

CO₂ Reduction by Mn Electrocatalyst in the Presence of Lewis Acid: A DFT Study on the Reaction Mechanism

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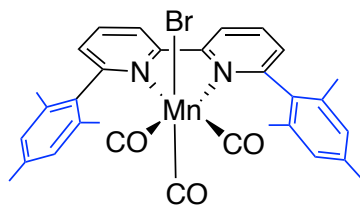
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(a)



(b)

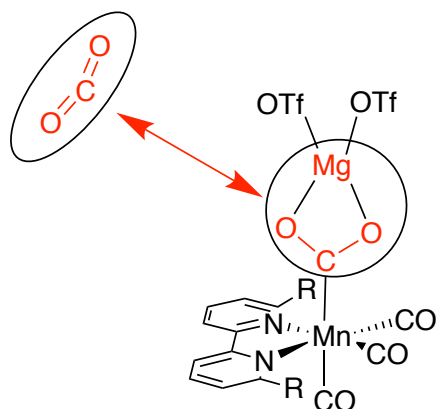


Figure S1. (a) Partitioning of the molecule into high- (black) and low- (blue) layers in ONIOM and (b) a schematic diagram showing the application of an artificial force between the highlighted atoms (red).

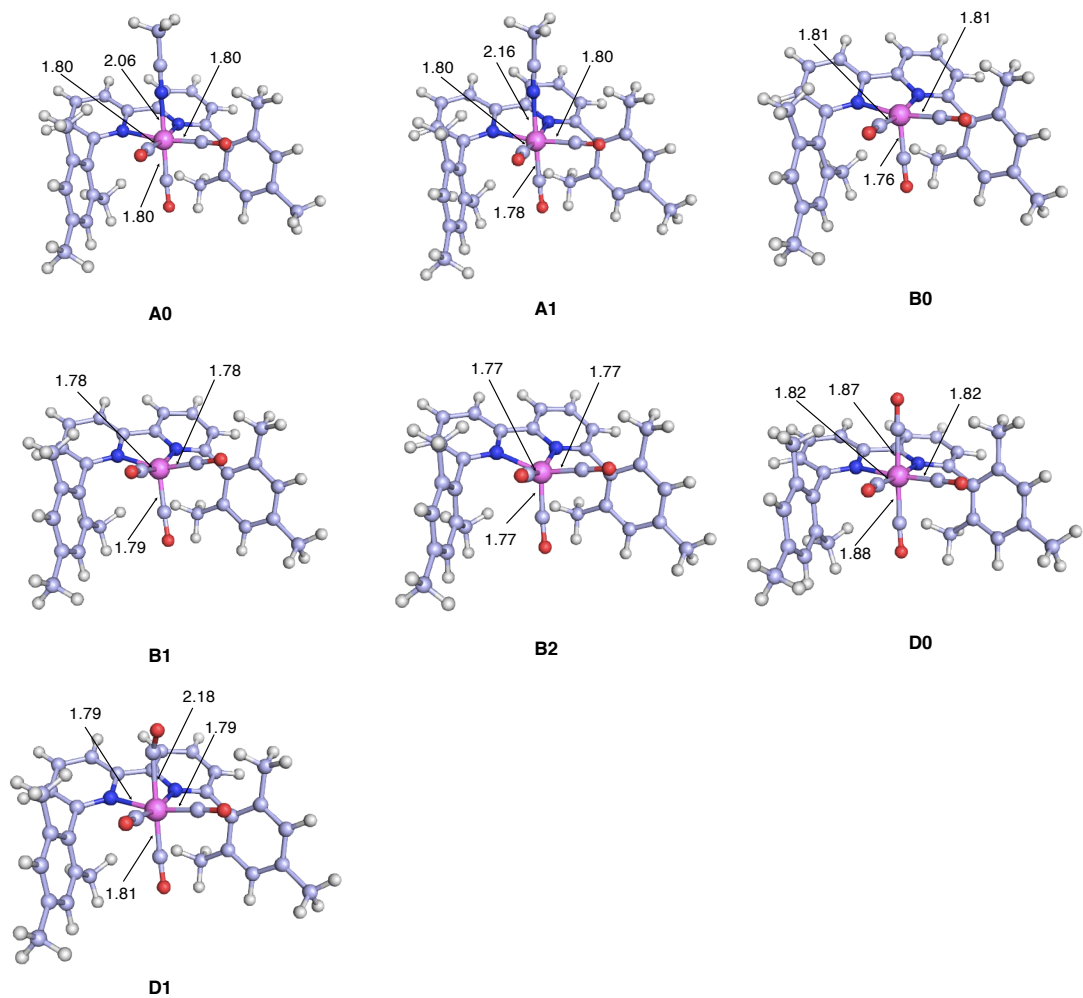


Figure S2. Optimized structures of complexes **A0**, **B0**, **D0**, and their reduced species, **A1**, **B1**, **B2**, and **D1**.

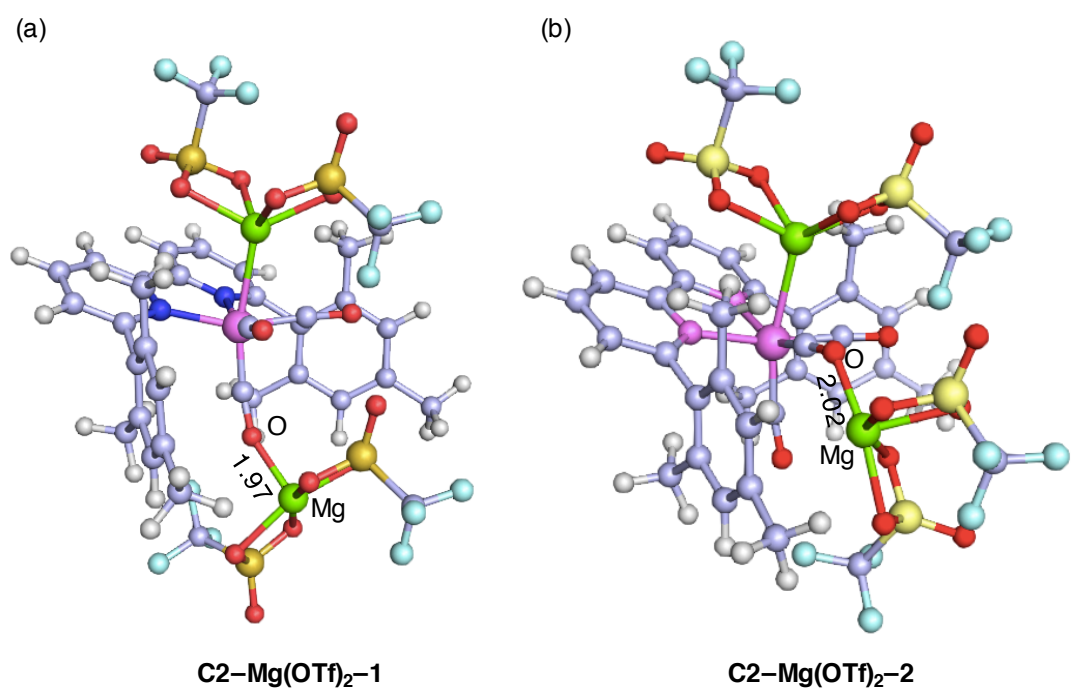
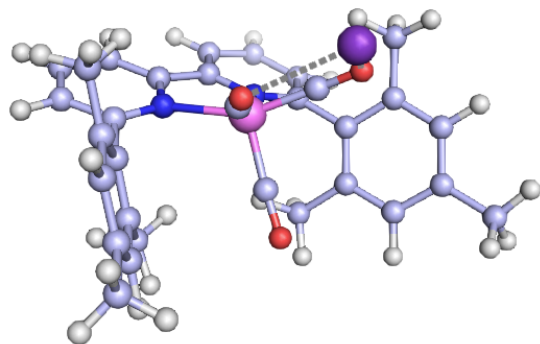


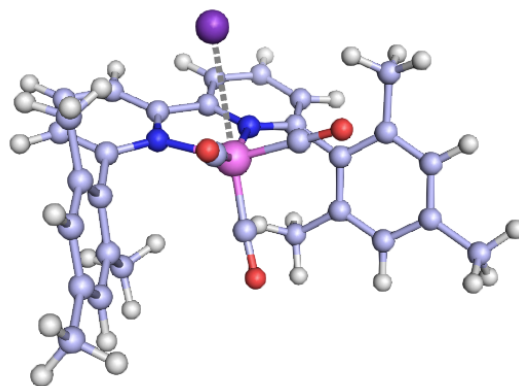
Figure S3. Mn complexes with two Mg(OTf)₂; (a) **C2-Mg(OTf)₂-1** and (b) **C2-Mg(OTf)₂-2**.

(a)



B1-K⁺

(b)



B2-K⁺

Figure S4. Mn complex with potassium cation; (a) **B1-K⁺** and (b) **B2-K⁺**.

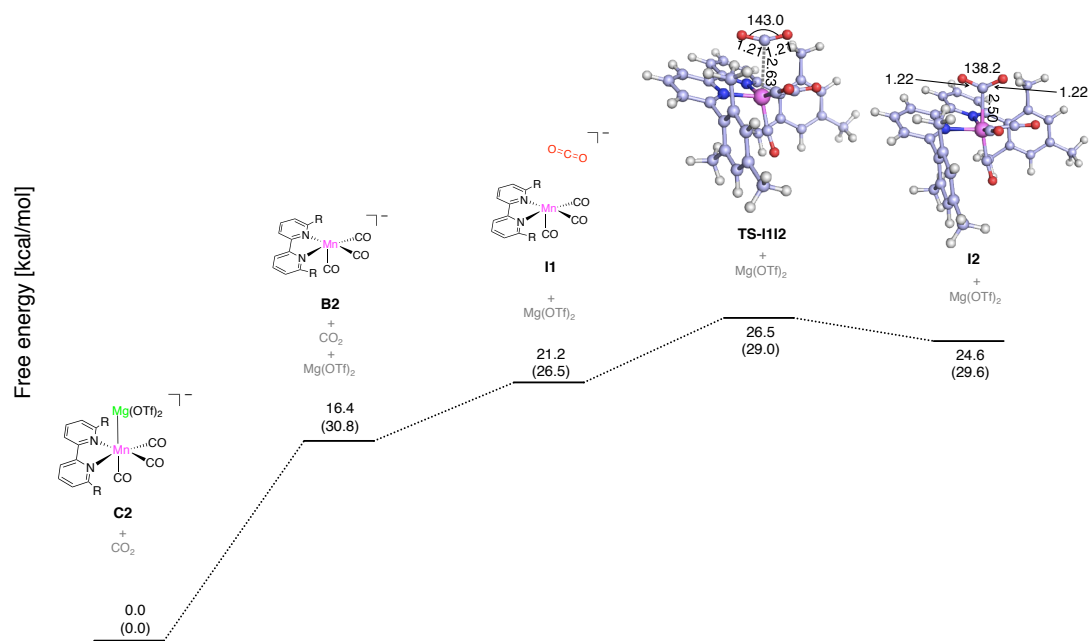


Figure S5. Free energy profile of Mg(OTf)₂ removal and CO₂ binding which occurs in a stepwise manner.

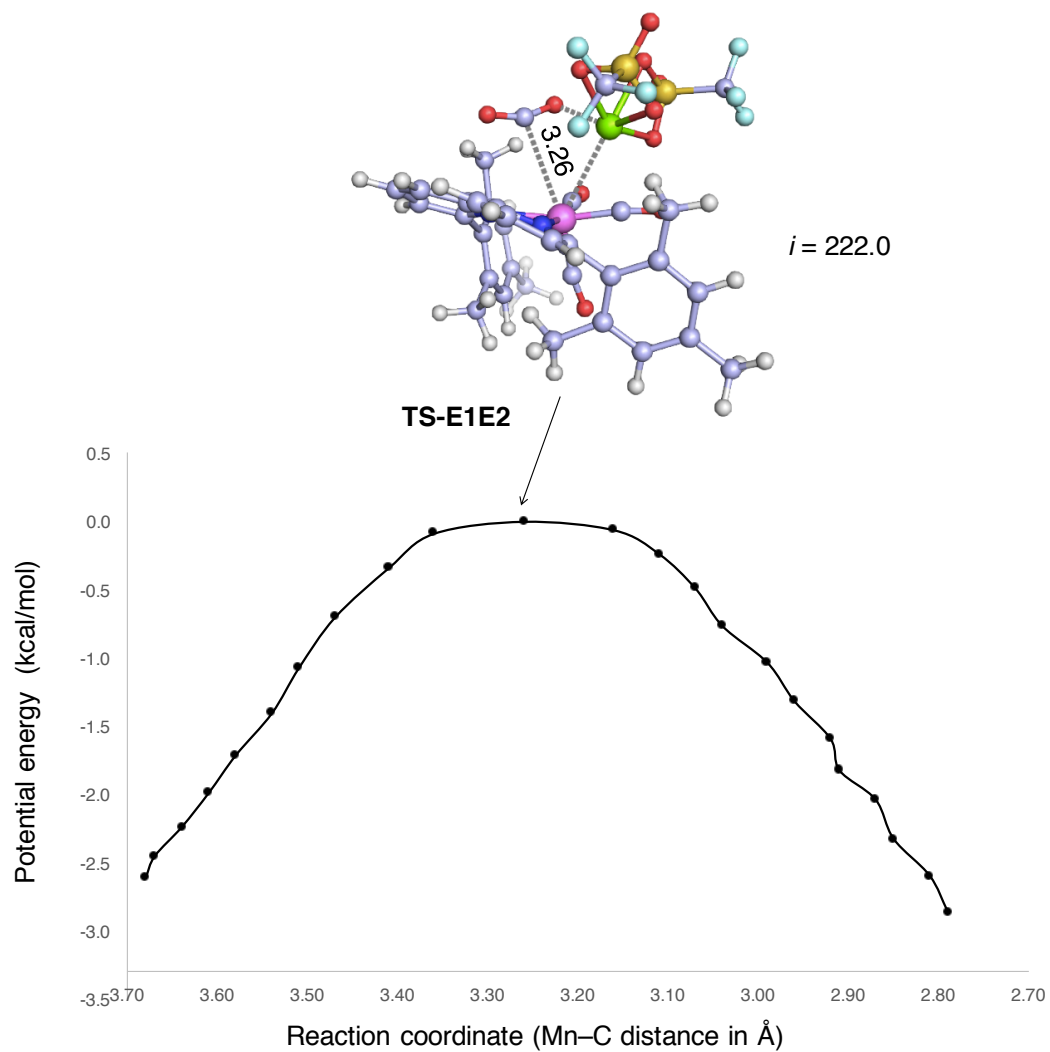


Figure S6. IRC path from the TS of 1st CO₂ binding. Imaginary frequency (i) of the TS is in cm⁻¹.

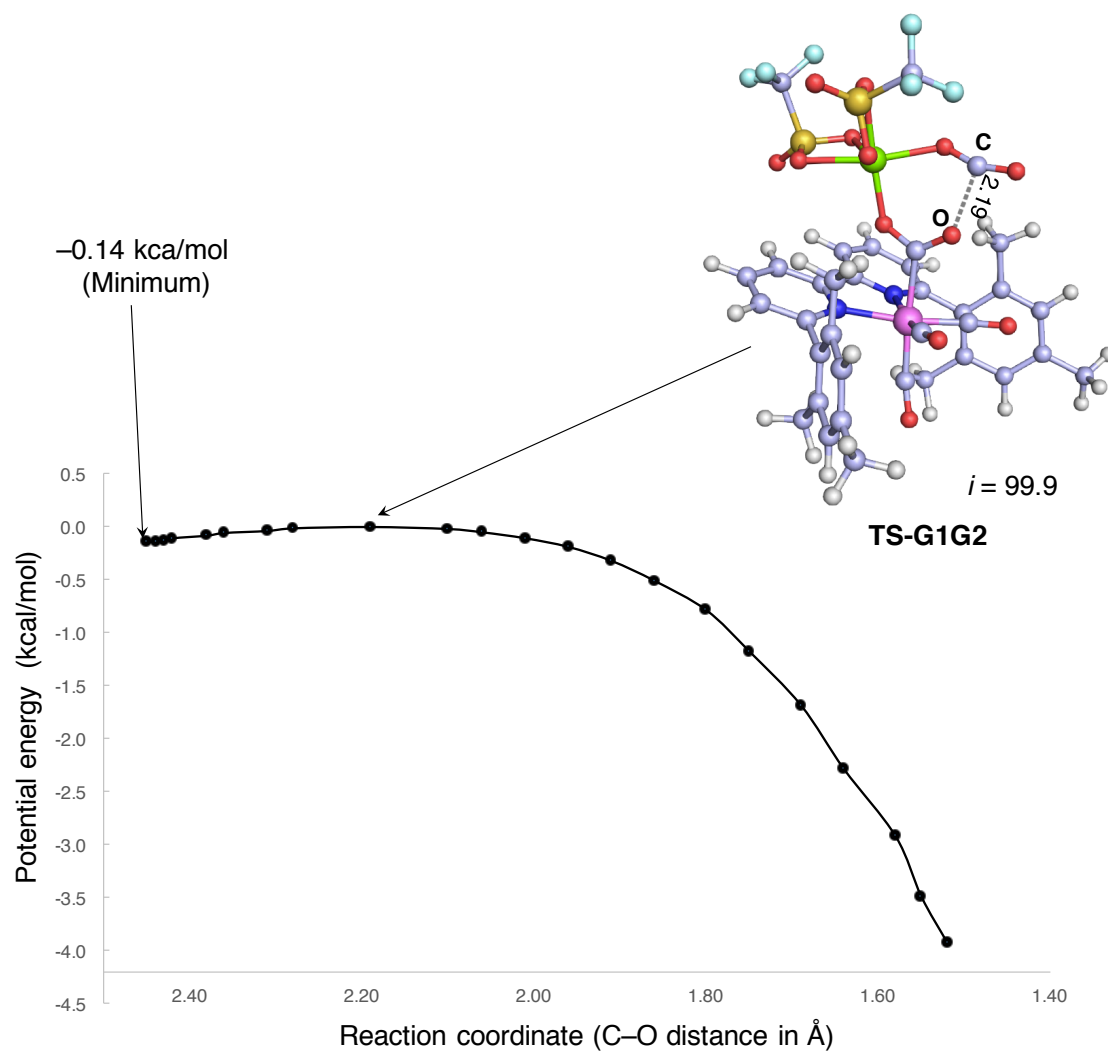


Figure S7. IRC path from the TS of 2nd CO₂ binding. Imaginary frequency (i) of the TS is in cm⁻¹.

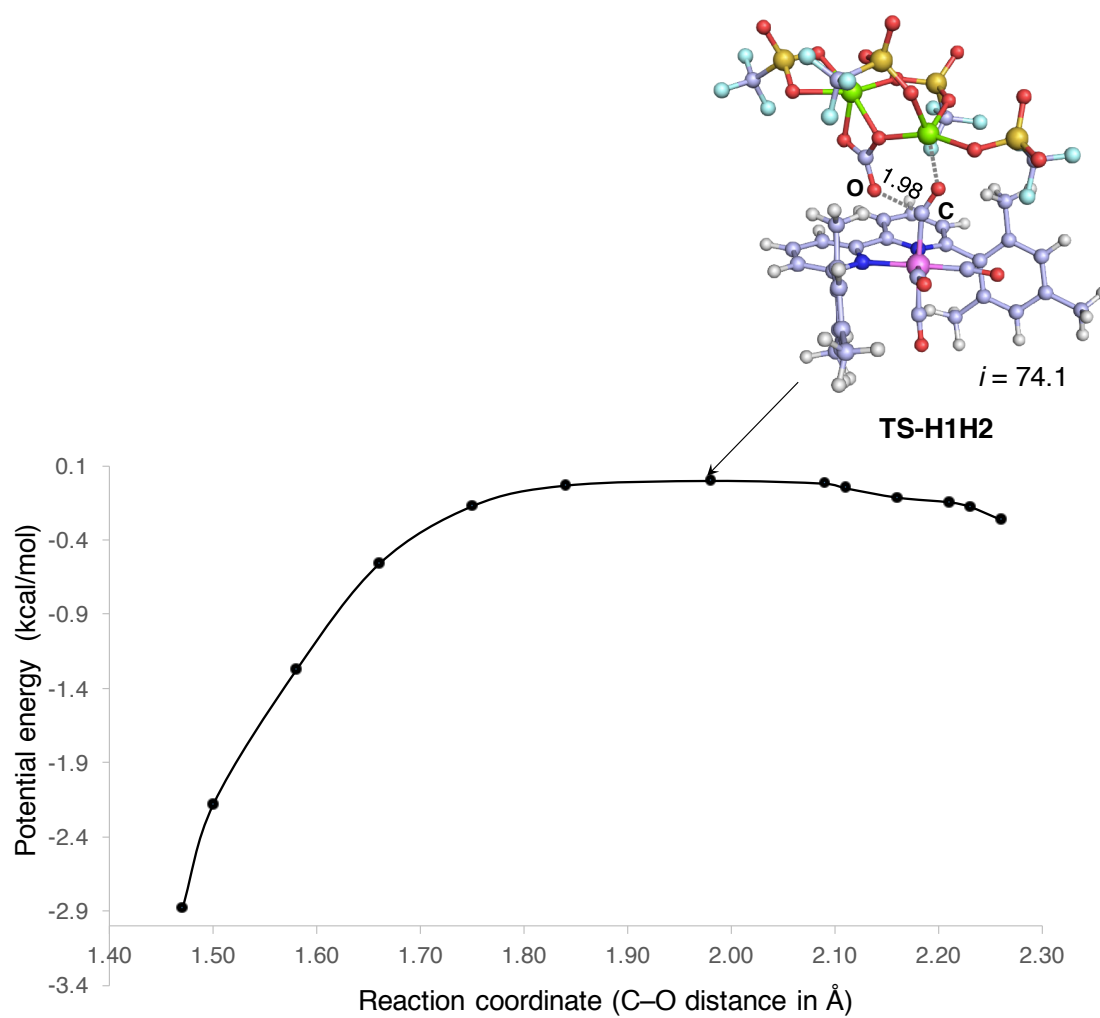


Figure S8. IRC path from the TS of C-O bond cleavage. Imaginary frequency (i) of the TS is in cm^{-1} .

