Molecular Structures of Magnesium Dichloride Sheets and Nanoballs

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Supporting Information

Used basis sets for Mg and Cl

Mg 0

S 8 1.00

68370.0 0.0002226

9661.0 0.001901

2041.0 0.011042

529.6 0.05005

159.17 0.1690

54.71 0.36695

21.236 0.4008

8.791 0.1487

SP 5 1.00

143.7 -0.00671 0.00807

31.27 -0.07927 0.06401

9.661 -0.08088 0.2092

3.726 0.2947 0.3460

1.598 0.5714 0.3731

SP 1 1.00

0.6696 1.0 1.0

SP 1 1.00

0.1886 1.0 1.0

D 1 1.00

0.3329 1.0

Cl 0

S 8 1.00

135320.0 0.000225

19440.0 0.00191

4130.0 0.01110

1074.0 0.04989

323.4 0.1703

111.1 0.3683

43.4 0.4036

18.18 0.1459

SP 6 1.00

324.8 -0.00763 0.00820

73.00 -0.0829 0.0605

23.71 -0.1046 0.2115

9.138 0.2540 0.3765

3.930 0.695 0.3967

1.329 0.399 0.186

SP 3 1.00

4.755 -0.3740 -0.0340

1.756 -0.4754 0.1617

0.785 1.3400 0.9250

SP 1 1.00

0.3122 1.0 1.0

SP 1 1.00

```

0.1453 1.0 1.0
D 1 1.00
0.3042 1.0
D 1 1.00
0.1173 1.0
****

```

Mg₄Cl₈ (Optimized)

Input Keywords:

```
#p opt hf/Gen geom=connectivity scfcyc=800
```

Input coordinates:

```

Cl      0.73353600  0.36384200 -2.99428000
Mg      -0.45105500 -0.00297900 -1.01409800
Cl      1.34793500  0.04659900  0.66749500
Mg      -0.49106300 -0.36922500  2.43220400
Cl      -1.93511000 -0.95537200  0.51758500
Cl      -0.16371700 -1.80075200  4.09084800
Cl      0.48339400  4.23372200 -4.27132100
Mg      0.81072100  2.80219100 -2.61267500
Cl      2.25476700  3.38833800 -0.69805500
Mg      0.77071200  2.43594100  0.83362400
Cl      -1.02827800  2.38636400 -0.84797000
Cl      -0.41387800  2.06912200  2.81380600

```

Output coordinates:

```

Cl      -2.037763 -2.064168 -1.041656
Mg      0.000146 -1.656635 -0.000058
Cl      1.030087 -0.000039 -1.511460
Mg      3.024245  0.000141  0.134139
Cl      2.037859 -2.064202  1.041697
Cl      5.104903  0.000035 -0.582753
Cl      -5.104904 -0.000035  0.582753
Mg      -3.024245 -0.000141 -0.134138
Cl      -2.037859  2.064202 -1.041697
Mg      -0.000146  1.656635  0.000058
Cl      -1.030087  0.000040  1.511460
Cl      2.037763  2.064168  1.041656

```

Mg₄Cl₈ (Frozen)

Input Keywords:

```
#p hf/Gen geom=connectivity scfcyc=800
```

Input coordinates:

```

Cl      -2.21636232  1.14758937 -1.36300000
Cl      -2.21636232  4.78858937 -1.36300000
Cl      -0.11436232 -2.49341063  1.36300000
Mg      -1.16536232 -0.67241063  0.00000000
Cl      -0.11436232  1.14758937  1.36300000
Cl      0.93663768 -0.67241063 -1.36300000
Mg      -1.16536232  2.96858937  0.00000000
Cl      0.93663768  2.96858937 -1.36300000
Cl      3.03863768 -4.31441063  1.36300000
Mg      1.98763768 -2.49341063  0.00000000
Cl      3.03863768 -0.67241063  1.36300000
Mg      1.98763768  1.14758937  0.00000000

```

Mg₆Cl₁₂ (Optimized)

Input Keywords:

#p opt hf/Gen geom=connectivity scfcyc=800

Input coordinates:

Cl	0.28851000	-4.23933100	-2.15690000
Mg	0.41032700	-2.00544600	-1.52100100
Cl	0.63901400	-2.53958900	0.85045700
Mg	-0.10082500	-4.92124100	0.18717800
Mg	-1.83380800	-1.89444500	1.09566600
Cl	1.13867300	0.19383400	-1.94615700
Cl	-1.88867200	-1.19769000	-1.29332600
Mg	-0.81515800	1.18051800	-0.86865500
Cl	0.96876900	-6.66993500	1.03806300
Mg	-2.54825600	4.20729300	0.03902300
Cl	-2.31427800	-4.21319700	0.87753100
Mg	-3.05741100	1.29230000	1.75001000
Cl	-0.33557600	3.49968500	-0.65344900
Cl	-0.75881300	0.48443100	1.52010300
Cl	-3.28858500	1.82519700	-0.62163100
Cl	-3.78533200	-0.90719600	2.17597500
Cl	-3.62019900	5.95513600	-0.81067600
Cl	-2.93494100	3.52645500	2.38439000

