Supplementary Information

A decomposition mechanism for Mn_2(DSBDC) metal-organic framework in the presence of water molecules

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S1. Adsorption configurations for the adsorption of three, four and five water molecules

S1.1. Three adsorbed water molecues

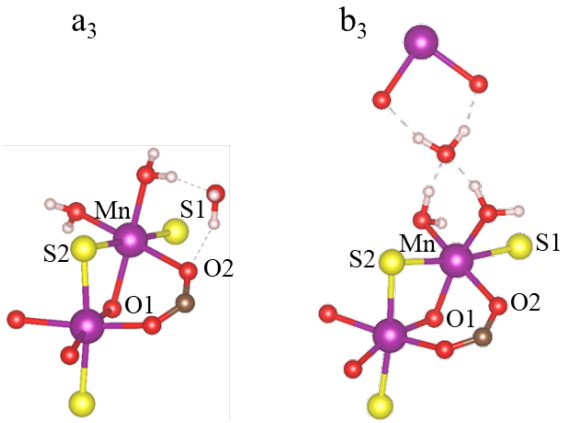

Figure S1. Configurations for the adsorption of three water molecules. The Mn, O, S, C, and H atoms are colored in purple, red, yellow, brown, and white.

Table S1. The adsorption energies E_{ads} (eV), the metal-linker bond lengths d (Å), and the angles θ and φ (°) for the adsorption of three water molecules.

$3H_2O$	E_{ads}	d_{Mn-O1}	d_{Mn-O2}	d_{Mn-S1}	d_{Mn-S2}	θ	φ
a_3	-0.53	2.29	2.31	2.56	2.55	178.7	85.6
b_3	-0.31	2.24	2.20	2.72	2.56	170.7	84.2

S1.2. Four adsorbed water molecules

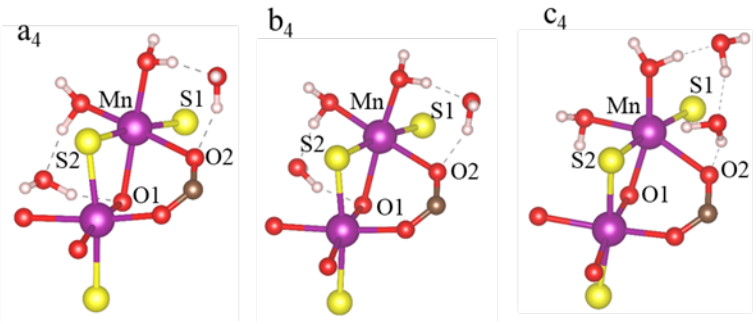

Figure S2. Configurations for the adsorption of four water molecules. The Mn, O, S, C, and H atoms are colored in purple, red, yellow, brown, and white.

Table S2. The adsorption energies E_{ads} (eV), the metal-linker bond lengths d (Å), and the angles θ and φ (°) for the adsorption of four water molecules.

$4H_2O$	E_{ads}	d_{Mn-O1}	d_{Mn-O2}	d_{Mn-S1}	d_{Mn-S2}	θ	φ
a_4	-0.58	2.37	2.39	2.55	2.56	173.9	83.0
b_4	-0.52	2.40	2.37	2.55	2.55	175.0	83.8
c_4	-0.36	2.35	2.40	2.54	2.58	174.1	82.5

S1.3. Five adsorbed water molecules

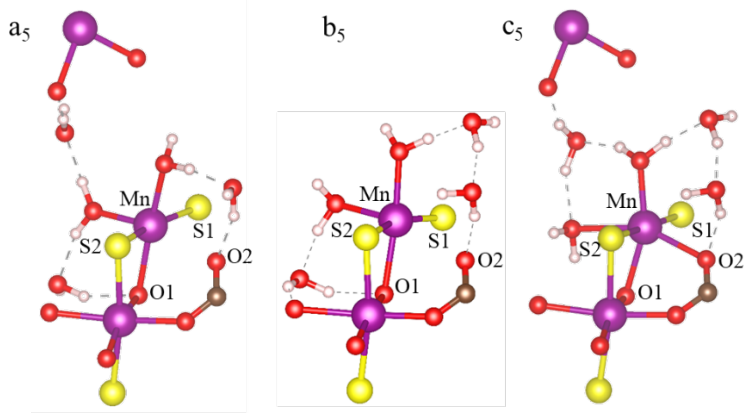

Figure S3. Configurations for the adsorption of five water molecules. The Mn, O, S, C, and H atoms are colored in purple, red, yellow, brown, and white.

Table S3. The adsorption energies E_{ads} (eV), the metal-linker bond lengths d (Å), and the angles θ and φ (°) for the adsorption of five water molecules.

$5H_2O$	E_{ads}	d_{Mn-O1}	d_{Mn-O2}	d_{Mn-S1}	d_{Mn-S2}	θ	φ
a_5	-0.50	2.33	2.54	2.56	2.55	167.9	80.7
b_5	-0.32	2.40	2.75	2.51	2.55	162.3	75.9
c_5	-0.19	2.32	2.31	2.57	2.60	177.4	69.1

S2. Optimized structures and energies at PBE-D3 level

S2.1. Water in the pore

Energy (eV): -816.13

Simulation cell vectors (Å):

a =	16.5453479131724741	-0.0128362548017865	-0.0410984844141151
b =	-5.9741385465123997	15.4557798010297009	0.0192601024933196
c =	-5.9696692819030144	-8.7762589586729387	12.7344044946325621

Fractional coordinates:

No.	Element	a	b	c
1	Mn	0.407347680	0.091008575	0.748556094
2	Mn	0.591388402	0.907506756	0.248095162
3	Mn	0.748996967	0.407553077	0.090659341
4	Mn	0.248986098	0.591591540	0.906395584
5	Mn	0.090926961	0.748905164	0.406397720
6	Mn	0.907187788	0.249592916	0.590032311
7	Mn	0.646217021	0.249320247	0.851914230
8	Mn	0.352135527	0.749722361	0.145107556
9	Mn	0.851907938	0.646232955	0.248529337
10	Mn	0.146084281	0.352915068	0.748218390
11	Mn	0.248758953	0.852430769	0.645400327
12	Mn	0.748632704	0.146740864	0.351679973
13	S	0.329383235	0.995346893	0.821809795
14	S	0.668724608	0.004220278	0.175297542
15	S	0.822838897	0.330236086	0.994853593
16	S	0.175470174	0.668946709	0.002296281
17	S	-0.004656522	0.822267590	0.328352285
18	S	0.003439560	0.176053617	0.666640400
19	S	0.675328204	0.503203566	0.167502034
20	S	0.322621084	0.495765105	0.828901324
21	S	0.503524153	0.167695603	0.675053363
22	S	0.495084602	0.829109263	0.321177385
23	S	0.167963241	0.675726802	0.502690126
24	S	0.829012039	0.322994977	0.494825685
25	O	0.559873283	0.136981663	0.873610824
26	O	0.438646896	0.862175516	0.123643921
27	O	0.874262751	0.560195604	0.136447332
28	O	0.123893682	0.438887133	0.860437284
29	O	0.136720839	0.874381850	0.558703024
30	O	0.862031885	0.125190713	0.436975343
31	O	0.623969185	0.361470791	0.937713157

32	O	0.374119179	0.637387793	0.058920448
33	O	0.361912647	0.937989641	0.623895468
34	O	0.636723636	0.059556304	0.373511339
35	O	0.938008386	0.624500972	0.360999978
36	O	0.059716471	0.374912564	0.636173265
37	O	0.653635871	0.253239671	0.049087869
38	O	0.344419021	0.746043013	0.948089471
39	O	0.049923855	0.653194347	0.252414504
40	O	0.948149871	0.344649298	0.744352022
41	O	0.253394844	0.049779145	0.652225755
42	O	0.746169450	0.949539373	0.343061057
43	O	0.448213693	0.245293592	0.843411805
44	O	0.549840268	0.753292621	0.152381537
45	O	0.245877028	0.843661056	0.448304039
46	O	0.753383889	0.152733152	0.548827386
47	O	0.844224698	0.448905029	0.245003270
48	O	0.153232522	0.550391295	0.752437033
49	O	0.482058341	0.492081701	0.395188796
50	C	0.535128205	0.076455326	0.979518243
51	C	0.462788289	0.922868968	0.017609884
52	C	0.980048269	0.535646449	0.075276917
53	C	0.017747480	0.463282662	0.921197781
54	C	0.076680868	0.980735892	0.533618005
55	C	0.923305950	0.019328433	0.461015739
56	C	0.517714537	0.422180774	0.961883225
57	C	0.479964352	0.576261974	0.034278076
58	C	0.422902655	0.962000921	0.517946344
59	C	0.576539637	0.034470353	0.479655149
60	C	0.962047909	0.518629729	0.422009548
61	C	0.034568640	0.480779342	0.575717871
62	C	0.426539320	0.995839134	0.914825582
63	C	0.571369613	0.003493200	0.082266491
64	C	0.915411448	0.427132454	0.994777195
65	C	0.082430084	0.571823500	0.001775050
66	C	-0.003799846	0.916129909	0.425114955
67	C	0.003644515	0.083739366	0.569557995
68	C	0.582393196	0.502738157	0.070386776
69	C	0.415319942	0.495751807	0.925784736
70	C	0.503439673	0.070533520	0.582539842
71	C	0.495895441	0.925981712	0.414910745
72	C	0.070673971	0.583187082	0.502450130
73	C	0.925947743	0.416098232	0.495223545
74	C	0.604783789	0.079397090	0.061600778
75	C	0.393105265	0.919975874	0.935555072
76	C	0.061830489	0.605284735	0.077829799
77	C	0.935824564	0.393695569	0.918563631

78	C	0.079632291	0.063029845	0.603084696
79	C	0.920598741	0.937284015	0.391472153
80	C	0.435780257	0.419556803	0.892304545
81	C	0.561795273	0.578817421	0.103854391
82	C	0.420094316	0.892445463	0.435821376
83	C	0.579476847	0.103992578	0.561879644
84	C	0.892366604	0.436801973	0.419362197
85	C	0.104171205	0.562749688	0.578507496
86	C	0.585081904	0.161811824	0.967171584
87	C	0.413066668	0.837476798	0.030018813
88	C	0.967827646	0.585240850	0.160963705
89	C	0.030141889	0.413383577	0.835729241
90	C	0.161805470	0.967991203	0.583714158
91	C	0.837630845	0.031642208	0.411425704
92	C	0.530181662	0.336725420	0.912107980
93	C	0.467731342	0.661888637	0.084062222
94	C	0.337328545	0.912316987	0.530302756
95	C	0.661778771	0.084449991	0.467033184
96	C	0.912483888	0.530898621	0.336436337
97	C	0.084697829	0.468447545	0.661017608
98	H	0.688182182	0.142199240	0.109309544
99	H	0.309678998	0.857284395	0.887967415
100	H	0.109362444	0.688671009	0.140437328
101	H	0.888119877	0.310342601	0.855810913
102	H	0.142298913	0.110640696	0.686413604
103	H	0.858113054	0.889819194	0.308079786
104	H	0.388132874	0.356844692	0.808964026
105	H	0.609341212	0.641406762	0.187214779
106	H	0.357308981	0.809091159	0.388080598
107	H	0.642208089	0.187349692	0.609544955
108	H	0.808881290	0.389345235	0.356879528
109	H	0.187596674	0.610437422	0.641224577
110	H	0.498723680	0.562506803	0.419766437
111	H	0.410660860	0.451388261	0.375713684