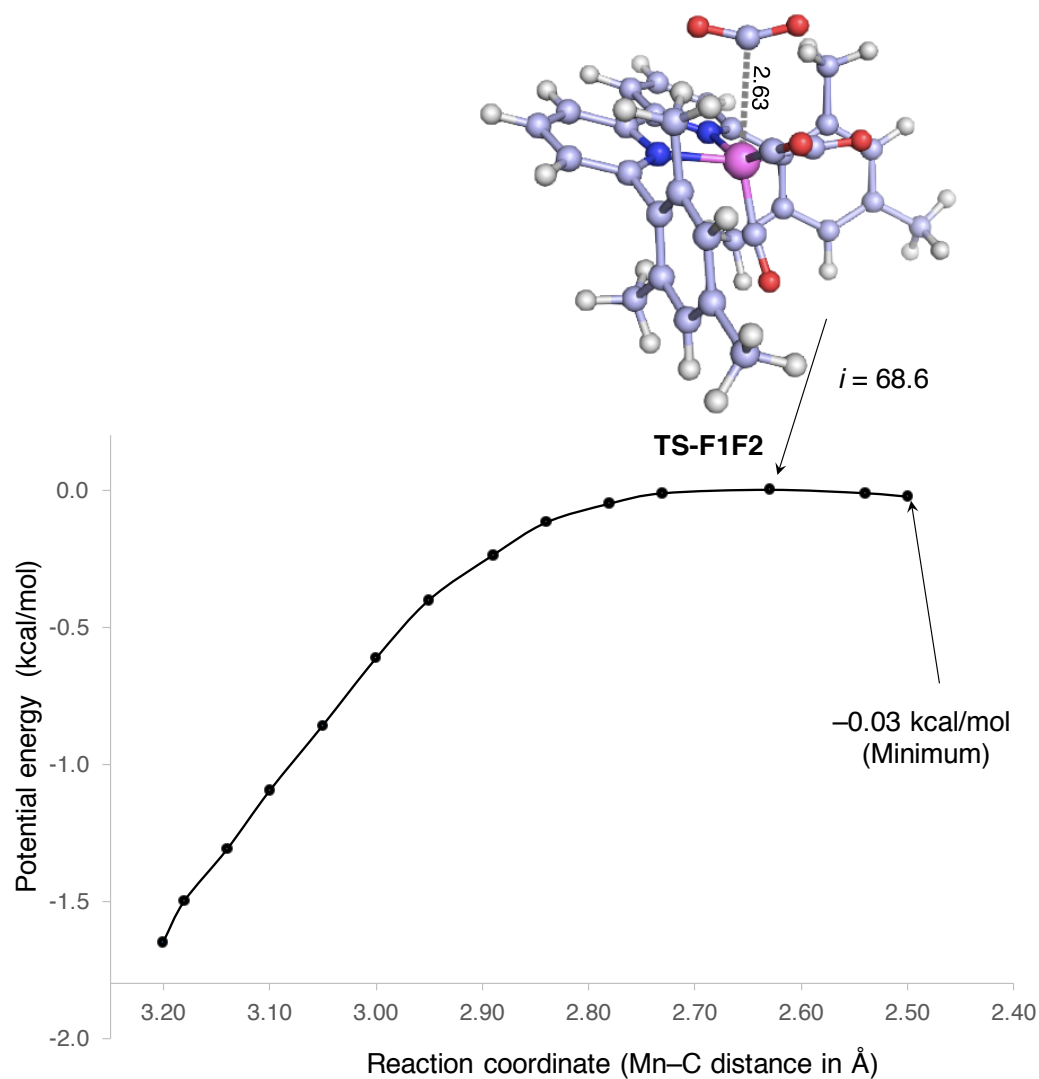


Figure S9. IRC path from the TS of CO₂ binding to Mn center in absence of Mg(OTf)₂. Imaginary frequency (i) of the TS is in cm⁻¹.

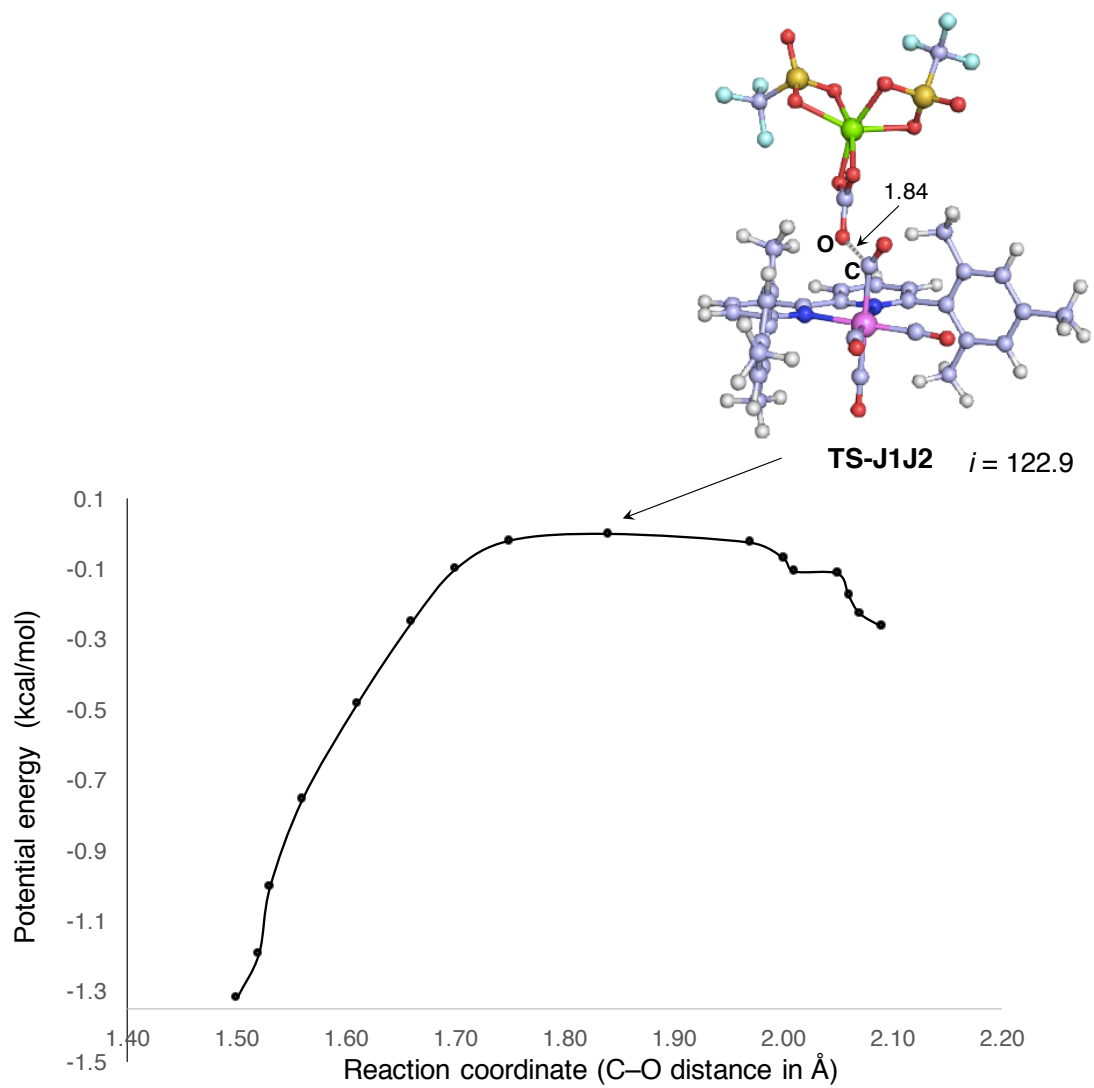


Figure S10. IRC path from the TS of C-O bond cleavage with one $\text{Mg}(\text{OTf})_2$. Imaginary frequency (i) of the TS is in cm^{-1} .

Table S1. Total electronic energy (E_{SCF}), thermal correction to enthalpy (H_{corr}), and thermal correction to free energy (G_{corr}). All are given in a.u.

label	E_{SCF}	E_{SCF}	H_{corr}	G_{corr}
Basis set	BS2 ^a	BS1 ^a	BS1 ^a	BS1 ^a
CO	-113.3252595	-113.2913502	0.0083030	-0.0141450
CO ₂	-188.6313683	-188.5751751	0.0153730	-0.0095790
CO ₂ ⁻	-188.6313683	-188.6098018	0.0126580	-0.0152630
MeCN	-132.7840434	-132.7447396	0.0499350	0.0214610
Mg(OTf) ₂	-2123.3545076	-2122.9732095	0.0767050	0.0107740
A0	-1770.7796922	-1770.3606184	0.6036510	0.4884050
A1	-1770.8841837	-1770.4591191	0.5993910	0.4848680
B0	-1637.9649130	-1637.5829816	0.5514620	0.4474210
B1	-1638.0974085	-1637.7125665	0.5494060	0.4428120
B2	-1638.2039204	-1637.8133096	0.5475310	0.4417100
D0	-1751.3299760	-1750.9176493	0.5618280	0.4513700
D1	-1751.4398737	-1751.0239031	0.5591670	0.4462930
A0-O1	-3894.1583214	-3893.3597461	0.6831090	0.5307280
A0-O2	-3894.1550466	-3893.3553081	0.6827600	0.5230850
A0-C1	-3894.1450762	-3893.3452191	0.6828020	0.5263110
A0-C3	-3894.1531112	-3893.3531025	0.6828480	0.5220250
A0-C4	-3894.1505410	-3893.3510293	0.6830070	0.5238880
A0-Z2	-3894.1534896	-3893.3531556	0.6833030	0.5245740
A1-C1	-3894.2623595	-3893.4574186	0.6797210	0.5205490
A1-C2	-3894.2638331	-3893.4580580	0.6790310	0.5206940
A1-C3	-3894.2577133	-3893.4520078	0.6795300	0.5151200
A1-C4	-3894.2555855	-3893.4502287	0.6772970	0.5183020
A1-Z2	-3894.2607441	-3893.4545509	0.6793700	0.5138170
B0-O1	-3761.3370940	-3760.5759763	0.6321250	0.4904760
B0-O2	-3761.3391128	-3760.5781818	0.6316940	0.4899990
B0-C1	-3761.3364897	-3760.5746719	0.6310550	0.4872920
B0-C2	-3761.3387887	-3760.5739811	0.6314920	0.4851440
B0-C3	-3761.3380300	-3760.5743449	0.6314610	0.4858240
B0-C4	-3761.3377645	-3760.5749574	0.6309910	0.4849190
B0-Z1	-3761.3376236	-3760.5736759	0.6321510	0.4881070
B0-Z2	-3761.3375161	-3760.5739608	0.6320830	0.4878230
B1-Mn	-3761.4826484	-3760.7169221	0.6283590	0.4826490
B1-O1	-3761.4809607	-3760.7173125	0.6289850	0.4817860
B1-O2	-3761.4829290	-3760.7197367	0.6292400	0.4851210
B1-C1	-3761.4683662	-3760.7036861	0.6286010	0.4834400
B1-C2	-3761.4672277	-3760.7024333	0.6287110	0.4828460
B1-C3	-3761.4698815	-3760.7032312	0.6286640	0.4780830

^aSee main text.

Table S1 (Continue) Total electronic energy (E_{SCF}), thermal correction to enthalpy (H_{corr}) and thermal correction to free energy (G_{corr}). All are given in a.u.

label	E_{SCF}	E_{SCF}	H_{corr}	G_{corr}
Basis set	BS2 ^a	BS1 ^a	BS1 ^a	BS1 ^a
B1-C4	-3761.4718289	-3760.7065658	0.6289010	0.4801100
B1-Z1	-3761.4700748	-3760.7031719	0.6290930	0.4809480
B1-Z2	-3761.4714318	-3760.7053581	0.6290770	0.4799480
B2-Mn	-3761.6100012	-3760.8386579	0.6266620	0.4778610
B2-O1	-3761.5960588	-3760.8276019	0.6272880	0.4803380
B2-O2	-3761.5954688	-3760.8271902	0.6277910	0.4846750
B2-C1	-3761.5843028	-3760.8134765	0.6265320	0.4773300
B2-C2	-3761.5833644	-3760.8125464	0.6267650	0.4798270
B2-C3	-3761.5830511	-3760.8115465	0.6272070	0.4781880
B2-C4	-3761.5824561	-3760.8108784	0.6271950	0.4790410
B2-Z1	-3761.5746630	-3760.8018202	0.6269220	0.4806190
B2-Z2	-3761.5818767	-3760.8103002	0.6274590	0.4806220
D0-O1	-3874.7076380	-3873.9156126	0.6415010	0.4930730
D0-O2	-3874.7006425	-3873.9095346	0.6412820	0.4934870
D0-C1	-3874.6970374	-3873.9040496	0.6409280	0.4868820
D0-C3	-3874.7027415	-3873.9102956	0.6414510	0.4854180
D0-C4	-3874.7025009	-3873.9097811	0.6416350	0.4905040
D0-Z2	-3874.7041786	-3873.9106943	0.6415570	0.4901280
D1-O1	-3874.8219865	-3874.0284421	0.6388400	0.4834100
D1-O2	-3874.8185955	-3874.0232639	0.6393950	0.4868180
D1-C1	-3874.8155788	-3874.0173300	0.6376810	0.4826300
D1-C2	-3874.8157025	-3874.0169834	0.6377760	0.4824410
D1-C3	-3874.8172574	-3874.0215751	0.6389360	0.4796160
D1-C4	-3874.8158597	-3874.0205228	0.6393600	0.4821120
D1-Z2	-3874.8168117	-3874.0208665	0.6394700	0.4837050
E1	-3950.2479538	-3949.4190766	0.6451800	0.4895430
TS-E1E2	-3950.2233823	-3949.3997418	0.6424810	0.4854220
E2	-3950.2653448	-3949.4431419	0.6449060	0.4893860
F	-3950.2809078	-3949.4600935	0.6452550	0.4906560
G1	-4138.9049242	-4138.0261091	0.6613420	0.4976190
TS_G1G2	-4138.9041040	-4138.0258693	0.6602370	0.4990980
G2	-4138.9124852	-4138.0359093	0.6619930	0.5001440
H1	-6262.3588739	-6261.0948859	0.7421140	0.5459680
TS-H1H2	-6262.3524183	-6261.0861671	0.7401760	0.5428400
C2-MgOTf2-1	-5884.9992883	-5883.8489641	0.7066090	0.5225290
C2-MgOTf2-2	-5885.0073345	-5883.8561451	0.7059380	0.5254670
B1-K+	-2237.9496194	-2237.5349910	0.5524510	0.4393230
B2-K+	-2238.0643128	-2237.6434134	0.5506700	0.4375520
I1	-1826.8433376	-1826.3973514	0.5640710	0.4478390
TS-I1I2	-1826.8381923	-1826.3937269	0.5628510	0.4510460
I2	-1826.8382908	-1826.3938055	0.5639860	0.4481800
TS-J1J2	-4138.8891484	-4138.0147049	0.6601470	0.4941130

^aSee main text.

Cartesian Coordinates

CO

C 0.000000 0.000000 -0.651859
O 0.000000 0.000000 0.488894

CO2

C 0.000000 0.000000 -0.000003
O 0.000000 0.000000 -1.168594
O 0.000000 0.000000 1.168596

CO2-

C 0.000000 0.358295 0.000000
O 1.147926 -0.134304 -0.000000
O -1.147926 -0.134417 0.000000

MeCN

C 1.172589 -0.000054 -0.000017
H 1.551077 0.639507 0.803382
H 1.550628 -1.015896 0.151842
H 1.550495 0.376142 -0.955789
C -0.271198 0.000193 0.000209
N -1.437221 -0.000083 -0.000084

MgOTf2

Mg 0.037014 -1.062702 -0.039102
S 2.065810 0.639404 -0.016402
O 2.367606 2.056605 -0.024902
O 1.365711 0.059702 -1.217002
O 1.325811 0.081302 1.169498
C 3.687212 -0.240591 0.019498
F 4.398311 0.091811 -1.053702
F 3.476016 -1.558492 0.019498
F 4.350411 0.099911 1.120398
S -2.610786 -0.867009 0.006098
O -1.680286 -0.955207 1.185398
O -3.820684 -1.664413 0.030198
O -1.720686 -0.968407 -1.203902
C -3.132091 0.901489 0.006798
F -3.788292 1.173887 1.130898
F -3.919092 1.136587 -1.038802
F -2.045693 1.673192 -0.071402

A0

Mn 0.001843 0.040425 0.555223
O 0.003918 -2.442141 -1.048106
O -1.825843 -1.329711 2.431574
O 1.833543 -1.321298 2.433404
N 1.318444 1.241101 -0.600421
N -1.324592 1.238979 -0.593424
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C -1.193024 -0.764734 1.638593
C 1.199235 -0.759144 1.639601
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C 3.444704 2.147509 -1.225979
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C 2.853291 3.348466 -1.586269
H 3.453692 4.175567 -1.957346
C 1.473807 3.465164 -1.502002
H 0.984802 4.378539 -1.824280
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H -3.483391 4.224290 -1.787989
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C 3.285593 -0.210785 -0.460926
C 3.117019 -1.263937 -1.382355
C 3.734427 -2.487057 -1.116903
H 3.599900 -3.306948 -1.824351
C 4.535875 -2.680275 0.011642
C 4.724474 -1.602841 0.880624
H 5.350599 -1.732249 1.764855
C 4.115651 -0.366878 0.663358
C 2.372467 -1.065768 -2.670395
H 2.984883 -0.497772 -3.385505
H 1.439459 -0.502958 -2.549448
H 2.128223 -2.025538 -3.137369
C 5.162242 -4.011511 0.290380
H 6.090763 -3.910233 0.863596
H 5.385150 -4.556795 -0.633860
H 4.490279 -4.649071 0.881557
C 4.310052 0.754779 1.639432
H 4.762476 0.392907 2.568992
H 3.360972 1.245815 1.895684
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C -3.102927 -1.253216 -1.397082
C -3.707655 -2.486012 -1.155794
H -3.559433 -3.292646 -1.875891
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C -4.712054 -1.649936 0.854909
H -5.334603 -1.803882 1.737628
C -4.116786 -0.401897 0.660896
C -2.351921 -1.026650 -2.676866
H -2.955630 -0.432352 -3.377819
H -2.116462 -1.975988 -3.169061
H -1.413253 -0.477699 -2.538155
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H -5.787175 -4.336681 -0.643044
H -5.759248 -4.049583 1.106082
H -4.389726 -4.834046 0.300695
C -4.324313 0.696245 1.660930
H -3.385393 1.209647 1.909981
H -4.749769 0.304491 2.591174
H -5.011604 1.467173 1.286104
N -0.003476 1.679548 1.809300
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C -0.019755 3.688041 3.457107
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H -0.893461 4.318436 3.263065
H -0.061928 3.329291 4.490335

A1

Mn -0.002011 0.067178 0.543816
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O -1.819809 -1.220277 2.484953
O 1.816977 -1.231910 2.476052
N 1.321877 1.221679 -0.592419
N -1.323638 1.227694 -0.589390
C -0.007595 -1.413148 -0.436596
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C 2.661220 1.079111 -0.768594
C 3.456658 2.099832 -1.267930
H 4.525037 1.930987 -1.380191
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H 3.472305 4.146567 -2.008168
C 1.499351 3.453577 -1.541924
H 1.015487 4.373209 -1.860952
C 0.713864 2.385622 -1.050225

C -0.711419 2.387816 -1.051068
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 H -3.462749 4.152589 -2.022346
 C -3.455155 2.110658 -1.269000
 H -4.524185 1.945300 -1.380263
 C -2.663387 1.089205 -0.765279
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 C 4.108897 -0.400027 0.652751
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 H 1.420468 -0.553522 -2.527745
 H 2.133207 -2.053571 -3.151130
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 H 5.777741 -4.028051 1.178039
 H 5.834945 -4.339442 -0.565373
 H 4.429679 -4.840057 0.364980
 C 4.304596 0.716408 1.635697
 H 4.682366 0.336852 2.591899
 H 3.368835 1.256894 1.832803
 H 5.024949 1.462163 1.272304
 C -3.296376 -0.221515 -0.467032
 C -3.136693 -1.282253 -1.383279
 C -3.753404 -2.503579 -1.113944
 H -3.621381 -3.326640 -1.819135
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 C -4.722465 -1.617212 0.890830
 H -5.336793 -1.746226 1.783850
 C -4.111640 -0.380550 0.665165
 C -2.383467 -1.089416 -2.666796
 H -2.975706 -0.497420 -3.379654
 H -2.158307 -2.049608 -3.143419
 H -1.439311 -0.549788 -2.526716
 C -5.198552 -4.018428 0.285319
 H -5.859977 -4.315005 -0.539404
 H -5.796630 -3.999436 1.203076
 H -4.454237 -4.819033 0.388362
 C -4.297459 0.738816 1.646697
 H -3.358117 1.274938 1.838761
 H -4.673169 0.363185 2.605253
 H -5.015505 1.487495 1.284708
 N 0.009413 1.806480 1.819586
 C 0.033525 2.629678 2.639763
 C 0.068136 3.655884 3.648366
 H 0.055786 3.203247 4.645063
 H 0.978506 4.254367 3.542199
 H -0.801538 4.312698 3.546713

B0

Mn 0.007063 0.161559 0.825545
 O -0.006760 -2.137728 -0.982850
 O -1.862565 -1.385620 2.528890
 O 1.881114 -1.390557 2.520318
 N 1.309925 1.514811 -0.070182
 N -1.312518 1.512622 -0.038650
 C 0.000084 -1.196241 -0.300560
 C -1.202641 -0.742213 1.824277
 C 1.222375 -0.744441 1.817145
 C 2.642491 1.389934 -0.277570
 C 3.436722 2.513261 -0.513875

H 4.502455 2.377057 -0.678772
 C 2.858546 3.773747 -0.552175
 H 3.466907 4.657317 -0.729158
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B1

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B2

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D0

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D1

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A0-O1

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A1-C1

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C	-3.865549	1.086605	0.504725	F	3.599817	-3.198182	1.563317
C	-2.099145	2.595959	0.757486	F	2.299615	-4.917213	1.267260
C	0.830624	1.776788	-0.671743	S	5.459848	-0.804648	-0.087454
C	2.095359	1.585463	-1.252360	O	4.717822	-1.401008	-1.248548
H	2.886789	2.299343	-1.038601	O	6.457295	-1.623732	0.575370
C	2.221604	0.644998	-2.325864	O	4.407730	-0.154794	0.767114
H	3.113211	0.626767	-2.951605	C	6.370251	0.617350	-0.830611
C	1.157869	-0.200868	-2.569726	F	7.273542	0.163508	-1.696647
H	1.223800	-0.924737	-3.377248	F	6.980421	1.312254	0.126488
C	-0.018571	-0.122259	-1.785328	F	5.509317	1.412238	-1.470876
C	-1.072744	-1.078941	-1.888082	N	-1.523665	-0.021071	1.449837
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H	0.003942	-2.482301	-3.143407	C	-0.706893	-1.394313	3.500300
C	-1.958954	-3.181430	-2.680773	H	-0.815415	-2.464801	3.294695
H	-1.853636	-4.106117	-3.244422	H	-1.299921	-1.142802	4.385721
C	-3.137622	-2.900622	-1.979962	H	0.346867	-1.175471	3.704668
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C	-3.246244	-1.712875	-1.263465	A1-C2			
C	0.657958	3.012771	0.138375	Mn	2.000912	0.807558	0.013314
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C	0.880872	4.246202	2.197367	O	2.679589	3.203541	-1.570918
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C	0.458115	5.421109	1.571820	N	1.576938	-0.991042	1.057043
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C	1.494555	1.812252	2.198811	C	-1.470422	2.834251	1.903749
H	2.567968	1.655810	2.015811	H	-1.928342	3.818754	1.870793
H	0.983410	0.910247	1.849508	C	-2.036474	1.787599	2.645311
H	1.360909	1.885246	3.284554	H	-2.961911	1.933104	3.200110
C	0.295437	6.690899	2.349013	C	-1.380986	0.570652	2.690174
H	0.484088	7.574932	1.728914	H	-1.734629	-0.207745	3.370656
H	0.967662	6.727487	3.213966	C	-0.159367	0.382018	1.968422
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H	-0.737285	4.973630	-2.266553	H	-0.461382	-1.710498	3.697576
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H	-2.715721	-2.514417	1.128298	C	-1.103671	3.621646	-1.414696
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H	-4.311215	-0.024969	-2.876119	H	1.424970	8.049333	-1.468740
H	-5.971314	0.598916	-2.877338	H	2.929023	7.162514	-1.694826
H	-5.636522	-1.048233	-3.414638	C	1.764269	4.037343	2.739303
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Mg	2.830293	-0.721755	-0.521695	H	1.071094	4.437315	3.493662
S	1.283076	-2.624108	0.517129	C	3.218015	-2.440682	-0.077664
O	-0.062368	-3.156923	0.628043	C	2.826157	-2.936473	-1.336717
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C	5.535316	-2.602595	-0.732220	C	1.908961	1.127308	-1.254601
H	6.592845	-2.476608	-0.491890	H	2.234592	2.167500	-1.334107
C	4.581338	-2.293841	0.238047	C	2.144823	0.248723	-2.330738
C	1.384155	-3.204619	-1.658670	C	1.675120	-1.064699	-2.219332
H	1.103601	-4.232072	-1.382253	H	1.882951	-1.771893	-3.023056
H	1.192656	-3.103964	-2.734263	C	0.936894	-1.492082	-1.112993
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C	6.211574	-3.336116	-3.044167	H	1.734510	1.648067	1.733941
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H	7.146990	-3.698047	-2.601499	H	0.895162	2.735999	0.623037
H	6.459420	-2.424882	-3.606859	C	2.856079	0.712321	-3.563311
C	5.019338	-1.836297	1.598165	H	3.526405	-0.058175	-3.960339
H	4.257762	-1.231432	2.101820	H	3.434083	1.625388	-3.385660
H	5.940927	-1.244679	1.542925	H	2.126195	0.939139	-4.352067
H	5.228389	-2.691457	2.257053	C	0.517785	-2.923819	-1.007635
C	3.208000	1.263508	1.243391	H	0.400879	-3.379673	-1.996830
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Mg	-2.737168	-0.637219	1.055111	H	1.283770	-3.502175	-0.471771
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O	-2.585143	-3.511316	-1.552865	C	-6.542164	1.357504	0.023727
O	-3.761241	-2.412762	0.404148	C	-7.294522	1.806130	-1.063582
O	-1.428718	-1.996069	0.099665	H	-7.558700	2.863900	-1.121732
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F	-2.157792	-4.071475	2.160364	H	-7.700807	-1.103078	-2.751041
F	-0.884710	-4.871024	0.588188	C	-6.625872	-0.900673	-0.903371
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F	-6.281194	0.849446	-1.548707	H	-9.183913	0.708888	-3.640533
F	-4.724706	-0.626227	-1.911150	H	-7.800358	1.701646	-4.091627
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A1-Z2

