

Busold, Strassner: A Density Functional Theory Study on the Mechanism of the Permanganate Oxidation of Substituted Alkenes

XYZ-Coordinates of all compounds, transition states and products. The numbering follows the scheme:

9ts3p2bs2.xyz = Compound 9, transition state, (3+2)pathway, basis set 2

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1edbs1.xyz

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9

C	-0.961353	0.007173	-1.674154
C	-0.987375	-0.124422	-0.345002
C	0.203838	-0.018113	0.527842
O	0.173274	-0.138663	1.736124
O	1.355274	0.230242	-0.149223
H	-0.036833	0.205891	-2.206972
H	-1.907638	-0.322850	0.195895
H	-1.868179	-0.080388	-2.265926
H	2.053602	0.276894	0.529681

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1edbs2.xyz

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9

C	-1.923169	0.119193	0.000003
C	-0.831240	-0.644647	-0.000041
C	0.552272	-0.122732	0.000095
O	1.537820	-0.823430	0.000001
O	0.625229	1.232924	-0.000042
H	-1.857359	1.200363	0.000164
H	-0.886925	-1.726679	-0.000126
H	-2.912961	-0.322498	0.000003
H	1.565673	1.461977	-0.000055

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1gs2p2bs1.xyz

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14

Mn	1.388540	0.040435	-0.006846
O	2.064286	-0.563507	1.332452
O	1.724755	1.596136	-0.002219
O	1.937317	-0.805302	-1.226994
O	-0.337056	0.512252	-0.966565
C	-0.275799	-0.807492	0.831852
H	-0.097369	-1.845883	1.110221
H	-0.499088	-0.177856	1.693932
C	-1.103004	-0.487349	-0.409065
H	-1.216878	-1.391583	-1.039824
C	-2.525682	-0.068935	-0.051337
O	-2.613492	1.198381	0.433143
O	-3.515308	-0.777424	-0.129660
H	-3.557279	1.302814	0.656858

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1gs3p2bs1.xyz

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14

C	-1.343295	0.274350	-0.776443
O	-1.611436	-0.304691	0.466716

C	0.914779	1.753932	0.260701
C	1.552758	0.869912	-0.594407
C	2.425613	-0.200141	-0.149801
O	3.159253	-0.879029	-0.858537
O	2.425402	-0.395162	1.212297
O	-0.875866	1.240864	0.630648
Mn	-1.442658	-0.174273	-0.012642
O	-2.654564	0.125170	-0.996901
O	-1.837083	-1.186450	1.146290

O	-0.169318	-0.718669	-0.836740
H	1.186218	1.753388	1.309941
H	1.522980	1.006315	-1.668018
H	0.587230	2.710787	-0.133112
H	3.028543	-1.149667	1.331812

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1ts3p2bs2.xyz

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14

C	0.919229	1.753870	0.269337
C	1.529405	0.852616	-0.588823
C	2.426704	-0.202973	-0.153771
O	3.147062	-0.872075	-0.875768
O	2.449512	-0.394641	1.205676
O	-0.874015	1.242906	0.630681
Mn	-1.449939	-0.175323	-0.010362
O	-2.650983	0.120604	-1.012455
O	-1.838907	-1.192730	1.148828
O	-0.147453	-0.695453	-0.818100
H	1.193086	1.749016	1.315371
H	1.497781	0.991714	-1.659616
H	0.590399	2.704656	-0.129691
H	3.033446	-1.152288	1.341630

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2edbs1.xyz

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12

C	-0.688963	0.198449	-2.547315
C	-0.718266	-0.309428	-1.315940
C	0.484887	-0.428400	-0.421880
C	0.215427	0.044646	0.995547
O	1.372088	0.274605	1.665136
O	-0.873227	0.180552	1.506996
H	0.227678	0.583045	-2.990482
H	-1.653305	-0.673351	-0.895310
H	-1.583055	0.248323	-3.162513
H	0.797954	-1.481570	-0.334057
H	1.349345	0.109598	-0.824805
H	1.111976	0.541105	2.567633

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2edbs2.xyz

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12

C	-0.355336	2.508425	-0.742619
C	0.108064	1.267937	-0.862603
C	0.567448	0.425508	0.292472
C	0.000571	-0.979530	0.276438
O	0.144619	-1.579011	1.485265
O	-0.493245	-1.537666	-0.669353
H	-0.448387	2.995730	0.223429
H	0.175887	0.805011	-1.842542
H	-0.659703	3.082597	-1.610016
H	1.659789	0.303490	0.264867
H	0.340627	0.892264	1.253686
H	-0.203691	-2.479718	1.401147

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2gs2p2bs1.xyz

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17

C	0.574764	1.468713	-0.445777
C	-0.680479	0.934691	0.219760
O	-0.151997	-0.092797	0.974442
Mn	1.656442	-0.197122	0.040322
O	1.235566	-1.510211	-0.741943
O	2.756505	0.556489	-0.878001
O	2.331454	-0.380299	1.468373
H	1.063399	2.287021	0.084831
H	0.600846	1.620288	-1.526163
H	-1.184015	1.698586	0.847263
C	-1.722860	0.431773	-0.824783
C	-2.913372	-0.229822	-0.187114
H	-2.086134	1.281957	-1.420912
H	-1.242106	-0.299147	-1.479177
O	-3.593405	0.622802	0.641490
O	-3.303926	-1.366816	-0.352652
H	-4.304925	0.073883	1.019922

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2gs3p2bs1.xyz

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17

C	-0.337664	-1.334974	-1.544541
C	-0.361171	-1.279671	-0.013481
C	1.071716	-1.399770	0.580814
C	1.017046	-1.423284	2.084118
O	1.593129	-0.338467	2.662996
O	0.520445	-2.305869	2.760806
O	0.063780	-0.075870	-2.015645
Mn	-0.499811	1.260923	-0.895617
O	-1.805017	1.935058	-1.475876
O	0.735936	2.108171	-0.387034
O	-0.919378	-0.040727	0.337567
H	0.341393	-2.120906	-1.926389
H	-1.357658	-1.588480	-1.896677
H	1.531654	-2.342211	0.255782
H	1.661983	-0.552725	0.224222
H	1.435963	-0.452680	3.619279

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2prod2p2bs2.xyz

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17

C	-0.490305	-1.362554	-0.487871
C	0.695855	-0.698735	0.172304
O	0.202981	0.579468	0.357071
Mn	-1.766067	0.169031	0.056634
O	-1.873135	1.548686	-0.731969
O	-2.848024	-0.821412	-0.633121
O	-2.082552	0.188338	1.608678
H	-0.885197	-2.289730	-0.080461
H	-0.501913	-1.342256	-1.576449
H	0.945812	-1.200101	1.125773
C	1.980788	-0.705562	-0.708439
C	3.123092	-0.023854	-0.011976
H	2.278771	-1.743314	-0.889818
H	1.759263	-0.207827	-1.653447
O	3.441375	1.180253	-0.558503
O	3.730182	-0.458366	0.942574
H	4.124207	1.561561	0.012894

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2prod3p2bs2.xyz

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17

C	0.424575	1.972118	-0.349605
C	-0.634228	1.096520	0.325137
C	-1.676906	0.566851	-0.697628
C	-2.767404	-0.204956	-0.009223
O	-2.791171	-1.519756	-0.344258
O	-3.574580	0.258410	0.768370
O	1.399987	1.127394	-0.913451
Mn	1.615285	-0.415316	0.061437
O	2.861149	-0.275067	1.028138
O	1.387436	-1.683921	-0.859222
O	0.047255	0.024685	0.930630
H	-0.003255	2.619489	-1.132014
H	-1.178517	1.660471	1.097245
H	0.877383	2.625177	0.415992
H	-2.154227	1.419103	-1.193046
H	-1.170430	-0.053968	-1.437017
H	-3.483077	-1.924078	0.199832

