3741.143599	9.39
170	96-3_b_Mn_CO5_A1A2D1BD1-Q-xqc.log	-3741.143599	9.39
171	120-3_a_Mn_CO5_A1A2D1BD1-Q-xqc.log	-3741.143598	9.39
172	168-3_a_Mn_CO5_A1A2BD1B-Q-xqc-freq.log	-3741.143598	9.39
173	142-3_b_Mn_CO5_A1A2BBB-Q-xqc.log	-3741.143596	9.39
174	33-2_b_Mn_CO5_pA1pA1pA1A2pD1-Q-xqc.log	-3741.140707	11.20
175	106-2_a_Mn_CO5_pA1pA1pA1A2A2-T-freq.log	-3741.138522	12.58
176	80-2_a_Mn_CO5_A1A1pA2BB-T-xqc.log	-3741.136391	13.91

177	2_a_Mn_CO5_A1A1A1pA2pD2----65	-3741.134863	14.87
178	1_a_Mn_CO5_A1A1BBB----12	-3741.134861	14.87
179	1_a_Mn_CO5_A1A2BBD1----25	-3741.134861	14.87
180	1_b_Mn_CO5_A1A1A1A2D2----34	-3741.134861	14.87
181	1_b_Mn_CO5_A1A1BBB----43	-3741.134861	14.87
182	1_b_Mn_CO5_A1A2BBD1----56	-3741.134861	14.87
183	1_b_Mn_CO5_A1A2D1BD2----61	-3741.134861	14.87
184	2_a_Mn_CO5_A1A1A1pA2pA2----64	-3741.134861	14.87
185	2_a_Mn_CO5_A1A1BBB----66	-3741.134861	14.87
186	2_a_Mn_CO5_A1A1pA2BB----85	-3741.134861	14.87
187	2_b_Mn_CO5_A1A1A1pA2pD2----124	-3741.134861	14.87
188	2_b_Mn_CO5_A1A1BBB----125	-3741.134861	14.87
189	2_b_Mn_CO5_A1A1pA2BB----144	-3741.134861	14.87
190	2_b_Mn_CO5_A1pA2BBD1----159	-3741.134861	14.87
191	3_a_Mn_CO5_A1A1A1A2D1----182	-3741.134861	14.87
192	4_b_Mn_CO5_x----241	-3741.134861	14.87
193	2_a_Mn_CO5_A1pA2BBD1----100	-3741.134859	14.87
194	2_b_Mn_CO5_A1A1A1pA2pA2----123	-3741.134859	14.87
195	13-3_a_Mn_CO5_A1A1A1A2B-Q-xqc.log	-3741.134486	15.11
196	215-2_a_Mn_CO5_pA1pA1A2pD1pD1-Q.log	-3741.134471	15.12
197	2_a_Mn_CO5_A1A1D1BD2----82	-3741.134169	15.31
198	2_a_Mn_CO5_A1A1pA2BpD2----87	-3741.134168	15.31
199	2_a_Mn_CO5_pA1pA1A2pD1D2----110	-3741.134168	15.31
200	2_b_Mn_CO5_A1A1D1BD2----141	-3741.134168	15.31
201	3_a_Mn_CO5_A1A2BBB----204	-3741.134168	15.31
202	3_b_Mn_CO5_A1A2D1BD1----239	-3741.134168	15.31
203	2_a_Mn_CO5_A1A1BBD2----68	-3741.134167	15.31
204	2_a_Mn_CO5_A1A1BD2B----74	-3741.134167	15.31
205	2_a_Mn_CO5_A1A1BD2D2----78	-3741.134167	15.31
206	2_a_Mn_CO5_A1A1pA2pD2pD2----91	-3741.134167	15.31
207	2_a_Mn_CO5_pA1A2BpD1B----103	-3741.134167	15.31
208	2_a_Mn_CO5_pA1pA1A2A2B----104	-3741.134167	15.31
209	2_a_Mn_CO5_pA1pA1A2A2pD1----105	-3741.134167	15.31
210	2_a_Mn_CO5_pA1pA1A2BB----106	-3741.134167	15.31
211	2_a_Mn_CO5_pA1pA1A2BpD1----108	-3741.134167	15.31
212	2_a_Mn_CO5_pA1pA1pA1A2A2----117	-3741.134167	15.31
213	2_a_Mn_CO5_pA1pA1pA1A2B----118	-3741.134167	15.31
214	2_b_Mn_CO5_A1A1BBD2----127	-3741.134167	15.31
215	2_b_Mn_CO5_A1A1BD2B----133	-3741.134167	15.31
216	2_b_Mn_CO5_A1A1pA2BpD2----146	-3741.134167	15.31
217	2_b_Mn_CO5_A1A1pA2pD2pD2----150	-3741.134167	15.31
218	2_b_Mn_CO5_pA1pA1A2A2pD1----164	-3741.134167	15.31
219	2_b_Mn_CO5_pA1pA1A2BB----165	-3741.134167	15.31

220	2_b_Mn_CO5_pA1pA1A2BpD1----167	-3741.134167	15.31
221	2_b_Mn_CO5_pA1pA1A2pD1D2----169	-3741.134167	15.31
222	2_b_Mn_CO5_pA1pA1pA1A2D2----178	-3741.134167	15.31
223	3_a_Mn_CO5_A1A1A2BD2----188	-3741.134167	15.31
224	3_a_Mn_CO5_A1A1A2D2D2----191	-3741.134167	15.31
225	3_a_Mn_CO5_A1A2BD1D1----207	-3741.134167	15.31
226	3_a_Mn_CO5_A1A2D1BD1----209	-3741.134167	15.31
227	3_a_Mn_CO5_A1A2D1BD2----210	-3741.134167	15.31
228	3_b_Mn_CO5_A1A1A1A2A2----211	-3741.134167	15.31
229	3_b_Mn_CO5_A1A1A2A2D1----215	-3741.134167	15.31
230	3_b_Mn_CO5_A1A1A2BD2----218	-3741.134167	15.31
231	3_b_Mn_CO5_A1A1A2D2D2----221	-3741.134167	15.31
232	2_a_Mn_CO5_pA1pA1pA1A2D2----119	-3741.134166	15.31
233	2_b_Mn_CO5_pA1pA1A2A2B----163	-3741.134166	15.31
234	3_b_Mn_CO5_A1A2BD1D1----237	-3741.134166	15.31
235	2_b_Mn_CO5_pA1pA1pA1A2B----177	-3741.134165	15.31
236	3_b_Mn_CO5_A1A2BBB----234	-3741.134164	15.31
237	1_b_Mn_CO5_A1A2BBB----55	-3741.134163	15.31
238	212-3_b_Mn_CO5_A1A1A1A2D2-Q.log	-3741.134136	15.33
239	9-3_a_Mn_CO5_A1A1A2A2B-Q.log	-3741.134131	15.33
240	94-2_b_Mn_CO5_A1A1D1BD2-Q-xqc.log	-3741.134131	15.33
241	137-3_b_Mn_CO5_A1A1A2A2D1-Q-xqc.log	-3741.134130	15.33
242	61-2_a_Mn_CO5_A1A2BD1D2-o-Q-xqc-freq.log	-3741.133082	15.99
243	2_b_Mn_CO5_A1A2BD1D2----155	-3741.132878	16.12
244	1_b_Mn_CO5_A1A1A2D2D2----42	-3741.132877	16.12
245	2_a_Mn_CO5_A1A1D2BD2-o----83	-3741.132877	16.12
246	2_a_Mn_CO5_A1A2BD1D2----96	-3741.132877	16.12
247	2_a_Mn_CO5_pA1pA1A2D2D2----109	-3741.132877	16.12
248	1_a_Mn_CO5_A1A1A2D2D2----11	-3741.132876	16.12
249	2_a_Mn_CO5_A1A1BBD1----67	-3741.132876	16.12
250	2_a_Mn_CO5_A1A1BD2D2-o----77	-3741.132876	16.12
251	2_a_Mn_CO5_A1pA2BD1B----101	-3741.132876	16.12
252	2_a_Mn_CO5_pA1pA1A2BD2----107	-3741.132876	16.12
253	2_b_Mn_CO5_A1A1BBD1----126	-3741.132876	16.12
254	2_b_Mn_CO5_A1A1BD2D2-o----136	-3741.132876	16.12
255	2_b_Mn_CO5_A1A1D2BD2-o----142	-3741.132876	16.12
256	2_b_Mn_CO5_A1pA2BD1B----160	-3741.132876	16.12
257	2_b_Mn_CO5_pA1pA1A2BD2----166	-3741.132876	16.12
258	3_b_Mn_CO5_A1A1A2BD1----217	-3741.132876	16.12
259	2_b_Mn_CO5_pA1pA1A2D2D2----168	-3741.132875	16.12
260	161-2_a_Mn_CO5_A1A2BD1D1-Q-xqc-freq.log	-3741.132695	16.23
261	18-3_a_Mn_CO5_A1A1D2BD2-Q-xqc-1-freq.log	-3741.132693	16.23
262	190-3_a_Mn_CO5_A1A1A1A2D2-Q-xqc-freq.log	-3741.132693	16.23

263	192-1_b_Mn_CO5_A1A2D1BD1-Q-xqc.log	-3741.132693	16.23
264	64-2_b_Mn_CO5_pA1A2BpD1B-Q-xqc.log	-3741.132693	16.23
265	25-2_a_Mn_CO5_A1A2BD1D1-o-Q-xqc-1-freq.log	-3741.132691	16.23
266	32-2_b_Mn_CO5_A1A2BD1D1-o-Q-xqc-1-freq.log	-3741.132689	16.24
267	214-2_a_Mn_CO5_A1A2D1BD1-Q.log	-3741.130604	17.54
268	208-2_a_Mn_CO5_pA1pA1BBpD1-Q-rpt.log	-3741.128691	18.74
269	216-2_b_Mn_CO5_A1A2D1BD1-Q-rupt.log	-3741.128688	18.75
270	23-3_b_Mn_CO5_A1A1A2A2B-Q-xqc.log	-3741.126986	19.81
271	55-1_b_Mn_CO5_A1A1D2BD2-Q-xqc-1.log	-3741.123642	21.91
272	31-2_a_Mn_CO5_A1A2D1BD2-Q.log	-3741.123641	21.91
273	227-3_b_Mn_CO5_A1A1A2D1D1-Q-xqc.log	-3741.123109	22.25
274	39-3_a_Mn_CO5_A1A1A2D1D1-Q-xqc.log	-3741.123109	22.25
275	2_a_Mn_CO5_A1A1BD1D2-o----72	-3741.123022	22.30
276	2_a_Mn_CO5_A1A1D1BD2-o----81	-3741.123022	22.30
277	2_a_Mn_CO5_A1A2BBB----92	-3741.123022	22.30
278	2_a_Mn_CO5_pA1A2BBpD1----102	-3741.123022	22.30
279	2_a_Mn_CO5_pA1pA1BBD2----113	-3741.123022	22.30
280	2_b_Mn_CO5_A1A1BD1D2-o----131	-3741.123022	22.30
281	2_b_Mn_CO5_A1A2BBB----151	-3741.123022	22.30
282	2_b_Mn_CO5_pA1pA1BBB----171	-3741.123022	22.30
283	2_b_Mn_CO5_pA1pA1BBD2----172	-3741.123022	22.30
284	46-1_a_Mn_CO5_A1A1BD1D1-Q-xqc.log	-3741.120652	23.79
285	218-1_b_Mn_CO5_A1A1BD1B-Q-freq.log	-3741.120651	23.79
286	107-2_a_Mn_CO5_pA1pA1pA1A2B-T-freq.log	-3741.120156	24.10
287	163-2_b_Mn_CO5_A1A1A1pA2D1-T.log	-3741.118971	24.84
288	204-2_b_Mn_CO5_pA1pA1BpD1B-Q.log	-3741.118444	25.17
289	149-2_b_Mn_CO5_A1A2BBB-Q-xqc.log	-3741.115184	27.22
290	82-2_a_Mn_CO5_A1A1A1pA2pA2-Q.log	-3741.115183	27.22
291	108-2_b_Mn_CO5_A1A1BBD2-Q-xqc.log	-3741.115076	27.29
292	132-2_b_Mn_CO5_pA1pA1A2D2D2-Q-xqc.log	-3741.115076	27.29
293	73-2_b_Mn_CO5_A1A1A1pA2pA2-Q.log	-3741.115076	27.29
294	84-2_a_Mn_CO5_pA1pA1A2pD1D2-Q-xqc-freq.log	-3741.115076	27.29
295	54-1_a_Mn_CO5_A1A1D1BD2-T-xqc.log	-3741.114324	27.76
296	146-2_a_Mn_CO5_pA1pA1A2D2D2-T-xqc.log	-3741.114308	27.77
297	231-1_b_Mn_CO5_A1A1D1BD2-T-xqc-freq.log	-3741.114308	27.77
298	47-2_a_Mn_CO5_A1A1BD1D2-Q-xqc.log	-3741.114245	27.81
299	159-2_a_Mn_CO5_A1A1A1pA2D1-T-freq.log	-3741.114220	27.83
300	171-2_b_Mn_CO5_A1A1pA2pA2D1-Q-xqc.log	-3741.112946	28.62
301	41-2_a_Mn_CO5_A1A1D2BD2-Q-xqc.log	-3741.112946	28.62
302	17-2_a_Mn_CO5_pA1pA1pA1A2pD1-T-xqc-1.log	-3741.112350	29.00
303	36-1_b_Mn_CO5_A1A1A1A2D1-T-xqc.log	-3741.112349	29.00
304	204-2_b_Mn_CO5_pA1pA1BpD1B-T.log	-3741.111356	29.62
305	207-2_a_Mn_CO5_pA1pA1BpD1B-T.log	-3741.111356	29.62
306	50-2_a_Mn_CO5_A1A1D1BD1-T-xqc.log	-3741.109027	31.08

307	169-3_b_Mn_CO5_A1A2BD1B-T-xqc-freq.log	-3741.108864	31.19
308	137-3_b_Mn_CO5_A1A1A2A2D1-T-xqc.log	-3741.108863	31.19
309	170-3_a_Mn_CO5_A1A1A2A2D1-T-xqc.log	-3741.108863	31.19
310	23-3_b_Mn_CO5_A1A1A2A2B-T.log	-3741.108863	31.19
311	104-2_a_Mn_CO5_pA1pA1A2BB-T-xqc.log	-3741.108600	31.35
312	203-2_a_Mn_CO5_pA1pA1BBB-Q-XQC.log	-3741.108315	31.53
313	207-2_a_Mn_CO5_pA1pA1BpD1B-Q.log	-3741.108315	31.53
314	223-2_b_Mn_CO5_A1A1pA2D1pD2-T-xqc.log	-3741.107873	31.81
315	221-2_b_Mn_CO5_pA1A2BBpD1-Q-xqc.log	-3741.107420	32.09
316	101-2_a_Mn_CO5_pA1A2BpD1B-Q-xqc-freq.log	-3741.107083	32.30
317	29-2_b_Mn_CO5_A1A1D1BD2-o-Q-xqc-1.log	-3741.107080	32.31
318	3_a_Mn_CO5_A1A1BBD2----194	-3741.106327	32.78
319	3_b_Mn_CO5_A1A1BBD2----224	-3741.106327	32.78
320	3_b_Mn_CO5_A1A1D2BD2----233	-3741.106327	32.78
321	122-2_a_Mn_CO5_A1A1BBD1-T-xqc.log	-3741.106235	32.84
322	187-1_a_Mn_CO5_A1A1BBD1-T-xqc.log	-3741.106235	32.84
323	141-2_b_Mn_CO5_pA1pA1pA1A2B-T-xqc-freq.log	-3741.106184	32.87
324	70-1_b_Mn_CO5_A1A1BBB-T-xqc.log	-3741.105850	33.08
325	19-1_b_Mn_CO5_A1A1BBD1-T-xqc-1.log	-3741.105849	33.08
326	84-2_a_Mn_CO5_pA1pA1A2pD1D2-T-xqc-freq.log	-3741.105646	33.21
327	2-2_a_Mn_CO5_A1A1D1BD2-Q-xqc.log	-3741.105068	33.57
328	112-2_b_Mn_CO5_pA1pA1A2A2pD1-Q-freq.log	-3741.104314	34.04
329	24-3_b_Mn_CO5_A1A2D1BD2-T-xqc-2.log	-3741.104269	34.07
330	153-3_b_Mn_CO5_A1A1D2BD2-T-xqc.log	-3741.104197	34.11
331	213-3_b_Mn_CO5_A1A1BBD1-T.log	-3741.104197	34.11
332	233-3_b_Mn_CO5_A1A1BD1D1-T-xqc.log	-3741.104197	34.11
333	234-3_b_Mn_CO5_A1A1D1BD2-T-xqc.log	-3741.104197	34.11
334	240-3_a_Mn_CO5_A1A1BD1D1-T-xqc-freq.log	-3741.104195	34.12
335	172-2_a_Mn_CO5_A1A1pA2pA2D1-T-xqc.log	-3741.104180	34.13
336	199-2_a_Mn_CO5_A1A1BD2D1-o-T-xqc.log	-3741.104177	34.13
337	62-2_b_Mn_CO5_A1A2BD1D2-o-T-xqc.log	-3741.104175	34.13
338	135-3_a_Mn_CO5_A1A2D1BD2-T-xqc.log	-3741.104157	34.14
339	136-3_b_Mn_CO5_A1A1A1A2A2-T-xqc.log	-3741.104157	34.14
340	175-3_a_Mn_CO5_A1A1A1A2A2-T-xqc.log	-3741.104157	34.14
341	201-2_b_Mn_CO5_pA1pA1BD2B-T-xqc.log	-3741.104157	34.14
342	179-1_a_Mn_CO5_A1A1A2D1D1-T-xqc.log	-3741.103633	34.47
343	183-1_b_Mn_CO5_A1A1A2D1D1-T-xqc.log	-3741.103633	34.47
344	75-3_a_Mn_CO5_A1A1A1A2D1-T-xqc-freq.log	-3741.103633	34.47
345	116-2_b_Mn_CO5_pA1pA1pA1A2D2-T.log	-3741.103489	34.56
346	88-2_b_Mn_CO5_A1A1BD1D2-o-Q-xqc-freq.log	-3741.102062	35.45
347	4-2_a_Mn_CO5_A1A1BD1D2-Q-xqc-1-freq.log	-3741.102061	35.45
348	190-3_a_Mn_CO5_A1A1A1A2D2-T-xqc.log	-3741.102012	35.49
349	7-2_b_Mn_CO5_pA1pA1pA1A2A2-Q.log	-3741.101469	35.83
350	219-1_b_Mn_CO5_A1A2BD1B-T-rupt.log	-3741.100782	36.26

351	24-3_b_Mn_CO5_A1A2D1BD2-Q-xqc.log	-3741.100763	36.27
352	48-1_a_Mn_CO5_A1A1BD2B-T-xqc-1.log	-3741.100017	36.74
353	18-3_a_Mn_CO5_A1A1D2BD2-T-xqc.log	-3741.100015	36.74
354	9-3_a_Mn_CO5_A1A1A2A2B-T-xqc.log	-3741.099902	36.81
355	174-1_b_Mn_CO5_A1A1A2A2B-Q-xqc.log	-3741.099436	37.10
356	2_b_Mn_CO5_A1A1A1pA2B----121	-3741.098231	37.86
357	2_a_Mn_CO5_A1A1pA2BD1----86	-3741.09823	37.86
358	2_b_Mn_CO5_A1A2D1BD1-o----156	-3741.098229	37.86
359	1_a_Mn_CO5_A1A1A1A2D1----3	-3741.098228	37.86
360	1_a_Mn_CO5_A1A2BD1D1----27	-3741.098228	37.86
361	1_b_Mn_CO5_A1A2BD1D1----58	-3741.098228	37.86
362	2_a_Mn_CO5_A1A1A1pA2B----62	-3741.098228	37.86
363	2_a_Mn_CO5_A1A1A1pA2D1----63	-3741.098228	37.86
364	2_a_Mn_CO5_A1A1BD1B----69	-3741.098228	37.86
365	2_a_Mn_CO5_A1A2BD1D1----94	-3741.098228	37.86
366	2_a_Mn_CO5_A1A2D1BD1-o----97	-3741.098228	37.86
367	2_b_Mn_CO5_A1A1A1pA2D1----122	-3741.098228	37.86
368	2_b_Mn_CO5_A1A1pA2BD1----145	-3741.098228	37.86
369	2_b_Mn_CO5_A1A2BD1D1----153	-3741.098228	37.86
370	2_a_Mn_CO5_A1A1pA2D1D1----88	-3741.098227	37.86
371	2_b_Mn_CO5_A1A1pA2D1D1----147	-3741.098226	37.86
372	10-1_a_Mn_CO5_A1A1A2A2D1-Q-xqc.log	-3741.098156	37.91
373	91-1_b_Mn_CO5_A1A1A2A2D1-Q.log	-3741.098154	37.91
374	218-1_b_Mn_CO5_A1A1BD1B-T.log	-3741.097561	38.28
375	215-2_a_Mn_CO5_pA1pA1A2pD1pD1-T.log	-3741.097110	38.56
376	64-2_b_Mn_CO5_pA1A2BpD1B-T-xqc.log	-3741.096579	38.89
377	1-1_a_Mn_CO5_A1A1BBB-T-xqc.log	-3741.096567	38.90
378	222-3_a_Mn_CO5_A1A1A2D1D2-Q-freq.log	-3741.095479	39.59
379	117-3_a_Mn_CO5_A1A1A2BD2-Q-xqc.log	-3741.095477	39.59
380	109-2_b_Mn_CO5_A1A1BD2B-Q-xqc.log	-3741.095475	39.59
381	196-3_b_Mn_CO5_A1A1BD2B-Q-xqc.log	-3741.095474	39.59
382	209-3_a_Mn_CO5_A1A1BD2B-Q.log	-3741.095474	39.59
383	210-3_a_Mn_CO5_A1A1BD2D1-Q.log	-3741.095474	39.59
384	28-3_b_Mn_CO5_A1A1A2D1D2-Q-xqc.log	-3741.095474	39.59
385	195-3_b_Mn_CO5_A1A1BD2D1-Q-xqc.log	-3741.095469	39.59
386	211-3_a_Mn_CO5_A1A1BD2D2-Q.log	-3741.095468	39.59
387	33-2_b_Mn_CO5_pA1pA1pA1A2pD1-T-xqc-1.log	-3741.095015	39.88
388	2-2_a_Mn_CO5_A1A1D1BD2-T-xqc-1.log	-3741.095013	39.88
389	206-2_b_Mn_CO5_A1A1BD1D1-o-T.log	-3741.095013	39.88
390	208-2_a_Mn_CO5_pA1pA1BBpD1-T-freq.log	-3741.095011	39.88
391	53-2_a_Mn_CO5_A1A1D1BD1-o-Q-xqc.log	-3741.093763	40.66
392	219-1_b_Mn_CO5_A1A2BD1B-Q.log	-3741.093343	40.93
393	101-2_a_Mn_CO5_pA1A2BpD1B-T-xqc.log	-3741.093094	41.08
394	2_b_Mn_CO5_pA1pA1pA1A2A2----176	-3741.092604	41.39

395	171-2_b_Mn_CO5_A1A1pA2pA2D1-T-xqc.log	-3741.092182	41.65
396	57-2_a_Mn_CO5_A1A1BD1D1-o-Q-xqc.log	-3741.092171	41.66
397	173-3_b_Mn_CO5_A1A1D1BD1-T-xqc.log	-3741.092128	41.69
398	152-3_b_Mn_CO5_A1A1BBD2-T-xqc.log	-3741.092127	41.69
399	235-3_a_Mn_CO5_A1A1BBB-T-xqc.log	-3741.092127	41.69
400	236-3_a_Mn_CO5_A1A1D1BD2-T-xqc.log	-3741.092127	41.69
401	238-3_a_Mn_CO5_A1A1BD1D2-T-xqc.log	-3741.092127	41.69
402	239-3_b_Mn_CO5_A1A1BD1B-T-xqc.log	-3741.092127	41.69
403	5-3_a_Mn_CO5_A1A1BBD2-T-xqc-1.log	-3741.092127	41.69
404	52-3_a_Mn_CO5_A1A1BD1B-T-xqc-1.log	-3741.092127	41.69
405	1_a_Mn_CO5_A1A2BBB----24	-3741.091176	42.29
406	71-1_b_Mn_CO5_A1A2BBD1-Q-xqc-freq.log	-3741.090979	42.41
407	14-1_a_Mn_CO5_A1A1A2BD2-T-xqc-1.log	-3741.090200	42.90
408	76-2_b_Mn_CO5_A1pA2BBD1-Q-xqc-rupt.log	-3741.090117	42.95
409	199-2_a_Mn_CO5_A1A1BD2D1-o-Q-xqc-freq.log	-3741.089654	43.24
410	133-2_a_Mn_CO5_A1A1D1BD2-o-T-xqc.log	-3741.089335	43.44
411	87-2_a_Mn_CO5_A1A2BD1D2-T-xqc-rupt.log	-3741.089019	43.64
412	145-2_a_Mn_CO5_A1A1D2BD2-o-Q-xqc.log	-3741.088929	43.70
413	3_a_Mn_CO5_A1A1A2A2B----184	-3741.088285	44.10
414	3_a_Mn_CO5_A1A2BD1B----206	-3741.088285	44.10
415	3_b_Mn_CO5_A1A1A2BB----216	-3741.088285	44.10
416	3_b_Mn_CO5_A1A2BD1B----236	-3741.088285	44.10
417	3_a_Mn_CO5_A1A1A2A2D1----185	-3741.088284	44.10
418	51-1_b_Mn_CO5_A1A1D1BD1-Q-xqc.log	-3741.087908	44.34
419	237-2_b_Mn_CO5_A1A1D1BD1-T-xqc.log	-3741.087900	44.34
420	172-2_a_Mn_CO5_A1A1pA2pA2D1-Q-xqc.log	-3741.087886	44.35
421	197-1_a_Mn_CO5_A1A1BD2D1-T-xqc.log	-3741.087696	44.47
422	74-2_a_Mn_CO5_A1pA2BBD1-T-xqc-rupt.log	-3741.087635	44.51
423	1_a_Mn_CO5_A1A1A2A2D1----5	-3741.087406	44.65
424	2_b_Mn_CO5_A1A1pA2pA2D1----149	-3741.087404	44.65
425	1_b_Mn_CO5_A1A1A2A2D1----36	-3741.087403	44.65
426	2_a_Mn_CO5_A1A1pA2pA2D1----90	-3741.087403	44.65
427	60-2_b_Mn_CO5_A1A1BD2D1-T-xqc.log	-3741.086485	45.23
428	85-3_b_Mn_CO5_A1A1A2BD2-Txqc.log	-3741.086483	45.23
429	8-1_a_Mn_CO5_A1A2BBB-Q-xqc-1-freq.log	-3741.086295	45.35
430	12-1_a_Mn_CO5_A1A1A2A2B-Q.log	-3741.085860	45.62
431	176-1_b_Mn_CO5_A1A1A2D1D2-T-xqc.log	-3741.085331	45.95
432	92-1_b_Mn_CO5_A1A1A2BD2-T.log	-3741.085331	45.95
433	15-1_a_Mn_CO5_A1A1A2D1D2-T-xqc.log	-3741.085330	45.95
434	174-1_b_Mn_CO5_A1A1A2A2B-T-xqc.log	-3741.085330	45.95
435	12-1_a_Mn_CO5_A1A1A2A2B-T-xqc.log	-3741.085329	45.95
436	35-3_b_Mn_CO5_A1A1A1A2D1-T-xqc-1-freq.log	-3741.085066	46.12
437	38-3_a_Mn_CO5_A1A2BBD1-T-xqc-1-freq.log	-3741.085064	46.12
438	120-3_a_Mn_CO5_A1A2D1BD1-T-xqc.log	-3741.085063	46.12

439	131-3_b_Mn_CO5_A1A1A2BD1-T-xqc.log	-3741.085058	46.12
440	168-3_a_Mn_CO5_A1A2BD1B-T-xqc.log	-3741.085058	46.12
441	39-3_a_Mn_CO5_A1A1A2D1D1-T-xqc.log	-3741.085058	46.12
442	13-3_a_Mn_CO5_A1A1A1A2B-T-xqc.log	-3741.085057	46.13
443	37-3_a_Mn_CO5_A1A1A2BD1-T-xqc-1.log	-3741.085057	46.13
444	90-3_b_Mn_CO5_A1A1A2BB-T-xqc.log	-3741.085057	46.13
445	21-3_a_Mn_CO5_A1A1A2BB-T-xqc.log	-3741.085056	46.13
446	227-3_b_Mn_CO5_A1A1A2D1D1-T.log	-3741.085056	46.13
447	96-3_b_Mn_CO5_A1A2D1BD1-T-xqc.log	-3741.085055	46.13
448	236-3_a_Mn_CO5_A1A1D1BD2-Q-freq.log	-3741.083686	46.99
449	93-1_b_Mn_CO5_A1A1A2BB-T.log	-3741.083639	47.01
450	206-2_b_Mn_CO5_A1A1BD1D1-o-Q.log	-3741.082812	47.53
451	189-1_b_Mn_CO5_A1A1BD2D2-Q-xqc-freq.log	-3741.081434	48.40
452	66-1_a_Mn_CO5_A1A1D2BD2-Q-xqc-freq.log	-3741.080704	48.86
453	3_a_Mn_CO5_A1A1D1BD1----201	-3741.080295	49.11
454	3_b_Mn_CO5_A1A1D1BD1----231	-3741.080294	49.11
455	47-2_a_Mn_CO5_A1A1BD1D2-T-xqc-rupt.log	-3741.079831	49.40
456	88-2_b_Mn_CO5_A1A1BD1D2-o-T-xqc.log	-3741.079573	49.57
457	205-2_b_Mn_CO5_pA1pA1BBpD1-T.log	-3741.079567	49.57
458	40-2_b_Mn_CO5_A1A1D2BD2-T-xqc-1.log	-3741.079251	49.77
459	66-1_a_Mn_CO5_A1A1D2BD2-T-xqc-1.log	-3741.079245	49.77
460	109-2_b_Mn_CO5_A1A1BD2B-T-xqc.log	-3741.079162	49.82
461	136-3_b_Mn_CO5_A1A1A1A2A2-Q-freq.log	-3741.079113	49.86
462	1_a_Mn_CO5_A1A1A2A2B----4	-3741.078644	50.15
463	1_b_Mn_CO5_A1A1A2A2B----35	-3741.078644	50.15
464	74-2_a_Mn_CO5_A1pA2BBD1-Q-xqc.log	-3741.078350	50.33
465	3_a_Mn_CO5_A1A1A1A2B----181	-3741.077692	50.75
466	3_a_Mn_CO5_A1A1A1A2A2----180	-3741.07769	50.75
467	1_a_Mn_CO5_A1A1A2BD2----8	-3741.077551	50.84
468	1_b_Mn_CO5_A1A1A2BD2----39	-3741.077551	50.84
469	1_b_Mn_CO5_A1A1A2D1D2----41	-3741.077551	50.84
470	1_a_Mn_CO5_A1A1A2D1D2----10	-3741.077549	50.84
471	15-1_a_Mn_CO5_A1A1A2D1D2-Q.log	-3741.077384	50.94
472	176-1_b_Mn_CO5_A1A1A2D1D2-Q-xqc.log	-3741.077384	50.94
473	226-2_a_Mn_CO5_A1A1pA2D1pD2-Q-xqc.log	-3741.077383	50.94
474	170-3_a_Mn_CO5_A1A1A2A2D1-Q-xqc-freq.log	-3741.077360	50.96
475	22-1_a_Mn_CO5_A1A1BBD2-Q.log	-3741.076635	51.41
476	110-2_b_Mn_CO5_A1A1pA2BpD2-Q.log	-3741.076634	51.41
477	193-1_b_Mn_CO5_A1A1BBD2-Q-xqc.log	-3741.076632	51.41
478	92-1_b_Mn_CO5_A1A1A2BD2-Q.log	-3741.076631	51.41
479	14-1_a_Mn_CO5_A1A1A2BD2-Q-xqc-1.log	-3741.076630	51.41
480	1_a_Mn_CO5_A1A1A1A2A2----1	-3741.076146	51.72
481	1_a_Mn_CO5_A1A1A2BB----6	-3741.076146	51.72
482	1_a_Mn_CO5_A1A1A2BD1----7	-3741.076146	51.72

483	1_a_Mn_CO5_A1A1A2D1D1----9	-3741.076146	51.72
484	1_b_Mn_CO5_A1A1A2BB----37	-3741.076146	51.72
485	1_b_Mn_CO5_A1A1A2BD1----38	-3741.076146	51.72
486	1_a_Mn_CO5_A1A1A1A2B----2	-3741.076145	51.72
487	1_b_Mn_CO5_A1A1A1A2A2----31	-3741.076145	51.72
488	1_b_Mn_CO5_A1A1A2D1D1----40	-3741.076145	51.72
489	1_b_Mn_CO5_A1A1A1A2B----32	-3741.076142	51.72
490	223-2_b_Mn_CO5_A1A1pA2D1pD2-Q.log	-3741.076107	51.74
491	54-1_a_Mn_CO5_A1A1D1BD2-Q-xqc-1-freq.log	-3741.076103	51.74
492	2_a_Mn_CO5_pA1pA1pA1A2pD1----120	-3741.075547	52.09
493	3_a_Mn_CO5_A1A1D2BD2----203	-3741.075522	52.11
494	121-1_a_Mn_CO5_A1A1A2D2D2-Q-xqc.log	-3741.074899	52.50
495	83-2_a_Mn_CO5_A1A1pA2BpD2-Q-xqc.log	-3741.074899	52.50
496	46-1_a_Mn_CO5_A1A1BD1D1-T-xqc-1.log	-3741.074869	52.52
497	1_b_Mn_CO5_A1A1BBD1----44	-3741.074544	52.72
498	1_b_Mn_CO5_A1A1BD1D1----47	-3741.074544	52.72
499	196-3_b_Mn_CO5_A1A1BD2B-T-xqc.log	-3741.074464	52.77
500	59-2_a_Mn_CO5_A1A1BD2D1-Q-xqc-1.log	-3741.074094	53.00
501	60-2_b_Mn_CO5_A1A1BD2D1-Q-xqc.log	-3741.074091	53.01
502	48-1_a_Mn_CO5_A1A1BD2B-Q-xqc.log	-3741.073780	53.20
503	98-2_a_Mn_CO5_A1A1BD2B-Q-xqc.log	-3741.073779	53.20
504	30-1_a_Mn_CO5_A1A1BD1B-T-xqc.log	-3741.073149	53.60
505	2_a_Mn_CO5_A1A1BD1D1----71	-3741.072543	53.98
506	2_b_Mn_CO5_A1A1BD1D1----130	-3741.072543	53.98
507	3_a_Mn_CO5_A1A1A2BB----186	-3741.0725	54.00
508	1_a_Mn_CO5_A1A1BBD1----13	-3741.072499	54.01
509	1_a_Mn_CO5_A1A1BD2D2----20	-3741.072499	54.01
510	1_b_Mn_CO5_A1A1BD2D2----51	-3741.072499	54.01
511	3_a_Mn_CO5_A1A1A1A2D2----183	-3741.072499	54.01
512	3_a_Mn_CO5_A1A1BD2B----198	-3741.072499	54.01
513	3_a_Mn_CO5_A1A1BD2D1----199	-3741.072499	54.01
514	3_a_Mn_CO5_A1A1BD2D2----200	-3741.072499	54.01
515	3_b_Mn_CO5_A1A1A1A2D2----213	-3741.072499	54.01
516	3_b_Mn_CO5_A1A1BBD1----223	-3741.072499	54.01
517	3_b_Mn_CO5_A1A1BD2B----228	-3741.072499	54.01
518	3_b_Mn_CO5_A1A1BD2D1----229	-3741.072499	54.01
519	3_b_Mn_CO5_A1A1BD2D2----230	-3741.072499	54.01
520	1_a_Mn_CO5_A1A1BBD2----14	-3741.072433	54.05
521	1_b_Mn_CO5_A1A1BBD2----45	-3741.072433	54.05
522	3_b_Mn_CO5_A1A1A2A2B----214	-3741.072161	54.22
523	117-3_a_Mn_CO5_A1A1A2BD2-T-xqc.log	-3741.071563	54.59
524	173-3_b_Mn_CO5_A1A1D1BD1-Q-xqc.log	-3741.070535	55.24
525	49-3_b_Mn_CO5_A1A1BBB-Q-xqc.log	-3741.070535	55.24

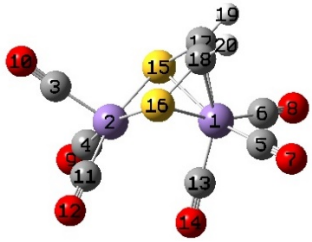
526	11-3_a_Mn_CO5_A1A1D1BD1-Q.log	-3741.070531	55.24
527	3_b_Mn_CO5_A1A2D1BD2----240	-3741.070513	55.25
528	225-1_a_Mn_CO5_A1A2D1BD2-Q-xqc.log	-3741.069950	55.60
529	2_a_Mn_CO5_A1A2BD1D1-o----93	-3741.069345	55.98
530	1_a_Mn_CO5_A1A2BD1B----26	-3741.069343	55.99
531	1_b_Mn_CO5_A1A2D1BD1----60	-3741.069343	55.99
532	2_a_Mn_CO5_A1A2D1BD1----98	-3741.069343	55.99
533	2_a_Mn_CO5_pA1pA1A2pD1pD1----111	-3741.069343	55.99
534	2_b_Mn_CO5_A1A2D1BD1----157	-3741.069343	55.99
535	2_b_Mn_CO5_pA1pA1A2pD1pD1----170	-3741.069342	55.99
536	1_a_Mn_CO5_A1A2D1BD1----29	-3741.06934	55.99
537	11-3_a_Mn_CO5_A1A1D1BD1-T-xqc-1.log	-3741.069318	56.00
538	2_b_Mn_CO5_A1A1BD1B----128	-3741.069219	56.06
539	191-1_a_Mn_CO5_A1A2BD1B-Q-xqc.log	-3741.068024	56.81
540	228-1_b_Mn_CO5_A1A2BD1D2-Q-xqc.log	-3741.068024	56.81
541	63-1_a_Mn_CO5_A1A1D1BD1-T-xqc-rupt.log	-3741.066635	57.69
542	3_b_Mn_CO5_A1A1A2D1D2----220	-3741.065708	58.27
543	1_a_Mn_CO5_A1A2D1BD2----30	-3741.065707	58.27
544	2_a_Mn_CO5_A1A1pA2D1pD2----89	-3741.065707	58.27
545	2_b_Mn_CO5_A1A1BD2D2----137	-3741.065707	58.27
546	2_b_Mn_CO5_A1A1pA2D1pD2----148	-3741.065707	58.27
547	3_a_Mn_CO5_A1A1A2D1D2----190	-3741.065707	58.27
548	203-2_a_Mn_CO5_pA1pA1BBB-T.log	-3741.065505	58.39
549	2_b_Mn_CO5_A1A1D1BD2-o----140	-3741.065296	58.53
550	20-2_a_Mn_CO5_A1A1BD1D1-T-xqc-1.log	-3741.064975	58.73
551	1_a_Mn_CO5_A1A1BD1B----15	-3741.06469	58.91
552	1_b_Mn_CO5_A1A1BD1B----46	-3741.06469	58.91
553	2_a_Mn_CO5_A1A2D1BD2----99	-3741.064446	59.06
554	2_b_Mn_CO5_pA1A2BBpD1----161	-3741.064443	59.06
555	2_b_Mn_CO5_A1A2D1BD2----158	-3741.064441	59.06
556	212-3_b_Mn_CO5_A1A1A1A2D2-T.log	-3741.064434	59.07
557	216-2_b_Mn_CO5_A1A2D1BD1-T.log	-3741.063378	59.73
558	2_b_Mn_CO5_A1A2BD1D1-o----152	-3741.063368	59.74
559	1_b_Mn_CO5_A1A2BD1B----57	-3741.063367	59.74
560	119-3_a_Mn_CO5_A1A2BD1D1-T-xqc.log	-3741.063172	59.86
561	142-3_b_Mn_CO5_A1A2BBB-T-xqc.log	-3741.063172	59.86
562	202-3_b_Mn_CO5_A1A2BD1D2-T.log	-3741.063172	59.86
563	95-3_a_Mn_CO5_A1A2BBB-T.log	-3741.063172	59.86
564	43-3_b_Mn_CO5_A1A2BBD1-T-xqc-1.log	-3741.063171	59.86
565	140-3_b_Mn_CO5_A1A2BD1D1-T-xqc.log	-3741.063170	59.86
566	220-2_b_Mn_CO5_A1A2D1BD2-T.log	-3741.062001	60.59
567	200-2_a_Mn_CO5_pA1pA1BD2B-T.log	-3741.060583	61.48
568	58-3_a_Mn_CO5_A1A2BD1D2-T-xqc-freq.log	-3741.058036	63.08

569	2_b_Mn_CO5_pA1pA1pA1A2pD1----179	-3741.057731	63.27
570	201-2_b_Mn_CO5_pA1pA1BD2B-Q-freq.log	-3741.056947	63.76
571	200-2_a_Mn_CO5_pA1pA1BD2B-Q.log	-3741.056944	63.77
572	1_b_Mn_CO5_A1A1BD2B-COdeplasat----49	-3741.056728	63.90
573	65-1_b_Mn_CO5_A1A1BD2D1-T-xqc.log	-3741.054829	65.09
574	128-2_b_Mn_CO5_A1A1D2BD2-o-Q-xqc-rupt.log	-3741.052708	66.42
575	123-2_a_Mn_CO5_A1A1BD2D2-o-Q-xqc.log	-3741.052366	66.64
576	224-2_b_Mn_CO5_A1A1BD2D2-Q-xqc.log	-3741.052366	66.64
577	49-3_b_Mn_CO5_A1A1BBB-T-xqc.log	-3741.052299	66.68
578	56-3_a_Mn_CO5_A1A1BBD1-T-xqc-1.log	-3741.052287	66.69
579	45-1_a_Mn_CO5_A1A2BD1D2-Q-xqc.log	-3741.051683	67.07
580	28-3_b_Mn_CO5_A1A1A2D1D2-T-xqc.log	-3741.050008	68.12
581	222-3_a_Mn_CO5_A1A1A2D1D2-T.log	-3741.050007	68.12
582	195-3_b_Mn_CO5_A1A1BD2D1-T-xqc.log	-3741.050006	68.12
583	209-3_a_Mn_CO5_A1A1BD2B-T.log	-3741.050006	68.12
584	210-3_a_Mn_CO5_A1A1BD2D1-T.log	-3741.050005	68.12
585	229-2_b_Mn_CO5_A1A1BD1D2-Q-freq.log	-3741.049180	68.64
586	232-3_b_Mn_CO5_A1A1BD1D2-T-freq.log	-3741.049149	68.66
587	3_b_Mn_CO5_A1A1A1A2D1----212	-3741.049138	68.66
588	44-1_a_Mn_CO5_A1A1BD1D2-Q-xqc-1-freq.log	-3741.047748	69.54
589	42-2_b_Mn_CO5_A1A1BD2D1-o-Q.log	-3741.047556	69.66
590	192-1_b_Mn_CO5_A1A2D1BD1-T-xqc.log	-3741.047169	69.90
591	214-2_a_Mn_CO5_A1A2D1BD1-T-freq.log	-3741.047163	69.90
592	32-2_b_Mn_CO5_A1A2BD1D1-o-T-xqc-1.log	-3741.047161	69.91
593	1_b_Mn_CO5_A1A1A1A2D1----33	-3741.046931	70.05
594	3_a_Mn_CO5_A1A1A2BD1----187	-3741.042193	73.02
595	202-3_b_Mn_CO5_A1A2BD1D2-Q-xqc.log	-3741.039751	74.56
596	58-3_a_Mn_CO5_A1A2BD1D2-Q-xqc.log	-3741.039750	74.56
597	3_a_Mn_CO5_A1A2BBD1----205	-3741.039325	74.82
598	198-2_b_Mn_CO5_A1A1D1BD1-o-T-xqc-freq.log	-3741.038286	75.47
599	51-1_b_Mn_CO5_A1A1D1BD1-T-xqc-CO_inversat.log	-3741.038285	75.48
600	3_a_Mn_CO5_A1A1A2D1D1----189	-3741.03784	75.75
601	3_b_Mn_CO5_A1A1A2D1D1----219	-3741.03784	75.75
602	2_b_Mn_CO5_A1A1D2BD2----143	-3741.037455	76.00
603	2_a_Mn_CO5_A1A1D2BD2----84	-3741.037453	76.00
604	2_b_Mn_CO5_A1A1BD2D1-o----134	-3741.037246	76.13
605	198-2_b_Mn_CO5_A1A1D1BD1-o-Q-freq.log	-3741.036783	76.42
606	3_b_Mn_CO5_A1A2BBD1----235	-3741.036739	76.45
607	228-1_b_Mn_CO5_A1A2BD1D2-T-xqc.log	-3741.033870	78.25
608	45-1_a_Mn_CO5_A1A2BD1D2-T-xqc-1.log	-3741.033089	78.74
609	1_a_Mn_CO5_A1A1BD1D2----17	-3741.032854	78.88
610	1_a_Mn_CO5_A1A2BD1D2----28	-3741.030713	80.23
611	1_b_Mn_CO5_A1A2BD1D2----59	-3741.030713	80.23
612	118-3_a_Mn_CO5_A1A1A2D2D2-T.log	-3741.029621	80.91

613	86-3_b_Mn_CO5_A1A1A2D2D2-T.log	-3741.029619	80.91
614	1_a_Mn_CO5_A1A1BD1D1----16	-3741.029143	81.21
615	118-3_a_Mn_CO5_A1A1A2D2D2-Q.log	-3741.029010	81.30
616	86-3_b_Mn_CO5_A1A1A2D2D2-Q-xqc.log	-3741.029009	81.30
617	2_a_Mn_CO5_A1A1BD1D2----73	-3741.028448	81.65
618	2_b_Mn_CO5_A1A1BD1D2----132	-3741.028448	81.65
619	1_b_Mn_CO5_A1A1BD1D2----48	-3741.028447	81.65
620	40-2_b_Mn_CO5_A1A1D2BD2-Q.log	-3741.025062	83.77
621	1_a_Mn_CO5_A1A1BD2B----18	-3741.024325	84.24
622	217-1_a_Mn_CO5_A1A2D1BD1-T.log	-3741.020656	86.54
623	226-2_a_Mn_CO5_A1A1pA2D1pD2-T-freq.log	-3741.020166	86.84
624	3_b_Mn_CO5_A1A1BBB----222	-3741.014929	90.13
625	3_b_Mn_CO5_A1A1D1BD2----232	-3741.014929	90.13
626	3_a_Mn_CO5_A1A1BBB----192	-3741.014928	90.13
627	3_a_Mn_CO5_A1A1D1BD2----202	-3741.014928	90.13
628	2_a_Mn_CO5_A1A1D1BD1----80	-3741.013538	91.00
629	2_b_Mn_CO5_A1A1D1BD1----139	-3741.013538	91.00
630	1_b_Mn_CO5_A1A1D1BD1----52	-3741.012338	91.76
631	3_a_Mn_CO5_A1A1BD1B----195	-3741.011808	92.09
632	3_a_Mn_CO5_A1A1BD1D2----197	-3741.011808	92.09
633	3_b_Mn_CO5_A1A1BD1B----225	-3741.011807	92.09
634	3_a_Mn_CO5_A1A1BD1D1----196	-3741.011806	92.09
635	3_b_Mn_CO5_A1A1BD1D1----226	-3741.011806	92.09
636	3_b_Mn_CO5_A1A1BD1D2----227	-3741.011806	92.09
637	2_a_Mn_CO5_A1A1D1BD1-o----79	-3741.011699	92.16
638	53-2_a_Mn_CO5_A1A1D1BD1-o-T-xqc.log	-3741.010870	92.68
639	1_a_Mn_CO5_A1A1D1BD2----22	-3741.010688	92.79
640	1_b_Mn_CO5_A1A1D1BD2----53	-3741.010688	92.79
641	1_b_Mn_CO5_A1A1D2BD2----54	-3741.009404	93.60
642	194-3_b_Mn_CO5_A1A1BD2D2-T-xqc-freq.log	-3741.007100	95.04
643	3_a_Mn_CO5_A1A1BBD1----193	-3741.00321	97.48
644	26-2_b_Mn_CO5_pA1pA1A2pD1pD1-T-xqc-1-freq.log	-3741.000724	99.04
645	29-2_b_Mn_CO5_A1A1D1BD2-o-T-xqc-1-freq.log	-3741.000142	99.41
646	2_a_Mn_CO5_A1A1BD1D1-o----70	-3740.99887	100.21
647	2_a_Mn_CO5_pA1pA1BBpD1----114	-3740.99887	100.21
648	2_a_Mn_CO5_pA1pA1BpD1B----116	-3740.99887	100.21
649	2_b_Mn_CO5_A1A1BD1D1-o----129	-3740.99887	100.21
650	2_b_Mn_CO5_pA1pA1BBpD1----173	-3740.99887	100.21
651	2_b_Mn_CO5_pA1pA1BpD1B----175	-3740.998869	100.21
652	2_a_Mn_CO5_pA1pA1BBB----112	-3740.998868	100.21
653	3_a_Mn_CO5_A1A2BD1D2----208	-3740.998622	100.36
654	3_b_Mn_CO5_A1A2BD1D2----238	-3740.998621	100.36
655	2_a_Mn_CO5_A1A1BD2D1----76	-3740.996156	101.91

656	2_b_Mn_CO5_A1A1BD2D1----135	-3740.99291	103.95
657	2_a_Mn_CO5_A1A2BD1D2-o----95	-3740.992274	104.35
658	44-1_a_Mn_CO5_A1A1BD1D2-T-xqc-freq.log	-3740.991063	105.11
659	2_b_Mn_CO5_A1A2BD1D2-o----154	-3740.989378	106.16
660	1_a_Mn_CO5_A1A1D1BD1----21	-3740.988715	106.58
661	2_b_Mn_CO5_pA1A2BpD1B----162	-3740.988172	106.92
662	1_b_Mn_CO5_A1A1BD2D1----50	-3740.981447	111.14
663	1_a_Mn_CO5_A1A1BD2D1----19	-3740.981446	111.14
664	1_a_Mn_CO5_A1A1D2BD2----23	-3740.973482	116.14
665	2_b_Mn_CO5_A1A1D1BD1-o----138	-3740.938506	138.09
666	2_a_Mn_CO5_A1A1BD2D1-o----75	-3740.936969	139.05
667	2_a_Mn_CO5_pA1pA1BD2B----115	-3740.936964	139.05
668	2_b_Mn_CO5_pA1pA1BD2B----174	-3740.936963	139.06

Table S4A. Distance table for the lowest-lying $H_2C_2S_2Mn_2(CO)_6$ structures after PBE0/6-311G(d,p) optimization followed by a single point CCSD(T) energy calculation. Provided are the absolute CCSD(T) energy (a.u.), relative energy (kcal/mol), symmetry and WBI.