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 H -6.357273 1.796457 0.388767
 C -7.531140 -1.911423 -3.930497
 H -8.225475 -1.145689 -4.293476
 H -8.077334 -2.863098 -3.886832
 H -6.746823 -2.039331 -4.687897
 C -4.554069 -3.043040 -0.048055
 H -3.698315 -2.557136 0.435566
 H -4.168376 -3.787919 -0.752388
 H -5.089952 -3.585355 0.744437
 C -2.507712 -0.733809 -1.138402
 O -2.333381 -1.620079 -1.876232
 Mg 3.656191 -0.203742 -0.463229
 S 5.908929 1.212857 -0.516443
 O 7.335182 0.959357 -0.428289
 O 5.065922 0.842872 0.675933
 O 5.168313 0.688946 -1.709927
 C 5.725436 3.044046 -0.636543
 F 6.222138 3.615680 0.458344
 F 4.434087 3.360914 -0.750791
 F 6.382088 3.485968 -1.706843
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 O 4.373632 -2.118722 -1.015790
 O 3.151052 -3.999291 0.158083
 O 3.268584 -1.636325 1.049591
 C 5.442962 -3.144558 1.171917
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 F 5.143117 -3.583520 2.392491
 F 6.193993 -2.047908 1.268952
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 H -4.373021 4.919550 2.578259
 H -2.633494 5.275990 2.434653
 C -3.297142 3.625801 1.346736

B0-O1

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 O 0.636065 -1.791256 -1.803658
 O -1.562618 0.342883 -0.216785
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 N 3.425542 0.770867 -0.425876
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 C -0.428673 0.662229 -0.268956
 C 0.782018 3.491045 0.918720
 C 1.175486 4.683469 1.529216
 H 0.407075 5.354787 1.903959
 C 2.519818 5.003978 1.626191
 H 2.839445 5.931617 2.094405
 C 3.452997 4.127435 1.094156
 H 4.510604 4.363029 1.143834
 C 3.019596 2.939217 0.511213
 C 3.959523 1.962921 -0.049982
 C 5.321792 2.223802 -0.169152
 H 5.727163 3.188827 0.115469
 C 6.159799 1.234108 -0.662954
 H 7.225049 1.421075 -0.773837
 C 5.622301 -0.004618 -0.971422
 H 6.254633 -0.825859 -1.298125

C 4.250078 -0.227404 -0.826564
 C -0.670075 3.246250 0.731310
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 H -3.422393 2.176171 2.411306
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 H -1.495622 1.865577 3.756098
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 H -0.896270 4.037107 -2.571237
 H 0.573727 4.027277 -1.578677
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 H 2.421127 -4.137050 0.844569
 C 2.885077 -4.268417 -1.257358
 C 3.375418 -3.561868 -2.358210
 H 3.414161 -4.052850 -3.331556
 C 3.806961 -2.239120 -2.256246
 C 3.100164 -1.612899 1.455847
 H 4.014988 -1.077080 1.741662
 H 2.868463 -2.337668 2.243657
 H 2.286708 -0.872245 1.458770
 C 2.456435 -5.696473 -1.385169
 H 3.212478 -6.374634 -0.966012
 H 2.306552 -5.982622 -2.431748
 H 1.525920 -5.890179 -0.838248
 C 4.276993 -1.504321 -3.475554
 H 5.357285 -1.309278 -3.456365
 H 3.784054 -0.527031 -3.573880
 H 4.066782 -2.079437 -4.383317
 C 1.191816 1.428350 -2.073769
 O 1.141466 1.825126 -3.162326

Mg -2.488122 -1.463157 0.531148

S -0.683476 -1.430808 2.467502
 O 0.381039 -0.550238 2.912162
 O -0.538212 -2.058692 1.106410
 O -2.089226 -0.895946 2.510763
 C -0.678678 -2.873785 3.619234
 F 0.496176 -3.492921 3.528498
 F -1.652695 -3.716791 3.281178
 F -0.868525 -2.448868 4.863932
 S -4.386795 -1.512500 -1.294668
 O -4.423859 -0.854555 0.060938
 O -5.479780 -2.399848 -1.642549
 O -2.983545 -2.044374 -1.425787
 C -4.482989 -0.116285 -2.500655
 F -5.677446 0.461595 -2.393096
 F -4.329111 -0.599599 -3.730819
 F -3.533472 0.780998 -2.254002

B0-O2

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 O -0.824983 -1.927212 -3.024652
 O -0.651065 1.929020 -2.924430
 N -3.243091 1.306667 -0.095537
 N -3.238118 -1.313807 -0.120383

C	-1.254285	-1.234787	-2.206428	F	5.244307	0.033095	-2.036267
C	-1.169588	1.248761	-2.147967	F	4.536280	1.094105	-3.797705
C	-3.106238	2.642118	0.092395	S	3.310567	0.006705	2.809256
C	-4.225398	3.444342	0.313387	O	3.072607	-1.184471	1.918542
H	-4.086646	4.512535	0.458405	O	4.496203	0.007278	3.642469
C	-5.486454	2.866628	0.376903	O	3.066235	1.201676	1.925075
H	-6.366736	3.480740	0.550088	C	1.864309	-0.004068	3.954250
C	-5.610036	1.488347	0.261644	F	0.741114	0.049793	3.241588
H	-6.581628	1.014482	0.359361	F	1.926720	1.052083	4.760414
C	-4.467340	0.725899	0.035135	F	1.876629	-1.124105	4.672392
C	-4.466256	-0.743954	0.009708				
C	-5.608181	-1.520249	0.189151	B0-C1			
H	-6.587353	-1.058043	0.264723	Mn	1.666253	0.213367	-0.165458
C	-5.474013	-2.899424	0.281394	O	3.029316	-1.110558	-2.437947
H	-6.352587	-3.524974	0.418573	O	-0.044712	1.125276	-2.411462
C	-4.205796	-3.464427	0.246003	N	0.398757	0.755436	1.409889
H	-4.060591	-4.532704	0.384166	N	2.553159	-0.748744	1.444554
C	-3.089830	-2.649611	0.057119	C	2.559140	-0.625100	-1.494943
C	-1.732966	3.188458	0.153635	C	0.579450	0.805735	-1.488208
C	-1.241551	4.051421	-0.842235	C	-0.600483	1.670965	1.399920
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H	0.491348	5.089158	-1.563213	H	-2.467995	2.302557	2.253141
C	0.929068	4.067151	0.280841	C	-1.711265	0.514079	3.202722
C	0.388916	3.277745	1.300604	H	-2.543335	0.415253	3.896559
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C	-0.934462	2.839572	1.263069	H	-0.629475	-1.171613	3.994087
C	-2.107202	4.508577	-1.977999	C	0.409427	-0.216944	2.359038
H	-2.743027	5.352755	-1.677166	C	1.634074	-1.026297	2.408341
H	-2.781576	3.721754	-2.337863	C	1.883844	-1.960497	3.409731
H	-1.500058	4.846653	-2.824444	H	1.135213	-2.174593	4.165796
C	2.357044	4.514966	0.326350	C	3.115900	-2.599087	3.441667
H	2.960768	3.876658	0.980933	H	3.334022	-3.331003	4.215425
H	2.439445	5.541951	0.708167	C	4.074761	-2.262051	2.497222
H	2.811098	4.512315	-0.671600	H	5.067205	-2.704803	2.519169
C	-1.505170	2.060179	2.410598	C	3.777016	-1.324096	1.507260
H	-0.838017	2.092872	2.376855	C	-0.484627	2.841903	0.502625
H	-1.671864	1.003121	2.163765	C	-1.465107	3.094975	-0.476793
H	-2.480967	2.458395	2.718590	C	-1.321433	4.215404	-1.296962
C	-1.711246	-3.178874	0.148378	H	-2.063366	4.391423	-2.077041
C	-1.189061	-4.051156	-0.823886	C	-0.253868	5.102642	-1.157410
C	0.147239	-4.441263	-0.715921	C	0.683072	4.852425	-0.150017
H	0.569416	-5.082836	-1.490955	H	1.511727	5.547649	-0.006590
C	0.956181	-4.033155	0.348279	C	0.586265	3.746516	0.692893
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H	0.983787	-2.940697	2.209153	H	-3.418978	2.326267	0.053257
C	-0.940114	-2.810057	1.272102	H	-2.326746	1.117655	-0.624374
C	-2.027347	-4.558462	-1.958786	H	-3.075917	2.322942	-1.676409
H	-2.593494	-5.450895	-1.657409	C	-0.123599	6.303564	-2.041371
H	-1.403829	-4.846589	-2.811758	H	-0.316379	7.229862	-1.483463
H	-2.762574	-3.824418	-2.308194	H	-0.830363	6.269391	-2.877501
C	2.385032	-4.471923	0.434344	H	0.889118	6.393504	-2.453134
H	2.862604	-4.483197	-0.552487	C	1.556834	3.604238	1.830691
H	2.463158	-5.492117	0.834909	H	2.001618	2.605761	1.904837
H	2.969746	-3.820281	1.092584	H	1.057023	3.790420	2.792019
C	-1.542586	-2.027110	2.401351	H	2.374623	4.326836	1.737182
H	-2.475322	-2.489541	2.751685	C	4.812951	-0.903078	0.538205
H	-1.804596	-0.999811	2.115403	C	5.268278	-1.806690	-0.438152
H	-0.855638	-1.970467	3.250759	C	6.250672	-1.383176	-1.335321
C	-0.499204	-0.020139	-0.131754	H	6.586512	-2.072903	-2.111058
O	0.537648	-0.020488	0.431549	C	6.799061	-0.100778	-1.277617
Mg	2.648057	0.009191	0.261329	C	6.353404	0.764919	-0.273558
S	2.652790	-0.019379	-2.375910	H	6.785776	1.763977	-0.196625
O	1.763777	-0.053192	-3.519848	C	5.376627	0.386562	0.646186
O	2.644076	-1.204561	-1.445092	C	4.688700	-3.185306	-0.552981
O	2.590705	1.186185	-1.473529	H	5.095961	-3.862805	0.210061
C	4.373502	0.009294	-3.047243	H	4.914113	-3.623864	-1.531015
F	4.577243	-1.079765	-3.781354	H	3.597839	-3.189802	-0.425057

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H 8.690233 0.814564 -1.765880
H 7.425710 1.096060 -2.955050
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Mg -3.335353 -1.413085 0.760536
S -1.231104 -2.551675 -0.397105
O 0.055710 -3.058441 0.045920
O -1.496506 -1.082522 -0.201944
O -2.471504 -3.238058 0.103637
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F -2.389376 -2.293225 -2.732008
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O -5.395037 -1.776838 0.911688
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F -5.503456 1.071356 1.308299

B0-C2

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H -2.893434 0.535428 3.616858
C -0.902346 -0.107980 3.102383
H -0.833570 -0.821256 3.917136
C 0.156433 0.062532 2.212702
C 1.358658 -0.777857 2.246231
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C 2.616526 -2.661599 3.033106
H 2.729827 -3.520333 3.690187
C 3.591042 -2.349706 2.099644
H 4.484068 -2.960151 1.993556
C 3.426842 -1.246057 1.257098
C -1.152649 2.619791 -0.131287
C -1.021541 2.140769 -1.452114
C -1.272481 3.015395 -2.511635
H -1.186442 2.637469 -3.531362
C -1.624816 4.348737 -2.305871
C -1.706548 4.810466 -0.988215
H -1.940318 5.860278 -0.804288
C -1.486259 3.973681 0.102369
C -0.580476 0.742153 -1.758827
H -0.986131 -0.001680 -1.066147
H 0.518849 0.668467 -1.708549
H -0.867109 0.455522 -2.776664
C -1.899240 5.265495 -3.456377
H -2.947624 5.592204 -3.463577
H -1.695186 4.781390 -4.417411

H -1.290889 6.176888 -3.398471
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C 7.551346 -0.498364 -2.729401
H 7.214731 -0.808691 -3.724406
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H 7.869895 0.550360 -2.798216
C 6.078991 -0.321310 2.068723
H 5.345574 0.368664 2.509712
H 7.070044 0.133987 2.166821
H 6.071146 -1.225632 2.691446
C 2.563471 2.214790 1.854929
O 2.924110 2.737915 2.829153
Mg -2.858117 -2.210148 0.995299

S -1.014371 -3.456651 -0.467541
O 0.054493 -4.430092 -0.348696
O -0.846904 -2.148817 0.254385
O -2.418174 -3.901277 -0.151829
C -1.108221 -3.008696 -2.258587
F 0.015840 -2.398423 -2.628863
F -2.140778 -2.195305 -2.468263
F -1.267952 -4.119508 -2.973577
S -4.866607 -1.026875 -0.282609
O -4.954949 -2.219447 0.629049
O -5.537013 -1.102090 -1.566160
O -3.416256 -0.629791 -0.271710
C -5.702991 0.321377 0.660712
F -7.011492 0.088316 0.705627
F -5.476560 1.488531 0.062165
F -5.219841 0.363362 1.904702

B0-C3

Mn 2.890028 -0.545875 0.527292
O 4.845977 0.560172 2.459170
O 1.317210 0.071878 2.959780
N 1.506332 -1.473387 -0.770269
N 4.039338 -0.825315 -1.203268
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C 1.830624 -0.198710 1.953318
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C -0.560527 -2.531274 -1.374954
H -1.617792 -2.665904 -1.160154
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H -0.522971 -3.811362 -3.108506
C 1.387882 -2.911079 -2.697179
H 1.878844 -3.375997 -3.545162
C 2.093642 -2.061117 -1.848176
C 3.495058 -1.700713 -2.089423
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H 3.766865 -2.879912 -3.877677
C 5.506831 -1.719652 -3.393866
H 6.083701 -2.076530 -4.243489
C 6.034442 -0.779937 -2.524282

H	7.023673	-0.359037	-2.683578	N	-4.052037	-1.073278	-1.066995
C	5.279872	-0.334474	-1.434926	C	-4.310378	-0.503802	1.800884
C	-0.507856	-1.012020	0.569300	C	-2.044994	-1.275723	2.223456
C	-0.764380	0.367252	0.477609	C	-0.250947	-2.000192	-0.448850
C	-1.534835	0.975913	1.486824	C	0.459743	-2.920421	-1.217874
H	-1.679551	2.061148	1.457353	H	1.530176	-3.023917	-1.058717
C	-2.008955	0.250618	2.598835	C	-0.206606	-3.674922	-2.173919
C	-1.747465	-1.120878	2.643982	H	0.328977	-4.406481	-2.773740
H	-2.124310	-1.706067	3.482968	C	-1.560186	-3.455230	-2.382171
C	-1.010800	-1.765746	1.649253	H	-2.091226	-4.001332	-3.155127
C	-0.235506	1.180071	-0.661817	C	-2.220741	-2.507387	-1.603631
H	-0.500216	0.743671	-1.633864	C	-3.604523	-2.089056	-1.853713
H	0.862092	1.223520	-0.626272	C	-4.380016	-2.614407	-2.883299
H	-0.609972	2.207607	-0.629677	H	-4.013909	-3.439277	-3.486007
C	-2.754770	0.934383	3.700476	C	-5.622853	-2.053621	-3.142819
H	-3.450820	0.252448	4.199435	H	-6.243761	-2.444042	-3.945353
H	-3.313686	1.805424	3.338726	C	-6.040029	-0.964988	-2.391691
H	-2.052081	1.300147	4.461110	H	-6.981927	-0.464349	-2.600711
C	-0.762109	-3.237155	1.744267	C	-5.237095	-0.483044	-1.356030
H	-1.028252	-3.617013	2.735382	C	0.467089	-1.144356	0.526850
H	0.289420	-3.484446	1.548735	C	1.046577	-1.722185	1.677035
H	-1.359451	-3.791541	1.008361	C	1.751248	-0.909710	2.564549
C	5.820192	0.742706	-0.578687	H	2.182077	-1.357169	3.460355
C	5.171275	1.994635	-0.547785	C	1.892035	0.467504	2.354992
C	5.740217	3.024371	0.203275	C	1.361395	1.010048	1.169095
H	5.245690	3.996573	0.219755	H	1.427533	2.087966	0.996524
C	6.919457	2.844985	0.928198	C	0.648434	0.220013	0.242176
C	7.533510	1.588933	0.891570	C	0.909834	-3.185344	1.955759
H	8.441668	1.421697	1.472765	H	1.561270	-3.774180	1.296739
C	7.010819	0.533990	0.147879	H	-0.114392	-3.541620	1.789779
C	3.889009	2.234061	-1.288352	H	1.192196	-3.416595	2.987576
H	3.922765	1.858964	-2.319205	C	2.590378	1.329327	3.359500
H	3.648478	3.301879	-1.320342	H	2.652448	2.370848	3.030303
H	3.038924	1.728619	-0.803662	H	3.605675	0.967264	3.565679
C	7.505335	3.955480	1.742882	H	2.052567	1.308306	4.315335
H	6.967414	4.897290	1.591162	C	0.194306	0.836195	-1.048055
H	8.561089	4.122553	1.494829	H	0.098945	1.922502	-0.957121
H	7.472114	3.721598	2.815339	H	-0.763504	0.438516	-1.398536
C	7.661184	-0.816370	0.202968	H	0.927803	0.632623	-1.842687
H	6.926478	-1.607328	0.409904	C	-5.647288	0.714399	-0.590030
H	8.420796	-0.849444	0.991020	C	-6.783434	0.657788	0.242769
H	8.157088	-1.086799	-0.738217	C	-7.149559	1.798652	0.953350
C	3.303283	-2.115988	1.202545	H	-8.010940	1.747127	1.621096
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Mg	-3.658473	0.619974	0.427452	C	-5.333091	3.033644	-0.008094
S	-4.579955	-1.851709	0.727947	H	-4.776009	3.964985	-0.120704
O	-4.336789	-3.099504	1.426197	C	-4.931846	1.918772	-0.748001
O	-3.537732	-1.377867	-0.248374	C	-7.560379	-0.613708	0.413561
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F	-5.813744	-3.064657	-1.229551	H	-6.904550	-1.485477	0.536675
F	-6.350711	-0.972710	-0.968959	C	-6.833924	4.194769	1.651278
F	-7.101616	-2.470620	0.418310	H	-7.891208	4.444316	1.496303
S	-5.009279	2.466178	-0.931282	H	-6.235925	5.074509	1.390481
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C	-4.017354	4.001074	-1.183359	H	-3.233389	2.959566	-1.565515
F	-4.666633	5.042169	-0.670479	H	-4.239687	2.142537	-2.768713
F	-3.812232	4.197755	-2.482675	C	-2.408956	0.719601	0.768904
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				S	4.827470	2.674495	-0.664700
B0-C4				O	6.181675	3.172201	-0.803628
Mn	-2.946872	-0.957693	0.686982	O	4.286807	2.465323	0.722523
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O 3.522198 -1.454372 -0.348464
O 4.338613 -2.983108 1.496681
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F 5.844304 -3.292138 -1.064592
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B0-Z1

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C 1.237371 4.600869 -1.509125
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H 0.417439 4.185138 -2.111583
H 2.169884 4.355999 -2.034297
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C -2.725029 -1.638201 1.481494
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H -2.061685 -0.776713 1.300964

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F -0.005206 -2.268007 2.743007
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F 5.752600 1.449337 0.027038
F 5.202133 0.538738 -1.867512