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2ts2p2bs1.xyz

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17

C	-0.394824	1.960005	0.080830
C	0.774018	1.350907	-0.327274
O	0.006517	-0.371600	-0.761366
Mn	-1.643823	-0.266296	0.045015
O	-1.688015	-0.277941	1.632672
O	-2.834015	0.421786	-0.744164
O	-1.157822	-1.719587	-0.608491
H	-1.027014	2.481905	-0.628461
H	-0.649405	2.062483	1.129666
H	1.148175	1.519856	-1.331596
C	1.776789	0.866393	0.694216
C	2.717362	-0.210245	0.202564
H	2.414836	1.694289	1.052921
H	1.247290	0.457250	1.558610
O	3.123532	-1.153507	0.848249
O	3.173372	0.024167	-1.059835
H	3.733061	-0.747272	-1.265051

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2ts2p2bs2.xyz

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17

C	-0.297518	2.031273	0.190287
C	0.825190	1.388629	-0.281092
O	0.003451	-0.269463	-0.713942
Mn	-1.699196	-0.269846	0.027964
O	-1.800040	-0.351469	1.611528
O	-2.859653	0.452949	-0.777344
O	-1.153677	-1.682081	-0.676192
H	-0.956848	2.561396	-0.483389
H	-0.534979	2.063383	1.246103
H	1.159269	1.574280	-1.295287
C	1.883592	0.878320	0.670948
C	2.790643	-0.136092	0.017013
H	2.533375	1.703640	0.997218
H	1.412631	0.442705	1.552248
O	3.371217	0.012633	-1.032705
O	2.957194	-1.252421	0.770500
H	3.507094	-1.853198	0.246312

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2ts3p2bs1.xyz

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17

C	0.045426	2.303112	-0.254739
C	-0.913150	1.452286	0.250690
C	-1.860212	0.722634	-0.672312
C	-2.679888	-0.318263	0.054376
O	-3.207796	-0.185961	1.139771
O	-2.857467	-1.448194	-0.682027
O	1.727438	1.164624	-0.540110
Mn	1.592906	-0.364591	0.041621
O	1.636814	-1.412521	-1.156063
O	0.082607	-0.305121	0.692425
O	2.677410	-0.627277	1.175914
H	0.085994	2.531784	-1.314605
H	-1.209918	1.512334	1.291166
H	0.546071	3.009276	0.398829
H	-2.587617	1.412628	-1.136574
H	-1.295876	0.242031	-1.475848
H	-3.386405	-2.036303	-0.110865

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2ts3p2bs2.xyz

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17

C	0.014891	2.285930	-0.248057
C	-0.934241	1.427766	0.263785
C	-1.961705	0.774250	-0.628405
C	-2.717998	-0.332829	0.065209
O	-3.196938	-0.277752	1.173124
O	-2.895559	-1.420764	-0.730705
O	1.734572	1.194752	-0.497717
Mn	1.627013	-0.359029	0.035384
O	1.777301	-1.374941	-1.184827
O	0.072594	-0.345104	0.586048
O	2.645635	-0.616125	1.234027
H	0.039848	2.520277	-1.304904
H	-1.171507	1.454619	1.318926
H	0.532945	2.973337	0.405996
H	-2.726334	1.504558	-0.935890
H	-1.490837	0.385272	-1.531832
H	-3.365973	-2.073568	-0.191676

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3edbs1.xyz

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15

C	3.281369	-0.046320	-0.434523
C	2.245343	-0.180256	0.394462
C	0.899199	0.465642	0.207734
C	-0.227507	-0.570482	0.083691
C	-1.597584	0.063538	-0.027576
O	-2.567090	-0.874320	-0.178659
O	-1.841100	1.249460	0.010510
H	3.218685	0.566067	-1.332062
H	2.355584	-0.805435	1.282864
H	4.232928	-0.536449	-0.246522
H	0.673345	1.121539	1.059172
H	0.906173	1.107267	-0.680380
H	-0.075698	-1.216108	-0.790360
H	-0.241856	-1.247377	0.948811

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H      -3.408553      -0.383349      -0.239062
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3edbs2.xyz
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C	3.282392	-0.051624	-0.429980
C	2.243477	-0.181462	0.391891
C	0.903008	0.471000	0.201370
C	-0.227571	-0.559094	0.084297
C	-1.597778	0.066858	-0.026583
O	-2.561231	-0.878301	-0.177681
O	-1.850363	1.244669	0.010939
H	3.225249	0.559303	-1.326099
H	2.349913	-0.804030	1.279852
H	4.227688	-0.545039	-0.234078
H	0.687903	1.129765	1.049963
H	0.916351	1.107245	-0.687336
H	-0.082004	-1.207916	-0.785345
H	-0.243717	-1.230076	0.950737
H	-3.409797	-0.414270	-0.239730
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3gs2p2bs1.xyz			
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C	0.670969	-1.662268	-0.817122
Mn	0.638856	-1.529883	1.226922
O	1.976504	-1.460539	2.084622
C	0.829202	-0.163347	-0.983572
C	-0.472870	0.539923	-1.423897
C	-0.340945	2.047902	-1.229336
O	-0.650876	-0.833186	1.833712
On	0.288989	-3.102743	1.074694
C	-1.581429	2.840033	-1.542100
H	1.558482	-2.255379	-1.041948
H	-0.239724	-2.152941	-1.164490
H	1.621758	0.092061	-1.725128
H	-0.712877	0.301679	-2.470284
H	-1.294524	0.169988	-0.799792
H	0.477980	2.463171	-1.835450
H	-0.048941	2.231682	-0.187155
O	-1.379469	4.184921	-1.378372
O	-2.660810	2.418576	-1.903658
H	-2.240510	4.590159	-1.591862
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3gs3p2bs1.xyz			
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C	1.263142	2.008323	-0.160801
O	1.831471	0.996137	-0.954734
Mn	1.819009	-0.620798	-0.093715
O	0.747334	0.148501	1.183089
C	0.186103	1.354488	0.710142
C	-1.099931	1.082260	-0.100940
C	-1.983862	0.049396	0.595174
C	-3.299960	-0.204089	-0.089803
O	-3.717513	0.303437	-1.110786
O	-4.056293	-1.122146	0.588557
O	3.256694	-0.932253	0.481825
O	0.974537	-1.697031	-0.894403
H	0.850220	2.807747	-0.804787

H	-0.070177	1.990492	1.580315
H	2.022719	2.476186	0.496278
H	-1.651613	2.017988	-0.266768
H	-0.811449	0.691942	-1.082936
H	-1.431275	-0.894862	0.662173
H	-2.201195	0.332332	1.635460
H	-4.865268	-1.217310	0.052133

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3ts2p2bs1.xyz

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C	-1.048459	1.961543	-0.189754
C	0.079778	1.432139	-0.783669
C	1.336567	1.175170	0.016736
C	2.195316	0.057845	-0.580130
O	-0.608506	-0.380410	-0.942809
Mn	-2.051506	-0.360047	0.200278
O	-1.573924	-1.814669	-0.461427
O	-1.754735	-0.254855	1.755928
O	-3.446503	0.158230	-0.345596
H	-1.867219	2.348666	-0.785634
H	-1.094378	2.140592	0.878750
H	0.205946	1.541151	-1.859802
H	1.938077	2.094427	0.097754
H	1.048131	0.897286	1.036476
H	2.452667	0.261941	-1.629161
H	1.596993	-0.861211	-0.602377
C	3.476449	-0.194859	0.165951
O	4.257768	-1.124654	-0.464407
O	3.842640	0.318010	1.204174
H	5.035611	-1.225935	0.115329