S2.2. a_0

Energy (eV): -801.88

Simulation cell vectors (Å):

a =	16.5693759918000012	0.0000000000000000	0.0000000000000000
b =	-5.9987501901000000	15.4453623109000002	0.0000000000000000
c =	-5.9987508955999997	-8.7651317318000004	12.7173867992999998

Fractional coordinates:

No.	Element	a	b	c
1	Mn	0.408041988	0.091958019	0.750000005
2	Mn	0.591958038	0.908041929	0.250000008
3	Mn	0.750000023	0.408041990	0.091958026
4	Mn	0.250000036	0.591958050	0.908041987
5	Mn	0.091958039	0.749999993	0.408042009
6	Mn	0.908042018	0.249999987	0.591958060
7	Mn	0.646837096	0.249999974	0.853162950
8	Mn	0.353162935	0.749999990	0.146837090
9	Mn	0.853162918	0.646837063	0.250000008
10	Mn	0.146837119	0.353162916	0.750000005
11	Mn	0.250000000	0.853162908	0.646837059
12	Mn	0.750000038	0.146837091	0.353162935
13	S	0.330785837	0.995994523	0.823387200
14	S	0.669214267	0.004005523	0.176612851
15	S	0.823387136	0.330785791	0.995994526
16	S	0.176612833	0.669214173	0.004005513
17	S	0.995994541	0.823387147	0.330785828
18	S	0.004005551	0.176612849	0.669214241
19	S	0.676612846	0.504005475	0.169214188
20	S	0.323387162	0.495994484	0.830785843
21	S	0.504005488	0.169214189	0.676612885
22	S	0.495994492	0.830785832	0.323387146
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24	S	0.830785805	0.323387160	0.495994510
25	O	0.560604259	0.137723733	0.875037326
26	O	0.439395788	0.862276195	0.124962706
27	O	0.875037338	0.560604217	0.137723730
28	O	0.124962726	0.439395809	0.862276311
29	O	0.137723735	0.875037322	0.560604224
30	O	0.862276231	0.124962719	0.439395845
31	O	0.624962754	0.362276285	0.939395823
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33	O	0.362276267	0.939395766	0.624962722
34	O	0.637723769	0.060604192	0.375037310
35	O	0.939395752	0.624962655	0.362276258
36	O	0.060604238	0.375037335	0.637723774
37	O	0.655257513	0.253642730	0.050713156
38	O	0.344742462	0.746357263	0.949286828
39	O	0.050713147	0.655257485	0.253642750
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41	O	0.253642757	0.050713150	0.655257514

42	O	0.746357306	0.949286797	0.344742442
43	O	0.449286870	0.246357273	0.844742495
44	O	0.550713138	0.753642676	0.155257545
45	O	0.246357292	0.844742458	0.449286850
46	O	0.753642713	0.155257532	0.550713182
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49	C	0.536332027	0.076897652	0.981028436
50	C	0.463667966	0.923102293	0.018971570
51	C	0.981028472	0.536332015	0.076897660
52	C	0.018971557	0.463667955	0.923102339
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54	C	0.923102323	0.018971563	0.463668019
55	C	0.518971595	0.423102317	0.963667997
56	C	0.481028458	0.576897698	0.036332025
57	C	0.423102326	0.963667936	0.518971573
58	C	0.576897716	0.036332038	0.481028458
59	C	0.963667993	0.518971606	0.423102361
60	C	0.036332030	0.481028435	0.576897708
61	C	0.427785077	0.996370273	0.916334884
62	C	0.572214927	0.003629684	0.083665138
63	C	0.916334852	0.427785091	0.996370375
64	C	0.083665128	0.572214882	0.003629683
65	C	0.996370224	0.916334854	0.427785099
66	C	0.003629709	0.083665135	0.572214932
67	C	0.583665119	0.503629670	0.072214903
68	C	0.416334902	0.496370301	0.927785152
69	C	0.503629704	0.072214890	0.583665163
70	C	0.496370315	0.927785099	0.416334869
71	C	0.072214923	0.583665135	0.503629710
72	C	0.927785067	0.416334854	0.496370322
73	C	0.605785084	0.079611067	0.063055817
74	C	0.394214910	0.920388888	0.936944182
75	C	0.063055825	0.605785092	0.079611077
76	C	0.936944250	0.394214944	0.920388983
77	C	0.079611089	0.063055800	0.605785092
78	C	0.920388919	0.936944158	0.394214939
79	C	0.436944228	0.420388957	0.894214993
80	C	0.563055783	0.579611053	0.105785076
81	C	0.420388942	0.894214913	0.436944203
82	C	0.579611092	0.105785077	0.563055828
83	C	0.894214982	0.436944199	0.420388967
84	C	0.105785066	0.563055790	0.579611064

85	C	0.586299213	0.162319717	0.968687890
86	C	0.413700842	0.837680287	0.031312168
87	C	0.968687797	0.586299170	0.162319738
88	C	0.031312197	0.413700872	0.837680331
89	C	0.162319781	0.968687875	0.586299217
90	C	0.837680299	0.031312167	0.413700852
91	C	0.531312192	0.337680312	0.913700868
92	C	0.468687804	0.662319683	0.086299173
93	C	0.337680318	0.913700866	0.531312195
94	C	0.662319712	0.086299154	0.468687836
95	C	0.913700787	0.531312128	0.337680278
96	C	0.086299192	0.468687831	0.662319754
97	H	0.689146845	0.142298994	0.110784103
98	H	0.310853239	0.857700999	0.889215947
99	H	0.110784098	0.689146797	0.142298998
100	H	0.889215904	0.310853224	0.857701033
101	H	0.142298997	0.110784087	0.689146830
102	H	0.857700992	0.889215882	0.310853220
103	H	0.389215907	0.357701012	0.810853179
104	H	0.610784120	0.642298976	0.189146796
105	H	0.357701004	0.810853192	0.389215932
106	H	0.642298997	0.189146787	0.610784137
107	H	0.810853214	0.389215920	0.357701017
108	H	0.189146803	0.610784106	0.642299051

S2.3. a_1

Energy (eV): -816.80

Simulation cell vectors (Å):

a =	16.5677265132188012	0.0511150271927081	-0.0165935637798475
b =	-5.9302247980505296	15.3695197175355034	-0.0331520035156543
c =	-6.0181281504725224	-8.7356184538044950	12.7695065877148419

Fractional coordinates:

No.	Element	a	b	c
1	Mn	0.411320983	0.089323617	0.757347751
2	Mn	0.593991435	0.906381704	0.258804033
3	Mn	0.752476181	0.409116193	0.100292542
4	Mn	0.249229604	0.591285023	0.916924622
5	Mn	0.093840997	0.748103991	0.414911989

6	Mn	0.908933365	0.249065066	0.601229872
7	Mn	0.649045865	0.248352334	0.861289828
8	Mn	0.353877266	0.749395826	0.155640931
9	Mn	0.853171871	0.652985032	0.269262961
10	Mn	0.146718398	0.351538967	0.760135526
11	Mn	0.252178418	0.850480985	0.653933661
12	Mn	0.750260552	0.146540420	0.361888137
13	S	0.332998976	0.994202159	0.830401663
14	S	0.670819659	0.003191856	0.186196939
15	S	0.825113145	0.330808386	0.005267148
16	S	0.177280922	0.670164544	0.014009281
17	S	0.003153846	0.825441380	0.337151004
18	S	0.004343476	0.173021946	0.676230688
19	S	0.672444031	0.495685504	0.172282571
20	S	0.321685099	0.494256213	0.837649397
21	S	0.506642808	0.167189299	0.684588230
22	S	0.497654047	0.827405726	0.330730994
23	S	0.170947963	0.673339543	0.511367335
24	S	0.831676981	0.323263637	0.505296767
25	O	0.563189175	0.135259802	0.882607396
26	O	0.441406078	0.862157920	0.134760775
27	O	0.876109264	0.563706380	0.149966856
28	O	0.125729933	0.438792186	0.872713388
29	O	0.141425597	0.874777564	0.568161804
30	O	0.862847532	0.123776887	0.446712728
31	O	0.625508526	0.360452043	0.944773996
32	O	0.375153423	0.636322284	0.068499170
33	O	0.365269493	0.936035280	0.632857507
34	O	0.639480176	0.058818425	0.383921850
35	O	0.942837056	0.624323356	0.371760655
36	O	0.060941286	0.374245438	0.648207268
37	O	0.656925783	0.252502330	0.057649481
38	O	0.345350769	0.746049572	0.959310473
39	O	0.051699329	0.653290372	0.261715030
40	O	0.950533400	0.343367950	0.756075555
41	O	0.258611577	0.050357882	0.660775995
42	O	0.749476209	0.947356018	0.355176649
43	O	0.450419106	0.243249156	0.850598215
44	O	0.550747329	0.750847220	0.163122475
45	O	0.249293461	0.842397343	0.457640361
46	O	0.755550478	0.152085859	0.559074484
47	O	0.846860365	0.448177251	0.254280893
48	O	0.153337855	0.550312379	0.763229328