B0-Z2

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H -0.490223 2.954008 1.242984
C 2.405545 2.712976 -2.786723
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C	1.348040	-2.021007	-1.451666
H	0.348328	-2.445387	-1.621150
H	1.787090	-2.587904	-0.620724
H	1.948307	-2.211745	-2.347075
C	-6.109297	0.165870	0.317889
C	-5.708637	1.515037	0.414705
C	-6.399466	2.473383	-0.329385
H	-6.097749	3.518529	-0.246963
C	-7.459310	2.133358	-1.170761
C	-7.821097	0.785442	-1.265393
H	-8.626059	0.495360	-1.942461
C	-7.171776	-0.205441	-0.533940
C	-4.552491	1.940691	1.270716
H	-4.531750	1.432990	2.242702
H	-4.575651	3.021057	1.449478
H	-3.589576	1.722318	0.781666
C	-8.186487	3.175448	-1.961425
H	-9.243739	3.232102	-1.670813
H	-8.172109	2.946288	-3.034646
H	-7.747453	4.169070	-1.822138
C	-7.544198	-1.644893	-0.732889
H	-6.655355	-2.270906	-0.895113
H	-8.198428	-1.758434	-1.603639
H	-8.074927	-2.069518	0.128957
C	-2.960095	-2.088197	-1.250014
O	-3.010396	-3.159004	-1.699525
Mg	3.885282	0.203998	-0.484710
S	4.361377	1.862249	1.516960
O	4.999745	1.826444	2.818625
O	3.149950	0.993109	1.311203
O	5.221786	1.636747	0.303410
C	3.711701	3.585305	1.310000
F	4.625505	4.457962	1.724460
F	2.599737	3.724173	2.030096
F	3.436981	3.816705	0.026674
S	5.246299	-2.058641	-0.837557
O	4.796731	-1.060156	-1.875075
O	5.004685	-3.461458	-1.115445
O	4.769276	-1.502612	0.472435
C	7.079299	-1.851344	-0.784158
F	7.602424	-2.261853	-1.936674
F	7.574187	-2.577379	0.214929
F	7.382757	-0.568357	-0.592052
B1-Mn			
Mn	-1.178190	-0.030584	-0.097360
O	-0.678971	-1.777972	2.234057
O	-0.890935	1.964261	2.066222
N	-1.007896	1.204638	-1.810052
N	-0.933852	-1.432084	-1.666292
C	-0.833118	-1.148951	1.256979
C	-0.964747	1.242201	1.147375
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H	-0.909108	4.362072	-2.977001
C	-0.083596	2.654873	-4.013321
H	0.292191	3.222134	-4.861443
C	0.049612	1.276106	-3.975036
H	0.523612	0.754301	-4.799150
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C	0.128151	-1.677528	-3.816491
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C	0.070912	-3.057524	-3.706854
H	0.478028	-3.691089	-4.491165
C	-0.548453	-3.609754	-2.595165
H	-0.663096	-4.685973	-2.490749
C	-1.057746	-2.780520	-1.594677
C	-1.982136	3.230066	-0.824051
C	-1.343420	4.140700	0.035860
C	-2.108772	4.819457	0.984402
H	-1.610258	5.510689	1.665975
C	-3.485084	4.616654	1.102288
C	-4.098893	3.720239	0.222130
H	-5.177725	3.566187	0.282247
C	-3.376044	3.031613	-0.752804
C	0.142146	4.341764	-0.017620
H	0.510366	4.797241	0.908287
H	0.442003	4.998025	-0.846399
H	0.678127	3.393347	-0.161502
C	-4.279871	5.322900	2.157018
H	-5.310693	5.507707	1.833315
H	-3.827504	6.282924	2.430650
H	-4.338465	4.724132	3.076612
C	-4.094593	2.169539	-1.749314
H	-5.132241	1.996255	-1.444845
H	-3.618454	1.191887	-1.891639
H	-4.116371	2.650987	-2.737648
C	-1.804439	-3.391996	-0.470002
C	-1.126947	-4.171175	0.485818
C	-1.864484	-4.781025	1.500006
H	-1.336681	-5.367643	2.253818
C	-3.251410	-4.639312	1.590853
C	-3.902604	-3.881007	0.614504
H	-4.988598	-3.779342	0.652299
C	-3.207006	-3.264820	-0.427456
C	0.367266	-4.299784	0.459624
H	0.738100	-4.749008	1.387300
H	0.858347	-3.323103	0.343630
H	0.717047	-4.926281	-0.372099
C	-4.015450	-5.267811	2.715239
H	-3.584261	-6.231802	3.009673
H	-5.067161	-5.427453	2.451941
H	-4.001760	-4.629533	3.609649
C	-3.962830	-2.559554	-1.515545
H	-3.529011	-1.587305	-1.778317
H	-5.006350	-2.394577	-1.226926
H	-3.966180	-3.157695	-2.438257
C	-2.935641	-0.086342	0.315796
O	-4.027520	-0.107045	0.728836
Mg	1.656689	0.055394	0.356154
S	3.048826	-0.096631	-1.915053
O	2.996386	-0.178596	-3.363046
O	2.512089	-1.250454	-1.118317
O	2.507040	1.141895	-1.257156
C	4.835982	-0.061712	-1.460742
F	5.430771	-1.179293	-1.868464
F	4.941213	0.033478	-0.129513
F	5.427413	0.988446	-2.023271
S	2.992230	0.320045	2.641426
O	2.412012	1.420156	1.798208
O	4.373636	0.450143	3.068282
O	2.590443	-0.957147	1.955889
C	1.991120	0.347544	4.191193
F	2.207660	1.495278	4.832359
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F	0.696989	0.240283	3.903645
B1-O1			
Mn	1.410245	0.804130	-0.627015
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N	1.762869	2.592518	0.399516	C	-0.823595	-2.775727	3.703461
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C	1.081045	-0.817088	-1.322883	F	-1.895566	-3.485168	3.349961
C	-0.307286	0.671092	-0.420253	F	-0.993244	-2.304099	4.935997
C	0.851995	3.554274	0.713080	S	-4.551444	-1.525287	-0.854759
C	1.234142	4.755742	1.306534	O	-4.392416	-0.657211	0.364207
H	0.465285	5.489307	1.537681	O	-5.697973	-2.412410	-0.908900
C	2.570508	5.000122	1.594590	O	-3.191309	-2.125299	-1.089957
H	2.882499	5.933944	2.055949	C	-4.778737	-0.328017	-2.243335
C	3.498540	4.022794	1.282459	F	-5.944770	0.297284	-2.089534
H	4.548573	4.184419	1.501823	F	-4.779550	-0.992279	-3.397255
C	3.074977	2.831636	0.688900	F	-3.794773	0.567365	-2.247515
C	4.009712	1.761540	0.348833				
C	5.383484	1.883341	0.566012	B1-O2			
H	5.796123	2.795213	0.984077	Mn	1.952122	0.115102	-0.885998
C	6.223517	0.831913	0.243376	O	1.191023	2.425754	-2.574133
H	7.296099	0.910191	0.403704	O	0.750555	-1.227158	-3.234464
C	5.660445	-0.326588	-0.275404	N	3.235052	-1.424568	-0.303264
H	6.275290	-1.188633	-0.523361	N	3.412113	1.123819	0.222305
C	4.283631	-0.407867	-0.476427	C	1.504493	1.554063	-1.861165
C	-0.595308	3.348095	0.445139	C	1.243428	-0.762227	-2.281685
C	-1.421406	2.873345	1.483799	C	3.009028	-2.761927	-0.376502
C	-2.787505	2.734053	1.244158	C	4.061037	-3.672909	-0.312910
H	-3.426893	2.352425	2.043133	H	3.842480	-4.735694	-0.385964
C	-3.357220	3.069145	0.010699	C	5.363253	-3.216796	-0.135765
C	-2.519735	3.561951	-0.990748	H	6.195481	-3.915608	-0.096480
H	-2.948237	3.838773	-1.956018	C	5.578748	-1.858393	0.039736
C	-1.146567	3.727513	-0.790565	H	6.578722	-1.482838	0.234420
C	-0.836896	2.518848	2.817127	C	4.494083	-0.983438	-0.027502
H	-0.395891	3.396153	3.310773	C	4.591021	0.444033	0.280044
H	-0.035326	1.774182	2.724435	C	5.773318	1.059013	0.693445
H	-1.596795	2.104572	3.487086	H	6.705735	0.503221	0.713156
C	-4.832168	2.933179	-0.214020	C	5.740290	2.385207	1.095849
H	-5.087406	2.989446	-1.278022	H	6.650559	2.886035	1.416779
H	-5.385363	3.733000	0.297714	C	4.517844	3.048194	1.123911
H	-5.216890	1.984883	0.179363	H	4.440787	4.069657	1.488905
C	-0.303654	4.359454	-1.857569	C	3.363464	2.396468	0.695619
H	-0.688361	4.136453	-2.858972	C	1.601096	-3.222985	-0.437942
H	0.742675	4.037887	-1.816604	C	1.085142	-3.836289	-1.592742
H	-0.301311	5.454107	-1.750822	C	-0.263290	-4.200488	-1.612040
C	3.739717	-1.692706	-0.983713	H	-0.672043	-4.650613	-2.518444
C	3.215569	-2.627925	-0.070613	C	-1.100469	-3.999232	-0.512104
C	2.794952	-3.867978	-0.549112	C	-0.544169	-3.451225	0.647897
H	2.381610	-4.591153	0.156509	H	-1.169320	-3.320400	1.533350
C	2.885417	-4.204464	-1.902380	C	0.794714	-3.066536	0.709070
C	3.422147	-3.263143	-2.783797	C	1.947631	-4.091461	-2.792761
H	3.500333	-3.508014	-3.844524	H	2.540620	-5.008995	-2.671867
C	3.856477	-2.010708	-2.348359	H	2.659085	-3.277699	-2.976415
C	3.098864	-2.289540	1.383755	H	1.339022	-4.216282	-3.694933
H	4.079077	-2.079905	1.835023	C	-2.554144	-4.354741	-0.577340
H	2.637430	-3.107963	1.947758	H	-3.140496	-3.543339	-1.031031
H	2.483289	-1.393423	1.539571	H	-2.974023	-4.532465	0.419033
C	2.387560	-5.526535	-2.399460	H	-2.726219	-5.248246	-1.189149
H	2.510717	-6.316177	-1.649070	C	1.358542	-2.531322	1.991452
H	2.903918	-5.837878	-3.314745	H	0.652081	-2.666178	2.817058
H	1.315467	-5.480311	-2.637562	H	1.590450	-1.459095	1.924543
C	4.413013	-1.015741	-3.322328	H	2.296680	-3.033323	2.263833
H	5.484040	-0.833076	-3.158494	C	2.034826	3.047416	0.801260
H	3.914910	-0.040080	-3.234184	C	1.684540	4.116364	-0.042302
H	4.292542	-1.362050	-4.354403	C	0.390086	4.635570	0.036668
C	1.384945	1.474754	-2.295512	H	0.104730	5.438208	-0.645669
O	1.293122	1.807755	-3.413210	C	-0.549167	4.145529	0.947053
Mg	-2.367260	-1.162694	0.578270	C	-0.150008	3.133025	1.824064
S	-0.589004	-1.372964	2.528604	H	-0.857032	2.754917	2.565666
O	0.586986	-0.660714	2.996386	C	1.130046	2.581751	1.777210
O	-0.525800	-2.038979	1.183305	C	2.661108	4.687095	-1.026925
O	-1.902599	-0.638699	2.552164	H	3.343807	5.400315	-0.543751

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H 3.287593 3.916352 -1.490856
C -1.936286 4.708460 1.003344
H -2.319755 4.937512 0.001930
H -1.966412 5.645275 1.576988
H -2.634120 4.012483 1.484016
C 1.533060 1.535429 2.772402
H 2.421957 1.843736 3.339981
H 1.790362 0.582006 2.291731
H 0.728692 1.343212 3.489506
C 0.478660 0.052598 0.035126
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Mg -2.580500 0.115409 0.215658
S -2.602516 0.791663 -2.329570
O -1.715277 1.100160 -3.432097
O -2.597177 1.711921 -1.136761
O -2.567632 -0.599516 -1.758549
C -4.320062 0.948247 -2.985930
F -4.533491 2.198875 -3.387714
F -5.194132 0.638605 -2.024331
F -4.483007 0.117039 -4.012006
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O -3.293520 0.790552 2.070089
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F -1.130787 -0.686636 3.332151
F -2.384916 -2.289143 4.089920
F -2.578276 -0.278747 4.900289

B1-C1

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O 3.122869 -1.075035 -2.438765
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H -2.732229 2.038302 1.702307
C -2.045325 0.204225 2.632307
H -2.957947 0.036008 3.206072
C -0.937538 -0.618316 2.812314
H -0.986959 -1.453090 3.504984
C 0.226764 -0.363481 2.085212
C 1.440759 -1.153300 2.227698
C 1.595537 -2.139586 3.204215
H 0.777408 -2.383061 3.875447
C 2.808903 -2.795500 3.318479
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H 4.834676 -2.873832 2.561123
C 3.651070 -1.429738 1.515902
C -0.539786 2.807664 0.357136
C -1.385972 3.142600 -0.717037
C -1.178635 4.352799 -1.385359
H -1.817872 4.597412 -2.235217
C -0.180778 5.248424 -1.004219
C 0.614594 4.915445 0.097861
H 1.378884 5.617001 0.437160
C 0.452256 3.718548 0.791780
C -2.483892 2.231194 -1.179940
H -3.385923 2.322649 -0.557737
H -2.183795 1.178307 -1.157729
H -2.780678 2.471891 -2.207021
C 0.029236 6.537685 -1.736259

H -0.066199 7.401167 -1.064977
H -0.693281 6.663320 -2.549933
H 1.035975 6.593314 -2.170817
C 1.278327 3.459372 2.017654
H 1.927357 2.581249 1.909574
H 0.644685 3.268515 2.895002
H 1.915957 4.320400 2.245505
C 4.791466 -0.983137 0.679661
C 5.309981 -1.824851 -0.317987
C 6.401201 -1.382080 -1.071245
H 6.789780 -2.025911 -1.862126
C 6.997940 -0.141621 -0.846089
C 6.484761 0.661547 0.178654
H 6.949819 1.627159 0.386011
C 5.397651 0.261133 0.952699
C 4.706496 -3.170469 -0.591643
H 5.048358 -3.922442 0.133400
H 4.985511 -3.530548 -1.588003
H 3.610890 -3.153325 -0.534634
C 8.160139 0.322571 -1.669362
H 8.490513 -0.448496 -2.373918
H 9.017484 0.593441 -1.039635
H 7.907662 1.218923 -2.251306
C 4.927478 1.119206 2.089655
H 3.844142 1.292438 2.060899
H 5.424129 2.095510 2.078852
H 5.142884 0.646290 3.058508
C 2.868377 1.777752 -0.348314
O 3.547414 2.716370 -0.532836
Mg -3.191903 -1.249581 0.659959

S -1.187157 -2.448083 -0.585063
O 0.124187 -2.942380 -0.207065
O -1.453550 -0.977103 -0.433481
O -2.391063 -3.119048 0.020408
C -1.322168 -2.704738 -2.404927
F -0.345376 -2.019508 -2.999021
F -2.501049 -2.264048 -2.838260
F -1.197244 -3.998204 -2.687963
S -5.717676 -0.982478 -0.063694
O -5.194995 -1.683528 1.162799
O -6.809079 -1.602542 -0.786894
O -4.491723 -0.577373 -0.835474
C -6.351574 0.622808 0.593729
F -7.416649 0.407124 1.358690
F -6.677219 1.423284 -0.416498
F -5.392991 1.203963 1.324232

B1-C2

Mn 1.763471 0.481417 -0.316313
O 3.180856 -0.912089 -2.498951
O 0.563958 1.619329 -2.758370
N 0.211091 0.854505 0.991172
N 2.143522 -0.876611 1.211805
C 2.664286 -0.405387 -1.576778
C 0.985567 1.214150 -1.742768
C -0.675491 1.895460 0.968393
C -1.879891 1.842693 1.660995
H -2.561968 2.686681 1.600650
C -2.189773 0.722622 2.445175
H -3.121076 0.674734 3.007211
C -1.239065 -0.289404 2.558178
H -1.421487 -1.133623 3.218241
C -0.035046 -0.188200 1.847395
C 1.045378 -1.148967 1.976751
C 0.993693 -2.245398 2.841843
H 0.094897 -2.451876 3.415709
C 2.100654 -3.066346 2.958310

H	2.082331	-3.931025	3.617204	O	-1.381007	0.325898	-2.802233
C	3.251213	-2.737190	2.244938	N	-1.526112	-1.378724	0.876011
H	4.161753	-3.322500	2.350206	N	-4.041534	-0.738461	1.247123
C	3.258173	-1.634760	1.395455	C	-4.235936	-0.226290	-1.653571
C	-0.317561	3.122737	0.223142	C	-1.905586	-0.102101	-1.841315
C	-1.057507	3.504259	-0.909157	C	-0.200950	-1.598848	0.676867
C	-0.705180	4.681168	-1.575224	C	0.565045	-2.351387	1.562001
H	-1.261369	4.964585	-2.470164	H	1.622650	-2.490888	1.350441
C	0.342044	5.491471	-1.137129	C	-0.023673	-2.891538	2.701391
C	1.039239	5.105770	0.013651	H	0.557488	-3.487726	3.400641
H	1.847039	5.737860	0.386868	C	-1.361239	-2.629893	2.938221
C	0.725611	3.940877	0.709838	H	-1.840781	-3.017372	3.831492
C	-2.183862	2.660027	-1.428823	C	-2.088554	-1.864306	2.023194
H	-3.111244	2.816331	-0.859208	C	-3.481774	-1.496410	2.237198
H	-1.954489	1.588026	-1.377131	C	-4.185261	-1.847046	3.390851
H	-2.403858	2.902677	-2.474257	H	-3.721791	-2.467392	4.151589
C	0.710041	6.746996	-1.865784	C	-5.478251	-1.383553	3.566228
H	0.636707	7.626378	-1.212583	H	-6.043926	-1.642690	4.457972
H	0.061075	6.917281	-2.731606	C	-6.017264	-0.542475	2.598801
H	1.746841	6.713717	-2.225190	H	-7.002249	-0.100686	2.729288
C	1.443206	3.616945	1.987195	C	-5.283411	-0.221298	1.458143
H	2.272701	4.311733	2.157404	C	0.488042	-0.967042	-0.476952
H	1.852016	2.598747	1.994999	C	0.775625	0.408035	-0.426201
H	0.765655	3.688785	2.849907	C	1.530249	0.979103	-1.469630
C	4.514633	-1.239337	0.715118	H	1.689981	2.063096	-1.472535
C	5.057421	-2.048021	-0.297400	C	1.964357	0.218206	-2.574264
C	6.249749	-1.650678	-0.909154	C	1.680128	-1.148873	-2.575814
H	6.657303	-2.264380	-1.714312	H	2.032566	-1.763808	-3.404451
C	6.923152	-0.490249	-0.528336	C	0.955562	-1.754401	-1.546340
C	6.381770	0.276340	0.509955	C	0.297035	1.257634	0.709365
H	6.904042	1.176747	0.838830	H	0.595364	0.843928	1.681852
C	5.194802	-0.079859	1.146769	H	-0.801164	1.310648	0.715169
C	4.372819	-3.305891	-0.743315	H	0.680862	2.279392	0.636828
H	4.573335	-4.141387	-0.058035	C	2.693407	0.862493	-3.711063
H	4.721935	-3.610771	-1.736039	H	3.360030	0.155561	-4.215675
H	3.283041	-3.191666	-0.790370	H	3.282598	1.727470	-3.384021
C	8.199383	-0.077579	-1.195016	H	1.978456	1.230173	-4.459469
H	8.457887	-0.746706	-2.022909	C	0.710674	-3.229554	-1.577586
H	9.040413	-0.080731	-0.488773	H	0.902311	-3.640664	-2.573977
H	8.133968	0.942812	-1.594098	H	-0.317366	-3.480954	-1.289468
C	4.694728	0.728924	2.307467	H	1.373309	-3.752690	-0.874558
H	3.646001	1.029597	2.189327	C	-5.845824	0.773038	0.514229
H	5.290798	1.638540	2.439078	C	-5.206355	2.022099	0.350821
H	4.751244	0.154848	3.243325	C	-5.804657	2.982488	-0.463820
C	2.978143	1.785814	-0.229377	H	-5.312625	3.949872	-0.580706
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Mg	-2.885079	-1.003503	0.481761	C	-7.618442	1.499310	-0.957122
S	-1.111820	-2.678756	-0.547785	H	-8.549400	1.283709	-1.484317
O	0.261187	-3.131135	-0.440566	C	-7.059715	0.508568	-0.147617
O	-1.361905	-1.250541	-0.946379	C	-3.900885	2.331617	1.019019
O	-2.032723	-2.919606	0.622435	H	-3.879071	2.010277	2.068394
C	-1.878787	-3.650722	-1.917085	H	-3.686526	3.405403	0.984879
F	-1.234315	-3.401846	-3.053457	H	-3.070841	1.807780	0.517685
F	-3.157680	-3.290558	-2.043554	C	-7.639038	3.803601	-1.980201
F	-1.808972	-4.948273	-1.636781	H	-6.930170	4.194748	-2.721063
S	-5.471809	-0.692873	0.024356	H	-7.966547	4.663479	-1.380288
O	-4.825161	-1.240103	1.270359	H	-8.514412	3.423442	-2.518096
O	-6.613674	-1.402610	-0.515841	C	-7.721455	-0.835459	-0.059912
O	-4.324291	-0.389178	-0.901629	H	-6.995045	-1.652253	-0.168914
C	-6.084730	0.972347	0.533900	H	-8.474864	-0.949080	-0.847143
F	-7.036963	0.832350	1.450953	H	-8.230843	-0.995084	0.899662
F	-6.570872	1.609111	-0.526815	C	-3.086474	-2.389292	-1.191205
F	-5.074983	1.677801	1.048520	O	-3.172806	-3.453524	-1.679789
				Mg	3.647452	0.594162	-0.454415
B1-C3				S	4.580859	-1.873608	-0.751277
Mn	-2.948342	-0.741818	-0.533802	O	4.325346	-3.127578	-1.434232
O	-4.982945	0.018628	-2.524658	O	3.563316	-1.395754	0.248100

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C 6.094234 -2.125138 0.271907
F 5.875157 -3.081326 1.170982
F 6.388519 -0.984306 0.902647
F 7.113989 -2.471956 -0.508620
S 5.044851 2.456337 0.852965
O 4.976292 2.251751 -0.633228
O 6.347690 2.681182 1.449339
O 4.182124 1.376739 1.444439
C 4.073061 4.000331 1.125490
F 4.718749 5.034466 0.593320
F 3.906035 4.201614 2.429912
F 2.877508 3.880297 0.540604

B1-C4

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H -6.820360 -0.824831 -2.688588
C -5.132016 -0.657302 -1.383675
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H 1.476442 2.169922 0.833762
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H -0.740213 0.402267 -1.233012
H 0.884893 -0.003141 -1.769675
C -5.587225 0.640453 -0.829124
C -6.731107 0.697571 -0.015703
C -7.148225 1.938239 0.473962
H -8.022325 1.979122 1.126128
C -6.470022 3.117574 0.167538
C -5.352952 3.037255 -0.671933
H -4.820129 3.950835 -0.942485
C -4.903242 1.822302 -1.185557
C -7.485284 -0.544427 0.356424

H -8.145645 -0.879554 -0.455542
H -8.115114 -0.371187 1.235998
H -6.814541 -1.382615 0.582811
C -6.920915 4.437081 0.714669
H -7.845365 4.339655 1.294382
H -7.100341 5.165959 -0.086263
H -6.160948 4.879828 1.372156
C -3.753428 1.795588 -2.148943
H -2.990354 1.058226 -1.870311
H -3.267522 2.775517 -2.209495
H -4.091729 1.529443 -3.160620
C -2.356920 1.012214 0.698134
O -2.028161 2.137227 0.763569
Mg 3.464965 0.510180 0.196723
S 4.928408 2.547886 -0.642234
O 6.315277 2.910523 -0.860111
O 4.481274 2.276671 0.767090
O 4.361052 1.417860 -1.459586
C 3.924063 4.008750 -1.155325
F 4.163936 4.286997 -2.433715
F 4.244832 5.056179 -0.400980
F 2.626182 3.734449 -1.000827
S 4.335738 -1.989172 0.298576
O 3.363774 -1.415833 -0.694008
O 3.989753 -3.251743 0.925975
O 4.714545 -0.839752 1.194031
C 5.862456 -2.303533 -0.689155
F 5.598535 -3.208493 -1.628488
F 6.821847 -2.758197 0.112901
F 6.264931 -1.171610 -1.264325

B1-Z1

Mn 1.647535 0.677260 -0.131338
O 2.583952 -0.747833 -2.537458
O 0.235125 1.834460 -2.440460
N 0.313943 1.097812 1.427805
N 2.301059 -0.621813 1.364522
C 2.269828 -0.251373 -1.520149
C 0.723001 1.423656 -1.454068
C -0.645738 2.062683 1.461983
C -1.669630 2.045941 2.406948
H -2.414254 2.838543 2.384623
C -1.717567 1.040724 3.370292
H -2.511794 1.013519 4.112885
C -0.704280 0.095948 3.382288
H -0.696148 -0.680157 4.141534
C 0.305396 0.152323 2.416067
C 1.423890 -0.779593 2.399018
C 1.609306 -1.746887 3.390394
H 0.891907 -1.849270 4.198386
C 2.715715 -2.574139 3.339012
H 2.872579 -3.339871 4.094981
C 3.638552 -2.379271 2.315313
H 4.546583 -2.975216 2.256467
C 3.423940 -1.392080 1.358416
C -0.578477 3.201736 0.515170
C -1.557215 3.358123 -0.482328
C -1.500770 4.482075 -1.310671
H -2.253992 4.597481 -2.091767
C -0.500621 5.445128 -1.181202
C 0.452628 5.274114 -0.170917
H 1.227933 6.030117 -0.033170
C 0.422254 4.181407 0.693658
C -2.597227 2.307043 -0.736263
H -3.052246 1.924167 0.187266
H -2.156031 1.444965 -1.258927
H -3.405865 2.686184 -1.370922

C -0.446819 6.638643 -2.084435
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 H -1.289687 6.655382 -2.783880
 H 0.478243 6.652491 -2.675762
 C 1.391929 4.104377 1.836267
 H 2.166777 4.873372 1.746646
 H 1.890527 3.129858 1.902416
 H 0.879923 4.260194 2.796760
 C 4.481360 -1.138627 0.348107
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 C 6.548261 -0.679697 -1.501016
 C 6.356336 0.176722 -0.410987
 H 7.020220 1.033490 -0.280566
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 H 3.889862 -3.648470 -1.902496
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 O -2.241350 -2.980182 0.639405
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 F -2.008203 -2.733772 -2.350054
 F -1.041138 -4.569083 -1.703591
 S -5.282372 -1.349358 -0.221640
 O -4.853279 -1.355616 1.221186
 O -6.066920 -2.473506 -0.695395
 O -4.054910 -0.968572 -1.000301
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B1-Z2