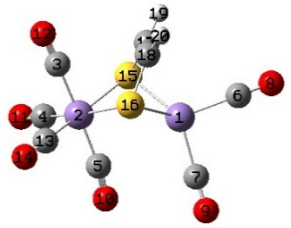
1S. -3852.23819729645 0.00 C_s
WBI 0.10

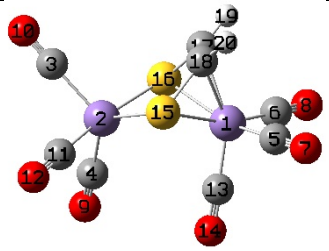
		1	2	3	4	5
1	Mn	0.000000				
2	Mn	2.802601	0.000000			
3	C	4.360323	1.758562	0.000000		
4	C	3.842570	1.794225	2.567581	0.000000	
5	C	1.785072	4.233791	5.754252	5.401215	0.000000
6	C	1.785075	4.233872	5.754328	4.762642	2.544245
7	O	2.926245	5.267177	6.744338	6.465881	1.141295
8	O	2.926257	5.267314	6.744475	5.584423	3.449156
9	O	4.741682	2.936187	3.492903	1.141978	6.295376
10	O	5.418430	2.901005	1.143596	3.502011	6.782850
11	C	3.842551	1.794229	2.567558	2.551500	4.762464
12	O	4.741646	2.936195	3.492871	3.457154	5.386429
13	C	1.796583	2.921652	4.679879	3.332736	2.584647
14	O	2.938301	3.539966	5.236882	3.517527	3.487121
15	S	2.391579	2.257313	3.147151	2.852793	4.134331
16	S	2.391579	2.257307	3.147146	4.017161	3.019205
17	C	2.118638	3.202063	4.044501	4.376161	3.362593
18	C	2.118642	3.202068	4.044506	4.761101	2.792757
19	H	2.869080	4.239522	4.993467	5.254305	3.879413
20	H	2.869085	4.239528	4.993474	5.834830	2.937713

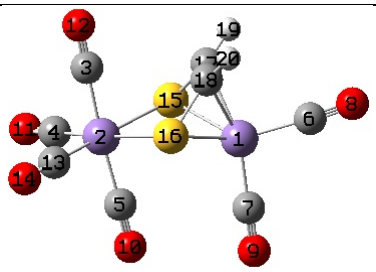
		6	7	8	9	10
6	C	0.000000				
7	O	3.449178	0.000000			
8	O	1.141303	4.163981	0.000000		
9	O	5.386673	7.351599	6.055815	0.000000	
10	O	6.782925	7.745715	7.745855	4.255759	0.000000
11	C	5.401295	5.584132	6.466026	3.457104	3.501972
12	O	6.295458	6.055420	7.351753	4.173082	4.255699
13	C	2.584642	3.507458	3.507479	4.006381	5.822655
14	O	3.487090	4.228079	4.228070	3.946073	6.368556
15	S	3.019290	5.260728	3.823705	3.664237	4.017213
16	S	4.134321	3.823560	5.260719	5.148728	4.017202
17	C	2.792752	4.350678	3.631501	5.306553	4.820816
18	C	3.362553	3.631501	4.350618	5.823408	4.820818
19	H	2.937683	4.757493	3.482340	6.089674	5.679430
20	H	3.879333	3.482383	4.757361	6.900201	5.679433

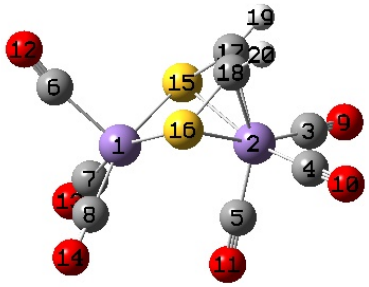
		11	12	13	14	15
11	C	0.000000				
12	O	1.141983	0.000000			
13	C	3.332834	4.006532	0.000000		
14	O	3.517716	3.946384	1.142109	0.000000	
15	S	4.017176	5.148750	3.317212	4.224596	0.000000
16	S	2.852678	3.664046	3.317285	4.224713	3.135232
17	C	4.761051	5.823324	3.770987	4.880999	1.741778
18	C	4.376078	5.306402	3.771018	4.881046	2.712187
19	H	5.834784	6.900123	4.543829	5.649223	2.443730
20	H	5.254207	6.089488	4.543875	5.649295	3.725919

		16	17	18	19	20

	16 S 0.000000 17 C 2.712172 0.000000 18 C 1.741772 1.378570 0.000000 19 H 3.725905 1.083900 2.157115 0.000000 20 H 2.443731 2.157118 1.083900 2.523131 0.000000
 2Q. -3852.20763094840 +19.18 C_1 WBI 0.01	1 2 3 4 5 1 Mn 0.000000 2 Mn 3.267977 0.000000 3 C 4.359256 1.854850 0.000000 4 C 4.594166 1.792856 2.579593 0.000000 5 C 3.096082 1.843340 3.697684 2.537258 0.000000 6 C 2.016833 5.193955 5.975331 6.443190 5.070985 7 C 2.004146 4.296754 5.835210 5.411119 3.183316 8 O 3.152330 6.303173 6.983105 7.509983 6.188052 9 O 3.140997 5.155906 6.801283 6.152724 3.766889 10 O 3.651820 2.975011 4.825136 3.366449 1.139790 11 O 5.567941 2.933487 3.466820 1.140788 3.427144 12 O 5.271629 2.988157 1.134072 3.465778 4.830037 13 C 4.592538 1.792971 2.584485 2.653848 2.544557 14 O 5.563856 2.933410 3.473259 3.594213 3.435334 15 S 2.461664 2.434071 2.966476 3.051089 3.172710 16 S 2.478366 2.430909 2.962544 4.215742 3.182919 17 C 2.645816 3.200517 3.011948 4.316910 4.307079 18 C 2.653188 3.197031 3.007136 4.706281 4.308727 19 H 3.447227 4.205164 3.774905 5.123492 5.320523 20 H 3.456137 4.202328 3.770629 5.724597 5.324308 6 7 8 9 10 6 C 0.000000 7 C 2.962189 0.000000 8 O 1.136657 3.871407 0.000000 9 O 3.865765 1.138200 4.617427 0.000000 10 O 5.481060 3.068218 6.549030 3.311935 0.000000 11 O 7.345106 6.282633 8.375491 6.954410 4.038347 12 O 6.704367 6.873836 7.636230 7.870376 5.954382 13 C 6.550200 5.228526 7.674532 5.872303 3.386078 14 O 7.497381 6.020354 8.615659 6.540536 4.064535 15 S 3.773420 4.053827 4.719301 5.111391 4.068940 16 S 4.010286 3.770725 5.048800 4.711944 4.093074 17 C 3.426691 4.632423 4.244893 5.768434 5.287721 18 C 3.539702 4.532155 4.403158 5.625233 5.294351 19 H 3.698665 5.427634 4.274425 6.562468 6.272938 20 H 3.886813 5.267646 4.556624 6.327426 6.284336 11 12 13 14 15 11 O 0.000000 12 O 4.156732 0.000000 13 C 3.592611 3.472634 0.000000 14 O 4.375302 4.166861 1.140637 0.000000 15 S 3.833297 3.759314 4.218414 5.354764 0.000000 16 S 5.352692 3.756505 3.037739 3.814866 3.208693 17 C 5.213886 3.470693 4.707294 5.742674 1.777959 18 C 5.743615 3.466309 4.307614 5.200984 2.730984 19 H 5.904241 3.989270 5.726042 6.754341 2.461588 20 H 6.754378 3.985242 5.114302 5.890589 3.742113 16 17 18 19 20 16 S 0.000000

	17 C 2.732261 0.000000 18 C 1.777032 1.340822 0.000000 19 H 3.743872 1.084707 2.122259 0.000000 20 H 2.461334 2.120110 1.084944 2.478019 0.000000
 3T. -3852.20319646607 +21.96 C_1 WBI 0.01	1 2 3 4 5 1 Mn 0.000000 2 Mn 3.264503 0.000000 3 C 4.803243 1.914702 0.000000 4 C 3.923787 1.869852 3.254924 0.000000 5 C 1.782425 4.691536 6.227139 5.388334 0.000000 6 C 1.781356 4.683385 6.065972 5.016175 2.545665 7 O 2.924769 5.712344 7.220504 6.417678 1.142451 8 O 2.923921 5.701496 6.991801 5.901997 3.455774 9 O 4.693449 3.006944 4.248925 1.137865 6.100176 10 O 5.808723 3.048517 1.134326 4.271570 7.215501 11 C 4.565729 1.809891 2.598657 2.484638 5.609401 12 O 5.531008 2.954044 3.484532 3.350680 6.380132 13 C 1.800580 3.562824 5.415935 3.355233 2.606642 14 O 2.941147 4.133065 6.023235 3.425235 3.541535 15 S 2.409080 2.341774 3.576685 3.773742 3.032003 16 S 2.402455 2.325982 3.215394 3.084907 4.144842 17 C 2.102063 3.213625 3.926159 4.481659 3.351502 18 C 2.096619 3.213271 4.058346 4.701081 2.774534 19 H 2.840929 4.233868 4.730329 5.426451 3.852872 20 H 2.837274 4.234046 4.928000 5.757750 2.901562 6 7 8 9 10 6 C 0.000000 7 O 3.455507 0.000000 8 O 1.142673 4.178083 0.000000 9 O 5.565326 7.099021 6.337057 0.000000 10 O 6.983716 8.189477 7.852837 5.180200 0.000000 11 C 6.172686 6.453061 7.248197 3.360284 3.524481 12 O 7.184117 7.111679 8.275063 4.008139 4.227455 13 C 2.605833 3.533281 3.532563 3.762426 6.523126 14 O 3.539843 4.300567 4.298534 3.501389 7.144545 15 S 4.152435 3.831647 5.281508 4.813261 4.539773 16 S 3.027603 5.273107 3.828184 3.942358 4.064483 17 C 2.782990 4.343640 3.625479 5.444184 4.656974 18 C 3.353046 3.617041 4.347625 5.736956 4.844411 19 H 2.911852 4.735503 3.460887 6.332864 5.309430 20 H 3.858995 3.449062 4.745529 6.791227 5.604441 11 12 13 14 15 11 C 0.000000 12 O 1.144215 0.000000 13 C 4.495943 5.314586 0.000000 14 O 4.778818 5.453097 1.140985 0.000000 15 S 2.959924 3.764704 3.290930 4.151534 0.000000 16 S 4.128186 5.269368 3.294517 4.157541 3.155015 17 C 4.809450 5.880975 3.744804 4.836059 2.730143 18 C 4.411865 5.346931 3.735838 4.826629 1.751465 19 H 5.865042 6.941012 4.516546 5.614996 3.742377 20 H 5.264450 6.102621 4.507779 5.605272 2.449993 16 17 18 19 20 16 S 0.000000 17 C 1.749253 0.000000

	18 C 2.718429 1.381308 0.000000 19 H 2.452504 1.083840 2.159814 0.000000 20 H 3.731468 2.156760 1.084082 2.521702 0.000000
 4T. -3852.20160687800 +22.96 C_1 WBI 0.01	1 2 3 4 5 1 Mn 0.000000 2 Mn 3.490476 0.000000 3 C 4.280953 1.845910 0.000000 4 C 4.862573 1.795169 2.607753 0.000000 5 C 3.473351 1.846584 3.690639 2.598265 0.000000 6 C 1.861721 5.295612 5.792847 6.637520 5.302744 7 C 1.830514 4.165203 5.498429 5.321039 3.245093 8 O 2.999449 6.402279 6.771267 7.731478 6.438410 9 O 2.971665 4.890373 6.403124 5.878091 3.595065 10 O 3.959269 2.981902 4.826473 3.492581 1.135859 11 O 5.845694 2.935803 3.505508 1.140769 3.497879 12 O 5.038733 2.980668 1.134813 3.523926 4.824605 13 C 4.865481 1.795191 2.606742 2.632981 2.598051 14 O 5.850420 2.935843 3.504173 3.565375 3.497784 15 S 2.398530 2.405924 2.952782 3.052316 3.041935 16 S 2.400578 2.406961 2.952709 4.195206 3.042203 17 C 2.063284 3.235083 3.106284 4.373561 4.172048 18 C 2.063075 3.235468 3.106992 4.775859 4.171637 19 H 2.808705 4.230609 3.850194 5.176278 5.189613 20 H 2.808586 4.231098 3.851068 5.786463 5.189061 6 7 8 9 10 6 C 0.000000 7 C 2.814960 0.000000 8 O 1.139180 3.793995 0.000000 9 O 3.757381 1.141163 4.603088 0.000000 10 O 5.658286 3.162733 6.759432 3.133312 0.000000 11 O 7.577296 6.208517 8.652109 6.677452 4.203503 12 O 6.338762 6.437573 7.213864 7.402312 5.960460 13 C 6.637476 5.325964 7.729849 5.884357 3.492006 14 O 7.578098 6.216202 8.650624 6.687236 4.202919 15 S 3.853452 3.442925 4.865593 4.361552 3.864266 16 S 3.848262 3.448550 4.857511 4.368913 3.863921 17 C 2.969889 3.790126 3.839588 4.903884 5.032531 18 C 2.965739 3.791164 3.834034 4.905581 5.031734 19 H 3.113583 4.517243 3.722172 5.621127 6.017022 20 H 3.106598 4.519017 3.711960 5.624016 6.015899 11 12 13 14 15 11 O 0.000000 12 O 4.240893 0.000000 13 C 3.566172 3.522296 0.000000 14 O 4.334778 4.238530 1.140768 0.000000 15 S 3.847122 3.721975 4.194433 5.332068 0.000000 16 S 5.332649 3.720984 3.056176 3.852740 3.140205 17 C 5.277754 3.528009 4.776733 5.825378 1.748597 18 C 5.823600 3.528569 4.376389 5.282233 2.726951 19 H 5.968599 4.026832 5.786971 6.830439 2.456039 20 H 6.829121 4.027499 5.179588 5.973999 3.740401 16 17 18 19 20 16 S 0.000000 17 C 2.727339 0.000000 18 C 1.748385 1.394846 0.000000

	19 H 3.740672 1.083975 2.170560 0.000000 20 H 2.455412 2.170501 1.083974 2.535192 0.000000
 5T. -3852.20100557159 +23.34 C_1 WBI 0.02	1 2 3 4 5 1 Mn 0.000000 2 Mn 3.005178 0.000000 3 C 4.431043 1.780968 0.000000 4 C 4.431974 1.780977 2.537833 0.000000 5 C 3.151175 1.801272 2.600086 2.599709 0.000000 6 C 2.017482 4.663584 6.035836 6.033421 5.147668 7 C 1.839147 4.059230 5.025661 5.603265 3.548234 8 C 1.837601 4.067500 5.612561 5.036170 3.562345 9 O 5.458969 2.923142 1.142282 3.444791 3.525091 10 O 5.460264 2.923146 3.444697 1.142277 3.524584 11 O 3.720819 2.942431 3.521025 3.520412 1.141160 12 O 3.138799 5.617345 6.944753 6.940671 6.243856 13 O 2.980060 4.963913 5.694696 6.495823 4.206209 14 O 2.978733 4.973798 6.508216 5.707546 4.223715 15 S 2.314541 2.417656 3.038321 4.156773 3.324313 16 S 2.315806 2.417749 4.157013 3.038649 3.323287 17 C 3.252155 2.107721 2.783145 3.351898 3.756492 18 C 3.252458 2.107284 3.352002 2.782335 3.755683 19 H 4.286736 2.850726 2.916450 3.858844 4.527630 20 H 4.287143 2.850536 3.859449 2.915641 4.526820 6 7 8 9 10 6 C 0.000000 7 C 2.992098 0.000000 8 C 2.972553 2.418896 0.000000 9 O 7.012240 5.857661 6.671398 0.000000 10 O 7.008920 6.661835 5.868819 4.161606 0.000000 11 O 5.731076 3.670311 3.686650 4.272328 4.271432 12 O 1.130621 4.006275 3.983198 7.887856 7.882065 13 O 3.920555 1.141512 3.258675 6.394208 7.543281 14 O 3.898051 3.258667 1.141701 7.556596 6.408098 15 S 3.312586 3.005966 4.087416 3.837531 5.284266 16 S 3.306564 4.086360 3.004913 5.284543 3.838051 17 C 4.055879 4.516062 4.870804 3.624164 4.342464 18 C 4.053888 4.870177 4.515773 4.342695 3.623411 19 H 4.948245 5.406990 5.943717 3.462747 4.739350 20 H 4.944983 5.942910 5.406507 4.740216 3.461862 11 12 13 14 15 11 O 0.000000 12 O 6.857678 0.000000 13 O 4.078411 4.825968 0.000000 14 O 4.100061 4.796950 3.851209 0.000000 15 S 4.207159 4.125623 3.864447 5.210218 0.000000 16 S 4.205638 4.116746 5.208223 3.861941 3.170961 17 C 4.857048 4.700566 5.489486 5.952656 1.751929 18 C 4.856086 4.697414 5.951740 5.488628 2.726119 19 H 5.629811 5.470829 6.302313 7.029665 2.447925 20 H 5.628710 5.465490 7.028355 6.300983 3.738325 16 17 18 19 20 16 S 0.000000 17 C 2.726405 0.000000 18 C 1.752024 1.375949 0.000000 19 H 3.738582 1.083998 2.153943 0.000000

	20 H 2.447897 2.153905 1.084003 2.517776 0.000000

Table S4B. Energy rank for all of the $H_2C_2S_2Mn_2(CO)_6$ optimized structures. PBE0/6-311G(d,p).

No	Initial structure	Final enery (a.u.)	ΔE (kcal/mol)
1	1_b_Mn_CO6_A1A1A1A2A2D2----38	-3854.421425	0.00
2	1_a_Mn_CO6_A1A1A1A2A2A2----2	-3854.421424	0.00
3	1_a_Mn_CO6_A1A1A1A2A2D2----5	-3854.421424	0.00
4	1_a_Mn_CO6_A1A1A1A2BD2----8	-3854.421424	0.00
5	1_a_Mn_CO6_A1A2BBBB----33	-3854.421424	0.00
6	1_b_Mn_CO6_A1A1A1A2A2A2----35	-3854.421424	0.00
7	1_b_Mn_CO6_A1A1A2BD1B----52	-3854.421424	0.00
8	2_a_Mn_CO6_A1A1A1A1pA2pA2----67	-3854.421424	0.00
9	2_a_Mn_CO6_A1A1A1A2A2A2----68	-3854.421424	0.00
10	2_a_Mn_CO6_A1A1A1pA2BB----69	-3854.421424	0.00
11	2_a_Mn_CO6_A1A1A1pA2BpD2----71	-3854.421424	0.00
12	2_a_Mn_CO6_A1A1A1pA2pA2B----73	-3854.421424	0.00
13	2_a_Mn_CO6_A1A1A1pA2pA2pD2----76	-3854.421424	0.00
14	2_a_Mn_CO6_A1A1A1pA2pD2pD2----77	-3854.421424	0.00
15	2_a_Mn_CO6_A1A1A2A2BB----78	-3854.421424	0.00
16	2_a_Mn_CO6_A1A1pA2BBB----79	-3854.421424	0.00
17	2_a_Mn_CO6_A1A2BBBB----99	-3854.421424	0.00
18	2_a_Mn_CO6_pA1pA1A2BBD2----103	-3854.421424	0.00
19	2_a_Mn_CO6_pA1pA1pA1A2BB----121	-3854.421424	0.00
20	2_a_Mn_CO6_pA1pA1pA1A2BD2----122	-3854.421424	0.00
21	2_a_Mn_CO6_pA1pA1pA1A2D2D2----124	-3854.421424	0.00
22	2_b_Mn_CO6_A1A1A1A2A2A2----130	-3854.421424	0.00
23	2_b_Mn_CO6_A1A1A1pA2BB----131	-3854.421424	0.00
24	2_b_Mn_CO6_A1A1A1pA2BpD2----133	-3854.421424	0.00
25	2_b_Mn_CO6_A1A1A1pA2pA2B----136	-3854.421424	0.00
26	2_b_Mn_CO6_A1A1A1pA2pA2pD2----139	-3854.421424	0.00
27	2_b_Mn_CO6_A1A1A1pA2pD2pD2----140	-3854.421424	0.00
28	2_b_Mn_CO6_A1A1A2A2BB----141	-3854.421424	0.00
29	2_b_Mn_CO6_A1A1pA2BBB----142	-3854.421424	0.00
30	2_b_Mn_CO6_A1A1pA2pA2BD1----156	-3854.421424	0.00
31	2_b_Mn_CO6_A1A2BBBB----162	-3854.421424	0.00
32	2_b_Mn_CO6_pA1pA1A2BBB----165	-3854.421424	0.00
33	2_b_Mn_CO6_pA1pA1A2BBD2----166	-3854.421424	0.00
34	2_b_Mn_CO6_pA1pA1A2BD2D2----169	-3854.421424	0.00
35	2_b_Mn_CO6_pA1pA1A2D2D2D2----173	-3854.421424	0.00
36	2_b_Mn_CO6_pA1pA1pA1A2BB----184	-3854.421424	0.00
37	2_b_Mn_CO6_pA1pA1pA1A2BD2----185	-3854.421424	0.00
38	2_b_Mn_CO6_pA1pA1pA1A2D2D2----187	-3854.421424	0.00

39	3_a_Mn_CO6_A1A1A1A2A2A2----193	-3854.421424	0.00
40	3_b_Mn_CO6_A1A1A1A2A2A2----226	-3854.421424	0.00
41	2_a_Mn_CO6_pA1pA1A2BBB----102	-3854.421423	0.00
42	102-2_a_Mn_CO6_A1A1pA2BBB-T-xqc.log	-3854.390158	19.62
43	100-2_a_Mn_CO6_A1A1A1pA2pA2pD2-T-xqc.log	-3854.390157	19.62
44	11-1_b_Mn_CO6_A1A1A1A1A2A2-T.log	-3854.390157	19.62
45	111-2_b_Mn_CO6_A1A1pA2pA2BD1-T-xqc.log	-3854.390157	19.62
46	118-2_a_Mn_CO6_A1A1A1pA2pA2D1-T.log	-3854.390157	19.62
47	119-2_a_Mn_CO6_A1A1pA2pA2BD1-T-xqc.log	-3854.390157	19.62
48	120-2_b_Mn_CO6_A1A1A1pA2pA2D1-T-xqc.log	-3854.390157	19.62
49	134-1_b_Mn_CO6_A1A1A1A2D2D2-T-xqc.log	-3854.390157	19.62
50	135-1_a_Mn_CO6_A1A1A1A2D2D2-T-xqc.log	-3854.390157	19.62
51	139-1_a_Mn_CO6_A1A1A1A2BD1-T-xqc.log	-3854.390157	19.62
52	142-3_a_Mn_CO6_A1A1A1A2A2B-T.log	-3854.390157	19.62
53	148-1_a_Mn_CO6_A1A1A1A1A2A2-T.log	-3854.390157	19.62
54	153-3_b_Mn_CO6_A1A1A1A2A2D2-T-xqc.log	-3854.390157	19.62
55	154-3_b_Mn_CO6_A1A1A2A2BB-T-xqc.log	-3854.390157	19.62
56	157-2_a_Mn_CO6_A1A1A1pA2BD1-T-xqc.log	-3854.390157	19.62
57	158-2_b_Mn_CO6_A1A1A1pA2BD1-T-xqc.log	-3854.390157	19.62
58	16-1_b_Mn_CO6_A1A1A2BBD1-T-xqc.log	-3854.390157	19.62
59	212-3_b_Mn_CO6_A1A1A2A2D1D2-T-xqc.log	-3854.390157	19.62
60	227-2_a_Mn_CO6_A1A1pA2BD1D1-T-xqc.log	-3854.390157	19.62
61	23-1_b_Mn_CO6_A1A1A1A2A2B-T.log	-3854.390157	19.62
62	25-1_a_Mn_CO6_A1A1A2A2D1D1-T-xqc.log	-3854.390157	19.62
63	46-1_a_Mn_CO6_A1A1A2A2D1D2-T-xqc-1.log	-3854.390157	19.62
64	70-1_b_Mn_CO6_A1A1A2D2D1D2-T-xqc.log	-3854.390157	19.62
65	8-1_a_Mn_CO6_A1A1A1A2A2D1-T.log	-3854.390157	19.62
66	82-2_b_Mn_CO6_A1A2BBBB-T-xqc.log	-3854.390157	19.62
67	89-1_b_Mn_CO6_A1A1A2BD1B-T-xqc.log	-3854.390157	19.62
68	9-1_b_Mn_CO6_A1A1A1A2A2D1-T-xqc.log	-3854.390157	19.62
69	91-2_a_Mn_CO6_A1A1A1pA2BB-T-xqc.log	-3854.390157	19.62
70	94-2_b_Mn_CO6_A1A1A1pA2BB-T-xqc.log	-3854.390157	19.62
71	95-2_b_Mn_CO6_A1A1A1pA2pA2pD2-T-xqc.log	-3854.390157	19.62
72	150-3_b_Mn_CO6_A1A1A1A2A2B-T-xqc.log	-3854.390156	19.62
73	81-2_a_Mn_CO6_A1A1A1pA2D1D1-T-xqc.log	-3854.390156	19.62
74	98-2_a_Mn_CO6_A1A1pA2BD1B-T-xqc.log	-3854.390156	19.62
75	222-1_a_Mn_CO6_A1A1A1A2D1D1-T-xqc.log	-3854.390155	19.62
76	122-2_b_Mn_CO6_A1A1A1A1pA2pA2-T.log	-3854.390154	19.62
77	1052_a_Mn_CO6_pA1pA1pA1A2BD2-T-xqc.log	-3854.385344	22.64
78	106-2_a_Mn_CO6_pA1pA1pA1A2D2D2-T-xqc.log	-3854.385344	22.64
79	107-2_b_Mn_CO6_A1A1A1A2A2A2-T.log	-3854.385344	22.64
80	116-2_b_Mn_CO6_pA1pA1pA1A2BD2-T-xqc.log	-3854.385344	22.64
81	14-2_a_Mn_CO6_pA1pA1pA1A2A2D2-T-xqc.log	-3854.385344	22.64
82	169-1_a_Mn_CO6_A1A1A2BBD2-T-xqc.log	-3854.385344	22.64

83	88-1_a_Mn_CO6_A1A2BBBB-T-xqc.log	-3854.385344	22.64
84	103-2_a_Mn_CO6_A1A2BBBB-T-xqc.log	-3854.385343	22.64
85	75-1_b_Mn_CO6_A1A1A2BBD2-T-xqc.log	-3854.385343	22.64
86	84-2_a_Mn_CO6_A1A1A1pA2BpD2-T.log	-3854.385342	22.64
87	117--2_b_Mn_CO6_pA1pA1pA1A2D2D2-T-xqc.log	-3854.385341	22.64
88	43-1_b_Mn_CO6_A1A2BBBB-T-xqc.log	-3854.385340	22.64
89	247-2_a_Mn_CO6_pA1pA1A2BD2B-T-xqc.log	-3854.385339	22.64
90	110-2_b_Mn_CO6_A1A1A2A2BB-T-xqc-freq.log	-3854.385338	22.64
91	164-2_b_Mn_CO6_pA1pA1A2A2pD1pD1-T-xqc-freq.log	-3854.385338	22.64
92	247-2_a_Mn_CO6_pA1pA1A2BD2B-T-xqc.log	-3854.385338	22.64
93	101-2_a_Mn_CO6_A1A1A1pA2pD2pD2-T-xqc-freq.log	-3854.385331	22.65
94	99-2_b_Mn_CO6_A1A1A1pA2pD2pD2-T-xqc-freq.log	-3854.385329	22.65
95	90-2_a_Mn_CO6_A1A1A1A2A2A2-T.log	-3854.384914	22.91
96	156-1_a_Mn_CO6_A1A1A1A2BB-Q-xqc.log	-3854.381848	24.83
97	45-1_b_Mn_CO6_A1A1A1A2BB-Q-xqc.log	-3854.381848	24.83
98	123-2_a_Mn_CO6_pA1pA1pA1A2A2B-T-xqc.log	-3854.381634	24.97
99	15-2_b_Mn_CO6_pA1pA1pA1A2A2D2-T-xqc.log	-3854.381634	24.97
100	124-2_b_Mn_CO6_pA1pA1pA1A2A2B-T.log	-3854.381617	24.98
101	87-2_a_Mn_CO6_A1A1A1A1pA2pA2-T.log	-3854.378614	26.86
102	195-1_a_Mn_CO6_A1A1A2BBB-Q-xqc.log	-3854.378309	27.06
103	27-2_a_Mn_CO6_A1A1pA2BBpD2-Q-xqc.log	-3854.378309	27.06
104	102-2_a_Mn_CO6_A1A1pA2BBB-Q-xqc.log	-3854.378308	27.06
105	108-2_b_Mn_CO6_A1A1A1pA2BpD2-Q-xqc.log	-3854.378308	27.06
106	117--2_b_Mn_CO6_pA1pA1pA1A2D2D2-Q-xqc.log	-3854.378308	27.06
107	143-1_b_Mn_CO6_A1A1A2BD2B-Q-xqc-freq.log	-3854.378308	27.06
108	84-2_a_Mn_CO6_A1A1A1pA2BpD2-Q-xqc.log	-3854.378308	27.06
109	91-2_a_Mn_CO6_A1A1A1pA2BB-Q-xqc-freq.log	-3854.378308	27.06
110	93-2_a_Mn_CO6_A1A1A2A2BB-Q-xqc.log	-3854.378308	27.06
111	94-2_b_Mn_CO6_A1A1A1pA2BB-Q-xqc.log	-3854.378308	27.06
112	78-3_b_Mn_CO6_A1A1A1A2A2D1-Q-xqc.log	-3854.378307	27.06
113	9-1_b_Mn_CO6_A1A1A1A2A2D1-Q-xqc.log	-3854.378307	27.06
114	2-1_a_Mn_CO6_A1A1A1A2A2A2-Q-xqc.log	-3854.378306	27.06
115	21-1_a_Mn_CO6_A1A1A2A2BB-Q.log	-3854.378306	27.06
116	8-1_a_Mn_CO6_A1A1A1A2A2D1-Q-xqc-freq.log	-3854.378306	27.06
117	106-2_a_Mn_CO6_pA1pA1pA1A2D2D2-Q-xqc.log	-3854.378305	27.06
118	124-2_b_Mn_CO6_pA1pA1pA1A2A2B--Q.log	-3854.378305	27.06
119	36-1_b_Mn_CO6_A1A1A2BBB-Q-xqc-freq.log	-3854.378305	27.06
120	11-1_b_Mn_CO6_A1A1A1A1A2A2-Q.log	-3854.378304	27.06
121	118-2_a_Mn_CO6_A1A1A1pA2pA2D1-Q.log	-3854.378304	27.06
122	120-2_b_Mn_CO6_A1A1A1pA2pA2D1-Q.log	-3854.378304	27.06
123	123-2_a_Mn_CO6_pA1pA1pA1A2A2B-Q.log	-3854.378304	27.06
124	141-1_b_Mn_CO6_A1A1A1A2BD1-Q.log	-3854.378304	27.06
125	148-1_a_Mn_CO6_A1A1A1A1A2A2-Q.log	-3854.378304	27.06
126	22-3_a_Mn_CO6_A1A1A1A2A2D1-Q.log	-3854.378304	27.06
127	23-1_b_Mn_CO6_A1A1A1A2A2B-Q.log	-3854.378304	27.06

128	77-1_a_Mn_CO6_A1A1A1A2A2B-Q.log	-3854.378304	27.06
129	87-2_a_Mn_CO6_A1A1A1A1pA2pA2-Q.log	-3854.378304	27.06
130	92-2_a_Mn_CO6_A1A1A1pA2pA2B-Q.log	-3854.378304	27.06
131	139-1_a_Mn_CO6_A1A1A1A2BD1-Q.log	-3854.378302	27.06
132	186-1_a_Mn_CO6_A1A1A2BD1B-Q-xqc.log	-3854.376959	27.90
133	89-1_b_Mn_CO6_A1A1A2BD1B-Q-xqc.log	-3854.376959	27.90
134	2_b_Mn_CO6_A1A1pA2BD1B----145	-3854.374966	29.15
135	1_a_Mn_CO6_A1A1A1A2A2D1----4	-3854.374965	29.15
136	1_b_Mn_CO6_A1A1A1A2A2D1----37	-3854.374965	29.15
137	1_b_Mn_CO6_A1A1A2D1D1D1----59	-3854.374965	29.15
138	2_a_Mn_CO6_A1A1A1pA2pA2D1----75	-3854.374965	29.15
139	2_a_Mn_CO6_A1A1pA2BD1B----82	-3854.374965	29.15
140	2_a_Mn_CO6_A1A1pA2pA2BD1----93	-3854.374965	29.15
141	2_b_Mn_CO6_A1A1A1pA2pA2D1----138	-3854.374965	29.15
142	200-1_b_Mn_CO6_A1A1A2A2D1D1-Q-xqc.log	-3854.374529	29.43
143	132-3_a_Mn_CO6_A1A1A1A2D1D2-Q-xqc.log	-3854.374527	29.43
144	128-3_b_Mn_CO6_A1A1A1A2BB-Q.log	-3854.374526	29.43
145	130-3_a_Mn_CO6_A1A1A2BD1D1-Q-xqc.log	-3854.374526	29.43
146	146-3_b_Mn_CO6_A1A1A2A2BD1-Q-xqc.log	-3854.374526	29.43
147	180-3_a_Mn_CO6_A1A1A1A1A2A2-Q.log	-3854.374526	29.43
148	183-3_b_Mn_CO6_A1A1A1A2D1D1-Q-xqc.log	-3854.374526	29.43
149	184-3_b_Mn_CO6_A1A1A1A2BD1-Q-xqc.log	-3854.374526	29.43
150	204-3_a_Mn_CO6_A1A1A2D1D1D2-Q-xqc.log	-3854.374526	29.43
151	232-3_b_Mn_CO6_A1A1A2D2D1D2-Q-xqc-freq.log	-3854.374526	29.43
152	235-3_a_Mn_CO6_A1A2BBBB-Q-xqc-freq.log	-3854.374526	29.43
153	30-3_b_Mn_CO6_A1A1A1A1A2A2-Q.log	-3854.374526	29.43
154	33-3_a_Mn_CO6_A1A1A1A2BD1-Q-xqc.log	-3854.374526	29.43
155	71-3_b_Mn_CO6_A1A1A2D1BD2-Q-xqc-freq.log	-3854.374526	29.43
156	110-2_b_Mn_CO6_A1A1A2A2BB-Q-xqc-freq.log	-3854.374525	29.43
157	126-3_b_Mn_CO6_A1A1A2BD1D1-Q-xqc.log	-3854.374525	29.43
158	129-3_a_Mn_CO6_A1A1A2D2D1D2-Q-xqc.log	-3854.374525	29.43
159	131-3_a_Mn_CO6_A1A1A2BBD2-Q-xqc-freq.log	-3854.374525	29.43
160	133-3_a_Mn_CO6_A1A1A1A2BB-Q.log	-3854.374525	29.43
161	137-3_b_Mn_CO6_A1A1A2D1D1D1-Q-xqc.log	-3854.374525	29.43
162	142-3_a_Mn_CO6_A1A1A1A2A2B-Q-xqc.log	-3854.374525	29.43
163	146-3_b_Mn_CO6_A1A1A2A2BD1-Q-xqc.log	-3854.374525	29.43
164	151-2_a_Mn_CO6_pA1pA1A2A2pD1pD1-Q-xqc-FREQ.log	-3854.374525	29.43
165	164-2_b_Mn_CO6_pA1pA1A2A2pD1pD1-Q-xqc.log	-3854.374525	29.43
166	170-1_b_Mn_CO6_A1A1A2BD2D2-Q-xqc.log	-3854.374525	29.43
167	188-3_a_Mn_CO6_A1A1A2D2BD2-Q-xqc.log	-3854.374525	29.43
168	19-3_a_Mn_CO6_A1A1A2D1D1D1-Q-xqc.log	-3854.374525	29.43
169	192-3_b_Mn_CO6_A1A1A2D2BD2-Q-xqc-freq.log	-3854.374525	29.43
170	199-3_b_Mn_CO6_A1A1A1A2D1D2-Q-xqc.log	-3854.374525	29.43
171	203-3_a_Mn_CO6_A1A1A2D1BD2-Q-xqc.log	-3854.374525	29.43

172	205-3_b_Mn_CO6_A1A1A2BBB-Q-xqc-freq.log	-3854.374525	29.43
173	209-3_b_Mn_CO6_A1A1A2BBD1-Q-xqc.log	-3854.374525	29.43
174	214-3_a_Mn_CO6_A1A1A2BBD1-Q-xqc.log	-3854.374525	29.43
175	233-3_b_Mn_CO6_A1A1A2BD1D2-Q-xqc.log	-3854.374525	29.43
176	31-2_b_Mn_CO6_pA1pA1A2pD1D2D2-Q-xqc-freq.log	-3854.374525	29.43
177	38-3_a_Mn_CO6_A1A1A2A2BB-Q-xqc.log	-3854.374525	29.43
178	41-3_a_Mn_CO6_A1A1A2BD1B-Q-xqc.log	-3854.374525	29.43
179	47-3_a_Mn_CO6_A1A1A2A2BD1-Q-xqc.log	-3854.374525	29.43
180	65-3_a_Mn_CO6_A1A1A2D1D2D1-Q-xqc.log	-3854.374525	29.43
181	76-2_a_Mn_CO6_pA1pA1A2BpD1D2-Q-xqc.log	-3854.374525	29.43
182	79-3_b_Mn_CO6_A1A1A2BBD2-Q-xqc.log	-3854.374525	29.43
183	197-3_a_Mn_CO6_A1A1A1A2D1D1-Q-xqc.log	-3854.374524	29.43
184	207-3_b_Mn_CO6_A1A1A2D1D1D2-Q-xqc.log	-3854.374524	29.43
185	55-3_b_Mn_CO6_A1A2BBBB-Q-xqc.log	-3854.374523	29.43
186	4-3_a_Mn_CO6_A1A1A1A2A2A2-Q.log	-3854.374517	29.44
187	1_b_Mn_CO6_A1A1A1A1A2A2----34	-3854.374476	29.46
188	2_a_Mn_CO6_pA1pA1A2D2BD2----109	-3854.374476	29.46
189	2_a_Mn_CO6_A1A1A1pA2D1D1----72	-3854.374475	29.46
190	2_b_Mn_CO6_A1A1A1pA2D1D1----134	-3854.374475	29.46
191	2_b_Mn_CO6_pA1pA1A2D2BD2----172	-3854.374475	29.46
192	2_b_Mn_CO6_A1A1A1A1pA2pA2----129	-3854.374474	29.46
193	92-2_a_Mn_CO6_A1A1A1pA2pA2B-T.log	-3854.374199	29.63
194	188-3_a_Mn_CO6_A1A1A2D2BD2-T-xqc.log	-3854.374186	29.64
195	38-3_a_Mn_CO6_A1A1A2A2BB-T-xqc.log	-3854.374185	29.64
196	2_a_Mn_CO6_pA1pA1pA1A2A2D2----119	-3854.374157	29.66
197	2_a_Mn_CO6_pA1pA1pA1A2A2B----118	-3854.374156	29.66
198	2_b_Mn_CO6_pA1pA1pA1A2A2B----181	-3854.374156	29.66
199	2_b_Mn_CO6_pA1pA1pA1A2A2D2----182	-3854.374156	29.66
200	107-2_b_Mn_CO6_A1A1A1A2A2A2-Q.log	-3854.370705	31.83
201	103-2_a_Mn_CO6_A1A2BBBB-Q-xqc-rupt.log	-3854.370703	31.83
202	88-1_a_Mn_CO6_A1A2BBBB-Q-xqc-rupt.log	-3854.370696	31.83
203	83-2_a_Mn_CO6_pA1pA1pA1A2BB-Q-xqc-freq.log	-3854.370685	31.84
204	1_a_Mn_CO6_A1A1A2BBD1----17	-3854.369992	32.27
205	1_b_Mn_CO6_A1A1A2BBD1----50	-3854.369992	32.27
206	2_b_Mn_CO6_A1A1pA2BBD1----143	-3854.369992	32.27
207	43-1_b_Mn_CO6_A1A2BBBB-Q-xqc.log	-3854.369519	32.57
208	82-2_b_Mn_CO6_A1A2BBBB-Q-xqc.log	-3854.369519	32.57
209	152-2_a_Mn_CO6_pA1pA1A2pD1BD2-Q-xqc-freq.log	-3854.369013	32.89
210	24-2_b_Mn_CO6_pA1pA1A2pD1BD2-Q-xqc-rupt.log	-3854.369004	32.89
211	241-2_b_Mn_CO6_pA1pA1A2BBpD1-T.log	-3854.368211	33.39
212	61-2_b_Mn_CO6_A1A1pA2BD1D1-T-xqc-rupt.log	-3854.368106	33.46
213	64-2_a_Mn_CO6_A1A1pA2pD2BpD2-T-xqc-rupt.log	-3854.368105	33.46
214	59-2_a_Mn_CO6_pA1pA1A2pD1pD1D2-Q-xqc-rupt.log	-3854.368054	33.49
215	195-1_a_Mn_CO6_A1A1A2BBB-T-xqc.log	-3854.367563	33.80

216	1-1_b_Mn_CO6_A1A1A1A2A2D2-T-xqc-freq.log	-3854.367562	33.80
217	208-1_b_Mn_CO6_A1A1A2D1BD1-T-xqc.log	-3854.367562	33.80
218	21-1_a_Mn_CO6_A1A1A2A2BB-T-xqc-freq.log	-3854.367561	33.80
219	27-2_a_Mn_CO6_A1A1pA2BBpD2-T-xqc-freq.log	-3854.367561	33.80
220	5-3_b_Mn_CO6_A1A1A1A2A2A2-T.log	-3854.367561	33.80
221	200-1_b_Mn_CO6_A1A1A2A2D1D1-T-xqc.log	-3854.367560	33.80
222	77-1_a_Mn_CO6_A1A1A1A2A2B-T.log	-3854.367560	33.80
223	86-1_b_Mn_CO6_A1A1A1A2A2A2-T-xqc.log	-3854.367560	33.80
224	3-1_a_Mn_CO6_A1A1A1A2A2D2-T.log	-3854.367559	33.80
225	149-1_b_Mn_CO6_A1A1A2A2BB-T.log	-3854.367558	33.80
226	2-1_a_Mn_CO6_A1A1A1A2A2A2-T.log	-3854.367558	33.80
227	30-3_b_Mn_CO6_A1A1A1A1A2A2-T.log	-3854.367556	33.80
228	4-3_a_Mn_CO6_A1A1A1A2A2A2-T.log	-3854.367556	33.80
229	112-2_b_Mn_CO6_pA1pA1A2BBB-T-xqc.log	-3854.366065	34.74
230	162-2_b_Mn_CO6_pA1pA1pA1A2A2pD1-T-xqc.log	-3854.366065	34.74
231	168-2_a_Mn_CO6_pA1pA1pA1A2A2pD1-T-xqc.log	-3854.366065	34.74
232	170-1_b_Mn_CO6_A1A1A2BD2D2-T-xqc.log	-3854.366065	34.74
233	174-2_b_Mn_CO6_pA1pA1A2A2BpD1-T-xqc.log	-3854.366065	34.74
234	176-2_a_Mn_CO6_A1A1pA2BpD2pD2-T-xqc.log	-3854.366065	34.74
235	28-2_b_Mn_CO6_A1A1pA2BpD2pD2-T-xqc.log	-3854.366065	34.74
236	32-2_a_Mn_CO6_pA1pA1pA1A2pD1D2-T-xqc.log	-3854.366065	34.74
237	37-1_a_Mn_CO6_A1A1A2D2D2D2-T-xqc.log	-3854.366065	34.74
238	40-2_b_Mn_CO6_pA1pA1pA1pA1A2A2-T.log	-3854.366065	34.74
239	44-1_b_Mn_CO6_A1A1A2D2D2D2-T-xqc.log	-3854.366065	34.74
240	6-2_a_Mn_CO6_pA1pA1A2BBB-T-xqc.log	-3854.366065	34.74
241	178-2_a_Mn_CO6_pA1pA1A2A2BpD1-T.log	-3854.366064	34.74
242	151-2_a_Mn_CO6_pA1pA1A2A2pD1pD1-T.log	-3854.366042	34.75
243	108-2_b_Mn_CO6_A1A1A1pA2BpD2-T-xqc.log	-3854.365013	35.40
244	96-2_b_Mn_CO6_A1A1pA2BBB-T-xqc-freq.log	-3854.365012	35.40
245	121-+2_b_Mn_CO6_A1A1A1pA2D1D1-T-xqc-freq-1.log	-3854.364708	35.59
246	1_a_Mn_CO6_A1A1A1A2D2D2----11	-3854.363822	36.15
247	1_b_Mn_CO6_A1A1A1A2D2D2----44	-3854.363822	36.15
248	3_a_Mn_CO6_A1A1A1A2A2D2----196	-3854.363822	36.15
249	3_a_Mn_CO6_A1A1A1A2BB----197	-3854.363822	36.15
250	3_a_Mn_CO6_A1A1A1A2BD2----199	-3854.363822	36.15
251	3_a_Mn_CO6_A1A1A1A2D1D2----201	-3854.363822	36.15
252	3_a_Mn_CO6_A1A1A1A2D2D2----202	-3854.363822	36.15
253	3_a_Mn_CO6_A1A1A2BBD2----209	-3854.363822	36.15
254	3_a_Mn_CO6_A1A1A2BD1D1----211	-3854.363822	36.15
255	3_a_Mn_CO6_A1A1A2D1D1D1----217	-3854.363822	36.15
256	3_a_Mn_CO6_A1A1A2D2D1D2----222	-3854.363822	36.15
257	3_b_Mn_CO6_A1A1A1A2BB----230	-3854.363822	36.15
258	3_b_Mn_CO6_A1A1A1A2BD2----232	-3854.363822	36.15
259	3_b_Mn_CO6_A1A1A1A2D2D2----235	-3854.363822	36.15

260	3_b_Mn_CO6_A1A1A2BBD2----242	-3854.363822	36.15
261	3_b_Mn_CO6_A1A1A2BD1D1----244	-3854.363822	36.15
262	3_b_Mn_CO6_A1A1A2D1D1D1----250	-3854.363822	36.15
263	3_a_Mn_CO6_A1A1A2BBB----207	-3854.36382	36.15
264	184-3_b_Mn_CO6_A1A1A1A2BD1-T-xqc.log	-3854.363245	36.51
265	193-1_a_Mn_CO6_A1A1A1A2D1D2-T.log	-3854.363245	36.51
266	79-3_b_Mn_CO6_A1A1A2BBD2-T-xqc.log	-3854.363245	36.51
267	131-3_a_Mn_CO6_A1A1A2BBD2-T-xqc.log	-3854.363244	36.51
268	132-3_a_Mn_CO6_A1A1A1A2D1D2-T-xqc.log	-3854.363244	36.51
269	161-1_a_Mn_CO6_A1A1A2BD2B-T-xqc.log	-3854.363244	36.51
270	180-3_a_Mn_CO6_A1A1A1A1A2A2-T.log	-3854.363244	36.51
271	183-3_b_Mn_CO6_A1A1A1A2D1D1-T-xqc.log	-3854.363244	36.51
272	197-3_a_Mn_CO6_A1A1A1A2D1D1-T.log	-3854.363244	36.51
273	33-3_a_Mn_CO6_A1A1A1A2BD1-T-xqc.log	-3854.363244	36.51
274	41-3_a_Mn_CO6_A1A1A2BD1B-T-xqc.log	-3854.363244	36.51
275	67-1_b_Mn_CO6_A1A1A1A2BD2-T-xqc.log	-3854.363244	36.51
276	194-1_b_Mn_CO6_A1A1A1A2D1D2-T-xqc.log	-3854.363243	36.51
277	20-3_b_Mn_CO6_A1A1A1A2BD2-T-xqc-freq.log	-3854.363243	36.51
278	97-2_b_Mn_CO6_pA1pA1pA1A2BB-T.log	-3854.363243	36.51
279	127-3_b_Mn_CO6_A1A1A1A2D2D2-T.log	-3854.363242	36.51
280	203-3_a_Mn_CO6_A1A1A2D1BD2-T.log	-3854.363235	36.51
281	199-3_b_Mn_CO6_A1A1A1A2D1D2-T.log	-3854.363202	36.54
282	145-3_a_Mn_CO6_A1A1A2A2D1D1-Q-xqc.log	-3854.362430	37.02
283	150-3_b_Mn_CO6_A1A1A1A2A2B-Q-xqc.log	-3854.362430	37.02
284	179-3_b_Mn_CO6_A1A1A2D2D2D2-Q-xqc.log	-3854.362430	37.02
285	189-3_a_Mn_CO6_A1A1A2BD2D2-Q-xqc.log	-3854.362430	37.02
286	198-3_a_Mn_CO6_A1A1A2D2D2D2-Q-xqc.log	-3854.362429	37.02
287	218-1_b_Mn_CO6_A1A1A2D2BD2-Q-xqc.log	-3854.362429	37.02
288	220-1_a_Mn_CO6_A1A1A2D2BD2-Q-xqc.log	-3854.362429	37.02
289	83-2_a_Mn_CO6_pA1pA1pA1A2BB-T.log	-3854.362406	37.04
290	182-2_b_Mn_CO6_pA1pA1pA1A2pD1D2-T-xqc.log	-3854.362404	37.04
291	80-3_a_Mn_CO6_A1A1A1A2D2D2-T-xqc.log	-3854.362404	37.04
292	128-3_b_Mn_CO6_A1A1A1A2BB-T-xqc.log	-3854.362403	37.04
293	138-3_a_Mn_CO6_A1A1A2BBB-T-xqc.log	-3854.362403	37.04
294	192-3_b_Mn_CO6_A1A1A2D2BD2-T-xqc.log	-3854.362403	37.04
295	209-3_b_Mn_CO6_A1A1A2BBD1-T-xqc.log	-3854.362403	37.04
296	133-3_a_Mn_CO6_A1A1A1A2BB-T.log	-3854.362402	37.04
297	217-2_a_Mn_CO6_A1A1pA2pD2pD2pD2-Q-xqc-rupt.log	-3854.361185	37.80
298	210-3_b_Mn_CO6_A1A1A2D1D2D1-Q.log	-3854.360314	38.35
299	138-3_a_Mn_CO6_A1A1A2BBB-Q-xqc-freq.log	-3854.360311	38.35
300	190-3_a_Mn_CO6_A1A1A2BD2B-Q.log	-3854.360311	38.35
301	125-1_a_Mn_CO6_A1A1A2BBD1-Q-xqc.log	-3854.360310	38.35
302	34-2_a_Mn_CO6_A1A1pA2D1BD1-Q-xqc-freq.log	-3854.360310	38.35
303	69-3_a_Mn_CO6_A1A1A2D1BD1-Q-xqc-freq.log	-3854.360310	38.35

304	196-2_a_Mn_CO6_A1A1pA2BBD1-Q-xqc.log	-3854.360309	38.35
305	206-3_b_Mn_CO6_A1A1A2BD1B-Q-xqc.log	-3854.360309	38.35
306	215-3_b_Mn_CO6_A1A1A2D1BD1-Q-xqc-freq.log	-3854.360309	38.35
307	227-2_a_Mn_CO6_A1A1pA2BD1D1-Q-xqc-freq.log	-3854.360309	38.35
308	96-2_b_Mn_CO6_A1A1pA2BBB-Q-xqc-freq.log	-3854.360309	38.35
309	13-2_b_Mn_CO6_pA1pA1A2D2BD2-T-xqc-rupt.log	-3854.360066	38.50
310	125-1_a_Mn_CO6_A1A1A2BBD1-T-xqc-rupt.log	-3854.359763	38.69
311	1_a_Mn_CO6_A1A1A1A2BD1----7	-3854.359395	38.92
312	1_a_Mn_CO6_A1A1A2A2BB----12	-3854.359395	38.92
313	1_a_Mn_CO6_A1A1A2A2BD1----13	-3854.359395	38.92
314	1_b_Mn_CO6_A1A1A1A2BD1----40	-3854.359395	38.92
315	1_b_Mn_CO6_A1A1A2A2BD1----46	-3854.359395	38.92
316	1_b_Mn_CO6_A1A1A2BD2B----55	-3854.359395	38.92
317	3_a_Mn_CO6_A1A1A1A2A2B----194	-3854.359395	38.92
318	3_a_Mn_CO6_A1A1A1A2A2D1----195	-3854.359395	38.92
319	3_a_Mn_CO6_A1A1A2A2D1D1----205	-3854.359395	38.92
320	3_b_Mn_CO6_A1A1A1A2A2D1----228	-3854.359395	38.92
321	3_b_Mn_CO6_A1A1A2A2BD1----237	-3854.359395	38.92
322	3_b_Mn_CO6_A1A1A2A2D1D1----238	-3854.359395	38.92
323	1_a_Mn_CO6_A1A1A1A1A2A2----1	-3854.359394	38.93
324	1_a_Mn_CO6_A1A1A1A2A2B----3	-3854.359394	38.93
325	1_b_Mn_CO6_A1A1A1A2A2B----36	-3854.359394	38.93
326	1_b_Mn_CO6_A1A1A2A2BB----45	-3854.359394	38.93
327	3_b_Mn_CO6_A1A1A1A2A2B----227	-3854.359394	38.93
328	2_b_Mn_CO6_pA1pA1A2pD1BD2----175	-3854.359264	39.01
329	2_a_Mn_CO6_pA1pA1A2A2pD1pD1----101	-3854.359263	39.01
330	2_a_Mn_CO6_pA1pA1A2pD1BD2----112	-3854.359248	39.02
331	54-2_a_Mn_CO6_A1A1pA2D1D1D1-Q-xqc.log	-3854.359080	39.12
332	97-2_b_Mn_CO6_pA1pA1pA1A2BB-Q-xqc-freq.log	-3854.358625	39.41
333	6-2_a_Mn_CO6_pA1pA1A2BBB-Q-xqc-freq.log	-3854.358609	39.42
334	158-2_b_Mn_CO6_A1A1A1pA2BD1-Q-xqc-rupt.log	-3854.357444	40.15
335	157-2_a_Mn_CO6_A1A1A1pA2BD1-Q-xqc-rupt.log	-3854.357412	40.17
336	3_b_Mn_CO6_A1A1A1A2A2D2----229	-3854.357336	40.22
337	3_b_Mn_CO6_A1A1A2A2BB----236	-3854.357336	40.22
338	1_a_Mn_CO6_A1A1A2D1BD1----24	-3854.357213	40.29
339	10-1_b_Mn_CO6_A1A1A2D1D1D1-Q-xqc-rupt.log	-3854.356203	40.93
340	16-1_b_Mn_CO6_A1A1A2BBD1-Q-xqc-rupt.log	-3854.356202	40.93
341	177-2_a_Mn_CO6_A1A1pA2D1BpD2-T-xqc.log	-3854.355827	41.16
342	1_a_Mn_CO6_A1A1A1A2BB----6	-3854.354955	41.71
343	2_a_Mn_CO6_A1A1A1pA2BD1----70	-3854.353988	42.32
344	2_b_Mn_CO6_A1A1A1pA2BD1----132	-3854.353988	42.32
345	2_a_Mn_CO6_A1A1pA2pA2D1D1----94	-3854.353987	42.32
346	2_b_Mn_CO6_A1A1A1pA2D1pD2----135	-3854.353987	42.32