Output coordinates:

Cl	-4.214212	-1.903096	-1.167017
Mg	-2.101453	-1.945134	-0.222008
Cl	-2.661718	-0.245337	1.445070
Mg	-4.719861	0.230608	-0.045070
Mg	-1.335314	1.392206	-0.034672
Cl	-0.227472	-3.206925	0.416682
Cl	-0.696800	-0.459655	-1.543229
Mg	1.335292	-1.392205	0.034753
Cl	-6.702344	0.527688	0.870635
Mg	4.719847	-0.230573	0.045062
Cl	-3.413626	2.047858	-0.958103
Mg	2.101443	1.945137	0.221893
Cl	3.413606	-2.047779	0.958222
Cl	0.696832	0.459717	1.543237
Cl	2.661748	0.245281	-1.445089
Cl	0.227454	3.206907	-0.416786
Cl	6.702363	-0.527862	-0.870508
Cl	4.214201	1.903177	1.166916

Mg₈Cl₁₆ (Optimized)

Input Keywords:

#p opt hf/Gen geom=connectivity scfcyc=900

Input coordinates:

Cl	3.87608500	-5.21315900	-4.18001000
Mg	3.79650900	-2.82826300	-3.95881900
Mg	3.48708000	-5.76721900	-1.89046800
Cl	4.26301200	-3.25946300	-1.47544900
Cl	1.21345800	-4.91795100	-1.25514300
Mg	2.01804100	-2.50188200	-0.78335100
Cl	1.55009900	-2.07247400	-3.26882600
Cl	4.59706600	-0.40985900	-3.48383800
Cl	4.10251600	-2.21789500	-6.31688000
Mg	4.01312200	0.06998500	-5.82199600
Cl	4.10815800	-6.02568000	0.57156900
Mg	3.20727700	-8.45055000	0.51163900
Cl	3.04037400	-8.11621900	-1.87131600
Mg	2.31981600	0.43463300	-2.85619100

Cl	1.72225900	-3.11194400	1.57666400
Mg	1.80583500	-5.39970800	1.08099400
Mg	2.59900100	3.11635600	-5.26054400
Cl	1.93099700	-0.11743400	-0.56527200
Cl	1.70684300	0.68919300	-5.32160700
Cl	4.66641000	2.24670600	-6.30166000
Cl	1.14768300	-7.57464600	1.56256600
Cl	4.37528700	-10.05467700	1.50794900
Cl	1.42906700	4.71610100	-6.26167700
Cl	2.75697400	2.78540900	-2.87629400

Output coordinates:

Cl	1.333540	-2.972772	0.360576
Mg	-0.622011	-1.684997	-0.152114
Mg	2.971148	-1.288124	0.030250
Cl	0.949918	-0.149338	-1.449682
Cl	2.531459	0.599395	1.603684
Mg	0.622006	1.685362	0.150056
Cl	-0.950168	0.149187	1.448451
Cl	-2.532079	-0.597423	-1.604742
Cl	-2.330099	-3.376067	0.342298
Mg	-4.071662	-1.946093	-0.255273
Cl	4.405067	0.224221	-1.448674
Mg	6.459393	-0.460281	-0.018881
Cl	5.008108	-2.116359	0.945027
Mg	-2.970638	1.287924	-0.028413
Cl	2.330421	3.375560	-0.347096
Mg	4.071583	1.946239	0.252684
Mg	-6.459C18	0.459903	0.021190
Cl	-1.333677	2.973441	-0.359953
Cl	-4.404631	-0.226992	1.448963
Cl	-6.193013	-1.695244	-1.141387
Cl	6.192595	1.696700	1.139975
Cl	8.370630	-0.921275	-1.017630
Cl	-8.370260	0.919358	1.020993
Cl	-5.008264	2.117654	-0.940451

Mg₉Cl₁₈ (Optimized)

Input Keywords:

#p opt hf/Gen geom=connectivity scfcyc=800

Input coordinates:

Cl	0.99934400	-12.83950400	-2.48846400
Cl	4.76936300	-13.00114600	-2.40629200
Cl	-2.64756300	-11.06766900	-0.34965800
Mg	-0.56650400	-11.95101700	-0.98195600
Cl	1.18368400	-10.51323400	-0.08442600
Cl	-0.62160700	-13.37151700	0.99671200
Mg	2.97268400	-12.06975700	-1.18590200
Cl	4.66476300	-10.51892200	-0.06151800
Cl	2.95935900	-13.37231500	0.96061900
Mg	6.52448300	-11.87596300	-1.14954800
Cl	6.77949600	-12.98101000	1.00444800
Mg	-2.45983800	-11.81524000	2.01444500
Cl	-0.58228300	-10.49385200	3.03074800
Mg	1.18848600	-11.93322600	1.99572200
Cl	2.99845600	-10.49472400	2.99477400
Cl	1.19336600	-13.35302100	4.07583100
Mg	4.83687500	-12.05080500	1.97703800
Cl	5.02468700	-12.79833500	4.34114400
Mg	-0.59573100	-11.79626000	5.17740000

Cl	1.37763400	-11.02692700	6.48004000
Mg	2.94350100	-11.91524400	4.97340200
Cl	8.20947800	-10.81997000	-2.14885700
Cl	-2.39240300	-10.86419900	6.39736100
Cl	-4.40270600	-10.88542700	2.98684300
Cl	-2.28764500	-13.34708900	4.05327200
Mg	-4.14746100	-11.98995600	5.14107900
Cl	-5.83222000	-13.04608100	6.14064300

Output coordinates:

Cl	-2.120532	3.972198	0.843403
Cl	-5.322350	1.996565	1.017426
Cl	2.120513	3.972199	-0.843401
Mg	-0.000005	3.446555	0.000013
Cl	-1.030943	1.795866	-1.454259
Cl	1.030960	1.795880	1.454294
Mg	-3.161885	1.842949	0.097575
Cl	-4.057910	-0.000049	-1.463404
Cl	-2.082055	0.000012	1.417206
Mg	-6.178092	-0.000011	-0.061698
Cl	-5.322327	-1.996503	1.0Cl558
Mg	3.161867	1.842949	-0.097594
Cl	2.082027	0.000019	-1.417191
Mg	-0.000004	-0.000001	0.000044
Cl	-1.030909	-1.795855	-1.454273
Cl	1.030894	-1.795844	1.454298
Mg	-3.161899	-1.842959	0.097591
Cl	-2.120546	-3.972215	0.843342
Mg	3.161931	-1.842944	-0.0976Cl
Cl	2.120568	-3.972204	-0.843303
Mg	0.000005	-3.446529	0.000016
Cl	-8.154353	-0.000049	-1.053227
Cl	5.322327	-1.996445	-1.017676
Cl	5.322350	1.996606	-1.017381
Cl	4.057918	-0.000106	1.463384
Mg	6.178101	-0.000006	0.061667
Cl	8.154356	-0.000076	1.053207

Mg₉Cl₁₈ (Frozen)

Input Keywords:

#p hf/Gen geom=connectivity scfcyc=800

Input coordinates:

Cl	-17.98247800	-7.95491400	-1.36300000
Cl	-17.98247800	-4.31391400	-1.36300000
Cl	-17.98247800	-0.67291400	-1.36300000
Cl	-15.88047800	-11.59591400	1.36300000
Mg	-16.93147800	-9.77491400	0.00000000
Cl	-15.88047800	-7.95491400	1.36300000
Cl	-14.82947800	-9.77491400	-1.36300000
Mg	-16.93147800	-6.13391400	0.00000000
Cl	-15.88047800	-4.31391400	1.36300000
Cl	-14.82947800	-6.13391400	-1.36300000
Mg	-16.93147800	-2.49291400	0.00000000
Cl	-14.82947800	-2.49291400	-1.36300000
Cl	-12.72747800	-13.41691400	1.36300000
Mg	-13.77847800	-11.59591400	0.00000000
Cl	-12.72747800	-9.77491400	1.36300000
Cl	-11.67547800	-11.59591400	-1.36300000
Mg	-13.77847800	-7.95491400	0.00000000
Cl	-12.72747800	-6.13391400	1.36300000

Cl	-11.67547800	-7.95491400	-1.36300000
Mg	-13.77847800	-4.31391400	0.00000000
Cl	-11.67547800	-4.31391400	-1.36300000
Cl	-9.57347800	-15.23691400	1.36300000
Mg	-10.62447800	-13.41691400	0.00000000
Cl	-9.57347800	-11.59591400	1.36300000
Mg	-10.62447800	-9.77491400	0.00000000
Cl	-9.57347800	-7.95491400	1.36300000
Mg	-10.62447800	-6.13391400	0.00000000

Mg₁₀Cl₂₀ (Optimized)

Input Keywords:

#p opt hf/Gen geom=connectivity scfcyc=800

Input coordinates:

Cl	4.31871400	-0.55454100	-2.62560900
Mg	4.19570200	1.81882900	-2.52351300
Mg	4.05186200	-0.97896600	-0.27499900
Cl	4.71782500	1.51288500	-0.00880300
Cl	1.75108000	-0.29298300	0.37834200
Mg	2.41683800	2.19852300	0.64398100
Cl	1.92224300	2.47919000	-1.85107500
Cl	4.88391700	4.28545500	-2.17174600
Cl	4.49364800	2.31991300	-4.91225700
Mg	4.28036300	4.61835300	-4.53133500
Cl	4.54657500	-1.26025000	2.21947700
Mg	3.89849500	-3.83383000	1.95178900
Cl	4.23485400	-3.38211600	-0.35478900
Mg	2.56727600	5.05187900	-1.58418600
Cl	2.15040300	1.77474100	2.99489100
Mg	2.27434700	-0.59844100	2.89331600
Mg	2.69823000	7.60566200	-4.13960900
Cl	2.23253400	4.60123700	0.72308200
Cl	1.94289100	5.13243100	-4.05915200
Cl	4.81393600	6.79737700	-5.13195200
Cl	1.58380200	-3.06417900	2.54270800
Mg	2.19088700	-3.39794100	4.90115700
Cl	3.57926300	-6.20066000	2.11097500
Cl	4.52702200	-3.91611200	4.42470800
Mg	3.76696900	-6.38799300	4.50599700
Cl	1.44162300	9.07527600	-5.23199700
Cl	2.88078800	7.41932700	-1.74416200
Cl	1.98183900	-1.09939300	5.28279900
Cl	5.02303800	-7.86034500	5.59525100
Cl	1.65513400	-5.57593900	5.50337700

Output coordinates:

Cl	-0.608157	-3.155993	0.236853
Mg	-2.505426	-1.795092	-0.188047
Mg	1.075766	-1.497314	-0.185148
Cl	-0.853532	-0.292296	-1.512715
Cl	0.853354	0.292926	1.512011
Mg	-1.075723	1.497437	0.184984
Cl	-2.694342	0.011152	1.445166
Cl	-4.366039	-0.621993	-1.605057
Cl	-4.288100	-3.409935	0.339413
Mg	-5.957010	-1.895504	-0.234632
Cl	2.694345	-0.012113	-1.445717
Mg	4.721356	-1.289701	0.038233
Cl	3.003836	-2.870696	0.328966
Mg	-4.721125	1.289538	-0.036426

Cl	0.608140	3.156018	-0.238594
Mg	2.505413	1.795304	0.186106
Mg	-8.234528	0.615000	0.053409
Cl	-3.003978	2.871217	-0.326695
Cl	-6.185984	-0.148535	1.461466
Cl	-8.076441	-1.555967	-1.095194
Cl	4.365726	0.623672	1.604447
Mg	5.956984	1.895621	0.232811
Cl	6.728759	-2.193388	0.951306
Cl	6.186236	0.146501	-1.461090
Mg	8.234633	-0.615259	-0.051700
Cl	-10.105523	1.158107	1.086059
Cl	-6.728804	2.194356	-0.947880
Cl	4.288241	3.409437	-0.343202
Cl	10.105770	-1.159595	-1.083426
Cl	8.076251	1.557105	1.094171

Mg₁₂Cl₂₄ (Optimized)

Input Keywords:

#p opt hf/Gen geom=connectivity scfcyc=800

Input coordinates:

Cl	2.67470500	-12.68479900	-5.56049900
Cl	-0.89476000	-10.75673800	-3.49273800
Mg	1.17238300	-11.74207100	-4.03356900
Cl	2.98117200	-10.39044400	-3.11849700
Cl	1.00287900	-13.14454100	-2.05363700
Mg	4.68476900	-12.03178000	-4.24767800
Cl	4.56573900	-13.37207900	-2.14005800
Cl	-2.74946400	-10.48166300	-0.20298700
Mg	-0.79099100	-11.47459100	-1.13734400
Cl	1.14531400	-10.32500800	-0.07422900
Cl	-0.87078400	-12.96598700	0.92393000
Mg	2.94504200	-11.80214800	-1.03394500
Cl	4.85150600	-10.60907600	0.03943500
Cl	2.83451300	-13.24907700	1.03716300
Mg	6.55427600	-12.22490600	-1.10013700
Cl	6.72685300	-13.09736300	1.16525000
Cl	-0.58656800	-10.20347000	3.10361000
Mg	1.03498000	-11.77162300	1.99682300
Cl	2.97673000	-10.42972300	3.01645200
Cl	0.99953900	-13.18438500	4.08108500
Mg	4.77053300	-12.10064000	2.10041700
Cl	4.87488000	-12.81639300	4.45610000
Mg	2.80672300	-11.83175000	4.99641700
Cl	8.42890600	-13.21706700	-2.16517400
Cl	6.41564200	-12.99232900	-5.53514600
Cl	-4.44834200	-10.35795400	3.12881000
Mg	-2.57476500	-11.35162600	2.06321700
Cl	-2.46477400	-12.97397500	4.04912400
Mg	-4.24766900	-11.57882900	5.21301100
Cl	-2.43483300	-10.58448900	6.49917500
Mg	-0.70504700	-11.54576600	5.21055300
Cl	1.30432900	-10.89158200	6.52453800
Cl	-5.96572800	-12.60444600	6.19116400
Mg	8.22795500	-11.99616000	-4.24971800
Cl	6.44403300	-10.60251700	-3.08616000
Cl	9.94516800	-10.97072300	-5.22924900