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 N -3.996674 0.866894 -1.179862
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 C -1.768826 -2.191741 -0.812133
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 H 1.779714 1.105084 -2.459292
 C 0.071078 2.052259 -3.394972
 H 0.651930 2.602053 -4.131095
 C -1.303503 2.203653 -3.324387
 H -1.812578 2.886293 -3.997982
 C -2.029965 1.473807 -2.380563
 C -3.462439 1.646030 -2.165764
 C -4.223705 2.588249 -2.859395
 H -3.773765 3.183378 -3.648241

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 H -7.099019 2.182270 -1.123333
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 C 1.276693 -1.485683 -0.820382
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 H 2.383887 -3.152756 -0.022546
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 C 1.116872 -0.620411 1.846494
 H 1.084352 -0.261584 2.874665
 C 0.521817 0.155296 0.842416
 C 1.382339 -1.966207 -2.234267
 H 2.190458 -1.453448 -2.771953
 H 0.456847 -1.781780 -2.790652
 H 1.594638 -3.038947 -2.264872
 C 2.389504 -2.645549 2.652203
 H 2.900631 -2.008471 3.383456
 H 3.109493 -3.367520 2.254269
 H 1.617165 -3.203601 3.197035
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 C -6.858701 -0.897951 2.661157
 C -5.876465 0.091197 2.783925
 H -5.512057 0.363164 3.776358
 C -5.353256 0.751659 1.674029
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 H -8.079333 -0.200481 -1.483020
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 H -6.563174 -1.012634 -1.862495
 C -7.392066 -1.597677 3.873524
 H -8.189378 -2.303255 3.615611
 H -7.796304 -0.885487 4.604612
 H -6.603989 -2.159864 4.391766
 C -4.366753 1.866405 1.862293
 H -3.500630 1.777516 1.194891
 H -3.995534 1.895094 2.892516
 H -4.828689 2.841091 1.648783
 C -2.529623 -0.694698 1.147618
 O -2.370457 -0.799927 2.305560
 Mg 3.197873 0.007871 0.475965

S 5.453016 -1.163860 -0.318308
 O 6.851027 -0.795080 -0.445017
 O 4.457298 -0.413813 -1.162247
 O 4.861393 -1.171592 1.062379
 C 5.345909 -2.943106 -0.902437
 F 6.448775 -3.255642 -1.574249
 F 4.291746 -3.103677 -1.701085
 F 5.226197 -3.751123 0.148808
 S 3.389933 2.545504 1.285765
 O 3.547846 1.320579 2.136727
 O 2.662520 3.675189 1.832447
 O 2.983867 2.040628 -0.072125
 C 5.125848 3.109380 1.026018
 F 5.661182 3.468637 2.189570
 F 5.151905 4.140268 0.185625
 F 5.833230 2.099202 0.507793

B2-Mn

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O -1.532812 -1.649490 2.054562
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 N -1.105527 -0.934174 -1.780880
 C -1.401974 -0.950650 1.113394
 C -0.718003 1.247777 1.284359
 C -0.326362 2.956205 -1.496613
 C 0.314187 3.682581 -2.492379
 H 0.447969 4.752873 -2.348150
 C 0.741991 3.057355 -3.663016
 H 1.241559 3.617798 -4.449675
 C 0.479837 1.711081 -3.805580
 H 0.768184 1.193663 -4.714538
 C -0.152327 1.008551 -2.771799
 C -0.464905 -0.399877 -2.872944
 C -0.134095 -1.164221 -3.998979
 H 0.401231 -0.707367 -4.824724
 C -0.478264 -2.498996 -4.051508
 H -0.215978 -3.112819 -4.909821
 C -1.214358 -3.021671 -2.988131
 H -1.572020 -4.049235 -3.007522
 C -1.540369 -2.229580 -1.895417
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 H -1.715802 6.855477 3.240691
 H -2.697893 5.478441 3.731037
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 H -4.191800 3.820190 -1.199704
 H -3.004542 2.631739 -1.768041
 H -2.936922 4.292656 -2.353784
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 H -5.732087 -2.769865 0.021098
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 H -0.276720 -4.676310 0.974935
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 H -6.200647 -4.699491 1.527669
 H -5.222606 -4.050795 2.841329
 C -4.354545 -1.500023 -1.916112
 H -3.736161 -0.599836 -2.019834
 H -5.373057 -1.183084 -1.665798
 H -4.392158 -1.973895 -2.907936
 C -2.979626 0.769508 0.063675
 O -4.073718 1.025679 0.422696
 Mg 1.232209 -0.409837 0.296802
 S 2.927141 -0.453342 -1.840732
 O 2.958756 -0.407896 -3.294440

O 2.198392 -1.599360 -1.198863
 O 2.521496 0.776900 -1.098549
 C 4.680529 -0.734103 -1.343705
 F 5.106605 -1.900162 -1.833564
 F 4.785355 -0.758308 -0.013355
 F 5.447749 0.246695 -1.822653
 S 2.592429 -1.097099 2.538513
 O 2.503166 0.253065 1.889999
 O 3.917445 -1.583917 2.892627
 O 1.705055 -2.003281 1.747687
 C 1.729975 -0.883949 4.154702
 F 0.467617 -0.510323 3.972964
 F 2.363788 0.046409 4.874218
 F 1.751200 -2.039798 4.824507

B2-O1

Mn 1.708269 0.782600 -0.659135
 O 0.737036 -1.721248 -1.859757
 O -1.207671 0.574299 -0.715804
 N 2.098634 2.449127 0.492383
 N 3.584375 0.343209 0.089582
 C 1.253558 -0.798707 -1.338422
 C -0.007204 0.763179 -0.560018
 C 1.258088 3.503838 0.744366
 C 1.690573 4.659489 1.373040
 H 0.973190 5.460774 1.539494
 C 3.016828 4.778213 1.806804
 H 3.367232 5.682101 2.299650
 C 3.856992 3.704300 1.613845
 H 4.883822 3.750446 1.964397
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 C 4.208441 1.386917 0.749624
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 H 7.308454 0.091624 1.312620
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 H -4.925538 4.152336 0.140746
 H -4.903675 2.397698 -0.004718
 C 0.238176 4.464499 -1.844184
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 C 2.816858 -4.324135 -2.021043
 C 3.508328 -3.351660 -2.746140
 H 3.684677 -3.504798 -3.812742
 C 3.980734 -2.183529 -2.145187

C 2.803573 -2.732446 1.440500
 H 3.734566 -2.738794 2.024938
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 H 2.325482 -1.759881 1.620372
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 H 2.313731 -6.425924 -2.029812
 H 2.846333 -5.795369 -3.602546
 H 1.234997 -5.419499 -2.991554
 C 4.723695 -1.159664 -2.951267
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 H 4.645652 -1.365957 -4.024577
 H 5.792949 -1.134489 -2.698081
 C 1.972948 1.461721 -2.271429
 O 1.984091 1.825234 -3.396257
 Mg -2.342415 -0.632251 0.347219
 S -1.057059 -1.493500 2.495466
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 O -0.901836 -2.015549 1.097554
 O -2.050244 -0.367392 2.399706
 C -2.005798 -2.829408 3.340771
 F -1.288255 -3.951301 3.350695
 F -3.147358 -3.043507 2.678704
 F -2.285518 -2.469832 4.591495
 S -4.643310 -1.107868 -0.877157
 O -4.388804 -0.157370 0.260492
 O -5.826963 -1.943831 -0.808157
 O -3.323261 -1.774538 -1.140565
 C -4.888318 0.005139 -2.329813
 F -5.989060 0.732963 -2.147650
 F -5.017944 -0.727218 -3.433737
 F -3.839126 0.818088 -2.458963

B2-O2

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 O -1.150210 2.203998 -2.837320
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 N -3.391553 -1.239034 -0.317786
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 H -4.051075 4.368261 1.330965
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 H -6.598975 0.922465 1.035428
 C -4.562524 0.703479 0.352929
 C -4.593647 -0.712529 0.102545
 C -5.723108 -1.520072 0.305415
 H -6.665433 -1.065667 0.600725
 C -5.631926 -2.886240 0.135771
 H -6.500678 -3.525728 0.273494
 C -4.370450 -3.434562 -0.142682
 H -4.225296 -4.512757 -0.176773
 C -3.274613 -2.609170 -0.322254
 C -1.826262 3.203225 0.455359
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 C -0.211368 4.687795 -0.556733
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 H 0.866981 -3.409734 1.579761
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 C -2.329249 -4.120106 -2.697887
 H -2.974918 -4.995695 -2.538123
 H -1.741399 -4.313091 -3.602142
 H -2.992055 -3.271274 -2.901471
 C 2.160905 -4.621863 -0.491543
 H 2.547224 -4.646657 -1.517222
 H 2.255068 -5.640864 -0.089707
 H 2.823649 -3.984825 0.106616
 C -1.598542 -2.439452 2.021519
 H -2.615886 -2.778859 2.257625
 H -1.645044 -1.342399 1.944730
 H -0.953780 -2.686177 2.871520
 C -0.537369 0.009104 0.010893
 O 0.574374 -0.069582 0.497624
 Mg 2.514598 0.002576 0.296576

S 2.938791 0.359507 -2.282014
 O 2.227541 0.519959 -3.535149
 O 2.811704 -0.951689 -1.558394
 O 2.765144 1.420851 -1.229329
 C 4.734487 0.454191 -2.694128
 F 5.045646 -0.502938 -3.565009
 F 5.455974 0.288533 -1.581877
 F 5.012087 1.643809 -3.222808
 S 3.472478 -0.426104 2.723766
 O 3.268029 -1.438562 1.630930
 O 4.717353 -0.472883 3.467714
 O 3.059158 0.892455 2.130686
 C 2.140546 -0.820098 3.939600
 F 0.953546 -0.803892 3.337041
 F 2.150351 0.083521 4.918027
 F 2.356622 -2.032663 4.447684

B2-C1

Mn 1.873853 0.591521 -0.272182
 O 2.954830 -0.984583 -2.518889
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 N 0.286155 0.723773 0.883104
 N 2.330278 -0.803400 1.207692
 C 2.561829 -0.396269 -1.576327
 C 1.188185 1.468497 -1.648807
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 C -1.938336 1.496335 1.480444
 H -2.692389 2.276322 1.400967
 C -2.187705 0.332367 2.280679
 H -3.071158 0.274422 2.917551
 C -1.071997 -0.480856 2.532157
 H -1.156444 -1.298251 3.244513
 C 0.126945 -0.280048 1.857641
 C 1.278058 -1.108234 2.039865
 C 1.346715 -2.160721 2.970824

H 0.488295 -2.384380 3.598785
 C 2.502180 -2.897232 3.087193
 H 2.573251 -3.715561 3.800403
 C 3.598884 -2.544780 2.286741
 H 4.547444 -3.070585 2.374125
 C 3.495611 -1.503741 1.379944
 C -0.481958 2.986577 0.191698
 C -1.247810 3.388711 -0.917954
 C -1.019930 4.647831 -1.481964
 H -1.603003 4.944899 -2.355879
 C -0.058720 5.521790 -0.976834
 C 0.668881 5.115725 0.148391
 H 1.400661 5.798032 0.586027
 C 0.465651 3.876146 0.751689
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 H -3.216900 2.470106 -0.970174
 H -1.922494 1.438949 -1.567968
 H -2.507895 2.791745 -2.555705
 C 0.185573 6.859504 -1.605844
 H 0.071591 7.675747 -0.880245
 H -0.506890 7.048611 -2.433740
 H 1.206590 6.938829 -2.002768
 C 1.208867 3.533058 2.007482
 H 1.903837 2.694771 1.860257
 H 0.521849 3.223545 2.807719
 H 1.785196 4.391415 2.370445
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 H 6.671423 -2.131008 -1.968442
 C 7.054666 -0.389902 -0.765077
 C 6.606053 0.355106 0.331005
 H 7.173177 1.231664 0.650842
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 H 4.749169 -4.013034 -0.217577
 H 4.681295 -3.436540 -1.885624
 H 3.363235 -3.069560 -0.759731
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 H 8.599431 -0.751844 -2.228502
 H 9.122155 0.231302 -0.847454
 H 8.108238 0.941584 -2.096636
 C 5.045837 0.793662 2.243740
 H 3.976275 1.038652 2.238825
 H 5.606651 1.732045 2.315061
 H 5.233678 0.223951 3.165318
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 Mg -2.931768 -0.968513 0.562518
 S -1.229495 -2.735346 -0.458828
 O 0.144996 -3.183522 -0.333574
 O -1.479281 -1.326135 -0.912773
 O -2.154373 -2.952291 0.706805
 C -1.975628 -3.755089 -1.802843
 F -1.327715 -3.535474 -2.945342
 F -3.260524 -3.422560 -1.955688
 F -1.891744 -5.045725 -1.486106
 S -5.500167 -0.651178 -0.088067
 O -4.950406 -1.356406 1.119102
 O -6.588507 -1.285994 -0.807917
 O -4.299705 -0.209124 -0.874555
 C -6.180846 0.927283 0.581701
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 F -6.526904 1.724917 -0.426718
 F -5.251872 1.537393 1.322384

B2-C2

Mn 1.765256 0.798222 -0.251779
 O 2.292000 -0.489526 -2.849922
 O 0.830741 2.722608 -2.267258
 N 0.302930 0.898839 1.050425
 N 2.238935 -0.804462 1.005852
 C 2.124977 -0.044420 -1.771226
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 C -0.668049 1.901506 1.186353
 C -1.867361 1.667377 1.813302
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 C -2.112050 0.426601 2.493310
 H -2.990777 0.310632 3.127651
 C -0.999006 -0.409472 2.657898
 H -1.069810 -1.277893 3.308587
 C 0.177026 -0.170315 1.954604
 C 1.297539 -1.055663 1.978189
 C 1.445182 -2.102638 2.907104
 H 0.687463 -2.253149 3.671513
 C 2.552285 -2.915765 2.853265
 H 2.687810 -3.724169 3.568482
 C 3.512075 -2.664460 1.861728
 H 4.408947 -3.275496 1.782394
 C 3.339276 -1.618417 0.970712
 C -0.337832 3.278623 0.748298
 C -1.095130 3.932926 -0.240453
 C -0.788734 5.256080 -0.571348
 H -1.369723 5.749150 -1.353191
 C 0.247188 5.953278 0.047771
 C 0.980145 5.290066 1.038810
 H 1.779237 5.823146 1.558226
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 H -3.130778 3.201012 -0.428745
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 H -2.385899 3.710526 -1.944725
 C 0.566943 7.369226 -0.323012
 H 0.491226 8.040938 0.542570
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 H 1.593441 7.466799 -0.700890
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 H 2.201387 2.597247 2.151443
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 C 5.428627 -1.907415 -2.160654
 H 5.421005 -2.470411 -3.095967
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 C 6.451273 -0.296830 -0.709490
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 C 5.449400 -0.486882 0.242104
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 H 3.442574 -4.026300 -0.878734
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 H 2.328651 -2.736537 -1.322772
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 H 7.452270 -1.447613 -3.782757
 H 8.531721 -0.864569 -2.502383
 H 7.482649 0.266612 -3.346248
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 H 4.538319 0.595454 1.885269
 H 6.212876 1.060127 1.534648
 H 5.862583 -0.467220 2.356693
 C 3.255968 1.754949 -0.177337
 O 4.156785 2.514348 -0.212947
 Mg -2.920527 -0.700094 0.660121
 S -1.969004 -2.896396 -0.524131

O -2.016244 -3.575649 -1.806331
O -3.257425 -2.753667 0.238661
O -1.309193 -1.552362 -0.464968
C -0.922294 -3.956623 0.571240
F -1.315108 -5.225699 0.476023
F -1.048076 -3.557589 1.838015
F 0.356776 -3.859720 0.207068
S -5.058378 0.517793 -0.385956
O -3.755606 0.199893 -1.062348
O -5.574263 1.869815 -0.513539
O -4.946540 -0.057590 0.995119
C -6.288617 -0.558780 -1.241088
F -6.363918 -0.208578 -2.524416
F -7.482191 -0.402330 -0.668904
F -5.924311 -1.836486 -1.154596

B2-C3

Mn 2.797607 -0.624566 -0.332809
O 4.803655 -1.458384 -2.322521
O 1.298451 -1.859952 -2.544819
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N 3.991052 -0.682586 1.348075
C 4.072238 -1.105470 -1.463173
C 1.833067 -1.365242 -1.611285
C 0.060063 -0.946202 1.054464
C -0.773211 -1.359723 2.073582
H -1.850347 -1.334762 1.915694
C -0.233144 -1.766207 3.307621
H -0.877452 -2.090124 4.121262
C 1.131331 -1.682152 3.468034
H 1.583084 -1.930981 4.424953
C 1.952198 -1.267762 2.404873
C 3.367318 -1.112012 2.511314
C 4.084630 -1.365485 3.694354
H 3.556710 -1.729912 4.571900
C 5.441435 -1.146339 3.744800
H 6.010088 -1.341638 4.651066
C 6.059731 -0.611595 2.600980
H 7.117422 -0.354368 2.607749
C 5.329809 -0.371103 1.452184
C -0.553426 -0.368276 -0.169608
C -1.211096 -1.193161 -1.104565
C -1.822914 -0.599277 -2.226205
H -2.306707 -1.240188 -2.964399
C -1.767664 0.787213 -2.454631
C -1.141906 1.585336 -1.482668
H -1.138700 2.668459 -1.610065
C -0.545448 1.036217 -0.344055
C -1.252643 -2.680642 -0.932150
H -2.029394 -2.985306 -0.219171
H -0.297851 -3.058875 -0.550659
H -1.463772 -3.178390 -1.884170
C -2.376816 1.392526 -3.679925
H -2.598875 2.454578 -3.535226
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C 6.020108 0.309440 0.324311
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C 7.418648 1.654240 -1.720641
C 6.499628 2.329853 -0.912999
H 6.325952 3.395084 -1.078255

C 5.810252 1.687401 0.117458
C 7.220231 -1.844806 -0.236363
H 7.891180 -2.017138 0.616997
H 7.690696 -2.298913 -1.115996
H 6.295343 -2.396332 -0.026732
C 8.164793 2.366845 -2.807787
H 8.171941 1.790224 -3.741204
H 9.216610 2.529450 -2.534218
H 7.728512 3.349313 -3.020690
C 4.910679 2.476360 1.021601
H 3.935079 1.992953 1.158983
H 4.736032 3.483597 0.626763
H 5.354093 2.585705 2.021923
C 2.644959 1.024440 -0.942291
O 2.547587 2.065859 -1.495992
Mg -3.470175 0.314833 -0.607959
S -3.874573 2.724953 0.438765
O -3.150122 3.967266 0.638146
O -3.342156 1.490407 1.116938
O -4.185472 2.311298 -0.968514
C -5.526100 2.965415 1.224737
F -5.361162 3.300035 2.503214
F -6.231489 1.836399 1.152957
F -6.183540 3.935805 0.592878
S -5.271481 -1.548302 0.053831
O -5.442031 -0.421582 -0.924680
O -6.324602 -1.764198 1.028597
O -3.861984 -1.429130 0.557804
C -5.227458 -3.066373 -0.995543
F -6.438469 -3.303726 -1.493846
F -4.837874 -4.102949 -0.255250
F -4.364374 -2.897719 -1.999345

B2-C4

Mn -2.837878 -0.704822 0.574639
O -4.914773 -0.590182 2.661703
O -1.489666 -1.576679 3.044816
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N -4.049685 -1.118191 -1.032267
C -4.148767 -0.624855 1.762148
C -1.972634 -1.243529 2.016562
C -0.168511 -1.687291 -0.624024
C 0.602011 -2.462845 -1.466567
H 1.677915 -2.500395 -1.305586
C 0.001702 -3.159791 -2.530944
H 0.596474 -3.771025 -3.205421
C -1.351890 -2.997533 -2.723257
H -1.843793 -3.474077 -3.567497
C -2.108057 -2.208058 -1.839794
C -3.503065 -1.949428 -2.000537
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H -3.810753 -3.160697 -3.760860
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C -6.126519 -1.205850 -2.269851
H -7.146403 -0.840028 -2.375256
C -5.344270 -0.694994 -1.251652
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C 1.784140 -0.630521 2.451848
H 2.241072 -1.094978 3.326755
C 1.861028 0.760835 2.302902
C 1.314702 1.323128 1.130239
H 1.385214 2.400409 0.972665
C 0.653855 0.537007 0.169089
C 1.067047 -2.921691 1.737829
H 1.795790 -3.435786 1.096881

H	0.080274	-3.331055	1.493992	C	1.752934	-1.618907	3.429451
H	1.302441	-3.179378	2.775808	H	1.045322	-1.701010	4.250249
C	2.515350	1.615743	3.343233	C	2.870226	-2.417294	3.403427
H	2.660589	2.641191	2.990198	H	3.062065	-3.144265	4.189608
H	3.488653	1.211484	3.647666	C	3.773839	-2.242891	2.340200
H	1.894126	1.658218	4.247197	H	4.688777	-2.829863	2.281906
C	0.175028	1.169895	-1.102842	C	3.531776	-1.298088	1.360275
H	0.085557	2.254754	-0.995236	C	-0.659422	3.185291	0.451373
H	-0.799254	0.772660	-1.407412	C	-1.609720	3.301605	-0.578866
H	0.879794	0.971224	-1.923039	C	-1.627778	4.458551	-1.362620
C	-5.903281	0.408419	-0.426891	H	-2.360292	4.536860	-2.168343
C	-6.923503	0.162783	0.505974	C	-0.724734	5.501587	-1.160715
C	-7.465554	1.236562	1.220054	C	0.201914	5.373176	-0.119927
H	-8.243066	1.037567	1.960274	H	0.901184	6.188520	0.077066
C	-7.029262	2.546151	1.027101	C	0.237395	4.246742	0.701640
C	-6.034638	2.772529	0.067615	C	-2.549169	2.176492	-0.900266
H	-5.697117	3.793624	-0.122318	H	-3.100065	1.826729	-0.017604
C	-5.476532	1.732519	-0.673399	H	-1.997124	1.311694	-1.298309
C	-7.420150	-1.228988	0.763333	H	-3.285782	2.469601	-1.657205
H	-8.150374	-1.550387	0.007175	C	-0.749629	6.730941	-2.017064
H	-7.915208	-1.295377	1.738987	H	-0.935129	7.635435	-1.422280
H	-6.605826	-1.963528	0.747912	H	-1.528876	6.672254	-2.785191
C	-7.610333	3.684594	1.809420	H	0.210161	6.887749	-2.526892
H	-8.398001	3.345677	2.491665	C	1.174375	4.206112	1.871706
H	-8.044375	4.448493	1.150576	H	1.846960	5.071285	1.870501
H	-6.845520	4.193675	2.411019	H	1.789060	3.296662	1.875662
C	-4.480771	2.033332	-1.753599	H	0.621494	4.215907	2.822033
H	-3.563601	1.439962	-1.643683	C	4.573808	-1.119275	0.313474
H	-4.200812	3.092843	-1.750300	C	4.659670	-2.025212	-0.755284
H	-4.889894	1.799907	-2.747081	C	5.687360	-1.873940	-1.691378
C	-2.427120	1.005665	0.706838	H	5.739841	-2.567448	-2.533146
O	-2.178651	2.137838	0.946972	C	6.632216	-0.853483	-1.590050
Mg	3.395708	0.389656	0.322678	C	6.543917	0.019936	-0.499260
S	4.778841	2.412684	-0.727336	H	7.285935	0.813370	-0.387081
O	6.170517	2.763270	-0.946568	C	5.541992	-0.105725	0.462208
O	4.280963	2.335978	0.682543	C	3.658904	-3.132345	-0.909568
O	4.264552	1.171521	-1.408145	H	3.645439	-3.511709	-1.937941
C	3.787291	3.771663	-1.483187	H	2.643442	-2.801354	-0.661585
F	4.090717	3.882887	-2.774846	H	3.885819	-3.982510	-0.250119
F	4.058282	4.918229	-0.862465	C	7.718940	-0.695589	-2.610220
F	2.486583	3.501526	-1.358056	H	7.659057	-1.466677	-3.386534
S	4.773931	-1.819968	0.865600	H	8.715732	-0.758450	-2.153556
O	3.725045	-1.634964	-0.197230	H	7.667672	0.282005	-3.107781
O	4.654472	-2.978974	1.731601	C	5.532437	0.789380	1.665761
O	4.932810	-0.473204	1.509619	H	4.525399	1.158442	1.898359
C	6.337119	-2.052905	-0.086398	H	6.184861	1.657804	1.521480
F	6.242496	-3.157207	-0.824468	H	5.888727	0.254006	2.557902
F	7.358136	-2.170311	0.760351	C	3.085012	2.085954	-0.116767
F	6.543546	-1.005589	-0.883332	O	3.881146	2.945170	-0.295340
B2-Z1				Mg	-2.941063	-0.992980	0.710893
Mn	1.813412	0.863723	-0.082095	S	-0.986012	-2.668441	0.076908
O	2.577924	-0.646786	-2.493442	O	0.208103	-3.192172	0.714207
O	0.496263	2.097057	-2.403037	O	-1.074877	-1.187388	-0.161760
N	0.361628	1.094615	1.330375	O	-2.314689	-3.047612	0.670220
N	2.398937	-0.518874	1.344638	C	-0.956678	-3.361636	-1.631273
C	2.324548	-0.106876	-1.470410	F	0.143628	-2.916372	-2.241038
C	0.947084	1.654802	-1.402944	F	-2.029031	-2.972428	-2.316655
C	-0.674526	2.009235	1.360935	F	-0.926931	-4.692006	-1.576782
C	-1.727971	1.917326	2.251300	S	-5.393022	-1.400690	-0.222537
H	-2.514208	2.668912	2.202368	O	-4.954612	-1.430078	1.216337
C	-1.771752	0.891080	3.219545	O	-6.199198	-2.505832	-0.705129
H	-2.596972	0.812467	3.923917	O	-4.166334	-1.028599	-1.006745
C	-0.688143	0.040371	3.281477	C	-6.464078	0.097787	-0.330010
H	-0.651255	-0.735575	4.042209	F	-7.552903	-0.080274	0.414777
C	0.374520	0.163991	2.368552	F	-6.818484	0.300986	-1.596428
C	1.520054	-0.684047	2.402224	F	-5.794605	1.162023	0.116450