49	O	0.815714521	0.730894198	0.380060963
50	C	0.538297120	0.075534375	0.989021142
51	C	0.465484555	0.922441463	0.028283523
52	C	0.979168606	0.537147328	0.084354934
53	C	0.018893141	0.464037630	0.931903565
54	C	0.082730372	0.982551209	0.542616924
55	C	0.928008339	0.020159999	0.470776642
56	C	0.518317044	0.420076435	0.968297607
57	C	0.479737161	0.573761355	0.042149605
58	C	0.425795125	0.960882312	0.527243218
59	C	0.579273737	0.033322226	0.489527191
60	C	0.965729838	0.516418872	0.430533595
61	C	0.036975673	0.479757441	0.585772798
62	C	0.429934710	0.995082419	0.924363097
63	C	0.573830378	0.002705995	0.092713280
64	C	0.916081111	0.428304769	0.004678280
65	C	0.082825698	0.572909846	0.012162018
66	C	0.004765662	0.920109423	0.433641088
67	C	0.006881275	0.083141227	0.579395939
68	C	0.581720601	0.498666794	0.077121958
69	C	0.415429882	0.494115122	0.933570075
70	C	0.506185390	0.069607993	0.591955235
71	C	0.498762901	0.924665308	0.424653623
72	C	0.073948500	0.580999525	0.511297517
73	C	0.928832216	0.415044661	0.504895663
74	C	0.607457341	0.078341036	0.071464033
75	C	0.396345777	0.919576213	0.945753628
76	C	0.060833260	0.606702071	0.086859195
77	C	0.936981849	0.394604261	0.929078121
78	C	0.083623582	0.062842720	0.612443806
79	C	0.928514885	0.941257992	0.400551430
80	C	0.436857978	0.418422293	0.899278311
81	C	0.561024141	0.575011854	0.110869991
82	C	0.423021531	0.891137956	0.445254032
83	C	0.582118318	0.103041085	0.571561050
84	C	0.895923557	0.434962150	0.428125307
85	C	0.106872313	0.561014179	0.588012666
86	C	0.588477861	0.160806755	0.976288197
87	C	0.415205083	0.837397702	0.041103701
88	C	0.967953324	0.586819967	0.171258677
89	C	0.031968944	0.413216304	0.847439283
90	C	0.167234161	0.968772994	0.592711766
91	C	0.840306024	0.030596845	0.421850232

92	C	0.531785836	0.335048951	0.918856138
93	C	0.468214133	0.659863279	0.093437117
94	C	0.340458677	0.910840567	0.539400059
95	C	0.664305431	0.083557348	0.477244837
96	C	0.916263217	0.529816595	0.345640134
97	C	0.085926337	0.468001115	0.672033320
98	H	0.690684572	0.140875015	0.119010350
99	H	0.313124107	0.857075599	0.898223029
100	H	0.108040744	0.690353176	0.149112144
101	H	0.890040552	0.310905100	0.867054274
102	H	0.145030964	0.109009893	0.695895174
103	H	0.867962932	0.895922781	0.316893268
104	H	0.389929302	0.356639258	0.815794220
105	H	0.608187441	0.637628855	0.194031696
106	H	0.360350500	0.807645894	0.397465965
107	H	0.644682968	0.186560005	0.619314550
108	H	0.812829414	0.387472713	0.365193527
109	H	0.189967751	0.608648471	0.650980366
110	H	0.832440487	0.802049713	0.404454227
111	H	0.743431277	0.685155596	0.355886240

S2.4. a_2

Energy (eV):

Simulation cell vectors (Å): = -831.65

a =	16.5839773914605608	0.0874979127047795	-0.0429252073667438
b =	-5.9022211251893131	15.3020395198382815	0.0119287476792093
c =	-6.0634317945648428	-8.6883899528903221	12.7588715312856564

Fractional coordinates:

No.	Element	a	b	c
1	Mn	0.412217197	0.087022127	0.755851150
2	Mn	0.594777655	0.903747713	0.259273715
3	Mn	0.752362680	0.408963195	0.099480383
4	Mn	0.248273095	0.590475028	0.916946020
5	Mn	0.090752952	0.747860327	0.413497873
6	Mn	0.907344858	0.248952491	0.600069632
7	Mn	0.648332876	0.247845604	0.859868601
8	Mn	0.353748243	0.748696032	0.156107024
9	Mn	0.845170756	0.655877928	0.256073875

10	Mn	0.145227221	0.351331619	0.759030427
11	Mn	0.252416901	0.849580065	0.653157992
12	Mn	0.748531624	0.146126617	0.360989348
13	S	0.334140614	0.993102016	0.829615285
14	S	0.671835478	0.001590970	0.187175313
15	S	0.824470160	0.330663951	0.003876051
16	S	0.177357899	0.670419389	0.013931186
17	S	0.011577565	0.832245530	0.340929770
18	S	0.003691920	0.172809135	0.675776447
19	S	0.669896200	0.487992508	0.172398622
20	S	0.321618593	0.493810737	0.839706699
21	S	0.505563330	0.165711974	0.682458235
22	S	0.497616590	0.825712494	0.331025394
23	S	0.167192087	0.672459544	0.508973907
24	S	0.828420169	0.323072018	0.503538012
25	O	0.564293086	0.133795062	0.881424955
26	O	0.442217558	0.860517089	0.134771147
27	O	0.873537176	0.563951242	0.144648005
28	O	0.124382832	0.438197553	0.871574573
29	O	0.142051701	0.875939211	0.570355630
30	O	0.862734990	0.124839060	0.446375349
31	O	0.623902204	0.359634411	0.942720216
32	O	0.373350379	0.633687489	0.070095899
33	O	0.365016746	0.934071654	0.631417560
34	O	0.638621007	0.056861346	0.382830483
35	O	0.936212399	0.625906405	0.367322039
36	O	0.058810380	0.374102311	0.646749796
37	O	0.658542051	0.250845737	0.056405787
38	O	0.346521646	0.744402473	0.959466682
39	O	0.048470744	0.651414559	0.259986800
40	O	0.949334791	0.343948292	0.754910089
41	O	0.260783539	0.051018164	0.660762086
42	O	0.751302967	0.948105698	0.355666736
43	O	0.449808322	0.239744726	0.850567806
44	O	0.549023259	0.746508072	0.162730298
45	O	0.248048121	0.840929503	0.456307078
46	O	0.754573773	0.151044758	0.558219430
47	O	0.848966637	0.450018439	0.253085802
48	O	0.152195529	0.550034024	0.762468450
49	O	0.800534440	0.732149092	0.359459160
50	O	0.766023540	0.694023431	0.144456683
51	C	0.539543196	0.073965780	0.988222560
52	C	0.466812139	0.920590046	0.027961949

53	C	0.978486003	0.536917164	0.083026939
54	C	0.018144804	0.464154171	0.930830325
55	C	0.085157629	0.985122445	0.544367772
56	C	0.930403168	0.022440952	0.470740389
57	C	0.514961399	0.414964149	0.969152784
58	C	0.475866785	0.567935707	0.044428733
59	C	0.424580460	0.959236433	0.525467191
60	C	0.578589665	0.031731019	0.488590892
61	C	0.961955393	0.520120752	0.430913957
62	C	0.033565682	0.481042296	0.585546122
63	C	0.431260029	0.993701730	0.923643093
64	C	0.575010779	0.000774276	0.092491669
65	C	0.915362885	0.428172929	0.003274714
66	C	0.082461863	0.572854846	0.011474750
67	C	0.009340534	0.924374889	0.434917672
68	C	0.007888509	0.084385936	0.579698955
69	C	0.576519610	0.490383182	0.078742846
70	C	0.412929435	0.490625217	0.935422488
71	C	0.505029069	0.067947581	0.590161609
72	C	0.498212403	0.923113476	0.423922378
73	C	0.070197115	0.582763069	0.510831718
74	C	0.925371437	0.417107806	0.504719554
75	C	0.608635219	0.076477358	0.070952218
76	C	0.397729685	0.917954530	0.945120474
77	C	0.060521089	0.606486066	0.086074009
78	C	0.936152748	0.394664309	0.927782002
79	C	0.084758405	0.064114593	0.613830994
80	C	0.932602627	0.945185455	0.400808147
81	C	0.434351374	0.414875639	0.900499922
82	C	0.555107974	0.566459363	0.113475704
83	C	0.422155779	0.889601611	0.443978331
84	C	0.581111801	0.101371299	0.570150640
85	C	0.892226377	0.438771999	0.428850075
86	C	0.103212391	0.562360389	0.587639736
87	C	0.589833765	0.159318551	0.975276506
88	C	0.416382244	0.835704499	0.041149793
89	C	0.965870797	0.586280401	0.168728082
90	C	0.030819442	0.413279361	0.846283397
91	C	0.168976142	0.970183053	0.594157080
92	C	0.841609204	0.031816929	0.421716552
93	C	0.530176077	0.331905887	0.918430796
94	C	0.465904793	0.655807452	0.094940808
95	C	0.339338821	0.909031100	0.537623952

96	C	0.663474208	0.082009430	0.476305194
97	C	0.913535381	0.532929589	0.344166286
98	C	0.083641156	0.468230170	0.671181093
99	H	0.784546450	0.702100494	0.396867671
100	H	0.791294591	0.699711728	0.101057124
101	H	0.691775948	0.138964661	0.118651063
102	H	0.314581678	0.855543571	0.897453475
103	H	0.108088576	0.690015056	0.148632720
104	H	0.888985721	0.311062621	0.865596178
105	H	0.145044320	0.109260973	0.697565088
106	H	0.872359724	0.899784738	0.316985753
107	H	0.388513684	0.354904632	0.816684633
108	H	0.601661122	0.626918975	0.197235070
109	H	0.359527358	0.806127073	0.396179035
110	H	0.643644575	0.184863254	0.617901475
111	H	0.809082003	0.391600309	0.366100487
112	H	0.186411182	0.609160044	0.650062172
113	H	0.844197858	0.809101690	0.407629475
114	H	0.689349319	0.646937900	0.098268503

S2.5. a_3

Energy (eV): -846.53

Simulation cell vectors (Å):

a =	16.4481557814500654	0.1450386539574471	-0.0582719401355663
b =	-5.8011028571030501	15.3433068873285006	-0.0443944641619118
c =	-6.0550026874942500	-8.7955558202775119	12.8302655307586466

Fractional coordinates:

No.	Element	a	b	c
1	Mn	0.412927252	0.080166475	0.755777800
2	Mn	0.594456041	0.899639318	0.257047492
3	Mn	0.752698837	0.403444817	0.098206719
4	Mn	0.247559055	0.587382534	0.915985774
5	Mn	0.091421523	0.741379774	0.411580661
6	Mn	0.907054795	0.245766228	0.599010537
7	Mn	0.649607198	0.240280632	0.859686045
8	Mn	0.352569292	0.746381177	0.154388155
9	Mn	0.840272330	0.652337948	0.256687799
10	Mn	0.145633427	0.347601472	0.757588495