347	1_a_Mn_CO6_A1A1A2A2D1D1----14	-3854.353873	42.39
348	3-1_a_Mn_CO6_A1A1A1A2A2D2-Q-xqc.log	-3854.353351	42.72
349	95-2_b_Mn_CO6_A1A1A1pA2pA2pD2-Q-xqc.log	-3854.353351	42.72
350	1-1_b_Mn_CO6_A1A1A1A2A2D2-Q.log	-3854.353349	42.72
351	147-3_b_Mn_CO6_A1A1A2A2D1D1-Q-xqc.log	-3854.351231	44.05
352	135-1_a_Mn_CO6_A1A1A1A2D2D2-Q-xqc.log	-3854.351029	44.17
353	136-2_b_Mn_CO6_A1A1pA2BBD1-T-xqc.log	-3854.350785	44.33
354	196-2_a_Mn_CO6_A1A1pA2BBD1-T-xqc.log	-3854.350785	44.33
355	2_a_Mn_CO6_pA1pA1A2BpD1D2----107	-3854.350448	44.54
356	2_a_Mn_CO6_pA1pA1pA1A2A2pD1----120	-3854.350448	44.54
357	2_a_Mn_CO6_pA1pA1pA1A2BpD1----123	-3854.350448	44.54
358	2_a_Mn_CO6_pA1pA1pA1pA1A2A2----127	-3854.350448	44.54
359	2_b_Mn_CO6_A1A1pA2pD2pD2pD2----161	-3854.350448	44.54
360	2_b_Mn_CO6_pA1pA1A2A2pD1pD1----164	-3854.350448	44.54
361	2_b_Mn_CO6_pA1pA1A2BpD1D2----170	-3854.350448	44.54
362	2_b_Mn_CO6_pA1pA1pA1A2A2pD1----183	-3854.350448	44.54
363	2_b_Mn_CO6_pA1pA1pA1A2BpD1----186	-3854.350446	44.54
364	1_a_Mn_CO6_A1A1A2BD2B----22	-3854.348616	45.69
365	1_a_Mn_CO6_A1A1A2BBD2----18	-3854.348615	45.69
366	1_b_Mn_CO6_A1A1A2BBD2----51	-3854.348615	45.69
367	1_b_Mn_CO6_A1A1A2BD2D2----56	-3854.348615	45.69
368	2_a_Mn_CO6_A1A1pA2BBpD2----81	-3854.348615	45.69
369	2_a_Mn_CO6_A1A1pA2BpD2pD2----86	-3854.348615	45.69
370	2_a_Mn_CO6_A1A1pA2D1pD2pD2----92	-3854.348615	45.69
371	2_a_Mn_CO6_A1A1pA2pA2D1pD2----95	-3854.348615	45.69
372	2_b_Mn_CO6_A1A1pA2BBpD2----144	-3854.348615	45.69
373	2_b_Mn_CO6_A1A1pA2BpD2pD2----149	-3854.348615	45.69
374	2_b_Mn_CO6_A1A1pA2D1pD2pD2----155	-3854.348615	45.69
375	2_b_Mn_CO6_A1A1pA2pA2D1pD2----158	-3854.348615	45.69
376	2_b_Mn_CO6_pA1pA1A2A2BpD1----163	-3854.348615	45.69
377	1_a_Mn_CO6_A1A1A2BD2D2----23	-3854.348614	45.69
378	2_a_Mn_CO6_A1A1pA2D1BpD2----88	-3854.348614	45.69
379	2_a_Mn_CO6_pA1pA1A2A2BpD1----100	-3854.348614	45.69
380	3_b_Mn_CO6_A1A1A2D2D2D2----256	-3854.348614	45.69
381	7-2_b_Mn_CO6_A1A1pA2BD1B-Q-xqc.log	-3854.346823	46.81
382	53-2_a_Mn_CO6_A1A1pA2D1pD2D1-Q-xqc.log	-3854.346541	46.99
383	2_b_Mn_CO6_A1A1pA2pA2D1D1-COdeplasat----157	-3854.345983	47.34
384	75-1_b_Mn_CO6_A1A1A2BBD2-Q.log	-3854.345485	47.65
385	18-3_a_Mn_CO6_A1A1A1A2BD2-T-freq.log	-3854.345369	47.73
386	3_b_Mn_CO6_A1A1A1A1A2A2----225	-3854.344137	48.50
387	3_a_Mn_CO6_A1A1A1A1A2A2----192	-3854.344136	48.50
388	2_b_Mn_CO6_pA1pA1A2pD1D2D2-COdeplasat----177	-3854.344079	48.54
389	2_a_Mn_CO6_pA1pA1A2pD1D2D2-COdeplasat----114	-3854.34406	48.55

390	2_a_Mn_CO6_pA1pA1pA1A2pD1D2----125	-3854.343367	48.98
391	2_b_Mn_CO6_pA1pA1pA1A2pD1D2----188	-3854.343367	48.98
392	3_a_Mn_CO6_A1A1A1A2BD1----198	-3854.343366	48.98
393	3_b_Mn_CO6_A1A1A1A2BD1----231	-3854.343365	48.98
394	3_b_Mn_CO6_A1A1A1A2D1D1----233	-3854.343365	48.98
395	63-2_b_Mn_CO6_pA1pA1A2pD1pD1pD1-Q-xqc-rupt.log	-3854.342823	49.32
396	231-2_a_Mn_CO6_pA1pA1A2pD1BpD1-Q.log	-3854.342675	49.42
397	37-1_a_Mn_CO6_A1A1A2D2D2D2-Q-xqc.log	-3854.342406	49.59
398	73-1_a_Mn_CO6_A1A1A2BD2D2-Q-xqc.log	-3854.342403	49.59
399	25-1_a_Mn_CO6_A1A1A2A2D1D1-Q-xqc.log	-3854.342402	49.59
400	2_a_Mn_CO6_A1A1pA2D1BD1----87	-3854.34117	50.36
401	2_b_Mn_CO6_A1A1pA2D1BD1----150	-3854.341169	50.36
402	145-3_a_Mn_CO6_A1A1A2A2D1D1-T-xqc.log	-3854.340593	50.72
403	146-3_b_Mn_CO6_A1A1A2A2BD1-T-xqc-freq.log	-3854.340589	50.73
404	198-3_a_Mn_CO6_A1A1A2D2D2D2-T-xqc.log	-3854.340588	50.73
405	1_a_Mn_CO6_A1A1A2BD1B----19	-3854.340482	50.79
406	57-2_b_Mn_CO6_pA1pA1A2pD1pD1D2-Q-xqc-rupt.log	-3854.340276	50.92
407	104-2_a_Mn_CO6_pA1pA1A2BBD2-Q-xqc.log	-3854.340056	51.06
408	113-2_b_Mn_CO6_pA1pA1A2BBD2-Q-xqc.log	-3854.340055	51.06
409	156-1_a_Mn_CO6_A1A1A1A2BB-T-xqc.log	-3854.338546	52.01
410	1_a_Mn_CO6_A1A1A2D2D1D2----31	-3854.338338	52.14
411	3_a_Mn_CO6_A1A1A2D1D2D2----220	-3854.338337	52.14
412	1_b_Mn_CO6_A1A1A2D2D1D2----64	-3854.338336	52.14
413	3_a_Mn_CO6_A1A1A2BD2B----213	-3854.338336	52.14
414	3_a_Mn_CO6_A1A1A2BD2D2----214	-3854.338336	52.14
415	3_a_Mn_CO6_A1A1A2D1BD1----215	-3854.338336	52.14
416	3_a_Mn_CO6_A1A1A2D2BD2----221	-3854.338336	52.14
417	3_b_Mn_CO6_A1A1A2BD2B----246	-3854.338336	52.14
418	3_b_Mn_CO6_A1A1A2BD2D2----247	-3854.338336	52.14
419	3_b_Mn_CO6_A1A1A2D1BD2----249	-3854.338336	52.14
420	3_b_Mn_CO6_A1A1A2D1D2D2----253	-3854.338336	52.14
421	3_b_Mn_CO6_A1A1A2D2BD2----254	-3854.338336	52.14
422	40-2_b_Mn_CO6_pA1pA1pA1pA1A2A2-Q.log	-3854.338161	52.25
423	2_a_Mn_CO6_A1A1pA2BBD1----80	-3854.337497	52.67
424	147-3_b_Mn_CO6_A1A1A2A2D1D1-T.log	-3854.336111	53.54
425	85-1_a_Mn_CO6_A1A1A1A2BD2-T.log	-3854.335752	53.76
426	1_a_Mn_CO6_A1A1A2BBB----16	-3854.335751	53.76
427	1_b_Mn_CO6_A1A1A2BBB----49	-3854.335751	53.76
428	1_a_Mn_CO6_A1A1A1A2D1D2----10	-3854.33575	53.76
429	1_b_Mn_CO6_A1A1A1A2BD2----41	-3854.33575	53.76
430	1_b_Mn_CO6_A1A1A1A2D1D2----43	-3854.33575	53.76
431	45-1_b_Mn_CO6_A1A1A1A2BB-T.log	-3854.335443	53.95
432	122-2_b_Mn_CO6_A1A1A1A1pA2pA2-Q.log	-3854.335057	54.20

433	17-3_a_Mn_CO6_A1A1A1A2A2D2-T.log	-3854.334479	54.56
434	1_a_Mn_CO6_A1A1A2D2D2D2-COdeplasat----32	-3854.334214	54.73
435	176-2_a_Mn_CO6_A1A1pA2BpD2pD2-Q-xqc.log	-3854.333397	55.24
436	241-2_b_Mn_CO6_pA1pA1A2BBpD1-Q-xqc.log	-3854.333397	55.24
437	90-2_a_Mn_CO6_A1A1A1A2A2A2-Q.log	-3854.333397	55.24
438	99-2_b_Mn_CO6_A1A1A1pA2pD2pD2-Q-xqc.log	-3854.333397	55.24
439	149-1_b_Mn_CO6_A1A1A2A2BB-Q.log	-3854.333150	55.39
440	1052_a_Mn_CO6_pA1pA1pA1A2BD2-Q.log	-3854.333053	55.45
441	26-2_b_Mn_CO6_pA1pA1pA1A2BpD1-Q-xqc-freq.log	-3854.333049	55.46
442	167-2_a_Mn_CO6_pA1pA1pA1A2BpD1-Q-xqc-freq.log	-3854.333041	55.46
443	3_a_Mn_CO6_A1A1A1A2D1D1----200	-3854.331228	56.60
444	3_a_Mn_CO6_A1A1A2D2D2D2----223	-3854.330512	57.05
445	3_b_Mn_CO6_A1A1A1A2D1D2----234	-3854.330512	57.05
446	3_a_Mn_CO6_A1A1A2A2BB----203	-3854.33051	57.05
447	1_b_Mn_CO6_A1A1A2A2D1D1----47	-3854.330508	57.05
448	185-2_b_Mn_CO6_A1A1pA2D1BD1-T-xqc-rupt.log	-3854.330281	57.19
449	2_b_Mn_CO6_pA1pA1pA1pA1A2A2----190	-3854.330032	57.35
450	101-2_a_Mn_CO6_A1A1A1pA2pD2pD2-Q-xqc.log	-3854.329785	57.51
451	78-3_b_Mn_CO6_A1A1A1A2A2D1-T.log	-3854.329331	57.79
452	22-3_a_Mn_CO6_A1A1A1A2A2D1-T.log	-3854.329327	57.79
453	172-2_b_Mn_CO6_A1A1pA2BBpD2-T-xqc.log	-3854.329104	57.93
454	155-1_a_Mn_CO6_A1A1A2D1BD1-T.log	-3854.329103	57.93
455	100-2_a_Mn_CO6_A1A1A1pA2pA2pD2-Q-xqc.log	-3854.328418	58.36
456	86-1_b_Mn_CO6_A1A1A1A2A2A2-Q.log	-3854.328418	58.36
457	5-3_b_Mn_CO6_A1A1A1A2A2A2-Q.log	-3854.328030	58.61
458	220-1_a_Mn_CO6_A1A1A2D2BD2-T-xqc-freq.log	-3854.327796	58.75
459	39-1_b_Mn_CO6_A1A1A2D1BD2-T-xqc.log	-3854.327796	58.75
460	66-1_a_Mn_CO6_A1A1A2D1BD2-T-xqc.log	-3854.327796	58.75
461	1_b_Mn_CO6_A1A1A2D1BD2----58	-3854.327542	58.91
462	1_b_Mn_CO6_A1A1A2D1D1D2----60	-3854.327542	58.91
463	2_b_Mn_CO6_A1A1pA2D1BpD2----151	-3854.327542	58.91
464	1_a_Mn_CO6_A1A1A2D1BD2----25	-3854.327541	58.91
465	177-2_a_Mn_CO6_A1A1pA2D1BpD2-Q-xqc-rupt.log	-3854.325973	59.90
466	13-2_b_Mn_CO6_pA1pA1A2D2BD2-Q-xqc-rupt.log	-3854.325798	60.01
467	134-1_b_Mn_CO6_A1A1A1A2D2D2-Q-xqc.log	-3854.325447	60.23
468	159-2_b_Mn_CO6_A1A1A1pA2D1pD2-Q.log	-3854.325280	60.33
469	15-2_b_Mn_CO6_pA1pA1pA1A2A2D2-Q.log	-3854.325089	60.45
470	14-2_a_Mn_CO6_pA1pA1pA1A2A2D2-Q-xqc.log	-3854.325088	60.45
471	49-2_b_Mn_CO6_A1A1pA2D1D1pD2-Q-xqc-rupt.log	-3854.323547	61.42
472	168-2_a_Mn_CO6_pA1pA1pA1A2A2pD1-Q-xqc.log	-3854.323285	61.58
473	168-2_a_Mn_CO6_pA1pA1pA1A2A2pD1-Q-xqc.log	-3854.323284	61.58
474	173-2_a_Mn_CO6_A1A1pA2pA2D1pD2-T-xqc.log	-3854.322201	62.26
475	74-2_b_Mn_CO6_A1A1pA2pA2D1pD2-T-xqc-freq.log	-3854.322201	62.26
476	160-2_a_Mn_CO6_A1A1pA2pA2D1D1-T-xqc.log	-3854.321955	62.42

477	3_a_Mn_CO6_A1A1A2D1BD2----216	-3854.321903	62.45
478	3_a_Mn_CO6_A1A1A2BD1B----210	-3854.321902	62.45
479	3_a_Mn_CO6_A1A1A2D1D1D2----218	-3854.321902	62.45
480	3_b_Mn_CO6_A1A1A2BBB----240	-3854.321902	62.45
481	3_b_Mn_CO6_A1A1A2BD1B----243	-3854.321902	62.45
482	3_b_Mn_CO6_A1A1A2D1D1D2----251	-3854.321902	62.45
483	141-1_b_Mn_CO6_A1A1A1A2BD1-T.log	-3854.321669	62.60
484	144-1_b_Mn_CO6_A1A1A2A2BD1-Q-xqc.log	-3854.321084	62.96
485	154-3_b_Mn_CO6_A1A1A2A2BB-Q-xqc.log	-3854.321084	62.96
486	211-3_a_Mn_CO6_A1A1A2A2D1D2-Q-xqc-freq.log	-3854.321084	62.96
487	212-3_b_Mn_CO6_A1A1A2A2D1D2-Q-xqc-freq.log	-3854.321084	62.96
488	213-1_b_Mn_CO6_A1A1A2A2D1D2-Q.log	-3854.321074	62.97
489	112-2_b_Mn_CO6_pA1pA1A2BBB-Q.log	-3854.321044	62.99
490	140-1_a_Mn_CO6_A1A1A2A2BD1-Q-freq.log	-3854.320203	63.52
491	67-1_b_Mn_CO6_A1A1A1A2BD2-Q.log	-3854.319983	63.66
492	85-1_a_Mn_CO6_A1A1A1A2BD2-Q.log	-3854.319983	63.66
493	17-3_a_Mn_CO6_A1A1A1A2A2D2-Q.log	-3854.319982	63.66
494	20-3_b_Mn_CO6_A1A1A1A2BD2-Q.log	-3854.319982	63.66
495	80-3_a_Mn_CO6_A1A1A1A2D2D2-Q-xqc.log	-3854.319982	63.66
496	18-3_a_Mn_CO6_A1A1A1A2BD2-Q.log	-3854.319981	63.66
497	181-2_a_Mn_CO6_pA1pA1A2pD1D2D2-Q-xqc-freq.log	-3854.319977	63.66
498	113-2_b_Mn_CO6_pA1pA1A2BBD2-T-xqc.log	-3854.319639	63.87
499	152-2_a_Mn_CO6_pA1pA1A2pD1BD2-T-xqc-freq.log	-3854.319638	63.87
500	51-2_a_Mn_CO6_pA1pA1A2BD2D2-T-xqc-freq.log	-3854.319638	63.87
501	153-3_b_Mn_CO6_A1A1A1A2A2D2-Q.log	-3854.318910	64.33
502	235-3_a_Mn_CO6_A1A2BBBB-T-opt-new-freq.log	-3854.318808	64.39
503	235-3_a_Mn_CO6_A1A2BBBB-T-xqc-freq-1.log	-3854.318804	64.40
504	29-2_b_Mn_CO6_A1A1pA2pA2D1D1-T-xqc-rupt.log	-3854.318044	64.87
505	1_b_Mn_CO6_A1A1A2D1BD1----57	-3854.317689	65.10
506	119-2_a_Mn_CO6_A1A1pA2pA2BD1-Q-xqc.log	-3854.317617	65.14
507	223-2_b_Mn_CO6_pA1pA1A2pD1BpD1-T.log	-3854.317400	65.28
508	231-2_a_Mn_CO6_pA1pA1A2pD1BpD1-T-xqc.log	-3854.317342	65.31
509	2_a_Mn_CO6_A1A1pA2BpD2B----85	-3854.317161	65.43
510	1_b_Mn_CO6_A1A2BBBB----66	-3854.315208	66.65
511	127-3_b_Mn_CO6_A1A1A1A2D2D2-Q-xqc.log	-3854.314260	67.25
512	187-3_a_Mn_CO6_A1A1A2D1D2D2-Q-xqc.log	-3854.314225	67.27
513	35-3_b_Mn_CO6_A1A1A2D1D2D2-Q-xqc.log	-3854.314225	67.27
514	211-3_a_Mn_CO6_A1A1A2A2D1D2-T.log	-3854.313877	67.49
515	111-2_b_Mn_CO6_A1A1pA2pA2BD1-Q.log	-3854.313856	67.50
516	47-3_a_Mn_CO6_A1A1A2A2BD1-T.log	-3854.312772	68.18
517	213-1_b_Mn_CO6_A1A1A2A2D1D2-T.log	-3854.312768	68.18
518	44-1_b_Mn_CO6_A1A1A2D2D2D2-Q-xqc-rupt.log	-3854.312465	68.37
519	1_b_Mn_CO6_A1A1A2D2D2D2----65	-3854.312171	68.56
520	1_b_Mn_CO6_A1A1A1A2BB----39	-3854.311816	68.78

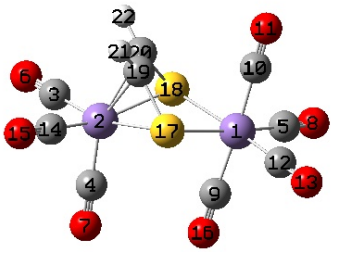
521	46-1_a_Mn_CO6_A1A1A2A2D1D2-Q.log	-3854.310526	69.59
522	173-2_a_Mn_CO6_A1A1pA2pA2D1pD2-Q.log	-3854.310524	69.59
523	1_a_Mn_CO6_A1A1A2A2D1D2----15	-3854.308431	70.90
524	3_a_Mn_CO6_A1A1A2D1D2D1----219	-3854.308431	70.90
525	3_b_Mn_CO6_A1A1A2BBD1----241	-3854.308431	70.90
526	3_b_Mn_CO6_A1A1A2D1D2D1----252	-3854.308431	70.90
527	3_a_Mn_CO6_A1A1A2A2BD1----204	-3854.30843	70.91
528	3_a_Mn_CO6_A1A1A2A2D1D2----206	-3854.30843	70.91
529	3_b_Mn_CO6_A1A1A2A2D1D2----239	-3854.30843	70.91
530	1_b_Mn_CO6_A1A1A2A2D1D2----48	-3854.308428	70.91
531	3_a_Mn_CO6_A1A1A2BBD1----208	-3854.308428	70.91
532	3_b_Mn_CO6_A1A1A2D1BD1----248	-3854.308428	70.91
533	2_a_Mn_CO6_pA1pA1pA1A2pD1pD1----126	-3854.307776	71.32
534	2_b_Mn_CO6_pA1pA1pA1A2pD1pD1----189	-3854.307776	71.32
535	224-2_b_Mn_CO6_A1A1pA2pD2BpD2-T-xqc.log	-3854.306805	71.93
536	205-3_b_Mn_CO6_A1A1A2BBB-T.log	-3854.306796	71.93
537	233-3_b_Mn_CO6_A1A1A2BD1D2-T-xqc.log	-3854.306794	71.93
538	137-3_b_Mn_CO6_A1A1A2D1D1D1-T-xqc.log	-3854.306792	71.93
539	126-3_b_Mn_CO6_A1A1A2BD1D1-T-xqc.log	-3854.306791	71.93
540	129-3_a_Mn_CO6_A1A1A2D2D1D2-T-xqc.log	-3854.306791	71.93
541	215-3_b_Mn_CO6_A1A1A2D1BD1-T-xqc.log	-3854.306791	71.93
542	232-3_b_Mn_CO6_A1A1A2D2D1D2-T-xqc.log	-3854.306791	71.93
543	69-3_a_Mn_CO6_A1A1A2D1BD1-T-xqc.log	-3854.306791	71.93
544	206-3_b_Mn_CO6_A1A1A2BD1B-T-xqc.log	-3854.306790	71.93
545	130-3_a_Mn_CO6_A1A1A2BD1D1-T.log	-3854.306784	71.94
546	214-3_a_Mn_CO6_A1A1A2BBD1-T.log	-3854.306783	71.94
547	237-2_b_Mn_CO6_A1A1pA2BpD2B-Q-xqc.log	-3854.306250	72.27
548	42-2_a_Mn_CO6_A1A1pA2BpD2B-Q-xqc.log	-3854.306250	72.27
549	63-2_b_Mn_CO6_pA1pA1A2pD1pD1pD1-T-xqc-rupt.log	-3854.305377	72.82
550	178-2_a_Mn_CO6_pA1pA1A2A2BpD1-Q-xqc.log	-3854.305346	72.84
551	174-2_b_Mn_CO6_pA1pA1A2A2BpD1-Q.log	-3854.305342	72.84
552	169-1_a_Mn_CO6_A1A1A2BBD2-Q-xqc-freq.log	-3854.304814	73.17
553	66-1_a_Mn_CO6_A1A1A2D1BD2-Q-xqc-freq.log	-3854.304814	73.17
554	39-1_b_Mn_CO6_A1A1A2D1BD2-Q-xqc-freq.log	-3854.304813	73.18
555	74-2_b_Mn_CO6_A1A1pA2pA2D1pD2-Q-xqc-freq.log	-3854.304812	73.18
556	2_a_Mn_CO6_A1A1pA2pD2pD2pD2----98	-3854.304566	73.33
557	2_a_Mn_CO6_A1A1pA2pD2BpD2----96	-3854.298709	77.01
558	162-2_b_Mn_CO6_pA1pA1pA1A2A2pD1-Q-freq.log	-3854.298461	77.16
559	186-1_a_Mn_CO6_A1A1A2BD1B-T.log	-3854.297942	77.49
560	216-2_b_Mn_CO6_pA1pA1pA1A2pD1pD1-T.log	-3854.297797	77.58
561	48-2_a_Mn_CO6_pA1pA1pA1A2pD1pD1-T.log	-3854.297796	77.58
562	243-2_b_Mn_pA1pA1A2BpD1B-T.log	-3854.297768	77.60
563	240-2_a_Mn_pA1pA1A2BpD1B-T.log	-3854.297767	77.60
564	114--2_b_Mn_CO6_pA1pA1A2BD2D2-T-xqc.log	-3854.297678	77.65

565	144-1_b_Mn_CO6_A1A1A2A2BD1-T.log	-3854.297666	77.66
566	140-1_a_Mn_CO6_A1A1A2A2BD1-T.log	-3854.297658	77.67
567	194-1_b_Mn_CO6_A1A1A1A2D1D2-Q-xqc-fneg-1.log	-3854.297312	77.88
568	194-1_b_Mn_CO6_A1A1A1A2D1D2-Q-xqc-fneg-4.log	-3854.297312	77.88
569	194-1_b_Mn_CO6_A1A1A1A2D1D2-Q-xqc-fneg-3.log	-3854.297305	77.89
570	1_b_Mn_CO6_A1A1A2D2BD2----63	-3854.296766	78.22
571	2_b_Mn_CO6_A1A1pA2pD2D1pD2----160	-3854.296766	78.22
572	1_a_Mn_CO6_A1A1A2D2BD2----30	-3854.296765	78.23
573	247-2_a_Mn_CO6_pA1pA1A2BD2B-Q-xqc-freq.log	-3854.296723	78.25
574	182-2_b_Mn_CO6_pA1pA1pA1A2pD1D2-Q-xqc-freq.log	-3854.295731	78.87
575	193-1_a_Mn_CO6_A1A1A1A2D1D2-Q-xqc-freq.log	-3854.295729	78.88
576	32-2_a_Mn_CO6_pA1pA1pA1A2pD1D2-Q-xqc-freq.log	-3854.295724	78.88
577	194-1_b_Mn_CO6_A1A1A1A2D1D2-Q-xqc-fneg-2-freq.log	-3854.295011	79.33
578	194-1_b_Mn_CO6_A1A1A1A2D1D2-Q-xqc-fneg.log	-3854.293921	80.01
579	1_b_Mn_CO6_A1A1A1A2D1D1----42	-3854.293843	80.06
580	1_a_Mn_CO6_A1A1A1A2D1D1----9	-3854.293842	80.06
581	204-3_a_Mn_CO6_A1A1A2D1D1D2-T-xqc.log	-3854.293442	80.31
582	51-2_a_Mn_CO6_pA1pA1A2BD2D2-Q-xqc.log	-3854.292684	80.79
583	51-2_a_Mn_CO6_pA1pA1A2BD2D2-Q-xqc.log	-3854.292683	80.79
584	243-2_b_Mn_pA1pA1A2BpD1B-Q.log	-3854.291828	81.32
585	240-2_a_Mn_pA1pA1A2BpD1B-Q.log	-3854.291820	81.33
586	207-3_b_Mn_CO6_A1A1A2D1D1D2-T-xqc.log	-3854.291052	81.81
587	179-3_b_Mn_CO6_A1A1A2D2D2D2-T-xqc.log	-3854.291045	81.81
588	161-1_a_Mn_CO6_A1A1A2BD2B-Q.log	-3854.290981	81.85
589	58-2_a_Mn_CO6_pA1pA1A2BBpD1-Q-xqc.log	-3854.290781	81.98
590	2_b_Mn_CO6_pA1pA1A2pD1pD1pD1----180	-3854.289739	82.63
591	2_b_Mn_CO6_pA1pA1A2pD1BpD1----176	-3854.289738	82.63
592	2_b_Mn_CO6_A1A1pA2pD2BpD2----159	-3854.289699	82.66
593	36-1_b_Mn_CO6_A1A1A2BBB-T-freq.log	-3854.289132	83.02
594	56-1_a_Mn_CO6_A1A1A2D1D2D1-Q-xqc-rupt.log	-3854.288532	83.39
595	1_a_Mn_CO6_A1A1A2BD1D1----20	-3854.287741	83.89
596	1_b_Mn_CO6_A1A1A2BD1D1----53	-3854.287741	83.89
597	187-3_a_Mn_CO6_A1A1A2D1D2D2-T-xqc.log	-3854.287478	84.05
598	190-3_a_Mn_CO6_A1A1A2BD2B-T-xqc.log	-3854.287478	84.05
599	210-3_b_Mn_CO6_A1A1A2D1D2D1-T.log	-3854.287478	84.05
600	35-3_b_Mn_CO6_A1A1A2D1D2D2-T-xqc.log	-3854.287478	84.05
601	65-3_a_Mn_CO6_A1A1A2D1D2D1-T-xqc-freq.log	-3854.287478	84.05
602	71-3_b_Mn_CO6_A1A1A2D1BD2-T-xqc.log	-3854.287478	84.05
603	72-3_b_Mn_CO6_A1A1A2BD2B-Q-xqc.log	-3854.287477	84.05
604	72-3_b_Mn_CO6_A1A1A2BD2B-T.log	-3854.287477	84.05
605	52-1_a_Mn_CO6_A1A1A2D1D1D2-Q-xqc.log	-3854.287332	84.14
606	201-1_b_Mn_CO6_A1A1A2D1D1D2-Q.log	-3854.287310	84.16
607	189-3_a_Mn_CO6_A1A1A2BD2D2-T-xqc.log	-3854.286398	84.73
608	2_b_Mn_CO6_A1A1pA2D1D1pD2----153	-3854.286232	84.83

609	2_a_Mn_CO6_A1A1pA2D1D1pD2----90	-3854.286231	84.84
610	2_a_Mn_CO6_A1A1pA2BD1D1----83	-3854.286046	84.95
611	2_a_Mn_CO6_pA1pA1A2BD2D2----106	-3854.286044	84.95
612	2_a_Mn_CO6_pA1pA1A2D2D2D2----110	-3854.286044	84.95
613	2_b_Mn_CO6_A1A1pA2BD1D1----146	-3854.286044	84.95
614	2_b_Mn_CO6_pA1pA1A2pD1D2pD1----178	-3854.284991	85.61
615	2_a_Mn_CO6_pA1pA1A2pD1D2pD1----115	-3854.28499	85.61
616	50-2_b_Mn_CO6_pA1pA1A2pD1D2pD1-Q.log	-3854.284848	85.70
617	2_a_Mn_CO6_A1A1pA2pD2D1pD2----97	-3854.283475	86.57
618	244-2_a_Mn_CO6_pA1pA1A2pD1pD1pD1-T-xqc.log	-3854.282696	87.05
619	1_a_Mn_CO6_A1A1A2D1D1D2----27	-3854.281023	88.10
620	2_b_Mn_CO6_A1A1pA2D1pD2D1-COdeplasat----154	-3854.279261	89.21
621	2_a_Mn_CO6_A1A1pA2D1pD2D1-COdeplasat----91	-3854.27693	90.67
622	218-1_b_Mn_CO6_A1A1A2D2BD2-T.log	-3854.276717	90.81
623	2_b_Mn_CO6_A1A1pA2BpD2B----148	-3854.276454	90.97
624	2_a_Mn_CO6_A1A1pA2D1D1D1----89	-3854.273917	92.56
625	2_b_Mn_CO6_A1A1pA2D1D1D1----152	-3854.273917	92.56
626	3_a_Mn_CO6_A1A2BBBB----224	-3854.271542	94.05
627	3_b_Mn_CO6_A1A2BBBB----257	-3854.271539	94.05
628	3_a_Mn_CO6_A1A1A2BD1D2----212	-3854.271177	94.28
629	3_b_Mn_CO6_A1A1A2BD1D2----245	-3854.271177	94.28
630	3_b_Mn_CO6_A1A1A2D2D1D2----255	-3854.271176	94.28
631	1_a_Mn_CO6_A1A1A2D1D2D1----28	-3854.269933	95.06
632	237-2_b_Mn_CO6_A1A1pA2BpD2B-T-xqc.log	-3854.269230	95.50
633	42-2_a_Mn_CO6_A1A1pA2BpD2B-T.log	-3854.268596	95.90
634	2_b_Mn_CO6_pA1pA1A2pD1pD1D2----179	-3854.268245	96.12
635	58-2_a_Mn_CO6_pA1pA1A2BBpD1-T-freq.log	-3854.267399	96.65
636	2_a_Mn_CO6_pA1pA1A2BBpD1----104	-3854.266351	97.31
637	2_a_Mn_CO6_pA1pA1A2BpD1pD1----108	-3854.266351	97.31
638	2_a_Mn_CO6_pA1pA1A2pD1BpD1----113	-3854.266351	97.31
639	2_a_Mn_CO6_pA1pA1A2pD1pD1D2----116	-3854.266351	97.31
640	2_a_Mn_pA1pA1A2BpD1B----128	-3854.266351	97.31
641	2_b_Mn_CO6_pA1pA1A2BBpD1----167	-3854.266351	97.31
642	2_b_Mn_CO6_pA1pA1A2BpD1pD1----171	-3854.266351	97.31
643	2_b_Mn_pA1pA1A2BpD1B----191	-3854.266351	97.31
644	2_a_Mn_CO6_pA1pA1A2pD1pD1pD1----117	-3854.26635	97.31
645	19-3_a_Mn_CO6_A1A1A2D1D1D1-T-xqc.log	-3854.259706	101.48
646	114--2_b_Mn_CO6_pA1pA1A2BD2D2-Q-freq.log	-3854.259175	101.81
647	1_b_Mn_CO6_A1A1A2BD1D2----54	-3854.257727	102.72
648	2_b_Mn_CO6_A1A1pA2BD1pD2----147	-3854.25752	102.85
649	2_a_Mn_CO6_A1A1pA2BD1pD2----84	-3854.257519	102.85
650	2_a_Mn_CO6_pA1pA1A2BD2B----105	-3854.25429	104.88
651	2_b_Mn_CO6_pA1pA1A2BD2B----168	-3854.254289	104.88

652	104-2_a_Mn_CO6_pA1pA1A2BBD2-T-freq.log	-3854.251733	106.48
653	1_a_Mn_CO6_A1A1A2D1D2D2----29	-3854.24489	110.78
654	1_b_Mn_CO6_A1A1A2D1D2D2----62	-3854.24489	110.78
655	1_a_Mn_CO6_A1A1A2D1D1D1----26	-3854.236256	116.20
656	1_b_Mn_CO6_A1A1A2D1D2D1----61	-3854.235714	116.54
657	216-2_b_Mn_CO6_pA1pA1pA1A2pD1pD1-Q.log	-3854.231313	119.30
658	48-2_a_Mn_CO6_pA1pA1pA1A2pD1pD1-Q.log	-3854.231309	119.30
659	136-2_b_Mn_CO6_A1A1pA2BBD1-Q-freq.log	-3854.227978	121.39
660	1_a_Mn_CO6_A1A1A2BD1D2----21	-3854.200954	138.35
661	202-2_b_Mn_CO6_A1A1pA2D1BpD2-Q-freq.log	-3854.194842	142.18
662	55-3_b_Mn_CO6_A1A2BBBB-T-freq.log	-3854.194375	142.48
663	53-2_a_Mn_CO6_A1A1pA2D1pD2D1-T-freq.log	-3854.194343	142.50
664	202-2_b_Mn_CO6_A1A1pA2D1BpD2-T-freq.log	-3854.193439	143.06
665	2_b_Mn_CO6_pA1pA1A2D2pD1D2----174	-3854.159703	164.23
666	2_a_Mn_CO6_pA1pA1A2D2pD1D2----111	-3854.159697	164.24

Table S5A. Distance table for the lowest-lying $H_2C_2S_2Mn_2(CO)_7$ structures after PBE0/6-311G(d,p) optimization followed by a single point CCSD(T) energy calculation. Provided are the absolute CCSD(T) energy (a.u.), relative energy (kcal/mol), symmetry and WBI.



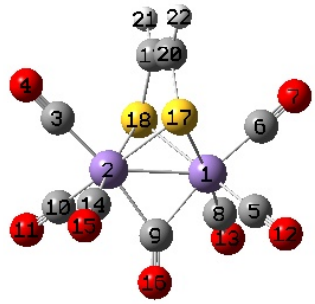
1S. -3965.41226130610 0.00 C_s
WBI 0.02

		1	2	3	4	5
1	Mn	0.000000				
2	Mn	3.592200	0.000000			
3	C	5.003219	1.785058	0.000000		
4	C	4.122411	1.805583	2.597678	0.000000	
5	C	1.798005	4.971292	6.047123	5.298185	0.000000
6	O	6.008314	2.927475	1.142587	3.523392	6.888793
7	O	4.793036	2.945459	3.513082	1.139884	5.796692
8	O	2.938190	5.952968	6.858205	6.192943	1.140336
9	C	1.848480	3.603607	4.954209	3.243614	2.599280
10	C	1.842808	4.349772	5.600504	5.441032	2.601706
11	O	2.978107	5.089465	6.205276	6.376242	3.516405
12	C	1.798000	4.971252	6.575916	5.298288	2.630060
13	O	2.938176	5.952890	7.617324	6.193075	3.562049
14	C	5.002808	1.785066	2.538861	2.597319	6.575631
15	O	6.007763	2.927496	3.447715	3.522918	7.642428
16	O	2.983010	4.092549	5.298535	3.198409	3.491031
17	S	2.400134	2.402670	4.143239	3.328266	4.189401
18	S	2.400200	2.402650	3.066998	3.328164	3.084036
19	C	3.241950	2.085054	3.325681	3.748925	4.781969
20	C	3.241960	2.085032	2.747388	3.748874	4.385032
21	H	4.224085	2.820650	3.822811	4.500305	5.778701
22	H	4.224106	2.820609	2.852911	4.500215	5.165771

		6	7	8	9	10
6	O	0.000000				
7	O	4.263673	0.000000			
8	O	7.599700	6.604053	0.000000		
9	C	5.944740	3.515358	3.497909	0.000000	
10	C	6.522526	6.304701	3.499002	3.689914	0.000000
11	O	7.051733	7.305578	4.231739	4.824562	1.135360
12	C	7.642837	5.796572	3.562034	2.599374	2.601693
13	O	8.705992	6.603872	4.329856	3.498029	3.498966
14	C	3.447690	3.512177	7.617115	4.953555	5.600404
15	O	4.167669	4.262389	8.705670	5.943824	6.522421
16	O	6.227232	3.083062	4.200365	1.135137	4.824962
17	S	5.269442	4.219110	5.325659	3.021361	2.972135
18	S	3.876703	4.219459	3.889296	3.021491	2.972014
19	C	4.313727	4.852637	5.827954	4.201127	3.097946
20	C	3.583741	4.852764	5.289104	4.201156	3.097885
21	H	4.700827	5.601279	6.819628	5.214519	3.819973
22	H	3.386637	5.601471	5.955132	5.214563	3.819896

		11	12	13	14	15
11	O	0.000000				
12	C	3.516389	0.000000			
13	O	4.231694	1.140329	0.000000		
14	C	6.205334	6.046420	6.857352	0.000000	
15	O	7.051867	6.887798	7.598469	1.142599	0.000000
16	O	5.959688	3.491234	4.200653	5.297834	6.226214
17	S	3.748653	3.083854	3.889051	3.066490	3.876047
18	S	3.748472	4.189447	5.325689	4.143296	5.269549

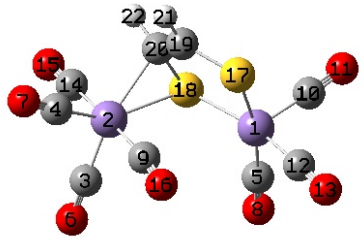
19	C	3.511088	4.384854	5.288832	2.747485	3.583909
20	C	3.510996	4.781858	5.827776	3.325994	4.314186
21	H	3.982815	5.165543	5.954778	2.853190	3.387077
22	H	3.982683	5.778593	6.819444	3.823369	4.701658
		16	17	18	19	20
16	O	0.000000				
17	S	3.841196	0.000000			
18	S	3.841245	3.057177	0.000000		
19	C	5.069313	1.751886	2.701684	0.000000	
20	C	5.069317	2.701663	1.751886	1.383608	0.000000
21	H	6.054773	2.465326	3.725062	1.083747	2.168828
22	H	6.054778	3.725048	2.465310	2.168829	1.083749
		21	22			
21	H	0.000000				
22	H	2.550798	0.000000			



2S. -3965.38622809209 +16.34 C_{2v}
WBI 0.17

		1	2	3	4	5
1	Mn	0.000000				
2	Mn	2.542349	0.000000			
3	C	4.075963	1.809842	0.000000		
4	O	5.125003	2.946374	1.136648	0.000000	
5	C	1.799266	3.714172	5.321600	6.381575	0.000000
6	C	1.809850	4.075923	5.246238	6.130078	2.556047
7	O	2.946368	5.124879	6.129949	6.916406	3.464505
8	C	1.799265	3.714319	5.321835	6.381847	2.649402
9	C	2.008129	2.008142	3.806091	4.940894	2.545264
10	C	3.714277	1.799265	2.556005	3.464392	4.926078
11	O	4.670867	2.938985	3.447124	4.165469	5.860899
12	O	2.938928	4.670766	6.251130	7.294033	1.139813
13	O	2.938955	4.670955	6.251467	7.294435	3.580672
14	C	3.714098	1.799267	2.556046	3.464427	4.152631
15	O	4.670632	2.938990	3.447192	4.165543	4.777363
16	O	2.990637	2.990642	4.708596	5.820145	3.047190
17	S	2.370996	2.370995	3.034172	3.838036	3.040965
18	S	2.371010	2.371010	3.034400	3.838337	4.160858
19	C	3.198159	3.198162	3.172038	3.630779	4.742470
20	C	3.198154	3.198158	3.171943	3.630640	4.356405
21	H	4.162645	4.162652	3.874156	4.092764	5.731034
22	H	4.162637	4.162644	3.874005	4.092525	5.107932
		6	7	8	9	10
6	C	0.000000				
7	O	1.136636	0.000000			
8	C	2.556015	3.464425	0.000000		
9	C	3.806093	4.940894	2.545067	0.000000	
10	C	5.321735	6.381652	4.153111	2.545084	0.000000
11	O	6.251286	7.294145	4.777977	3.384210	1.139872
12	O	3.447055	4.165495	3.580663	3.384454	5.860879
13	O	3.447087	4.165469	1.139841	3.384180	4.778075
14	C	5.321532	6.381467	4.926005	2.545177	2.649483
15	O	6.251010	7.293890	5.860726	3.384305	3.580864
16	O	4.708625	5.820202	3.046829	1.152454	3.046854
17	S	3.034149	3.837942	4.160852	3.234877	4.160844
18	S	3.034299	3.838086	3.041021	3.234541	3.040940
19	C	3.171910	3.630440	4.356381	4.462860	4.356325
20	C	3.171846	3.630370	4.742431	4.462967	4.742400
21	H	3.874008	4.092363	5.107899	5.458677	5.107841

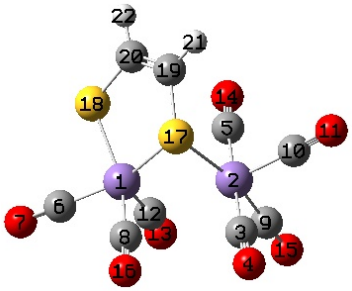
22	H	3.873908	4.092247	5.730974	5.458843	5.730953
		11	12	13	14	15
11	O	0.000000				
12	O	6.766609	0.000000			
13	O	5.184128	4.348896	0.000000		
14	C	3.580882	4.777508	5.860830	0.000000	
15	O	4.349279	5.183375	6.766438	1.139874	0.000000
16	O	3.601709	3.602205	3.601644	3.047080	3.601989
17	S	5.297241	3.849882	5.297233	3.040949	3.849846
18	S	3.849804	5.297207	3.849991	4.160855	5.297257
19	C	5.267960	5.789525	5.268091	4.742497	5.789613
20	C	5.789464	5.268069	5.789525	4.356431	5.268134
21	H	5.901043	6.775694	5.901199	5.731075	6.775816
22	H	6.775628	5.901186	6.775669	5.107974	5.901269
		16	17	18	19	20
16	O	0.000000				
17	S	4.286281	0.000000			
18	S	4.285826	3.044112	0.000000		
19	C	5.605121	2.684238	1.780194	0.000000	
20	C	5.605274	1.780203	2.684229	1.325839	0.000000
21	H	6.584736	3.720401	2.466088	1.083595	2.133980
22	H	6.584984	2.466091	3.720394	2.133985	1.083595
		21	22			
21	H	0.000000				
22	H	2.549104	0.000000			



3S. -3965.37261476952 +24.88 C_1
WBI 0.03

		1	2	3	4	5
1	Mn	0.000000				
2	Mn	3.750049	0.000000			
3	C	4.583621	1.795385	0.000000		
4	C	5.238208	1.787490	2.685017	0.000000	
5	C	1.792419	4.270874	4.428669	5.946197	0.000000
6	O	5.349962	2.935791	1.140611	3.633746	4.861720
7	O	6.258584	2.928475	3.642152	1.141599	7.043734
8	O	2.934930	4.913003	4.682077	6.601612	1.142620
9	C	3.221987	1.846567	2.532050	2.556943	3.914147
10	C	1.762170	5.190814	6.104482	6.717339	2.564997
11	O	2.904328	6.193132	7.141265	7.714796	3.497385
12	C	1.794338	5.088536	5.711004	6.346324	2.575773
13	O	2.935924	6.051654	6.568777	7.181634	3.486479
14	C	4.991522	1.851580	2.537699	2.589877	5.288752
15	O	5.920696	2.986411	3.423976	3.496396	6.113351
16	O	3.503769	2.978557	3.365557	3.421651	4.179759
17	S	2.307732	3.910547	5.322965	4.746954	4.075344
18	S	2.293877	2.375682	3.466561	4.033379	2.879923
19	C	3.154153	2.998462	4.713222	3.616551	4.712049
20	C	3.210095	2.191864	3.904123	3.186283	4.376427
21	H	4.202990	3.631786	5.388655	3.754725	5.792465
22	H	4.216145	2.717389	4.384376	3.387349	5.280871
		6	7	8	9	10
6	O	0.000000				
7	O	4.444153	0.000000			
8	O	4.861642	7.707951	0.000000		
9	C	3.417955	3.445414	4.657784	0.000000	
10	C	6.851076	7.733879	3.495383	4.936536	0.000000
11	O	7.879928	8.720207	4.256947	6.052785	1.143160

12	C	6.331276	7.255412	3.488112	3.959671	2.550829
13	O	7.105960	8.018829	4.214901	4.715851	3.480644
14	C	3.418292	3.486935	5.758363	3.696159	6.078228
15	O	4.102176	4.207816	6.487970	4.829935	6.828655
16	O	4.033104	4.106441	4.898644	1.137549	5.234815
17	S	6.316928	5.495858	5.208898	3.219448	3.144954
18	S	4.392173	5.126513	3.681866	3.133524	3.153636
19	C	5.825482	4.330489	5.772530	3.052786	4.037736
20	C	5.017100	4.087456	5.300764	3.031556	4.099013
21	H	6.516874	4.205063	6.853714	3.708293	4.999117
22	H	5.481810	4.147131	6.134993	3.920261	4.895188
		11	12	13	14	15
11	O	0.000000				
12	C	3.479551	0.000000			
13	O	4.236454	1.141770	0.000000		
14	C	6.904471	6.579301	7.628063	0.000000	
15	O	7.548777	7.578656	8.653989	1.134981	0.000000
16	O	6.363669	3.692186	4.203524	4.823326	5.954756
17	S	3.996356	2.876673	3.672402	5.270073	6.241347
18	S	4.012766	4.062534	5.194322	2.926135	3.717499
19	C	4.835125	4.298564	5.216316	4.024309	4.912111
20	C	4.895056	4.750650	5.802705	2.785197	3.613701
21	H	5.708459	5.187303	6.006829	4.507872	5.312788
22	H	5.549903	5.803609	6.863333	2.610933	3.158017
		16	17	18	19	20
16	O	0.000000				
17	S	3.410624	0.000000			
18	S	4.040114	3.211356	0.000000		
19	C	3.694122	1.685471	2.718401	0.000000	
20	C	3.981497	2.729819	1.759649	1.388098	0.000000
21	H	4.272046	2.380497	3.720517	1.088960	2.133263
22	H	4.925132	3.659090	2.461395	2.123755	1.086101
		21	22			
21	H	0.000000				
22	H	2.444117	0.000000			



4S. -3965.36674206271 +28.56 C_1
WBI 0.15

		1	2	3	4	5
1	Mn	0.000000				
2	Mn	2.838430	0.000000			
3	C	3.529172	1.853168	0.000000		
4	O	4.356864	2.985497	1.134141	0.000000	
5	C	3.271553	1.859588	3.712623	4.844036	0.000000
6	C	1.794283	4.496800	5.014760	5.679199	4.732684
7	O	2.933504	5.596020	6.046173	6.634514	5.763373
8	C	1.792479	3.293359	2.939207	3.338936	4.485534
9	C	3.978126	1.803673	2.569343	3.449575	2.589435
10	C	4.458429	1.774995	2.558178	3.427619	2.567447
11	O	5.534472	2.914599	3.445526	4.112136	3.452385
12	C	1.769546	2.690458	3.584140	4.471456	2.929907
13	O	2.908269	3.330449	4.227814	5.068840	3.348251
14	O	4.021134	2.990338	4.842334	5.972008	1.132788
15	O	4.908834	2.942156	3.454277	4.135731	3.481752
16	O	2.933214	4.044120	3.153565	3.147940	5.463547
17	S	2.278321	2.311156	2.928745	3.764475	3.021963
18	S	2.220508	4.130165	5.360568	6.308196	3.529536
19	C	3.217480	3.362155	4.498308	5.413326	3.067059

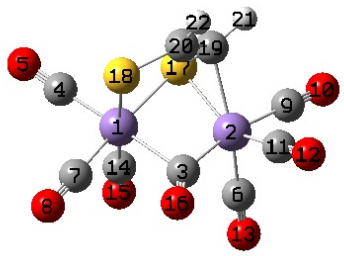
20	C	3.175065	4.056257	5.373368	6.341482	3.330478
21	H	4.249855	3.906517	4.953140	5.805324	3.606768
22	H	4.202900	5.003974	6.399029	7.377835	4.024929

		6	7	8	9	10
6	C	0.000000				
7	O	1.139262	0.000000			
8	C	2.523985	3.420369	0.000000		
9	C	5.264941	6.219426	4.257599	0.000000	
10	C	6.196142	7.315633	4.817055	2.618718	0.000000
11	O	7.294794	8.421572	5.858421	3.562054	1.140389
12	C	2.415362	3.306583	2.665133	2.958219	4.433948
13	O	3.185435	3.824899	3.640090	2.949862	4.954121
14	O	5.273613	6.213664	5.442014	3.462667	3.441249
15	O	5.986019	6.835070	5.106246	1.138492	3.540658
16	O	3.403496	4.097109	1.142529	4.855900	5.402227
17	S	3.984566	5.097208	2.852471	4.088637	3.121890
18	S	2.723221	3.512206	3.917551	5.351671	5.384421
19	C	4.696411	5.727922	4.365974	5.049588	3.771457
20	C	4.259016	5.156079	4.675966	5.556430	4.768124
21	H	5.770614	6.803655	5.244567	5.578871	3.822118
22	H	5.107348	5.895829	5.741668	6.432375	5.537644