B2-Z2

Mn -2.743913 -0.652830 -0.506068
 O -4.772784 -2.771784 -0.788984
 O -1.192564 -3.148745 -0.681622
 N -1.406043 0.545776 -1.449790
 N -3.925837 0.934680 -1.108879
 C -4.021068 -1.865208 -0.683713
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D0-O1

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C	3.918105	-1.898363	2.255881	H	3.164361	-5.071481	-1.636358
H	4.603867	-2.466724	2.896013	H	3.258078	-3.349632	-1.990227
H	3.019987	-1.706136	2.860529	H	2.410020	-4.439042	-3.104721
H	4.386579	-0.931365	2.041835	C	-2.409048	-4.636498	-1.819587
C	2.146737	-6.112672	0.212269	H	-3.267436	-4.362244	-1.195865
H	2.397546	-6.754930	-0.639781	H	-2.447035	-5.721428	-1.983120
H	1.050304	-6.096929	0.285403	H	-2.542929	-4.168063	-2.803058
H	2.521692	-6.587374	1.125807	C	0.096353	-2.657431	2.065966
C	3.412431	-2.296513	-2.789643	H	-0.926080	-2.516183	2.430425
H	3.355386	-1.203455	-2.829546	H	0.621774	-1.697832	2.161751
H	2.653031	-2.701813	-3.467716	H	0.603247	-3.347184	2.755428
H	4.392275	-2.571806	-3.205340	C	1.774888	3.062841	0.879586
C	1.053317	0.209562	-1.899960	C	2.010679	4.064719	-0.078595
O	0.857601	0.008134	-3.013701	C	0.923119	4.784014	-0.574724
C	1.794278	0.820101	1.735019	H	1.098344	5.537000	-1.344509
O	2.076266	1.033833	2.828394	C	-0.381391	4.543944	-0.136995
Mg	-3.144914	-0.873136	0.444781	C	-0.580010	3.581966	0.857625
S	-3.022551	-0.739388	-2.213751	H	-1.587149	3.405991	1.238941
O	-2.432189	0.110306	-3.230295	C	0.478203	2.845999	1.391594
O	-4.009993	-0.100874	-1.268975	C	3.391564	4.317830	-0.605341
O	-2.102140	-1.547351	-1.348242	H	4.008897	4.868780	0.117408
C	-4.036899	-1.994475	-3.109355	H	3.359436	4.909774	-1.526251
F	-5.018434	-1.383347	-3.767593	H	3.926283	3.383069	-0.823795
F	-4.559215	-2.852790	-2.232475	C	-1.542300	5.266594	-0.745148
F	-3.266398	-2.655521	-3.969013	H	-1.259090	6.260853	-1.108590
S	-2.724103	-1.314622	3.036840	H	-2.369225	5.379504	-0.034869
O	-2.100709	-2.004572	1.854616	H	-1.937036	4.711105	-1.608173
O	-3.227401	-2.148950	4.110978	C	0.234551	1.925379	2.551520
O	-3.655289	-0.292210	2.445678	H	0.558218	2.399786	3.489073
C	-1.312664	-0.346162	3.779977	H	0.784431	0.977917	2.487787
F	-1.570340	-0.096350	5.058060	H	-0.830064	1.693172	2.654038
F	-1.134538	0.810089	3.139012	C	0.391250	-0.049678	0.083112
F	-0.197648	-1.071935	3.681177	O	-0.747136	-0.077129	0.322286
				Mg	-2.945514	-0.549242	-0.237165
D0-O2				S	-2.833655	0.179264	-2.794310
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O	1.705845	2.221663	-2.387895	O	-2.023087	-0.883266	-2.098903
O	1.154283	-1.478786	-2.947851	O	-3.723109	0.746739	-1.724733
N	2.832772	-1.632092	0.720803	C	-1.607621	1.523140	-3.090416
N	3.014170	0.965626	1.120257	F	-0.614203	1.061986	-3.846218
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C	2.564149	-2.951251	0.597624	S	-3.396037	-0.193276	2.355646
C	3.403369	-3.910348	1.168732	O	-3.221276	-1.488376	1.600525
H	3.157255	-4.961716	1.043167	O	-2.619954	-0.026201	3.569591
C	4.511281	-3.511153	1.900686	O	-3.322976	0.877915	1.307761
H	5.181862	-4.245603	2.339674	C	-5.169488	-0.217148	2.866941
C	4.726951	-2.155748	2.103185	F	-5.939258	-0.373320	1.790302
H	5.558128	-1.820148	2.714654	F	-5.470735	0.932103	3.464353
C	3.864400	-1.234398	1.513535	F	-5.373150	-1.226958	3.707959
C	3.947375	0.208623	1.758344	C	3.872066	-0.125273	-1.282088
C	4.861046	0.770769	2.647075	O	4.905522	-0.173409	-1.777367
H	5.608430	0.152695	3.133631				
C	4.797322	2.130280	2.914045	D0-C1			
H	5.504862	2.589647	3.599703	Mn	2.096492	0.913049	-0.035817
C	3.793266	2.881013	2.322736	O	4.692299	0.966435	-1.459817
H	3.670693	3.937366	2.547901	O	2.066052	3.206232	-1.910030
C	2.902020	2.277804	1.432291	N	0.208430	1.005541	0.948448
C	1.302522	-3.370789	-0.052124	N	2.200621	-0.770119	1.262971
C	1.312112	-4.012382	-1.303635	C	3.726949	0.820346	-0.835240
C	0.097294	-4.412205	-1.858809	C	1.941483	2.352949	-1.135663
H	0.097502	-4.873929	-2.847304	C	-0.749958	1.950998	0.792062
C	-1.115576	-4.220567	-1.191173	C	-1.950821	1.891651	1.504675
C	-1.089495	-3.631090	0.075985	H	-2.693715	2.668674	1.340695
H	-2.021538	-3.519030	0.632126	C	-2.159546	0.881651	2.430001

H	-3.074392	0.839633	3.016773	O	-7.183697	-1.368605	-0.587723
C	-1.170537	-0.074882	2.600146	O	-4.829908	-0.480353	-0.905818
H	-1.308134	-0.866140	3.328302	C	-6.394877	0.692346	0.885115
C	0.000148	0.002196	1.843262	F	-7.219211	0.417144	1.890346
C	1.075618	-0.983000	1.994393	F	-6.984731	1.524735	0.034151
C	0.946567	-2.085142	2.839696	F	-5.284352	1.259139	1.361941
H	0.037553	-2.245132	3.408887				
C	1.983896	-2.996844	2.936819	D0-C3			
H	1.895234	-3.867322	3.581982	Mn	-2.797535	0.024477	-0.223120
C	3.134783	-2.769113	2.201126	O	-4.461798	1.778375	-1.935547
H	3.983717	-3.446177	2.253981	O	-1.006244	1.410033	-2.127503
C	3.229118	-1.643637	1.379721	N	-1.498511	-1.202783	0.946307
C	-0.536943	3.129630	-0.084459	N	-4.167899	-0.917535	1.108044
C	-1.032680	3.130049	-1.403953	C	-3.942476	1.052316	-1.197245
C	-0.895345	4.286129	-2.167767	C	-1.599158	0.808232	-1.332539
H	-1.266202	4.285304	-3.193809	C	-0.154980	-1.319123	0.832113
C	-0.288462	5.439295	-1.659246	C	0.584392	-2.153570	1.670406
C	0.158081	5.423611	-0.337494	H	1.661243	-2.210790	1.529997
H	0.609618	6.322427	0.085494	C	-0.060824	-2.891130	2.649450
C	0.028008	4.293089	0.471772	H	0.496008	-3.547571	3.313243
C	-1.677754	1.908183	-1.980941	C	-1.435615	-2.777677	2.764105
H	-2.565257	1.602893	-1.408588	H	-1.960506	-3.349948	3.520422
H	-0.998494	1.046351	-1.973959	C	-2.134049	-1.929032	1.904294
H	-1.991649	2.077307	-3.016191	C	-3.589941	-1.776485	1.989942
C	-0.106193	6.650672	-2.519169	C	-4.343163	-2.476665	2.931773
H	-0.026777	7.565343	-1.921156	H	-3.864525	-3.155119	3.628537
H	-0.931878	6.772361	-3.229788	C	-5.716257	-2.301624	2.977571
H	0.814743	6.574517	-3.114062	H	-6.317176	-2.840393	3.705835
C	0.427224	4.366476	1.916086	C	-6.300522	-1.424662	2.079806
H	1.293015	5.022804	2.058270	H	-7.373146	-1.248425	2.077455
H	0.664981	3.389740	2.350481	C	-5.509906	-0.739716	1.154410
H	-0.391180	4.783673	2.520161	C	0.590029	-0.567549	-0.209888
C	4.512304	-1.409375	0.673130	C	1.112761	0.700658	0.080506
C	4.769297	-2.051136	-0.552990	C	1.875737	1.354791	-0.908530
C	6.014636	-1.867290	-1.153024	H	2.201555	2.382391	-0.727238
H	6.212483	-2.348231	-2.112362	C	2.108485	0.773111	-2.168877
C	7.005681	-1.076180	-0.567644	C	1.629359	-0.524256	-2.393563
C	6.735783	-0.480480	0.667095	H	1.837900	-1.010935	-3.346659
H	7.506390	0.123533	1.148953	C	0.878106	-1.205149	-1.437241
C	5.509737	-0.643840	1.310928	C	0.902065	1.366289	1.405555
C	3.741417	-2.924682	-1.207752	H	1.805981	1.287658	2.026289
H	3.879232	-3.977877	-0.923655	H	0.087070	0.914565	1.978738
H	3.816735	-2.876875	-2.300273	H	0.693183	2.435364	1.283525
H	2.717308	-2.658445	-0.925365	C	2.835033	1.518293	-3.243336
C	8.313626	-0.847330	-1.258733	H	3.630667	0.911475	-3.692148
H	8.588230	-1.692615	-1.899824	H	3.270234	2.451176	-2.872231
H	9.126719	-0.676704	-0.543934	H	2.140616	1.774570	-4.053913
H	8.265398	0.040821	-1.904462	C	0.436793	-2.611063	-1.690117
C	5.302114	-0.064419	2.678899	H	0.408760	-2.833838	-2.761481
H	4.252328	0.157360	2.898841	H	-0.546945	-2.828858	-1.260457
H	5.880241	0.856279	2.814792	H	1.141980	-3.316388	-1.228325
H	5.637508	-0.770439	3.452183	C	-6.191058	0.200242	0.230932
C	2.848905	1.994715	1.291452	C	-6.414766	1.529083	0.642576
O	3.360710	2.679452	2.062925	C	-7.120546	2.379278	-0.208091
C	1.408240	-0.189431	-1.395446	H	-7.281809	3.414250	0.097782
O	1.070981	-0.815946	-2.300233	C	-7.625345	1.942226	-1.434994
Mg	-3.412061	-1.497623	0.238588	C	-7.424896	0.608163	-1.797645
S	-1.229001	-2.746929	-0.552101	H	-7.824526	0.246761	-2.746563
O	0.167828	-2.960572	-0.227936	C	-6.722332	-0.278614	-0.982591
O	-1.667290	-1.347469	-0.899440	C	-5.946860	2.030493	1.976597
O	-2.265389	-3.241261	0.424707	H	-6.758735	1.984659	2.716326
C	-1.562556	-3.697872	-2.099124	H	-5.628323	3.077724	1.919580
F	-0.749711	-3.265839	-3.057174	H	-5.118065	1.444856	2.388197
F	-2.830490	-3.504214	-2.466664	C	-8.336981	2.887433	-2.351888
F	-1.355867	-4.991706	-1.880635	H	-8.818033	3.703503	-1.801010
S	-5.959753	-0.875711	0.008937	H	-9.100059	2.376828	-2.950339
O	-5.305710	-1.719516	1.074192	H	-7.634326	3.349474	-3.059574

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 C -3.010529 -1.394602 -1.425985
 O -3.131297 -2.244107 -2.192871
 C -2.589290 1.404436 1.027864
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 Mg 3.984208 0.397574 -0.292854
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 F 5.429827 3.640065 2.649774
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D0-C4

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 C 3.617494 2.126218 -1.490534
 C 4.387136 3.011923 -2.244499
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 H -2.103217 -2.461440 0.216588
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 C -0.407942 2.157123 2.399454
 H -0.965401 3.002630 1.973430
 H 0.651899 2.358687 2.202105
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 H -3.438366 -1.923913 3.506353
 H -1.866307 -2.711785 3.597558
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H -0.990261 -1.913997 -1.855992
 H -0.032602 -0.425214 -2.037279
 H -1.779068 -0.366210 -2.177091
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 H 9.006591 -3.520869 1.848650
 H 8.552717 -4.480548 0.422608
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 H 4.797601 -0.996568 -2.748638
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 O -4.396444 -1.551558 -1.376775
 O -5.121111 -2.213448 0.804146
 C -6.862063 -2.507419 -1.177716
 F -6.945052 -2.803921 -2.472498
 F -7.296104 -1.264620 -0.978686
 F -7.610082 -3.355520 -0.476114
 S -4.856992 1.993870 -0.202948
 O -5.598766 0.941556 0.573451
 O -5.588678 2.756143 -1.194796
 O -3.570916 1.335325 -0.627305
 C -4.309391 3.194622 1.091330
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 F -3.416311 4.034020 0.567499
 F -3.743871 2.528184 2.100949

D0-Z2

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 H 1.910563 -0.722388 2.078772
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 H 0.937010 -1.968848 4.030648
 C -1.070051 -1.768816 3.282373
 H -1.516783 -2.283051 4.125494
 C -1.868333 -1.277767 2.249146
 C -3.328500 -1.410584 2.276168
 C -3.985151 -2.071317 3.313492
 H -3.423048 -2.531096 4.118500
 C -5.368525 -2.142076 3.311188
 H -5.895662 -2.656397 4.110708
 C -6.060297 -1.535643 2.276516

H	-7.146511	-1.548524	2.238363	O	-1.557568	0.370966	0.501690
C	-5.364279	-0.889690	1.251700	N	1.772715	2.624689	-0.448760
C	0.642620	0.322154	0.036146	N	3.582209	0.545635	-0.592536
C	0.773699	1.720082	0.135914	C	1.196490	-1.464306	0.337412
C	1.426775	2.417070	-0.886002	C	-0.392879	0.502024	0.279742
H	1.514740	3.501048	-0.809043	C	0.923317	3.638879	-0.170449
C	2.005295	1.760687	-1.970291	C	1.383489	4.943922	0.025314
C	1.927972	0.351391	-2.011086	H	0.663886	5.732019	0.236450
H	2.312669	-0.178399	-2.887473	C	2.741631	5.219343	-0.065847
C	1.228866	-0.378806	-1.035607	H	3.118026	6.225839	0.102801
C	0.330031	2.461558	1.356046	C	3.607418	4.186083	-0.388367
H	1.164685	2.514239	2.070298	H	4.677469	4.360126	-0.463256
H	-0.501082	1.979140	1.880104	C	3.085371	2.904702	-0.588302
H	0.045081	3.491660	1.118107	C	3.966258	1.788535	-0.962479
C	2.718823	2.504643	-3.055244	C	5.150293	2.028502	-1.664969
H	3.753375	2.150851	-3.164731	H	5.397754	3.036902	-1.984813
H	2.745115	3.580152	-2.856887	C	5.982355	0.963215	-1.969629
H	2.230017	2.345199	-4.024536	H	6.904283	1.120918	-2.524905
C	1.059731	-1.857819	-1.184659	C	5.618369	-0.305307	-1.538928
H	0.016276	-2.095548	-1.433231	H	6.256409	-1.167097	-1.721594
H	1.301173	-2.405159	-0.266049	C	4.416724	-0.487368	-0.849950
H	1.679930	-2.251245	-1.996419	C	-0.541323	3.387679	-0.127403
C	-6.161169	-0.226743	0.190067	C	-1.240466	3.518817	1.089321
C	-6.529623	1.124287	0.366328	C	-2.623040	3.337877	1.095430
C	-7.347169	1.723311	-0.590216	H	-3.159148	3.416560	2.043611
H	-7.625070	2.770760	-0.462642	C	-3.335191	3.046545	-0.071704
C	-7.843935	1.010909	-1.686311	C	-2.621831	2.937899	-1.266846
C	-7.500581	-0.335420	-1.809594	H	-3.158959	2.710747	-2.188945
H	-7.882363	-0.908152	-2.656454	C	-1.236729	3.107565	-1.319955
C	-6.660674	-0.971311	-0.893708	C	-0.519694	3.813998	2.371677
C	-6.125737	1.891426	1.590388	H	-0.164225	4.852470	2.416268
H	-6.859979	1.747056	2.396009	H	0.366045	3.178226	2.500021
H	-6.077991	2.967156	1.388929	H	-1.174685	3.656474	3.235313
H	-5.157956	1.577127	1.996390	C	-4.819964	2.851813	-0.032744
C	-8.703924	1.683804	-2.710323	H	-5.234405	2.699414	-1.034805
H	-9.349122	2.447577	-2.260993	H	-5.327425	3.714725	0.418005
H	-9.337452	0.965841	-3.242938	H	-5.096658	1.979100	0.574512
H	-8.089780	2.193055	-3.466076	C	-0.524842	3.035410	-2.638075
C	-6.257274	-2.394456	-1.138586	H	-1.183053	2.645664	-3.421871
H	-5.762698	-2.857926	-0.277939	H	0.367086	2.400506	-2.597518
H	-5.562121	-2.455754	-1.988463	H	-0.179655	4.029105	-2.958785
H	-7.122936	-3.013588	-1.402560	C	4.087764	-1.845449	-0.345337
C	-2.713641	-1.853320	-0.931430	C	4.253529	-2.133666	1.024675
O	-2.695064	-2.941640	-1.303775	C	3.998657	-3.429200	1.473050
Mg	4.022855	0.150371	-0.810423	H	4.121962	-3.651305	2.534657
S	4.962237	1.676091	1.146184	C	3.594141	-4.445544	0.603794
O	5.615935	1.575913	2.436603	C	3.464555	-4.140274	-0.751589
O	3.576344	1.109610	1.014036	H	3.152480	-4.921179	-1.447460
O	5.709397	1.181412	-0.063014	C	3.710865	-2.857988	-1.245851
C	4.712601	3.481442	0.826317	C	4.756320	-1.098018	1.986426
F	5.840249	4.144506	1.064809	H	5.850450	-1.003582	1.925219
F	3.746322	3.934968	1.623260	H	4.511724	-1.364984	3.020552
F	4.354449	3.668460	-0.445398	H	4.349712	-0.101054	1.788376
S	4.719850	-2.399453	-1.054932	C	3.272024	-5.813810	1.119885
O	4.922393	-1.291866	-2.054434	H	3.889398	-6.078595	1.986258
O	4.161297	-3.647841	-1.539420	H	3.410318	-6.582341	0.350791
O	4.061508	-1.744099	0.126864	H	2.224236	-5.873881	1.447212
C	6.422987	-2.806113	-0.471349	C	3.573613	-2.589462	-2.715784
F	7.129698	-3.288332	-1.490862	H	3.294001	-1.552232	-2.929497
F	6.347035	-3.722329	0.491235	H	2.819421	-3.243914	-3.167988
F	7.018409	-1.713943	0.002818	H	4.517440	-2.776229	-3.247821
C	-2.865149	1.653745	0.379141	C	1.001940	-0.048084	-1.809792
O	-2.944803	2.744641	0.737361	O	0.797647	-0.312788	-2.921019
D1-O1				C	1.745746	0.698816	1.746196
Mn	1.317402	0.300317	-0.014427	O	2.000016	0.961889	2.848191
O	0.879227	-2.558431	0.589847	Mg	-3.185368	-0.842255	0.346441
				S	-3.177981	-0.874025	-2.302808

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D1-O2

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C 1.661676 -0.286646 -3.684362
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C -4.047730 0.559909 3.238628
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C -4.901225 -0.505111 3.533736
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H -6.034175 -2.127854 2.686336
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C -2.772715 2.029366 1.655695
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H 1.712014 -5.677543 -2.354965

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O 3.634497 1.566386 1.183091
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C 3.654281 -0.525164 2.821658
F 4.764620 -1.068141 2.322879
F 2.600362 -0.997370 2.157551
F 3.544161 -0.845508 4.108867
S 0.253024 3.335583 -0.708417
O 0.245020 3.788241 0.729646
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O 1.359617 2.331527 -0.807433
C 0.884076 4.781994 -1.660377
F 0.026786 5.795234 -1.564037
F 1.013398 4.425868 -2.938109
F 2.070626 5.159238 -1.184208

D1-C1

Mn 2.060130 0.984549 0.057418
O 4.685315 1.323055 -1.265704
O 1.951249 3.428041 -1.609162
N 0.146898 0.893157 0.948698
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C 3.714646 1.063424 -0.683551
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C -1.165501 -0.343203 2.600365
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C 0.024097 -0.180822 1.850011
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C 1.112873 -2.192863 2.826856
H 0.225281 -2.412049 3.411922
C 2.197415 -3.031207 2.893149
H 2.178837 -3.907432 3.537775
C 3.323686 -2.741513 2.112702
H 4.206413 -3.375564 2.131347
C 3.324149 -1.614442 1.298735
C -0.796521 2.939251 -0.049656
C -1.218006 3.006371 -1.392175
C -1.145691 4.229135 -2.056464
H -1.460626 4.278363 -3.100114
C -0.676017 5.386576 -1.428161
C -0.301688 5.301397 -0.087209
H 0.043658 6.198340 0.429925
C -0.367899 4.100419 0.622682