Output coordinates:

Cl	4.591141	3.980320	-0.951625
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Cl	0.464570	4.946416	0.658091
Mg	2.406852	3.887700	-0.130374
Cl	3.072653	2.125449	1.401662
Cl	1.047830	2.446807	-1.526629
Mg	5.189246	1.712250	-0.130521
Cl	3.764411	0.107247	-1.420131
Cl	-3.134291	3.776907	0.834994
Mg	-1.009560	3.086035	0.010453
Cl	-0.333396	1.106010	1.360300
Cl	-2.370144	1.481896	-1.436397
Mg	1.731712	0.482867	0.024122
Cl	2.370307	-1.482230	1.436411
Cl	0.333346	-1.105962	-1.360096
Mg	4.479167	-1.898765	-0.075344
Cl	3.134223	-3.776685	-0.835708
Cl	-3.764572	-0.107139	1.420152
Mg	-1.731794	-0.482971	-0.023770
Cl	-1.047878	-2.446620	1.526808
Cl	-3.072733	-2.125696	-1.401431
Mg	1.009663	-3.086076	-0.010588
Cl	-0.464555	-4.946519	-0.657554
Mg	-2.406897	-3.887771	0.130842
Cl	6.610847	-2.438058	-0.944087
Cl	7.360685	1.456600	-0.996777
Cl	-6.610823	2.437923	0.944094
Mg	-4.479178	1.898795	0.075066
Cl	-5.681322	0.214618	-1.484500
Mg	-7.797893	0.639099	-0.144769
Cl	-7.360704	-1.456693	0.996355
Mg	-5.189150	-1.712240	0.130340
Cl	-4.591153	-3.980C16	0.952142
Cl	-9.714370	0.976365	-1.197756
Mg	7.797895	-0.639061	0.144561
Cl	5.681398	-0.214467	1.484292
Cl	9.714484	-0.976215	1.197380

Mg₁₅Cl₃₀ (Optimized)

Input Keywords:

#p opt hf/Gen geom=connectivity scfcyc=800

Input coordinates:

Mg	3.61265600	-5.47589500	-1.21093300
Cl	4.06415900	-3.23901200	-1.76912600
Cl	1.26920800	-4.89881600	-0.87711300
Mg	1.99797900	-2.41754400	-0.69373400
Cl	4.03664900	-5.80487000	1.16182100
Mg	3.49245000	-8.34158200	0.83275000
Cl	3.84764900	-7.77472100	-1.56532500
Cl	2.17735800	-2.84333800	1.75461800
Mg	1.61009100	-5.30113500	1.64627200
Mg	-0.24402500	-2.27748400	2.22078600
Cl	2.25359100	-0.06657200	-1.04486100
Cl	-0.45309000	-1.85298500	-0.27351400
Mg	0.18510400	0.66117100	-0.03394400
Cl	1.11234600	-7.73865000	1.29519000
Mg	1.30233200	-8.23472300	3.76184600
Cl	3.58639500	-10.69979700	0.76155900
Cl	3.82373600	-8.47573800	3.35299600
Mg	3.50187000	-10.99460400	3.17739400
Mg	-1.78575300	3.68355100	0.68365300