11	Mn	0.252588501	0.843490364	0.651953552
12	Mn	0.746973367	0.141909949	0.359893451
13	S	0.333725240	0.987378594	0.828048798
14	S	0.672103358	0.997627884	0.186570420
15	S	0.827092016	0.325916477	0.004001764
16	S	0.174901447	0.667409665	0.012704167
17	S	0.010863994	0.824411721	0.338826324
18	S	0.003750396	0.169324143	0.673557451
19	S	0.668523399	0.480227561	0.170736956
20	S	0.322702033	0.490306944	0.839635586
21	S	0.505788401	0.159301140	0.683493813
22	S	0.497439275	0.821177391	0.327567916
23	S	0.166780635	0.665499809	0.507809918
24	S	0.826996108	0.319591044	0.502506110
25	O	0.565672024	0.126875059	0.880960467
26	O	0.441502352	0.857772662	0.133642206
27	O	0.872772728	0.559845292	0.145560442
28	O	0.124009546	0.435209467	0.869682378
29	O	0.141225586	0.868258163	0.566940901
30	O	0.862968412	0.122033254	0.445395953
31	O	0.623462128	0.351857954	0.941516011
32	O	0.373206970	0.631153075	0.068813521
33	O	0.366517472	0.927071804	0.631056998
34	O	0.636770531	0.052537612	0.380818168
35	O	0.933832229	0.620132276	0.369464230
36	O	0.058895178	0.370725377	0.646018593
37	O	0.660772910	0.244819817	0.055581054
38	O	0.344787624	0.741234881	0.958630646
39	O	0.047901854	0.642282961	0.259540134
40	O	0.948211989	0.341584024	0.753242485
41	O	0.260461975	0.043374057	0.660488827
42	O	0.752303058	0.945077615	0.353015319
43	O	0.448820508	0.232432878	0.850464942
44	O	0.549742322	0.742400626	0.160448209
45	O	0.249657984	0.832087247	0.456194458
46	O	0.753331292	0.148685378	0.555837779
47	O	0.854625132	0.446065048	0.251799926
48	O	0.150880044	0.546743004	0.761744787
49	O	0.762979782	0.692896181	0.147891875
50	O	0.799109611	0.728905884	0.361222625
51	O	0.894216541	0.711091091	0.516352644
52	C	0.540096262	0.068584298	0.987302929
53	C	0.466253223	0.916775751	0.027278981

54	C	0.977385611	0.532474376	0.081964329
55	C	0.017090095	0.460943523	0.929319137
56	C	0.085346821	0.979147500	0.542113763
57	C	0.931972699	0.019550276	0.468761693
58	C	0.514062081	0.408228885	0.968366245
59	C	0.475426496	0.562737336	0.043872400
60	C	0.425785367	0.952841747	0.525524056
61	C	0.577926718	0.027028221	0.486716660
62	C	0.961384390	0.513696271	0.429785348
63	C	0.032812934	0.476767795	0.584792684
64	C	0.431288517	0.988703322	0.922650747
65	C	0.574948744	0.996446828	0.091730838
66	C	0.915520383	0.423712317	0.002349600
67	C	0.080638660	0.569667688	0.010135079
68	C	0.010453432	0.919410932	0.432939366
69	C	0.008614180	0.080538606	0.577612572
70	C	0.574994630	0.483111729	0.077759217
71	C	0.413044928	0.485872915	0.934946149
72	C	0.505280680	0.061835863	0.590043797
73	C	0.498432277	0.918155048	0.422125234
74	C	0.069999798	0.576827892	0.510083995
75	C	0.924231573	0.412541687	0.503684976
76	C	0.609071993	0.071308074	0.070094901
77	C	0.397254476	0.913894760	0.944358488
78	C	0.058508122	0.602785018	0.084844113
79	C	0.935990805	0.390770884	0.926419220
80	C	0.084944615	0.058848836	0.611596052
81	C	0.934695024	0.942131537	0.398909477
82	C	0.434079041	0.409158321	0.899851935
83	C	0.553607358	0.559854126	0.112920451
84	C	0.423448194	0.883813448	0.443304396
85	C	0.580444921	0.096044570	0.569073500
86	C	0.891063245	0.433024677	0.427357599
87	C	0.102937146	0.557378489	0.587073103
88	C	0.591310938	0.153210183	0.974603069
89	C	0.415324118	0.832547037	0.040287303
90	C	0.964814597	0.580361649	0.168382736
91	C	0.029951565	0.410495412	0.844574958
92	C	0.168426249	0.962946560	0.592141617
93	C	0.842653009	0.029013574	0.419851050
94	C	0.529393564	0.324585505	0.917720169
95	C	0.465996231	0.651902646	0.093662377
96	C	0.340955645	0.901595198	0.537682153

97	C	0.662120443	0.078271530	0.474105812
98	C	0.914197042	0.526794700	0.343599967
99	C	0.082992850	0.464651246	0.670565327
100	H	0.692644034	0.133240963	0.117777582
101	H	0.313671975	0.852020110	0.896690477
102	H	0.105424841	0.686354281	0.147459563
103	H	0.889609536	0.307135915	0.864237178
104	H	0.144543228	0.103044089	0.695190678
105	H	0.875162319	0.897664791	0.315187366
106	H	0.388698155	0.349450626	0.816121257
107	H	0.599354379	0.619322904	0.196827102
108	H	0.361661070	0.800100129	0.395647382
109	H	0.642213276	0.179757135	0.616767552
110	H	0.807652594	0.385452158	0.364170656
111	H	0.186396972	0.604362472	0.649780032
112	H	0.787979382	0.698223548	0.104417918
113	H	0.685825808	0.648588763	0.102738242
114	H	0.828275396	0.803504993	0.389054157
115	H	0.826678974	0.724852226	0.423370260
116	H	0.853184972	0.658502204	0.523427828
117	H	0.922703085	0.680210799	0.480887584

S2.6. b_3

Energy (eV): -846.37

Simulation cell vectors (Å):

a =	16.3982771923479369	0.0216401680702027	-0.0127927812418133
b =	-5.8998461294108706	15.4950505470244408	-0.0414819073739848
c =	-5.9349951883375658	-8.7952615253237063	12.8562935563740162

Fractional coordinates:

No.	Element	a	b	c
1	Mn	0.409190004	0.079838137	0.755479601
2	Mn	0.589669905	0.901004945	0.253302939
3	Mn	0.747069945	0.399254992	0.098332605
4	Mn	0.244217731	0.583825132	0.910479927
5	Mn	0.089547625	0.739036765	0.409731324
6	Mn	0.907965584	0.248160525	0.597411223
7	Mn	0.647548423	0.240165274	0.859931942
8	Mn	0.346784624	0.742577700	0.150117792

9	Mn	0.838740958	0.637844730	0.256900511
10	Mn	0.145803172	0.348400725	0.754271743
11	Mn	0.247358487	0.842201982	0.649230006
12	Mn	0.748331694	0.143270962	0.357355582
13	S	0.329968541	0.983422947	0.826695995
14	S	0.668578305	0.996119323	0.182982371
15	S	0.823958494	0.323633571	0.003140842
16	S	0.170866831	0.663372504	0.006861859
17	S	0.012410173	0.825342221	0.339093929
18	S	0.002695036	0.170468588	0.668763781
19	S	0.658351743	0.472740850	0.168826953
20	S	0.324419525	0.490700976	0.839959422
21	S	0.505405342	0.158375903	0.683478232
22	S	0.494775186	0.823490548	0.324496053
23	S	0.168707320	0.667201809	0.507457772
24	S	0.827244805	0.318376308	0.500492194
25	O	0.560996843	0.125707979	0.879181025
26	O	0.438559311	0.850645101	0.127631031
27	O	0.872125429	0.552312552	0.146966374
28	O	0.119924579	0.432796778	0.863944479
29	O	0.132769372	0.864290886	0.565030829
30	O	0.871270690	0.130397059	0.443327991
31	O	0.620806645	0.349543565	0.942475721
32	O	0.361406873	0.622150654	0.063189796
33	O	0.362862028	0.928434911	0.630081126
34	O	0.639070317	0.052154254	0.379550691
35	O	0.939001697	0.614655298	0.363334896
36	O	0.059761161	0.371554882	0.643939289
37	O	0.656106585	0.240698488	0.053533266
38	O	0.343537848	0.736693924	0.953397339
39	O	0.049174745	0.645279461	0.257310815
40	O	0.944097726	0.339552597	0.749336114
41	O	0.254250973	0.038279279	0.661862101
42	O	0.760343060	0.955552244	0.346883345
43	O	0.445063788	0.231844629	0.845633038
44	O	0.537598856	0.730330768	0.164880427
45	O	0.247978590	0.834124351	0.455935176
46	O	0.754296635	0.146734851	0.553459797
47	O	0.844119829	0.439036003	0.250689029
48	O	0.152416737	0.546350596	0.758343442
49	O	0.770960568	0.680190501	0.149735282
50	O	0.828989029	0.718147183	0.389864111
51	O	0.723117994	0.768591735	0.279810433

52	C	0.535976115	0.064958437	0.984252663
53	C	0.462978960	0.912368767	0.022715790
54	C	0.976266508	0.528744727	0.080761250
55	C	0.013487969	0.457874956	0.925416262
56	C	0.082162156	0.977505659	0.541015211
57	C	0.939378039	0.027588295	0.465248335
58	C	0.509497902	0.404899678	0.966489022
59	C	0.463836043	0.551846922	0.043413611
60	C	0.424650376	0.954104514	0.525111122
61	C	0.577831414	0.027541016	0.485421591
62	C	0.962548424	0.510788370	0.426710278
63	C	0.034000533	0.475856033	0.582203128
64	C	0.427345464	0.984409060	0.919581724
65	C	0.571327051	0.993336159	0.087728913
66	C	0.913268271	0.420762635	0.001134957
67	C	0.077504687	0.565844142	0.005822112
68	C	0.013085698	0.922192260	0.431602886
69	C	0.009697127	0.083109395	0.574356437
70	C	0.564587501	0.473986779	0.075607154
71	C	0.408875189	0.481937280	0.934246689
72	C	0.505169797	0.062162239	0.589858897
73	C	0.496888227	0.919720142	0.420408351
74	C	0.070925949	0.575537976	0.507271180
75	C	0.925581279	0.410826807	0.501384807
76	C	0.605141097	0.068311070	0.066586793
77	C	0.393765793	0.908918887	0.940284439
78	C	0.056649763	0.598535902	0.081892492
79	C	0.932833755	0.388189185	0.924002316
80	C	0.081352649	0.057228668	0.609283940
81	C	0.944773732	0.952046132	0.397259112
82	C	0.432167357	0.408074736	0.898686716
83	C	0.536546378	0.543764788	0.110693749
84	C	0.421623421	0.885649033	0.442131512
85	C	0.581040210	0.096019537	0.568598538
86	C	0.892642173	0.430245835	0.424951208
87	C	0.103831589	0.556668304	0.584183887
88	C	0.586767351	0.150249367	0.972310533
89	C	0.412874067	0.827218416	0.034647396
90	C	0.964856766	0.577444820	0.167957071
91	C	0.025904471	0.407988873	0.839991732
92	C	0.162151335	0.958979141	0.591815733
93	C	0.852197691	0.039067344	0.416283106
94	C	0.525978713	0.323025373	0.915639664