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3ts2p2bs2.xyz

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C	-0.914433	2.013791	-0.180637
C	0.171457	1.390689	-0.756852
C	1.462953	1.178013	-0.000503
C	2.261285	-0.017081	-0.522317
O	-0.566802	-0.371405	-0.757040
Mn	-2.170448	-0.346910	0.181166
O	-1.613519	-1.823845	-0.370927
O	-2.093108	-0.191877	1.759128
O	-3.459349	0.181813	-0.579024
H	-1.737969	2.376414	-0.780306
H	-0.954839	2.202913	0.885056
H	0.259808	1.423341	-1.839878
H	2.079516	2.084101	-0.069329
H	1.239013	1.032843	1.059425
H	2.453183	0.068314	-1.598407
H	1.662810	-0.927042	-0.411483
C	3.583263	-0.218164	0.159163
O	4.295639	-1.239998	-0.407243
O	4.032246	0.400719	1.095653
H	5.111675	-1.314871	0.108278

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3ts3p2bs1.xyz

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C	-0.805291	2.326148	0.045956
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C	0.181814	1.608863	-0.597526
C	1.438930	1.182357	0.127895
C	2.183404	0.047962	-0.579135
C	3.467774	-0.351973	0.093607
O	3.911712	0.060347	1.146281
O	4.149510	-1.293082	-0.628447
O	-2.232258	1.000929	0.653402
Mn	-2.020152	-0.517268	0.067205
O	-1.772972	-1.544570	1.257434
O	-3.227507	-0.915825	-0.890035
H	-0.683346	2.620379	1.083441
H	0.233556	1.642690	-1.682862
H	-1.525877	2.901498	-0.525040
H	2.124403	2.036857	0.250274
H	1.171931	0.855293	1.139389
H	1.518141	-0.821203	-0.641037
H	2.418398	0.308386	-1.620959
H	4.939089	-1.491467	-0.091185

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3ts3p2bs2.xyz

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C	-0.807577	2.335493	0.055681
C	0.185070	1.623368	-0.586339
C	1.444329	1.198300	0.133933
C	2.196293	0.081340	-0.589552
C	3.460078	-0.354492	0.092102
O	3.905733	0.040269	1.143984
O	4.119179	-1.313646	-0.628765
O	-2.236875	1.001107	0.645122
Mn	-2.019855	-0.524681	0.066338
O	-1.745827	-1.543300	1.262283
O	-0.638640	-0.283290	-0.804217
O	-3.224462	-0.940941	-0.892039
H	-0.695225	2.617321	1.095014
H	0.229891	1.656922	-1.669574
H	-1.530789	2.900268	-0.516833
H	2.113174	2.061100	0.257606
H	1.184341	0.864515	1.142294
H	1.538636	-0.786831	-0.694647
H	2.458064	0.373005	-1.613972
H	4.896279	-1.554893	-0.104241

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4edbs1.xyz

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12

C	-0.592115	0.033176	-1.727794
C	-0.611347	-0.043709	-0.390672
C	0.649489	0.047322	0.400151
O	1.768218	0.209355	-0.352634
C	-1.861973	-0.223779	0.428592
O	0.695327	-0.015604	1.613513
H	0.332624	0.163230	-2.278796
H	-1.510103	-0.032987	-2.306073
H	-1.991360	0.606757	1.131687
H	-2.744735	-0.282675	-0.214244
H	-1.804312	-1.135139	1.034387
H	2.505205	0.252742	0.284342

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4edbs2.xyz

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12

C	-1.038167	1.496426	0.000007
C	-0.696818	0.203792	-0.000038
C	0.736814	-0.207237	-0.000158
O	1.612965	0.830194	0.000044
C	-1.686506	-0.928782	0.000027
O	1.110040	-1.357916	0.000035
H	-0.292360	2.280182	-0.000036
H	-2.080458	1.796337	0.000087
H	-1.547376	-1.567845	0.876025
H	-2.708387	-0.547063	0.000083
H	-1.547473	-1.567861	-0.875974
H	2.500067	0.442831	0.000149

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4gs2p2bs1.xyz

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17

C	0.173664	0.112407	1.150148
C	1.061885	0.450105	-0.048852
C	2.385334	-0.327157	0.028384
O	3.491921	0.140175	0.241512
Mn	-1.486562	-0.097167	-0.024791
O	0.253785	-0.013186	-1.074975
O	-2.183612	-0.218058	1.430565
O	-1.830765	-1.446993	-0.789614
O	-2.014788	1.249906	-0.672917
O	2.225700	-1.667018	-0.139480
H	0.009817	0.868479	1.918650
H	0.327633	-0.879932	1.573374
C	1.361254	1.955116	-0.161232
H	3.125429	-2.028503	-0.034290
H	0.405657	2.487670	-0.164784
H	1.988728	2.317453	0.661098
H	1.876041	2.162562	-1.105679

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4gs3p2bs1.xyz

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17

C	0.599804	-0.139726	-2.121980
C	0.788880	0.319628	-0.665189
C	2.224021	0.790702	-0.456385
O	2.899987	1.384634	-1.281457
C	-0.163917	1.501850	-0.324625
O	-1.433723	0.960716	-0.106063
Mn	-1.340747	-0.709360	0.641285
O	0.449015	-0.714846	0.221239
O	2.704545	0.557521	0.790925
O	-2.106326	-1.764201	-0.255111
O	-1.566728	-0.614409	2.200543
H	0.215520	2.014695	0.580404
H	-0.191877	2.243048	-1.142004
H	1.188852	-1.045767	-2.303954
H	-0.456798	-0.385116	-2.261714
H	0.905327	0.630762	-2.837275
H	3.590750	0.966343	0.780890

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4ts2p2bs1.xyz

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17

C	-0.300617	0.112508	-1.467701
Mn	1.533122	-0.112704	0.058096
O	2.195781	1.217383	-0.498263
C	-1.226084	0.506100	-0.496039
C	-2.246812	-0.477887	-0.090878
O	-2.341116	-1.640051	-0.454191
O	-3.182384	0.043107	0.771728
O	-0.040466	0.034199	0.991680
O	1.570054	-0.190961	1.720918
O	1.940297	-1.479035	-0.627755
H	0.207507	0.854958	-2.071264
H	-0.336508	-0.900093	-1.849885
C	-1.425385	1.971001	-0.183628
H	-3.747695	-0.722803	0.978257
H	-0.459020	2.479216	-0.259148
H	-2.127759	2.450527	-0.883121
H	-1.808506	2.108341	0.829297

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4ts2p2bs2.xyz

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17

C	-0.389413	0.126782	-1.516889
Mn	1.580571	-0.112045	0.062584
O	2.212420	1.238103	-0.484719
C	-1.255678	0.502986	-0.497746
C	-2.280462	-0.484879	-0.079740
O	-2.405340	-1.624610	-0.476273
O	-3.167431	0.028758	0.831858
O	-0.046904	0.011907	0.936933
O	1.578555	-0.198175	1.725720
O	2.000030	-1.470036	-0.636370
H	0.157674	0.871466	-2.077222
H	-0.399160	-0.888819	-1.886691
C	-1.467643	1.962705	-0.168777
H	-3.744246	-0.711982	1.063163
H	-0.540852	2.508080	-0.355435
H	-2.263195	2.399848	-0.785567
H	-1.735965	2.089373	0.878874

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4ts3p2bs1.xyz

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17

C	0.878890	0.375907	1.663744
C	1.475277	0.636785	0.440257
C	1.444819	2.020620	-0.162504
C	2.266776	-0.431957	-0.164046
O	2.905130	-0.050300	-1.322990
O	2.448071	-1.562095	0.273324
O	-0.998698	0.011490	1.440741
Mn	-1.589316	-0.177504	-0.090174
O	-2.608885	0.996876	-0.422500
O	-2.236792	-1.617831	-0.259064
O	-0.260893	-0.038581	-0.998678
H	1.103203	-0.565014	2.152290
H	0.619772	1.204806	2.314056
H	1.538171	1.978162	-1.249073
H	0.486492	2.497664	0.069197
H	2.252968	2.664073	0.222423
H	3.354259	-0.866700	-1.605915