Cl	-0.81044400	-4.72774200	2.03059100
Cl	-0.03508900	-2.69975700	4.71517300
Mg	-2.10131700	0.74318200	2.79224700
Mg	-0.67057400	-5.21288900	4.47785800
Mg	-2.48706700	-2.13605500	5.13623900
Cl	0.34260800	3.04171500	-0.26816400
Cl	0.32093500	0.17271000	2.41294100
Cl	-2.29640100	1.13997000	0.34801700
Cl	-2.66642800	-1.71299900	2.68684100
Cl	1.81059000	-5.69020500	4.09188600
Cl	-0.82590500	-7.59344000	4.71356100
Cl	4.91035500	-12.35012800	4.24578000
Cl	1.22292100	-10.60684300	3.89509100
Cl	-2.73993300	-4.48699400	5.48848500
Cl	-1.70555000	6.05558800	0.55190800
Cl	-1.60069400	3.18179800	3.14896300
Cl	-4.30890300	3.92510600	1.08858800
Mg	-3.98545200	6.44262300	1.26777800
Mg	-3.97971500	3.78760800	3.60957200
Cl	-1.76076900	0.34436800	5.31826500
Cl	-4.52629600	1.25073800	3.27662600
Cl	-4.55653900	-1.31643600	6.20588200
Mg	-4.10458000	0.92040600	5.64943700
Cl	-4.07116100	6.14556100	3.68379200
Cl	-4.34075700	3.21859800	6.00603000
Cl	-5.39014800	7.80201700	0.19927100

Output coordinates:

Mg	4.612380	-3.931664	0.191257
Cl	2.802920	-5.209255	-0.573788
Cl	3.097729	-2.637247	1.578443
Mg	1.140158	-3.503719	0.073832
Cl	5.060041	-2.130143	-1.368406
Mg	7.129848	-1.465818	0.134151
Cl	6.796089	-3.774126	0.996273
Cl	1.564029	-1.486822	-1.328255
Mg	3.550387	-0.618475	-0.001569
Mg	0.000004	0.000009	0.000021
Cl	-0.865318	-4.541229	-0.701493
Cl	-0.423481	-2.048143	1.475570
Mg	-2.436216	-2.845079	-0.016707
Cl	5.546414	-0.018662	1.422197
Mg	6.030941	2.038085	0.048Mg5
Cl	9.272279	-0.967640	0.965192
Cl	7.390703	0.477880	-1.511864
Mg	9.467978	1.146081	-0.210515
Mg	-6.031001	-2.038105	-0.048672
Cl	1.976933	0.797370	1.372362
Cl	0.423507	2.048116	-1.475391
Mg	-3.550486	0.618474	0.002363
Mg	2.436187	2.845135	0.016588
Mg	-1.140275	3.503733	-0.073454
Cl	-4.505859	-3.745983	-0.816225
Cl	-1.976910	-0.797209	-1.372102
Cl	-3.953648	-1.378175	1.438619
Cl	-1.563947	1.486727	1.328598
Cl	3.953517	1.377833	-1.438548
Cl	4.505938	3.746244	0.815508
Cl	11.322318	1.667719	-1.300098
Cl	8.107668	2.812482	0.879727
Cl	0.865262	4.541196	0.701660
Cl	-8.107642	-2.812458	-0.880505

Cl	-5.546131	0.018861	-1.422220
Cl	-7.390874	-0.478005	1.511348
Mg	-9.468088	-1.146166	0.209681
Mg	-7.129927	1.465715	-0.134387
Cl	-3.097630	2.637611	-1.577936
Cl	-5.059985	2.129900	1.368819
Cl	-2.802960	5.209200	0.574796
Mg	-4.612331	3.93Cl32	-0.190551
Cl	-9.272Cl3	0.967570	-0.965929
Cl	-6.796021	3.774161	-0.995702
Cl	-11.322454	-1.667731	1.299240

Mg₁₆Cl₃₂ (Optimized)

Input Keywords:

#p Opt hf/Gen geom=connectivity scfcyc=800

Input coordinates:

Cl	-0.95067100	-12.67149000	-5.62423400
Cl	2.82993900	-12.85379600	-5.64914800
Mg	-2.47409500	-11.75514100	-4.08670100
Cl	-0.68229500	-10.37633800	-3.18373300
Cl	-2.60405100	-13.19364300	-2.12683800
Mg	1.05041200	-11.99154600	-4.32902900
Cl	2.86013800	-10.53584000	-3.27188900
Cl	1.01006000	-13.25283700	-2.19598600
Mg	4.70347800	-12.04856900	-4.30863200
Cl	4.63534900	-13.37384500	-2.17064000
Cl	-2.53761200	-10.37946600	-0.07827100
Mg	-0.74208800	-11.81554400	-1.09869400
Cl	1.11067700	-10.49723600	-0.06626700
Cl	-0.78512700	-13.20100500	0.97886700
Mg	2.92363200	-11.85707100	-1.14668000
Cl	4.75964700	-10.60153100	0.00159900
Cl	2.86235400	-13.31794700	0.99215100
Mg	6.54803300	-12.11235200	-1.13024500
Cl	6.76903100	-12.98873200	1.13649700
Cl	-0.68601700	-10.44540300	3.10900800
Mg	1.06587400	-11.88145300	2.01206300
Cl	2.92817200	-10.50273900	3.03935400
Cl	1.00907100	-13.32117800	4.09703700
Mg	4.75498700	-12.11925000	2.05320000
Cl	4.87462000	-12.87462100	4.41086800
Mg	2.79964900	-11.94064500	4.99970900
Cl	8.51425500	-12.95928000	-2.15095700
Cl	6.55041900	-12.89112500	-5.53509200
Cl	-4.54840700	-10.81982800	-3.49750900
Cl	-6.44452500	-10.70878200	-0.22340300
Mg	-4.43028300	-11.57728100	-1.14039100
Cl	-4.43481100	-13.09663600	0.91008800
Mg	-6.22357600	-11.58604000	2.04301800
Cl	-4.31072700	-10.32601600	3.08415900
Mg	-2.59926800	-11.84255300	2.05957800
Cl	-2.53465100	-13.16370400	4.18492500
Mg	-4.37858900	-11.65267300	5.22176100
Cl	-2.50535000	-10.84592600	6.56195800
Mg	-0.72503900	-11.70670800	5.24201300
Cl	1.27543900	-11.02551000	6.53713900
Cl	-6.22568000	-10.81272300	6.44950300
Cl	-8.18919000	-10.73980200	3.06511500
Mg	8.25148600	-11.74989000	-4.23667700