95	C	0.453535182	0.639641922	0.092735817
96	C	0.338836126	0.903233858	0.537271696
97	C	0.663056417	0.077637659	0.472611052
98	C	0.913104698	0.522007685	0.340492585
99	C	0.084186953	0.464640441	0.667770410
100	H	0.688472405	0.131136417	0.114334851
101	H	0.310414551	0.846158157	0.892422805
102	H	0.103613828	0.681485375	0.144218241
103	H	0.885942615	0.305178895	0.861889264
104	H	0.137133113	0.098606200	0.692869104
105	H	0.892869832	0.914076819	0.313725701
106	H	0.390958605	0.352728508	0.814997383
107	H	0.573204378	0.593223701	0.194300617
108	H	0.358877960	0.802706272	0.394300193
109	H	0.643753061	0.178987913	0.616591210
110	H	0.809340700	0.382653567	0.362294552
111	H	0.187154896	0.604544858	0.646862853
112	H	0.836242114	0.733613588	0.165240979
113	H	0.750066489	0.720244140	0.189817140
114	H	0.785785078	0.743306639	0.362951816
115	H	0.896513865	0.779878903	0.452733417
116	H	0.752786492	0.844928037	0.316259107
117	H	0.647077075	0.738253387	0.232240948

S2.7. a_4

Energy (eV): -861.45

Simulation cell vectors (Å):

a =	16.4383958286577503	0.2226256532406143	-0.0897959786069950
b =	-5.7263921302814085	15.2734126942352830	-0.0653228637348406
c =	-6.1156672151428291	-8.8271574957866932	12.8874809319032035

Fractional coordinates:

No.	Element	a	b	c
1	Mn	0.415573963	0.078494627	0.755743949
2	Mn	0.596155483	0.900421026	0.258585316

3	Mn	0.756327305	0.404111224	0.100817003
4	Mn	0.247859132	0.588709126	0.916641869
5	Mn	0.092816146	0.741668690	0.413008464
6	Mn	0.907121729	0.247386597	0.600111645
7	Mn	0.651773268	0.239766504	0.860359854
8	Mn	0.353605393	0.748970873	0.155178076
9	Mn	0.838931449	0.659699397	0.255964034
10	Mn	0.145812068	0.348121009	0.758300390
11	Mn	0.255579321	0.842274718	0.651848972
12	Mn	0.747015126	0.144089795	0.362026396
13	S	0.336490399	0.986615612	0.827436532
14	S	0.674409346	0.999685292	0.189989706
15	S	0.829989824	0.328233389	0.005212015
16	S	0.175735753	0.669741056	0.013412741
17	S	0.014801915	0.826453655	0.341543089
18	S	0.003968069	0.169752643	0.674273777
19	S	0.672473531	0.482046497	0.171389017
20	S	0.322946923	0.490767373	0.841025148
21	S	0.507633764	0.159302360	0.684853315
22	S	0.498165974	0.821250312	0.327348831
23	S	0.167387292	0.663574190	0.507145133
24	S	0.826920157	0.322495704	0.504158996
25	O	0.569211171	0.126014870	0.881547171
26	O	0.443686888	0.860066887	0.135395926
27	O	0.876345790	0.563683799	0.145426971
28	O	0.124287266	0.436423560	0.869945455
29	O	0.145478349	0.870026459	0.569121973
30	O	0.862936434	0.123120748	0.446961403
31	O	0.624751848	0.353726384	0.939803629
32	O	0.373897573	0.632788883	0.069966189
33	O	0.369254123	0.925694706	0.631195914
34	O	0.636986286	0.053354829	0.381856682
35	O	0.933946022	0.621339397	0.369268123
36	O	0.058729837	0.371841741	0.647265175
37	O	0.663918727	0.245033403	0.055434104
38	O	0.345496011	0.743111560	0.960695182
39	O	0.049738593	0.639309143	0.261547831
40	O	0.948354196	0.343559282	0.753960346
41	O	0.264399638	0.045588301	0.662201011
42	O	0.754188387	0.945357954	0.354370861
43	O	0.452293284	0.230779394	0.854808898
44	O	0.550761801	0.741823001	0.161364570
45	O	0.251608027	0.830495476	0.456779385

46	O	0.753427371	0.150734324	0.556661280
47	O	0.858616176	0.447357803	0.252746506
48	O	0.151033441	0.548539435	0.762794109
49	O	0.761295842	0.699067621	0.149710933
50	O	0.798234400	0.733523978	0.361657330
51	O	0.896823690	0.716440082	0.515482972
52	O	0.745044237	0.567565268	-0.01567614
53	C	0.543156808	0.068745222	0.987940313
54	C	0.468778666	0.918056365	0.028983810
55	C	0.981222092	0.534764597	0.083847096
56	C	0.018296340	0.463001970	0.930081373
57	C	0.088812401	0.981352107	0.544404743
58	C	0.934458435	0.021432134	0.470240083
59	C	0.514170672	0.407052307	0.969383141
60	C	0.474255312	0.561054172	0.044788791
61	C	0.427380738	0.952188327	0.525968565
62	C	0.578683329	0.027531729	0.487282776
63	C	0.961818793	0.515048151	0.430743670
64	C	0.032798090	0.478405667	0.586017195
65	C	0.434351673	0.988736415	0.922936559
66	C	0.577460712	0.997832701	0.093874664
67	C	0.918232923	0.425836503	0.003506760
68	C	0.082551037	0.571979454	0.011311325
69	C	0.014516523	0.922006679	0.435393866
70	C	0.010354894	0.081898211	0.579080056
71	C	0.574973518	0.481696696	0.078415116
72	C	0.412374337	0.484818763	0.935873363
73	C	0.506669489	0.061537167	0.590796684
74	C	0.499486078	0.918302691	0.422425531
75	C	0.070524007	0.577123037	0.510595278
76	C	0.924123044	0.414801796	0.505101409
77	C	0.611835681	0.072118087	0.071662415
78	C	0.400128022	0.914521192	0.945170934
79	C	0.061862232	0.605300871	0.086862336
80	C	0.937539706	0.392672032	0.927074429
81	C	0.087419938	0.060632606	0.613539114
82	C	0.938605586	0.944979188	0.400778856
83	C	0.433528864	0.407734302	0.900755323
84	C	0.551956272	0.557352865	0.113642416
85	C	0.424937179	0.883417413	0.443530901
86	C	0.581331313	0.096314161	0.569870321
87	C	0.891113685	0.435299297	0.428749301
88	C	0.103258097	0.558120457	0.587890777

89	C	0.594508864	0.152855832	0.974835394
90	C	0.417164684	0.834410059	0.042196946
91	C	0.968646243	0.581733790	0.170020129
92	C	0.030393512	0.412233307	0.845047784
93	C	0.172309139	0.965015823	0.594271481
94	C	0.844114999	0.030098973	0.421256654
95	C	0.530740210	0.324112255	0.918911916
96	C	0.466080646	0.651652717	0.094655528
97	C	0.343000129	0.900287395	0.537956654
98	C	0.662425354	0.079418563	0.474886842
99	C	0.915710495	0.528376512	0.344359161
100	C	0.082950689	0.466218429	0.671774689
101	H	0.695433553	0.134043892	0.119700961
102	H	0.316546141	0.852654562	0.897211812
103	H	0.109119131	0.689069816	0.149721572
104	H	0.890645308	0.308891059	0.864391716
105	H	0.146562736	0.104529457	0.697096097
106	H	0.880336542	0.901326541	0.316954743
107	H	0.388371817	0.348172432	0.817138398
108	H	0.597064376	0.616268218	0.197499863
109	H	0.363365298	0.799406184	0.395548566
110	H	0.642835040	0.180320791	0.617797964
111	H	0.807598876	0.388292150	0.365849451
112	H	0.186796530	0.604434328	0.650308949
113	H	0.747635249	0.652921200	0.080089568
114	H	0.693319348	0.686321648	0.135326141
115	H	0.825775690	0.808220102	0.389693046
116	H	0.827568633	0.729449950	0.423618867
117	H	0.857725598	0.666271608	0.525805566
118	H	0.923327165	0.683054671	0.478935423
119	H	0.802119116	0.565771660	0.030786216
120	H	0.683721056	0.496383432	0.947348225

S2.8. b_4

Energy (eV): -861.36

Simulation cell vectors (Å):

a =	16.5420203051497232	0.1265644170458857	-0.0603159928604408
b =	-5.8513069220698535	15.2919010283681942	-0.0091781729180366
c =	-6.0816263459189939	-8.7274838508418231	12.7770776592694677

Fractional coordinates:

No.	Element	a	b	c
1	Mn	0.414445498	0.082127676	0.755520578
2	Mn	0.596401001	0.898840781	0.258390951
3	Mn	0.753780427	0.405427287	0.099716546
4	Mn	0.249678830	0.586723175	0.916563701
5	Mn	0.091858753	0.743995074	0.412475567
6	Mn	0.908143716	0.244985838	0.599265356
7	Mn	0.650157180	0.243171837	0.859338285
8	Mn	0.355209701	0.745926253	0.156058339
9	Mn	0.838678513	0.659482380	0.257009035
10	Mn	0.146550380	0.347257699	0.758389845
11	Mn	0.253879534	0.845612593	0.653293057
12	Mn	0.748129879	0.141668924	0.359838498
13	S	0.336295587	0.990000900	0.829611970
14	S	0.673443054	0.996907372	0.186834086
15	S	0.827186384	0.328165472	0.004197562
16	S	0.178362160	0.667892896	0.013639507
17	S	0.012891167	0.827010796	0.339204126
18	S	0.004665540	0.168632267	0.674220861
19	S	0.672372297	0.483477305	0.173333137
20	S	0.323473974	0.489762753	0.840366379
21	S	0.506627251	0.160367238	0.681962955
22	S	0.499455104	0.820674636	0.329916959
23	S	0.167195719	0.667735398	0.508649844
24	S	0.827919468	0.319269168	0.502520043
25	O	0.567127287	0.129563080	0.881712473
26	O	0.443824535	0.856893413	0.134313484
27	O	0.874181178	0.563713752	0.141801868
28	O	0.125312315	0.434757955	0.870781824
29	O	0.143400024	0.870960097	0.568457026
30	O	0.863599586	0.121574232	0.445320121
31	O	0.626557931	0.355280319	0.943700561
32	O	0.373768088	0.629679852	0.070045281
33	O	0.366353818	0.928342326	0.630507885
34	O	0.638749751	0.051863671	0.381538262
35	O	0.934145017	0.623129143	0.370221052
36	O	0.059443513	0.370097835	0.645972860
37	O	0.662930583	0.246639628	0.056986070
38	O	0.346714164	0.740712943	0.958784888
39	O	0.046556690	0.639475646	0.260237318
40	O	0.949959025	0.341612537	0.753898342