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4ts3p2bs2.xyz

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17

C	0.818795	0.533150	1.638992
C	1.464037	0.620174	0.413693
C	1.547902	1.922283	-0.342322
C	2.268281	-0.527014	-0.009580
O	2.980212	-0.284222	-1.162071
O	2.393328	-1.596866	0.560025
O	-1.049188	0.181637	1.388492
Mn	-1.608538	-0.133784	-0.139628
O	-2.554065	1.051307	-0.628124
O	-2.306542	-1.561835	-0.203300
O	-0.220925	-0.129090	-0.975887
H	0.994753	-0.341336	2.250414
H	0.561444	1.446187	2.159906
H	1.477590	1.755475	-1.417001
H	0.718927	2.570500	-0.049682
H	2.489364	2.451463	-0.142135
H	3.434719	-1.116713	-1.348584

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5edbs1.xyz

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12

C	-0.671380	0.000111	-2.678644
C	-0.690761	-0.000098	-1.183162
C	0.391421	-0.000068	-0.394367
C	0.250370	-0.000364	1.076156
O	1.462875	0.000325	1.691662
O	-0.792657	-0.000118	1.701474
H	-1.665165	-0.000313	-0.695266
H	1.401059	0.000142	-0.795881
H	0.347968	0.000360	-3.077029
H	-1.198443	-0.879089	-3.072974
H	-1.198777	0.879222	-3.072723
H	1.273716	0.000530	2.648890

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5edbs2.xyz

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12

C	-2.754856	-0.147997	0.000027
C	-1.335598	0.315246	-0.000008
C	-0.263207	-0.481916	-0.000042
C	1.101487	0.081099	-0.000082
O	2.040451	-0.903683	0.000036
O	1.399687	1.253539	0.000023
H	-1.162008	1.389298	-0.000009
H	-0.349343	-1.562862	-0.000043
H	-2.833130	-1.236758	0.000006
H	-3.284452	0.240299	0.877046
H	-3.284512	0.240338	-0.876941
H	2.905386	-0.467762	0.000099

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5gs2p2bs1.xyz

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17

C	-0.310116	0.886879	-0.430242
C	-1.080409	0.020657	0.560203
C	-2.510289	-0.232307	0.100095
O	-3.489302	0.402193	0.456773

Mn	1.404611	-0.227842	0.011174
O	-0.277598	-1.103417	0.593787
O	2.029725	0.704883	-1.150272
O	1.885021	-1.716743	-0.332676
O	1.875212	0.327212	1.416438
O	-2.618902	-1.218796	-0.828788
C	-0.197886	2.378528	-0.229211
H	-0.517775	0.595786	-1.462507
H	-1.169792	0.548907	1.530237
H	-3.566407	-1.223025	-1.061512
H	0.576044	2.789342	-0.884576
H	-1.150710	2.886455	-0.454610
H	0.072326	2.613375	0.806464

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5gs3p2bs1.xyz

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17

scf done: -1758.467440

C	-0.766518	-1.147851	-2.317800
C	-0.734379	-1.163181	-0.782523
O	0.592092	-1.225515	-0.317853
Mn	1.345324	0.440439	-0.163602
O	-0.361858	1.129369	-0.238196
C	-1.339672	0.139855	-0.195829
C	-1.888038	-0.144101	1.204661
O	-2.829356	-0.886407	1.434493
O	-1.242399	0.505056	2.196629
O	2.146022	0.795680	-1.480565
O	1.971534	0.647527	1.269881
H	-1.292653	-2.041158	-0.417341
H	-2.226703	0.443822	-0.781726
H	-0.230020	-0.264890	-2.680940
H	-0.253569	-2.037373	-2.701804
H	-1.793739	-1.137798	-2.708819
H	-1.673057	0.192452	3.014471

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5ts2p2bs1.xyz

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17

C	0.386972	1.384169	0.283890
Mn	-1.367300	-0.380730	0.078902
O	-2.340553	0.620375	-0.672157
C	1.290001	0.654187	-0.491700
C	2.373196	-0.102204	0.146692
O	2.538320	-0.312739	1.337062
O	3.280850	-0.573201	-0.770936
O	0.188287	-0.890335	-0.760260
O	-1.303638	-1.878025	-0.642893
O	-1.469295	-0.447966	1.655774
C	-0.285019	2.631783	-0.219653
H	0.463590	1.260871	1.359672
H	1.441845	0.908346	-1.535730
H	3.908361	-1.086844	-0.230915
H	-1.242182	2.799662	0.281363
H	0.355685	3.513272	-0.041365
H	-0.487461	2.570473	-1.293669

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5ts2p2bs2.xyz

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17

C	0.504511	1.461428	0.307521
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Mn	-1.411489	-0.387174	0.083888
O	-2.380761	0.696953	-0.553484
C	1.328437	0.659873	-0.471364
C	2.376460	-0.163730	0.159352
O	3.244380	-0.674045	-0.772063
O	0.166342	-0.782457	-0.816853
O	-1.354457	-1.816253	-0.768297
O	-1.447009	-0.577243	1.654719
C	-0.162412	2.695703	-0.215769
H	0.528069	1.308303	1.380524
H	1.507714	0.921628	-1.507095
H	3.846745	-1.243442	-0.273689
H	-1.155317	2.829969	0.217346
H	0.438884	3.583744	0.035260
H	-0.277056	2.659565	-1.301433

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5ts3p2bs1.xyz

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17

C	0.537750	2.848706	-0.123484
C	0.935150	1.483736	0.382602
C	1.531541	0.562672	-0.467681
C	2.336488	-0.519261	0.061477
O	2.945405	-1.257666	-0.929138
O	2.549066	-0.793438	1.237269
O	-0.843162	0.922789	0.801040
Mn	-1.500163	-0.364372	-0.005946
O	-2.666824	0.134519	-0.964181
O	-1.985324	-1.471916	1.022863
O	-0.249405	-0.896592	-0.873916
H	1.228048	1.418923	1.426618
H	1.508973	0.688284	-1.542965
H	0.061466	2.767391	-1.106583
H	-0.174342	3.324083	0.557081
H	1.416973	3.503606	-0.220315
H	3.419325	-1.949678	-0.434163

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5ts3p2bs2.xyz

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17

C	0.582511	2.848128	-0.119361
C	0.941441	1.476057	0.388878
C	1.516323	0.536072	-0.456557
C	2.344870	-0.533070	0.065168
O	2.956320	-1.253493	-0.937290
O	2.566103	-0.809686	1.231903
O	-0.845782	0.936969	0.779779
Mn	-1.518501	-0.359206	-0.006208
O	-2.659030	0.137352	-1.001228
O	-2.026691	-1.444567	1.038712
O	-0.239863	-0.903532	-0.835400
H	1.222974	1.405564	1.433815
H	1.500012	0.664461	-1.529501
H	0.149313	2.789093	-1.120896
H	-0.145514	3.325767	0.538678
H	1.476891	3.482482	-0.167714
H	3.439534	-1.954683	-0.479770

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6edbs1.xyz

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15

C	-0.165931	0.000201	-1.764641
C	-0.193597	0.000019	-0.256739
C	1.112065	0.000068	0.466368
O	1.270433	-0.000048	1.672597
C	-1.291795	-0.000198	0.521302
C	-2.727147	-0.000323	0.098615
O	2.172286	0.000277	-0.386921
H	-1.113940	-0.000318	1.595492
H	-2.864999	0.000246	-0.985397
H	-3.243714	-0.879202	0.507903
H	-3.244165	0.877817	0.508902
H	0.366296	-0.877851	-2.148256
H	-1.172223	0.000195	-2.189515
H	0.366212	0.878392	-2.148050
H	2.963212	0.000297	0.184082