		11	12	13	14	15
11	O	0.000000				
12	C	5.566324	0.000000			
13	O	6.053315	1.151001	0.000000		
14	O	4.125774	3.616527	3.856430	0.000000	
15	O	4.320503	3.616208	3.250963	4.158417	0.000000
16	O	6.372460	3.635640	4.474682	6.474993	5.610760
17	S	3.955784	3.492122	4.555957	3.889884	5.220068
18	S	6.300418	3.218812	4.079734	3.694863	6.272028
19	C	4.368746	4.362959	5.332553	3.462303	6.149997
20	C	5.453185	4.271201	5.172621	3.421070	6.584530
21	H	4.139495	5.326769	6.255586	3.910684	6.670538
22	H	6.098130	5.199044	6.011519	3.838882	7.421227

		16	17	18	19	20
16	O	0.000000				
17	S	3.658446	0.000000			
18	S	5.016749	3.107670	0.000000		
19	C	5.282062	1.755344	2.698478	0.000000	
20	C	5.707261	2.669745	1.741226	1.336439	0.000000
21	H	6.068578	2.444288	3.722629	1.083994	2.142569
22	H	6.771508	3.692724	2.424190	2.120617	1.085619

		21	22
21	H	0.000000	
22	H	2.519515	0.000000



5S. -3965.36663886164 +28.63 C_1
WBI 0.14

		1	2	3	4	5
1	Mn	0.000000				
2	Mn	2.781132	0.000000			
3	C	2.248764	1.931651	0.000000		
4	C	1.786514	4.373523	4.005952	0.000000	
5	O	2.926098	5.443351	5.137463	1.139951	0.000000
6	C	3.502996	1.798896	2.553737	5.097621	6.169685
7	C	1.799294	4.069279	2.663981	2.545127	3.462681
8	O	2.939433	5.057075	3.435738	3.443118	4.173907
9	C	4.301675	1.822197	3.734507	5.617084	6.559092

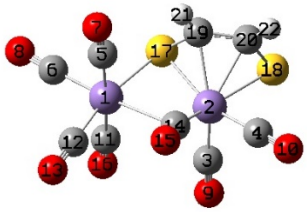
10	O	5.350004	2.958944	4.865196	6.538131	7.406131
11	C	4.179407	1.788361	2.436445	5.853753	6.941719
12	O	5.188955	2.927674	3.269720	6.860503	7.943406
13	O	4.315866	2.939296	3.427641	5.817898	6.851823
14	C	1.792777	3.259575	3.091280	2.580968	3.502219
15	O	2.934834	3.991467	3.983825	3.484676	4.224321
16	O	3.096728	2.973030	1.149591	4.744473	5.842604
17	S	2.278483	2.253347	3.308973	2.989160	3.809767
18	S	2.365401	3.634866	2.908085	2.976541	3.766053
19	C	3.049916	2.198699	3.170044	4.010679	4.851135
20	C	3.074802	3.011013	3.138351	3.914365	4.712131
21	H	4.102997	2.828186	4.097375	4.954865	5.702466
22	H	4.137684	3.816459	3.938819	4.900870	5.612545

		6	7	8	9	10
6	C	0.000000				
7	C	4.391756	0.000000			
8	O	5.214957	1.140214	0.000000		
9	C	2.497598	5.784114	6.809802	0.000000	
10	O	3.377927	6.882709	7.918865	1.136847	0.000000
11	C	2.707418	5.069319	5.862888	2.544119	3.444131
12	O	3.671213	5.902070	6.582417	3.439632	4.147652
13	O	1.140621	4.959134	5.644531	3.366863	4.034474
14	C	3.061308	2.568866	3.481128	4.427798	5.344224
15	O	3.318669	3.475739	4.203102	4.878957	5.660304
16	O	3.287664	2.844582	3.251321	4.704356	5.809792
17	S	3.449738	4.074431	5.214063	2.830769	3.643215
18	S	5.024902	2.941900	3.730730	5.120441	6.147464
19	C	3.954019	4.589931	5.646893	2.827419	3.662404
20	C	4.736786	4.220661	5.143550	4.071442	4.972755
21	H	4.528430	5.674312	6.730681	2.790700	3.334589
22	H	5.574811	5.133240	5.961628	4.677439	5.470728

		11	12	13	14	15
11	C	0.000000				
12	O	1.140194	0.000000			
13	O	3.645307	4.463042	0.000000		
14	C	4.850176	5.930551	3.469644	0.000000	
15	O	5.560331	6.633400	3.368337	1.142197	0.000000
16	O	2.933681	3.441591	3.944592	3.879333	4.689788
17	S	3.861013	4.935416	4.425202	2.906605	3.727902
18	S	4.291551	4.976950	6.031813	4.156971	5.299139
19	C	3.032817	3.881351	5.082130	4.241818	5.190905
20	C	3.470631	4.117185	5.858730	4.670929	5.752664
21	H	3.356065	4.047523	5.632715	5.155526	6.018501
22	H	3.850140	4.231827	6.704332	5.751723	6.831313

		16	17	18	19	20
16	O	0.000000				
17	S	4.441471	0.000000			
18	S	3.407103	3.266352	0.000000		
19	C	4.157429	1.774474	2.721596	0.000000	
20	C	3.869577	2.747644	1.667359	1.396862	0.000000
21	H	5.052540	2.449891	3.671089	1.085895	2.124421
22	H	4.501031	3.724639	2.371720	2.134750	1.089497

		21	22
21	H	0.000000	
22	H	2.410307	0.000000



6S. -3965.36392487062 +30.33 C_1
WBI 0.15

		1	2	3	4	5
1	Mn	0.000000				
2	Mn	2.884091	0.000000			
3	C	3.473171	1.806300	0.000000		
4	C	4.421198	1.798284	2.557371	0.000000	
5	C	1.852516	3.600861	4.813943	4.842334	0.000000
6	C	1.781411	4.504701	4.973976	6.149393	2.522713
7	O	2.985910	4.442287	5.820314	5.481284	1.135845
8	O	2.920902	5.583102	6.009160	7.261734	3.399964
9	O	4.259182	2.943834	1.139251	3.449666	5.777390
10	O	5.476115	2.936759	3.469195	1.138597	5.773986
11	C	1.849775	3.340478	2.913230	4.853778	3.700272
12	C	1.807962	4.022104	4.266757	5.115589	2.600609
13	O	2.946054	4.950488	5.046628	5.808407	3.492735
14	C	2.501902	1.793182	2.789771	2.341972	2.825955
15	O	3.182499	2.911634	3.744825	2.977039	3.131631
16	O	2.982407	4.088568	3.183483	5.484957	4.830107
17	S	2.319026	2.333881	3.275293	4.081193	3.048103
18	S	4.843228	2.366637	3.087149	2.834722	5.424230
19	C	3.124813	2.091823	3.754981	3.320990	2.971380
20	C	4.233080	2.134670	3.693862	2.731532	4.241866
21	H	3.287530	2.867288	4.598208	3.884421	2.486985
22	H	5.008815	2.886447	4.484998	2.893655	4.711816

		6	7	8	9	10
6	C	0.000000				
7	O	3.376033	0.000000			
8	O	1.139860	4.037732	0.000000		
9	O	5.600898	6.826674	6.566064	0.000000	
10	O	7.227074	6.307098	8.348580	4.173303	0.000000
11	C	2.530305	4.830383	3.412717	3.236717	5.900686
12	C	2.635811	3.487073	3.572489	4.842871	5.986879
13	O	3.557641	4.187040	4.329815	5.495801	6.552758
14	C	4.256108	3.582464	5.388202	3.776926	3.200792
15	O	4.815109	3.658695	5.911020	4.610332	3.523660
16	O	3.390102	5.957126	4.061971	3.104980	6.480974
17	S	3.096706	3.912594	3.929622	4.173566	5.203114
18	S	6.112609	6.105258	7.022193	3.870579	3.594296
19	C	4.234645	3.478333	5.127665	4.850692	4.302246
20	C	5.502739	4.704973	6.424326	4.742759	3.546638
21	H	4.251625	2.671017	5.087716	5.716954	4.760808
22	H	6.319823	4.966743	7.246566	5.534087	3.412751

		11	12	13	14	15
11	C	0.000000				
12	C	2.573331	0.000000			
13	O	3.464398	1.138103	0.000000		
14	C	3.460371	2.888177	3.609355	0.000000	
15	O	4.236616	2.950405	3.344086	1.155517	0.000000
16	O	1.134308	3.462198	4.159988	4.382112	5.144643
17	S	2.905385	4.104037	5.236341	3.316076	4.378003
18	S	5.016489	6.274516	7.264938	4.089338	5.130971
19	C	4.236158	4.658445	5.707594	2.923441	3.852123
20	C	5.039149	5.659480	6.654984	3.378497	4.300738
21	H	4.754105	4.637707	5.620997	3.103417	3.778483
22	H	5.974338	6.279299	7.199700	3.781691	4.493775

		16	17	18	19	20

	16 O 0.000000 17 S 3.721659 0.000000 18 S 5.497541 3.117262 0.000000 19 C 5.162751 1.760529 2.719190 0.000000 20 C 5.820631 2.703560 1.722125 1.387165 0.000000 21 H 5.784525 2.494403 3.722804 1.083315 2.158735 22 H 6.797068 3.707548 2.453288 2.128868 1.087633 21 22 21 H 0.000000 22 H 2.464952 0.000000

Table S5B. Energy rank for all of the $H_2C_2S_2Mn_2(CO)_7$ optimized structures. PBE0/6-311G(d,p).

No	**Initial structure**	**Final energy (a.u.)**	ΔE (kcal/mol)
1	2_b_Mn_CO7_A1A1A1pA2pA2pA2D1----173	-3967.657845	0.00
2	2_b_Mn_CO7_A1A1A1A2A2A2B----155	-3967.657842	0.00
3	2_a_Mn_CO7_A1A1A1pA2BD1pD2----89	-3967.657841	0.00
4	2_a_Mn_CO7_A1A1A1pA2BpD2B----90	-3967.657841	0.00
5	2_b_Mn_CO7_pA1pA1pA1A2A2BB----199	-3967.657841	0.00
6	2_a_Mn_CO7_A1A1A1A1pA2pA2B----79	-3967.65784	0.00
7	2_a_Mn_CO7_A1A1A1A1pA2pA2pA2----81	-3967.65784	0.00
8	2_a_Mn_CO7_A1A1A1A2A2A2B----83	-3967.65784	0.00
9	2_a_Mn_CO7_A1A1A1pA2BBB----84	-3967.65784	0.00
10	2_a_Mn_CO7_A1A1A1pA2pA2BD1----97	-3967.65784	0.00
11	2_a_Mn_CO7_A1A1A1pA2pA2BpD2----98	-3967.65784	0.00
12	2_a_Mn_CO7_A1A1A1pA2pA2pA2D1----101	-3967.65784	0.00
13	2_a_Mn_CO7_A1A1pA2BBBB----108	-3967.65784	0.00
14	2_a_Mn_CO7_pA1pA1pA1A2A2BB----127	-3967.65784	0.00
15	2_a_Mn_CO7_pA1pA1pA1A2A2D2D2----130	-3967.65784	0.00
16	2_a_Mn_CO7_pA1pA1pA1A2BBB----133	-3967.65784	0.00
17	2_a_Mn_CO7_pA1pA1pA1A2BD2B----136	-3967.65784	0.00
18	2_a_Mn_CO7_pA1pA1pA1A2D2BD2----141	-3967.65784	0.00
19	2_b_Mn_CO7_A1A1A1A1pA2pA2B----151	-3967.65784	0.00
20	2_b_Mn_CO7_A1A1A1A1pA2pA2pA2----153	-3967.65784	0.00
21	2_b_Mn_CO7_A1A1A1A1pA2pA2pD2----154	-3967.65784	0.00
22	2_b_Mn_CO7_A1A1A1pA2BBB----156	-3967.65784	0.00
23	2_b_Mn_CO7_A1A1A1pA2BBpD2----158	-3967.65784	0.00
24	2_b_Mn_CO7_A1A1A1pA2pA2BpD2----170	-3967.65784	0.00
25	2_b_Mn_CO7_A1A1pA2BBBB----180	-3967.65784	0.00
26	2_b_Mn_CO7_pA1pA1pA1A2A2D2D2----202	-3967.65784	0.00
27	2_b_Mn_CO7_pA1pA1pA1A2BBD2----205	-3967.65784	0.00
28	2_b_Mn_CO7_pA1pA1pA1A2BD2B----207	-3967.65784	0.00
29	2_a_Mn_CO7_A1A1A1A1pA2pA2pD2----82	-3967.657839	0.00
30	1_a_Mn_CO7_A1A1A1A2BD2B----19	-3967.638907	11.88
31	1_b_Mn_CO7_A1A1A2A2BBB----68	-3967.638907	11.88
32	1_a_Mn_CO7_A1A1A1A2A2A2B----5	-3967.638906	11.88
33	1_a_Mn_CO7_A1A1A1A2A2A2D1----6	-3967.638906	11.88
34	1_a_Mn_CO7_A1A1A1A2BD2D2----20	-3967.638906	11.88
35	1_a_Mn_CO7_A1A1A2A2BBB----29	-3967.638906	11.88
36	1_b_Mn_CO7_A1A1A1A1A2A2A2----40	-3967.638906	11.88
37	1_b_Mn_CO7_A1A1A1A2A2A2B----44	-3967.638906	11.88
38	1_b_Mn_CO7_A1A1A1A2A2BB----46	-3967.638906	11.88
39	1_b_Mn_CO7_A1A1A1A2BD2D2----59	-3967.638906	11.88
40	1_a_Mn_CO7_A1A1A1A1A2A2A2----1	-3967.638905	11.89

41	1_b_Mn_CO7_A1A1A1A2A2A2D1----45	-3967.638905	11.89
42	1_b_Mn_CO7_A1A1A2A2BBD1----69	-3967.638905	11.89
43	1_a_Mn_CO7_A1A1A1A2A2BB----7	-3967.638904	11.89
44	2_a_Mn_CO7_pA1pA1pA1A2A2A2pD1----126	-3967.638904	11.89
45	1_b_Mn_CO7_A1A1A1A2BD2B----58	-3967.638902	11.89
46	2_b_Mn_CO7_pA1pA1pA1A2pD1D2D2-COdeplasat----216	-3967.6328	15.72
47	2_a_Mn_CO7_A1A1A1pA2D1pD2pD2-COdeplasat----96	-3967.632787	15.72
48	2_b_Mn_CO7_pA1pA1pA1A2A2BD2-COdeplasat----200	-3967.632728	15.76
49	2_b_Mn_CO7_A1A1A1pA2D1pD2pD2-COdeplasat----168	-3967.632717	15.77
50	2_b_Mn_CO7_pA1pA1pA1A2D2D2D2-COdeplasat----213	-3967.632713	15.77
51	2_a_Mn_CO7_A1A1A1pA2pA2D1pD2-COdeplasat----100	-3967.632702	15.78
52	2_a_Mn_CO7_A1A1A1pA2BpD2pD2-COdeplasat----91	-3967.632656	15.81
53	2_b_Mn_CO7_A1A1A1pA2pA2pD2pD2-COdeplasat----174	-3967.632642	15.82
54	2_b_Mn_CO7_pA1pA1pA1A2D2BD2-COdeplasat----212	-3967.632639	15.82
55	2_a_Mn_CO7_pA1pA1pA1A2D2D2D2-COdeplasat----142	-3967.632633	15.82
56	2_a_Mn_CO7_A1A1A1pA2pA2pD2pD2----102	-3967.625388	20.37
57	2_a_Mn_CO7_A1A1pA2pA2BBD1----109	-3967.625388	20.37
58	2_a_Mn_CO7_pA1pA1pA1A2A2BD2----128	-3967.625388	20.37
59	2_a_Mn_CO7_pA1pA1pA1A2BD2D2----137	-3967.625388	20.37
60	2_b_Mn_CO7_A1A1A2A2BBB----178	-3967.625388	20.37
61	2_b_Mn_CO7_pA1pA1pA1A2BD2D2----208	-3967.625388	20.37
62	2_a_Mn_CO7_A1A1A2A2BBB----106	-3967.625387	20.37
63	2_a_Mn_CO7_pA1pA1pA1A2BBD2----134	-3967.625387	20.37
64	2_b_Mn_CO7_A1A1A1pA2BpD2pD2----163	-3967.625387	20.37
65	2_b_Mn_CO7_A1A1A1pA2D1BpD2----164	-3967.625387	20.37
66	2_a_Mn_CO7_A1A1A1pA2D1BpD2----92	-3967.625386	20.37
67	2_b_Mn_CO7_A1A1pA2pA2BBD1----181	-3967.625384	20.37
68	2_b_Mn_CO7_A1A1A1pA2pA2D1pD2-COdeplasat----172	-3967.624218	21.10
69	2_b_Mn_CO7_pA1pA1pA1A2A2A2pD1----198	-3967.623303	21.68
70	2_b_Mn_CO7_pA1pA1pA1pA1A2A2A2----220	-3967.623303	21.68
71	3_a_Mn_CO7_A1A1A2A2D1BD1----255	-3967.615909	26.32
72	3_a_Mn_CO7_A1A1A1A2BBB----234	-3967.615908	26.32
73	3_a_Mn_CO7_A1A1A1A2BBD1----235	-3967.615907	26.32
74	3_a_Mn_CO7_A1A1A2A2D1D1D1----257	-3967.615907	26.32
75	3_b_Mn_CO7_A1A1A1A2BBD1----274	-3967.615907	26.32
76	3_b_Mn_CO7_A1A1A1A2D1BD2----281	-3967.615907	26.32
77	3_b_Mn_CO7_A1A1A1A2D2D2D2----288	-3967.615907	26.32
78	3_b_Mn_CO7_A1A1A2A2BBB----289	-3967.615907	26.32
79	3_a_Mn_CO7_A1A1A1A2D1BD2----242	-3967.615906	26.32
80	3_a_Mn_CO7_A1A1A1A2D2D2D2----249	-3967.615904	26.32
81	1_a_Mn_CO7_A1A1A1A2A2D2D2----12	-3967.615796	26.39
82	1_a_Mn_CO7_A1A1A1A2BBD2----15	-3967.615796	26.39
83	1_a_Mn_CO7_A1A1A1A2D2BD2----26	-3967.615796	26.39
84	1_b_Mn_CO7_A1A1A1A2A2D2D2----51	-3967.615796	26.39
85	1_b_Mn_CO7_A1A1A1A2BBD2----54	-3967.615796	26.39

86	3_a_Mn_CO7_A1A1A1A1A2A2D2----225	-3967.615796	26.39
87	3_a_Mn_CO7_A1A1A1A2A2D2D2----233	-3967.615796	26.39
88	3_a_Mn_CO7_A1A1A1A2BD1B----237	-3967.615796	26.39
89	3_b_Mn_CO7_A1A1A1A2A2BB----267	-3967.615796	26.39
90	3_b_Mn_CO7_A1A1A1A2A2D1D2----271	-3967.615796	26.39
91	1_a_Mn_CO7_A1A1A1A2A2BD2----9	-3967.615795	26.39
92	1_a_Mn_CO7_A1A1A1A2BBB----13	-3967.615795	26.39
93	1_b_Mn_CO7_A1A1A1A2A2BD2----48	-3967.615795	26.39
94	1_b_Mn_CO7_A1A1A1A2D2BD2----65	-3967.615795	26.39
95	3_a_Mn_CO7_A1A1A1A1A2A2B----223	-3967.615795	26.39
96	3_a_Mn_CO7_A1A1A1A2A2BB----228	-3967.615795	26.39
97	3_a_Mn_CO7_A1A1A1A2A2BD2----230	-3967.615795	26.39
98	3_a_Mn_CO7_A1A1A1A2A2D1D2----232	-3967.615795	26.39
99	3_a_Mn_CO7_A1A1A1A2BD2B----240	-3967.615795	26.39
100	3_a_Mn_CO7_A1A1A1A2D1D2D2----246	-3967.615795	26.39
101	3_b_Mn_CO7_A1A1A1A2A2A2B----265	-3967.615795	26.39
102	3_b_Mn_CO7_A1A1A1A2A2D2D2----272	-3967.615795	26.39
103	3_b_Mn_CO7_A1A1A1A2BBB----273	-3967.615795	26.39
104	3_b_Mn_CO7_A1A1A1A2BD2B----279	-3967.615795	26.39
105	3_b_Mn_CO7_A1A1A1A2D1D2D2----285	-3967.615795	26.39
106	3_a_Mn_CO7_A1A1A1A2A2BD1----229	-3967.613907	27.57
107	3_b_Mn_CO7_A1A1A1A2A2BD1----268	-3967.613907	27.57
108	3_b_Mn_CO7_A1A1A1A1A2A2D2----264	-3967.610086	29.97
109	67-2_b_Mn_CO7_pA1pA1pA1A2BBD2-T-xqc-freq.log	-3967.607082	31.85
110	54-2_b_Mn_CO7_A1A1A1pA2BBpD2-T-xqc.log	-3967.607080	31.86
111	58-2_b_Mn_CO7_A1A1A1A1pA2pA2B-T-xqc.log	-3967.607080	31.86
112	61-2_a_Mn_CO7_pA1pA1pA1A2A2BB-T.log	-3967.607063	31.87
113	48-2_b_Mn_CO7_pA1pA1pA1A2A2BB-T-freq.log	-3967.604585	33.42
114	45-2_a_Mn_CO7_A1A1pA2BBBB-T-xqc.log	-3967.603851	33.88
115	60-2_a_Mn_CO7_A1A1A1pA2pA2pA2D1-T.log	-3967.603850	33.88
116	50-2_a_Mn_CO7_A1A1A1A1pA2pA2pA2-T.log	-3967.603849	33.88
117	57-2_b_Mn_CO7_A1A1A1A1pA2pA2pA2-T.log	-3967.603848	33.88
118	65-2_b_Mn_CO7_A1A1pA2BBBB-T-xqc-freq.log	-3967.603848	33.88
119	68-2_b_Mn_CO7_pA1pA1pA1A2BD2B-T-xqc.log	-3967.603847	33.88
120	49-2_a_Mn_CO7_A1A1A1pA2BpD2B-T-xqc-freq.log	-3967.603839	33.89
121	228-2_b_Mn_CO7_A1A1A1pA2BpD2B-T-xqc-freq.log	-3967.603838	33.89
122	62-2_a_Mn_CO7_pA1pA1pA1A2A2D2D2-T-xqc-freq.log	-3967.603426	34.15
123	66-2_b_Mn_CO7_pA1pA1pA1A2A2D2D2-T-xqc-freq.log	-3967.603426	34.15
124	208-3_b_Mn_CO7_A1A1A1A2BD1B-T-xqc.log	-3967.602302	34.85
125	133-3_b_Mn_CO7_A1A1A1A1A2A2B-T.log	-3967.602129	34.96
126	200-3_b_Mn_CO7_A1A1A1A1A2A2B-T.log	-3967.602129	34.96
127	104-3_a_Mn_CO7_A1A1A1A1A2A2D2-T-xqc.log	-3967.602128	34.96
128	106-3_b_Mn_CO7_A1A1A1A2A2BB-T-xqc.log	-3967.602128	34.96
129	112-3_a_Mn_CO7_A1A1A1A2A2D1D2-T-xqc-freq.log	-3967.602128	34.96
130	113-3_a_Mn_CO7_A1A1A1A2BD2B-T-xqc.log	-3967.602128	34.96

131	172-3_a_Mn_CO7_A1A1A1A2BD1B-T-xqc-freq.log	-3967.602128	34.96
132	179-3_a_Mn_CO7_A1A1A1A2BD2B-T-xqc.log	-3967.602128	34.96
133	209-3_a_Mn_CO7_A1A1A1A2D2D1D2-T-xqc.log	-3967.602128	34.96
134	221-3_a_Mn_CO7_A1A1A1A2D2BD2-T-xqc.log	-3967.602128	34.96
135	222-3_b_Mn_CO7_A1A1A1A2BBD2-T-xqc.log	-3967.602128	34.96
136	24-1_a_Mn_CO7_A1A1A1A2A2D1D2-T-xqc.log	-3967.602128	34.96
137	256-3_b_Mn_CO7_A1A1A2A2D1D2D1-T-xqc.log	-3967.602128	34.96
138	276-1_a_Mn_CO7_A1A1A2A2BD1D1-T-xqc.log	-3967.602128	34.96
139	291-3_a_Mn_CO7_A1A1A2A2BBD1-T-xqc.log	-3967.602128	34.96
140	103-1_b_Mn_CO7_A1A1A1A2BBD2-T-xqc.log	-3967.602127	34.96
141	111-3_a_Mn_CO7_A1A1A1A2A2BD2-T-xqc.log	-3967.602127	34.96
142	117-3_b_Mn_CO7_A1A1A1A2BBB-T-xqc.log	-3967.602127	34.96
143	123-3_a_Mn_CO7_A1A1A1A2A2A2B-T-xqc.log	-3967.602127	34.96
144	129-3_a_Mn_CO7_A1A1A1A1A2A2D1-T-xqc.log	-3967.602127	34.96
145	135-3_a_Mn_CO7_A1A1A1A2BD1D2-T-xqc.log	-3967.602127	34.96
146	143-1_b_Mn_CO7_A1A1A1A2A2D1D2-T-xqc.log	-3967.602127	34.96
147	152-1_a_Mn_CO7_A1A1A1A2A2BD2-T-xqc-freq.log	-3967.602127	34.96
148	165-1_b_Mn_CO7_A1A1A1A2A2D1D2-T-xqc-freq.log	-3967.602127	34.96
149	170-1_b_Mn_CO7_A1A1A1A2BBD2-T-xqc.log	-3967.602127	34.96
150	171-3_a_Mn_CO7_A1A1A1A1A2A2D2-T-xqc.log	-3967.602127	34.96
151	173-3_b_Mn_CO7_A1A1A1A2A2BB-T-xqc.log	-3967.602127	34.96
152	176-3_a_Mn_CO7_A1A1A1A2A2BB-T.log	-3967.602127	34.96
153	178-3_a_Mn_CO7_A1A1A1A2A2D1D2-T.log	-3967.602127	34.96
154	182-3_b_Mn_CO7_A1A1A1A2A2D2D2-T-xqc.log	-3967.602127	34.96
155	184-3_b_Mn_CO7_A1A1A1A2BD2B-T-xqc.log	-3967.602127	34.96
156	189-3_a_Mn_CO7_A1A1A1A2A2A2B-T-xqc.log	-3967.602127	34.96
157	193-3_b_Mn_CO7_A1A1A1A2A2BD1-T-xqc.log	-3967.602127	34.96
158	194-3_a_Mn_CO7_A1A1A1A2A2BD1-T-xqc.log	-3967.602127	34.96
159	197-3_a_Mn_CO7_A1A1A1A1A2A2D1-T-xqc.log	-3967.602127	34.96
160	223-3_b_Mn_CO7_A1A1A1A2BD2D2-T-xqc.log	-3967.602127	34.96
161	224-3_b_Mn_CO7_A1A1A1A2D2BD2-T-xqc.log	-3967.602127	34.96
162	225-3_b_Mn_CO7_A1A1A2A2BBD1-T-xqc.log	-3967.602127	34.96
163	38-1_b_Mn_CO7_A1A1A1A2A2BD2-T-xqc.log	-3967.602127	34.96
164	118-3_b_Mn_CO7_A1A1A1A2BD2B-T-xqc.log	-3967.602126	34.96
165	121-3_b_Mn_CO7_A1A1A1A2A2BD1-T-xqc.log	-3967.602126	34.96
166	196-3_b_Mn_CO7_A1A1A1A2A2D1D2-T-xqc.log	-3967.602126	34.96
167	220-3_a_Mn_CO7_A1A1A1A2BD2D2-T-xqc-freq.log	-3967.602126	34.96
168	43-1_a_Mn_CO7_A1A1A2A2BBB-T-xqc.log	-3967.602126	34.96
169	75-1_b_Mn_CO7_A1A1A1A2BD2B-T-xqc.log	-3967.602126	34.96
170	110-3_a_Mn_CO7_A1A1A1A2A2BB-T.log	-3967.602125	34.96
171	116-3_b_Mn_CO7_A1A1A1A2A2D2D2-T.log	-3967.602125	34.96
172	109-3_a_Mn_CO7_A1A1A1A1A2A2B-T.log	-3967.602123	34.97
173	175-3_a_Mn_CO7_A1A1A1A1A2A2B-T.log	-3967.602123	34.97
174	110-3_a_Mn_CO7_A1A1A1A2A2BB-Q-xqc.log	-3967.602047	35.01
175	118-3_b_Mn_CO7_A1A1A1A2BD2B-Q-xqc.log	-3967.602047	35.01

176	105-3_a_Mn_CO7_A1A1A1A2BD1B-Q-xqc.log	-3967.602045	35.02
177	117-3_b_Mn_CO7_A1A1A1A2BBB-Q-xqc-1-freq.log	-3967.602045	35.02
178	117-3_b_Mn_CO7_A1A1A1A2BBB-Q-xqc-1.log	-3967.602045	35.02
179	123-3_a_Mn_CO7_A1A1A1A2A2A2B-Q-xqc-freq.log	-3967.602045	35.02
180	170-1_b_Mn_CO7_A1A1A1A2BBD2-Q-xqc.log	-3967.602045	35.02
181	189-3_a_Mn_CO7_A1A1A1A2A2A2B-Q-xqc-freq.log	-3967.602045	35.02
182	295-3_a_Mn_CO7_A1A1A2A2D1BD2-Q-xqc-freq.log	-3967.602045	35.02
183	111-3_a_Mn_CO7_A1A1A1A2A2BD2-Q-xqc.log	-3967.602044	35.02
184	129-3_a_Mn_CO7_A1A1A1A1A2A2D1-Q.log	-3967.602044	35.02
185	177-3_a_Mn_CO7_A1A1A1A2A2BD2-Q-xqc-freq.log	-3967.602044	35.02
186	198-3_b_Mn_CO7_A1A1A1A2A2D1D1-Q-xqc.log	-3967.602044	35.02
187	20-1_a_Mn_CO7_A1A1A1A2BBD2-Q-xqc.log	-3967.602044	35.02
188	208-3_b_Mn_CO7_A1A1A1A2BD1B-Q-xqc-f.log	-3967.602044	35.02
189	232-1_a_Mn_CO7_A1A1A1A2BD1B-Q-xqc.log	-3967.602044	35.02
190	39-1_a_Mn_CO7_A1A1A1A2BBB-Q-xqc.log	-3967.602044	35.02
191	103-1_b_Mn_CO7_A1A1A1A2BBD2-Q-xqc.log	-3967.602043	35.02
192	113-3_a_Mn_CO7_A1A1A1A2BD2B-Q-xqc-freq.log	-3967.602043	35.02
193	131-3_b_Mn_CO7_A1A1A1A2A2D1D1-Q-xqc.log	-3967.602043	35.02
194	137-1_b_Mn_CO7_A1A1A1A2BBB-Q.log	-3967.602043	35.02
195	154-1_b_Mn_CO7_A1A1A1A2BBB-Q-xqc-freq.log	-3967.602043	35.02
196	172-3_a_Mn_CO7_A1A1A1A2BD1B-Q-xqc.log	-3967.602043	35.02
197	183-3_b_Mn_CO7_A1A1A1A2BBB-Q-xqc-1.log	-3967.602043	35.02
198	211-1_b_Mn_CO7_A1A1A1A1A2A2D2-Q-xqc.log	-3967.602043	35.02
199	218-3_b_Mn_CO7_A1A1A1A2A2BD2-Q-xqc-freq.log	-3967.602043	35.02
200	222-3_b_Mn_CO7_A1A1A1A2BBD2-Q-xqc-freq.log	-3967.602042	35.02
201	146-1_b_Mn_CO7_A1A1A1A2BBB-Q.log	-3967.602041	35.02
202	176-3_a_Mn_CO7_A1A1A1A2A2BB-Q.log	-3967.602041	35.02
203	151-1_b_Mn_CO7_A1A1A1A2BBD2-Q.log	-3967.601926	35.09
204	52-2_a_Mn_CO7_A1A1A1pA2BBB-T-xqc-freq.log	-3967.601887	35.11
205	55-2_b_Mn_CO7_A1A1A1pA2BBB-T-xqc.log	-3967.601887	35.11
206	130-3_b_Mn_CO7_A1A1A1A1A2A2D1-Q-xqc-freq.log	-3967.601795	35.17
207	134-3_a_Mn_CO7_A1A1A1A2A2D1D1-Q-xqc-freq.log	-3967.601795	35.17
208	262-2_a_Mn_CO7_A1A1A1pA2BD1D1-T-xqc-rupt.log	-3967.601477	35.37
209	16-2_b_Mn_CO7_A1A1A1pA2pA2D1pD2-T-xqc-rupt.log	-3967.601467	35.38
210	12-2_a_Mn_CO7_A1A1A1pA2pA2D1pD2-T-xqc-rupt.log	-3967.601452	35.39
211	141-2_b_Mn_CO7_A1A1A1pA2BBD1-T.log	-3967.600912	35.73
212	149-3_a_Mn_CO7_A1A1A1A2A2D1D1-Q-freq.log	-3967.600816	35.79
213	131-3_b_Mn_CO7_A1A1A1A2A2D1D1-T-xqc-freq.log	-3967.599988	36.31
214	134-3_a_Mn_CO7_A1A1A1A2A2D1D1-T-xqc-freq.log	-3967.599988	36.31
215	198-3_b_Mn_CO7_A1A1A1A2A2D1D1-T-xqc-freq.log	-3967.599988	36.31
216	149-3_a_Mn_CO7_A1A1A1A2A2D1D1-T-xqc.log	-3967.599987	36.31
217	1-2_b_Mn_CO7_A1A1A1pA2pA2pA2D1-T.log	-3967.598258	37.39
218	7-1_a_Mn_CO7_A1A1A1A1A2A2A2-T.log	-3967.598258	37.39
219	0-1_b_Mn_CO7_A1A1A1A1A2A2A2-T.log	-3967.598257	37.39
220	136-1_b_Mn_CO7_A1A1A1A1A2A2B-T.log	-3967.598257	37.39

221	153-1_a_Mn_CO7_A1A1A1A1A2A2B-T.log	-3967.598257	37.39
222	199-1_a_Mn_CO7_A1A1A1A1A2A2B-T-xqc.log	-3967.598257	37.39
223	132-1_a_Mn_CO7_A1A1A1A1A2A2B-T.log	-3967.598255	37.39
224	2-2_b_Mn_CO7_A1A1A1A2A2A2B-T.log	-3967.598255	37.39
225	70-1_b_Mn_CO7_A1A1A1A2A2A2B-T.log	-3967.598255	37.39
226	6-1_a_Mn_CO7_A1A1A1A2A2A2B-T.log	-3967.598254	37.39
227	147-1_b_Mn_CO7_A1A1A1A1A2A2B-T.log	-3967.598250	37.40
228	15-2_b_Mn_CO7_pA1pA1pA1A2BD2D2-T-xqc-1.log	-3967.598148	37.46
229	99-2_b_Mn_CO7_A1A1A1pA2pD2BpD2-T-xqc.log	-3967.598139	37.47
230	203-2_b_Mn_CO7_A1A1A1pA2pD2BpD2-T-xqc.log	-3967.598138	37.47
231	130-3_b_Mn_CO7_A1A1A1A1A2A2D1-T.log	-3967.598056	37.52
232	155-1_b_Mn_CO7_A1A1A1A1A2A2D1-T.log	-3967.598056	37.52
233	195-3_b_Mn_CO7_A1A1A1A1A2A2D1-T.log	-3967.598056	37.52
234	144-1_b_Mn_CO7_A1A1A1A1A2A2D1-T.log	-3967.598055	37.52
235	139-1_b_Mn_CO7_A1A1A1A1A2A2D1-T.log	-3967.598054	37.52
236	2_a_Mn_CO7_A1A1pA2pA2BD1D1----111	-3967.597556	37.83
237	2_b_Mn_CO7_A1A1pA2pA2BD1D1----183	-3967.597555	37.83
238	2_b_Mn_CO7_A1A1pA2pA2D1D1D1----186	-3967.597554	37.83
239	51-2_a_Mn_CO7_A1A1A1A2A2A2B-T-freq.log	-3967.597549	37.84
240	218-3_b_Mn_CO7_A1A1A1A2A2BD2-T-freq.log	-3967.596672	38.39
241	69-2_a_Mn_CO7_A1A1A1A1pA2pA2pD2-T.log	-3967.596628	38.41
242	20-1_a_Mn_CO7_A1A1A1A2BBD2-T-xqc-freq.log	-3967.595149	39.34
243	27-1_a_Mn_CO7_A1A1A1A1A2A2D2--T.log	-3967.595149	39.34
244	107-3_b_Mn_CO7_A1A1A1A2A2D1D2-T.log	-3967.595148	39.34
245	293-3_a_Mn_CO7_A1A1A1A1A2A2A2-T.log	-3967.595148	39.34
246	35-1_b_Mn_CO7_A1A1A1A2D1BD2-T-xqc.log	-3967.595147	39.34
247	296-3_a_Mn_CO7_A1A1A2BBBB-T-xqc.log	-3967.595145	39.34
248	39-1_a_Mn_CO7_A1A1A1A2BBB-T-xqc.log	-3967.595145	39.34
249	211-1_b_Mn_CO7_A1A1A1A1A2A2D2-T-xqc.log	-3967.595142	39.35
250	65-2_b_Mn_CO7_A1A1pA2BBBB-Q-xqc-freq.log	-3967.593673	40.27
251	11-2_b_Mn_CO7_pA1pA1pA1A2A2BD2-Q-xqc.log	-3967.593512	40.37
252	2-2_b_Mn_CO7_A1A1A1A2A2A2B-Q.log	-3967.593512	40.37
253	6-1_a_Mn_CO7_A1A1A1A2A2A2B-Q.log	-3967.593512	40.37
254	70-1_b_Mn_CO7_A1A1A1A2A2A2B-Q.log	-3967.593512	40.37
255	42-1_a_Mn_CO7_A1A1A1A2BD2D2-Q-xqc.log	-3967.593511	40.37
256	71-1_b_Mn_CO7_A1A1A1A2A2BB-Q-xqc.log	-3967.593511	40.37
257	45-2_a_Mn_CO7_A1A1pA2BBBB-Q-xqc-freq.log	-3967.593510	40.37
258	51-2_a_Mn_CO7_A1A1A1A2A2A2B-Q.log	-3967.593510	40.37
259	8-1_b_Mn_CO7_A1A1A1A2A2A2D1-Q-xqc.log	-3967.593510	40.37
260	88-1_a_Mn_CO7_A1A1A1A2D1D1D1-Q.log	-3967.593509	40.37
261	73-1_a_Mn_CO7_A1A1A1A2A2BB-Q-xqc-freq.log	-3967.593506	40.37
262	1-2_b_Mn_CO7_A1A1A1pA2pA2pA2D1-Q.log	-3967.593225	40.55
263	50-2_a_Mn_CO7_A1A1A1A1pA2pA2pA2-Q.log	-3967.593225	40.55
264	60-2_a_Mn_CO7_A1A1A1pA2pA2pA2D1-Q-xqc.log	-3967.593225	40.55
265	57-2_b_Mn_CO7_A1A1A1A1pA2pA2pA2-Q.log	-3967.593224	40.55

266	7-1_a_Mn_CO7_A1A1A1A1A2A2A2-Q.log	-3967.593213	40.56
267	151-1_b_Mn_CO7_A1A1A1A2BBD2-T-xqc.log	-3967.593082	40.64
268	19-3_b_Mn_CO7_A1A1A1A2D1BD2-T-xqc-1.log	-3967.593082	40.64
269	105-3_a_Mn_CO7_A1A1A1A2BD1B-T.log	-3967.593065	40.65
270	183-3_b_Mn_CO7_A1A1A1A2BBB-T.log	-3967.593059	40.65
271	2_a_Mn_CO7_A1A1A1A1pA2pA2D1----80	-3967.593044	40.66
272	2_a_Mn_CO7_A1A1A1pA2pA2D1D1----99	-3967.593044	40.66
273	2_b_Mn_CO7_A1A1A1pA2pA2BD1----169	-3967.593044	40.66
274	2_b_Mn_CO7_A1A1A1A1pA2pA2D1----152	-3967.593043	40.66
275	168-1_a_Mn_CO7_A1A1A1A2A2D2D2-Q-xqc-freq.log	-3967.593027	40.67
276	101-1_a_Mn_CO7_A1A1A1A2A2D2D2-Q-xqc-freq.log	-3967.592831	40.80
277	108-1_a_Mn_CO7_A1A1A1A2A2BD2-T-xqc.log	-3967.592780	40.83
278	174-1_a_Mn_CO7_A1A1A1A2A2BD2-T-xqc.log	-3967.592780	40.83
279	21-3_a_Mn_CO7_A1A1A1A2A2D2D2-T-xqc-1.log	-3967.592780	40.83
280	265-2_b_Mn_CO7_pA1pA1A2A2BpD1B-T-xqc.log	-3967.592621	40.93
281	61-2_a_Mn_CO7_pA1pA1pA1A2A2BB-Q-xqc.log	-3967.592430	41.05
282	241-2_b_Mn_CO7_pA1pA1pA1pA1A2A2D2-T.log	-3967.592339	41.11
283	5-1_b_Mn_CO7_A1A1A2A2BBB-Q-xqc-freq.log	-3967.592237	41.17
284	150-1_a_Mn_CO7_A1A1A1A2A2D2D2-Q-xqc-freq.log	-3967.592236	41.17
285	43-1_a_Mn_CO7_A1A1A2A2BBB-Q-xqc.log	-3967.592236	41.17
286	14-2_a_Mn_CO7_A1A1A1pA2pA2pD2pD2-T-xqc.log	-3967.591746	41.48
287	140-1_a_Mn_CO7_A1A1A2A2BD1B--T-xqc.log	-3967.591745	41.48
288	156-1_a_Mn_CO7_A1A1A2A2BD1B-T.log	-3967.591745	41.48
289	42-1_a_Mn_CO7_A1A1A1A2BD2D2-T-xqc.log	-3967.591745	41.48
290	73-1_a_Mn_CO7_A1A1A1A2A2BB-T-xqc.log	-3967.591745	41.48
291	32-1_a_Mn_CO7_A1A1A1A2BBD1-T-xqc.log	-3967.591182	41.83
292	41-1_a_Mn_CO7_A1A1A1A2A2A2D1-T-xqc.log	-3967.591178	41.83
293	8-1_b_Mn_CO7_A1A1A1A2A2A2D1-T.log	-3967.591178	41.83
294	88-1_a_Mn_CO7_A1A1A1A2D1D1D1-T.log	-3967.591178	41.83
295	85-1_b_Mn_CO7_A1A1A1A2D1D1D1-T.log	-3967.591177	41.83
296	95-1_b_Mn_CO7_A1A1A1A2D1D2D1-T.log	-3967.591177	41.83
297	71-1_b_Mn_CO7_A1A1A1A2A2BB-T-xqc.log	-3967.591176	41.84
298	138-1_b_Mn_CO7_A1A1A1A2BBD1-T.log	-3967.591172	41.84
299	108-1_a_Mn_CO7_A1A1A1A2A2BD2-Q-xqc-freq.log	-3967.591006	41.94
300	116-3_b_Mn_CO7_A1A1A1A2A2D2D2-Q-xqc-freq.log	-3967.591005	41.94
301	174-1_a_Mn_CO7_A1A1A1A2A2BD2-Q-xqc-freq.log	-3967.591004	41.94
302	38-1_b_Mn_CO7_A1A1A1A2A2BD2-Q-xqc-freq.log	-3967.591004	41.94
303	107-3_b_Mn_CO7_A1A1A1A2A2D1D2-Q-xqc-freq.log	-3967.591003	41.94
304	112-3_a_Mn_CO7_A1A1A1A2A2D1D2-Q-xqc-freq.log	-3967.591003	41.94
305	184-3_b_Mn_CO7_A1A1A1A2BD2B-Q-xqc-freq.log	-3967.591003	41.94
306	115-3_b_Mn_CO7_A1A1A1A2A2A2B-Q-xqc-freq.log	-3967.591000	41.95
307	196-3_b_Mn_CO7_A1A1A1A2A2D1D2-Q-xqc-freq.log	-3967.591000	41.95
308	223-3_b_Mn_CO7_A1A1A1A2BD2D2-Q-xqc.log	-3967.591000	41.95
309	100-3_a_Mn_CO7_A1A1A1A2D2D2D2-Q-xqc-freq.log	-3967.590999	41.95
310	224-3_b_Mn_CO7_A1A1A1A2D2BD2-Q-xqc-freq.log	-3967.590999	41.95

311	181-3_b_Mn_CO7_A1A1A1A2A2A2B-Q-xqc-freq.log	-3967.590998	41.95
312	178-3_a_Mn_CO7_A1A1A1A2A2D1D2-Q-xqc-freq.log	-3967.590997	41.95
313	133-3_b_Mn_CO7_A1A1A1A1A2A2B-Q.log	-3967.590996	41.95
314	200-3_b_Mn_CO7_A1A1A1A1A2A2B-Q.log	-3967.590996	41.95
315	21-3_a_Mn_CO7_A1A1A1A2A2D2D2-Q.log	-3967.590996	41.95
316	109-3_a_Mn_CO7_A1A1A1A1A2A2B-Q.log	-3967.590995	41.95
317	121-3_b_Mn_CO7_A1A1A1A2A2BD1-Q-xqc.log	-3967.590995	41.95
318	175-3_a_Mn_CO7_A1A1A1A1A2A2B-Q.log	-3967.590995	41.95
319	179-3_a_Mn_CO7_A1A1A1A2BD2B-Q.log	-3967.590995	41.95
320	106-3_b_Mn_CO7_A1A1A1A2A2BB-Q.log	-3967.590994	41.95
321	173-3_b_Mn_CO7_A1A1A1A2A2BB-Q.log	-3967.590994	41.95
322	135-3_a_Mn_CO7_A1A1A1A2BD1D2-Q-xqc.log	-3967.590993	41.95
323	193-3_b_Mn_CO7_A1A1A1A2A2BD1-Q.log	-3967.590993	41.95
324	194-3_a_Mn_CO7_A1A1A1A2A2BD1-Q.log	-3967.590991	41.95
325	2_b_Mn_CO7_pA1pA1pA1A2pD1BD2----215	-3967.590489	42.27
326	158-1_a_Mn_CO7_A1A1A1A2A2BD1-T-xqc.log	-3967.590085	42.52
327	115-3_b_Mn_CO7_A1A1A1A2A2A2B-T-xqc.log	-3967.590084	42.52
328	162-1_b_Mn_CO7_A1A1A1A2A2BD1-Q-rupt.log	-3967.589923	42.62
329	201-1_b_Mn_CO7_A1A1A1A2A2BD1-Q.log	-3967.589923	42.62
330	146-1_b_Mn_CO7_A1A1A1A2A2BD1-Q.log	-3967.589922	42.62
331	138-1_b_Mn_CO7_A1A1A1A2BBD1-Q.log	-3967.589920	42.62
332	149-1_b_Mn_CO7_A1A1A1A2BBD1-Q.log	-3967.589918	42.62
333	32-1_a_Mn_CO7_A1A1A1A2BBD1-Q-xqc.log	-3967.589918	42.62
334	181-3_b_Mn_CO7_A1A1A1A2A2A2B-T.log	-3967.589915	42.63
335	125-2_b_Mn_CO7_A1A1A1pA2pA2BD1-T.log	-3967.589602	42.82
336	3_a_Mn_CO7_A1A1A1A2A2A2B----226	-3967.588198	43.70
337	1_a_Mn_CO7_A1A1A1A2A2D1D2----11	-3967.588197	43.70
338	101-1_a_Mn_CO7_A1A1A1A2A2D2D2-T-xqc-freq.log	-3967.588082	43.78
339	168-1_a_Mn_CO7_A1A1A1A2A2D2D2-T-xqc.log	-3967.588082	43.78
340	3_a_Mn_CO7_A1A1A1A1A2A2D1----224	-3967.588057	43.79
341	3_b_Mn_CO7_A1A1A1A1A2A2D1----263	-3967.588057	43.79
342	3_b_Mn_CO7_A1A1A1A2A2D1D1----270	-3967.588056	43.79
343	1_a_Mn_CO7_A1A1A1A1A2A2B----2	-3967.588053	43.80
344	3_b_Mn_CO7_A1A1A1A1A2A2B----262	-3967.588053	43.80
345	3_a_Mn_CO7_A1A1A1A2A2D1D1----231	-3967.58805	43.80
346	1_a_Mn_CO7_A1A1A1A2D1BD2----21	-3967.58733	44.25
347	1_b_Mn_CO7_A1A1A1A2D1BD2----60	-3967.58733	44.25
348	3_a_Mn_CO7_A1A1A1A2BD1D2----239	-3967.58733	44.25
349	2_b_Mn_CO7_A1A1A1pA2pA2D1D1-COdeplasat----171	-3967.586357	44.86
350	2_b_Mn_CO7_A1A1A1pA2pD2D1pD2-COdeplasat----176	-3967.586203	44.96
351	2_a_Mn_CO7_A1A1A1pA2pD2D1pD2-COdeplasat----104	-3967.586191	44.96
352	2_b_Mn_CO7_A1A1A1pA2BD1pD2-COdeplasat----161	-3967.586119	45.01
353	248-3_a_Mn_CO7_A1A1A1A2BD1D1-Q-xqc-rupt.log	-3967.585814	45.20
354	237-3_b_Mn_CO7_A1A1A1A2D1D1D2-Q-xqc-rupt.log	-3967.585804	45.21
355	180-3_a_Mn_CO7_A1A1A1A2D1D2D2-Q-xqc-rupt.log	-3967.585590	45.34

356	69-2_a_Mn_CO7_A1A1A1A1pA2pA2pD2-Q.log	-3967.584668	45.92
357	11-2_b_Mn_CO7_pA1pA1pA1A2A2BD2-T-xqc.log	-3967.584641	45.94
358	40-1_b_Mn_CO7_A1A1A1A2A2D2D2-Q-freq.log	-3967.584553	45.99
359	2_b_Mn_CO7_A1A1A1pA2BD1B----159	-3967.58407	46.29
360	279-1_b_Mn_CO7_A1A1A2BBBB-Q-xqc-rupt.log	-3967.583988	46.35
361	53-2_a_Mn_CO7_A1A1A1pA2pA2BpD2-T-xqc.log	-3967.583755	46.49
362	44-2_b_Mn_CO7_A1A1A1pA2pA2BpD2-T-xqc-freq.log	-3967.583754	46.49
363	1_a_Mn_CO7_A1A1A1A1A2A2D2----4	-3967.583198	46.84
364	1_b_Mn_CO7_A1A1A1A1A2A2B----41	-3967.583198	46.84
365	1_b_Mn_CO7_A1A1A1A2BBB----52	-3967.583198	46.84
366	3_b_Mn_CO7_A1A1A1A1A2A2A2----261	-3967.583198	46.84
367	1_a_Mn_CO7_A1A1A1A1A2A2D1----3	-3967.582209	47.46
368	1_b_Mn_CO7_A1A1A1A1A2A2D1----42	-3967.582208	47.46
369	49-2_a_Mn_CO7_A1A1A1pA2BpD2B-Q-xqc-freq.log	-3967.581051	48.19
370	249-3_b_Mn_CO7_A1A1A1A2BD1D1-Q-xqc-rupt.log	-3967.579942	48.88
371	1_a_Mn_CO7_A1A1A2A2BBD1----30	-3967.57957	49.12
372	1_a_Mn_CO7_A1A1A2A2BD1B----31	-3967.57957	49.12
373	1_b_Mn_CO7_A1A1A2A2BD1B----70	-3967.57957	49.12
374	120-3_a_Mn_CO7_A1A1A1A2A2BD1-Q-freq.log	-3967.579007	49.47
375	195-3_b_Mn_CO7_A1A1A1A1A2A2D1-Q-freq.log	-3967.577542	50.39
376	155-1_b_Mn_CO7_A1A1A1A1A2A2D1-Q-xqc.log	-3967.576364	51.13
377	204-2_b_Mn_CO7_A1A1A1pA2pD2pD2pD2-T-xqc-rupt.log	-3967.576334	51.15
378	122-3_b_Mn_CO7_A1A1A1A1A2A2D2-T.log	-3967.575491	51.68
379	192-3_b_Mn_CO7_A1A1A1A1A2A2D2-T.log	-3967.575491	51.68
380	1_a_Mn_CO7_A1A1A1A2D2D1D2-COdeplasat----27	-3967.575418	51.72
381	241-2_b_Mn_CO7_pA1pA1pA1pA1A2A2D2-Q.log	-3967.575163	51.88
382	277-1_a_Mn_CO7_A1A1A2BBBB-Q-xqc-freq.log	-3967.575161	51.89
383	177-3_a_Mn_CO7_A1A1A1A2A2BD2-T-freq.log	-3967.575056	51.95
384	3_a_Mn_CO7_A1A1A1A2BD1D1-COdeplasat----238	-3967.575044	51.96
385	237-3_b_Mn_CO7_A1A1A1A2D1D1D2-T-xqc-rupt.log	-3967.574920	52.04
386	3_b_Mn_CO7_A1A1A1A2BD1D1-COdeplasat----277	-3967.574882	52.06
387	72-1_b_Mn_CO7_A1A1A1A2BD2D2-T-xqc-rupt.log	-3967.574347	52.40
388	2_a_Mn_CO7_A1A1A1pA2BBD1----85	-3967.574317	52.41
389	2_b_Mn_CO7_A1A1A1pA2BBD1----157	-3967.574317	52.41
390	236-3_a_Mn_CO7_A1A1A1A2D1D1D2-T-xqc-rupt.log	-3967.574076	52.57
391	156-1_a_Mn_CO7_A1A1A2A2BD1B-Q.log	-3967.573873	52.69
392	84-2_b_Mn_CO7_pA1pA1A2BBBB-Q-xqc-freq.log	-3967.573272	53.07
393	270-2_a_Mn_CO7_pA1pA1A2BBBB-Q-xqc.log	-3967.573271	53.07
394	1_a_Mn_CO7_A1A1A1A2A2BD1----8	-3967.571875	53.95
395	1_a_Mn_CO7_A1A1A1A2BBD1----14	-3967.571875	53.95
396	1_a_Mn_CO7_A1A1A2A2BD1D2----33	-3967.571875	53.95
397	1_b_Mn_CO7_A1A1A1A2A2D1D1----49	-3967.571875	53.95
398	1_b_Mn_CO7_A1A1A1A2BBD1----53	-3967.571875	53.95
399	1_a_Mn_CO7_A1A1A1A2A2D1D1----10	-3967.571874	53.95