C	-1.723609	1.791649	-2.106528	C	-1.469447	-0.017201	2.578790
H	-2.610070	1.366392	-1.615502	H	-1.611532	-0.907290	3.197692
H	-0.975993	0.989953	-2.132065	C	-0.218771	0.194591	1.920723
H	-1.999118	2.027899	-3.139866	C	0.850177	-0.737162	1.978342
C	-0.561533	6.674633	-2.182715	C	0.878076	-1.801384	2.911509
H	-0.542461	7.539622	-1.510343	H	0.116900	-1.855740	3.685546
H	-1.388862	6.806217	-2.890126	C	1.870367	-2.747003	2.849496
H	0.364979	6.704294	-2.773165	H	1.896094	-3.569950	3.561510
C	-0.043073	4.091075	2.087755	C	2.851748	-2.632906	1.851604
H	0.745533	4.814088	2.325799	H	3.641218	-3.372448	1.743617
H	0.275189	3.108653	2.452328	C	2.821160	-1.549859	0.979237
H	-0.924418	4.373943	2.681179	C	-0.663903	3.653031	0.611040
C	4.557725	-1.342679	0.515471	C	-1.257790	4.070932	-0.595644
C	4.728944	-1.942041	-0.748491	C	-1.011141	5.362331	-1.056033
C	5.924642	-1.730537	-1.434384	H	-1.460292	5.677755	-1.999487
H	6.053514	-2.182282	-2.419690	C	-0.189326	6.252002	-0.357882
C	6.960903	-0.965468	-0.892148	C	0.370509	5.822800	0.845713
C	6.782254	-0.418601	0.379457	H	0.994127	6.509868	1.420338
H	7.585907	0.170587	0.824978	C	0.134524	4.543061	1.356214
C	5.599128	-0.596557	1.098468	C	-2.094151	3.129293	-1.404300
C	3.676832	-2.834162	-1.336722	H	-2.969311	2.769747	-0.849588
H	3.837735	-3.879404	-1.034556	H	-1.526872	2.232002	-1.687239
H	3.702090	-2.811945	-2.432424	H	-2.447317	3.605947	-2.325271
H	2.665385	-2.571797	-1.011671	C	0.091981	7.619528	-0.899416
C	8.217773	-0.718408	-1.667928	H	0.515034	8.280048	-0.134464
H	8.492257	-1.582668	-2.284128	H	-0.814215	8.092337	-1.297296
H	9.062012	-0.482408	-1.010243	H	0.812030	7.577668	-1.728386
H	8.097187	0.132422	-2.353284	C	0.654211	4.186610	2.718185
C	5.472516	-0.014457	2.475528	H	1.546844	4.770358	2.968503
H	4.430602	0.103977	2.790981	H	0.900102	3.124813	2.823083
H	5.961502	0.964923	2.541035	H	-0.100625	4.406947	3.486962
H	5.955245	-0.660607	3.222593	C	3.877717	-1.482728	-0.063391
C	2.651738	1.958635	1.533553	C	3.645824	-2.076362	-1.319513
O	3.040343	2.564025	2.434414	C	4.675558	-2.077041	-2.261225
C	1.494523	-0.059345	-1.403646	H	4.495518	-2.528174	-3.238800
O	1.247024	-0.648262	-2.362268	C	5.925005	-1.516330	-1.987402
Mg	-2.849230	-0.874905	0.528100	C	6.137846	-0.959392	-0.724049
S	-1.092514	-2.559900	-0.536754	H	7.111705	-0.525975	-0.488520
O	0.274685	-3.023658	-0.387779	C	5.138297	-0.940127	0.249270
O	-1.308753	-1.106418	-0.860567	C	2.335314	-2.732404	-1.642047
O	-2.077416	-2.869226	0.553574	H	2.367757	-3.808883	-1.418698
C	-1.757797	-3.429820	-2.020230	H	2.092471	-2.637498	-2.707311
F	-1.042345	-3.082043	-3.088097	H	1.502532	-2.317956	-1.064327
F	-3.032121	-3.084614	-2.209175	C	6.999250	-1.484851	-3.030525
F	-1.680644	-4.746439	-1.840899	H	6.889212	-2.301981	-3.752614
S	-5.452371	-1.108940	0.066510	H	7.999633	-1.550183	-2.586917
O	-4.728631	-1.524329	1.313541	H	6.966836	-0.546701	-3.602431
O	-6.400996	-2.039082	-0.516362	C	5.429288	-0.372779	1.607329
O	-4.394845	-0.534633	-0.838604	H	4.524105	-0.046668	2.130416
C	-6.428113	0.366315	0.592358	H	6.113564	0.481734	1.544831
F	-7.393693	-0.010420	1.427268	H	5.912144	-1.120535	2.252715
F	-6.964178	0.951645	-0.475629	C	2.756441	2.024119	1.143015
F	-5.624606	1.232538	1.214200	O	3.473005	2.542682	1.884451
D1-C2				C	0.569725	0.292924	-1.355323
Mn	1.671821	1.179026	-0.115058	O	-0.081974	-0.181576	-2.178514
O	3.931398	1.076138	-2.020492	Mg	-2.620746	-1.371537	0.877453
O	1.564312	3.640722	-1.748163	S	-1.491622	-3.389661	-0.438094
N	-0.027148	1.343839	1.152121	O	-1.180146	-3.828542	-1.785293
N	1.853902	-0.603145	1.035445	O	-2.937619	-3.258854	-0.051088
C	3.095480	0.983050	-1.218752	O	-0.832083	-2.137912	0.066129
C	1.488963	2.720208	-1.042997	C	-0.836436	-4.688634	0.695727
C	-0.962463	2.317444	1.193949	F	-1.410445	-5.858658	0.426142
C	-2.178914	2.164345	1.864546	F	-1.102784	-4.350029	1.960750
H	-2.891162	2.984368	1.864512	F	0.481710	-4.791144	0.537715
C	-2.442852	0.965523	2.548028	S	-4.459544	0.156403	-0.253476
H	-3.388644	0.817652	3.066622	O	-3.020978	-0.008893	-0.658968
				O	-4.983371	1.504998	-0.127179

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C -5.406572 -0.615148 -1.637054
F -5.173688 0.065127 -2.758715
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D1-C3

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C -2.469400 0.840010 -3.613197
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H -3.370828 0.231948 -3.753212
H -1.778120 0.577888 -4.425230
C 0.254841 2.478539 0.275691
H 0.367890 3.349883 -0.376799
H 1.246331 2.192285 0.646678
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C 6.128246 0.478688 0.172868
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H 8.209907 -0.341701 -2.387346
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C 7.340398 -1.712727 -0.257132
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H 7.714664 -2.248973 -1.136326
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C 7.818168 2.144380 -3.432012
H 8.390517 1.399770 -3.996135
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H 7.041042 2.546420 -4.094449
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O -4.572495 1.982413 -1.094442
C -5.398603 3.155757 1.126238
F -4.969547 3.674084 2.275106
F -6.171895 2.100216 1.378953
F -6.103294 4.069333 0.462056
S -6.099956 -1.448638 -0.448300
O -5.412361 -0.950239 -1.685219
O -7.543379 -1.331230 -0.373002
O -5.295913 -0.901522 0.701818
C -5.724759 -3.254882 -0.423183
F -6.320041 -3.848889 -1.453898
F -6.165978 -3.785974 0.714164
F -4.404737 -3.434630 -0.511821

D1-C4

Mn -3.131400 -0.369617 0.971145
O -5.355129 0.706414 2.596680
O -1.573993 0.052682 3.441865
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H 0.760042 -2.050339 3.882233
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H 3.435732 2.103073 3.365778
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H	-0.554672	0.769850	-1.555812	C	5.083071	1.426512	0.564084
H	0.743278	-0.316652	-2.031492	C	-0.789658	-0.253118	0.282101
C	-5.682408	0.736894	-1.042305	C	-1.408399	-1.482250	0.612283
C	-6.811610	0.670825	-0.206256	C	-1.985230	-2.247036	-0.413661
C	-7.371216	1.858238	0.261367	H	-2.452828	-3.197982	-0.161093
H	-8.232610	1.806448	0.929825	C	-1.941756	-1.850393	-1.757018
C	-6.840933	3.106885	-0.078195	C	-1.328652	-0.623141	-2.057218
C	-5.734450	3.144263	-0.928895	H	-1.320499	-0.270494	-3.088262
H	-5.316322	4.109509	-1.219970	C	-0.741221	0.178901	-1.067068
C	-5.153097	1.978441	-1.435181	C	-1.421242	-2.009387	2.014763
C	-7.369555	-0.655071	0.215586	H	-2.216848	-1.556720	2.619400
H	-7.847543	-1.185848	-0.619398	H	-0.471623	-1.806278	2.525009
H	-8.119749	-0.536435	1.005056	H	-1.584793	-3.091243	2.013282
H	-6.581443	-1.320541	0.597445	C	-2.554373	-2.688629	-2.830804
C	-7.447767	4.366386	0.460342	H	-3.054187	-2.070070	-3.584514
H	-7.374796	4.410869	1.555091	H	-3.280945	-3.396831	-2.420498
H	-8.516130	4.435494	0.217861	H	-1.779577	-3.266965	-3.350782
H	-6.953508	5.257482	0.058118	C	-0.138222	1.493426	-1.456740
C	-4.024996	2.063356	-2.420741	H	0.957157	1.439526	-1.466037
H	-3.230176	1.334758	-2.218752	H	-0.403156	2.290430	-0.752768
H	-3.574712	3.061703	-2.424172	H	-0.466314	1.787770	-2.459114
H	-4.380004	1.859079	-3.441278	C	5.780346	0.599764	-0.453615
C	-2.562637	1.312046	0.440495	C	6.784801	-0.301261	-0.066610
O	-2.187269	2.394958	0.237262	C	7.455957	-1.024268	-1.054803
C	-3.484026	-2.085770	1.546633	H	8.220832	-1.742073	-0.753758
O	-3.697881	-3.160489	1.939505	C	7.155982	-0.873405	-2.409415
Mg	3.730998	0.450812	0.148655	C	6.165412	0.047081	-2.768677
S	5.617670	2.201753	-0.482098	H	5.926046	0.192135	-3.823913
O	7.063582	2.284577	-0.560236	C	5.482608	0.802262	-1.815403
O	4.994127	1.993500	0.868491	C	7.097053	-0.520656	1.383020
O	4.924563	1.226794	-1.394685	H	7.590821	0.350949	1.834632
C	4.979265	3.850483	-1.008554	H	7.758893	-1.382875	1.519444
F	5.371058	4.106140	-2.253841	H	6.184310	-0.700474	1.969572
F	5.450596	4.787440	-0.189705	C	7.876996	-1.665918	-3.456609
F	3.645242	3.852414	-0.956374	H	7.180555	-2.257386	-4.065028
S	4.299068	-2.142829	0.260212	H	8.602733	-2.355909	-3.012489
O	3.459651	-1.454907	-0.778004	H	8.419449	-1.012947	-4.153099
O	3.781154	-3.367767	0.844556	C	4.493088	1.846068	-2.242924
O	4.743405	-1.054201	1.199071	H	3.579957	1.839002	-1.634779
C	5.841666	-2.617448	-0.635798	H	4.202011	1.712237	-3.290192
F	5.533252	-3.441135	-1.634976	H	4.920710	2.854501	-2.145917
F	6.671727	-3.228842	0.205453	C	2.662175	-0.705875	-1.298862
F	6.430219	-1.527614	-1.125020	O	2.499843	-0.709644	-2.451586
D1-Z2				Mg	-3.346661	0.013844	-0.560959
Mn	2.876685	-0.932697	0.527036	S	-5.580558	-1.218574	0.207210
O	5.031482	-2.925548	0.155705	O	-6.987517	-0.880919	0.322936
O	1.073469	-3.254544	0.258691	O	-4.609268	-0.453151	1.065208
N	1.141076	0.855436	1.172693	O	-4.977326	-1.207587	-1.168114
N	3.824573	1.105620	0.937313	C	-5.438368	-2.996388	0.783720
C	4.280832	-2.039685	0.299020	F	-6.519815	-3.322812	1.483672
C	1.705662	-2.274362	0.381253	F	-4.362359	-3.146688	1.554738
C	-0.161217	0.576243	1.341639	F	-5.336514	-3.801227	-0.272029
C	-0.886410	1.043976	2.439281	S	-3.572419	2.607846	-1.172465
H	-1.944224	0.808064	2.536678	O	-3.807963	1.436608	-2.082044
C	-0.235016	1.818629	3.392503	O	-2.867746	3.758240	-1.706399
H	-0.769497	2.182488	4.266906	O	-3.081231	2.017515	0.118860
C	1.107349	2.126747	3.209989	C	-5.273229	3.188441	-0.758521
H	1.640085	2.724182	3.945014	F	-5.869557	3.662082	-1.849720
C	1.759785	1.637112	2.075330	F	-5.208679	4.145023	0.164465
C	3.169472	1.949848	1.774108	F	-5.982444	2.161919	-0.279314
C	3.766779	3.098863	2.292167	C	2.880848	-1.208767	2.351140
H	3.198392	3.764642	2.935323	O	2.871980	-1.418387	3.495865
C	5.078147	3.396471	1.951127	E1			
H	5.566306	4.284111	2.347000	Mn	-1.339478	-0.367694	0.223599
C	5.736927	2.555184	1.068354	O	-0.318143	-2.432289	2.055196
H	6.753855	2.762468	0.742758	O	-0.426180	1.225854	2.532531

N	-1.772105	1.159701	-1.144812	C	1.865060	3.841383	-1.273906
N	-1.001373	-1.282063	-1.608721	F	1.880529	4.822518	-0.368941
C	-0.681904	-1.660185	1.243104	F	0.600393	3.546226	-1.575165
C	-0.784716	0.665348	1.549201	F	2.485429	4.254898	-2.379951
C	-2.399879	2.346379	-0.894878	S	3.845633	-1.231670	1.196064
C	-2.549919	3.317265	-1.878534	O	2.403662	-0.851137	1.424439
H	-3.059340	4.243930	-1.621492	O	4.402423	-0.624781	-0.020274
C	-2.082821	3.089814	-3.172360	O	4.120360	-2.644610	1.446070
H	-2.197961	3.841646	-3.949657	C	4.672187	-0.341861	2.578991
C	-1.502291	1.867105	-3.449567	F	4.208206	-0.774619	3.756563
H	-1.170955	1.634210	-4.457348	F	4.459225	0.974197	2.493466
C	-1.369760	0.915429	-2.431943	F	5.991314	-0.563749	2.531630
C	-0.873539	-0.425175	-2.674179	C	2.789866	-1.311049	-2.250721
C	-0.324996	-0.828907	-3.895654	O	1.980694	-1.473762	-1.414827
H	-0.180037	-0.104590	-4.692238	O	3.573197	-1.187939	-3.100709
C	0.026248	-2.154319	-4.084476				
H	0.466215	-2.488294	-5.021172	TS-E1E2			
C	-0.268389	-3.058391	-3.063585	Mn	-1.107785	0.308310	0.187397
H	-0.111994	-4.126503	-3.201765	O	-1.381256	-2.516385	1.004847
C	-0.798116	-2.615463	-1.857526	O	1.173327	0.391108	2.065516
C	-3.027690	2.585130	0.432455	N	-0.768375	2.173717	-0.701904
C	-2.398146	3.391132	1.394595	N	-2.419170	0.293539	-1.447794
C	-3.047773	3.624304	2.609318	C	-1.278808	-1.415718	0.608461
H	-2.548335	4.234996	3.363787	C	0.319219	0.374940	1.245966
C	-4.310165	3.096486	2.884036	C	-0.168985	3.278933	-0.165834
C	-4.935431	2.335059	1.891264	C	0.187591	4.368704	-0.954257
H	-5.933272	1.931370	2.074293	H	0.672852	5.218178	-0.478122
C	-4.322654	2.080617	0.664720	C	-0.105978	4.380961	-2.315852
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H	-0.619038	4.417804	2.039771	H	-1.159401	3.342809	-3.867902
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F -5.825699 -1.173148 -3.442532
F -3.684388 -1.476992 -3.643641
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F -5.641265 -0.470360 3.679142
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G2

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H	-0.014448	-4.390450	3.208982	O	-2.712451	-2.255886	0.359353
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H	-0.172908	-2.022895	3.896447	F	-5.437395	-3.047281	2.437557
C	1.005515	-1.302049	2.235962	F	-5.437680	-2.498648	0.344662
C	0.913932	0.117826	2.592945	F	-5.772875	-0.983573	1.863607
C	0.196749	0.539635	3.714164	C	-0.885959	0.074423	-2.811088
H	-0.318672	-0.177657	4.343496	O	-1.810980	-0.575658	-2.254921
C	0.135056	1.888470	4.019582	O	-0.787324	0.553612	-3.921558
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C	0.801399	2.780148	3.195137	H1			
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H	5.734928	-4.169087	-1.404232	N	-1.458913	2.984688	-0.675840
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C	1.902976	-3.572152	-1.644361	C	-3.753999	0.300222	-2.621592
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H	5.041920	-3.847128	-4.524437	H	-1.361389	2.435934	-4.711205
H	4.168628	-5.376718	-4.515515	C	-2.091146	1.932016	-2.741434
H	5.693605	-5.213326	-3.618407	C	-1.271258	2.911195	-2.019704
C	0.425111	-3.338727	-1.746433	C	-0.341056	3.713254	-2.680160
H	0.109120	-3.237366	-2.790902	H	-0.195152	3.624059	-3.750755
H	0.113545	-2.432178	-1.213111	C	0.416333	4.619009	-1.955868
H	-0.150690	-4.167314	-1.308518	H	1.157530	5.241451	-2.451451
C	2.197053	3.325568	1.246012	C	0.193487	4.723194	-0.592779
C	3.533998	3.653018	1.534878	H	0.741279	5.437594	0.017081
C	4.146902	4.676208	0.807938	C	-0.756233	3.904793	0.024059
H	5.186788	4.926405	1.025508	C	-4.774879	-0.469248	-1.865762
C	3.457126	5.403223	-0.164039	C	-6.022466	0.125351	-1.603335
C	2.119199	5.079918	-0.405249	C	-6.996374	-0.628648	-0.943656
H	1.562590	5.638129	-1.160230	H	-7.961851	-0.167242	-0.728955
C	1.475133	4.048725	0.276664	C	-6.775480	-1.956194	-0.573035
C	4.276915	2.975598	2.648195	C	-5.542840	-2.535347	-0.889554
H	5.359477	3.004799	2.481524	H	-5.349917	-3.572842	-0.609356
H	3.982469	1.928483	2.779206	C	-4.538274	-1.816327	-1.532536
H	4.084423	3.477446	3.607738	C	-6.344409	1.508866	-2.085601
C	4.134993	6.488193	-0.943289	H	-6.688340	1.484049	-3.129905
H	5.039429	6.846677	-0.438979	H	-5.481133	2.183314	-2.059974
H	3.471076	7.345489	-1.107214	H	-7.146304	1.962088	-1.492814
H	4.438526	6.132166	-1.937649	C	-7.820517	-2.736509	0.162720
C	0.066747	3.679587	-0.080034	H	-8.813785	-2.286141	0.057029
H	-0.441181	4.500352	-0.598484	H	-7.596959	-2.779887	1.237824
H	-0.536643	3.402956	0.793272	H	-7.874537	-3.774212	-0.187681
H	0.044316	2.811610	-0.756711	C	-3.205361	-2.442032	-1.801741
C	0.492320	0.116356	-0.692441	H	-3.195957	-3.498821	-1.514871
O	0.367473	0.232726	-2.031210	H	-2.415430	-1.935236	-1.231969
O	-0.511754	0.037736	0.043913	H	-2.918230	-2.374691	-2.860189
Mg	-2.434852	-0.266375	-0.407949	C	-1.009076	4.117154	1.471487
S	-4.429366	1.495587	-0.804865	C	-2.071117	4.961970	1.853612
O	-5.425995	2.166482	0.018152	C	-2.264564	5.224650	3.210132
O	-4.531674	0.008904	-0.936117	H	-3.090267	5.873512	3.507246
O	-2.991254	1.821011	-0.549995	C	-1.408715	4.712449	4.189637
C	-4.732191	2.119263	-2.511542	C	-0.336923	3.919556	3.777743
F	-4.633851	3.452032	-2.525715	H	0.347210	3.515633	4.526090
F	-5.961356	1.771021	-2.903200	C	-0.123179	3.604103	2.434802
F	-3.844280	1.611761	-3.364429	C	-2.924623	5.649487	0.829074
S	-3.249950	-1.775584	1.674581	H	-2.421385	6.551341	0.450990

H	-3.881375	5.968028	1.256660	H	-1.265982	2.306017	-4.722226
H	-3.135321	5.023377	-0.044992	C	-2.110067	1.837314	-2.791715
C	-1.645309	4.993363	5.641489	C	-1.392483	2.882157	-2.053474
H	-2.133513	5.962740	5.794286	C	-0.527065	3.765731	-2.696808
H	-0.710736	4.984093	6.213993	H	-0.371129	3.705567	-3.768033
H	-2.300323	4.233019	6.089377	C	0.149091	4.720883	-1.956461
C	0.985623	2.663654	2.071437	H	0.837852	5.409245	-2.440226
H	1.378232	2.821393	1.058586	C	-0.080004	4.782777	-0.592028
H	0.642999	1.617494	2.120729	H	0.415659	5.522695	0.031657
H	1.817817	2.751991	2.776810	C	-0.972903	3.891045	0.007019
C	-1.050102	0.194942	0.022611	C	-4.705752	-0.691633	-2.005120
O	-0.790299	-0.821119	0.668947	C	-6.003147	-0.170001	-1.848297
O	1.923462	0.509553	-1.919156	C	-6.967765	-0.959322	-1.217010
C	1.227965	0.255278	-0.919947	H	-7.971444	-0.553037	-1.080988
O	-0.069013	0.621123	-0.936262	C	-6.687501	-2.251163	-0.769947
O	1.745191	-0.301059	0.119461	C	-5.404117	-2.763123	-0.987095
Mg	3.554653	-0.486923	-0.931912	H	-5.163459	-3.772790	-0.648119
S	5.644969	1.109013	-1.373120	C	-4.409623	-2.009201	-1.603889
O	6.999135	1.270882	-0.870482	C	-6.382478	1.170649	-2.403874
O	4.511863	1.401989	-0.442566	H	-6.724293	1.074120	-3.444594
O	5.310804	-0.191576	-2.048956	H	-5.549310	1.881794	-2.417053
C	5.468275	2.352960	-2.721597	H	-7.204873	1.620678	-1.837001
F	5.675550	3.576452	-2.232842	C	-7.722588	-3.063136	-0.055417
F	4.243497	2.293321	-3.244926	H	-8.732720	-2.673685	-0.223600
F	6.363751	2.103789	-3.677824	H	-7.547713	-3.055722	1.029537
S	2.181881	-3.398649	-1.347933	H	-7.701998	-4.113958	-0.368252
O	3.035418	-2.261332	-1.795348	C	-3.033708	-2.567173	-1.787215
O	1.617298	-3.209457	0.017582	H	-2.971203	-3.603102	-1.438255
O	2.718217	-4.720967	-1.614409	H	-2.294556	-1.983772	-1.224719
C	0.709903	-3.202851	-2.443170	H	-2.712702	-2.543218	-2.837638
F	-0.112973	-4.240712	-2.319253	C	-1.214371	4.044854	1.464588
F	1.098851	-3.101570	-3.712436	C	-2.218114	4.929066	1.904663
F	0.053201	-2.083415	-2.099810	C	-2.373371	5.132427	3.276778
Mg	0.958368	-1.754950	1.305476	H	-3.158989	5.806123	3.623137
S	4.112885	-1.552581	2.138583	C	-1.540100	4.514658	4.212722
O	4.968698	-2.486500	2.848980	C	-0.531113	3.669787	3.744877
O	2.657759	-1.660242	2.451579	H	0.125717	3.173633	4.461539
O	4.396227	-1.434528	0.679925	C	-0.353249	3.420020	2.384958
C	4.527670	0.122693	2.782788	C	-3.067543	5.693480	0.932969
F	4.471277	0.120792	4.115515	H	-2.587289	6.644493	0.660730
F	3.656301	1.016799	2.313362	H	-4.044288	5.939445	1.364319
F	5.757778	0.461146	2.396037	H	-3.236511	5.152108	-0.004294
S	-0.702368	-4.173819	2.750080	C	-1.742180	4.727401	5.681178
O	-1.560155	-4.295347	3.925957	H	-2.256725	5.672608	5.887793
O	0.199079	-5.280272	2.433340	H	-0.791020	4.726402	6.226213
O	-0.051496	-2.817409	2.655019	H	-2.355738	3.925714	6.115485
C	-1.862277	-4.104297	1.320853	C	0.718812	2.480101	1.922767
F	-2.489348	-5.275522	1.161527	H	0.476643	2.017597	0.959142
F	-1.173662	-3.839639	0.198876	H	0.885917	1.677024	2.651951
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TS-H1H2				C	-1.308155	0.164794	0.198525
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O	-4.655206	-0.637637	1.192182	O	0.041618	0.684604	-1.147722
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C	-4.300466	2.523845	-0.027337	S	5.787519	0.998483	-1.438547
C	-2.722842	1.661691	1.802435	O	7.158969	1.094987	-0.961204
C	-3.954081	0.077143	0.603144	O	4.695314	1.421035	-0.514196
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H	-4.151312	-0.858530	-4.571409	F	5.952996	3.421386	-2.402188
C	-2.662078	0.685879	-4.826881	F	4.462323	2.176155	-3.374627
H	-2.540912	0.538551	-5.897328	F	6.572045	1.857133	-3.780700
C	-1.948523	1.672336	-4.167180	S	2.296189	-3.438675	-1.154659
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C2-MgOTf2-1