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6edbs2.xyz

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15

C	0.345156	1.734051	0.000011
C	0.218550	0.232436	0.000031
C	-1.153191	-0.355519	0.000095
O	-1.433405	-1.532986	-0.000015
C	1.233103	-0.647695	0.000004
C	2.700292	-0.366578	-0.000034
O	-2.121048	0.602081	-0.000048
H	0.952972	-1.697973	0.000033
H	2.944270	0.695518	-0.000367
H	3.171372	-0.825835	0.876454
H	3.171438	-0.826414	-0.876176
H	-0.142991	2.168213	0.876646
H	1.387724	2.050108	-0.000072
H	-0.143139	2.168208	-0.876544
H	-2.969480	0.135245	-0.000116

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6gs2p2bs1.xyz

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20

C	-0.221327	0.666726	-0.753975
C	-1.045285	0.092782	0.408160
C	-2.385149	-0.425386	-0.132571
O	-3.461539	0.145169	-0.058411
Mn	1.494796	-0.240294	0.027627
O	-0.194868	-0.941131	0.787768
O	2.138878	0.328554	-1.340542
O	1.996187	-1.759334	0.128522
O	1.948985	0.691867	1.224859
O	-2.276904	-1.608999	-0.792285
C	-0.129530	2.148635	-1.034173
H	-0.370349	0.073940	-1.658356
C	-1.316867	1.077395	1.558357
H	-3.178767	-1.777687	-1.123818
H	-0.359293	1.461597	1.918967
H	-1.965211	1.906598	1.256594
H	-1.803558	0.541857	2.380948
H	0.654188	2.332656	-1.774718
H	-1.081556	2.540113	-1.431306
H	0.117700	2.718354	-0.133053

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6gs3p2bs1.xyz

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20

C	-2.013391	1.127034	1.339600
C	-1.068851	0.359631	0.393819
O	0.038380	-0.093055	1.117475
Mn	1.518646	-0.357820	0.055841
O	1.731597	-1.894768	-0.232308
C	-0.524164	1.178701	-0.810267
O	0.574598	0.440219	-1.298925
C	-1.901119	-0.799833	-0.196416
O	-2.849618	-0.659183	-0.951046
C	-0.072869	2.597203	-0.435460
O	-1.521037	-2.023333	0.229777
O	2.708440	0.579856	0.511838
H	-1.293017	1.240716	-1.596334
H	0.661515	2.550386	0.375532
H	0.419507	3.043920	-1.306889
H	-0.907104	3.247041	-0.138980
H	-2.333682	0.465715	2.153672
H	-1.476600	1.969027	1.784922
H	-2.901389	1.494021	0.812719
H	-2.111853	-2.639664	-0.242784

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6ts2p2bs1.xyz

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20

C	-0.287060	2.498655	0.552079
C	0.325803	1.133958	0.715440
C	1.234303	0.547153	-0.179054
C	2.256390	-0.343163	0.410033
O	3.188701	-0.775474	-0.502231
Mn	-1.506651	-0.370412	0.002898
O	-1.916494	-0.512192	1.525441
O	-2.208572	0.771364	-0.846984
O	0.115904	-0.985246	-0.596322
O	-1.454839	-1.823401	-0.807749
O	2.355499	-0.684225	1.578731
H	0.376253	0.758368	1.732269
C	1.437439	1.104031	-1.568619
H	3.749125	-1.376862	0.020354
H	-1.202593	2.579435	1.145611
H	0.414237	3.275087	0.906870
H	-0.549305	2.723662	-0.484154
H	0.460218	1.319099	-2.011344
H	2.028966	2.033008	-1.564205
H	1.946540	0.378103	-2.204220

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6ts2p2bs2.xyz

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20

C	-0.174436	2.549401	0.499259
C	0.440777	1.201295	0.721324
C	1.264740	0.527688	-0.181914
C	2.277381	-0.385084	0.411905
O	3.148819	-0.889664	-0.518520
Mn	-1.569555	-0.364461	0.010148
O	-1.978940	-0.483598	1.536498
O	-2.228660	0.792916	-0.855877
O	0.099611	-0.945475	-0.542504
O	-1.490937	-1.822828	-0.795408

O	2.407826	-0.672147	1.583772
H	0.463947	0.836860	1.741480
C	1.488502	1.051516	-1.581223
H	3.710494	-1.502572	-0.024800
H	-1.020669	2.698953	1.172376
H	0.565005	3.339004	0.712028
H	-0.534966	2.688395	-0.520120
H	0.537016	1.379212	-2.002383
H	2.185176	1.900447	-1.590349
H	1.889332	0.268709	-2.221725

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6ts3p2bs1.xyz

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20

C	-1.544389	0.816283	1.655940
C	-1.468406	0.433893	0.198117
C	-0.900242	1.277944	-0.755133
C	-0.711711	2.754526	-0.512021
C	-2.137318	-0.762857	-0.303411
O	-2.776457	-1.492336	0.674812
O	-2.224899	-1.131188	-1.469992
O	0.991692	0.921110	-0.851438
Mn	1.642472	-0.315061	0.032444
O	2.569500	0.273567	1.183026
O	2.405875	-1.331929	-0.918586
O	0.330376	-1.005131	0.674196
H	-1.071737	0.985032	-1.786038
H	-0.266251	2.945368	0.468742
H	-0.049902	3.184279	-1.269384
H	-1.677397	3.282329	-0.555537
H	-1.802060	-0.047636	2.269788
H	-0.569298	1.183416	1.996177
H	-2.290270	1.605479	1.846426
H	-3.131184	-2.253223	0.181625

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6ts3p2bs2.xyz

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20

C	-1.560363	0.802228	1.650593
C	-1.452094	0.419165	0.196830
C	-0.900593	1.274519	-0.756881
C	-0.718618	2.749057	-0.512524
C	-2.148003	-0.764510	-0.307593
O	-2.793542	-1.476956	0.678064
O	-2.243386	-1.129916	-1.467253
O	0.995873	0.911603	-0.861472
Mn	1.658723	-0.314663	0.032773
O	2.565730	0.289662	1.195244
O	2.430052	-1.343475	-0.904117
O	0.322231	-0.982359	0.659782
H	-1.071629	0.982280	-1.786092
H	-0.236045	2.942772	0.446897
H	-0.097402	3.187892	-1.295100
H	-1.691413	3.259511	-0.515224
H	-1.677271	-0.081911	2.274066
H	-0.653406	1.317823	1.974480
H	-2.414172	1.469337	1.838107
H	-3.164379	-2.242341	0.219005

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7edbs1.xyz

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15

C	1.189354	0.000515	-1.596679
C	1.179423	0.000216	-0.091595
C	2.539530	0.000317	0.559110
C	0.071652	-0.000098	0.678631
C	-1.325102	-0.000300	0.206679
O	-1.743900	0.000014	-0.938158
O	-2.181183	-0.000743	1.267141
H	0.177632	-0.000264	1.759681
H	1.735420	0.880131	-1.964718
H	1.736978	-0.877961	-1.965099
H	0.184586	-0.000198	-2.015156
H	2.478703	0.000300	1.651178
H	3.117105	-0.879122	0.243518
H	3.116981	0.879841	0.243532
H	-3.075891	-0.000789	0.878320

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7edbs2.xyz

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15

C	1.430603	1.388060	-0.000071
C	1.177081	-0.092702	-0.000011
C	2.414135	-0.950869	0.000020
C	-0.036524	-0.676688	0.000042
C	-1.340080	0.007250	0.000023
O	-1.574196	1.196856	0.000076
O	-2.351678	-0.908902	-0.000073
H	-0.101740	-1.758670	0.000093
H	2.029602	1.657822	0.877459
H	2.030700	1.657594	-0.876913
H	0.514054	1.970208	-0.000660
H	2.180125	-2.016233	0.000255
H	3.031043	-0.729492	-0.878044
H	3.031252	-0.729145	0.877847
H	-3.179342	-0.406025	-0.000075