400	1_a_Mn_CO7_A1A1A2A2D1D1D1----36	-3967.571874	53.95
401	1_b_Mn_CO7_A1A1A1A2A2BD1----47	-3967.571874	53.95
402	1_b_Mn_CO7_A1A1A1A2A2D1D2----50	-3967.571873	53.95
403	2_a_Mn_CO7_A1A1A1pA2pD2BpD2----103	-3967.571029	54.48
404	2_b_Mn_CO7_A1A1A1pA2pD2BpD2----175	-3967.571029	54.48
405	2_b_Mn_CO7_A1A1A1pA2pD2pD2pD2----177	-3967.571029	54.48
406	2_a_Mn_CO7_A1A1A1pA2pD2pD2pD2----105	-3967.571028	54.48
407	2_a_Mn_CO7_pA1pA1pA1A2BBpD1----135	-3967.571026	54.48
408	1_b_Mn_CO7_A1A1A1A2BD1B-COdeplasat----55	-3967.570929	54.54
409	2_b_Mn_CO7_pA1pA1pA1A2D2pD1D2-COdeplasat----214	-3967.570569	54.77
410	2_a_Mn_CO7_pA1pA1pA1A2D2pD1D2-COdeplasat----143	-3967.570563	54.77
411	2_a_Mn_CO7_A1A1A1pA2BD1B----87	-3967.569916	55.18
412	3_b_Mn_CO7_A1A1A1A2BD1B----276	-3967.569158	55.65
413	3_a_Mn_CO7_A1A1A1A2D2D1D2----248	-3967.569157	55.65
414	41-1_a_Mn_CO7_A1A1A1A2A2A2D1-Q-xqc.log	-3967.569040	55.73
415	74-2_a_Mn_CO7_pA1pA1pA1A2A2A2pD1-Q-xqc.log	-3967.569040	55.73
416	17-2_b_Mn_CO7_pA1pA1pA1A2A2A2pD1-Q-freq.log	-3967.568572	56.02
417	2_b_Mn_CO7_pA1pA1pA1A2BpD1D2----210	-3967.568046	56.35
418	2_a_Mn_CO7_pA1pA1pA1A2pD1D2D2-COdeplasat----145	-3967.567667	56.59
419	267-2_a_Mn_CO7_pA1pA1pA1A2BpD1B-Q-xqc-rupt.log	-3967.566662	57.22
420	1_b_Mn_CO7_A1A1A1A1A2A2D2----43	-3967.566229	57.49
421	3_a_Mn_CO7_A1A1A1A2A2A2D1----227	-3967.566209	57.50
422	3_b_Mn_CO7_A1A1A1A2A2A2D1----266	-3967.566209	57.50
423	3_b_Mn_CO7_A1A1A2A2D1D1D1----296	-3967.566209	57.50
424	3_a_Mn_CO7_A1A1A2A2BBB----250	-3967.566208	57.50
425	3_a_Mn_CO7_A1A1A2A2BD1D1----253	-3967.566208	57.50
426	3_b_Mn_CO7_A1A1A2A2D1D1D2----297	-3967.566208	57.50
427	2_b_Mn_CO7_pA1pA1pA1A2BBpD1-COdeplasat----206	-3967.566189	57.52
428	268-2_a_Mn_CO7_pA1pA1pA1pA1A2A2B-T.log	-3967.564973	58.28
429	247-1_a_Mn_CO7_A1A1A1A2D2D1D2-Q.log	-3967.564094	58.83
430	279-1_b_Mn_CO7_A1A1A2BBBB-T-xqc.log	-3967.563875	58.97
431	270-2_a_Mn_CO7_pA1pA1A2BBBB-T-xqc.log	-3967.563874	58.97
432	277-1_a_Mn_CO7_A1A1A2BBBB-T-xqc.log	-3967.563873	58.97
433	84-2_b_Mn_CO7_pA1pA1A2BBBB-T-xqc.log	-3967.563872	58.97
434	3_b_Mn_CO7_A1A1A1A2A2BD2----269	-3967.562965	59.54
435	3_a_Mn_CO7_A1A1A1A2BBD2----236	-3967.562964	59.54
436	3_a_Mn_CO7_A1A1A1A2BD2D2----241	-3967.562964	59.54
437	3_a_Mn_CO7_A1A1A1A2D2BD2----247	-3967.562964	59.54
438	3_b_Mn_CO7_A1A1A1A2BBD2----275	-3967.562964	59.54
439	3_b_Mn_CO7_A1A1A1A2BD2D2----280	-3967.562964	59.54
440	3_b_Mn_CO7_A1A1A1A2D2BD2----286	-3967.562964	59.54
441	3_b_Mn_CO7_A1A1A2A2BBD1----290	-3967.562963	59.54
442	2_a_Mn_CO7_pA1pA1A2A2pD1pD1pD1----124	-3967.562011	60.14
443	2_a_Mn_CO7_pA1pA1pA1A2A2pD1pD1----132	-3967.562011	60.14
444	197-3_a_Mn_CO7_A1A1A1A1A2A2D1-Q-freq.log	-3967.561654	60.36

445	2_a_Mn_CO7_pA1pA1pA1A2pD1pD1D2-COdeplasat----147	-3967.56156	60.42
446	2_b_Mn_CO7_A1A1A1pA2BpD2B----162	-3967.561118	60.70
447	2_a_Mn_CO7_pA1pA1pA1A2BpD1D2----139	-3967.56091	60.83
448	74-2_a_Mn_CO7_pA1pA1pA1A2A2A2pD1-T-freq.log	-3967.560748	60.93
449	2_b_Mn_CO7_pA1pA1pA1A2pD1pD1D2-COdeplasat----218	-3967.559902	61.46
450	235-2_a_Mn_CO7_A1A1A1pA2BBpD2-T-xqc.log	-3967.559522	61.70
451	1_a_Mn_CO7_A1A1A1A2BD1B----16	-3967.559214	61.89
452	2_a_Mn_CO7_pA1pA1pA1A2pD1BD2----144	-3967.559007	62.02
453	2_b_Mn_CO7_pA1pA1A2A2pD1pD1pD1----196	-3967.558974	62.04
454	216-3_a_Mn_CO7_A1A1A2A2BD1D1-Q-xqc.log	-3967.558417	62.39
455	214-3_b_Mn_CO7_A1A1A2A2D1D1D1-Q-xqc.log	-3967.558376	62.42
456	256-3_b_Mn_CO7_A1A1A2A2D1D2D1-Q-xqc.log	-3967.558376	62.42
457	257-3_a_Mn_CO7_A1A1A2A2BD1B-Q.log	-3967.558376	62.42
458	296-3_a_Mn_CO7_A1A1A2BBBB-Q-xqc.log	-3967.558376	62.42
459	212-3_a_Mn_CO7_A1A1A1A2A2A2D1-Q.log	-3967.558375	62.42
460	213-3_b_Mn_CO7_A1A1A1A2A2A2D1-Q.log	-3967.558375	62.42
461	215-3_a_Mn_CO7_A1A1A2A2BBB-Q-xqc.log	-3967.558375	62.42
462	217-3_b_Mn_CO7_A1A1A2A2D1D1D2-Q-xqc.log	-3967.558375	62.42
463	225-3_b_Mn_CO7_A1A1A2A2BBD1-Q-xqc.log	-3967.558375	62.42
464	258-3_a_Mn_CO7_A1A1A2A2D1D1D2-Q-xqc.log	-3967.558375	62.42
465	259-3_b_Mn_CO7_A1A1A2A2BD1B-Q-xqc.log	-3967.558375	62.42
466	261-3_b_Mn_CO7_A1A1A2A2BD1D2-Q-xqc.log	-3967.558375	62.42
467	292-3_b_Mn_CO7_A1A1A2A2D1BD2-Q-xqc.log	-3967.558375	62.42
468	260-3_b_Mn_CO7_A1A1A2A2BD1D1-Q-xqc.log	-3967.558374	62.42
469	297-3_b_Mn_CO7_A1A1A2BBBB-Q-xqc.log	-3967.558373	62.42
470	291-3_a_Mn_CO7_A1A1A2A2BBD1-Q.log	-3967.558364	62.43
471	104-3_a_Mn_CO7_A1A1A1A1A2A2D2-Q.log	-3967.557957	62.68
472	171-3_a_Mn_CO7_A1A1A1A1A2A2D2-Q.log	-3967.557957	62.68
473	152-1_a_Mn_CO7_A1A1A1A2A2BD2-Q-xqc.log	-3967.557953	62.68
474	2_a_Mn_CO7_A1A1A1pA2BBpD2----86	-3967.557437	63.01
475	122-3_b_Mn_CO7_A1A1A1A1A2A2D2-Q.log	-3967.556880	63.36
476	192-3_b_Mn_CO7_A1A1A1A1A2A2D2-Q.log	-3967.556880	63.36
477	24-1_a_Mn_CO7_A1A1A1A2A2D1D2-Q-xqc.log	-3967.556127	63.83
478	139-1_b_Mn_CO7_A1A1A1A1A2A2D1-Q.log	-3967.554738	64.70
479	144-1_b_Mn_CO7_A1A1A1A1A2A2D1-Q-xqc.log	-3967.554737	64.70
480	3_a_Mn_CO7_A1A1A1A2D1D1D2-COdeplasat----244	-3967.554736	64.70
481	3_b_Mn_CO7_A1A1A1A2D1D1D2-COdeplasat----283	-3967.554732	64.70
482	13-2_b_Mn_CO7_A1A1A1pA2pA2pD2pD2-Q-xqc.log	-3967.554729	64.71
483	1_b_Mn_CO7_A1A1A2A2D1D2D1-COdeplasat----77	-3967.554415	64.90
484	1_b_Mn_CO7_A1A1A2A2D1D1D1-COdeplasat----75	-3967.553726	65.34
485	2_a_Mn_CO7_pA1pA1pA1pA1A2A2D2----150	-3967.55367	65.37
486	2_b_Mn_CO7_pA1pA1pA1pA1A2A2D2----221	-3967.553669	65.37
487	28-1_a_Mn_CO7_A1A1A1A1A2A2D1-Q.log	-3967.553601	65.41

488	132-1_a_Mn_CO7_A1A1A1A1A2A2B-Q-xqc.log	-3967.553548	65.45
489	136-1_b_Mn_CO7_A1A1A1A1A2A2B-Q-xqc.log	-3967.553548	65.45
490	143-1_b_Mn_CO7_A1A1A1A2A2D1D2-Q-xqc-freq.log	-3967.553548	65.45
491	202-1_b_Mn_CO7_A1A1A1A2A2D1D2-Q-xqc.log	-3967.553548	65.45
492	199-1_a_Mn_CO7_A1A1A1A1A2A2B-Q-xqc.log	-3967.553547	65.45
493	147-1_b_Mn_CO7_A1A1A1A1A2A2B-Q-xqc.log	-3967.553545	65.45
494	153-1_a_Mn_CO7_A1A1A1A1A2A2B-Q.log	-3967.553544	65.45
495	0-1_b_Mn_CO7_A1A1A1A1A2A2A2-Q.log	-3967.553268	65.62
496	63-2_a_Mn_CO7_pA1pA1pA1A2BBB-T-xqc.log	-3967.553240	65.64
497	58-2_b_Mn_CO7_A1A1A1A1pA2pA2B-Q-xqc-freq.log	-3967.552749	65.95
498	66-2_b_Mn_CO7_pA1pA1pA1A2A2D2D2-Q-xqc.log	-3967.552746	65.95
499	48-2_b_Mn_CO7_pA1pA1pA1A2A2BB-Q.log	-3967.552743	65.95
500	1_a_Mn_CO7_A1A1A1A2BD1D2----18	-3967.552557	66.07
501	1_b_Mn_CO7_A1A1A1A2D2D1D2----66	-3967.552557	66.07
502	1_b_Mn_CO7_A1A1A1A2BD1D2----57	-3967.552556	66.07
503	276-1_a_Mn_CO7_A1A1A2A2BD1D1-Q-xqc.log	-3967.552184	66.30
504	278-1_b_Mn_CO7_A1A1A2A2BD1D1-Q.log	-3967.552177	66.31
505	2_a_Mn_CO7_A1A1pA2pA2D1BD1-COdeplasat----113	-3967.552164	66.32
506	2_b_Mn_CO7_A1A1pA2pA2D1BD1-COdeplasat----185	-3967.552116	66.35
507	14-2_a_Mn_CO7_A1A1A1pA2pA2pD2pD2-Q-xqc.log	-3967.551563	66.69
508	297-3_b_Mn_CO7_A1A1A2BBBB-T-xqc.log	-3967.551490	66.74
509	290-3_b_Mn_CO7_A1A1A2A2D1BD1--T-xqc.log	-3967.551489	66.74
510	268-2_a_Mn_CO7_pA1pA1pA1pA1A2A2B-Q.log	-3967.550974	67.06
511	3_b_Mn_CO7_A1A1A2A2D1D2D1----298	-3967.550632	67.28
512	3_a_Mn_CO7_A1A1A2A2BD1B----252	-3967.550631	67.28
513	3_a_Mn_CO7_A1A1A2A2D1D1D2----258	-3967.550631	67.28
514	3_b_Mn_CO7_A1A1A2A2BD1B----291	-3967.550631	67.28
515	3_b_Mn_CO7_A1A1A2A2BD1D1----292	-3967.550631	67.28
516	3_b_Mn_CO7_A1A1A2A2BD1D2----293	-3967.550631	67.28
517	150-1_a_Mn_CO7_A1A1A1A2A2D2D2-T-xqc.log	-3967.549719	67.85
518	2_a_Mn_CO7_A1A1A1pA2BD1D1----88	-3967.549682	67.87
519	2_a_Mn_CO7_A1A1pA2pA2D1D1D1----114	-3967.549682	67.87
520	2_b_Mn_CO7_A1A1A1pA2BD1D1----160	-3967.549682	67.87
521	298-1_b_Mn_CO7_A1A1A1A2D2D2D2-T-xqc-freq.log	-3967.549625	67.91
522	185-3_b_Mn_CO7_A1A1A1A2D1D2D2-T.log	-3967.549485	68.00
523	119-3_b_Mn_CO7_A1A1A1A2D1D2D2-T-xqc.log	-3967.549484	68.00
524	53-2_a_Mn_CO7_A1A1A1pA2pA2BpD2-Q-xqc-freq.log	-3967.548800	68.43
525	44-2_b_Mn_CO7_A1A1A1pA2pA2BpD2-Q-xqc-freq.log	-3967.548799	68.43
526	124-2_b_Mn_CO7_A1A1A1A1pA2pA2D1-Q.log	-3967.547454	69.27
527	188-2_b_Mn_CO7_A1A1A1A1pA2pA2D1-Q.log	-3967.547450	69.27
528	120-3_a_Mn_CO7_A1A1A1A2A2BD1-T-freq.log	-3967.546108	70.12
529	2_b_Mn_CO7_pA1pA1A2A2BpD1B----190	-3967.545875	70.26
530	2_b_Mn_CO7_pA1pA1pA1A2BpD1B----209	-3967.545875	70.26
531	2_a_Mn_CO7_pA1pA1pA1A2BpD1B----138	-3967.545874	70.26
532	2_a_Mn_CO7_pA1pA1pA1pA1A2A2B----149	-3967.545874	70.26

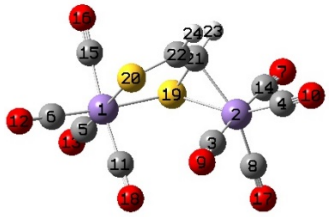
533	56-2_b_Mn_CO7_A1A1A1A1pA2pA2pD2-Q.log	-3967.544457	71.15
534	62-2_a_Mn_CO7_pA1pA1pA1A2A2D2D2-Q-xqc-rupt.log	-3967.544242	71.29
535	219-3_a_Mn_CO7_A1A1A1A2BBD2-Q-xqc.log	-3967.543893	71.51
536	293-3_a_Mn_CO7_A1A1A1A1A2A2A2-Q.log	-3967.543893	71.51
537	216-3_a_Mn_CO7_A1A1A2A2BD1D1-T.log	-3967.543353	71.84
538	261-3_b_Mn_CO7_A1A1A2A2BD1D2-T-xqc.log	-3967.543350	71.85
539	295-3_a_Mn_CO7_A1A1A2A2D1BD2-T-xqc.log	-3967.543350	71.85
540	258-3_a_Mn_CO7_A1A1A2A2D1D1D2-T-xqc.log	-3967.543349	71.85
541	260-3_b_Mn_CO7_A1A1A2A2BD1D1-T-xqc.log	-3967.543349	71.85
542	2_b_Mn_CO7_pA1pA1pA1A2BBB----204	-3967.541803	72.82
543	16-2_b_Mn_CO7_A1A1A1pA2pA2D1pD2-Q-xqc-rupt.log	-3967.541786	72.83
544	2_a_Mn_CO7_pA1pA1A2BBBB----125	-3967.541399	73.07
545	2_a_Mn_CO7_A1A1A2A2D1BD2----107	-3967.541396	73.07
546	2_b_Mn_CO7_pA1pA1pA1A2A2pD1D2----203	-3967.541396	73.07
547	2_a_Mn_CO7_pA1pA1A2A2BpD1pD1----120	-3967.541395	73.07
548	2_a_Mn_CO7_pA1pA1A2A2pD1pD1D2----123	-3967.541395	73.07
549	2_b_Mn_CO7_pA1pA1A2A2BpD1pD1----192	-3967.541395	73.07
550	2_b_Mn_CO7_pA1pA1pA1A2A2BpD1----201	-3967.541395	73.07
551	2_b_Mn_CO7_pA1pA1pA1A2pD1pD1pD1----219	-3967.541395	73.07
552	1_a_Mn_CO7_A1A1A2A2BD1D1----32	-3967.541394	73.07
553	1_a_Mn_CO7_A1A1A2BBBB----39	-3967.541394	73.07
554	1_b_Mn_CO7_A1A1A2A2BD1D1----71	-3967.541394	73.07
555	1_b_Mn_CO7_A1A1A2BBBB----78	-3967.541394	73.07
556	2_a_Mn_CO7_pA1pA1pA1A2BpD1pD1----140	-3967.541394	73.07
557	2_b_Mn_CO7_pA1pA1A2A2pD1pD1D2----195	-3967.541394	73.07
558	2_a_Mn_CO7_pA1pA1pA1A2A2BpD1----129	-3967.541393	73.07
559	2_b_Mn_CO7_pA1pA1pA1A2BpD1pD1----211	-3967.541393	73.07
560	2_a_Mn_CO7_pA1pA1A2A2BpD1B----118	-3967.541392	73.08
561	2_b_Mn_CO7_A1A1A2A2D1BD2----179	-3967.541392	73.08
562	37-2_a_Mn_CO7_A1A1A1A1pA2pA2D1-Q.log	-3967.541152	73.23
563	15-2_b_Mn_CO7_pA1pA1pA1A2BD2D2-Q-xqc-rupt.log	-3967.541089	73.27
564	5-1_b_Mn_CO7_A1A1A2A2BBB-T.log	-3967.540364	73.72
565	257-3_a_Mn_CO7_A1A1A2A2BD1B-T-freq.log	-3967.540001	73.95
566	267-2_a_Mn_CO7_pA1pA1pA1A2BpD1B-T-xqc.log	-3967.539918	74.00
567	212-3_a_Mn_CO7_A1A1A1A2A2A2D1-T.log	-3967.539786	74.08
568	217-3_b_Mn_CO7_A1A1A2A2D1D1D2-T-xqc.log	-3967.539785	74.08
569	213-3_b_Mn_CO7_A1A1A1A2A2A2D1-T.log	-3967.539782	74.09
570	98-3_b_Mn_CO7_A1A1A1A2BD1D2-T-xqc-rupt.log	-3967.539629	74.18
571	148-3_a_Mn_CO7_A1A1A1A2BD1D2-T-xqc.log	-3967.539582	74.21
572	2_a_Mn_CO7_A1A1pA2pA2BD1B----110	-3967.539487	74.27
573	2_a_Mn_CO7_pA1pA1A2A2BBpD1----117	-3967.539487	74.27
574	2_b_Mn_CO7_A1A1pA2pA2BD1B----182	-3967.539487	74.27
575	2_b_Mn_CO7_pA1pA1A2A2BBpD1----189	-3967.539487	74.27
576	271-2_b_Mn_CO7_pA1pA1pA1A2A2pD1D2-T.log	-3967.539484	74.27
577	282-2_a_Mn_CO7_pA1pA1pA1A2A2BpD1-T-xqc.log	-3967.539484	74.27

578	299-2_b_Mn_CO7_pA1pA1pA1A2A2BpD1-T.log	-3967.539484	74.27
579	219-3_a_Mn_CO7_A1A1A1A2BBD2-T-xqc.log	-3967.538662	74.79
580	18-3_a_Mn_CO7_A1A1A2A2D1BD1-T.log	-3967.538105	75.14
581	252-2_a_Mn_CO7_A1A1A1pA2pD2D1pD2-Q-xqc-rupt.log	-3967.538069	75.16
582	259-3_b_Mn_CO7_A1A1A2A2BD1B-T.log	-3967.537840	75.30
583	292-3_b_Mn_CO7_A1A1A2A2D1BD2-T-xqc.log	-3967.537587	75.46
584	154-1_b_Mn_CO7_A1A1A1A2BBB-T.log	-3967.537089	75.78
585	146-1_b_Mn_CO7_A1A1A1A2BBB-T.log	-3967.537088	75.78
586	137-1_b_Mn_CO7_A1A1A1A2BBB-T.log	-3967.537084	75.78
587	3_b_Mn_CO7_A1A1A2A2D1BD1----294	-3967.536994	75.84
588	3_a_Mn_CO7_A1A1A2A2BBD1----251	-3967.536993	75.84
589	67-2_b_Mn_CO7_pA1pA1pA1A2BBD2-Q.log	-3967.536985	75.84
590	3_b_Mn_CO7_A1A1A2A2D1BD2----295	-3967.536892	75.90
591	3_a_Mn_CO7_A1A1A1A1A2A2A2----222	-3967.536891	75.90
592	3_a_Mn_CO7_A1A1A2A2D1BD2----256	-3967.536891	75.90
593	3_a_Mn_CO7_A1A1A2BBBB----260	-3967.536891	75.90
594	3_b_Mn_CO7_A1A1A2BBBB----299	-3967.536891	75.90
595	124-2_b_Mn_CO7_A1A1A1A1pA2pA2D1-T.log	-3967.536664	76.04
596	188-2_b_Mn_CO7_A1A1A1A1pA2pA2D1-T.log	-3967.536664	76.04
597	1_b_Mn_CO7_A1A1A1A2D2D2D2----67	-3967.535352	76.87
598	244-2_b_Mn_CO7_pA1pA1pA1A2BBpD1-T.log	-3967.531078	79.55
599	166-2_b_Mn_CO7_A1A1A1pA2pD2BpD2-T-xqc.log	-3967.530958	79.62
600	142-1_a_Mn_CO7_A1A1A1A2A2BD1-T.log	-3967.530825	79.71
601	201-1_b_Mn_CO7_A1A1A1A2A2BD1-T.log	-3967.530824	79.71
602	162-1_b_Mn_CO7_A1A1A1A2A2BD1-T-xqc.log	-3967.530820	79.71
603	141-1_a_Mn_CO7_A1A1A1A2A2BD1-T.log	-3967.530817	79.71
604	37-2_a_Mn_CO7_A1A1A1A1pA2pA2D1-T.log	-3967.530079	80.17
605	146-1_b_Mn_CO7_A1A1A1A2A2BD1-T-freq.log	-3967.530047	80.19
606	144-1_a_Mn_CO7_A1A1A2A2BD1D2-T-xqc-rupt.log	-3967.529648	80.44
607	140-1_a_Mn_CO7_A1A1A2A2BD1D2-T-xqc-rupt.log	-3967.529647	80.45
608	284-2_a_Mn_CO7_pA1pA1A2A2BpD1B-Q-freq.log	-3967.528993	80.86
609	2_a_Mn_CO7_pA1pA1A2A2BpD1D2----119	-3967.528857	80.94
610	2_b_Mn_CO7_pA1pA1A2A2BpD1D2----191	-3967.528857	80.94
611	2_b_Mn_CO7_pA1pA1A2BBBB----197	-3967.528857	80.94
612	251-2_b_Mn_CO7_A1A1A1pA2pD2D1pD2-Q-xqc-rupt.log	-3967.528345	81.26
613	1_b_Mn_CO7_A1A1A2A2D1BD1-COdeplasat----73	-3967.52761	81.72
614	2_b_Mn_CO7_pA1pA1A2A2pD1BpD1-COdeplasat----193	-3967.527502	81.79
615	1_a_Mn_CO7_A1A1A2A2D1BD1-COdeplasat----34	-3967.527305	81.92
616	81-2_a_Mn_CO7_pA1pA1pA1A2A2pD1D2-T.log	-3967.526929	82.15
617	221-3_a_Mn_CO7_A1A1A1A2D2BD2-Q-xqc.log	-3967.526385	82.49
618	165-1_b_Mn_CO7_A1A1A1A2A2D1D2-Q-xqc.log	-3967.526371	82.50
619	299-2_b_Mn_CO7_pA1pA1pA1A2A2BpD1-Q-xqc.log	-3967.526371	82.50
620	190-2_b_Mn_CO7_A1A1pA2pA2BD1D1-T-xqc-freq.log	-3967.525651	82.95
621	127-2_b_Mn_CO7_A1A1pA2pA2BD1D1-T-xqc.log	-3967.525650	82.95
622	128-2_a_Mn_CO7_A1A1pA2pA2BD1D1-T.log	-3967.525636	82.96

623	191-2_a_Mn_CO7_A1A1pA2pA2BD1D1-T.log	-3967.525627	82.97
624	282-2_a_Mn_CO7_pA1pA1pA1A2A2BpD1-Q.log	-3967.525187	83.24
625	9-1_b_Mn_CO7_A1A1A2A2BBD1-Q-xqc.log	-3967.525187	83.24
626	29-1_a_Mn_CO7_A1A1A2A2BBD1-T-xqc.log	-3967.525127	83.28
627	9-1_b_Mn_CO7_A1A1A2A2BBD1-T.log	-3967.524701	83.55
628	1_b_Mn_CO7_A1A1A1A2D1D1D1----61	-3967.52378	84.13
629	28-1_a_Mn_CO7_A1A1A1A1A2A2D1-T-xqc.log	-3967.523764	84.14
630	28-1_a_Mn_CO7_A1A1A1A1A2A2D1-T-xqc.log	-3967.523763	84.14
631	1_a_Mn_CO7_A1A1A1A2D2D2D2----28	-3967.522998	84.62
632	3_a_Mn_CO7_A1A1A1A2D1D2D1----245	-3967.52279	84.75
633	3_b_Mn_CO7_A1A1A1A2D1D2D1----284	-3967.522789	84.75
634	2_a_Mn_CO7_pA1pA1pA1A2A2pD1D2----131	-3967.522637	84.84
635	3_a_Mn_CO7_A1A1A1A2D1D1D1----243	-3967.52252	84.92
636	3_b_Mn_CO7_A1A1A1A2D1D1D1----282	-3967.52252	84.92
637	1_a_Mn_CO7_A1A1A1A2D1D1D2----23	-3967.52181	85.36
638	1_b_Mn_CO7_A1A1A2A2BD1D2----72	-3967.520886	85.94
639	1_b_Mn_CO7_A1A1A2A2D1D1D2----76	-3967.520886	85.94
640	1_a_Mn_CO7_A1A1A2A2D1D1D2----37	-3967.520884	85.94
641	1_b_Mn_CO7_A1A1A1A2D1D1D2-COdeplasat----62	-3967.518889	87.20
642	271-2_b_Mn_CO7_pA1pA1pA1A2A2pD1D2-Q.log	-3967.518700	87.31
643	29-1_a_Mn_CO7_A1A1A2A2BBD1-Q.log	-3967.518689	87.32
644	145-1_b_Mn_CO7_A1A1A1A2A2D1D1-T-freq.log	-3967.518597	87.38
645	215-3_a_Mn_CO7_A1A1A2A2BBB-T.log	-3967.517144	88.29
646	3_a_Mn_CO7_A1A1A2A2BD1D2----254	-3967.515176	89.53
647	3_a_Mn_CO7_A1A1A2A2D1D2D1----259	-3967.515175	89.53
648	1_b_Mn_CO7_A1A1A1A2BD1D1----56	-3967.514243	90.11
649	2_a_Mn_CO7_pA1pA1A2A2pD1BpD1----121	-3967.513899	90.33
650	149-1_b_Mn_CO7_A1A1A1A2BBD1-T-freq.log	-3967.513821	90.38
651	78-2_a_Mn_CO7_pA1pA1A2A2BpD1D2-T-xqc-freq.log	-3967.510832	92.25
652	227-2_a_Mn_CO7_pA1pA1pA1A2A2pD1pD1-Q.log	-3967.509050	93.37
653	1_a_Mn_CO7_A1A1A1A2D1D1D1----22	-3967.506695	94.85
654	2_b_Mn_CO7_A1A1A1pA2D1pD2D1----167	-3967.504608	96.16
655	2_a_Mn_CO7_A1A1A1pA2D1pD2D1----95	-3967.504607	96.16
656	1_a_Mn_CO7_A1A1A2A2D1BD2----35	-3967.503681	96.74
657	1_b_Mn_CO7_A1A1A2A2D1BD2----74	-3967.503669	96.75
658	2_a_Mn_CO7_pA1pA1pA1A2pD1pD1pD1-COdeplasat----148	-3967.500956	98.45
659	2_a_Mn_CO7_A1A1A1pA2D1D1pD2-COdeplasat----94	-3967.497814	100.42
660	159-1_a_Mn_CO7_A1A1A2A2BD1D2-T-xqc.log	-3967.497184	100.82
661	2_b_Mn_CO7_A1A1A1pA2D1D1pD2----166	-3967.496734	101.10
662	3_b_Mn_CO7_A1A1A1A2D2D1D2----287	-3967.496441	101.28
663	3_b_Mn_CO7_A1A1A1A2BD1D2----278	-3967.49644	101.28
664	202-1_b_Mn_CO7_A1A1A1A2A2D1D2-T-freq.log	-3967.495775	101.70
665	265-2_b_Mn_CO7_pA1pA1A2A2BpD1B-Q-freq.log	-3967.493049	103.41
666	214-3_b_Mn_CO7_A1A1A2A2D1D1D1-T.log	-3967.487773	106.72

667	2_a_Mn_CO7_A1A1pA2pA2D1D1pD2----115	-3967.486972	107.22
668	2_b_Mn_CO7_A1A1pA2pA2D1D1pD2----187	-3967.486971	107.23
669	2_b_Mn_CO7_A1A1A1pA2D1D1D1-COdeplasat----165	-3967.484786	108.60
670	2_a_Mn_CO7_A1A1A1pA2D1D1D1-COdeplasat----93	-3967.484433	108.82
671	2_a_Mn_CO7_A1A1pA2pA2BD1pD2----112	-3967.482112	110.27
672	2_b_Mn_CO7_A1A1pA2pA2BD1pD2----184	-3967.48211	110.28
673	236-3_a_Mn_CO7_A1A1A1A2D1D1D2-Q-xqc-rupt.log	-3967.481931	110.39
674	1_a_Mn_CO7_A1A1A1A2D1D2D2----25	-3967.481908	110.40
675	1_b_Mn_CO7_A1A1A1A2D1D2D2----64	-3967.481908	110.40
676	1_a_Mn_CO7_A1A1A1A2BD1D1----17	-3967.478215	112.72
677	2_b_Mn_CO7_pA1pA1A2A2pD1D2pD1----194	-3967.475567	114.38
678	2_a_Mn_CO7_pA1pA1A2A2pD1D2pD1----122	-3967.475566	114.38
679	286-2_a_Mn_CO7_A1A1pA2pA2BD1B-T-freq.log	-3967.469893	117.94
680	280-2_a_Mn_CO7_pA1pA1pA1A2BpD1pD1-T.log	-3967.469606	118.12
681	283-2_b_Mn_CO7_pA1pA1pA1A2BpD1pD1-T.log	-3967.468701	118.69
682	1_a_Mn_CO7_A1A1A1A2D1D2D1----24	-3967.467496	119.45
683	1_b_Mn_CO7_A1A1A1A2D1D2D1----63	-3967.467496	119.45
684	2_b_Mn_CO7_pA1pA1pA1A2pD1D2pD1-COdeplasat----217	-3967.464	121.64
685	2_a_Mn_CO7_A1A1pA2pA2D1pD2D1----116	-3967.453752	128.07
686	2_b_Mn_CO7_A1A1pA2pA2D1pD2D1----188	-3967.453752	128.07
687	290-3_b_Mn_CO7_A1A1A2A2D1BD1--Q-freq.log	-3967.451727	129.34
688	1_a_Mn_CO7_A1A1A2A2D1D2D1----38	-3967.449487	130.75
689	239-1_b_Mn_CO7_A1A1A2A2D1D1D1-Q-xqc.log	-3967.439803	136.82
690	272-2_a_Mn_CO7_pA1pA1A2A2BpD1pD1-T-freq.log	-3967.438700	137.52
691	2_a_Mn_CO7_pA1pA1pA1A2pD1D2pD1----146	-3967.436456	138.92
692	169-1_a_Mn_CO7_A1A1A1A2D2BD2-T-freq.log	-3967.433205	140.96
693	232-1_a_Mn_CO7_A1A1A1A2BD1B-T-freq.log	-3967.432546	141.38
694	80-1_a_Mn_CO7_A1A1A1A2D2D2D2-T-freq.log	-3967.424193	146.62
695	205-2_a_Mn_CO7_A1A1A1pA2pD2pD2pD2-T-freq.log	-3967.420074	149.20
696	79-1_a_Mn_CO7_A1A1A2A2D1BD1-T-freq.log	-3967.413137	153.56
697	204-2_b_Mn_CO7_A1A1A1pA2pD2pD2pD2-Q-freq.log	-3967.386979	169.97

Table S6A. Distance table for the lowest-lying $H_2C_2S_2Mn_2(CO)_8$ structures after PBE0/6-311G(d,p) optimization followed by a single point CCSD(T) energy calculation. Provided are the absolute CCSD(T) energy (a.u.), relative energy (kcal/mol), and symmetry.



1S. -4078.55830452676 0.00 C_1
WBI 0.02

		1	2	3	4	5
1	Mn	0.000000				
2	Mn	4.145294	0.000000			
3	C	3.880612	1.844136	0.000000		
4	C	5.681279	1.786820	2.513933	0.000000	
5	C	1.796147	5.052416	5.093764	6.780943	0.000000
6	C	1.795880	5.768517	5.105226	7.165487	2.615446
7	O	6.078464	2.984608	4.824420	3.443540	6.441010
8	C	5.002819	1.795641	2.547375	2.715080	5.470224
9	O	4.264401	2.975976	1.137024	3.349258	5.551902
10	O	6.719748	2.929320	3.399307	1.142881	7.895284
11	C	1.841659	3.930898	3.123333	5.398777	2.580907
12	O	2.936553	6.840869	6.027645	8.167814	3.540226
13	O	2.936791	5.840140	6.014896	7.612425	1.140677
14	C	5.212821	1.848906	3.690409	2.552623	5.756313
15	C	1.850565	4.967903	5.134432	6.383068	2.621023
16	O	2.985109	5.697706	6.042032	7.002275	3.543174
17	O	5.755375	2.936559	3.435758	3.673423	5.978216
18	O	2.977156	4.236632	3.179141	5.562659	3.460743
19	S	2.395566	2.370034	3.210268	4.044865	3.000309
20	S	2.394694	3.927902	3.248906	4.819788	4.187709
21	C	3.265052	2.157236	2.999952	3.193705	4.455788
22	C	3.205601	2.935097	2.946174	3.610798	4.791638
23	H	4.196234	2.688089	3.872482	3.371783	5.229141
24	H	4.250827	3.502001	3.489454	3.653470	5.866428

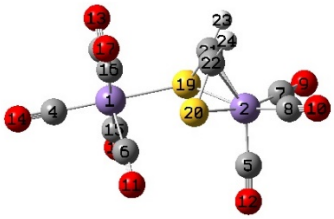
		6	7	8	9	10
6	C	0.000000				
7	O	7.863826	0.000000			
8	C	6.566721	3.439816	0.000000		
9	O	5.137297	5.947352	3.409241	0.000000	
10	O	8.129388	4.131368	3.674635	4.014483	0.000000
11	C	2.605920	6.348725	4.242093	3.219040	6.423083
12	O	1.140720	8.998938	7.611363	5.905040	9.089171
13	O	3.538961	6.898503	6.026130	6.495342	8.746432
14	C	6.976602	1.136027	2.549814	4.816436	3.439170
15	C	2.623076	6.239150	6.153862	5.667676	7.356374
16	O	3.546129	6.578433	6.995794	6.625071	7.915182
17	O	7.240576	4.129262	1.141211	4.091874	4.491298
18	O	3.515918	6.771975	4.139011	3.033542	6.533219
19	S	4.188003	3.690258	3.381327	4.145280	5.147389
20	S	2.989345	6.263172	5.299136	3.426031	5.601410
21	C	4.830682	3.605780	3.846474	3.939234	4.115518
22	C	4.378204	4.900698	4.624528	3.555408	4.360912
23	H	5.752153	3.164553	4.353416	4.855502	4.143842
24	H	5.262633	5.267958	5.246342	3.991673	4.141392

		11	12	13	14	15
11	C	0.000000				
12	O	3.505854	0.000000			
13	O	3.478524	4.292783	0.000000		
14	C	5.353002	8.102349	6.337583	0.000000	

15	C	3.689642	3.525848	3.520214	5.585387	0.000000
16	O	4.822791	4.273377	4.265214	6.067874	1.134736
17	O	4.771074	8.247211	6.378272	3.437423	7.023560
18	O	1.136210	4.233316	4.162307	5.751593	4.825261
19	S	3.055845	5.327346	3.791094	2.894332	2.896737
20	S	3.085535	3.775827	5.327085	5.286825	2.895194
21	C	4.014174	5.889849	5.383246	2.764766	3.336164
22	C	3.937675	5.300657	5.858612	3.995700	3.325950
23	H	5.065662	6.798601	6.065570	2.602194	3.906399
24	H	4.926816	6.087948	6.935126	4.436197	4.203055

		16	17	18	19	20
16	O	0.000000				
17	O	7.903939	0.000000			
18	O	5.958186	4.448103	0.000000		
19	S	3.648243	4.281457	3.868418	0.000000	
20	S	3.647226	6.273222	3.934431	3.276380	0.000000
21	C	3.826179	4.952364	4.801519	1.765610	2.747194
22	C	3.843206	5.727076	4.732504	2.738438	1.678659
23	H	4.124028	5.450946	5.850517	2.469951	3.656833
24	H	4.538567	6.369756	5.645555	3.732497	2.366660

		21	22	23	24
21	C	0.000000			
22	C	1.393938	0.000000		
23	H	1.085826	2.126797	0.000000	
24	H	2.129751	1.089609	2.445787	0.000000

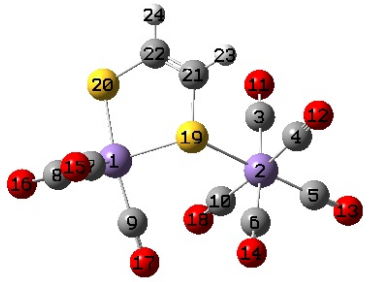


2S. -4078.55596155993 +1.47 C_1
WBI 0.03

		1	2	3	4	5
1	Mn	0.000000				
2	Mn	4.287921	0.000000			
3	C	1.850324	5.167189	0.000000		
4	C	1.799481	5.984749	2.659442	0.000000	
5	C	4.760036	1.797080	5.998758	6.268901	0.000000
6	C	1.873764	3.937670	3.719160	2.647798	3.831665
7	C	5.289123	1.786239	5.744876	7.072073	2.634573
8	C	5.933444	1.782007	6.812948	7.556481	2.618354
9	O	6.126403	2.930166	6.359442	7.908922	3.565817
10	O	7.019995	2.924814	7.892727	8.603696	3.550297
11	O	2.999274	4.242214	4.844207	3.513460	3.712143
12	O	5.306364	2.937681	6.681027	6.637685	1.141821
13	O	2.983789	5.918802	1.133558	3.587297	6.883726
14	O	2.938374	7.084963	3.566932	1.138897	7.293146
15	C	1.851304	4.850190	2.609398	2.632699	4.848477
16	C	1.865132	4.402617	2.609222	2.614981	5.301553
17	O	2.993092	4.926227	3.446439	3.481772	5.992821
18	O	2.984629	5.478358	3.499592	3.549416	5.233095
19	S	2.430802	2.398854	2.886012	4.226938	3.325553
20	S	3.794882	2.358434	5.047539	5.070861	3.137315
21	C	3.528544	2.101157	3.773815	5.225418	3.748406
22	C	3.987994	2.115404	4.623390	5.508744	3.699122
23	H	4.293120	2.867475	4.100534	5.953383	4.574133
24	H	4.974104	2.867493	5.440589	6.416851	4.494605

		6	7	8	9	10
6	C	0.000000				
7	C	5.278553	0.000000			
8	C	5.385046	2.524988	0.000000		
9	O	6.261671	1.143996	3.426133	0.000000	

10	O	6.402928	3.432383	1.142958	4.139565	0.000000
11	O	1.132197	5.655619	5.473217	6.662553	6.403874
12	O	4.123499	3.580579	3.567806	4.350994	4.339564
13	O	4.850708	6.266825	7.515490	6.736560	8.569771
14	O	3.546582	8.204495	8.619846	9.040904	9.644978
15	C	2.607948	5.423426	6.608668	6.054063	7.742938
16	C	2.688056	5.689871	5.712200	6.637804	6.659097
17	O	3.637833	6.272273	5.976226	7.233943	6.799352
18	O	3.494674	5.797740	7.224372	6.278279	8.355413
19	S	3.084042	2.941386	4.130686	3.727024	5.255802
20	S	3.079531	4.122067	3.000423	5.258572	3.808158
21	C	4.063919	2.828820	3.314475	3.691538	4.295854
22	C	4.044909	3.435017	2.790028	4.449765	3.626825
23	H	5.073303	3.029798	3.806672	3.619379	4.662333
24	H	5.068331	3.958315	2.938013	4.869529	3.479701
		11	12	13	14	15
11	O	0.000000				
12	O	3.737676	0.000000			
13	O	5.975226	7.613657	0.000000		
14	O	4.221432	7.582122	4.326221	0.000000	
15	C	3.425879	5.127658	3.499653	3.536448	0.000000
16	C	3.652564	6.036364	3.498673	3.507035	3.714753
17	O	4.466368	6.789076	4.131484	4.177689	4.842358
18	O	4.101410	5.340303	4.201234	4.277699	1.133342
19	S	3.927543	4.187193	3.620121	5.364926	2.900388
20	S	3.294603	3.962663	5.964270	6.017762	5.035774
21	C	4.821657	4.835102	4.314386	6.327992	4.538293
22	C	4.600758	4.769759	5.292531	6.543766	5.261147
23	H	5.878959	5.679189	4.368160	7.038680	5.209676
24	H	5.578675	5.576573	5.987141	7.409812	6.313577
		16	17	18	19	20
16	C	0.000000				
17	O	1.132263	0.000000			
18	O	4.847504	5.974841	0.000000		
19	S	3.128508	3.980686	3.646122	0.000000	
20	S	3.152445	3.376862	5.952889	3.259304	0.000000
21	C	3.234305	3.615758	5.377673	1.757318	2.737336
22	C	3.215552	3.313166	6.183389	2.763122	1.722451
23	H	3.960899	4.214234	5.982817	2.449963	3.733274
24	H	3.959653	3.776408	7.242514	3.747095	2.445684
		21	22	23	24	
21	C	0.000000				
22	C	1.392376	0.000000			
23	H	1.084344	2.157384	0.000000		
24	H	2.129767	1.087228	2.453839	0.000000	



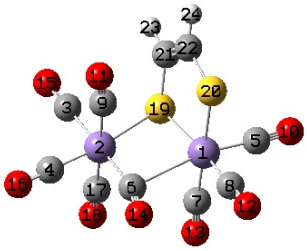
3S. -4078.54975251884 +5.37 C_1

		1	2	3	4	5
1	Mn	0.000000				
2	Mn	4.089544	0.000000			
3	C	4.517220	1.858585	0.000000		
4	C	5.127628	1.857582	2.642837	0.000000	
5	C	5.756877	1.802903	2.657937	2.648468	0.000000
6	C	4.286669	1.862412	3.715461	2.633910	2.660702
7	C	1.759732	5.191526	5.885599	5.833306	6.904991
8	C	1.789224	5.623153	5.890374	6.851452	7.140261
9	C	1.777902	3.872280	4.873884	5.179242	5.255627

WBI 0.02	10 C 3.614380 1.858772 2.568688 3.713308 2.626276 11 O 5.103585 2.989549 1.131179 3.550641 3.565655 12 O 5.947347 2.989842 3.533178 1.132385 3.572588 13 O 6.846213 2.940857 3.562921 3.548099 1.137963 14 O 4.760887 2.992760 4.843686 3.516166 3.587005 15 O 2.903157 6.074623 6.857314 6.496464 7.778516 16 O 2.931616 6.661737 6.858201 7.962924 8.097035 17 O 2.927571 4.135735 5.391230 5.517707 5.215151 18 O 3.836487 2.989046 3.425790 4.843852 3.501231 19 S 2.321564 2.434848 3.036545 2.902030 4.235302 20 S 2.243993 4.971806 4.533786 5.722212 6.622805 21 C 3.243282 3.355153 2.953559 3.347930 4.998922 22 C 3.174429 4.378398 3.689007 4.639562 6.000347 23 H 4.282054 3.554151 3.043121 2.998147 5.002745 24 H 4.203178 5.222931 4.262134 5.296568 6.735631 6 7 8 9 10 6 C 0.000000 7 C 4.914595 0.000000 8 C 5.782397 2.553526 0.000000 9 C 3.454812 2.542248 2.560161 0.000000 10 C 2.661062 5.057240 4.686164 3.083757 0.000000 11 O 4.845510 6.541037 6.318090 5.694754 3.435824 12 O 3.530977 6.446911 7.713095 6.111093 4.844163 13 O 3.563825 8.007400 8.160291 6.241938 3.526759 14 O 1.130582 5.066501 6.152189 3.665896 3.568169 15 O 5.601447 1.144519 3.475745 3.483941 6.095172 16 O 6.807450 3.482703 1.142514 3.471623 5.555132 17 O 3.330450 3.482623 3.476129 1.149993 3.224156 18 O 3.582613 5.373615 4.479559 3.168020 1.131985 19 S 2.932348 3.072513 4.097598 2.950248 3.109668 20 S 5.827215 3.252095 2.794569 3.962092 4.707773 21 C 4.429649 4.017288 4.790013 4.436261 4.151901 22 C 5.493311 4.026572 4.331737 4.720391 4.735123 23 H 4.696297 4.921087 5.869428 5.339308 4.720864 24 H 6.460217 4.960797 5.186888 5.792659 5.648964 11 12 13 14 15 11 O 0.000000 12 O 4.262392 0.000000 13 O 4.295528 4.299936 0.000000 14 O 5.972939 4.227722 4.321377 0.000000 15 O 7.529485 6.974366 8.874363 5.584573 0.000000 16 O 7.208802 8.842753 9.073560 7.131549 4.228923 17 O 6.296883 6.475230 6.077933 3.293904 4.255013 18 O 4.084137 5.974503 4.211643 4.323857 6.450213 19 S 3.831837 3.637999 5.372380 3.672658 3.907464 20 S 4.632704 6.388616 7.701367 6.542032 4.152633 21 C 3.268864 3.798250 6.082535 5.283725 4.771947 22 C 3.704058 5.114692 7.069615 6.329369 4.809513 23 H 3.278514 3.166588 6.015068 5.565310 5.561729 24 H 4.018080 5.629800 7.754621 7.326602 5.649624 16 17 18 19 20 16 O 0.000000 17 O 4.200511 0.000000 18 O 5.165197 3.187540 0.000000 19 S 5.234929 3.767530 3.955665 0.000000

20	S	3.594382	5.089646	4.939921	3.155194	0.000000
21	C	5.848767	5.377379	4.949812	1.754973	2.720580
22	C	5.257724	5.785599	5.297978	2.672414	1.738999
23	H	6.933058	6.196112	5.631184	2.452654	3.734943
24	H	6.011163	6.863585	6.193420	3.687875	2.419055

		21	22	23	24
21	C	0.000000			
22	C	1.338160	0.000000		
23	H	1.084886	2.137175	0.000000	
24	H	2.107418	1.086356	2.485667	0.000000



4S. -4078.54442218261 +8.71 C_1
WBI 0.07

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5	C	1.760392	4.699284	5.683982	6.358011	0.000000
6	C	2.627923	1.891856	3.736076	2.515934	4.365464
7	C	1.786930	3.465557	4.731017	4.819401	2.517641
8	C	1.795032	4.208791	5.815289	5.381231	2.544290
9	C	3.603498	1.868161	2.603253	2.591144	5.138487
10	O	2.901976	5.784862	6.627651	7.473427	1.142273
11	O	4.404371	2.992776	3.448759	3.426082	5.811928
12	O	2.936790	5.129832	6.822400	6.081787	3.460171
13	O	2.932186	4.175944	5.332793	5.316941	3.397976
14	O	3.294174	2.987983	4.818574	3.163986	4.911252
15	O	5.335039	2.978808	1.134311	3.531563	6.492613
16	O	5.719138	2.928002	3.524467	1.138549	7.447008
17	C	3.605474	1.858472	2.592925	2.593829	4.975971
18	O	4.345788	2.989348	3.456807	3.482075	5.502280
19	S	2.262803	2.521624	2.764894	4.291883	3.057290
20	S	2.296472	3.932745	4.916789	5.355591	2.904170
21	C	3.189893	3.446136	3.327071	5.063601	3.702391
22	C	3.165773	3.952956	4.252102	5.465969	3.617074
23	H	4.221444	4.071945	3.439068	5.564861	4.617449
24	H	4.205348	4.852868	4.973605	6.230535	4.511490