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H 3.549524 0.656937 -5.873753
H 3.239935 1.926397 -4.695542
C 1.823821 -2.755180 -2.491039
H 1.427443 -2.831331 -1.470104
H 2.917894 -2.746415 -2.429417
H 1.530258 -3.677840 -3.012425
C 1.250149 -0.769182 0.040519
O 2.452780 -0.670430 0.047777
Mg -2.956638 0.422305 0.004212

S -4.954324 -1.407873 0.009173
O -5.287980 -2.822699 0.040498
O -4.237718 -0.877964 -1.194370
O -4.269909 -0.818941 1.205447
C -6.574177 -0.529174 -0.033413
F -7.251931 -0.877973 -1.127131
F -6.368170 0.791998 -0.051861
F -7.291703 -0.840726 1.046106
S -3.924861 2.940581 -0.052790
O -3.586880 2.133570 1.163987
O -5.201433 3.637627 -0.067972
O -3.591732 2.073462 -1.229159
C -2.658870 4.281220 -0.093722
F -1.432185 3.775680 -0.071991
F -2.825977 5.078177 0.965753
F -2.819605 5.000438 -1.208297
Mg 4.106026 0.420158 0.029549
S 5.960250 -1.469159 -0.002702
O 7.405181 -1.602969 -0.021514
O 5.304791 -0.812892 -1.186440
O 5.333155 -0.830340 1.205967
C 5.306253 -3.197666 -0.012068
F 5.669154 -3.790804 -1.148523
F 3.979049 -3.198946 0.079247
F 5.818282 -3.862667 1.022074
S 3.023862 2.815133 -0.024791
O 3.393748 2.009912 1.192891
O 1.739125 3.481901 -0.041274
O 3.392299 1.950886 -1.201404
C 4.298144 4.149231 -0.062541
F 4.152190 4.941257 0.997685
F 4.159510 4.867016 -1.175226
F 5.518275 3.605009 -0.040040

C2-MgOTf2-2

Mn 1.079050 -1.105504 -0.448924
O 0.430530 -1.309988 2.422364
O -1.109292 0.840175 -0.203964
N 1.688254 -0.641596 -2.408065
N 3.101179 -1.716549 -0.470710
C 0.780356 -1.249943 1.304563
C -0.150709 0.100523 -0.351083
C 0.907017 -0.160741 -3.415828

C	1.445760	0.277095	-4.621479
H	0.771085	0.659764	-5.384151
C	2.817689	0.212533	-4.843286
H	3.251484	0.555786	-5.779332
C	3.611503	-0.318514	-3.846573
H	4.683256	-0.398824	-3.992672
C	3.030827	-0.744201	-2.646580
C	3.813895	-1.334502	-1.574959
C	5.198283	-1.510617	-1.673501
H	5.729347	-1.175175	-2.557567
C	5.891193	-2.099539	-0.634228
H	6.969918	-2.226855	-0.682609
C	5.158891	-2.568305	0.452455
H	5.644061	-3.102445	1.266719
C	3.778924	-2.400386	0.498715
C	-0.573505	-0.100616	-3.283576
C	-1.195190	1.146824	-3.102460
C	-2.591764	1.218980	-3.119465
H	-3.067599	2.191148	-2.996943
C	-3.389304	0.084290	-3.320170
C	-2.742819	-1.145308	-3.488885
H	-3.342603	-2.038252	-3.661747
C	-1.349897	-1.255782	-3.498760
C	-0.389935	2.387177	-2.858671
H	-0.026547	2.828909	-3.797058
H	0.494404	2.184436	-2.241612
H	-0.990184	3.149545	-2.348327
C	-4.881246	0.198864	-3.415185
H	-5.177502	0.568020	-4.406725
H	-5.287763	0.906490	-2.681420
H	-5.370293	-0.768356	-3.261587
C	-0.712993	-2.572775	-3.825691
H	-1.374971	-3.407731	-3.570796
H	0.239201	-2.723188	-3.304941
H	-0.502085	-2.638586	-4.903012
C	3.041966	-3.086529	1.589705
C	3.111687	-2.615404	2.909517
C	2.486100	-3.346584	3.922015
H	2.525509	-2.969415	4.945564
C	1.793149	-4.527601	3.656707
C	1.757842	-4.989874	2.336078
H	1.246103	-5.927632	2.110879
C	2.388645	-4.303057	1.299289
C	3.813624	-1.330043	3.229856
H	4.899901	-1.468462	3.328421
H	3.453557	-0.907066	4.174655
H	3.662821	-0.575860	2.447350
C	1.096142	-5.280285	4.748523
H	1.398820	-4.927014	5.740570
H	1.299842	-6.357021	4.693625
H	0.005646	-5.165690	4.679478
C	2.440054	-4.899796	-0.076230
H	2.197731	-4.172639	-0.860752
H	1.743484	-5.740220	-0.169229
H	3.447642	-5.280187	-0.299224
C	0.140009	-2.612570	-0.692829
O	-0.598969	-3.525988	-0.683467
Mg	2.068637	1.247313	0.347042
S	4.324420	2.079997	-0.893435
O	5.347132	1.703505	-1.855412
O	4.219987	1.283445	0.373619
O	2.923828	2.262258	-1.390570
C	4.812465	3.757783	-0.303819
F	6.034552	3.709242	0.226574
F	3.951323	4.180925	0.625599
F	4.808756	4.616472	-1.323444
S	1.290546	2.887596	2.339855
O	0.972173	3.010972	0.878848
O	1.763003	4.079766	3.025637
O	2.094843	1.633086	2.483791
C	-0.322480	2.484712	3.139091
F	-0.837324	1.374332	2.618479
F	-1.174755	3.493706	2.957633
F	-0.129328	2.304010	4.448405
Mg	-3.066070	0.386386	-0.379218
S	-4.223971	-1.837777	0.510070
O	-5.057130	-2.099489	1.672890
O	-2.802470	-1.432259	0.742210
O	-4.758561	-0.884195	-0.523525
C	-4.123253	-3.458372	-0.366156
F	-3.516412	-4.345578	0.422182
F	-3.445693	-3.343409	-1.505358
F	-5.358968	-3.885902	-0.638427
S	-4.260264	2.532893	0.732964
O	-3.918501	2.288397	-0.712331
O	-3.903745	3.827344	1.288270
O	-3.834845	1.302818	1.465928
C	-6.104740	2.496747	0.755957
F	-6.573051	3.540452	0.069068
F	-6.536165	2.570617	2.015834
F	-6.558713	1.373969	0.202255
B1-K+			
Mn	0.007668	0.075239	0.370647
O	0.099934	-1.506093	-2.144776
O	-1.709274	-1.997817	1.545769
O	1.645658	-1.882362	1.828107
N	1.325132	1.696175	0.213451
N	-1.299083	1.704533	0.218066
C	0.079194	-0.804272	-1.208485
C	-1.129895	-1.093181	1.045724
C	1.098104	-1.027278	1.216573
C	2.669529	1.647577	0.026643
C	3.466460	2.778432	0.192502
H	4.539385	2.690535	0.038589
C	2.885255	3.994418	0.531909
H	3.494579	4.884521	0.668797
C	1.507278	4.059039	0.659191
H	1.025252	5.005535	0.882467
C	0.748171	2.901092	0.483543
C	-0.713581	2.901500	0.506468
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C	-2.847802	3.990865	0.654222
H	-3.453022	4.874006	0.844087
C	-3.438021	2.789950	0.278467
H	-4.514017	2.709919	0.143008
C	-2.647406	1.664154	0.056126
C	3.291224	0.373524	-0.409016
C	3.148663	-0.037943	-1.750406
C	3.746103	-1.231723	-2.150668
H	3.627809	-1.556607	-3.186073
C	4.495778	-2.015950	-1.266535
C	4.651223	-1.564977	0.044349
H	5.235745	-2.159836	0.748332
C	4.069034	-0.374907	0.489359
C	2.419866	0.812191	-2.748875
H	2.997868	1.714764	-2.993943
H	1.446175	1.156294	-2.377915
H	2.248949	0.265884	-3.682671
C	5.122495	-3.296366	-1.726691
H	5.643604	-3.807666	-0.909949
H	5.850798	-3.121255	-2.529586
H	4.373695	-3.988266	-2.133514

C 4.260819 0.072532 1.907902
H 4.616050 -0.752167 2.535567
H 3.332939 0.456997 2.350205
H 5.001935 0.880734 1.981410
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C -3.106106 0.007632 -1.755783
C -3.723195 -1.164727 -2.188664
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C -4.706494 -1.497994 -0.028074
H -5.325440 -2.086842 0.651022
C -4.101079 -0.333638 0.451617
C -2.330439 0.849896 -2.725171
H -2.858932 1.789562 -2.940678
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H -1.340930 1.129488 -2.342852
C -5.178536 -3.188762 -1.837254
H -5.885215 -2.977180 -2.650685
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H -4.441645 -3.893918 -2.242887
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H -3.353832 0.384682 2.352245
H -4.719669 -0.739871 2.470619
H -4.982647 0.933905 1.969984
K -0.091892 -3.653216 3.022619

B2-K+

Mn -0.000299 -0.157215 0.364394
O 0.001152 -2.648019 -1.207382
O -1.757294 -1.315923 2.422820
O 1.755914 -1.312292 2.425561
N 1.289936 1.279721 -0.353975
N -1.291161 1.279977 -0.349868
C 0.001221 -1.602053 -0.659342
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C 1.131050 -0.809460 1.557237
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C 3.446663 2.284799 -0.800885
H 4.524499 2.148772 -0.865203
C 2.862000 3.532477 -1.081725
H 3.474243 4.394343 -1.335981
C 1.489445 3.611099 -1.082382
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H -0.999368 4.548589 -1.321884
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H -3.478636 4.404334 -1.291571
C -3.449504 2.288946 -0.779709
H -4.527683 2.153940 -0.840295
C -2.666107 1.194977 -0.468394
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H 3.838775 -2.997271 -2.086002
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C 4.818229 -1.620380 0.849097
H 5.432852 -1.835153 1.725405
C 4.149929 -0.394072 0.778397
C 2.495427 -0.731972 -2.644242
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H 6.009613 -4.108379 -0.949005

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H 4.614334 0.103965 2.819951
H 3.359492 1.127713 2.100092
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C -3.242721 -1.054163 -1.389678
C -3.914126 -2.270453 -1.280879
H -3.833109 -2.990154 -2.098112
C -4.704177 -2.582326 -0.167609
C -4.819100 -1.627554 0.841401
H -5.434837 -1.847000 1.715767
C -4.152402 -0.400005 0.777134
C -2.491328 -0.721534 -2.644195
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H -2.409937 -1.595361 -3.300277
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H -6.073475 -3.945007 0.794300
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C -4.303678 0.586200 1.897179
H -3.367341 1.119837 2.104167
H -4.616598 0.087139 2.821287
H -5.058749 1.352044 1.670351
K 0.003536 2.471247 2.242709

II

Mn 0.013168 -0.158246 0.230481
O 0.148090 -2.580224 -1.433465
O -1.735283 -1.596846 2.107322
O 1.683454 -1.210837 2.416393
N 1.313138 1.279370 -0.484003
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C 3.462878 2.280590 -0.965085
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H 3.476910 4.376370 -1.553133
C 1.499203 3.599827 -1.225158
H 1.000636 4.528059 -1.491675
C 0.730396 2.482664 -0.848849
C -0.696644 2.492432 -0.812237
C -1.466528 3.628031 -1.121118
H -0.967130 4.559159 -1.376390
C -2.840633 3.566936 -1.103432
H -3.447775 4.439771 -1.332320
C -3.431455 2.318488 -0.836487
H -4.511567 2.190543 -0.885488
C -2.650731 1.217452 -0.542370
C 3.367087 -0.103965 -0.396050
C 3.375250 -1.057404 -1.435401
C 4.064472 -2.254752 -1.249422
H 4.060708 -2.995413 -2.052024
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H 2.624893 -1.672958 -3.359200
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C -4.184194 0.581114 1.870337
H -3.203003 1.030875 2.072064
H -4.515316 0.073419 2.783750
H -4.880874 1.411859 1.689726
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O -0.571997 1.080090 3.739944
O 0.188031 2.752213 2.290697

TS-III2

Mn 0.013922 -0.111796 0.351633
O 0.205104 -2.398228 -1.492289
O -1.761889 -1.822801 1.946943
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N 1.323340 1.329951 -0.372157
N -1.288411 1.331362 -0.342134
C 0.152569 -1.410275 -0.846594
C -1.144304 -1.083749 1.271944
C 1.113744 -0.814692 1.551586
C 2.680294 1.244555 -0.502289
C 3.465255 2.345687 -0.812895
H 4.542947 2.215130 -0.888126
C 2.870043 3.588702 -1.050334
H 3.472170 4.459941 -1.298789
C 1.495092 3.668814 -1.001611
H 0.998073 4.608197 -1.225243
C 0.737360 2.535729 -0.667227
C -0.703931 2.540772 -0.643592
C -1.462550 3.687476 -0.917877
H -0.964110 4.631259 -1.119504
C -2.839845 3.620191 -0.929810
H -3.442914 4.502888 -1.129746
C -3.433352 2.368642 -0.731716
H -4.512205 2.242788 -0.800654
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C 3.357911 -0.071988 -0.371092
C 3.350500 -0.957589 -1.464544
C 4.038362 -2.168363 -1.356415
H 4.023482 -2.859992 -2.201045
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C 4.782678 -1.591833 0.847517
H 5.341605 -1.834638 1.753605
C 4.100791 -0.376084 0.783071
C 2.672250 -0.587983 -2.750165
H 3.254147 0.166597 -3.299334
H 1.675731 -0.159928 -2.584736

H 2.561136 -1.458735 -3.405671
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H 5.479232 -4.355571 -1.057670
H 5.007551 -4.476951 0.642374
H 6.518196 -3.685178 0.213682
C 4.153308 0.581336 1.936708
H 4.457206 0.072326 2.858234
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C -2.498475 -0.547728 -2.743379
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H -2.419181 -1.389579 -3.440362
H -1.482517 -0.202211 -2.512597
C -5.490241 -3.799904 -0.352856
H -4.806748 -4.655709 -0.431676
H -6.184607 -3.879627 -1.199893
H -6.071822 -3.922375 0.567680
C -4.193895 0.507610 1.900873
H -3.189309 0.818823 2.220323
H -4.673013 0.004613 2.748605
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C -0.229498 1.426187 2.474141
O -0.651790 0.804996 3.426480
O 0.125982 2.529001 2.117615

I2

Mn 0.013516 -0.101721 0.378976
O 0.207815 -2.355585 -1.510046
O -1.759823 -1.876496 1.904231
O 1.712964 -1.403079 2.399863
N 1.329039 1.338627 -0.355991
N -1.289422 1.340091 -0.332396
C 0.155492 -1.377500 -0.851213
C -1.144699 -1.110661 1.259814
C 1.117149 -0.831773 1.559065
C 2.683067 1.251314 -0.487888
C 3.469238 2.354927 -0.792939
H 4.546762 2.224933 -0.870126
C 2.873377 3.597232 -1.021517
H 3.474663 4.470088 -1.266429
C 1.497719 3.678527 -0.968356
H 1.001355 4.619559 -1.185574
C 0.742598 2.544135 -0.636444
C -0.702632 2.549500 -0.614415
C -1.457779 3.698689 -0.882428
H -0.959211 4.644693 -1.071975
C -2.835944 3.630789 -0.902028
H -3.437358 4.515836 -1.096603
C -3.431186 2.380263 -0.716916
H -4.509949 2.255988 -0.788645
C -2.649092 1.262787 -0.461834
C 3.357972 -0.067342 -0.366262
C 3.347858 -0.945033 -1.469092
C 4.028534 -2.157956 -1.370826
H 4.011612 -2.841735 -2.221948
C 4.743912 -2.511054 -0.220798
C 4.774301 -1.604262 0.838723
H 5.331620 -1.857722 1.742610
C 4.097261 -0.382649 0.784131

C	2.673556	-0.558410	-2.751920	C	-1.178562	4.861892	-0.540828
H	3.259003	0.201357	-3.290008	H	-0.439620	5.137740	-1.295200
H	1.677824	-0.129269	-2.584765	C	-0.941264	3.736745	0.252597
H	2.561956	-1.420949	-3.418021	C	-4.051430	3.811150	2.469443
C	5.453340	-3.828332	-0.135617	H	-3.626567	3.912053	3.478063
H	6.074270	-4.012968	-1.021534	H	-4.389517	2.770209	2.382099
H	4.743127	-4.664187	-0.074581	H	-4.935109	4.455868	2.416630
H	6.099862	-3.882962	0.747409	C	-2.575228	6.824706	-1.274221
C	4.153724	0.563453	1.946693	H	-1.646586	7.215147	-1.705542
H	4.455247	0.044491	2.863412	H	-3.074342	7.639387	-0.736258
H	3.183464	1.040670	2.135067	H	-3.230372	6.553450	-2.114051
H	4.876964	1.373842	1.776909	C	0.343846	2.975641	0.113723
C	-3.327335	-0.057558	-0.400409	H	1.128842	3.421264	0.742082
C	-3.256353	-0.917142	-1.516327	H	0.713857	2.992542	-0.918303
C	-3.949043	-2.127228	-1.479488	H	0.245249	1.929945	0.424233
H	-3.887250	-2.795203	-2.341020	C	-3.590373	-2.962033	-0.776497
C	-4.740968	-2.491568	-0.384517	C	-4.983476	-3.131407	-0.886690
C	-4.818278	-1.608577	0.692673	C	-5.528465	-3.403253	-2.140920
H	-5.422013	-1.878732	1.561164	H	-6.609929	-3.518672	-2.231861
C	-4.121088	-0.398000	0.706534	C	-4.728423	-3.525158	-3.279955
C	-2.499622	-0.518801	-2.748774	C	-3.346100	-3.389529	-3.135194
H	-3.003109	0.306731	-3.272380	H	-2.703584	-3.500491	-4.010464
H	-2.418601	-1.355448	-3.451774	C	-2.756175	-3.120955	-1.899116
H	-1.484324	-0.171930	-2.517164	C	-5.869000	-3.038523	0.319745
C	-5.483491	-3.793243	-0.378047	H	-5.827105	-3.958355	0.920609
H	-4.799642	-4.648139	-0.463276	H	-6.915379	-2.885250	0.034122
H	-6.178096	-3.867013	-1.225369	H	-5.576824	-2.220862	0.989808
H	-6.064504	-3.922704	0.541876	C	-5.340212	-3.768124	-4.625019
C	-4.170552	0.490117	1.913827	H	-6.282271	-4.323342	-4.549311
H	-3.159276	0.744194	2.263893	H	-4.664631	-4.324239	-5.285169
H	-4.696768	0.000797	2.741366	H	-5.569340	-2.819522	-5.130894
H	-4.683658	1.440296	1.712298	C	-1.263555	-3.056812	-1.773321
C	-0.239360	1.355620	2.398485	H	-0.855926	-4.031793	-1.467321
O	-0.696121	0.766577	3.369610	H	-0.929776	-2.328314	-1.025132
O	0.127759	2.485568	2.107362	H	-0.794298	-2.798330	-2.729687
TS-J1J2				C	-1.349086	0.242615	-0.956310
Mn	-3.096176	0.342569	0.071219	O	-0.887328	0.511258	-1.998618
O	-5.708146	0.525313	1.501639	O	1.968447	-0.532437	0.966003
O	-4.471312	-0.354146	-2.438936	C	1.144764	-0.490768	-0.029748
O	-3.686835	2.821744	-1.405808	O	-0.132703	-0.477560	0.226737
N	-2.039753	0.976078	1.804208	O	1.626517	-0.470756	-1.221731
N	-2.689791	-1.516037	1.016561	Mg	3.468463	-0.412171	-0.378324
C	-4.678373	0.445406	0.968522	S	5.318999	-2.252135	0.272058
C	-3.926060	-0.220983	-1.418159	O	6.632912	-2.710142	-0.155518
C	-3.392877	1.925774	-0.721901	O	4.177653	-2.438758	-0.675584
C	-1.643451	2.229989	2.120137	O	5.214682	-0.861911	0.814682
C	-0.953630	2.502509	3.304830	C	4.881779	-3.325285	1.703704
H	-0.651789	3.527208	3.508353	F	4.842746	-4.601658	1.312331
C	-0.661628	1.476688	4.187077	F	3.688650	-2.985791	2.192592
H	-0.124846	1.669009	5.113032	F	5.798460	-3.193891	2.666209
C	-1.060030	0.191600	3.857351	S	4.444907	1.746523	-1.660051
H	-0.827214	-0.629923	4.525394	O	3.930522	2.696872	-2.636788
C	-1.739719	-0.035231	2.660683	O	3.804822	1.734124	-0.309877
C	-2.121278	-1.390427	2.244445	O	4.590736	0.322410	-2.093369
C	-1.880284	-2.496576	3.059448	C	6.172746	2.297898	-1.337170
H	-1.444272	-2.372697	4.044333	F	6.866234	2.297079	-2.479204
C	-2.195174	-3.766189	2.603736	F	6.774231	1.488105	-0.466013
H	-2.008822	-4.638837	3.225156	F	6.159423	3.537606	-0.838585
C	-2.743406	-3.894064	1.338912				
H	-2.996068	-4.868460	0.927612				
C	-2.988682	-2.756132	0.565890				
C	-1.906129	3.374252	1.209461				
C	-3.053487	4.166728	1.409495				
C	-3.242466	5.287593	0.604551				
H	-4.136727	5.896233	0.749757				
C	-2.322990	5.645131	-0.386833				