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7gs2p2bs1.xyz

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20

C	-0.324325	2.276468	-0.810306
C	0.209375	1.098525	-0.012108
Mn	-1.298432	-0.389160	0.084789
O	-2.333325	-0.867277	-1.035478
C	1.049327	0.154046	-0.891150
O	0.120594	-0.793633	-1.253048
C	2.307362	-0.364140	-0.186803
O	2.172035	-1.589488	0.369087
O	3.360554	0.249558	-0.117711
O	-2.060815	0.793539	0.888112
O	-0.869304	-1.485857	1.139523
C	0.708851	1.478860	1.369621
H	1.459228	0.705287	-1.763754
H	3.036347	-1.762666	0.788337
H	-1.144396	2.766615	-0.278668
H	0.477779	3.015663	-0.981509
H	-0.694875	1.947492	-1.787499
H	-0.092721	1.963220	1.934114
H	1.036798	0.601438	1.935270
H	1.561172	2.174666	1.294571

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7gs3p2bs1.xyz

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20

C	-0.288498	-1.748416	-1.942293
C	-0.580182	-1.087488	-0.586741
C	0.659073	-0.985753	0.372983
C	1.965710	-0.804934	-0.396962
O	2.579976	-2.016978	-0.629976
C	-1.696901	-1.853630	0.154273
O	2.468073	0.222044	-0.790500
O	-1.003307	0.234104	-0.823447
Mn	-0.718469	1.348045	0.602695
O	-2.019173	1.412356	1.501464
O	0.044593	2.657563	0.170593
O	0.441666	0.076834	1.248415
H	0.767553	-1.928312	0.935871
H	-1.212582	-1.775078	-2.532121
H	0.445426	-1.158776	-2.501662
H	0.088803	-2.772872	-1.833529
H	-1.904890	-1.355001	1.105784
H	-2.612613	-1.828699	-0.448368
H	-1.427872	-2.902307	0.343778
H	3.368075	-1.786144	-1.157096

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7ts2p2bs1.xyz

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20

C	0.473804	1.312818	-0.201230
Mn	-1.493653	-0.409335	0.104616
O	-2.327736	0.283363	-1.051247
C	1.244892	0.245960	-0.689988
C	2.385881	-0.349699	0.023239
O	2.723376	-0.222696	1.189488
O	3.140562	-1.126162	-0.822712
O	0.101829	-1.205875	-0.356281
O	-1.457965	-2.066169	-0.010858
O	-1.706387	0.117596	1.583100
C	-0.154814	2.257837	-1.197448
C	0.616258	1.843792	1.202864
H	1.299652	0.124241	-1.766728
H	3.823971	-1.504133	-0.240026
H	-1.114303	2.639595	-0.836066
H	0.510829	3.124064	-1.366018
H	-0.338938	1.770834	-2.158774
H	-0.292189	2.375772	1.500633
H	0.804559	1.046904	1.919839
H	1.462167	2.551392	1.255201

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7ts2p2bs2.xyz

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20

C	0.607530	1.358385	-0.201767
Mn	-1.564443	-0.393421	0.105065
O	-2.360828	0.340790	-1.055463
C	1.272705	0.222058	-0.674761
C	2.395161	-0.427378	0.032574
O	2.749427	-0.302186	1.185743
O	3.094373	-1.244816	-0.819699
O	0.071786	-1.148911	-0.356537
O	-1.520490	-2.054364	-0.036815

O	-1.749312	0.131646	1.589869
C	-0.010754	2.302516	-1.196706
C	0.726565	1.865340	1.206310
H	1.321659	0.096709	-1.749375
H	3.761756	-1.675456	-0.267702
H	-0.971399	2.684046	-0.843782
H	0.655883	3.168449	-1.344463
H	-0.177901	1.825733	-2.163187
H	-0.171221	2.421403	1.484473
H	0.878332	1.062632	1.922492
H	1.587092	2.549203	1.284227

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7ts3p2bs1.xyz

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20

C	1.440133	1.748231	1.301130
C	0.967496	1.342675	-0.080672
C	0.672209	2.502044	-1.015782
C	1.415301	0.162588	-0.689036
C	2.161885	-0.896451	-0.042864
O	2.469111	-1.031235	1.138011
O	2.597993	-1.835017	-0.955316
O	-0.854282	1.081748	0.420449
Mn	-1.642814	-0.329440	0.052765
O	-2.164727	-1.032322	1.377158
O	-0.460770	-1.192418	-0.628588
O	-2.801737	-0.046426	-0.997364
H	1.311436	0.058836	-1.761848
H	0.777008	2.518680	1.707073
H	1.460618	0.891620	1.972971
H	2.459180	2.161331	1.248532
H	0.182781	2.149500	-1.929027
H	0.009037	3.226683	-0.533627
H	1.602595	3.018817	-1.297700
H	3.040833	-2.498622	-0.396954

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7ts3p2bs2.xyz

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20

C	1.449187	1.751548	1.302668
C	0.973837	1.337796	-0.072754
C	0.695538	2.494291	-1.013314
C	1.400398	0.146124	-0.676440
C	2.167016	-0.903327	-0.036615
O	2.462162	-1.043152	1.139223
O	2.622660	-1.823143	-0.959816
O	-0.846567	1.071088	0.429392
Mn	-1.657349	-0.327179	0.051145
O	-2.175078	-1.048944	1.370414
O	-0.459434	-1.171651	-0.639316
O	-2.812202	-0.020247	-1.001699
H	1.309486	0.049441	-1.748665
H	0.800481	2.539919	1.690539
H	1.452086	0.912015	1.992471
H	2.473167	2.143108	1.240060
H	0.240193	2.144923	-1.941980
H	0.016494	3.211433	-0.547917
H	1.632446	3.011740	-1.258741
H	3.061169	-2.503297	-0.431262

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8edbs1.xyz

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18

C	-1.393496	-1.623620	0.005487
C	-1.189780	-0.121457	0.001163
C	-2.491713	0.641940	-0.001260
C	0.028974	0.480426	-0.000757
C	1.260044	-0.352398	-0.001689
O	1.339616	-1.569418	-0.008653
C	0.263712	1.977172	-0.002055
O	2.393051	0.409441	0.006824
H	-2.462146	-1.861257	0.023871
H	-0.944845	-2.093764	-0.874871
H	-0.912678	-2.095087	0.867397
H	-2.388831	1.726849	-0.011928
H	-3.090321	0.348579	-0.874585
H	-3.084749	0.365107	0.881282
H	0.844779	2.280576	-0.880382
H	-0.664056	2.549311	0.000200
H	0.848840	2.280775	0.873428
H	3.126220	-0.233655	0.004893

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8edbs2.xyz

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18

C	1.399236	-1.621518	-0.049668
C	1.187633	-0.123868	-0.009232
C	2.484531	0.643618	0.013970
C	-0.029486	0.476044	0.006200
C	-1.260980	-0.354654	0.011725
O	-1.343484	-1.563114	0.081238
C	-0.257799	1.972811	0.018703
O	-2.392268	0.408224	-0.064448
H	2.456738	-1.847469	-0.202525
H	1.078685	-2.090431	0.884697
H	0.814903	-2.099000	-0.836454
H	2.378242	1.720267	0.117904
H	3.106421	0.281032	0.840193
H	3.048908	0.441779	-0.904059
H	-0.822597	2.275320	0.904855
H	0.671571	2.536318	0.003256
H	-0.851523	2.280324	-0.845887
H	-3.134144	-0.213618	-0.046485

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8gs2p2bs1.xyz

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23

C	0.441097	2.329657	0.454326
C	-0.088115	1.099267	-0.266717
Mn	1.378049	-0.428050	-0.015522
O	2.290944	-0.898411	1.216781
C	-1.035304	0.243640	0.600651
O	-0.104795	-0.518059	1.286437
C	-2.023850	-0.597896	-0.241395
O	-1.966788	-1.921359	0.025207
O	-2.857409	-0.148980	-1.011533
O	2.297111	0.613282	-0.845534
O	0.909135	-1.578741	-0.996054
C	-0.378701	1.372964	-1.730177
C	-1.951729	1.013610	1.588726
H	-2.647967	-2.310999	-0.555234