41	O	0.262613446	0.046346961	0.661544991
42	O	0.753930069	0.944246656	0.353971848
43	O	0.452051309	0.235258632	0.849012840
44	O	0.550092551	0.740710379	0.162829381
45	O	0.249622452	0.833768847	0.455086637
46	O	0.755149534	0.147803194	0.557096341
47	O	0.858264517	0.449900656	0.252503803
48	O	0.151977202	0.546226477	0.762219548
49	O	0.762668102	0.698624238	0.149638699
50	O	0.801043596	0.733641757	0.365443273
51	O	0.900837926	0.717080486	0.520531377
52	O	0.786914201	0.609688970	-0.00080837
53	C	0.542038889	0.069898245	0.988130428
54	C	0.468152630	0.916732363	0.027622015
55	C	0.979835874	0.534068466	0.082431636
56	C	0.019213640	0.461613463	0.930141369
57	C	0.087673307	0.981581621	0.543044300
58	C	0.933816851	0.020331209	0.468976050
59	C	0.516227285	0.409576371	0.969778234
60	C	0.475268723	0.561179976	0.045453668
61	C	0.426238154	0.953392141	0.524980996
62	C	0.579599160	0.026834015	0.487624585
63	C	0.962148206	0.516263813	0.430898297
64	C	0.033343598	0.477111301	0.585183382
65	C	0.433365280	0.990135887	0.923562776
66	C	0.576694779	0.996368630	0.092096672
67	C	0.916947705	0.425142369	0.002578973
68	C	0.083476812	0.570506730	0.011050552
69	C	0.013046870	0.922001879	0.433578420
70	C	0.010157929	0.081184703	0.578229779
71	C	0.576264726	0.483446304	0.079394226
72	C	0.413731560	0.485287563	0.936113297
73	C	0.506234924	0.062435871	0.589568038
74	C	0.499819064	0.917890654	0.423154483
75	C	0.070579188	0.578755022	0.511037961
76	C	0.924916039	0.413296694	0.504069711
77	C	0.610870573	0.071880808	0.070660818
78	C	0.399293768	0.914553424	0.944925901
79	C	0.061664727	0.604154302	0.085860852
80	C	0.937510287	0.391747940	0.926928879
81	C	0.086875146	0.060475262	0.612614375
82	C	0.937148441	0.944061318	0.398993109
83	C	0.435775460	0.409893410	0.900974282

84	C	0.553278958	0.558313991	0.114686059
85	C	0.424152548	0.883915596	0.443489621
86	C	0.581942713	0.096287307	0.569307457
87	C	0.891832539	0.434976455	0.428181153
88	C	0.103412057	0.558327677	0.587726661
89	C	0.593135541	0.155149523	0.975545784
90	C	0.417378352	0.832007821	0.040650702
91	C	0.966211643	0.581487879	0.167903663
92	C	0.031741651	0.410537813	0.845375277
93	C	0.170679508	0.965741292	0.593359091
94	C	0.843985049	0.028729788	0.420125267
95	C	0.532328071	0.327402646	0.918460710
96	C	0.466198123	0.650192702	0.095421267
97	C	0.340921138	0.902733353	0.536799722
98	C	0.663998870	0.077655594	0.475140143
99	C	0.915751232	0.530273139	0.344650066
100	C	0.083676329	0.464256081	0.670787603
101	H	0.694346802	0.133739761	0.118310763
102	H	0.315830989	0.852693504	0.897240659
103	H	0.109396240	0.687810826	0.148790823
104	H	0.890566900	0.308034045	0.864618757
105	H	0.146248126	0.104532041	0.696485118
106	H	0.878039431	0.899599025	0.314889853
107	H	0.391215991	0.351034084	0.817000469
108	H	0.598145432	0.616838897	0.198890976
109	H	0.362090698	0.800151401	0.395812394
110	H	0.643915637	0.180057627	0.616938011
111	H	0.808548052	0.387683297	0.365055850
112	H	0.186726513	0.604905905	0.650317928
113	H	0.768652271	0.672452618	0.088676272
114	H	0.687953248	0.667866951	0.120019424
115	H	0.827945021	0.807865878	0.392532166
116	H	0.831272572	0.730401641	0.428210135
117	H	0.861135246	0.665606175	0.529726722
118	H	0.926480847	0.684422772	0.482656637
119	H	0.817257179	0.580414020	0.034517273
120	H	0.841106747	0.654572368	0.996158258

S2.9. c_4

Energy (eV): -861.22

Simulation cell vectors (Å):

a =	16.5231976499016078	0.0882621881236604	-0.0550212311221351
b =	-5.8799323922778353	15.3134974931303294	-0.0164955430365376
c =	-6.0507939842934464	-8.7225149954500480	12.7673909494337678

Fractional coordinates:

No.	Element	a	b	c
1	Mn	0.409706727	0.074852562	0.746901075
2	Mn	0.593214850	0.892755485	0.249833347
3	Mn	0.750158257	0.399168400	0.091069005
4	Mn	0.245512191	0.580529297	0.907744910
5	Mn	0.085131542	0.736134669	0.402813027
6	Mn	0.904085689	0.239313257	0.590143325
7	Mn	0.645403163	0.237061132	0.850489527
8	Mn	0.350635051	0.740145445	0.147549131
9	Mn	0.833255434	0.651646482	0.242766000
10	Mn	0.142070656	0.341059724	0.748890228
11	Mn	0.248505491	0.837867374	0.643296551
12	Mn	0.743731656	0.136367308	0.350768619
13	S	0.330989765	0.981884745	0.820226020
14	S	0.669867353	0.991569948	0.178000979
15	S	0.822019127	0.320530260	0.994578565
16	S	0.173982008	0.661462051	0.004360383
17	S	0.007797755	0.820074525	0.329442668
18	S	-0.000309060	0.162004091	0.664167298
19	S	0.666838571	0.476049985	0.166482445
20	S	0.320224161	0.483673958	0.832371624
21	S	0.501510226	0.154298534	0.673193755
22	S	0.495079746	0.814866394	0.321370786
23	S	0.162801625	0.660985377	0.497813876
24	S	0.824174751	0.313462539	0.494236698
25	O	0.562553010	0.123432329	0.872967481
26	O	0.440810541	0.850216578	0.125683604
27	O	0.868940912	0.554694303	0.133766482
28	O	0.121529952	0.428547342	0.861846412
29	O	0.136441988	0.863143860	0.560122388
30	O	0.859019065	0.115940460	0.435783093
31	O	0.622322047	0.350890585	0.935017541
32	O	0.369655931	0.624114854	0.061910397
33	O	0.361125948	0.921923094	0.621239495
34	O	0.635925100	0.044648839	0.373159500

35	O	0.927129182	0.614120742	0.358425046
36	O	0.055792336	0.364205379	0.636846798
37	O	0.656000636	0.240971221	0.048006121
38	O	0.343718094	0.734038682	0.950000270
39	O	0.043114085	0.636542103	0.250750814
40	O	0.945920816	0.334509635	0.744991389
41	O	0.257386687	0.038390508	0.653266438
42	O	0.753642809	0.937675582	0.338823502
43	O	0.448189651	0.228218770	0.842653516
44	O	0.546790546	0.733346365	0.156975039
45	O	0.243528678	0.829330302	0.446117584
46	O	0.751296042	0.142379090	0.549099256
47	O	0.852637772	0.440763076	0.242517212
48	O	0.149619553	0.540415831	0.753059942
49	O	0.769007862	0.733827334	0.305066479
50	O	0.843021613	0.817940336	0.502244470
51	O	0.753470160	0.640841086	0.090771194
52	O	0.813500426	0.629872444	0.449617727
53	C	0.537210829	0.063540411	0.979244360
54	C	0.464357220	0.910286097	0.018766579
55	C	0.974798557	0.527144517	0.073116979
56	C	0.015004052	0.454847993	0.921180798
57	C	0.083257706	0.974984246	0.534257256
58	C	0.933796213	0.018213383	0.458881223
59	C	0.510883537	0.402319366	0.962297518
60	C	0.469499213	0.553332176	0.037765428
61	C	0.420918784	0.947627720	0.515683025
62	C	0.575336122	0.020914207	0.479074087
63	C	0.958001563	0.509247521	0.421126612
64	C	0.030038135	0.471047473	0.575978916
65	C	0.428534095	0.982948910	0.914478223
66	C	0.572910839	0.990614079	0.083323992
67	C	0.912217928	0.418161501	0.993477205
68	C	0.079016830	0.563820861	0.001864843
69	C	0.011483436	0.918165363	0.424542133
70	C	0.006678294	0.075903902	0.568702617
71	C	0.569750025	0.475353327	0.072312769
72	C	0.408970208	0.478371506	0.928176920
73	C	0.501330996	0.056673713	0.580574563
74	C	0.495194058	0.911963110	0.414373826
75	C	0.066603835	0.571966855	0.500978366
76	C	0.921336619	0.407069048	0.495160444
77	C	0.606650543	0.066300873	0.061961606

78	C	0.394893899	0.907306022	0.935866709
79	C	0.056755266	0.597350263	0.076420626
80	C	0.933133701	0.384786286	0.917985557
81	C	0.081905472	0.053631218	0.603728469
82	C	0.939950323	0.944638589	0.389940257
83	C	0.431012363	0.402997472	0.893192231
84	C	0.545740479	0.549191447	0.107031062
85	C	0.418883205	0.878011861	0.434286191
86	C	0.577581984	0.090535309	0.560677962
87	C	0.887852803	0.428263808	0.419066327
88	C	0.099980691	0.552124229	0.577993761
89	C	0.587634039	0.149072663	0.966687854
90	C	0.414183352	0.825434078	0.031903099
91	C	0.961343052	0.575112333	0.158680974
92	C	0.027698140	0.403877517	0.836521727
93	C	0.165046472	0.958069586	0.584982123
94	C	0.842616708	0.024085136	0.408464356
95	C	0.527815565	0.320968835	0.910897154
96	C	0.461865807	0.643301010	0.088238360
97	C	0.335267894	0.897173485	0.527500658
98	C	0.660368095	0.071447965	0.466931062
99	C	0.910528561	0.522126203	0.334255495
100	C	0.080604763	0.458451617	0.661602312
101	H	0.690137037	0.128857251	0.109744633
102	H	0.311419180	0.844779736	0.888113495
103	H	0.103977023	0.681115125	0.138953748
104	H	0.886374182	0.300980712	0.855849430
105	H	0.139751843	0.096428011	0.687875052
106	H	0.884935108	0.904278874	0.305706523
107	H	0.387089477	0.344554468	0.809104644
108	H	0.590045756	0.607264213	0.191075445
109	H	0.356429741	0.794234906	0.386445354
110	H	0.640000798	0.174291967	0.608477148
111	H	0.804233246	0.381197814	0.356682126
112	H	0.183564537	0.598954197	0.640332186
113	H	0.748767946	0.775037527	0.282887850
114	H	0.800492695	0.773343628	0.383745731
115	H	0.839330867	0.754397688	0.498735894
116	H	0.916640705	0.877040707	0.551561071
117	H	0.676968648	0.592532114	0.050380812
118	H	0.775449503	0.603222312	0.052835012
119	H	0.865812210	0.631629469	0.433943210
120	H	0.746541267	0.580758317	0.380307946