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7	C	2.964598	0.000000			
8	C	2.907584	2.579490	0.000000		
9	C	2.652139	4.701867	4.496732	0.000000	
10	O	5.504815	3.434818	3.469662	6.181609	0.000000
11	O	3.571459	5.694737	5.123350	1.130950	6.793319
12	O	3.577630	3.499271	1.141786	5.304750	4.206135
13	O	3.695760	1.146622	3.479049	5.636234	4.116936
14	O	1.140636	3.490238	2.915724	3.514054	6.015741
15	O	4.869724	5.682409	6.868996	3.480587	7.346273
16	O	3.382965	5.806256	6.285282	3.480724	8.570938
17	C	2.706519	3.006426	4.743331	3.725947	5.972697
18	O	3.627825	3.312344	5.412983	4.855945	6.402797
19	S	3.511144	2.952243	4.040119	3.199579	3.899886
20	S	3.696555	4.083221	2.844538	3.241036	3.696126
21	C	4.460722	4.449473	4.751896	3.130289	4.357332
22	C	4.498607	4.784088	4.332748	3.139850	4.252500
23	H	5.352563	5.326522	5.828033	3.739986	5.145518
24	H	5.422418	5.858719	5.209792	3.747299	5.001723

		11	12	13	14	15
11	O	0.000000				
12	O	5.822454	0.000000			
13	O	6.680235	4.212768	0.000000		
14	O	4.254497	3.220459	4.082889	0.000000	
15	O	4.119987	7.901654	6.226164	5.946522	0.000000
16	O	4.106878	6.869634	6.205086	3.752478	4.248218
17	C	4.848508	5.651047	3.207148	3.587571	3.489101
18	O	5.976181	6.272163	3.112178	4.346772	4.156796
19	S	4.060967	5.176571	3.815792	4.578165	3.452192
20	S	3.445591	3.631719	5.228307	4.270950	5.740035
21	C	3.537596	5.812474	5.431676	5.479244	3.744602
22	C	3.246941	5.256866	5.881414	5.345852	4.797047
23	H	4.032958	6.895156	6.223934	6.414239	3.514910
24	H	3.535837	6.035830	6.960359	6.216325	5.372761

		16	17	18	19	20
16	O	0.000000				
17	C	3.482390	0.000000			
18	O	4.178294	1.131894	0.000000		
19	S	5.423952	3.038884	3.807730	0.000000	
20	S	6.361626	5.233475	6.194717	3.158094	0.000000
21	C	6.142307	4.536416	5.419023	1.741556	2.705207
22	C	6.503683	5.301960	6.268451	2.679329	1.718788
23	H	6.590580	5.064296	5.879020	2.432248	3.718344
24	H	7.203628	6.300595	7.286589	3.691166	2.405611

		21	22	23	24
21	C	0.000000			
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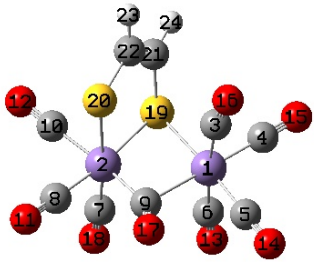
23	H	1.084015	2.144287	0.000000	
24	H	2.116115	1.086589	2.493438	0.000000



5S. -4078.54222826389 +10.09 C_1
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4	C	1.793182	4.322296	2.539582	0.000000	
5	C	1.799506	4.083764	2.562496	2.631784	0.000000
6	C	1.847174	3.353875	3.716511	2.540389	2.527337
7	C	3.360308	1.796273	4.734613	4.745852	4.456139
8	C	4.204984	1.799124	4.677255	5.916394	5.021932
9	C	2.229495	1.936975	2.788923	4.012817	2.662388
10	C	4.330500	1.822021	4.839143	5.559041	5.834758
11	O	5.228005	2.937192	5.597583	6.977119	5.830334
12	O	5.378816	2.956220	5.801895	6.464769	6.941065
13	O	2.979105	4.166988	4.842675	3.393869	3.386954
14	O	2.938360	5.076117	3.445369	3.543630	1.138954
15	O	2.931602	5.373259	3.408776	1.138679	3.565283
16	O	2.994203	4.391933	1.132496	3.348673	3.378711
17	O	3.078432	2.978705	3.344504	4.778735	2.847855
18	O	4.168562	2.935787	5.724599	5.385540	5.089444
19	S	2.341090	2.305927	3.112156	2.904906	4.138396
20	S	3.755998	2.376552	3.126096	5.001347	4.934935
21	C	3.354611	3.207955	3.070902	3.643059	5.027887
22	C	3.822259	3.193251	3.058325	4.470268	5.289857
23	H	4.758659	4.236280	3.696622	5.226029	6.118893
24	H	4.056192	4.235124	3.733156	3.879197	5.699100

	6	7	8	9	10
6 C	0.000000				
7 C	2.862351	0.000000			
8 C	4.668638	2.566001	0.000000		
9 C	3.096387	2.815883	2.391719	0.000000	
10 C	4.752920	2.620372	2.512885	3.720581	0.000000
11 O	5.645766	3.478910	1.138127	3.211570	3.396518
12 O	5.748848	3.545227	3.407388	4.844247	1.134363
13 O	1.134969	3.205525	5.341082	4.015500	5.403000
14 O	3.404118	5.355409	5.786245	3.443402	6.867611
15 O	3.429541	5.738361	7.017713	5.148813	6.461052
16 O	4.825169	5.787738	5.415839	3.663501	5.597985
17 O	3.884083	3.716171	2.841906	1.151652	4.675719
18 O	3.177446	1.141529	3.444927	3.761750	3.493043
19 S	2.968410	2.990837	4.096938	3.396295	2.831731
20 S	5.133229	4.167434	2.921412	3.001481	2.770380
21 C	4.542277	4.460053	4.756267	4.215142	3.294237
22 C	5.251349	4.800416	4.348347	4.054137	3.245891
23 H	6.271753	5.871827	5.225753	4.990767	4.128332
24 H	5.138698	5.325300	5.820011	5.219052	4.169734

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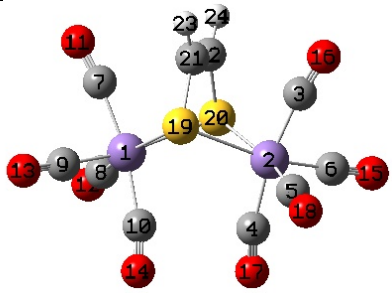
11 O	0.000000				
12 O	4.091878	0.000000			
13 O	6.247228	6.324889	0.000000		
14 O	6.460604	7.988216	4.051121	0.000000	
15 O	8.092487	7.281539	4.074548	4.308022	0.000000
16 O	6.241376	6.481709	5.942361	4.043019	3.991968
17 O	3.304804	5.769879	4.712171	3.270784	5.891267
18 O	4.165247	4.233431	3.106231	5.889629	6.299428
19 S	5.232139	3.607258	3.811331	5.276778	3.676630
20 S	3.692377	3.490127	6.150116	5.856506	5.925036
21 C	5.805770	3.799018	5.484034	6.125375	4.205436
22 C	5.260984	3.735193	6.272314	6.313207	5.149306
23 H	6.038084	4.431203	7.306636	7.086887	5.775198
24 H	6.872291	4.499994	6.009019	6.779099	4.154186

	16	17	18	19	20
16 O	0.000000				
17 O	4.011103	0.000000			
18 O	6.811432	4.533251	0.000000		
19 S	4.027855	4.530171	3.846243	0.000000	
20 S	3.445181	3.666786	5.301210	3.250078	0.000000
21 C	3.540825	5.227731	5.429700	1.762138	2.731018
22 C	3.268226	4.906256	5.881409	2.710945	1.730950
23 H	3.585858	5.737030	6.952668	3.715505	2.403091
24 H	4.062109	6.228490	6.206995	2.434543	3.737978

	21	22	23	24
21 C	0.000000			
22 C	1.339929	0.000000		
23 H	2.103110	1.086896	0.000000	
24 H	1.083633	2.135440	2.473566	0.000000



6S. -4078.53989534414 +11.55 C_2
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6	C	5.028489	1.791384	2.484936	2.428147	2.683566
7	C	1.858282	4.722124	5.224952	5.192735	6.077747
8	C	1.799218	4.845910	6.077862	4.376878	6.227805
9	C	1.791382	5.028391	6.052222	4.910235	5.853311
10	C	1.840537	3.605112	5.192654	2.772255	4.376689
11	O	2.987368	5.678114	5.929006	6.280816	7.047029
12	O	2.938242	5.753358	7.016483	5.111092	7.178108
13	O	2.931516	6.022062	6.990032	5.878437	6.657259
14	O	2.964323	4.207955	5.910391	3.008590	4.622277
15	O	6.022212	2.931518	3.343927	3.302818	3.630984
16	O	5.678083	2.987368	1.135583	4.796333	3.397895
17	O	4.208059	2.964323	4.782066	1.138380	3.432677
18	O	5.753150	2.938237	3.445962	3.444678	1.139633
19	S	2.448887	2.518515	3.037792	3.465198	3.193737
20	S	2.518526	2.448915	3.190674	3.060967	4.219121
21	C	3.089829	3.120887	2.769795	4.504970	4.215693
22	C	3.120891	3.089836	2.836487	4.368313	4.596606
23	H	3.976440	4.018980	3.293073	5.501801	4.861547
24	H	4.018991	3.976447	3.407341	5.287387	5.490986

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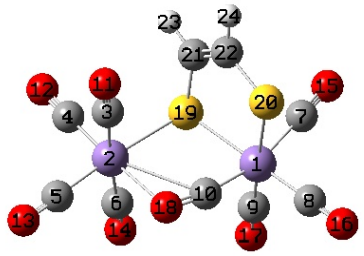
7	C	6.052362	0.000000			
8	C	5.853612	2.554190	0.000000		
9	C	6.603711	2.484940	2.683548	0.000000	
10	C	4.910241	3.682330	2.558735	2.428143	0.000000
11	O	6.942899	1.135583	3.397907	3.311908	4.796331
12	O	6.545466	3.445932	1.139633	3.638514	3.444733
13	O	7.651197	3.343950	3.630973	1.140523	3.302796
14	O	5.380437	4.782069	3.432703	3.174563	1.138380
15	O	1.140523	6.990235	6.657660	7.651253	5.878491
16	O	3.311926	5.928997	7.047150	6.942727	6.280722
17	O	3.174560	5.910508	4.622515	5.380493	3.008651
18	O	3.638556	7.016284	7.178018	6.545029	5.110812
19	S	4.281722	3.190544	4.219117	3.197114	3.061016
20	S	3.197214	3.037924	3.193817	4.281736	3.465097
21	C	4.518005	2.836412	4.596576	4.087250	4.368331
22	C	4.087242	2.769853	4.215687	4.518048	4.504933
23	H	5.375254	3.407226	5.490930	4.669505	5.287429
24	H	4.669484	3.293173	4.861530	5.375331	5.501758

		11	12	13	14	15
11	O	0.000000				
12	O	4.081528	0.000000			
13	O	3.938472	4.438887	0.000000		
14	O	5.879093	4.123557	3.789875	0.000000	
15	O	7.835480	7.225906	8.718157	6.289485	0.000000
16	O	6.483478	7.979810	7.835232	7.015943	3.938472
17	O	7.016077	5.170421	6.289499	2.893508	3.789895
18	O	7.979598	8.138694	7.225334	5.170077	4.438930
19	S	4.084825	5.344542	4.012051	3.895619	5.409401

20 S	3.871653	3.971076	5.409418	4.461769	4.012187
21 C	3.365859	5.631711	4.937978	5.376572	5.511470
22 C	3.260943	5.102779	5.511530	5.573020	4.937966
23 H	3.656003	6.520955	5.353855	6.266413	6.335916
24 H	3.459881	5.614640	6.336028	6.587192	5.353822
	16	17	18	19	20
16 O	0.000000				
17 O	5.879092	0.000000			
18 O	4.081545	4.123496	0.000000		
19 S	3.871466	4.461899	3.970950	0.000000	
20 S	4.085000	3.895552	5.344530	2.960882	0.000000
21 C	3.260854	5.573065	5.102783	1.793955	2.675362
22 C	3.365969	5.376543	5.631748	2.675366	1.793948
23 H	3.459714	6.587248	5.614666	2.498304	3.718989
24 H	3.656193	6.266348	6.521034	3.718995	2.498296
	21	22	23	24	
21 C	0.000000				
22 C	1.330492	0.000000			
23 H	1.084537	2.141630	0.000000		
24 H	2.141631	1.084538	2.563247	0.000000	



7S. -4078.53512121492 +14.55 C_1
WBI 0.02

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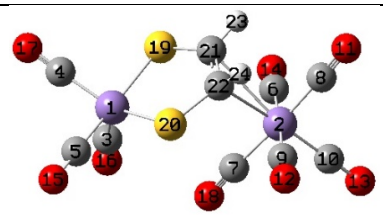
1 Mn	0.000000				
2 Mn	3.784203	0.000000			
3 C	4.352998	1.866635	0.000000		
4 C	5.079533	1.787427	2.604264	0.000000	
5 C	5.267292	1.807850	2.632093	2.621360	0.000000
6 C	3.976702	1.858367	3.723233	2.586134	2.631712
7 C	1.875542	5.117416	5.534182	5.988769	6.800409
8 C	1.802137	5.273826	5.715752	6.754077	6.483025
9 C	1.793194	4.164242	5.350901	5.315311	5.497048
10 C	1.771606	2.721241	3.333388	4.391781	3.809412
11 O	5.040664	2.997298	1.131016	3.504320	3.525002
12 O	6.020663	2.926205	3.491316	1.139108	3.553039
13 O	6.292190	2.946138	3.529915	3.536779	1.138310
14 O	4.507756	2.991224	4.855980	3.473260	3.541218
15 O	3.007640	6.046606	6.383067	6.712657	7.784683
16 O	2.941446	6.290903	6.671703	7.835460	7.363039
17 O	2.935670	4.756611	6.177574	5.761913	5.927451
18 O	2.920856	2.275181	2.868601	4.061331	2.868552
19 S	2.398574	2.430436	3.076672	3.019075	4.235473
20 S	2.385165	4.572914	4.088822	5.740231	5.968251
21 C	3.237038	3.399739	2.982853	3.730771	5.072483
22 C	3.190238	4.177842	3.432227	4.846219	5.715701
23 H	4.273558	3.805390	3.257186	3.627834	5.385933
24 H	4.228908	5.030428	3.977042	5.532447	6.461719
	6	7	8	9	10
6 C	0.000000				
7 C	5.246171	0.000000			
8 C	5.372908	2.711967	0.000000		
9 C	3.499867	2.681690	2.605355	0.000000	
10 C	3.191049	3.614311	2.683733	2.620308	0.000000
11 O	4.854236	6.088216	6.273084	6.254210	4.111923
12 O	3.478485	6.711034	7.750493	6.194287	5.486977
13 O	3.529311	7.890672	7.376072	6.458137	4.731038
14 O	1.133296	5.648322	5.766255	3.567336	3.932858

15	O	6.159984	1.132706	3.652479	3.622731	4.734460
16	O	6.357781	3.635059	1.139524	3.529247	3.610630
17	O	3.652008	3.593068	3.517799	1.142496	3.546410
18	O	2.976774	4.731575	3.734447	3.547196	1.163306
19	S	2.960436	2.975105	4.195991	3.042447	2.712559
20	S	5.576454	2.827883	2.932736	4.176018	2.948317
21	C	4.527934	3.349214	4.807215	4.469950	3.630969
22	C	5.407454	3.264755	4.369616	4.785821	3.664682
23	H	4.970434	4.223279	5.880470	5.353103	4.595375
24	H	6.390162	4.117117	5.244097	5.853848	4.662024

		11	12	13	14	15
11	O	0.000000				
12	O	4.203890	0.000000			
13	O	4.238280	4.299281	0.000000		
14	O	5.986917	4.172713	4.259052	0.000000	
15	O	6.861658	7.307938	8.895023	6.506797	0.000000
16	O	7.161942	8.853916	8.177821	6.690777	4.420037
17	O	7.156061	6.566789	6.810692	3.353715	4.372118
18	O	3.681422	5.199011	3.680229	3.831181	5.837074
19	S	3.893788	3.784706	5.373167	3.729935	3.738343
20	S	4.225972	6.610442	6.949228	6.396579	3.553228
21	C	3.293950	4.304407	6.165580	5.417237	3.845157
22	C	3.459019	5.513575	6.755205	6.316810	3.750647
23	H	3.434123	3.926797	6.442068	5.852186	4.541193
24	H	3.701687	6.084596	7.449594	7.332364	4.406987

		16	17	18	19	20
16	O	0.000000				
17	O	4.265671	0.000000			
18	O	4.536510	4.300196	0.000000		
19	S	5.332805	3.856286	3.266915	0.000000	
20	S	3.704501	5.318028	3.739541	3.311993	0.000000
21	C	5.865276	5.424599	4.128519	1.768847	2.749875
22	C	5.292860	5.864564	4.253454	2.726091	1.732912
23	H	6.942730	6.219654	4.958541	2.440344	3.747848
24	H	6.069953	6.934926	5.162799	3.722872	2.398139

		21	22	23	24
21	C	0.000000			
22	C	1.338523	0.000000		
23	H	1.084528	2.127799	0.000000	
24	H	2.092564	1.087614	2.445998	0.000000



8S. -4078.53270224220 +16.07 C_1
WBI 0.01

		1	2	3	4	5
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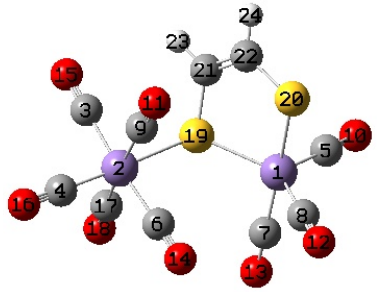
2	Mn	4.666356	0.000000			
3	C	1.758880	4.981112	0.000000		
4	C	1.783014	6.245968	2.531243	0.000000	
5	C	1.789542	5.778583	2.556871	2.570210	0.000000
6	C	4.829528	1.858633	4.815303	6.077242	6.298408
7	C	3.845814	1.874606	3.659353	5.500685	4.696497
8	C	5.871733	1.846935	6.488446	7.281432	7.093911
9	C	5.124572	1.863897	5.705039	6.844262	5.741460
10	C	6.221798	1.802817	6.189646	7.821929	7.202803
11	O	6.743893	2.981397	7.480033	8.046540	7.994762
12	O	5.706801	2.995127	6.389614	7.432390	6.027544
13	O	7.265989	2.940670	7.089897	8.865705	8.180876
14	O	5.299469	2.990835	5.085592	6.297622	6.880456

15	O	2.932736	6.643954	3.479225	3.486791	1.143201
16	O	2.904618	5.425401	1.147181	3.475404	3.483795
17	O	2.926841	7.306319	3.475100	1.144658	3.485159
18	O	3.836423	3.001466	3.226905	5.419184	4.418165
19	S	2.297332	3.988316	3.010636	2.884275	4.078901
20	S	2.241893	3.448373	3.499420	3.863501	2.781664
21	C	3.159238	2.782842	4.090341	4.239545	4.725594
22	C	3.196358	2.327554	4.282891	4.639966	4.351060
23	H	4.199197	3.069146	5.062745	5.098681	5.794752
24	H	4.136395	2.713800	5.344010	5.491524	5.131467
		6	7	8	9	10
6	C	0.000000				
7	C	2.611690	0.000000			
8	C	2.629450	3.718959	0.000000		
9	C	3.721242	2.639906	2.641506	0.000000	
10	C	2.611726	2.640050	2.635777	2.631920	0.000000
11	O	3.521308	4.852106	1.134609	3.539687	3.561177
12	O	4.852557	3.536239	3.533363	1.131351	3.533759
13	O	3.512943	3.538932	3.535421	3.521938	1.137912
14	O	1.133381	3.490967	3.533502	4.853950	3.485649
15	O	7.311190	5.481088	7.985083	6.368892	7.976329
16	O	5.080313	3.908339	7.041312	6.263808	6.362127
17	O	7.004799	6.606552	8.250345	7.954030	8.888766
18	O	3.484173	1.129890	4.847247	3.543681	3.496000
19	S	3.466135	3.906651	4.734185	5.105683	5.592100
20	S	4.424781	3.131283	4.482041	3.238579	5.060582
21	C	2.718278	3.409253	3.169520	3.820072	4.512079
22	C	3.184275	2.962986	2.893917	2.686277	4.116605
23	H	2.715688	4.115769	2.855596	4.250959	4.635235
24	H	3.788221	3.760792	2.640102	2.638182	4.369800
		11	12	13	14	15
11	O	0.000000				
12	O	4.249041	0.000000			
13	O	4.287226	4.239721	0.000000		
14	O	4.243906	5.985290	4.194886	0.000000	
15	O	8.888204	6.484154	8.904082	7.936720	0.000000
16	O	8.075209	6.983235	7.134748	5.211680	4.228119
17	O	8.953355	8.540897	9.931203	7.109912	4.219211
18	O	5.980802	4.263546	4.200009	4.167028	5.093092
19	S	5.442094	5.980112	6.661741	3.666048	5.219602
20	S	5.327760	3.627153	6.132070	5.290717	3.577960
21	C	3.835931	4.713746	5.629340	3.301215	5.792724
22	C	3.670691	3.430778	5.249622	4.086530	5.274999
23	H	3.261275	5.173110	5.698071	3.139525	6.862671
24	H	3.164882	3.186595	5.459479	4.724158	5.961454
		16	17	18	19	20
16	O	0.000000				
17	O	4.252630	0.000000			
18	O	3.237778	6.506273	0.000000		
19	S	3.837272	3.684336	4.340565	0.000000	
20	S	4.474174	4.948630	3.546898	3.175036	0.000000
21	C	4.910103	5.128700	4.220784	1.679037	2.729203
22	C	5.152542	5.652535	3.829862	2.719876	1.769614
23	H	5.809064	5.874893	5.026704	2.377881	3.727033
24	H	6.232662	6.448466	4.704220	3.613128	2.425305

	21	22	23	24	
21 C	0.000000				
22 C	1.404735	0.000000			
23 H	1.089069	2.157431	0.000000		
24 H	2.114558	1.089630	2.442812	0.000000	



9T. -4078.52216533389 +22.68 C_1
WBI 0.002

	1	2	3	4	5
1 Mn	0.000000				
2 Mn	4.085291	0.000000			
3 C	5.153649	1.854025	0.000000		
4 C	5.727367	1.801472	2.650876	0.000000	
5 C	1.926395	5.616854	6.309244	7.363003	0.000000
6 C	3.545045	1.853974	3.704713	2.626745	5.336832
7 C	1.810493	4.291087	5.561979	5.761907	2.656408
8 C	1.849629	4.893705	6.332417	6.199484	3.257714
9 C	4.169735	1.861873	2.634545	2.675075	5.813911
10 O	3.057946	6.628804	7.156609	8.398313	1.133584
11 O	4.606164	2.992309	3.525749	3.593204	6.210827
12 O	2.990302	5.659844	7.216611	6.752944	4.265591
13 O	2.958632	4.778737	6.091796	6.058579	3.560310
14 O	3.713272	2.986375	4.837815	3.511467	5.525833
15 O	5.985243	2.987202	1.133299	3.577641	6.928768
16 O	6.807897	2.940019	3.553331	1.138557	8.479408
17 C	4.586063	1.855185	2.619612	2.673285	5.783067
18 O	5.178879	2.987085	3.511078	3.609419	6.133587
19 S	2.381395	2.440081	2.923602	4.240453	3.397892
20 S	2.305351	4.798273	5.466503	6.335281	3.125940
21 C	3.199757	3.399677	3.217895	5.036591	3.885770
22 C	3.130052	4.309960	4.386407	5.880363	3.735929
23 H	4.235705	3.715542	2.947320	5.193787	4.756185
24 H	4.160712	5.150463	4.971105	6.604159	4.561074

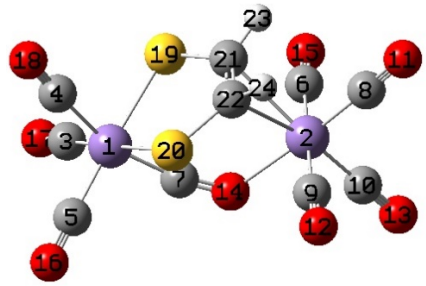
	6	7	8	9	10
6 C	0.000000				
7 C	3.431724	0.000000			
8 C	3.697550	2.478757	0.000000		
9 C	2.607804	5.023355	4.721995	0.000000	
10 O	6.443572	3.609959	4.270490	6.840776	0.000000
11 O	3.499310	5.726201	4.971804	1.130444	7.206518
12 O	4.234771	3.365448	1.140845	5.379013	5.195475
13 O	3.813323	1.148379	3.342702	5.787793	4.349949
14 O	1.133111	3.380557	3.328929	3.496461	6.639225
15 O	4.836413	6.467836	7.294967	3.527673	7.666352
16 O	3.528815	6.776808	7.138610	3.580561	9.523619
17 C	2.623667	4.100473	5.549334	3.708542	6.685624
18 O	3.516029	4.360010	6.175597	4.836641	6.936041
19 S	3.078336	3.029794	3.941391	2.999546	4.308285
20 S	4.668630	4.111128	2.980334	3.963567	3.933392
21 C	4.324870	4.468365	4.703334	3.070295	4.610474
22 C	4.862852	4.765773	4.365000	3.507648	4.416913
23 H	4.992720	5.360050	5.774860	3.476931	5.355158
24 H	5.828792	5.832374	5.288989	4.144274	5.079882

	11	12	13	14	15
11 O	0.000000				
12 O	5.521448	0.000000			
13 O	6.587186	4.010413	0.000000		
14 O	4.200887	3.602462	3.627178	0.000000	

15	O	4.234777	8.221024	7.006225	5.969458	0.000000
16	O	4.328480	7.586524	6.990377	4.226294	4.309191
17	C	4.837045	6.357161	4.185689	3.519486	3.511741
18	O	5.963403	6.978978	4.179700	4.228397	4.217004
19	S	3.772152	5.010975	3.852286	3.906107	3.662667
20	S	3.829844	3.807564	5.256671	4.980809	6.107032
21	C	3.392139	5.738991	5.439914	5.171859	3.589423
22	C	3.446075	5.311691	5.860022	5.520924	4.783783
23	H	3.795958	6.808867	6.249984	5.948430	2.971957
24	H	3.856163	6.164267	6.932716	6.502989	5.179674

		16	17	18	19	20
16	O	0.000000				
17	C	3.584700	0.000000			
18	O	4.358174	1.132206	0.000000		
19	S	5.378630	2.932708	3.665298	0.000000	
20	S	7.368005	5.936077	6.767533	3.269721	0.000000
21	C	6.117312	4.375920	5.192257	1.765526	2.741623
22	C	6.929328	5.474289	6.328643	2.716042	1.733902
23	H	6.214223	4.594636	5.362855	2.450166	3.741917
24	H	7.597687	6.392277	7.260592	3.715323	2.411159

		21	22	23	24
21	C	0.000000			
22	C	1.342185	0.000000		
23	H	1.084981	2.128669	0.000000	
24	H	2.095752	1.087421	2.445569	0.000000



10S. -4078.51817129178 +25.18
C_s
WBI 0.02

		1	2	3	4	5
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2	Mn	4.240970	0.000000			
3	C	1.799863	5.365181	0.000000		
4	C	1.871245	5.555209	2.713617	0.000000	
5	C	1.799863	5.365117	2.614146	2.713608	0.000000
6	C	4.648009	1.869202	5.243841	5.881488	6.104802
7	C	1.768471	2.941897	2.700807	3.584676	2.700832
8	C	5.669180	1.785270	6.881669	6.644815	6.881555
9	C	4.647908	1.869205	6.104709	5.881432	5.243601
10	C	5.579912	1.805920	6.453292	7.124045	6.453257
11	O	6.656045	2.925392	7.895719	7.458850	7.895585
12	O	5.276676	3.000005	6.823278	6.412526	5.557293
13	O	6.548325	2.943456	7.297339	8.169403	7.297323
14	O	2.915689	2.184861	3.729329	4.677149	3.729351
15	O	5.276810	3.000006	5.557609	6.412599	6.823434
16	O	2.940397	6.228996	3.534931	3.640200	1.140711
17	O	2.940400	6.229099	1.140713	3.640220	3.534910
18	O	3.003589	6.447165	3.665097	1.133708	3.665087
19	S	2.385774	3.577807	2.972802	2.930496	4.184219
20	S	2.385757	3.577798	4.184206	2.930482	2.972674
21	C	3.194162	2.455766	4.382891	3.786327	4.778340
22	C	3.194163	2.455756	4.778392	3.786329	4.382804
23	H	4.236705	2.838854	5.293392	4.636350	5.855064
24	H	4.236705	2.838842	5.855114	4.636350	5.293293

		6	7	8	9	10
6	C	0.000000				
7	C	3.489539	0.000000			
8	C	2.590293	4.629822	0.000000		
9	C	3.737906	3.489450	2.590302	0.000000	

10	C	2.578169	3.957631	2.613379	2.578191	0.000000
11	O	3.478601	5.731096	1.140465	3.478611	3.545855
12	O	4.867542	4.254249	3.474388	1.132536	3.444159
13	O	3.461428	4.850002	3.522718	3.461469	1.137620
14	O	2.870825	1.165883	3.967861	2.870770	2.846854
15	O	1.132540	4.254362	3.474386	4.867547	3.444142
16	O	7.098475	3.633242	7.755517	5.863377	7.168777
17	O	5.863700	3.633211	7.755700	7.098391	7.168837
18	O	6.735473	4.695372	7.354549	6.735441	8.094237
19	S	3.200549	2.701026	4.564483	4.758259	5.108999
20	S	4.758270	2.701065	4.564411	3.200512	5.109021
21	C	2.659545	3.001534	3.039425	3.500650	4.217257
22	C	3.500598	3.001551	3.039373	2.659595	4.217263
23	H	2.689199	4.016286	2.798098	4.023340	4.487657
24	H	4.023238	4.016310	2.798003	2.689324	4.487671
		11	12	13	14	15
11	O	0.000000				
12	O	4.168477	0.000000			
13	O	4.283398	4.124574	0.000000		
14	O	5.106228	3.734742	3.691629	0.000000	
15	O	4.168474	5.995429	4.124530	3.734808	0.000000
16	O	8.769678	5.995197	7.928155	4.532382	7.849855
17	O	8.769897	7.849691	7.928185	4.532353	5.995629
18	O	8.062196	7.215471	9.168160	5.761149	7.215509
19	S	5.393930	5.698843	6.154830	3.287305	3.548480
20	S	5.393833	3.548441	6.154869	3.287365	5.698857
21	C	3.801688	4.440416	5.342513	3.174999	3.377364
22	C	3.801623	3.377435	5.342527	3.175025	4.440352
23	H	3.293497	4.971655	5.573815	4.036798	3.217638
24	H	3.293369	3.217813	5.573843	4.036837	4.971529
		16	17	18	19	20
16	O	0.000000				
17	O	4.282255	0.000000			
18	O	4.440629	4.440655	0.000000		
19	S	5.323820	3.760393	3.674373	0.000000	
20	S	3.760205	5.323810	3.674365	3.316747	0.000000
21	C	5.842141	5.310017	4.449703	1.737270	2.759602
22	C	5.309876	5.842225	4.449707	2.759606	1.737276
23	H	6.922497	6.137083	5.144917	2.407210	3.706815
24	H	6.136915	6.922581	5.144919	3.706812	2.407223
		21	22	23	24	
21	C	0.000000				
22	C	1.386086	0.000000			
23	H	1.087473	2.122071	0.000000		
24	H	2.122067	1.087472	2.395653	0.000000	

Table S6B. Energy rank for all of the $H_2C_2S_2Mn_2(CO)_8$ optimized structures. PBE0/6-311G(d,p).

No	Initial structure	Final energy (a.u.)	ΔE (kcal/mol)
1	2_b_Mn_CO8_A1A1A1pA2pA2BpD2pD2----156	-4080.871399	0.00
2	2_a_Mn_CO8_A1A1pA2pA2BBBB----103	-4080.871398	0.00
3	2_b_Mn_CO8_A1A1pA2pA2BBBB----168	-4080.871398	0.00
4	2_a_Mn_CO8_A1A1A1pA2pA2BpD2B----88	-4080.871397	0.00
5	2_a_Mn_CO8_pA1pA1pA1pA1A2A2BB----129	-4080.871397	0.00
6	2_b_Mn_CO8_pA1pA1pA1A2A2BBB----172	-4080.871397	0.00
7	2_b_Mn_CO8_pA1pA1pA1A2BBBB----190	-4080.871397	0.00
8	2_b_Mn_CO8_pA1pA1pA1pA1A2A2D2D2----197	-4080.871397	0.00
9	2_a_Mn_CO8_A1A1A1pA2pA2BpD2pD2----90	-4080.871396	0.00
10	2_a_Mn_CO8_pA1pA1pA1A2BBBB----125	-4080.871396	0.00
11	2_b_Mn_CO8_A1A1A1pA2pA2BBB----148	-4080.871396	0.00
12	2_b_Mn_CO8_pA1pA1pA1pA1A2A2A2B----191	-4080.871396	0.00
13	2_b_Mn_CO8_pA1pA1pA1pA1A2A2BB----194	-4080.871396	0.00
14	2_a_Mn_CO8_A1A1A1A1pA2pA2pA2B----77	-4080.871395	0.00
15	2_a_Mn_CO8_A1A1A1pA2pA2pA2BB----97	-4080.871395	0.00
16	2_a_Mn_CO8_pA1pA1pA1pA1A2A2A2B----126	-4080.871395	0.00
17	2_b_Mn_CO8_A1A1A1A1pA2pA2pA2B----143	-4080.871395	0.00
18	2_b_Mn_CO8_A1A1A1A1pA2pA2pA2pD2----145	-4080.871395	0.00
19	2_b_Mn_CO8_pA1pA1pA1pA1A2A2A2D2----192	-4080.871395	0.00
20	2_a_Mn_CO8_A1A1A1A1pA2pA2pA2pD2----79	-4080.871394	0.00
21	2_b_Mn_CO8_A1A1A1pA2pA2pA2BB----162	-4080.871394	0.00
22	2_a_Mn_CO8_pA1pA1pA1A2A2D2D2D2_COdeplasat----117	-4080.869319	1.31
23	2_b_Mn_CO8_pA1pA1pA1A2A2D2D2D2_COdeplasat----182	-4080.869288	1.32
24	1_b_Mn_CO8_A1A1A1A2A2A2BD1_COdeplasat----47	-4080.869211	1.37
25	2_a_Mn_CO8_A1A1A1A1A1pA2pA2pA2_COdeplasat----70	-4080.869188	1.39
26	2_a_Mn_CO8_A1A1A1A1A2A2A2A2_COdeplasat----71	-4080.869186	1.39
27	2_b_Mn_CO8_A1A1A1A1A2A2A2A2_COdeplasat----137	-4080.869168	1.40
28	2_b_Mn_CO8_A1A1A1pA2pA2pA2D1D1_COdeplasat----164	-4080.869156	1.41
29	2_a_Mn_CO8_A1A1A1pA2pA2pA2D1D1_COdeplasat----99	-4080.869116	1.43
30	2_a_Mn_CO8_A1A1A1A1pA2pA2BpD2_COdeplasat----74	-4080.869085	1.45
31	2_b_Mn_CO8_A1A1A1A1pA2pA2BpD2_COdeplasat----140	-4080.869057	1.47
32	2_b_Mn_CO8_A1A1A1A1pA2pA2pA2D1_COdeplasat----144	-4080.868814	1.62
33	2_a_Mn_CO8_A1A1A1A1pA2pA2pA2D1_COdeplasat----78	-4080.868743	1.67
34	2_b_Mn_CO8_pA1pA1pA1A2A2D2BD2_COdeplasat----181	-4080.868727	1.68
35	2_a_Mn_CO8_pA1pA1pA1A2A2BD2B_COdeplasat----110	-4080.868722	1.68
36	2_a_Mn_CO8_A1A1A1A1pA2pA2BB----72	-4080.868403	1.88
37	2_b_Mn_CO8_A1A1A1A1pA2pA2BB----138	-4080.868402	1.88
38	2_b_Mn_CO8_A1A1A1A1A1pA2pA2pA2----136	-4080.868401	1.88
39	2_b_Mn_CO8_A1A1A1pA2pA2D1pD2pD2----161	-4080.868401	1.88
40	2_a_Mn_CO8_A1A1A1pA2pA2BBB----82	-4080.8684	1.88

41	2_a_Mn_CO8_pA1pA1pA1A2A2BBB----107	-4080.8684	1.88
42	2_b_Mn_CO8_A1A1A1pA2BBBB----147	-4080.8684	1.88
43	2_a_Mn_CO8_pA1pA1pA1A2A2BBpD1_COdeplasat----109	-4080.86828	1.96
44	2_a_Mn_CO8_A1A1A1pA2pA2BD1B_COdeplasat----85	-4080.867882	2.21
45	2_b_Mn_CO8_A1A1A1pA2pA2BD1B_COdeplasat----151	-4080.867843	2.23
46	2_b_Mn_CO8_pA1pA1pA1A2A2BD2B_COdeplasat----175	-4080.86706	2.72
47	2_b_Mn_CO8_pA1pA1pA1A2A2BBD2_COdeplasat----173	-4080.86503	4.00
48	1_b_Mn_CO8_A1A1A1A2A2A2D1D1_COdeplasat----48	-4080.863296	5.08
49	1_a_Mn_CO8_A1A1A1A1A2A2A2D1----4	-4080.859075	7.73
50	3_b_Mn_CO8_A1A1A1A1A2A2A2D2----237	-4080.858688	7.98
51	1_b_Mn_CO8_A1A1A1A1A2A2D2D2----45	-4080.858687	7.98
52	1_b_Mn_CO8_A1A1A1A2A2BD2B----56	-4080.858687	7.98
53	3_a_Mn_CO8_A1A1A1A2A2BD2D1----220	-4080.858686	7.98
54	1_a_Mn_CO8_A1A1A1A1A1A2A2A2----1	-4080.858685	7.98
55	1_a_Mn_CO8_A1A1A1A1A2A2BD1----7	-4080.858685	7.98
56	1_a_Mn_CO8_A1A1A1A2A2A2D1D2----15	-4080.858685	7.98
57	1_a_Mn_CO8_A1A1A1A2A2BBB----16	-4080.858685	7.98
58	1_a_Mn_CO8_A1A1A2A2BBBB----35	-4080.858685	7.98
59	1_b_Mn_CO8_A1A1A1A1A2A2BB----41	-4080.858685	7.98
60	1_b_Mn_CO8_A1A1A1A1A2A2BD2----42	-4080.858685	7.98
61	1_b_Mn_CO8_A1A1A1A2A2D1BD2----60	-4080.858685	7.98
62	1_b_Mn_CO8_A1A1A1A2BBBB----68	-4080.858685	7.98
63	1_b_Mn_CO8_A1A1A2A2BBBB----69	-4080.858685	7.98
64	3_a_Mn_CO8_A1A1A1A1A1A2A2A2----201	-4080.858685	7.98
65	3_a_Mn_CO8_A1A1A1A1A2A2A2A2----202	-4080.858685	7.98
66	3_a_Mn_CO8_A1A1A1A1A2A2A2B----203	-4080.858685	7.98
67	3_a_Mn_CO8_A1A1A1A1A2A2A2D2----205	-4080.858685	7.98
68	3_a_Mn_CO8_A1A1A1A1A2A2D1D2----208	-4080.858685	7.98
69	3_a_Mn_CO8_A1A1A1A2A2A2BB----210	-4080.858685	7.98
70	3_a_Mn_CO8_A1A1A1A2A2BBD2----215	-4080.858685	7.98
71	3_a_Mn_CO8_A1A1A1A2A2BD2B----219	-4080.858685	7.98
72	3_b_Mn_CO8_A1A1A1A1A2A2A2B----235	-4080.858685	7.98
73	1_a_Mn_CO8_A1A1A1A1A2A2A2B----3	-4080.858684	7.98
74	1_a_Mn_CO8_A1A1A1A1A2A2BB----6	-4080.858684	7.98
75	1_a_Mn_CO8_A1A1A1A1A2A2BD2----8	-4080.858684	7.98
76	1_a_Mn_CO8_A1A1A1A2A2D1BD2----26	-4080.858684	7.98
77	1_b_Mn_CO8_A1A1A1A1A1A2A2A2----36	-4080.858684	7.98
78	1_b_Mn_CO8_A1A1A1A2A2BBB----50	-4080.858684	7.98
79	2_a_Mn_CO8_pA1pA1pA1pA1pA1A2A2A2----135	-4080.858684	7.98
80	3_a_Mn_CO8_A1A1A1A2A2BBB----213	-4080.858684	7.98
81	3_b_Mn_CO8_A1A1A1A2A2A2BB----242	-4080.858684	7.98
82	3_b_Mn_CO8_A1A1A1A2A2BBB----245	-4080.858684	7.98
83	3_b_Mn_CO8_A1A1A1A2A2BD2B----251	-4080.858684	7.98
84	3_a_Mn_CO8_A1A1A1A2A2BBD1----214	-4080.858683	7.98
85	1_a_Mn_CO8_A1A1A1A2BBBB----34	-4080.85659	9.29

86	1_a_Mn_CO8_A1A1A1A2A2BD2B_COdeplasat----22	-4080.850521	13.10
87	1_b_Mn_CO8_A1A1A1A2A2BBD2_COdeplasat----52	-4080.850344	13.21
88	1_a_Mn_CO8_A1A1A1A2A2A2BB_COdeplasat----13	-4080.850339	13.22
89	1_b_Mn_CO8_A1A1A1A2A2BD2D2_COdeplasat----58	-4080.85008	13.38
90	1_b_Mn_CO8_A1A1A1A1A2A2A2D1_COdeplasat----39	-4080.849946	13.46
91	1_a_Mn_CO8_A1A1A1A1A2A2A2D2----5	-4080.849279	13.88
92	1_b_Mn_CO8_A1A1A1A1A2A2A2D2----40	-4080.849279	13.88
93	1_b_Mn_CO8_A1A1A1A2A2A2D1D2_COdeplasat----49	-4080.84757	14.95
94	2_b_Mn_CO8_pA1pA1pA1A2A2A2BpD1----169	-4080.844485	16.89
95	2_a_Mn_CO8_pA1pA1pA1A2A2A2pD1pD1----106	-4080.844482	16.89
96	2_b_Mn_CO8_pA1pA1pA1pA1pA1A2A2A2----200	-4080.844481	16.89
97	2_a_Mn_CO8_pA1pA1pA1A2A2A2BpD1----104	-4080.844478	16.89
98	2_a_Mn_CO8_pA1pA1pA1pA1A2A2A2pD1----128	-4080.844478	16.89
99	2_b_Mn_CO8_pA1pA1pA1pA1A2A2A2pD1----193	-4080.844478	16.89
100	2_b_Mn_CO8_A1A1A1pA2pA2BpD2B----154	-4080.844475	16.90
101	2_b_Mn_CO8_pA1pA1pA1A2A2A2pD1pD1----171	-4080.844475	16.90
102	2_a_Mn_CO8_pA1pA1pA1pA1A2A2BD2_COdeplasat----130	-4080.843872	17.27
103	2_a_Mn_CO8_A1A1A1pA2pA2pD2BpD2_COdeplasat----100	-4080.843824	17.30
104	2_b_Mn_CO8_A1A1A1pA2pA2pD2BpD2_COdeplasat----165	-4080.843759	17.34
105	2_b_Mn_CO8_pA1pA1pA1pA1A2A2BD2_COdeplasat----195	-4080.843605	17.44
106	2_b_Mn_CO8_A1A1A1A1pA2pA2pD2pD2_COdeplasat----146	-4080.843582	17.46
107	2_a_Mn_CO8_A1A1A1A1pA2pA2pD2pD2_COdeplasat----80	-4080.843513	17.50
108	2_b_Mn_CO8_A1A1A1A1pA2pA2D1pD2_COdeplasat----142	-4080.84293	17.86
109	1_b_Mn_CO8_A1A1A1A1A2A2A2B----38	-4080.842813	17.94
110	1_b_Mn_CO8_A1A1A1A2A2A2BB----46	-4080.842813	17.94
111	1_a_Mn_CO8_A1A1A1A1A2A2A2A2----2	-4080.842812	17.94
112	1_b_Mn_CO8_A1A1A1A1A2A2A2A2----37	-4080.842812	17.94
113	2_a_Mn_CO8_A1A1A1pA2pA2pA2BD1----98	-4080.838991	20.34
114	2_a_Mn_CO8_pA1pA1pA1pA1A2A2D2D2----132	-4080.838991	20.34
115	2_a_Mn_CO8_A1A1A1pA2pA2BpD2D1----89	-4080.83899	20.34
116	2_a_Mn_CO8_pA1pA1pA1pA1A2A2A2D2----127	-4080.83899	20.34
117	2_b_Mn_CO8_A1A1A1pA2pA2pA2BD1----163	-4080.83899	20.34
118	2_b_Mn_CO8_pA1pA1pA1A2A2A2pD1D2----170	-4080.83899	20.34
119	2_a_Mn_CO8_pA1pA1pA1A2A2BBD2_COdeplasat----108	-4080.836865	21.67
120	2_a_Mn_CO8_A1A1A1pA2pA2D1BpD2_COdeplasat----92	-4080.836783	21.72
121	2_a_Mn_CO8_pA1pA1pA1A2A2A2pD1D2_COdeplasat----105	-4080.834538	23.13
122	1_a_Mn_CO8_A1A1A1A1A2A2A2D1----4-T	-4080.832111	24.65
123	1_a_Mn_CO8_A1A1A1A2BBBB----34-T	-4080.832109	24.65
124	1_a_Mn_CO8_A1A1A1A1A2A2A2D2----5-T	-4080.830128	25.90
125	1_b_Mn_CO8_A1A1A1A1A2A2A2B----38-T	-4080.830128	25.90
126	3_b_Mn_CO8_A1A1A1A2A2BD2D2----253	-4080.828291	27.05
127	3_b_Mn_CO8_A1A1A1A1A2A2A2A2----234	-4080.827846	27.33
128	3_a_Mn_CO8_A1A1A1A2A2D1D2D2----227	-4080.827573	27.50
129	3_b_Mn_CO8_A1A1A1A2A2BBD1----246	-4080.827572	27.50
130	3_b_Mn_CO8_A1A1A1A1A2A2D2D2----241	-4080.827386	27.62

131	3_b_Mn_CO8_A1A1A1A2A2D1D2D2----259	-4080.827384	27.62
132	3_b_Mn_CO8_A1A1A1A2A2D1BD2----255	-4080.827383	27.62
133	1_a_Mn_CO8_A1A1A1A2A2D2D2D2_COdeplasat----33	-4080.82731	27.67
134	1_b_Mn_CO8_A1A1A1A2A2D2D2D2_COdeplasat----67	-4080.82724	27.71
135	1_a_Mn_CO8_A1A1A1A2A2D1BD1_COdeplasat----25	-4080.826942	27.90
136	1_a_Mn_CO8_A1A1A1A2A2BBD2_COdeplasat----18	-4080.826711	28.04
137	1_a_Mn_CO8_A1A1A1A1A2A2D2D2_COdeplasat----11	-4080.826261	28.32
138	2_b_Mn_CO8_A1A1A1pA2pA2BpD2pD2----156-T	-4080.82596	28.51
139	2_a_Mn_CO8_A1A1A1A1pA2pA2BB----72-T	-4080.823811	29.86
140	3_b_Mn_CO8_A1A1A1A1A2A2A2D2----237-T	-4080.823463	30.08
141	2_b_Mn_CO8_A1A1A1pA2pA2BBpD2----150	-4080.822617	30.61
142	2_a_Mn_CO8_A1A1A1pA2pA2BBpD2----84	-4080.822616	30.61
143	2_a_Mn_CO8_pA1pA1pA1A2A2pD1D2D2----121	-4080.822616	30.61
144	8-19-mn-T	-4080.82209	30.94
145	2_a_Mn_CO8_A1A1A1pA2BBBB----81	-4080.819403	32.63
146	3_a_Mn_CO8_A1A1A1A1A2A2A2D1----204	-4080.815083	35.34
147	3_a_Mn_CO8_A1A1A1A1A2A2BB----206	-4080.815083	35.34
148	3_b_Mn_CO8_A1A1A1A2A2A2D1D2----244	-4080.815083	35.34
149	3_a_Mn_CO8_A1A1A1A2A2A2D1D2----212	-4080.815082	35.34
150	3_b_Mn_CO8_A1A1A1A1A2A2A2D1----236	-4080.815082	35.34
151	2_a_Mn_CO8_A1A1A1A1pA2pA2D1pD2----76	-4080.814715	35.57
152	1_a_Mn_CO8_A1A1A1A1A2A2A2D1----4-Q	-4080.814445	35.74
153	1_a_Mn_CO8_A1A1A1A2A2D2BD2----31	-4080.81317	36.54
154	1_b_Mn_CO8_A1A1A1A2A2D1D2D2----64	-4080.81317	36.54
155	1_b_Mn_CO8_A1A1A1A2A2D2BD2----65	-4080.81317	36.54
156	3_b_Mn_CO8_A1A1A1A2A2A2D1D1----243	-4080.812532	36.94
157	3_a_Mn_CO8_A1A1A1A1A2A2D2D2----209	-4080.812531	36.94
158	3_a_Mn_CO8_A1A1A1A2A2D1BD2----223	-4080.812531	36.94
159	3_b_Mn_CO8_A1A1A1A1A2A2BB----238	-4080.812531	36.94
160	3_b_Mn_CO8_A1A1A1A2A2D1D2D1----258	-4080.812531	36.94
161	3_a_Mn_CO8_A1A1A1A2A2D1BD1----222	-4080.81253	36.94
162	3_b_Mn_CO8_A1A1A1A1A2A2D1D2----240	-4080.81253	36.94
163	3_b_Mn_CO8_A1A1A1A2A2BBD2----247	-4080.81253	36.94
164	1_a_Mn_CO8_A1A1A1A2A2D1D2D2----30	-4080.812523	36.95
165	8-12-mn-T	-4080.812385	37.03
166	2_b_Mn_CO8_pA1pA1pA1A2A2A2BpD1----169-T	-4080.812384	37.03
167	3_b_Mn_CO8_A1A1A1A1A1A2A2A2----233	-4080.810403	38.28
168	2_a_Mn_CO8_A1A1A1pA2pA2pA2BD1----98-T-xqc	-4080.807796	39.91
169	2_a_Mn_CO8_A1A1A1A1pA2pA2BB----72-Q	-4080.806771	40.55
170	3_b_Mn_CO8_A1A1A1A2A2D2D2D2----262	-4080.806676	40.61
171	1_a_Mn_CO8_A1A1A1A2A2A2D1D1----14	-4080.806592	40.67
172	2_b_Mn_CO8_pA1pA1pA1pA1A2A2pD1D2----198	-4080.803318	42.72
173	2_a_Mn_CO8_pA1pA1pA1pA1A2A2BpD1----131	-4080.803317	42.72
174	2_b_Mn_CO8_pA1pA1pA1pA1A2A2BpD1----196	-4080.803317	42.72
175	2_a_Mn_CO8_pA1pA1pA1pA1A2A2pD1D2----133	-4080.80331	42.73