H	1.324147	2.707582	-0.067507
H	-0.317658	3.130774	0.478067
H	0.729437	2.098914	1.484540
H	0.523502	1.770766	-2.204717
H	-0.681396	0.474949	-2.271390
H	-1.188697	2.113787	-1.835265
H	-2.503710	0.291911	2.203360
H	-1.342621	1.624576	2.258952
H	-2.672231	1.649675	1.062334

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8gs3p2bs1.xyz

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23

C	-0.763199	0.980007	-1.794041
C	-0.843381	-0.245762	0.463975
C	-0.914365	-0.079057	1.997260
C	-1.308030	2.323156	0.270928
C	-2.180712	-0.810580	-0.012513
O	-2.078857	-1.863005	-0.860786
O	-3.277307	-0.372618	0.301127
O	0.847466	1.331518	-0.046185
Mn	1.814568	-0.221777	-0.010767
O	2.629010	-0.341751	1.339213
O	2.477377	-0.481541	-1.421911
O	0.214959	-1.109230	0.144007
H	-0.360445	1.871461	-2.288454
H	-0.224849	0.107277	-2.172813
H	-1.827181	0.892279	-2.052328
H	-1.034864	2.518314	1.312063
H	-1.049648	3.214885	-0.313538
H	-2.390384	2.161656	0.212406
H	-0.948924	-1.074350	2.454809
H	0.004334	0.411969	2.329250
H	-1.789229	0.490660	2.323288
H	-3.005674	-2.070023	-1.087548

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8ts2p2bs1.xyz

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23

C	-0.399671	1.280949	0.140697
Mn	1.594188	-0.389179	-0.153076
O	2.185408	-0.091540	1.290774
C	-1.179423	0.161742	0.516379
C	-2.321146	-0.269466	-0.330661
O	-2.668477	0.161093	-1.420154
O	-3.071623	-1.260936	0.254129
O	-0.060296	-1.193539	-0.209726
O	1.538440	-2.009836	-0.516914
O	2.083488	0.517021	-1.357907
C	0.220927	2.193438	1.174581
C	-0.484584	1.894493	-1.236584
C	-1.200693	-0.280976	1.968486
H	-3.738696	-1.460545	-0.427218
H	1.161574	2.608794	0.799576
H	-0.459713	3.042699	1.370157
H	0.434835	1.701276	2.122755
H	0.391411	2.525450	-1.413480
H	-0.528772	1.136794	-2.017312
H	-1.390434	2.514012	-1.329868
H	-1.654309	-1.267633	2.056224
H	-0.174476	-0.346246	2.338959

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H      -1.764112      0.415707      2.608102
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8ts2p2bs2.xyz
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    23
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C	-0.523494	1.330840	0.092489
Mn	1.669705	-0.379657	-0.136158
O	2.247718	0.044969	1.282109
C	-1.211346	0.169937	0.502042
C	-2.319349	-0.363113	-0.345697
O	-2.680583	0.019586	-1.439944
O	-3.000563	-1.385692	0.262849
O	-0.022845	-1.142482	-0.111925
O	1.589837	-2.031667	-0.372599
O	2.108579	0.448440	-1.416387
C	0.070692	2.282852	1.097464
C	-0.580097	1.869203	-1.310420
C	-1.274685	-0.180884	1.977948
H	-3.642648	-1.676732	-0.399009
H	0.955679	2.771127	0.684639
H	-0.664469	3.074224	1.323935
H	0.359165	1.810046	2.032840
H	0.292798	2.497300	-1.498724
H	-0.610366	1.081212	-2.057597
H	-1.485091	2.479959	-1.446823
H	-1.640649	-1.195930	2.106832
H	-0.277293	-0.128729	2.413870
H	-1.937234	0.500711	2.528220

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.:ts3p2bs1.xyz
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23
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C	-1.078329	1.624416	-1.560978
C	-0.902246	1.325855	-0.085373
C	-0.855099	2.570304	0.785009
C	-1.361573	0.122182	0.487411
C	-2.081599	-0.870082	-0.304719
O	-2.355806	-0.848783	-1.501471
C	-1.261328	-0.079283	1.984673
O	-2.563288	-1.922165	0.449385
O	1.029959	1.178032	-0.117186
Mn	1.746373	-0.313434	-0.065352
O	2.502115	-0.605478	-1.431246
O	0.468692	-1.290294	0.101664
O	2.687813	-0.414413	1.211968
H	-0.511308	2.525862	-1.817308
H	-0.723067	0.794243	-2.169862
H	-2.134692	1.786960	-1.812689
H	-0.513648	2.358038	1.799533
H	-0.176466	3.308793	0.348532
H	-1.858490	3.020930	0.849174
H	-1.418342	-1.126384	2.241646
H	-0.258770	0.197568	2.329813
H	-1.994778	0.521031	2.546591
H	-2.984601	-2.486733	-0.222684

[illegible]

C	-1.107059	1.644880	-1.551396
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C	-0.912873	1.322645	-0.085810
C	-0.883943	2.557612	0.794952
C	-1.348365	0.103887	0.477022
C	-2.071854	-0.886536	-0.319137
O	-2.333652	-0.869641	-1.511305
C	-1.293429	-0.094180	1.975407
O	-2.556201	-1.932165	0.442232
O	1.024602	1.178704	-0.115082
Mn	1.763305	-0.304812	-0.063214
O	2.524768	-0.594076	-1.430513
O	0.466501	-1.265652	0.098132
O	2.692046	-0.410476	1.226687
H	-0.519392	2.530668	-1.803270
H	-0.803557	0.820482	-2.190270
H	-2.163408	1.849975	-1.763760
H	-0.515197	2.350604	1.797720
H	-0.239898	3.317198	0.348598
H	-1.898394	2.972046	0.879304
H	-1.334400	-1.151851	2.222711
H	-0.358278	0.302027	2.376136
H	-2.124848	0.408065	2.490611
H	-2.964631	-2.522297	-0.204856

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9edbs1.xyz

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21

C	-1.596878	-0.000052	-1.798914
C	-1.612825	-0.000148	-0.261750
C	-0.226522	-0.000066	0.338869
C	0.948997	0.000162	-0.303674
C	2.214270	0.000227	0.460190
O	2.330115	0.000022	1.670928
C	-2.351284	-1.260455	0.251194
C	-2.351505	1.259967	0.251349
O	3.293190	0.000398	-0.368553
H	-0.187939	-0.000165	1.429296
H	1.032284	0.000323	-1.385266
H	-3.386047	-1.268246	-0.111767
H	-1.859823	-2.175524	-0.097658
H	-2.378056	-1.287894	1.346825
H	-3.386196	1.267755	-0.111820
H	-2.378502	1.287139	1.346981
H	-1.860053	2.175161	-0.097184
H	-2.621439	0.000068	-2.187953
H	-1.090039	0.887346	-2.195030
H	-1.090214	-0.887496	-2.195146
H	4.074074	0.000373	0.216138

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9edbs2.xyz

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21

C	1.854584	1.527696	-0.000005
C	1.632910	0.007707	0.000016
C	0.172903	-0.374645	-0.000080
C	-0.887832	0.438488	-0.000167
C	-2.257825	-0.113711	-0.000292
O	-2.569724	-1.282562	0.000060
C	2.282913	-0.613270	1.259769
C	2.283101	-0.613331	-1.259609
O	-3.188026	0.880739	0.000132
H	-0.028029	-1.445369	-0.000079

H	-0.802336	1.517757	-0.000164
H	3.358486	-0.413258	1.266426
H	2.141244	-1.697429	1.285767
H	3.358682	-0.413363	-1.266092
H	2.141392	-1.697487	-1.285599
H	1.852217	-0.193890	-2.172583
H	2.925039	1.750791	0.000105
H	1.418067	1.997128	-0.885956
H	1.417871	1.997182	0.885821
H	-4.057010	0.452737	0.000373