S2.10. a_5

Energy (eV): -876.28

Simulation cell vectors (Å):

a =	16.5311364529102178	0.2302137648885437	-0.1416887193303515
b =	-5.7573844226525406	15.2018860918589755	-0.0113026893444288
c =	-6.1889845838433537	-8.7644165878533613	12.8877204318586145

Fractional coordinates:

No.	Element	a	b	c
1	Mn	0.415692012	0.081355654	0.760520352
2	Mn	0.594901885	0.902734687	0.268413113
3	Mn	0.756101738	0.402974312	0.105854975
4	Mn	0.248332587	0.586849715	0.922469310
5	Mn	0.091084517	0.742103336	0.416433531
6	Mn	0.908163913	0.247701023	0.606838801
7	Mn	0.651738296	0.242951441	0.865822554
8	Mn	0.354756897	0.746938743	0.161594747
9	Mn	0.836431351	0.657532656	0.244401546
10	Mn	0.146998279	0.347493832	0.764538384
11	Mn	0.255345416	0.842948971	0.656009251
12	Mn	0.746877596	0.146280155	0.369414807
13	S	0.336514571	0.986894560	0.831543827
14	S	0.673411242	0.000561349	0.197541681
15	S	0.829158891	0.324631511	0.009117076
16	S	0.177206211	0.666920811	0.019428082
17	S	0.015160906	0.829790591	0.345290950
18	S	0.004361557	0.168462843	0.679055563
19	S	0.676479926	0.485407390	0.177860672
20	S	0.322856191	0.491535303	0.846710708
21	S	0.507897907	0.159848169	0.688591116
22	S	0.498690849	0.820888843	0.335444082
23	S	0.167600683	0.664301492	0.512347935
24	S	0.827705117	0.324111928	0.511274678
25	O	0.568246625	0.126991422	0.886135404
26	O	0.443301486	0.860385214	0.142297273
27	O	0.876942199	0.558289126	0.145964653
28	O	0.125413138	0.433994885	0.876332736

29	O	0.143926118	0.869454038	0.572548103
30	O	0.862272830	0.124058852	0.452607222
31	O	0.627125811	0.352760659	0.950899621
32	O	0.375892224	0.631479933	0.077352441
33	O	0.368634832	0.927028400	0.636005419
34	O	0.637508675	0.054711760	0.389301173
35	O	0.934694636	0.620301349	0.370678927
36	O	0.059109940	0.372795644	0.654538241
37	O	0.665527971	0.243427851	0.060755474
38	O	0.345532946	0.742697304	0.967983274
39	O	0.050738311	0.640162398	0.266516593
40	O	0.949571547	0.341797768	0.760526508
41	O	0.263430030	0.045170278	0.665523874
42	O	0.753648504	0.946059690	0.360231767
43	O	0.451992533	0.234570432	0.853188748
44	O	0.550857970	0.744509584	0.166293296
45	O	0.250866696	0.832424871	0.461432352
46	O	0.754689331	0.150498216	0.563898593
47	O	0.860382280	0.445869589	0.257347253
48	O	0.150595347	0.549423560	0.769946414
49	O	0.767670224	0.669427128	0.116643031
50	O	0.789521197	0.731393506	0.342937162
51	O	0.867710389	0.698786457	0.490791208
52	O	0.772319971	0.547447596	-0.040273893
53	O	0.696720416	0.791570801	0.118735506
54	C	0.542480025	0.067614414	0.991889893
55	C	0.467851967	0.917716143	0.034724436
56	C	0.984297626	0.530983819	0.090177969
57	C	0.020490119	0.459716070	0.936819552
58	C	0.088242975	0.981743927	0.547966924
59	C	0.934463178	0.022511012	0.474633912
60	C	0.517214476	0.409709141	0.975013285
61	C	0.477787101	0.563730628	0.050325097
62	C	0.427382099	0.952561553	0.531286892
63	C	0.579763785	0.027556776	0.494409798
64	C	0.962548746	0.515650598	0.435962520
65	C	0.033257273	0.479719929	0.592728615
66	C	0.433638601	0.988262173	0.927416190
67	C	0.576482788	-0.002890847	0.099023236
68	C	0.920215317	0.422019999	0.009460487
69	C	0.085158954	0.568673489	0.018006200
70	C	0.014335503	0.923726426	0.438939432
71	C	0.010328700	0.081877659	0.583439744

72	C	0.579032350	0.485009856	0.083832108
73	C	0.414411397	0.486568770	0.941576699
74	C	0.507266412	0.061911332	0.596314557
75	C	0.499973186	0.918312163	0.429413459
76	C	0.071090594	0.577911806	0.516200440
77	C	0.924720757	0.416122061	0.511556505
78	C	0.611106144	0.070801227	0.075929155
79	C	0.399239208	0.914230436	0.950442307
80	C	0.065301582	0.601694761	0.093705983
81	C	0.939692934	0.389138291	0.933583310
82	C	0.087178411	0.060347751	0.617436029
83	C	0.938906991	0.947420479	0.404866464
84	C	0.435863231	0.410234035	0.906505503
85	C	0.557368661	0.561522545	0.118945044
86	C	0.424990613	0.883556527	0.449669972
87	C	0.582574241	0.096415663	0.576406205
88	C	0.891790930	0.436213996	0.434449002
89	C	0.103773825	0.559287707	0.594268436
90	C	0.594480288	0.152316485	0.979213471
91	C	0.416687488	0.834337567	0.048909151
92	C	0.970289436	0.578835086	0.174277837
93	C	0.031898746	0.409721615	0.851611996
94	C	0.171301809	0.964753416	0.597651687
95	C	0.843755128	0.030904152	0.426546161
96	C	0.532736030	0.326439854	0.924069705
97	C	0.467408040	0.651968514	0.099961900
98	C	0.342384377	0.901402518	0.542726380
99	C	0.663477775	0.079810020	0.482447911
100	C	0.916906503	0.527975042	0.348139909
101	C	0.083074393	0.467302860	0.678841292
102	H	0.694657319	0.132617836	0.123759095
103	H	0.315619008	0.852665364	0.902752282
104	H	0.113014165	0.685390405	0.156850013
105	H	0.892197689	0.305413557	0.870733911
106	H	0.146417321	0.103482805	0.700940795
107	H	0.880922325	0.905498906	0.321091614
108	H	0.390218998	0.350599068	0.822989293
109	H	0.605158614	0.622071866	0.202441392
110	H	0.363062994	0.799521363	0.401691366
111	H	0.644487075	0.180428446	0.624478402
112	H	0.808381537	0.388985534	0.371142153
113	H	0.187236610	0.605653463	0.656931379
114	H	0.762565818	0.631051655	0.051820976

115	H	0.745703392	0.719185413	0.114953167
116	H	0.819951797	0.807344160	0.376088656
117	H	0.811565352	0.720566673	0.401289659
118	H	0.817200549	0.639359417	0.484228670
119	H	0.903129434	0.672525207	0.462945279
120	H	0.809989137	0.536426018	0.012594837
121	H	0.823427157	0.583114269	0.948740713
122	H	0.715067091	0.860634323	0.130870185
123	H	0.646810583	0.772989834	0.137770950

S2.11. b_5

Energy (eV): -876.13

Simulation cell vectors (Å):

a =	16.2520329306972897	0.1113689530405717	-0.0095152054329613
b =	-5.7623174257870495	15.4887556755020839	-0.1538936231344209
c =	-5.9284673175192681	-8.9346647819967853	12.8782268263472410

Fractional coordinates:

No.	Element	a	b	c
1	Mn	0.410145669	0.069061551	0.749519333
2	Mn	0.593172944	0.892828585	0.245577263
3	Mn	0.752191326	0.397500448	0.095333692
4	Mn	0.245045987	0.580610096	0.903933937
5	Mn	0.082993993	0.728808344	0.404751623
6	Mn	0.903177110	0.239778180	0.587724504
7	Mn	0.647707664	0.229652678	0.852541593
8	Mn	0.348357786	0.742192849	0.143628282
9	Mn	0.825505284	0.658164588	0.236030773
10	Mn	0.142409372	0.340473199	0.744492240
11	Mn	0.247898196	0.833554158	0.643272415
12	Mn	0.743448836	0.135034105	0.350070136
13	S	0.329982010	0.977549995	0.820689923
14	S	0.671452880	0.992043989	0.176815089
15	S	0.826545750	0.320993031	0.997588306
16	S	0.170323075	0.660913939	0.001163302
17	S	0.010188179	0.814345537	0.332244009
18	S	-0.001317826	0.163615345	0.661757447
19	S	0.669469891	0.481579863	0.166737164
20	S	0.322166987	0.481346992	0.829053453

21	S	0.502515786	0.149506743	0.678210771
22	S	0.493084979	0.813387658	0.314413578
23	S	0.164338554	0.656612312	0.498660645
24	S	0.823042002	0.312207755	0.492987566
25	O	0.564925494	0.117899264	0.874392508
26	O	0.439830046	0.851633434	0.123715642
27	O	0.870862820	0.555459828	0.136806812
28	O	0.120588504	0.429300938	0.856904283
29	O	0.135420929	0.859758413	0.561766717
30	O	0.859066935	0.113780011	0.433455875
31	O	0.619043802	0.342767523	0.932653676
32	O	0.369610556	0.626717546	0.057634138
33	O	0.362755135	0.917076174	0.622583835
34	O	0.633515141	0.043002018	0.370285928
35	O	0.928224081	0.608492206	0.360696945
36	O	0.056018815	0.362788707	0.633993412
37	O	0.654954383	0.238700429	0.047917415
38	O	0.343476571	0.734281098	0.948688873
39	O	0.044687908	0.629889131	0.253416822
40	O	0.943587285	0.336046543	0.742029371
41	O	0.257562909	0.034266129	0.656518992
42	O	0.754751893	0.935936752	0.335553100
43	O	0.445817351	0.220527979	0.850814000
44	O	0.547799227	0.734582310	0.148140569
45	O	0.244001975	0.822354134	0.448536867
46	O	0.748815345	0.143075300	0.545337415
47	O	0.852649354	0.435384328	0.242790883
48	O	0.150445381	0.539012833	0.750217521
49	O	0.765979125	0.740961425	0.312337232
50	O	0.847719051	0.819330624	0.509109714
51	O	0.749717074	0.673620861	0.110355534
52	O	0.816217536	0.631106012	0.451617170
53	O	0.741002731	0.535229128	0.956200467
54	C	0.537861599	0.061665340	0.980210312
55	C	0.464659095	0.909751786	0.018107527
56	C	0.977336657	0.526399541	0.075226250
57	C	0.013815295	0.455008619	0.919098500
58	C	0.083950940	0.972216884	0.535392065
59	C	0.935502718	0.017239100	0.458043655
60	C	0.508071153	0.397541160	0.961922496
61	C	0.469410435	0.553246855	0.033475262
62	C	0.421174515	0.943105362	0.516402887
63	C	0.573391502	0.018598431	0.476258729