176	2_a_Mn_CO8_A1A1A1A1pA2pA2BD1----73	-4080.802557	43.20
177	2_b_Mn_CO8_pA1pA1pA1A2A2D2pD1D2_COdeplasat----183	-4080.801332	43.97
178	2_a_Mn_CO8_pA1pA1pA1A2A2BD2pD1_COdeplasat----112	-4080.80095	44.21
179	2_b_Mn_CO8_pA1pA1pA1A2A2BBpD1----174	-4080.800602	44.43
180	1_a_Mn_CO8_A1A1A1A2A2D1D1D2_COdeplasat----28	-4080.800029	44.79
181	1_b_Mn_CO8_A1A1A1A2A2D1D1D2_COdeplasat----62	-4080.800001	44.80
182	1_a_Mn_CO8_A1A1A1A1A2A2D1D1_COdeplasat----9	-4080.799643	45.03
183	3_b_Mn_CO8_A1A1A1A1A2A2D1D1_COdeplasat----239	-4080.79929	45.25
184	1_b_Mn_CO8_A1A1A1A2A2BBD1-2----51	-4080.799205	45.30
185	2_b_Mn_CO8_pA1pA1pA1pA1A2A2pD1pD1_COdeplasat----199	-4080.798928	45.48
186	2_b_Mn_CO8_pA1pA1pA1A2A2pD1pD1D2----188	-4080.798926	45.48
187	2_a_Mn_CO8_pA1pA1pA1A2A2pD1pD1D2----123	-4080.798925	45.48
188	1_b_Mn_CO8_A1A1A1A1A2A2D1D2_COdeplasat----44	-4080.798683	45.63
189	1_a_Mn_CO8_A1A1A1A1A2A2D1D2_COdeplasat----10	-4080.798677	45.63
190	3_a_Mn_CO8_A1A1A1A2A2D1D1D2_COdeplasat----225	-4080.798068	46.02
191	2_a_Mn_CO8_A1A1A1A1pA2pA2D1D1_COdeplasat----75	-4080.797276	46.51
192	3_b_Mn_CO8_A1A1A1A1A2A2A2A2----234-T	-4080.797135	46.60
193	3_a_Mn_CO8_A1A1A1A2A2D1D2D2----227-T	-4080.797086	46.63
194	3_b_Mn_CO8_A1A1A1A2A2D2BD2----260	-4080.795231	47.80
195	3_a_Mn_CO8_A1A1A1A2A2A2D1D1----211	-4080.79523	47.80
196	3_a_Mn_CO8_A1A1A1A2A2D1D2D1----226	-4080.79523	47.80
197	3_a_Mn_CO8_A1A1A1A2A2D2BD2----228	-4080.79523	47.80
198	3_b_Mn_CO8_A1A1A1A2A2BD2D1----252	-4080.79523	47.80
199	3_b_Mn_CO8_A1A1A1A2A2D1BD1----254	-4080.79523	47.80
200	3_a_Mn_CO8_A1A1A1A2BBBB----231	-4080.794506	48.25
201	3_a_Mn_CO8_A1A1A2A2BBBB----232	-4080.794506	48.25
202	3_b_Mn_CO8_A1A1A1A2BBBB----263	-4080.794506	48.25
203	3_b_Mn_CO8_A1A1A2A2BBBB----264	-4080.794506	48.25
204	8-12-mn-Q	-4080.792779	49.33
205	2_b_Mn_CO8_pA1pA1pA1A2A2A2BpD1----169-Q	-4080.792775	49.34
206	1_b_Mn_CO8_A1A1A1A2A2BD1B----53	-4080.791761	49.97
207	1_a_Mn_CO8_A1A1A1A2A2BD1B----19	-4080.791755	49.98
208	1_a_Mn_CO8_A1A1A1A1A2A2A2D2----5-Q	-4080.791499	50.14
209	1_b_Mn_CO8_A1A1A1A1A2A2D1D1----43	-4080.791293	50.27
210	2_a_Mn_CO8_A1A1A1pA2pA2pD2pD2pD2----102	-4080.791182	50.34
211	2_b_Mn_CO8_A1A1A1pA2pA2pD2pD2pD2----167	-4080.791182	50.34
212	3_a_Mn_CO8_A1A1A1A2A2BD2D2----221	-4080.790241	50.93
213	3_a_Mn_CO8_A1A1A1A2A2D2D2D2----230	-4080.790241	50.93
214	3_b_Mn_CO8_A1A1A1A2A2BD1B----248	-4080.788053	52.30
215	3_a_Mn_CO8_A1A1A1A2A2BD1B----216	-4080.788052	52.30
216	2_a_Mn_CO8_A1A1A1pA2pA2BBD1----83	-4080.787068	52.92
217	2_b_Mn_CO8_A1A1A1pA2pA2BpD2D1----155	-4080.787066	52.92
218	2_b_Mn_CO8_A1A1A1pA2pA2BBD1----149	-4080.787065	52.92
219	1_a_Mn_CO8_A1A1A1A2A2D1D1D1_COdeplasat----27	-4080.783574	55.11
220	1_b_Mn_CO8_A1A1A1A2A2D1D2D1_COdeplasat----63	-4080.783546	55.13

221	1_b_Mn_CO8_A1A1A1A2A2BD2D1_COdeplasat----57	-4080.782814	55.59
222	1_a_Mn_CO8_A1A1A1A2A2BD2D1_COdeplasat----23	-4080.782793	55.60
223	1_a_Mn_CO8_A1A1A1A2A2BD1D1_COdeplasat----20	-4080.782762	55.62
224	1_b_Mn_CO8_A1A1A1A2A2BD1D1_COdeplasat----54	-4080.782727	55.64
225	2_a_Mn_CO8_pA1pA1pA1pA1A2A2pD1pD1----134	-4080.781773	56.24
226	2_b_Mn_CO8_A1A1A1A1pA2pA2BD1_COdeplasat----139	-4080.781538	56.39
227	2_b_Mn_CO8_A1A1A1A1pA2pA2D1D1_COdeplasat----141	-4080.781536	56.39
228	1_b_Mn_CO8_A1A1A1A2A2D1BD1----59	-4080.780803	56.85
229	2_b_Mn_CO8_pA1pA1pA1A2A2BpD1D2----179	-4080.776545	59.52
230	2_a_Mn_CO8_pA1pA1pA1A2A2BpD1D2----114	-4080.776544	59.52
231	1_b_Mn_CO8_A1A1A1A1A2A2A2B----38-Q	-4080.772541	62.03
232	3_b_Mn_CO8_A1A1A1A2A2BD2D2----253-Q	-4080.772269	62.21
233	3_a_Mn_CO8_A1A1A1A2A2D1D2D2----227-Q	-4080.77199	62.38
234	2_b_Mn_CO8_A1A1A1pA2pA2BpD2pD2----156-Q	-4080.771989	62.38
235	2_b_Mn_CO8_A1A1A1pA2pA2BD1D1----152	-4080.771626	62.61
236	1_a_Mn_CO8_A1A1A1A2A2BBD1_COdeplasat----17	-4080.771205	62.87
237	2_a_Mn_CO8_pA1pA1pA1A2A2BD2D2----111	-4080.770829	63.11
238	2_b_Mn_CO8_pA1pA1pA1A2A2BD2D2----176	-4080.770829	63.11
239	3_a_Mn_CO8_A1A1A1A2A2D1D1D1----224	-4080.768621	64.49
240	3_b_Mn_CO8_A1A1A1A1A2A2A2A2----234-Q	-4080.764398	67.14
241	2_b_Mn_CO8_A1A1A1pA2pA2BD1pD2----153	-4080.763117	67.95
242	2_a_Mn_CO8_A1A1A1pA2pA2D1D1pD2----94	-4080.763116	67.95
243	3_b_Mn_CO8_A1A1A1A2A2BD2D2----253-T	-4080.762841	68.12
244	3_b_Mn_CO8_A1A1A1A2A2D1D1D2----257	-4080.760718	69.45
245	2_a_Mn_CO8_pA1pA1pA1A2A2BpD1pD1----115	-4080.76042	69.64
246	2_a_Mn_CO8_pA1pA1pA1A2A2BpD1B----113	-4080.760419	69.64
247	1_b_Mn_CO8_A1A1A1A2A2D1D1D1----61	-4080.756992	71.79
248	3_a_Mn_CO8_A1A1A1A2A2BD1D1----217	-4080.756624	72.02
249	2_a_Mn_CO8_A1A1A1pA2pA2BD1D1----86	-4080.756558	72.06
250	2_a_Mn_CO8_A1A1A1pA2pA2pA2BD1----98-Q	-4080.754123	73.59
251	2_b_Mn_CO8_pA1pA1pA1A2A2BpD1pD1_COdeplasat----180	-4080.752909	74.35
252	2_b_Mn_CO8_pA1pA1pA1A2A2BpD1B_COdeplasat----178	-4080.752907	74.35
253	2_a_Mn_CO8_pA1pA1pA1A2A2pD1BD2_COdeplasat----119	-4080.752761	74.45
254	3_b_Mn_CO8_A1A1A1A2A2D1D1D1----256	-4080.751621	75.16
255	2_a_Mn_CO8_A1A1A1pA2pA2D1D1D1_COdeplasat----93	-4080.751438	75.28
256	2_a_Mn_CO8_A1A1A1pA2pA2D1pD2pD2----96	-4080.750806	75.67
257	3_b_Mn_CO8_A1A1A1A2A2BD1D1----249	-4080.749915	76.23
258	2_a_Mn_CO8_pA1pA1pA1A2A2pD1pD1pD1----124	-4080.748544	77.09
259	3_b_Mn_CO8_A1A1A1A2A2BD1D2----250	-4080.747356	77.84
260	1_a_Mn_CO8_A1A1A1A2A2D1D2D1----29	-4080.74538	79.08
261	2_a_Mn_CO8_A1A1A1pA2pA2D1BD1----91	-4080.743129	80.49
262	2_b_Mn_CO8_A1A1A1pA2pA2D1BD1----157	-4080.743126	80.49
263	3_a_Mn_CO8_A1A1A1A2A2BD1D2----218	-4080.742846	80.67
264	3_a_Mn_CO8_A1A1A1A2A2D2D1D2----229	-4080.739251	82.92
265	3_b_Mn_CO8_A1A1A1A2A2D2D1D2----261	-4080.739251	82.92

266	2_b_Mn_CO8_pA1pA1pA1A2A2BD2pD1----177	-4080.738742	83.24
267	3_a_Mn_CO8_A1A1A1A1A2A2D1D1----207	-4080.734937	85.63
268	2_b_Mn_CO8_pA1pA1pA1A2A2pD1BD2_COdeplasat----184	-4080.7342	86.09
269	2_b_Mn_CO8_pA1pA1pA1A2A2pD1pD1pD1_COdeplasat----189	-4080.732718	87.02
270	2_a_Mn_CO8_pA1pA1pA1A2A2pD1BpD1----120	-4080.730434	88.46
271	2_b_Mn_CO8_pA1pA1pA1A2A2pD1BpD1----185	-4080.730434	88.46
272	2_a_Mn_CO8_A1A1A1pA2pA2BD1pD2_COdeplasat----87	-4080.726593	90.87
273	1_b_Mn_CO8_A1A1A1A2A2BD1D2----55	-4080.726429	90.97
274	1_a_Mn_CO8_A1A1A1A2A2BD1D2----21	-4080.726428	90.97
275	1_a_Mn_CO8_A1A1A1A2A2BD2D2----24	-4080.722613	93.36
276	2_b_Mn_CO8_pA1pA1pA1A2A2pD1D2D2----186	-4080.722142	93.66
277	1_a_Mn_CO8_A1A1A1A2A2D2D1D2----32	-4080.720419	94.74
278	1_b_Mn_CO8_A1A1A1A2A2D2D1D2----66	-4080.720419	94.74
279	2_b_Mn_CO8_A1A1A1pA2pA2D1pD2D1----160	-4080.715526	97.81
280	2_a_Mn_CO8_pA1pA1pA1A2A2D2BD2----116	-4080.713412	99.14
281	2_a_Mn_CO8_A1A1A1pA2pA2D1pD2D1----95	-4080.709796	101.41
282	2_a_Mn_CO8_A1A1A1pA2pA2pD2D1pD2----101	-4080.705731	103.96
283	2_b_Mn_CO8_A1A1A1pA2pA2pD2D1pD2----166	-4080.705731	103.96
284	2_a_Mn_CO8_pA1pA1pA1A2A2D2pD1D2----118	-4080.704933	104.46
285	2_b_Mn_CO8_A1A1A1pA2pA2D1BpD2----158	-4080.700441	107.28
286	2_b_Mn_CO8_A1A1A1pA2pA2D1D1pD2_COdeplasat----159	-4080.69811	108.74
287	2_b_Mn_CO8_pA1pA1pA1A2A2pD1D2pD1----187	-4080.695389	110.45
288	2_a_Mn_CO8_pA1pA1pA1A2A2pD1D2pD1_COdeplasat----122	-4080.6332	149.47

Table S7. CO dissociation energies for $H_2C_2S_2Mn_2(CO)_n$ systems.

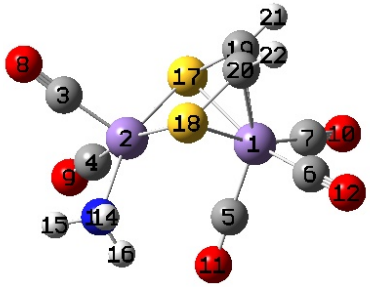
Reaction	ΔE, kcal/mol	ΔG, kcal/mol
$H_2C_2S_2Mn_2(CO)_8$ (**MnS8-1S**) → $H_2C_2S_2Mn_2(CO)_7$ (**MnS7-1S**) + CO	2.4	-7.0
$H_2C_2S_2Mn_2(CO)_7$ (**MnS7-1S**) → $H_2C_2S_2Mn_2(CO)_6$ (**MnS6-1S**) + CO	16.8	6.6
$H_2C_2S_2Mn_2(CO)_6$ (**MnS6-1S**) → $H_2C_2S_2Mn_2(CO)_5$ (**MnS5-7S**) + CO	48.3	37.8
$H_2C_2S_2Mn_2(CO)_5$ (**MnS5-1Q**)→ $H_2C_2S_2Mn_2(CO)_4$ (**MnS4-1Q**)+ CO	8.6	-2.0

Table S8. Orbital energies and HOMO/LUMO gaps for $H_2C_2S_2Mn_2(CO)_n$ systems.

	Name	LUMO (Hartree)	HOMO (Hartree)	Gap (Hartree)	Gap (eV)
1	MnS4-1Q	-0.05764	-0.25500	0.19736	5.37
2	MnS4-2Q	-0.07161	-0.24510	0.17349	4.72
3	MnS4-3T	-0.10465	-0.24287	0.13822	3.76
4	MnS4-4T	-0.11325	-0.24730	0.13405	3.65
1	MnS5-1Q	-0.06910	-0.22582	0.15672	4.26
2	MnS5-2T	-0.06714	-0.25301	0.18587	5.06
3	MnS5-3Q	-0.11381	-0.22744	0.11363	3.09
4	MnS5-4Q	-0.07133	-0.21759	0.14626	3.98
5	MnS5-5T	-0.08524	-0.25424	0.16900	4.60
6	MnS5-6Q	-0.10155	-0.23639	0.13484	3.67
7	MnS5-7S	-0.11157	-0.25544	0.14387	3.91
8	MnS5-8Q	-0.08931	-0.23019	0.14088	3.83
9	MnS5-9S	-0.09528	-0.24757	0.15229	4.14
10	MnS5-10T	-0.07930	-0.23838	0.15908	4.33
11	MnS5-11Q	-0.07557	-0.21332	0.13775	3.75
12	MnS5-12S	-0.11509	-0.24938	0.13429	3.65
13	MnS5-13S	-0.09435	-0.24707	0.15272	4.16
14	MnS5-14T	-0.07958	-0.23833	0.15875	4.32
15	MnS5-15Q	-0.09535	-0.22604	0.13069	3.56
1	MnS6-1S	-0.08765	-0.26573	0.17808	4.85
2	MnS6-2Q	-0.06765	-0.22332	0.15567	4.24
3	MnS6-3T	-0.06850	-0.24063	0.17213	4.68
4	MnS6-4T	-0.07378	-0.25129	0.17751	4.83
5	MnS6-5T	-0.06313	-0.22740	0.16427	4.47
1	MnS7-1S	-0.08334	-0.26316	0.17982	4.89
2	MnS7-2S	-0.09909	-0.24581	0.14672	3.99
3	MnS7-3S	-0.11312	-0.25991	0.14679	3.99
4	MnS7-4S	-0.12644	-0.25154	0.12510	3.40
5	MnS7-5S	-0.10728	-0.25736	0.15008	4.08
6	MnS7-6S	-0.11098	-0.23702	0.12604	3.43
1	MnS8-1S	-0.09752	-0.25036	0.15284	4.16
2	MnS8-2S	-0.08914	-0.23020	0.14106	3.84
3	MnS8-3S	-0.09886	-0.22765	0.12879	3.50
4	MnS8-4S	-0.09948	-0.23172	0.13224	3.60
5	MnS8-5S	-0.10509	-0.22699	0.12190	3.32
6	MnS8-6S	-0.08334	-0.25190	0.16856	4.59
7	MnS8-7S	-0.10651	-0.21377	0.10726	2.92
8	MnS8-8S	-0.10379	-0.23930	0.13551	3.69

9	MnS8-9T	-0.09037	-0.20806	0.11769	3.20
10	MnS8-10S	-0.10310	-0.22025	0.11715	3.19

Table S9. Distance table for the lowest-lying $H_2C_2S_2Mn_2(CO)_5$•NH_3 structures after PBE0/6-311G(d,p) optimization followed by a single point CCSD(T) energy calculation. Provided are the absolute energy (a.u.) and relative energy (kcal/mol).



1S. -3795.49266504963 0.0 C_1
WBI 0.06

		1	2	3	4	5
1	Mn	0.000000				
2	Mn	2.835250	0.000000			
3	C	4.385277	1.739608	0.000000		
4	C	3.918206	1.772103	2.498289	0.000000	
5	C	1.781857	2.903615	4.639678	3.420443	0.000000
6	C	1.780917	4.290816	5.787753	5.494680	2.577471
7	C	1.785981	4.228582	5.760263	4.805462	2.608651
8	O	5.455624	2.890983	1.152498	3.427345	5.791209
9	O	4.851882	2.922552	3.411601	1.150511	4.155530
10	O	2.927801	5.248097	6.741842	5.608074	3.538982
11	O	2.929618	3.477333	5.140568	3.593970	1.148719
12	O	2.923868	5.333033	6.783611	6.566345	3.502098
13	N	3.924045	2.089649	2.874627	2.773628	3.227400
14	H	4.183115	2.687681	3.272078	3.714226	3.693230
15	H	4.847124	2.629278	2.916290	2.844529	4.084010
16	H	3.876324	2.641326	3.753593	3.018720	2.756547
17	S	2.394190	2.222840	3.160403	2.856746	3.311004
18	S	2.388411	2.282188	3.151407	4.028161	3.236099
19	C	2.121055	3.200430	4.067725	4.395438	3.757522
20	C	2.114913	3.223157	4.071822	4.787758	3.725208
21	H	2.865120	4.234998	5.020716	5.274142	4.541239
22	H	2.865047	4.263037	5.018838	5.862491	4.498566

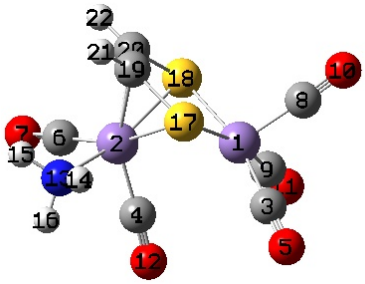
		6	7	8	9	10
6	C	0.000000				
7	C	2.550786	0.000000			
8	O	6.824843	6.807156	0.000000		
9	O	6.427249	5.473592	4.150068	0.000000	
10	O	3.460301	1.141885	7.763637	6.123726	0.000000
11	O	3.475010	3.554612	6.276786	4.111369	4.319757
12	O	1.143014	3.458716	7.792533	7.492238	4.180285
13	N	4.776460	5.452235	3.794317	3.634139	6.503743
14	H	4.731278	5.848445	4.068113	4.627087	6.948561
15	H	5.784219	6.308231	3.634231	3.491038	7.324087
16	H	4.571571	5.240675	4.733224	3.725504	6.232934
17	S	4.130482	3.008498	4.051729	3.694161	3.808487
18	S	3.040092	4.137426	4.029338	5.172600	5.266856
19	C	3.352361	2.810957	4.862581	5.349991	3.655990
20	C	2.781681	3.382910	4.862466	5.870383	4.380322
21	H	3.853449	2.958056	5.728633	6.136541	3.516066
22	H	2.921083	3.912705	5.718545	6.949352	4.807263

		11	12	13	14	15
11	O	0.000000				
12	O	4.212799	0.000000			
13	N	3.232206	5.567852	0.000000		
14	H	3.778685	5.379896	1.017079	0.000000	
15	H	3.943851	6.579912	1.014754	1.622633	0.000000
16	H	2.460983	5.302191	1.017992	1.626945	1.623744
17	S	4.230869	5.258635	4.232287	4.763974	4.821549
18	S	4.091425	3.854158	2.972876	2.772129	3.835842

19 C	4.874568	4.341730	4.953183	5.169294	5.723513
20 C	4.818257	3.623418	4.531281	4.482183	5.385934
21 H	5.667574	4.729656	6.025013	6.245875	6.791301
22 H	5.584435	3.466454	5.381396	5.182662	6.262340

	16	17	18	19	20
16 H	0.000000				
17 S	4.544696	0.000000			
18 S	3.458427	3.115311	0.000000		
19 C	5.282896	1.743966	2.704882	0.000000	
20 C	4.905057	2.713439	1.741343	1.381182	0.000000
21 H	6.314735	2.451805	3.719088	1.084057	2.156473
22 H	5.730444	3.728955	2.448056	2.161887	1.083542

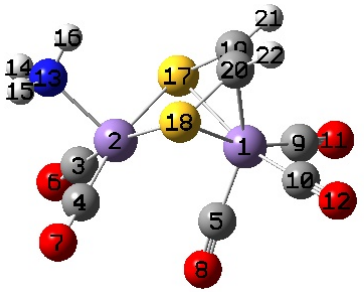
	21	22
21 H	0.000000	
22 H	2.525014	0.000000



2S. -3795.49165154984 +0.6 C_1
WBI 0.08

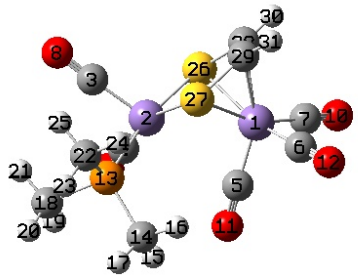
	1	2	3	4	5
1 Mn	0.000000				
2 Mn	2.745827	0.000000			
3 C	1.789850	3.771563	0.000000		
4 C	2.866318	1.778329	3.273257	0.000000	
5 O	2.933900	4.669788	1.144074	3.951565	0.000000
6 C	4.200432	1.771370	5.331933	2.532266	6.213793
7 O	5.255774	2.919271	6.409528	3.453989	7.277232
8 C	1.756562	4.304918	2.573299	4.622210	3.503060
9 C	1.790066	3.791794	2.549780	3.265680	3.459889
10 O	2.900402	5.367864	3.510485	5.766515	4.270092
11 O	2.933122	4.699543	3.457157	3.944778	4.178263
12 O	3.501059	2.927485	3.482223	1.149769	3.916775
13 N	4.381052	2.076849	4.791222	2.797090	5.351772
14 H	4.384620	2.602209	4.552839	3.290892	4.997813
15 H	5.164418	2.663538	5.733804	3.639072	6.333513
16 H	4.843788	2.642691	5.025161	2.727235	5.446515
17 S	2.277430	2.393725	2.865443	3.354052	3.671963
18 S	2.261125	2.382866	4.016262	3.289201	5.149582
19 C	3.206071	2.123292	4.374012	3.777434	5.302800
20 C	3.197964	2.126753	4.750101	3.759154	5.812100
21 H	4.247835	2.894003	5.261349	4.571546	6.096097
22 H	4.235510	2.889016	5.823420	4.533649	6.888172

	6	7	8	9	10
6 C	0.000000				
7 O	1.148048	0.000000			
8 C	5.731849	6.751439	0.000000		
9 C	4.744323	5.593722	2.560897	0.000000	
10 O	6.768579	7.764303	1.144822	3.493788	0.000000
11 O	5.380843	6.080072	3.484321	1.143060	4.242901
12 O	3.425626	4.151622	5.191125	3.444130	6.322009
13 N	2.769978	3.623534	5.881721	5.582044	6.905681
14 H	3.676117	4.598618	5.729654	5.778456	6.690504
15 H	2.899636	3.535711	6.591047	6.383724	7.570528
16 H	3.051513	3.757060	6.453492	5.829705	7.525300
17 S	4.119873	5.252259	3.136294	4.038787	3.999587
18 S	3.048865	3.879053	3.140186	2.850639	4.009183
19 C	3.342441	4.333613	4.041707	4.760815	4.819944
20 C	2.809614	3.661096	4.035294	4.367985	4.814058
21 H	3.860980	4.730653	4.992319	5.837561	5.678744

	22 H 2.973988 3.531393 4.986949 5.244942 5.676209 11 12 13 14 15 11 O 0.000000 12 O 3.864796 0.000000 13 N 6.490712 3.658656 0.000000 14 H 6.765072 4.101226 1.017272 0.000000 15 H 7.285104 4.521492 1.015930 1.634602 0.000000 16 H 6.635289 3.313884 1.015310 1.626313 1.622216 17 S 5.173474 4.287780 3.104836 2.737016 3.746836 18 S 3.661825 4.195523 4.410651 4.783144 4.841861 19 C 5.824756 4.902453 2.953341 2.949098 3.160610 20 C 5.299925 4.873622 3.614793 3.931603 3.763849 21 H 6.904141 5.693779 3.049864 2.935708 2.962810 22 H 6.081118 5.637873 4.140012 4.569092 4.038705 16 17 18 19 20 16 H 0.000000 17 S 3.855460 0.000000 18 S 5.022905 3.158633 0.000000 19 C 3.911103 1.745615 2.717011 0.000000 20 C 4.460920 2.717998 1.740447 1.376176 0.000000 21 H 4.064841 2.449435 3.727144 1.084813 2.151134 22 H 4.980160 3.729904 2.438861 2.152539 1.084341 21 22 21 H 0.000000 22 H 2.509971 0.000000
 3S. -3795.48818784938 +2.8 C_s WBI 0.06	1 2 3 4 5 1 Mn 0.000000 2 Mn 2.806496 0.000000 3 C 3.877211 1.770340 0.000000 4 C 3.877351 1.770337 2.505122 0.000000 5 C 1.800157 2.874071 3.338495 3.338735 0.000000 6 O 4.802907 2.920900 1.150577 3.413094 4.048024 7 O 4.803109 2.920897 3.413099 1.150578 4.048377 8 O 2.941274 3.496661 3.529910 3.530193 1.142351 9 C 1.781107 4.226776 4.795594 5.419602 2.583598 10 C 1.781107 4.226758 5.419427 4.795730 2.583606 11 O 2.923594 5.260210 5.618977 6.481468 3.507028 12 O 2.923595 5.260190 6.481288 5.619114 3.507043 13 N 4.544581 2.043893 2.808980 2.808948 4.914247 14 H 5.173662 2.625981 2.753113 3.413496 5.425486 15 H 5.173469 2.625963 3.413881 2.753180 5.425520 16 H 4.570610 2.564292 3.573267 3.573506 5.294049 17 S 2.394927 2.296405 2.902362 4.042591 3.312107 18 S 2.394943 2.296365 4.042524 2.902320 3.312118 19 C 2.112830 3.242859 4.417849 4.793536 3.765296 20 C 2.112830 3.242847 4.793503 4.417844 3.765293 21 H 2.858014 4.281751 5.303324 5.866874 4.536126 22 H 2.858013 4.281734 5.866834 5.303306 4.536120 6 7 8 9 10 6 O 0.000000 7 O 4.121714 0.000000 8 O 3.995828 3.996272 0.000000 9 C 5.453421 6.342544 3.475994 0.000000 10 C 6.342286 5.453647 3.476008 2.543892 0.000000 11 O 6.126246 7.396117 4.213757 1.142634 3.449884

12	O	7.395843	6.126484	4.213783	3.449881	1.142634
13	N	3.696254	3.696195	5.508121	5.926756	5.926817
14	H	3.374429	4.252863	5.931080	6.372349	6.689040
15	H	4.253400	3.374502	5.931237	6.688856	6.372145
16	H	4.490291	4.490584	6.042205	5.912541	5.912783
17	S	3.724152	5.186358	4.227999	3.011412	4.136398
18	S	5.186278	3.724113	4.228012	4.136417	3.011420
19	C	5.364038	5.870835	4.879161	2.789323	3.360691
20	C	5.870791	5.364038	4.879159	3.360704	2.789305
21	H	6.157259	6.947596	5.642560	2.929836	3.869891
22	H	6.947541	6.157244	5.642555	3.869903	2.929809
		11	12	13	14	15
11	O	0.000000				
12	O	4.165301	0.000000			
13	N	6.912463	6.912552	0.000000		
14	H	7.271829	7.723498	1.015100	0.000000	
15	H	7.723313	7.271626	1.015101	1.626049	0.000000
16	H	6.878035	6.878378	1.016260	1.625915	1.625921
17	S	3.814611	5.264759	3.278824	3.552740	4.214234
18	S	5.264779	3.814617	3.278961	4.214477	3.552427
19	C	3.630502	4.351335	4.118977	4.669590	4.903787
20	C	4.351355	3.630476	4.119030	4.904205	4.669153
21	H	3.477291	4.749504	5.049880	5.511479	5.870011
22	H	4.749527	3.477251	5.049959	5.870462	5.511003
		16	17	18	19	20
16	H	0.000000				
17	S	3.196991	0.000000			
18	S	3.197553	3.161000	0.000000		
19	C	3.707696	1.746591	2.723423	0.000000	
20	C	3.707914	2.723424	1.746590	1.381353	0.000000
21	H	4.544898	2.449067	3.733740	1.084186	2.155573
22	H	4.545224	3.733742	2.449065	2.155574	1.084187
		21	22			
21	H	0.000000				
22	H	2.512780	0.000000			

Table S10. Distance table for the lowest-lying $H_2C_2S_2Mn_2(CO)_5$•PMe_3 structures after PBE0/6-311G(d,p) optimization followed by a single point CCSD(T) energy calculation. Provided are the absolute energy (a.u.) and relative energy (kcal/mol).

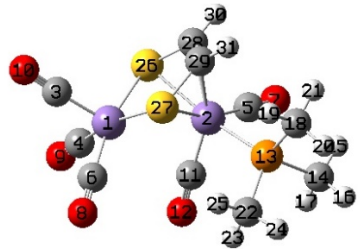


1S. -4199.38040842987 0.0 C_1
WBI 0.06

		1	2	3	4	5
1	Mn	0.000000				
2	Mn	2.855043	0.000000			
3	C	4.414063	1.737165	0.000000		
4	C	3.826550	1.767123	2.513817	0.000000	
5	C	1.790597	2.996358	4.726366	3.269092	0.000000
6	C	1.781764	4.257297	5.807733	5.339733	2.595171
7	C	1.779846	4.304599	5.792806	4.811801	2.565440
8	O	5.495307	2.889845	1.153230	3.451543	5.878072
9	O	4.708360	2.917685	3.447367	1.150666	3.880656
10	O	2.922265	5.344890	6.778452	5.662111	3.487917
11	O	2.934812	3.617237	5.278523	3.423534	1.144716
12	O	2.924931	5.281006	6.798122	6.389156	3.522090
13	P	4.321302	2.252866	2.830533	2.848818	3.845046
14	C	4.511907	3.517394	4.568742	3.912933	3.577166
15	H	4.463137	3.693968	4.919258	3.666123	3.150939
16	H	4.053004	3.688968	4.905382	4.433449	3.342760
17	H	5.582682	4.458491	5.276007	4.775709	4.638965
18	C	5.855474	3.451235	3.447126	3.159427	5.099556
19	H	5.860285	3.624918	3.851089	2.808493	4.860791
20	H	6.653855	4.410651	4.404299	4.217674	5.825464
21	H	6.269527	3.577813	3.032722	3.296145	5.736086
22	C	5.358846	3.445730	3.418671	4.466072	5.293058
23	H	6.254628	4.408033	4.378821	5.212861	5.994177
24	H	5.018646	3.628684	3.822894	4.953795	5.199411
25	H	5.788037	3.559185	2.987468	4.568608	5.899881
26	S	2.385680	2.243745	3.113808	2.872837	3.260524
27	S	2.406787	2.256015	3.234259	3.967278	3.377276
28	C	2.115681	3.207841	4.071968	4.386613	3.744372
29	C	2.116582	3.219315	4.126985	4.755104	3.782281
30	H	2.857247	4.243412	5.010690	5.271359	4.496957
31	H	2.863886	4.255830	5.086098	5.825047	4.558303

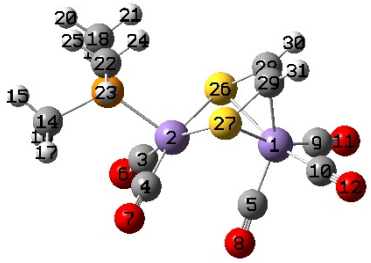
		6	7	8	9	10
6	C	0.000000				
7	C	2.545159	0.000000			
8	O	6.871234	6.833873	0.000000		
9	O	6.206521	5.427382	4.205589	0.000000	
10	O	3.452638	1.142552	7.787068	6.133603	0.000000
11	O	3.509996	3.460539	6.412021	3.750524	4.195426
12	O	1.143249	3.455552	7.839655	7.242299	4.174418
13	P	5.102566	5.924919	3.659789	3.661430	7.005615
14	C	4.760548	5.981908	5.475874	4.523583	7.010596
15	H	4.806777	5.697129	5.893183	4.065990	6.633341
16	H	3.954682	5.551281	5.863945	5.178477	6.594205
17	H	5.706563	7.057835	6.052820	5.285404	8.078873
18	C	6.789737	7.288207	3.930218	3.471507	8.288152
19	H	6.885518	7.099452	4.426767	2.789948	8.014465
20	H	7.390504	8.131028	4.794390	4.472969	9.145572
21	H	7.359860	7.701574	3.221201	3.601617	8.696347
22	C	5.845896	7.107054	3.862703	5.340906	8.239001

23	H	6.597369	7.986057	4.734592	5.959602	9.111182
24	H	5.258943	6.796990	4.340813	5.937757	7.939308
25	H	6.474663	7.513828	3.127452	5.438731	8.634545
26	S	4.130213	3.039292	4.002288	3.706176	3.852911
27	S	3.016947	4.134252	4.145579	5.099342	5.258379
28	C	3.378470	2.766400	4.882221	5.333672	3.599936
29	C	2.792981	3.324718	4.950490	5.825481	4.304579
30	H	3.901920	2.885668	5.730087	6.127461	3.416129
31	H	2.941834	3.824188	5.828841	6.897417	4.686596
		11	12	13	14	15
11	O	0.000000				
12	O	4.259647	0.000000			
13	P	3.998911	5.845963	0.000000		
14	C	3.404208	5.253168	1.832824	0.000000	
15	H	2.665679	5.350224	2.429785	1.091798	0.000000
16	H	3.375640	4.308938	2.428654	1.092700	1.769142
17	H	4.364089	6.077658	2.445797	1.093501	1.782513
18	C	4.949058	7.558894	1.828123	2.854439	3.103343
19	H	4.527990	7.698898	2.427610	3.111036	2.964763
20	H	5.582587	8.045863	2.444483	2.976822	3.332579
21	H	5.713453	8.193835	2.415208	3.819595	4.125880
22	C	5.601160	6.408043	1.831734	2.858640	3.828587
23	H	6.144203	7.054400	2.449703	2.991018	3.989260
24	H	5.654980	5.710052	2.436582	3.113884	4.138489
25	H	6.285003	7.119668	2.412988	3.820823	4.699959
26	S	4.149985	5.260608	4.473645	5.449771	5.406892
27	S	4.306170	3.814207	3.150723	3.850897	4.370717
28	C	4.849164	4.375500	5.201383	5.987153	6.121244
29	C	4.901973	3.634758	4.757874	5.408496	5.740713
30	H	5.590816	4.796795	6.279931	7.022138	7.105744
31	H	5.677634	3.492783	5.593908	6.099133	6.496719
		16	17	18	19	20
16	H	0.000000				
17	H	1.780784	0.000000			
18	C	3.824059	2.975978	0.000000		
19	H	4.134583	3.342732	1.091716	0.000000	
20	H	3.976122	2.684867	1.092982	1.784014	0.000000
21	H	4.698763	3.971012	1.092761	1.768173	1.782239
22	C	3.104267	2.977921	2.830268	3.807972	2.956817
23	H	3.346397	2.697662	2.952295	3.962589	2.662146
24	H	2.964040	3.337573	3.809830	4.704713	3.962821
25	H	4.122131	3.975071	3.053733	4.076126	3.297399
26	S	5.397259	6.488541	5.573971	5.531539	6.587546
27	S	3.390526	4.732823	4.893963	5.342543	5.568091
28	C	5.622390	7.016200	6.645141	6.784652	7.554044
29	C	4.875404	6.363882	6.410232	6.722507	7.187562
30	H	6.619417	8.062210	7.692781	7.788070	8.619773
31	H	5.425310	6.997452	7.313157	7.684521	8.019549
		21	22	23	24	25
21	H	0.000000				
22	C	3.050546	0.000000			
23	H	3.280501	1.093285	0.000000		
24	H	4.079170	1.092046	1.781797	0.000000	
25	H	2.869559	1.092713	1.783382	1.768648	0.000000
26	S	5.597118	5.560794	6.579025	5.523290	5.568737

	27 S 5.141271 3.435238 4.428292 2.902940 3.743480 28 C 6.724002 5.899564 6.950315 5.535660 5.961849 29 C 6.570200 5.139495 6.156404 4.574148 5.303891 30 H 7.744202 6.965549 8.020044 6.566789 6.996012 31 H 7.492098 5.750348 6.720507 5.024456 5.938583 26 27 28 29 30 26 S 0.000000 27 S 3.109640 0.000000 28 C 1.743012 2.704430 0.000000 29 C 2.711601 1.746134 1.379643 0.000000 30 H 2.448018 3.721192 1.084105 2.157408 0.000000 31 H 3.728336 2.452735 2.162871 1.083526 2.530789 31 31 H 0.000000
 2S. -4199.38027195004 +0.1 C_1 WBI 0.08	1 2 3 4 5 1 Mn 0.000000 2 Mn 2.756445 0.000000 3 C 1.757019 4.323558 0.000000 4 C 1.791392 3.786949 2.564398 0.000000 5 C 4.219093 1.763881 5.751059 4.762974 0.000000 6 C 1.788872 3.773175 2.573626 2.551015 5.346683 7 O 5.277578 2.912596 6.771926 5.620705 1.148808 8 O 2.933201 4.663465 3.506870 3.464212 6.222408 9 O 2.934369 4.688067 3.489472 1.142989 5.397449 10 O 2.901087 5.390061 1.144972 3.497848 6.789062 11 C 2.873843 1.773182 4.629028 3.227180 2.523673 12 O 3.512889 2.923190 5.199169 3.393257 3.414248 13 P 4.520359 2.248559 6.057534 5.662441 2.871762 14 C 5.981422 3.466869 7.630005 6.794980 3.120259 15 H 6.354837 3.652853 7.957282 7.154776 2.867222 16 H 6.824289 4.419018 8.442043 7.706217 4.203755 17 H 5.936608 3.601558 7.661632 6.476301 3.113608 18 C 5.604251 3.506814 6.852388 7.033461 4.098494 19 H 5.311471 3.688077 6.350715 6.901919 4.648151 20 H 6.526130 4.447687 7.802037 7.912415 4.919070 21 H 5.979166 3.684673 7.178164 7.378820 3.933599 22 C 4.826506 3.438554 6.300765 5.901629 4.398159 23 H 4.741218 3.581627 6.305187 5.511023 4.433587 24 H 5.906772 4.402635 7.340696 6.988126 5.172907 25 H 4.420995 3.587542 5.698680 5.670821 4.890746 26 S 2.260009 2.380332 3.148140 2.853453 3.051849 27 S 2.264902 2.391744 3.146059 4.023238 4.103920 28 C 3.198413 2.117510 4.055109 4.367831 2.778062 29 C 3.208790 2.122564 4.065213 4.761716 3.314625 30 H 4.235175 2.873226 5.007892 5.243301 2.923935 31 H 4.247558 2.895798 5.011677 5.836274 3.830267 6 7 8 9 10 6 C 0.000000 7 O 6.430553 0.000000 8 O 1.144414 7.293630 0.000000 9 O 3.458118 6.107745 4.183302 0.000000 10 O 3.509583 7.785326 4.273224 4.249581 0.000000 11 C 3.304431 3.444558 3.986121 3.887298 5.773400 12 O 3.536763 4.136640 3.985643 3.781367 6.328534 13 P 4.838295 3.690142 5.339361 6.541716 7.097410

14	C	6.321755	3.396567	6.766606	7.489812	8.712322
15	H	6.955535	2.856414	7.525246	7.834875	9.012697
16	H	6.977448	4.441276	7.290416	8.416902	9.508477
17	H	6.204178	3.299290	6.612231	7.036029	8.783879
18	C	5.961698	4.791049	6.431136	8.019242	7.745650
19	H	5.588851	5.480873	6.030647	7.959477	7.151400
20	H	6.688871	5.502430	7.018314	8.870118	8.699700
21	H	6.610839	4.463072	7.208075	8.348479	8.038050
22	C	4.441952	5.248612	4.544245	6.744335	7.323038
23	H	4.207485	5.239081	4.225635	6.220924	7.373019
24	H	5.453727	5.902709	5.442054	7.811325	8.335094
25	H	3.844234	5.866971	3.867293	6.596367	6.644664
26	S	4.012169	3.883048	5.144364	3.666309	4.021940
27	S	2.847493	5.235426	3.649520	5.156383	4.017229
28	C	4.742555	3.625922	5.799343	5.299448	4.843382
29	C	4.365905	4.301525	5.286818	5.824511	4.852731
30	H	5.815082	3.470944	6.874244	6.078955	5.709185
31	H	5.248861	4.692448	6.073795	6.901857	5.708383
		11	12	13	14	15
11	C	0.000000				
12	O	1.150877	0.000000			
13	P	2.832356	3.634436	0.000000		
14	C	3.631388	4.123942	1.829584	0.000000	
15	H	4.126339	4.733366	2.427412	1.091823	0.000000
16	H	4.530845	4.919780	2.442848	1.092772	1.783762
17	H	3.263618	3.492157	2.424085	1.092567	1.767225
18	C	4.555833	5.431795	1.832398	2.841883	3.082313
19	H	4.823789	5.737562	2.430177	3.813308	4.114244
20	H	5.259985	5.999486	2.442615	2.947912	3.291998
21	H	4.978632	5.937571	2.431578	3.094639	2.936745
22	C	3.261678	3.637212	1.829662	2.847020	3.818445
23	H	2.839632	2.885718	2.422583	3.084160	4.111180
24	H	4.270475	4.560654	2.449198	2.979080	3.976410
25	H	3.556396	3.997954	2.419681	3.815499	4.698688
26	S	3.249138	4.148659	4.605349	5.738397	5.714638
27	S	3.373695	4.319302	3.289532	5.065714	5.439557
28	C	3.731299	4.843828	3.859776	5.072789	4.906465
29	C	3.780436	4.910080	3.211361	4.741641	4.759280
30	H	4.492682	5.590696	4.380909	5.322310	4.932031
31	H	4.582496	5.710688	3.314272	4.759411	4.688981
		16	17	18	19	20
16	H	0.000000				
17	H	1.780388	0.000000			
18	C	2.967267	3.814685	0.000000		
19	H	3.958079	4.698944	1.092185	0.000000	
20	H	2.657736	3.953694	1.093425	1.776213	0.000000
21	H	3.333979	4.117418	1.092613	1.777691	1.778184
22	C	2.959141	3.096608	2.841521	3.067991	2.967631
23	H	3.300934	2.935490	3.812201	4.097377	3.962563
24	H	2.676905	3.341180	2.961248	3.284851	2.672221
25	H	3.963048	4.115180	3.086399	2.913126	3.333229
26	S	6.744433	5.764402	5.563622	5.505018	6.605232
27	S	5.720375	5.419030	3.750979	3.211787	4.684107
28	C	5.991212	5.418857	4.318771	4.239008	5.404175
29	C	5.497540	5.254736	3.347427	3.029711	4.431585

30	H	6.241240	5.725267	4.646813	4.692590	5.703433
31	H	5.374781	5.464966	2.851496	2.459988	3.903489
		21	22	23	24	25
21	H	0.000000				
22	C	3.816768	0.000000			
23	H	4.700719	1.092131	0.000000		
24	H	3.969054	1.093281	1.781730	0.000000	
25	H	4.108953	1.091954	1.768893	1.783616	0.000000
26	S	5.522328	5.665742	5.701367	6.688693	5.570454
27	S	4.188829	3.710021	4.143567	4.639990	3.134119
28	C	4.083471	5.227457	5.578288	6.113199	5.149526
29	C	3.307601	4.390174	4.938276	5.212244	4.150355
30	H	4.158058	5.947982	6.337872	6.748608	5.981474
31	H	2.636076	4.566464	5.299155	5.208302	4.351462
		26	27	28	29	30
26	S	0.000000				
27	S	3.142725	0.000000			
28	C	1.738763	2.709560	0.000000		
29	C	2.716741	1.744344	1.377248	0.000000	
30	H	2.436546	3.723248	1.084063	2.153464	0.000000
31	H	3.726911	2.450088	2.154119	1.083034	2.515849
		31				
31	H	0.000000				



3S. -4199.37926041001 +0.7 C_1
WBI 0.06

		1	2	3	4	5
1	Mn	0.000000				
2	Mn	2.832507	0.000000			
3	C	3.848850	1.765479	0.000000		
4	C	3.861119	1.766021	2.508593	0.000000	
5	C	1.799394	2.924580	3.321462	3.342541	0.000000
6	O	4.754487	2.916919	1.151443	3.422137	4.000442
7	O	4.768843	2.917226	3.422408	1.151210	4.026844
8	O	2.940668	3.540199	3.509469	3.533286	1.142013
9	C	1.781054	4.256008	4.771667	5.412131	2.588216
10	C	1.780998	4.257339	5.397548	4.786485	2.587304
11	O	2.923756	5.289162	5.596895	6.477005	3.512929
12	O	2.923699	5.291224	6.462034	5.612714	3.512118
13	P	4.833021	2.193349	2.811269	2.827304	5.114243
14	C	6.254965	3.425875	3.321493	3.259594	6.095044
15	H	7.174003	4.377009	4.322972	4.281446	7.138780
16	H	6.371988	3.592157	2.923225	3.520489	6.014518
17	H	6.350321	3.586902	3.633259	2.862156	6.025248
18	C	5.629166	3.410515	3.575822	4.512004	6.144271
19	H	5.734058	3.566918	3.205247	4.716775	6.053827
20	H	6.667374	4.365226	4.505887	5.247233	7.178171
21	H	5.304379	3.571962	4.021965	4.935905	6.118101
22	C	5.599043	3.412840	4.522113	3.700128	6.177741
23	H	5.689472	3.573932	4.782079	3.366130	6.113270
24	H	5.267820	3.571272	4.910268	4.173093	6.149551
25	H	6.642292	4.366858	5.250103	4.608161	7.205381
26	S	2.396147	2.273834	2.862181	4.007173	3.313311
27	S	2.397015	2.272737	4.001902	2.855822	3.311253
28	C	2.114488	3.228259	4.382233	4.760491	3.765711
29	C	2.114323	3.228027	4.759124	4.379858	3.764418
30	H	2.858071	4.265801	5.264404	5.833912	4.534958
31	H	2.857501	4.265552	5.831811	5.260957	4.532698

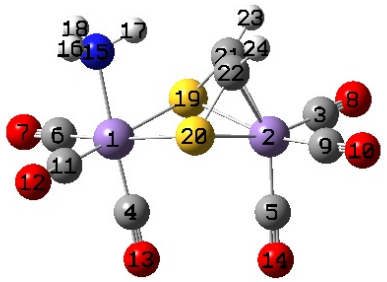
	6	7	8	9	10
6 O	0.000000				
7 O	4.140328	0.000000			
8 O	3.940134	3.972523	0.000000		
9 C	5.401284	6.317524	3.487549	0.000000	
10 C	6.298504	5.419633	3.485849	2.540501	0.000000
11 O	6.073147	7.374860	4.229699	1.142841	3.446963
12 O	7.354421	6.093304	4.227791	3.446613	1.142847
13 P	3.644342	3.666510	5.638570	6.203204	6.220611
14 C	3.731944	3.643613	6.316121	7.604108	7.586513
15 H	4.662356	4.601693	7.398988	8.518786	8.509508
16 H	3.009624	3.928056	6.111528	7.545727	7.807409
17 H	4.094724	2.918887	6.142681	7.816726	7.493406
18 C	4.112336	5.424456	6.746784	6.645227	7.211255
19 H	3.471134	5.641583	6.553288	6.545359	7.424178
20 H	4.948652	6.037094	7.748729	7.723670	8.198144
21 H	4.667037	5.941913	6.868935	6.215812	6.862928
22 C	5.436012	4.290926	6.811911	7.143522	6.660741
23 H	5.727658	3.712046	6.666486	7.360050	6.530269
24 H	5.906088	4.882937	6.931950	6.762375	6.255061
25 H	6.038614	5.103303	7.803130	8.132559	7.743795
26 S	3.678922	5.148618	4.223592	3.023383	4.135995
27 S	5.142897	3.670123	4.220059	4.137267	3.026031
28 C	5.320274	5.830958	4.877118	2.790371	3.359192
29 C	5.830314	5.315899	4.875304	3.360698	2.789154
30 H	6.107402	6.907663	5.640892	2.927144	3.867951
31 H	6.906016	6.101247	5.637739	3.869791	2.924635

	11	12	13	14	15
11 O	0.000000				
12 O	4.162271	0.000000			
13 P	7.179943	7.204881	0.000000		
14 C	8.558808	8.533599	1.827185	0.000000	
15 H	9.462062	9.448769	2.446594	1.092990	0.000000
16 H	8.419595	8.802249	2.418720	1.092533	1.782253
17 H	8.825072	8.353407	2.420260	1.092265	1.783570
18 C	7.450120	8.267896	1.830731	2.840032	2.973712
19 H	7.253384	8.528171	2.416809	3.070037	3.317677
20 H	8.528998	9.226335	2.448016	2.965293	2.684083
21 H	6.976717	7.908420	2.428660	3.813645	3.977115
22 C	8.183453	7.486903	1.830987	2.844598	2.971436
23 H	8.454794	7.252852	2.418540	3.076557	3.312688
24 H	7.780380	7.051007	2.427650	3.816718	3.975902
25 H	9.141722	8.571059	2.448040	2.971684	2.684028
26 S	3.828642	5.264025	3.525998	5.063970	5.828207
27 S	5.265473	3.832039	3.559601	5.026721	5.807149
28 C	3.630898	4.348925	4.445526	6.183602	6.878023
29 C	4.351107	3.629346	4.457749	6.170594	6.870646
30 H	3.473238	4.747068	5.368990	7.123625	7.763954
31 H	4.750148	3.469880	5.387766	7.103258	7.752341

	16	17	18	19	20
16 H	0.000000				
17 H	1.768618	0.000000			
18 C	3.069392	3.812210	0.000000		
19 H	2.897703	4.090208	1.092553	0.000000	
20 H	3.302150	3.971756	1.093466	1.783188	0.000000

21	H	4.093529	4.699250	1.091706	1.767839	1.784696
22	C	3.814202	3.087624	2.862979	3.826189	2.993319
23	H	4.099686	2.919936	3.826752	4.697306	3.988999
24	H	4.698371	4.108993	3.115410	4.133716	3.355251
25	H	3.971637	3.325991	2.990662	3.987467	2.709171
26	S	5.068344	5.555018	3.638435	3.598288	4.714920
27	S	5.531279	4.970113	4.784214	5.297622	5.614235
28	C	6.421526	6.557589	4.673911	4.940370	5.642469
29	C	6.587940	6.347859	5.108850	5.573935	5.994571
30	H	7.325284	7.566760	5.330320	5.546305	6.260500
31	H	7.590736	7.232808	6.015924	6.552683	6.832741
		21	22	23	24	25
21	H	0.000000				
22	C	3.114973	0.000000			
23	H	4.134751	1.092483	0.000000		
24	H	2.973307	1.091786	1.767911	0.000000	
25	H	3.349955	1.093515	1.783449	1.784494	0.000000
26	S	3.226682	4.651416	5.172701	4.371572	5.491971
27	S	4.564804	3.659065	3.536895	3.308868	4.745206
28	C	3.995563	4.969079	5.395811	4.347196	5.874005
29	C	4.534388	4.589732	4.779737	3.912691	5.580736
30	H	4.515779	5.847532	6.347317	5.135542	6.680554
31	H	5.366055	5.250883	5.370015	4.451912	6.204568
		26	27	28	29	30
26	S	0.000000				
27	S	3.134369	0.000000			
28	C	1.744410	2.714667	0.000000		
29	C	2.714643	1.744558	1.380223	0.000000	
30	H	2.448264	3.728366	1.084032	2.157886	0.000000
31	H	3.728211	2.448681	2.157740	1.084035	2.522077
		31				
31	H	0.000000				

Table S11. Distance table for the lowest-lying $H_2C_2S_2Mn_2(CO)_6 \bullet NH_3$ structures after PBE0/6-311G(d,p) optimization followed by a single point CCSD(T) energy calculation. Provided are the absolute energy (a.u.) and relative energy (kcal/mol).