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9gs2p2bs1.xyz

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26

C	0.891273	1.754616	0.068527
C	0.429163	0.313270	0.306913
Mn	-1.661019	-0.304327	0.015761
O	-1.978936	0.814970	-1.065889
C	0.795690	-0.839496	-0.607084
O	-0.390470	-1.582807	-0.608051
C	1.996322	-1.622095	-0.098024
O	1.697095	-2.498100	0.894561
O	3.146905	-1.473537	-0.478943
O	-1.888317	0.210228	1.509813
O	-2.653307	-1.562954	-0.197837
H	0.545907	0.030311	1.354565
H	1.074321	-0.494956	-1.615818
H	2.559566	-2.873949	1.152730
C	0.010250	2.713329	0.896246
C	2.359235	1.876622	0.557707
C	0.830262	2.176013	-1.412764
H	1.097370	3.237483	-1.512526
H	1.534194	1.602777	-2.028327
H	-0.177569	2.026761	-1.808948
H	2.737179	2.898053	0.402871
H	2.435362	1.650057	1.629218
H	3.014578	1.182532	0.019864
H	0.387159	3.743515	0.819881
H	-1.022483	2.683013	0.539832
H	0.002940	2.426614	1.954271

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9gs3p2bs1.xyz

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26

C	-2.255735	0.349825	-1.286752
C	-2.178445	0.356198	0.252402
C	-0.708757	0.194196	0.770075
O	-0.203550	-1.096824	0.533262
Mn	0.955497	-1.236269	-0.873100
O	0.907442	0.597125	-0.971016
C	0.307393	1.190025	0.136317
C	1.301387	1.649900	1.206890
O	0.990019	2.273366	2.208588
C	-2.990559	-0.833635	0.800457
O	2.585165	1.319583	0.950965
O	0.230584	-1.898785	-2.117665
O	2.371584	-1.732601	-0.392094
H	-0.752780	0.359518	1.860593
H	-0.201728	2.122325	-0.165302
H	-4.038944	-0.773017	0.476227
H	-2.559907	-1.774257	0.448876

H	-2.977201	-0.848043	1.898997
H	-3.833986	1.759276	0.505062
H	-2.736355	1.693077	1.898810
H	-2.252356	2.549571	0.428513
H	-3.305714	0.382058	-1.612794
H	-1.744776	1.217455	-1.719561
H	-1.783791	-0.544629	-1.702268
H	3.080592	1.646468	1.725409

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9ts2p2bs1.xyz

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26

C	-2.047944	0.709656	-0.019941
C	-0.569559	0.734850	0.347968
C	0.436844	1.276085	-0.453066
C	1.576710	1.964705	0.175342
O	2.338495	2.635133	-0.748143
O	1.862486	2.008409	1.359366
O	1.449656	-0.292461	-0.775374
Mn	0.493340	-1.611860	0.080332
O	0.554355	-1.712511	1.655486
O	-0.772163	-2.242778	-0.650007
O	1.918892	-2.025955	-0.664692
H	-0.358339	0.714620	1.414094
H	0.240488	1.553659	-1.482359
H	3.072298	3.001575	-0.222194
C	-2.801378	-0.314349	0.854193
C	-2.607272	2.124225	0.297402
C	-2.289196	0.397924	-1.509254
H	-3.367309	0.371040	-1.719202
H	-1.848702	1.164631	-2.158729
H	-1.853221	-0.571423	-1.763715
H	-3.882748	-0.254127	0.667749
H	-2.455828	-1.326511	0.634735
H	-2.631268	-0.114850	1.920111
H	-3.687744	2.165875	0.096307
H	-2.449529	2.386107	1.351061
H	-2.114582	2.888631	-0.315155

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9ts2p2bs2.xyz

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26

C	-2.198268	-0.057706	-0.025080
C	-0.850882	0.528594	0.359931
C	-0.066811	1.351115	-0.438850
C	0.737491	2.425728	0.177630
O	1.221201	3.292557	-0.768262
O	0.957295	2.607013	1.355084
O	1.454814	0.274151	-0.710800
Mn	1.089995	-1.366094	0.078768
O	1.121300	-1.476973	1.657030
O	0.155616	-2.372224	-0.722266
O	2.587000	-1.170860	-0.620481
H	-0.641277	0.558312	1.424976
H	-0.326487	1.517830	-1.475698
H	1.779097	3.915693	-0.282582
C	-2.494323	-1.328468	0.798263
C	-3.258251	1.016057	0.353218
C	-2.315923	-0.372527	-1.526808
H	-3.308094	-0.784405	-1.742642
H	-2.193997	0.526177	-2.139297

H	-1.562868	-1.103785	-1.824376
H	-3.525629	-1.656678	0.624157
H	-1.815002	-2.134157	0.521190
H	-2.374974	-1.134254	1.868767
H	-4.266869	0.638663	0.146070
H	-3.201267	1.266818	1.416842
H	-3.108502	1.936063	-0.218869

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9ts3p2bs1.xyz

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26

C	-1.683510	-1.573036	-1.309368
C	-2.125600	-0.926346	0.018409
C	-2.211852	-2.010137	1.111457
C	-3.529015	-0.297047	-0.157551
C	-1.169059	0.190963	0.450802
C	-0.778363	1.199968	-0.419391
C	-0.341854	2.483426	0.098888
O	-0.120141	3.404641	-0.899175
O	-0.203393	2.812895	1.270611
O	0.385447	-0.866466	0.885662
Mn	1.770482	-0.674498	-0.000891
O	2.023286	-1.967155	-0.896899
O	2.993942	-0.337830	0.950608
O	1.401571	0.593489	-0.928545
H	-1.255169	0.488880	1.492965
H	-0.902076	1.121975	-1.490698
H	-2.952670	-2.773804	0.837099
H	-1.239923	-2.486205	1.253388
H	-2.518714	-1.573618	2.071470
H	-4.265963	-1.065414	-0.431552
H	-3.870112	0.178702	0.771154
H	-3.523127	0.468655	-0.941183
H	-2.348052	-2.410277	-1.563342
H	-1.726932	-0.857637	-2.138897
H	-0.657665	-1.944378	-1.239441
H	0.188177	4.192238	-0.416251

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9ts3p2bs2.xyz

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26

C	-1.683667	-1.661230	-1.277359
C	-2.133588	-0.961931	0.018275
C	-2.260002	-2.004604	1.146126
C	-3.521274	-0.313419	-0.205333
C	-1.167134	0.149471	0.442238
C	-0.775236	1.164403	-0.418411
C	-0.399830	2.467390	0.100591
O	-0.214741	3.391226	-0.903087
O	-0.280400	2.803699	1.265788
O	0.397515	-0.921729	0.812432
Mn	1.815121	-0.641643	0.000088
O	2.123197	-1.860039	-0.979847
O	2.996644	-0.336814	1.018286
O	1.422341	0.679802	-0.847761
H	-1.236901	0.436208	1.487072
H	-0.893307	1.088075	-1.488799
H	-2.990492	-2.774416	0.872579
H	-1.298090	-2.479153	1.339110
H	-2.599493	-1.533422	2.075224
H	-4.263578	-1.082387	-0.450288

H	-3.862399	0.212368	0.692413
H	-3.490907	0.409553	-1.024592
H	-2.411958	-2.430726	-1.558170
H	-1.608024	-0.958202	-2.111430
H	-0.708573	-2.132078	-1.147519
H	0.073623	4.195612	-0.451046

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mnbs1.xyz

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5

Mn	0.000000	0.000000	0.000000
O	0.533181	0.754013	-1.305999
O	0.533153	-1.508045	0.000000
O	-1.599516	0.000020	0.000000
O	0.533182	0.754012	1.305999

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mnbs2.xyz

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5

Mn	0.000010	-0.000041	-0.000009
O	-1.393407	0.177215	0.768658
O	1.208135	0.241191	1.022791
O	0.094846	-1.482291	-0.598247
O	0.090396	1.064012	-1.193174

28