64	C	0.958182283	0.503658268	0.420192595
65	C	0.030287731	0.468256653	0.574248448
66	C	0.428706671	0.980498672	0.914847693
67	C	0.573697448	0.990441445	0.083121842
68	C	0.914520686	0.417692682	0.994755685
69	C	0.077844317	0.563763301	0.000371673
70	C	0.013811260	0.915118162	0.426063388
71	C	0.006953863	0.075492636	0.567554284
72	C	0.568634531	0.474711702	0.070669424
73	C	0.408382949	0.475449232	0.924788213
74	C	0.500982683	0.052129682	0.581820116
75	C	0.493888650	0.909666745	0.410964658
76	C	0.067270252	0.567260322	0.500332466
77	C	0.921054575	0.403915939	0.493607603
78	C	0.607588737	0.065553499	0.062681048
79	C	0.394984823	0.905710404	0.935551091
80	C	0.057495509	0.597028542	0.077288339
81	C	0.933550307	0.384554112	0.917085789
82	C	0.081792686	0.052417636	0.603565726
83	C	0.943106823	0.942552938	0.390439234
84	C	0.428423806	0.397153110	0.891679659
85	C	0.545263435	0.550300105	0.103868833
86	C	0.418783018	0.874676661	0.432763344
87	C	0.575987354	0.087040012	0.560054455
88	C	0.887562357	0.423512958	0.417734799
89	C	0.100720066	0.548593364	0.576719887
90	C	0.588355735	0.145907213	0.967639765
91	C	0.413872942	0.825786097	0.030494552
92	C	0.963930878	0.573149417	0.161926708
93	C	0.025988870	0.404713441	0.832957977
94	C	0.164842520	0.954380222	0.586999258
95	C	0.843733602	0.022697697	0.406317498
96	C	0.524475513	0.313732047	0.912797678
97	C	0.462151368	0.644702455	0.082176269
98	C	0.336109515	0.891531650	0.529099138
99	C	0.657920370	0.070419890	0.463574022
100	C	0.911025729	0.516835373	0.335014230
101	C	0.081004430	0.456720118	0.659079541
102	H	0.691481599	0.128321217	0.110844277
103	H	0.311137892	0.842956972	0.887427321
104	H	0.104442839	0.680654184	0.140313416
105	H	0.886920129	0.300967732	0.854223227
106	H	0.138410413	0.095736078	0.687542947

107	H	0.889461395	0.901491889	0.306359477
108	H	0.383738768	0.335952368	0.808300656
109	H	0.590240257	0.611037713	0.187290235
110	H	0.356892024	0.790897510	0.384445274
111	H	0.637798117	0.170805133	0.608321130
112	H	0.803524227	0.376137603	0.355447500
113	H	0.184702745	0.595889241	0.639043583
114	H	0.753726436	0.790452627	0.300265753
115	H	0.799812115	0.775968498	0.390797698
116	H	0.843506118	0.754858465	0.502464555
117	H	0.922404141	0.876557465	0.555193790
118	H	0.679651461	0.659408252	0.091136871
119	H	0.740124837	0.623042510	0.044003323
120	H	0.865681342	0.629448413	0.430861407
121	H	0.746637766	0.582322763	0.385253556
122	H	0.800829467	0.541930978	0.008832673
123	H	0.681602131	0.466400290	0.928428912

S2.12. c_5

Energy (eV): -875.99

Simulation cell vectors (Å):

a =	16.5437257025207956	0.0935259736027929	-0.0640662978071175
b =	-5.8823606108367663	15.3128076896244210	0.0110298305744028
c =	-6.0679181671869289	-8.7049204211183646	12.7710241905378421

Fractional coordinates:

No.	Element	a	b	c
1	Mn	0.408881064	0.074855829	0.747200601
2	Mn	0.593410645	0.896147661	0.253482039
3	Mn	0.749274811	0.396793243	0.091411375
4	Mn	0.244826730	0.580809893	0.908776547
5	Mn	0.085850632	0.738629949	0.403878962
6	Mn	0.904769882	0.240350753	0.591671254
7	Mn	0.644941458	0.237046526	0.851197337
8	Mn	0.350709255	0.740416594	0.148981920
9	Mn	0.835373145	0.646152770	0.244013637
10	Mn	0.142453510	0.341798013	0.750290665
11	Mn	0.248454754	0.838290610	0.643696955
12	Mn	0.745280296	0.138118125	0.352768290

13	S	0.331130556	0.981314677	0.820694248
14	S	0.669912341	0.992094624	0.180133786
15	S	0.821728347	0.320195604	0.994803163
16	S	0.174197096	0.661419485	0.005693300
17	S	0.005888972	0.821013219	0.329947933
18	S	0.001001079	0.163596017	0.667241419
19	S	0.663928025	0.471844648	0.165083653
20	S	0.320227729	0.485051402	0.833891843
21	S	0.501377711	0.154942917	0.674085075
22	S	0.495610934	0.816537563	0.323168568
23	S	0.162728703	0.661912240	0.498442997
24	S	0.825128074	0.314915926	0.495926456
25	O	0.561903341	0.122862721	0.872965239
26	O	0.439849868	0.851334845	0.127579793
27	O	0.871306385	0.552649328	0.136263216
28	O	0.121419969	0.429151811	0.862693214
29	O	0.136608184	0.863612034	0.560253974
30	O	0.861948933	0.119801077	0.438519931
31	O	0.621617210	0.351063214	0.935488916
32	O	0.368981675	0.622267651	0.064953076
33	O	0.361102315	0.922710421	0.621896088
34	O	0.635524098	0.048210999	0.374810020
35	O	0.927478898	0.614409874	0.358598916
36	O	0.056600961	0.365929886	0.638993707
37	O	0.657049686	0.239178956	0.048027568
38	O	0.345092213	0.734187891	0.952680628
39	O	0.045770637	0.637291335	0.253116499
40	O	0.945962253	0.335574128	0.746099027
41	O	0.256687194	0.038716115	0.654377434
42	O	0.752181913	0.943220165	0.349637714
43	O	0.447902310	0.228122448	0.843979461
44	O	0.543484857	0.734563118	0.149348205
45	O	0.244060385	0.830655794	0.446883575
46	O	0.751622071	0.143538011	0.550317739
47	O	0.851307972	0.440682795	0.243908409
48	O	0.150313439	0.541884373	0.754653647
49	O	0.769430529	0.725724524	0.294791314
50	O	0.836349500	0.819095421	0.492658487
51	O	0.746355581	0.617735060	0.072654936
52	O	0.812925860	0.633396815	0.450820462
53	O	0.728274766	0.785959933	0.160357966
54	C	0.537212675	0.062494884	0.979426897
55	C	0.464395103	0.910261494	0.020193351

56	C	0.976882297	0.526466863	0.075516780
57	C	0.015273042	0.455050321	0.922290286
58	C	0.082525295	0.975387075	0.535300680
59	C	0.933173136	0.019420208	0.462036693
60	C	0.510066962	0.402133387	0.962624957
61	C	0.469182685	0.553172726	0.038274843
62	C	0.421334845	0.948904656	0.516854590
63	C	0.575665705	0.022689410	0.480457124
64	C	0.958499981	0.510286888	0.422410034
65	C	0.030807724	0.472484202	0.577597706
66	C	0.428644027	0.982194987	0.914881999
67	C	0.572811193	0.990480875	0.084766427
68	C	0.912941805	0.417981316	0.994808802
69	C	0.079909643	0.563597115	0.003454122
70	C	0.009734163	0.918814421	0.425843187
71	C	0.006994892	0.076852782	0.571444976
72	C	0.568449860	0.474244974	0.072613529
73	C	0.408903855	0.478768289	0.928707215
74	C	0.501433472	0.057769201	0.581640272
75	C	0.495885721	0.913872427	0.415950022
76	C	0.067013886	0.573161867	0.502122262
77	C	0.922194055	0.408444872	0.496926447
78	C	0.606491786	0.065491817	0.062579503
79	C	0.395080718	0.906943314	0.936797200
80	C	0.058717381	0.596660906	0.078815885
81	C	0.933282730	0.385054641	0.918896385
82	C	0.082110828	0.054279654	0.605491409
83	C	0.938235722	0.945765648	0.392127671
84	C	0.430715567	0.403480891	0.893491281
85	C	0.545021952	0.548643097	0.107615513
86	C	0.419652723	0.879708481	0.435765374
87	C	0.577588251	0.091870153	0.561796909
88	C	0.888624712	0.429471760	0.420635848
89	C	0.100493892	0.553391609	0.579308100
90	C	0.587693109	0.147748814	0.966618284
91	C	0.414343584	0.825947804	0.033985954
92	C	0.964100743	0.574375158	0.161307197
93	C	0.027686967	0.404481565	0.837433561
94	C	0.164505866	0.958519031	0.585602577
95	C	0.842630171	0.027224423	0.413808110
96	C	0.527071338	0.320777862	0.911560652
97	C	0.460033674	0.642545975	0.086747058
98	C	0.335573779	0.898267546	0.528347173

99	C	0.660556365	0.073708868	0.468378454
100	C	0.910419917	0.522470727	0.335229317
101	C	0.081366959	0.459943889	0.663366174
102	H	0.689878465	0.127781978	0.110158107
103	H	0.311714092	0.844609189	0.889122104
104	H	0.106414876	0.680071953	0.141850701
105	H	0.885851004	0.301622207	0.856127386
106	H	0.140688109	0.096896077	0.689343591
107	H	0.881809138	0.905756625	0.308378549
108	H	0.386926159	0.345490386	0.809454094
109	H	0.589874832	0.606693177	0.191629538
110	H	0.357491544	0.796044626	0.388082641
111	H	0.639722023	0.175520162	0.609444547
112	H	0.805103427	0.382381770	0.358277578
113	H	0.183996697	0.600166208	0.641542573
114	H	0.757268321	0.761651276	0.258586077
115	H	0.797661953	0.771988454	0.371205903
116	H	0.834672887	0.757747791	0.492780127
117	H	0.908902432	0.879813636	0.544071865
118	H	0.676787313	0.551978816	0.030288643
119	H	0.788218172	0.597007661	0.052875173
120	H	0.866194511	0.635008611	0.437138515
121	H	0.746724512	0.582742140	0.381115741
122	H	0.726610294	0.730951723	0.108887315
123	H	0.655237937	0.760166033	0.137630210