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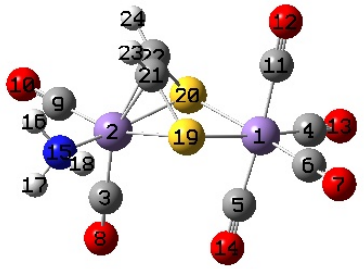
		1	2	3	4	5
1	Mn	0.000000				
2	Mn	3.575881	0.000000			
3	C	4.987336	1.782201	0.000000		
4	C	1.789278	3.617052	4.968285	0.000000	
5	C	4.076235	1.809612	2.596616	3.247855	0.000000
6	C	1.784187	4.954655	6.035103	2.542761	5.250986
7	O	2.929435	5.948574	6.860236	3.459963	6.160921
8	O	5.994580	2.925460	1.143461	5.960861	3.522745
9	C	4.985335	1.782383	2.537475	4.955133	2.598082
10	O	5.991536	2.925577	3.447760	5.942996	3.525225
11	C	1.783562	4.957230	6.557745	2.541420	5.264693
12	O	2.928758	5.952699	7.611905	3.462419	6.183112
13	O	2.931853	4.106127	5.316626	1.142925	3.200139
14	O	4.744780	2.948802	3.506904	3.525395	1.139277
15	N	2.120392	4.487007	5.708328	3.908895	5.617257
16	H	2.691952	5.224705	6.564839	4.422463	6.317853
17	H	2.651076	4.060664	5.187762	4.351943	5.447839
18	H	2.683128	5.085124	6.088966	4.409538	6.201782
19	S	2.411886	2.413578	3.068340	3.057518	3.339239
20	S	2.411600	2.413039	4.150773	3.037786	3.342904
21	C	3.268271	2.079751	2.739397	4.219645	3.745908
22	C	3.269098	2.079499	3.319962	4.213888	3.747418
23	H	4.261991	2.807755	2.834439	5.237778	4.490673
24	H	4.263363	2.806789	3.802714	5.229134	4.492235

		6	7	8	9	10
6	C	0.000000				
7	O	1.145400	0.000000			
8	O	6.880760	7.606350	0.000000		
9	C	6.553931	7.606771	3.447638	0.000000	
10	O	7.620528	8.694673	4.169174	1.143418	0.000000
11	C	2.586476	3.515785	7.624992	6.034091	6.877687
12	O	3.516167	4.272267	8.700295	6.860156	7.603650
13	O	3.443659	4.171389	6.249199	5.291864	6.214994
14	O	5.744851	6.567145	4.256104	3.509643	4.260792
15	N	2.791567	3.632615	6.615459	5.717957	6.628342
16	H	3.340428	4.120149	7.510274	6.278129	7.095251
17	H	3.599369	4.473733	6.064005	5.147338	6.006232
18	H	2.720940	3.285839	6.887546	6.449554	7.406444
19	S	3.092804	3.903379	3.874399	4.152010	5.278581
20	S	4.188198	5.329998	5.277443	3.065458	3.870376
21	C	4.408317	5.317432	3.575241	3.322728	4.311171
22	C	4.799353	5.849597	4.308465	2.739742	3.574869
23	H	5.209950	6.006669	3.366461	3.808075	4.685220
24	H	5.807721	6.851949	4.679265	2.834507	3.365866

		11	12	13	14	15
11	C	0.000000				
12	O	1.145444	0.000000			
13	O	3.433172	4.162682	0.000000		
14	O	5.764499	6.599622	3.089184	0.000000	

15	N	2.791787	3.628179	5.051740	6.499280	0.000000
16	H	2.697146	3.243489	5.542559	7.167966	1.015248
17	H	3.519648	4.363028	5.473845	6.438060	1.016799
18	H	3.446872	4.260542	5.533113	7.064433	1.015322
19	S	4.187081	5.328218	3.888039	4.233300	3.099994
20	S	3.090199	3.899256	3.853065	4.239223	3.122087
21	C	4.790976	5.836686	5.091681	4.850650	3.166224
22	C	4.400679	5.304424	5.080226	4.853016	3.176989
23	H	5.797155	6.835402	6.081600	5.591284	3.853355
24	H	5.201075	5.990407	6.063736	5.594262	3.870282
		16	17	18	19	20
16	H	0.000000				
17	H	1.629002	0.000000			
18	H	1.627918	1.628246	0.000000		
19	S	4.070854	2.977017	3.291448	0.000000	
20	S	3.478515	2.889022	4.041535	3.085035	0.000000
21	C	4.007768	2.499588	3.563477	1.751618	2.711493
22	C	3.749038	2.453627	3.896530	2.712594	1.751627
23	H	4.687903	3.077238	4.065195	2.466745	3.731043
24	H	4.279543	3.009762	4.590799	3.732060	2.467425
		21	22	23	24	
21	C	0.000000				
22	C	1.389612	0.000000			
23	H	1.084580	2.169374	0.000000		
24	H	2.169693	1.084630	2.540643	0.000000	



2S. -3908.66425444307 +13.2 C_1
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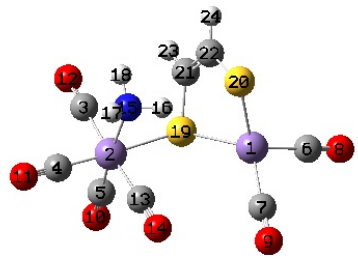
2	Mn	3.580562	0.000000			
3	C	4.138358	1.793241	0.000000		
4	C	1.794203	4.937406	5.234325	0.000000	
5	C	1.847702	3.570641	3.255676	2.604897	0.000000
6	C	1.795052	4.972305	5.387019	2.629467	2.605081
7	O	2.936676	5.962046	6.314018	3.562766	3.506839
8	O	4.816778	2.939253	1.146867	5.700239	3.547288
9	C	5.054444	1.760180	2.536961	6.121861	5.025186
10	O	6.107413	2.910993	3.468139	7.041741	6.080822
11	C	1.841546	4.326382	5.434136	2.608263	3.686627
12	O	2.977349	5.059961	6.358895	3.527205	4.821242
13	O	2.935499	5.913606	6.098262	1.141434	3.506174
14	O	2.983011	4.047070	3.199700	3.503123	1.135777
15	N	5.112189	2.085883	2.827079	6.713044	4.982027
16	H	5.781932	2.669462	3.661924	7.376185	5.859311
17	H	5.746723	2.657361	2.761643	7.281868	5.309551
18	H	4.947860	2.603086	3.326802	6.659569	4.876338
19	S	2.403604	2.434414	3.470585	4.188833	3.008780
20	S	2.399738	2.381319	3.216527	3.064715	3.017027
21	C	3.249025	2.081029	3.776443	4.783467	4.182660
22	C	3.240244	2.063937	3.682038	4.374608	4.182461
23	H	4.226820	2.840487	4.564749	5.774706	5.199536
24	H	4.218315	2.806693	4.408695	5.149457	5.197249
		6	7	8	9	10
6	C	0.000000				
7	O	1.141752	0.000000			
8	O	5.934878	6.794999	0.000000		
9	C	6.611692	7.649190	3.439145	0.000000	

10	O	7.716712	8.770970	4.181873	1.151348	0.000000
11	C	2.607195	3.506829	6.303262	5.594240	6.544365
12	O	3.525712	4.245083	7.292891	6.167469	7.028574
13	O	3.562650	4.331546	6.455063	6.944680	7.778985
14	O	3.500419	4.214605	3.113283	5.372538	6.375746
15	N	6.062746	6.832259	3.726897	2.782048	3.632482
16	H	6.775481	7.548341	4.582232	2.906657	3.532510
17	H	6.665056	7.404987	3.403718	3.085642	3.796308
18	H	5.617172	6.261614	4.179374	3.678720	4.600050
19	S	3.082628	3.888606	4.412317	4.129158	5.254039
20	S	4.187040	5.325204	4.062528	3.154858	4.022980
21	C	4.394865	5.302300	4.901032	3.236275	4.207248
22	C	4.779943	5.828493	4.770402	2.712647	3.558468
23	H	5.172278	5.965726	5.698154	3.700695	4.526570
24	H	5.771405	6.814463	5.478293	2.806547	3.334062
		11	12	13	14	15
11	C	0.000000				
12	O	1.135901	0.000000			
13	O	3.508021	4.247105	0.000000		
14	O	4.822398	5.956922	4.217858	0.000000	
15	N	5.737345	6.348339	7.769097	5.270377	0.000000
16	H	6.146956	6.606248	8.424605	6.222189	1.015455
17	H	6.573368	7.257796	8.306458	5.386443	1.014902
18	H	5.549755	6.157788	7.764183	5.201989	1.017878
19	S	2.964127	3.735443	5.326182	3.820240	3.097524
20	S	2.952523	3.722140	3.866150	3.834852	4.418704
21	C	3.098600	3.504650	5.829745	5.038805	2.924670
22	C	3.082299	3.486464	5.277765	5.042817	3.618943
23	H	3.807847	3.958452	6.815375	6.029388	3.014606
24	H	3.794480	3.943358	5.936657	6.031170	4.165450
		16	17	18	19	20
16	H	0.000000				
17	H	1.622276	0.000000			
18	H	1.634853	1.628548	0.000000		
19	S	3.713196	3.867804	2.702361	0.000000	
20	S	4.894225	5.028113	4.739267	3.077264	0.000000
21	C	3.113344	3.884203	2.938205	1.758796	2.707920
22	C	3.788512	4.452749	3.938589	2.710493	1.751728
23	H	2.885526	4.028287	2.952542	2.473397	3.728997
24	H	4.099524	4.981776	4.614481	3.733420	2.461393
		21	22	23	24	
21	C	0.000000				
22	C	1.384037	0.000000			
23	H	1.084524	2.166903	0.000000		
24	H	2.168557	1.084097	2.545746	0.000000	



3Q. -3908.65209223838 +20.9 C_1
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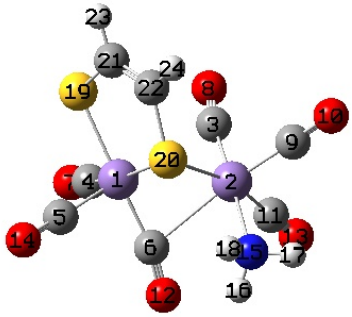
2	Mn	4.155727	0.000000			
3	C	5.186049	1.850897	0.000000		
4	C	5.770641	1.790845	2.625717	0.000000	
5	C	4.856398	1.805856	2.587920	2.619471	0.000000
6	C	2.002027	5.876378	6.674494	7.578806	6.203461
7	C	1.979411	4.821191	6.311045	6.112602	5.306238
8	O	3.139655	6.932136	7.637325	8.654035	7.124663
9	O	3.120231	5.520310	7.149318	6.599003	5.890870

10	O	5.545126	2.944882	3.482167	3.549568	1.139159
11	O	6.846402	2.933714	3.527529	1.142916	3.543631
12	O	6.010941	2.986657	1.135803	3.547746	3.488790
13	C	3.686800	1.849148	3.698029	2.607416	2.588739
14	O	3.887643	2.984736	4.834161	3.497940	3.476058
15	N	4.072595	2.105082	2.806616	2.815150	3.906157
16	H	3.279691	2.655817	3.527614	3.660319	4.349631
17	H	4.806268	2.703520	3.490578	2.799522	4.472532
18	H	4.527358	2.662314	2.663169	3.349850	4.389792
19	S	2.450229	2.433792	2.943374	4.223740	2.970663
20	S	2.383675	4.580271	5.226770	5.946167	5.931243
21	C	3.096567	3.363977	3.163722	4.964493	4.361881
22	C	3.037039	4.157648	4.184494	5.628513	5.421768
23	H	4.106092	3.808966	3.047002	5.289694	4.620266
24	H	4.041429	5.016194	4.751518	6.364285	6.316957
		6	7	8	9	10
6	C	0.000000				
7	C	2.975255	0.000000			
8	O	1.137881	3.901548	0.000000		
9	O	3.896097	1.141273	4.672636	0.000000	
10	O	6.638684	5.869106	7.450957	6.369204	0.000000
11	O	8.684151	7.053054	9.766540	7.434757	4.304879
12	O	7.346993	7.303469	8.239495	8.192307	4.194418
13	C	5.478606	3.571013	6.559273	4.001006	3.479994
14	O	5.581328	3.163583	6.627307	3.283469	4.173259
15	N	5.983347	4.935135	7.093306	5.698118	5.042973
16	H	5.203528	4.193086	6.317168	5.008951	5.450537
17	H	6.772713	5.390606	7.898268	6.009245	5.602456
18	H	6.306612	5.675413	7.370019	6.525776	5.504246
19	S	3.743364	3.865712	4.716380	4.879419	3.728698
20	S	3.756320	3.777024	4.730220	4.759769	6.880284
21	C	4.234508	4.907608	5.127599	6.005785	5.208053
22	C	4.195779	4.845569	5.089883	5.934556	6.344197
23	H	5.017146	5.927188	5.792131	7.023802	5.376058
24	H	4.976943	5.854431	5.750972	6.935051	7.239423
		11	12	13	14	15
11	O	0.000000				
12	O	4.272159	0.000000			
13	C	3.510688	4.833068	0.000000		
14	O	4.211865	5.969181	1.136477	0.000000	
15	N	3.668109	3.661968	2.782748	3.650567	0.000000
16	H	4.554552	4.376973	2.866739	3.546281	1.029064
17	H	3.386220	4.314788	3.062351	3.762665	1.015209
18	H	4.140239	3.242836	3.712674	4.635742	1.015502
19	S	5.366145	3.699588	3.072123	3.899229	3.124890
20	S	6.914702	5.880390	4.541641	4.930203	3.363652
21	C	6.038184	3.543991	4.328619	5.199667	3.069014
22	C	6.644231	4.583696	4.802544	5.520034	3.180526
23	H	6.315191	3.070561	5.083472	6.044175	3.694092
24	H	7.317720	4.935427	5.801750	6.543349	3.851645
		16	17	18	19	20
16	H	0.000000				
17	H	1.641750	0.000000			
18	H	1.604657	1.628304	0.000000		
19	S	2.929672	4.085007	3.369079	0.000000	

20	S	2.401502	3.960193	3.473312	3.403910	0.000000
21	C	2.809488	4.060527	2.798995	1.775135	2.782930
22	C	2.608028	4.026419	2.874087	2.762715	1.754265
23	H	3.660682	4.664522	3.206518	2.446102	3.766394
24	H	3.380949	4.604592	3.306411	3.743851	2.422503

		21	22	23	24
21	C	0.000000			
22	C	1.344544	0.000000		
23	H	1.085712	2.113469	0.000000	
24	H	2.086814	1.087927	2.402189	0.000000



4S. -3908.64050608605 +28.2 C_1

		1	2	3	4	5
1	Mn	0.000000				
2	Mn	2.643483	0.000000			
3	C	2.736951	1.797740	0.000000		
4	C	1.799214	3.787791	3.261657	0.000000	
5	C	1.762845	4.103205	4.495834	2.624609	0.000000
6	C	1.786059	2.459576	3.273537	2.508593	2.457963
7	O	2.939750	4.731064	3.997853	1.140556	3.555527
8	O	3.455975	2.933448	1.142939	3.531081	5.193445
9	C	4.209293	1.777179	2.519880	5.375243	5.674339
10	O	5.276271	2.919737	3.426042	6.448135	6.722263
11	C	3.828044	1.793330	2.501838	4.327399	5.248519
12	O	2.929888	3.150420	4.156373	3.352514	3.250839
13	O	4.786371	2.936407	3.396470	4.988861	6.144701
14	O	2.903528	5.147569	5.634085	3.566265	1.141535
15	N	3.793355	2.116677	3.913213	5.140183	4.548515
16	H	3.946724	2.666884	4.374035	5.075229	4.497502
17	H	4.733630	2.687086	4.428421	6.046632	5.556061
18	H	3.816424	2.655515	4.386689	5.371187	4.283281
19	S	2.247061	4.136621	3.425564	2.777821	3.003584
20	S	2.278576	2.347997	3.177108	4.050331	3.063707
21	C	3.156044	4.189470	3.743875	4.280920	3.906378
22	C	3.194546	3.546613	3.626547	4.711503	3.978244
23	H	4.189704	5.170712	4.554881	5.135272	4.849498
24	H	4.230290	4.175424	4.378867	5.783869	4.935610

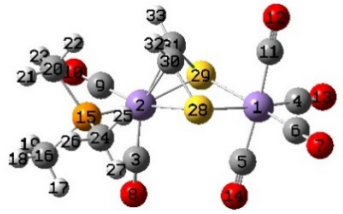
		6	7	8	9	10
6	C	0.000000				
7	O	3.412274	0.000000			
8	O	4.186149	4.017226	0.000000		
9	C	4.224012	6.272250	3.363644	0.000000	
10	O	5.361383	7.324427	4.059690	1.143232	0.000000
11	C	3.005507	4.969861	3.330061	2.580916	3.519528
12	O	1.158190	4.040505	5.066227	4.815855	5.924421
13	O	3.783114	5.435850	4.001649	3.498102	4.264165
14	O	3.366430	4.335248	6.324950	6.688592	7.713876
15	N	2.895125	6.119227	5.047646	2.833014	3.686441
16	H	2.628678	5.968377	5.484903	3.674746	4.576041
17	H	3.847547	6.995549	5.520764	2.801091	3.400157
18	H	3.182668	6.426087	5.524140	3.307966	4.077623
19	S	4.027095	3.566685	3.575261	5.153766	5.979696
20	S	3.037744	5.182885	4.118702	3.171646	4.010759
21	C	4.801923	5.189824	4.016359	4.688718	5.278037
22	C	4.508253	5.755008	4.200742	3.839540	4.376436
23	H	5.871449	5.936906	4.629136	5.466387	5.905200
24	H	5.402883	6.828538	4.933837	4.056134	4.333771

	11	12	13	14	15
11 C	0.000000				
12 O	3.179558	0.000000			
13 O	1.143083	3.689331	0.000000		
14 O	6.272727	3.923326	7.136516	0.000000	
15 N	2.782913	2.992271	3.632291	5.296465	0.000000
16 H	2.890639	2.343029	3.538982	5.159943	1.017811
17 H	3.035879	3.843265	3.721969	6.293821	1.015072
18 H	3.703277	3.396820	4.618668	4.898893	1.019393
19 S	5.480650	5.166819	6.452503	3.840931	5.623813
20 S	4.109699	3.976443	5.244327	3.899338	2.921409
21 C	5.818031	5.940253	6.898410	4.655471	5.499795
22 C	5.305211	5.563935	6.435747	4.735312	4.532446
23 H	6.764704	7.015406	7.825085	5.501958	6.515707
24 H	5.922922	6.395394	7.048080	5.602966	4.923718

	16	17	18	19	20
16 H	0.000000				
17 H	1.631622	0.000000			
18 H	1.639379	1.630858	0.000000		
19 S	6.005598	6.457390	5.502474	0.000000	
20 S	3.571657	3.665537	2.538441	3.155240	0.000000
21 C	6.126730	6.183772	5.210919	1.734403	2.677245
22 C	5.274636	5.124888	4.148568	2.709087	1.748550
23 H	7.182540	7.146022	6.205005	2.412691	3.693882
24 H	5.770223	5.352578	4.453389	3.725039	2.435302

	21	22	23	24
21 C	0.000000			
22 C	1.339264	0.000000		
23 H	1.086117	2.116497	0.000000	
24 H	2.138115	1.083657	2.500544	0.000000

Table S12. Distance table for the lowest-lying H2C2S2Mn2(CO)6•PMe3 structures after PBE0/6-311G(d,p) optimization followed by a single point CCSD(T) energy calculation. Provided are the absolute energy (a.u.) and relative energy (kcal/mol).



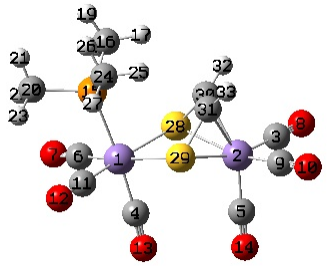
1S. -4312.56193475793 0.0 C_1
WBI 0.01

		1	2	3	4	5
1	Mn	0.000000				
2	Mn	3.600003	0.000000			
3	C	4.137198	1.786437	0.000000		
4	C	1.795467	4.963945	5.290877	0.000000	
5	C	1.848767	3.599396	3.259251	2.606332	0.000000
6	C	1.795136	4.987555	5.338170	2.628707	2.602357
7	O	2.936799	5.975290	6.245741	3.561545	3.503247
8	O	4.808883	2.933634	1.147251	5.782827	3.531091
9	C	5.019387	1.757376	2.546206	6.063948	4.966872
10	O	6.057291	2.909470	3.475129	6.950777	5.991213
11	C	1.840012	4.339531	5.432970	2.607831	3.686426
12	O	2.976126	5.070316	6.358697	3.528602	4.821445
13	O	2.936690	5.940898	6.177156	1.141389	3.507317
14	O	2.983803	4.080864	3.210779	3.504887	1.135606
15	P	5.436748	2.239250	2.913501	7.016090	5.343958
16	C	6.758961	3.445863	3.220168	8.213668	6.230504
17	H	6.606070	3.621525	2.873547	8.013313	5.805510
18	H	7.666480	4.405294	4.283394	9.190799	7.193169
19	H	7.066162	3.577231	3.331347	8.376592	6.532507
20	C	6.612248	3.435856	4.516309	8.144938	6.868126
21	H	7.547699	4.399601	5.275640	9.135322	7.724787
22	H	6.363234	3.614608	4.999521	7.904986	6.906411
23	H	6.916612	3.560184	4.606259	8.300686	7.144883
24	C	5.774869	3.504122	3.995106	7.520876	5.716423
25	H	5.427404	3.671472	4.498558	7.212059	5.685769
26	H	6.865375	4.443435	4.862129	8.612744	6.782506
27	H	5.572313	3.684930	3.748549	7.291136	5.241534
28	S	2.400720	2.424668	3.360278	4.186775	3.007180
29	S	2.395850	2.389654	3.291936	3.071575	3.013280
30	C	3.251869	2.079510	3.734371	4.787718	4.191891
31	C	3.242025	2.071398	3.714964	4.378133	4.190860
32	H	4.220900	2.845892	4.517291	5.769253	5.206752
33	H	4.217028	2.813880	4.465830	5.147969	5.204170

		6	7	8	9	10
6	C	0.000000				
7	O	1.141793	0.000000			
8	O	5.847072	6.672111	0.000000		
9	C	6.587769	7.630400	3.464738	0.000000	
10	O	7.682120	8.743881	4.209723	1.152454	0.000000
11	C	2.603226	3.502516	6.302064	5.592039	6.544216
12	O	3.518858	4.236278	7.295494	6.183973	7.057732
13	O	3.562796	4.331342	6.577350	6.875581	7.667328
14	O	3.493648	4.205127	3.095395	5.308755	6.271425
15	P	6.435868	7.219456	3.760228	2.770498	3.555307
16	C	7.753545	8.511118	3.581995	3.402712	3.824380
17	H	7.485336	8.189996	2.926796	3.835562	4.365221
18	H	8.555544	9.244713	4.595764	4.348019	4.663645
19	H	8.249670	9.096324	3.661995	2.991338	3.113555
20	C	7.693343	8.492915	5.416461	3.321689	3.693811

21	H	8.507963	9.233200	6.060147	4.287789	4.561085
22	H	7.388935	8.165372	6.006553	3.723996	4.181347
23	H	8.185558	9.072663	5.486591	2.890356	2.943550
24	C	6.280327	6.814374	4.668039	4.518289	5.376582
25	H	5.808831	6.291849	5.295485	4.859810	5.779201
26	H	7.330438	7.810646	5.443489	5.210919	5.925025
27	H	5.901951	6.354448	4.221784	4.885867	5.816458
28	S	3.086852	3.895192	4.261730	4.137821	5.274104
29	S	4.182642	5.320629	4.176071	3.093140	3.944079
30	C	4.396599	5.303477	4.847897	3.295726	4.291517
31	C	4.781255	5.829588	4.821609	2.740478	3.598894
32	H	5.161255	5.952707	5.630860	3.812363	4.684249
33	H	5.769968	6.812961	5.567150	2.858112	3.411217
		11	12	13	14	15
11	C	0.000000				
12	O	1.136215	0.000000			
13	O	3.508107	4.249724	0.000000		
14	O	4.821983	5.956957	4.219660	0.000000	
15	P	5.997556	6.565315	8.059116	5.635828	0.000000
16	C	7.594770	8.259815	9.192686	6.205477	1.829990
17	H	7.672375	8.451265	8.973422	5.607367	2.427404
18	H	8.409432	9.010634	10.197872	7.168353	2.449810
19	H	7.887902	8.540386	9.283238	6.494460	2.419175
20	C	6.734795	7.035255	9.158474	7.296073	1.833746
21	H	7.689445	7.971877	10.170954	8.082903	2.455197
22	H	6.204103	6.355975	8.924360	7.485371	2.436904
23	H	7.043761	7.337125	9.241267	7.551193	2.417828
24	C	6.286915	6.819702	8.638116	6.001030	1.830994
25	H	5.677728	6.094272	8.346737	6.147427	2.434182
26	H	7.315988	7.784518	9.729229	7.008824	2.442696
27	H	6.347998	7.014099	8.399465	5.381121	2.422088
28	S	2.962266	3.732242	5.323750	3.818833	3.436909
29	S	2.957227	3.732556	3.875078	3.835243	4.587343
30	C	3.098694	3.502267	5.833394	5.051117	3.094561
31	C	3.083878	3.489133	5.280443	5.055848	3.721330
32	H	3.791777	3.935656	6.809194	6.042512	3.120739
33	H	3.792555	3.943260	5.933566	6.044187	4.172955
		16	17	18	19	20
16	C	0.000000				
17	H	1.092035	0.000000			
18	H	1.093044	1.782629	0.000000		
19	H	1.092738	1.768215	1.780990	0.000000	
20	C	2.828784	3.806344	2.958018	3.052254	0.000000
21	H	2.958864	3.967769	2.671592	3.291461	1.093308
22	H	3.808665	4.703228	3.965869	4.079963	1.092182
23	H	3.050680	4.074637	3.293384	2.869664	1.092504
24	C	2.850372	3.103801	2.976359	3.817360	2.859724
25	H	3.825967	4.124833	3.985684	4.705587	3.131344
26	H	2.975420	3.343385	2.687727	3.970181	2.968021
27	H	3.082472	2.938321	3.313023	4.106996	3.825201
28	S	4.971925	4.970101	5.707592	5.510988	4.617179
29	S	5.786178	5.867549	6.776847	5.749903	5.459920
30	C	4.836691	5.189230	5.542980	5.154570	3.637333

31	C	5.243774	5.609485	6.076943	5.285093	4.145030
32	H	4.940835	5.451912	5.464460	5.319199	3.191984
33	H	5.626052	6.144384	6.398305	5.518460	4.155972
		21	22	23	24	25
21	H	0.000000				
22	H	1.778603	0.000000			
23	H	1.781898	1.768923	0.000000		
24	C	2.990109	3.119275	3.822263	0.000000	
25	H	3.370501	2.998722	4.149210	1.091621	0.000000
26	H	2.685427	3.330570	3.964460	1.093400	1.784480
27	H	3.982438	4.144460	4.695587	1.091958	1.761638
28	S	5.422756	4.372023	5.182004	3.448936	3.027137
29	S	6.517538	5.332395	5.408751	5.651223	5.523307
30	C	4.599283	3.177344	4.025091	3.674699	3.213253
31	C	5.215649	3.794429	4.171458	4.760918	4.478040
32	H	4.056481	2.475091	3.717307	3.478411	2.847843
33	H	5.231060	3.731846	3.975374	5.368480	5.093587
		26	27	28	29	30
26	H	0.000000				
27	H	1.784045	0.000000			
28	S	4.523952	3.395569	0.000000		
29	S	6.663292	5.741612	3.054858	0.000000	
30	C	4.616398	4.097996	1.755677	2.703448	0.000000
31	C	5.679978	5.155977	2.702998	1.751086	1.385753
32	H	4.259031	4.131767	2.471031	3.726858	1.084183
33	H	6.173550	5.911175	3.727885	2.462850	2.171942
		31	32	33		
31	C	0.000000				
32	H	2.171551	0.000000			
33	H	1.083867	2.555789	0.000000		



2S. -4312.55179544788 +6.4 C_1
WBI 0.01

		1	2	3	4	5
1	Mn	0.000000				
2	Mn	3.593675	0.000000			
3	C	5.003977	1.782831	0.000000		
4	C	1.804612	3.578723	4.927095	0.000000	
5	C	4.099536	1.808013	2.595015	3.212933	0.000000
6	C	1.778301	4.945051	6.020532	2.543422	5.238597
7	O	2.925130	5.925755	6.826290	3.450284	6.127491
8	O	6.010514	2.926412	1.143790	5.919672	3.521867
9	C	5.004394	1.782954	2.536903	4.923143	2.596173
10	O	6.011453	2.926523	3.446562	5.914546	3.523163
11	C	1.777002	4.954590	6.555908	2.542306	5.251324
12	O	2.924349	5.942859	7.604180	3.454331	6.151801
13	O	2.944040	4.085603	5.288716	1.141413	3.181274
14	O	4.770620	2.947760	3.504914	3.498786	1.139849
15	P	2.343742	4.900864	6.125966	4.145207	6.002248
16	C	3.606467	5.281619	6.034979	5.310625	6.626776
17	H	3.854085	4.697882	5.296012	5.458018	6.218597
18	H	3.699311	5.474288	6.054753	5.237186	6.656388
19	H	4.540078	6.286567	7.024066	6.292684	7.682572
20	C	3.475597	6.612162	7.838502	5.078164	7.507633
21	H	4.451151	7.342258	8.502968	6.120044	8.387966
22	H	3.621880	6.865792	7.964210	5.058394	7.630021
23	H	3.589254	6.910657	8.297155	5.004621	7.645809
24	C	3.570791	5.394434	6.740381	5.247179	6.677134

25	H	3.788810	4.797792	6.084851	5.354304	6.234740
26	H	4.517700	6.352957	7.583567	6.248336	7.709280
27	H	3.666956	5.707441	7.225411	5.162589	6.792224
28	S	2.411647	2.408358	3.070665	3.020561	3.338862
29	S	2.411053	2.406764	4.143895	3.013672	3.340776
30	C	3.282189	2.082521	2.739387	4.194947	3.749271
31	C	3.281715	2.083529	3.320611	4.193400	3.751990
32	H	4.275610	2.805767	2.825371	5.209762	4.486761
33	H	4.274946	2.807199	3.801992	5.207561	4.491068

		6	7	8	9	10
6	C	0.000000				
7	O	1.147028	0.000000			
8	O	6.864385	7.567826	0.000000		
9	C	6.548975	7.590421	3.447015	0.000000	
10	O	7.618183	8.681870	4.167330	1.143774	0.000000
11	C	2.603974	3.545158	7.623694	6.034104	6.880034
12	O	3.543273	4.318496	8.693828	6.850505	7.595637
13	O	3.422797	4.129711	6.219194	5.280445	6.207853
14	O	5.733271	6.530652	4.254468	3.506880	4.256986
15	P	2.871196	3.656355	7.026520	6.116826	7.013863
16	C	3.757240	4.254244	6.708695	6.566594	7.484454
17	H	4.330901	4.949586	5.915986	5.865765	6.741664
18	H	3.395506	3.658445	6.640027	6.946656	7.946349
19	H	4.599615	4.978177	7.661211	7.464276	8.317324
20	C	3.211762	3.548478	8.715743	7.870437	8.763370
21	H	4.242424	4.498970	9.337669	8.519532	9.362927
22	H	2.802150	2.802668	8.777800	8.288174	9.257835
23	H	3.446823	3.834583	9.249431	8.072827	8.917872
24	C	4.557669	5.415383	7.684010	6.133547	6.798297
25	H	5.035239	5.982501	7.010558	5.334256	5.922249
26	H	5.262264	5.980808	8.460934	7.072173	7.699526
27	H	4.741324	5.633930	8.243995	6.327048	6.926043
28	S	3.077324	3.879398	3.879628	4.146206	5.272991
29	S	4.179150	5.321205	5.270440	3.070735	3.880911
30	C	4.410376	5.315039	3.574149	3.322673	4.310979
31	C	4.803533	5.853305	4.307959	2.744148	3.580101
32	H	5.212509	6.004262	3.354939	3.804095	4.681366
33	H	5.816074	6.862762	4.678035	2.832350	3.364209

		11	12	13	14	15
11	C	0.000000				
12	O	1.147530	0.000000			
13	O	3.418384	4.130711	0.000000		
14	O	5.747472	6.558696	3.075140	0.000000	
15	P	2.838993	3.608512	5.280234	6.864568	0.000000
16	C	4.573735	5.415180	6.423250	7.583748	1.829585
17	H	5.023658	5.932938	6.547300	7.252256	2.433076
18	H	4.833259	5.740635	6.286658	7.540227	2.420801
19	H	5.253272	5.948589	7.415640	8.650789	2.436119
20	C	3.272236	3.629865	6.120565	8.242021	1.830928
21	H	4.258787	4.514889	7.183241	9.183380	2.442575
22	H	3.623774	4.067936	6.034298	8.295104	2.429051
23	H	2.825815	2.860366	5.969863	8.295790	2.426863
24	C	3.560416	3.980623	6.345268	7.606530	1.829532
25	H	4.062883	4.590696	6.425359	7.234512	2.436504
26	H	4.459888	4.770350	7.359339	8.659556	2.437553

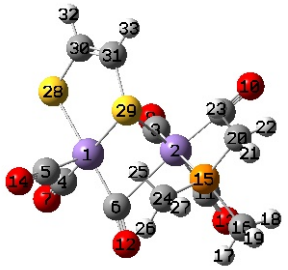
27	H	3.147189	3.291753	6.188022	7.629791	2.416498
28	S	4.179861	5.323139	3.860016	4.236162	3.467142
29	S	3.090707	3.899907	3.848152	4.239795	3.444073
30	C	4.808234	5.859953	5.078240	4.855363	3.577263
31	C	4.418568	5.327324	5.075198	4.858757	3.565451
32	H	5.819948	6.867794	6.061818	5.587925	4.239061
33	H	5.221627	6.018111	6.057256	5.593499	4.220607

		16	17	18	19	20
16	C	0.000000				
17	H	1.090500	0.000000			
18	H	1.092364	1.768194	0.000000		
19	H	1.093282	1.781013	1.783735	0.000000	
20	C	2.832267	3.803796	3.110921	2.901278	0.000000
21	H	2.956787	3.933538	3.366334	2.608931	1.092817
22	H	3.066484	4.107728	2.948538	3.223192	1.091974
23	H	3.807213	4.693673	4.127240	3.915682	1.092163
24	C	2.871769	3.091292	3.838089	3.025087	2.828024
25	H	3.131620	2.957686	4.139954	3.405995	3.807705
26	H	2.996512	3.309740	4.008285	2.741014	2.928666
27	H	3.833133	4.116689	4.707843	4.011251	3.063305
28	S	3.534701	3.239787	3.373846	4.624596	4.971729
29	S	4.531024	4.256921	5.031991	5.387847	5.029630
30	C	3.428836	2.684883	3.712966	4.381167	5.360319
31	C	3.922592	3.264058	4.482635	4.758231	5.383164
32	H	3.626388	2.681419	3.868079	4.462357	5.971073
33	H	4.451840	3.676883	5.152808	5.122775	6.008613

		21	22	23	24	25
21	H	0.000000				
22	H	1.781238	0.000000			
23	H	1.780408	1.769002	0.000000		
24	C	2.943214	3.804160	3.066462	0.000000	
25	H	3.944977	4.700937	4.097840	1.090544	0.000000
26	H	2.625598	3.933469	3.274197	1.093182	1.782444
27	H	3.294675	4.089102	2.899703	1.092544	1.767013
28	S	5.726737	4.951423	5.495956	4.676967	4.465126
29	S	5.753443	5.553106	5.075560	3.525858	3.095118
30	C	5.894877	5.640148	5.920897	4.139562	3.557519
31	C	5.904801	5.887397	5.746741	3.583092	2.818806
32	H	6.370612	6.217738	6.652063	4.724032	4.074842
33	H	6.387338	6.625435	6.365150	3.797159	2.819164

		26	27	28	29	30
26	H	0.000000				
27	H	1.783005	0.000000			
28	S	5.494885	5.208926	0.000000		
29	S	4.596356	3.527007	3.055794	0.000000	
30	C	4.901556	4.799641	1.749591	2.701632	0.000000
31	C	4.460160	4.044584	2.701363	1.750644	1.385952
32	H	5.317127	5.518247	2.466657	3.724640	1.084779
33	H	4.547179	4.263700	3.724048	2.468358	2.169272

		31	32	33
31	C	0.000000		
32	H	2.169521	0.000000	
33	H	1.084733	2.546688	0.000000



3S. -4312.51773452689 +27.7 C_1
WBI 0.11

		1	2	3	4	5
1	Mn	0.000000				
2	Mn	2.599637	0.000000			
3	C	2.650372	1.810004	0.000000		
4	C	1.799009	3.769257	3.169230	0.000000	
5	C	1.763486	4.042650	4.410202	2.625268	0.000000
6	C	1.795953	2.432303	3.180630	2.482360	2.470436
7	O	2.939700	4.725089	3.917111	1.140718	3.553009
8	O	3.402103	2.939604	1.142976	3.447037	5.141303
9	C	4.149068	1.772977	2.522437	5.322675	5.613661
10	O	5.214606	2.917296	3.420710	6.383383	6.667515
11	C	3.775176	1.782329	2.499129	4.304272	5.175214
12	O	2.931233	3.173271	4.066990	3.267888	3.257559
13	O	4.737824	2.926803	3.397281	4.971557	6.071428
14	O	2.904708	5.080783	5.549450	3.568895	1.142034
15	P	4.096867	2.362953	4.171533	5.471424	4.795829
16	C	5.420426	3.562865	5.207369	6.441544	6.102736
17	H	5.242928	3.715354	5.209254	6.010925	5.851103
18	H	5.905298	3.706624	5.179388	6.847760	6.823416
19	H	6.243555	4.519754	6.228905	7.344175	6.720531
20	C	5.397375	3.522442	5.186746	6.957580	6.075766
21	H	6.225946	4.489283	6.212279	7.778677	6.699566
22	H	5.881272	3.664952	5.155738	7.347345	6.796586
23	H	5.200469	3.651393	5.176699	6.888785	5.799149
24	C	4.218149	3.591008	5.292418	5.634183	4.191340
25	H	3.869955	3.697055	5.254241	5.446950	3.645672
26	H	4.058492	3.810378	5.377958	5.211158	3.858960
27	H	5.305579	4.531436	6.287514	6.716287	5.180411
28	S	2.254719	4.106219	3.358274	2.770062	3.034415
29	S	2.281542	2.356873	3.209894	4.059442	3.021794
30	C	3.154777	4.149605	3.704090	4.270583	3.927532
31	C	3.188661	3.513168	3.618518	4.703111	3.976078
32	H	4.189543	5.128931	4.515860	5.124462	4.879974
33	H	4.224329	4.147566	4.390091	5.776085	4.931170

		6	7	8	9	10
6	C	0.000000				
7	O	3.377316	0.000000			
8	O	4.091143	3.931877	0.000000		
9	C	4.200293	6.227912	3.343481	0.000000	
10	O	5.343321	7.263415	4.022734	1.144792	0.000000
11	C	2.922619	4.966284	3.302639	2.570813	3.508968
12	O	1.157272	3.924252	4.942772	4.856015	5.975683
13	O	3.686200	5.440764	3.971765	3.488903	4.252627
14	O	3.376196	4.334036	6.275454	6.626738	7.661158
15	P	3.246102	6.456632	5.291972	2.935114	3.729435
16	C	4.108424	7.253947	6.227506	3.989349	4.633494
17	H	3.690275	6.712557	6.182793	4.504970	5.291723
18	H	4.703469	7.613996	6.100930	3.736828	4.199566
19	H	4.927263	8.177491	7.274195	4.850225	5.384211
20	C	4.933591	8.002759	6.242728	3.181803	3.453054
21	H	5.600025	8.815743	7.286143	4.245312	4.463488
22	H	5.458554	8.349094	6.114506	2.826300	2.791701
23	H	5.082907	7.986913	6.210085	3.287526	3.516328
24	C	3.315794	6.632011	6.428791	4.550167	5.385597
25	H	3.423894	6.508306	6.369267	4.658270	5.482478

26	H	2.839634	6.109489	6.473869	5.069181	6.017778
27	H	4.367878	7.698291	7.428926	5.257935	5.957743
28	S	4.039444	3.554519	3.548886	5.078926	5.888131
29	S	3.088032	5.194436	4.179408	3.185972	4.032396
30	C	4.821834	5.177696	4.025571	4.604346	5.177314
31	C	4.536349	5.747202	4.236933	3.779356	4.311536
32	H	5.889226	5.923165	4.639250	5.371483	5.785429
33	H	5.434559	6.821605	4.987190	4.006938	4.280517
		11	12	13	14	15
11	C	0.000000				
12	O	3.116371	0.000000			
13	O	1.144509	3.582078	0.000000		
14	O	6.190100	3.929854	7.050987	0.000000	
15	P	2.938901	3.405058	3.727698	5.499877	0.000000
16	C	3.137627	3.765694	3.360942	6.759272	1.827759
17	H	2.999957	3.089653	3.034481	6.486095	2.420080
18	H	2.980844	4.442830	3.008554	7.581403	2.430105
19	H	4.229324	4.509800	4.417281	7.245271	2.435956
20	C	4.286798	5.213657	5.047941	6.708102	1.827675
21	H	5.095118	5.715766	5.739111	7.202733	2.435236
22	H	4.203667	5.755617	4.864826	7.532602	2.430744
23	H	4.798487	5.555022	5.703370	6.391494	2.416186
24	C	4.343220	3.316443	5.097426	4.544136	1.829618
25	H	4.826006	3.715829	5.724098	3.918077	2.427884
26	H	4.306592	2.557190	4.942788	4.148243	2.426140
27	H	5.152788	4.229800	5.803288	5.401993	2.427625
28	S	5.443917	5.163179	6.423113	3.881767	5.900156
29	S	4.104460	4.073653	5.238611	3.842823	3.126903
30	C	5.769812	5.972774	6.856115	4.688288	5.700536
31	C	5.262228	5.627177	6.396304	4.736179	4.685749
32	H	6.713360	7.043375	7.779831	5.549920	6.697725
33	H	5.883154	6.474162	7.010200	5.600350	5.012331
		16	17	18	19	20
16	C	0.000000				
17	H	1.092276	0.000000			
18	H	1.092146	1.770327	0.000000		
19	H	1.092755	1.782163	1.781815	0.000000	
20	C	2.863152	3.829560	3.103293	2.995212	0.000000
21	H	2.991795	3.991802	3.339231	2.712682	1.092885
22	H	3.107060	4.126558	2.951236	3.348056	1.091697
23	H	3.826954	4.702057	4.123147	3.991166	1.092099
24	C	2.848090	3.089501	3.821972	2.958729	2.852671
25	H	3.822781	4.094362	4.712526	3.983392	3.138859
26	H	3.029906	2.871012	4.068092	3.222633	3.814668
27	H	3.005206	3.385563	3.992064	2.705072	2.918961
28	S	7.407273	7.367282	7.762621	8.234456	6.789460
29	S	4.893099	5.178628	5.354299	5.531670	3.728722
30	C	7.395096	7.607557	7.690090	8.133954	6.122384
31	C	6.450857	6.806268	6.754858	7.106349	4.881912
32	H	8.402310	8.653121	8.647669	9.133261	6.966391
33	H	6.790340	7.292500	7.038654	7.353229	4.802527
		21	22	23	24	25
21	H	0.000000				
22	H	1.781459	0.000000			
23	H	1.782570	1.772308	0.000000		

24	C	2.964603	3.825947	3.088120	0.000000	
25	H	3.372153	4.159249	2.980919	1.091607	0.000000
26	H	3.935577	4.699609	4.123763	1.090718	1.777237
27	H	2.615759	3.926946	3.250517	1.093096	1.781368
28	S	7.714680	7.153973	6.312236	6.106702	5.506851
29	S	4.593236	4.278488	3.209645	3.371842	2.756478
30	C	7.062280	6.432134	5.440624	6.020616	5.299590
31	C	5.802038	5.222871	4.135762	5.059091	4.339218
32	H	7.907132	7.210998	6.214310	7.042720	6.283091
33	H	5.678254	5.076506	3.913992	5.435251	4.693786

		26	27	28	29	30
26	H	0.000000				
27	H	1.779956	0.000000			
28	S	6.134124	7.144001	0.000000		
29	S	3.826624	4.294213	3.166365	0.000000	
30	C	6.349299	6.944814	1.734423	2.683287	0.000000
31	C	5.565159	5.899130	2.709975	1.751525	1.339105
32	H	7.410414	7.930662	2.412144	3.698804	1.086351
33	H	6.103068	6.134888	3.724933	2.435574	2.136589

		31	32	33
31	C	0.000000		
32	H	2.116445	0.000000	
33	H	1.083760	2.498050	0.000000

Table S13. Harmonic ν(CO) vibrational frequencies and infrared intensities (in parantheses, in km/mol) for the $H_2C_2S_2Mn_2(CO)_n$.

1	MnS4-1Q	1957(443) 1970(649) 1972(1392) 2032(721)
2	MnS4-2Q	1933(331) 1938(765) 1988(2237) 2020(458)
3	MnS4-3T	1833(386) 1948(1883) 1963(707) 2012(693)
4	MnS4-4T	1920(463) 1965(684) 1965(1128) 2030(719)
1	MnS5-1Q	1852(360) 1981(688) 1986(2138) 2000(726) 2051(476)
2	MnS5-2T	1919(887) 1967(343) 1974(669) 2004(1607) 2038(488)
3	MnS5-3Q	1953(295) 1983(1059) 1988(958) 2000(599) 2059(672)
4	MnS5-4Q	1862(379) 1977(679) 1989(633) 1998(1927) 2044(508)
5	MnS5-5T	1942(630) 1966(808) 1968(675) 1995(1682) 2036(476)
6	MnS5-6Q	1890(450) 1958(140) 1986(1057) 2007(1602) 2042(550)
7	MnS5-7S	1945(368) 1964(562) 1969(690) 1982(1732) 2035(593)
8	MnS5-8Q	1873(343) 1970(534) 1993(838) 2008(1573) 2040(554)
9	MnS5-9S	1933(671) 1961(410) 1975(614) 1982(1800) 2032(609)
10	MnS5-10T	1916(358) 1950(904) 1970(722) 2000(1891) 2031(379)
11	MnS5-11Q	1869(423) 1938(393) 1971(2530) 2009(768) 2051(576)
12	MnS5-12S	1939(690) 1961(130) 1979(657) 1987(1664) 2034(706)
13	MnS5-13S	1788(308) 1963(457) 1978(865) 1997(1999) 2029(299)
14	MnS5-14T	1916(358) 1950(904) 1970(722) 2000(1891) 2031(379)
15	MnS5-15Q	1660(317) 1986(716) 2009(446) 2010(1053) 2071(539)
1	MnS6-1S	1964(469) 1971(343) 1978(923) 1981(681) 2021(1534) 2048(362)
2	MnS6-2Q	1880(369) 1972(636) 1983(830) 2000(706) 2007(1524) 2054(529)
3	MnS6-3T	1955(385) 1968(857) 1969(349) 1985(950) 2013(1598) 2043(370)
4	MnS6-4T	1947(755) 1983(731) 1994(515) 2005(496) 2011(1820) 2079(266)
5	MnS6-5T	1955(385) 1968(849) 1969(356) 1985(950) 2013(1597) 2043(371)
1	MnS7-1S	1964(631) 1977(395) 1984(749) 2002(1216) 2007(335) 2033(1311) 2079(225)
2	MnS7-2S	1893(339) 1980(0) 1987(1357) 1997(8) 2001(1074) 2038(2038) 2063(108)
3	MnS7-3S	1890(252) 1969(147) 1988(763) 1993(510) 1998(817) 2029(1907) 2061(315)
4	MnS7-4S	1945(235) 1967(164) 1986(585) 2004(1021) 2007(708) 2019(1389) 2079(400)
5	MnS7-5S	1890(252) 1969(147) 1988(766) 1993(507) 1998(817) 2029(1907) 2061(314)
6	MnS7-6S	1900(232) 1985(144) 1991(647) 2000(1066) 2012(649) 2029(1220) 2079(435)
1	MnS8-1S	1973(716) 1979(389) 1984(1027) 1995(327) 2005(1540) 2006(401) 2058(1010) 2081(127)
2	MnS8-2S	1965(576) 1976(649) 2005(465) 2012(1011) 2019(908) 2029(1572) 2039(68) 2095(371)
3	MnS8-3S	1925(561) 1959(655) 2012(1143) 2014(242) 2029(1171) 2035(1094) 2056(58) 2110(306)
4	MnS8-4S	1880(305) 1969(185) 2003(419) 2009(1179) 2012(774) 2015(405) 2047(1386) 2083(314)
5	MnS8-5S	1880(304) 1969(185) 2003(416) 2009(1182) 2012(774) 2015(403) 2047(1387) 2083(314)
6	MnS8-6S	1969(381) 1982(3) 1984(1493) 1995(1651) 1999(191) 2001(134) 2060(1142) 2078(79)
7	MnS8-7S	1819(729) 1979(329) 1985(641) 2008(661) 2011(684) 2017(1101) 2059(904) 2082(273)
8	MnS8-8S	1950(739) 1961(615) 2008(672) 2016(1123) 2020(1112) 2025(1017) 2051(139) 2102(347)
9	MnS8-9T	1942(452) 1965(580) 2003(993) 2004(5) 2010(1735) 2019(1405) 2031(41) 2084(661)
10	MnS8-10S	1834(649) 1978(681) 1985(519) 2008(530) 2008(1158) 2013(750) 2055(1341) 2075(180)

Table S14. Mulliken charges and spin densities $H_2C_2S_2Mn_2(CO)_n$ (n=5, 6, 7).

	Charge	Spin density
MnS5-1Q	1 Mn 1.06	4.24
	2 Mn 0.64	0.05
MnS5-2T	1 Mn 0.65	0.06
	2 Mn 0.88	2.48
MnS5-3Q	1 Mn 0.56	-0.24
	2 Mn 1.11	4.39
MnS5-4Q	1 Mn 0.58	0.07
	2 Mn 1.09	4.18
MnS6-1S	1 Mn 0.64	
	2 Mn 0.67	
MnS7-1S	1 Mn 0.65	
	2 Mn 0.72	
MnS7-2S	1 Mn 0.62	
	2 Mn 0.627	

Table S15. TD-DFT-derived spectra: main contributors to the lowest-energy maxima in $H_2C_2S_2Mn_2(CO)_6$ and $H_2C_2S_2Mn_2(CO)_6 \cdot NH_3$. Orbital transitions marked in **bold** are discussed in the main text of the manuscript.

Wavelength (nm)	Oscillator strength	Molecular orbitals, coefficients
$(HC)_2S_2Mn_2(CO)_6$		
489.92	0.0033	HOMO-5 -> LUMO -0.13452
		HOMO -> LUMO 0.61644
		HOMO -> LUMO+2 -0.20493
		HOMO ->LUMO+15 -0.14890
464.47	0.0064	HOMO-4 -> LUMO -0.12364
		HOMO-3 -> LUMO -0.20530
		HOMO-1 -> LUMO 0.57626
		HOMO-1 -> LUMO+2 -0.17916
		HOMO-1 ->LUMO+15 -0.14717
$(HC)_2S_2Mn_2(CO)_6 .NH_3$		
357.50 nm	0.0126	HOMO-4 -> LUMO+3 0.15996
		HOMO-3 -> LUMO+2 -0.11098
		HOMO-3 -> LUMO+3 0.11619
		HOMO-3 ->LUMO+5 -0.13454
		HOMO-3 ->LUMO+6 0.10631
		HOMO-2 -> LUMO+2 -0.10703
		HOMO-1 -> LUMO+1 -0.16827
		HOMO-1 -> LUMO+4 0.11364
		HOMO -> LUMO+1 -0.24104
		HOMO -> LUMO+2 0.41212
		HOMO ->LUMO+4 -0.12812
		HOMO ->LUMO+18 -0.14625