Cl	6.34979300	-10.49726600	-3.10784000
Cl	9.91077400	-10.59540100	-5.17610000
Mg	-7.92621500	-11.95236100	5.14920500
Cl	-6.02467500	-13.20312800	4.01875400
Cl	-9.58550300	-13.10839600	6.08676000

Output coordinates:

Cl	-2.11622700	-5.81443300	-0.84044600
Cl	-5.41006100	-3.94397700	-0.91506700
Mg	-0.00003100	-5.24800600	0.00009400
Cl	-1.04618200	-3.61550900	1.45961600
Cl	1.04609300	-3.61555800	-1.45954300
Mg	-3.19097100	-3.70477700	-0.11283000
Cl	-4.19135800	-1.89491700	1.40372600
Cl	-2.11875400	-1.86906300	-1.38521300
Mg	-6.34028300	-1.84620100	-0.08804400
Cl	-5.24358600	-0.00004900	-1.40506300
Cl	2.11897300	-1.86929200	1.38528400
Mg	0.00014800	-1.80709600	0.00009000
Cl	-1.05450400	-0.00002200	1.37728200
Cl	1.05442600	0.00008700	-1.37704900
Mg	-3.21278100	-0.00009000	0.07117900
Cl	-4.19129000	1.89479800	1.40369900
Cl	-2.11882900	1.86918800	-1.38521100
Mg	-6.34031800	1.84616500	-0.08802500
Cl	-5.41024700	3.94412200	-0.91469900
Cl	2.11882200	1.86913900	1.38531900
Mg	-0.00003100	1.80714500	0.00020800
Cl	-1.04612900	3.61561200	1.45958800
Cl	1.04624800	3.61548200	-1.45953200
Mg	-3.19103400	3.70473500	-0.11281800
Cl	-2.11624800	5.81435000	-0.84064900
Mg	-0.00003900	5.24801700	-0.00013800
Cl	-8.54846500	1.97199500	-0.91900500
Cl	-8.54850700	-1.97223200	-0.91874800
Cl	2.11620100	-5.81445100	0.84054200
Cl	5.41025400	-3.94413600	0.91459200
Mg	3.19095500	-3.70482800	0.11283000
Cl	4.19122100	-1.89478400	-1.40375200
Mg	6.34041000	-1.84618500	0.08819300
Cl	5.24352100	0.00014100	1.40507600
Mg	3.21295100	0.00007600	-0.07142900
Cl	4.19149600	1.89491600	-1.40379800
Mg	6.34018900	1.84624100	0.08789300
Cl	5.40997600	3.94395400	0.91514700
Mg	3.19087300	3.70487500	0.11303100
Cl	2.11611000	5.81457000	0.84045100
Cl	8.54854600	1.97248800	0.91818400
Cl	8.54851400	-1.97184500	0.91926400
Mg	-9.34924300	-0.00003100	0.22441400
Cl	-7.16701600	0.00003700	1.51610900
Cl	-11.27130200	0.00001500	1.32345700
Mg	9.34921500	0.00001600	-0.22455400
Cl	7.16697100	-0.00034400	-1.51611800
Cl	11.27132700	-0.00032300	-1.32350700

Mg₁₆Cl₃₂ (Frozen)

Input Keywords:

#p hf/Gen geom=connectivity scfcyc=800

Input coordinates:

Cl	-17.98247800	-7.95491400	-1.36300000
Cl	-17.98247800	-4.31391400	-1.36300000
Cl	-17.98247800	-0.67291400	-1.36300000
Cl	-17.98247800	2.96808600	-1.36300000
Cl	-15.88047800	-11.59591400	1.36300000
Mg	-16.93147800	-9.77491400	0.00000000
Cl	-15.88047800	-7.95491400	1.36300000
Cl	-14.82947800	-9.77491400	-1.36300000
Mg	-16.93147800	-6.13391400	0.00000000
Cl	-15.88047800	-4.31391400	1.36300000
Cl	-14.82947800	-6.13391400	-1.36300000
Mg	-16.93147800	-2.49291400	0.00000000
Cl	-15.88047800	-0.67291400	1.36300000
Cl	-14.82947800	-2.49291400	-1.36300000
Mg	-16.93147800	1.14808600	0.00000000
Cl	-14.82947800	1.14808600	-1.36300000
Cl	-12.72747800	-13.41691400	1.36300000
Mg	-13.77847800	-11.59591400	0.00000000
Cl	-12.72747800	-9.77491400	1.36300000
Cl	-11.67547800	-11.59591400	-1.36300000
Mg	-13.77847800	-7.95491400	0.00000000
Cl	-12.72747800	-6.13391400	1.36300000
Cl	-11.67547800	-7.95491400	-1.36300000
Mg	-13.77847800	-4.31391400	0.00000000
Cl	-12.72747800	-2.49291400	1.36300000
Cl	-11.67547800	-4.31391400	-1.36300000
Mg	-13.77847800	-0.67291400	0.00000000
Cl	-11.67547800	-0.67291400	-1.36300000
Cl	-9.57347800	-15.23691400	1.36300000
Mg	-10.62447800	-13.41691400	0.00000000
Cl	-9.57347800	-11.59591400	1.36300000
Cl	-8.52247800	-13.41691400	-1.36300000
Mg	-10.62447800	-9.77491400	0.00000000
Cl	-9.57347800	-7.95491400	1.36300000
Cl	-8.52247800	-9.77491400	-1.36300000
Mg	-10.62447800	-6.13391400	0.00000000
Cl	-9.57347800	-4.31391400	1.36300000
Cl	-8.52247800	-6.13391400	-1.36300000
Mg	-10.62447800	-2.49291400	0.00000000
Cl	-8.52247800	-2.49291400	-1.36300000
Cl	-6.42047800	-17.05791400	1.36300000
Mg	-7.47147800	-15.23691400	0.00000000
Cl	-6.42047800	-13.41691400	1.36300000
Mg	-7.47147800	-11.59591400	0.00000000
Cl	-6.42047800	-9.77491400	1.36300000
Mg	-7.47147800	-7.95491400	0.00000000
Cl	-6.42047800	-6.13391400	1.36300000
Mg	-7.47147800	-4.31391400	0.00000000

Mg₂₀Cl₄₀ (Optimized)

Input Keywords:

#p opt hf/Gen geom=connectivity scfcyc=800

Input coordinates:

Cl	3.86720600	-5.22515600	-4.04885500
Mg	3.82811400	-2.83995100	-3.95472100
Mg	3.58767000	-5.69641900	-1.68110600
Cl	4.23795300	-3.17810600	-1.45979100
Cl	1.28508500	-4.99149200	-1.04358400
Mg	1.87132900	-2.55152100	-0.87228700

Cl	1.51459200	-2.16869300	-3.36524800
Cl	4.43104300	-0.31164200	-3.56782500
Cl	4.19532500	-2.23086500	-6.32184900
Mg	3.98631100	0.07917100	-5.92916700
Cl	4.03040700	-5.92618700	0.83840900
Mg	3.43465000	-8.45467400	0.73212000
Cl	3.65953300	-8.08281600	-1.65480700
Mg	2.00371700	0.30357700	-3.09367300
Cl	2.15413400	-2.90013100	1.59376500
Mg	1.68250800	-5.36602600	1.47530800
Mg	-0.21949300	-2.30414500	2.10140600
Mg	2.35366800	3.17080000	-5.40018100
Cl	2.32436200	-0.08521600	-0.65749200
Cl	-0.54112100	-1.91599800	-0.33507300
Mg	-0.08857600	0.55024300	-0.12123400
Cl	1.64508300	0.64438100	-5.58321900
Cl	4.42556700	2.32076200	-6.46811500
Cl	1.06953200	-7.78963800	1.28783900
Mg	1.36481500	-8.18971300	3.75121700
Cl	3.49115600	-10.82653700	0.84528500
Cl	3.86217300	-8.44514300	3.26041600
Mg	3.53714000	-10.96410800	3.26319100
Mg	-1.80442200	3.69577700	0.68804300
Cl	-0.79038200	-4.74594000	1.97776200
Cl	0.14003700	-2.64480900	4.59084000
Mg	-2.04357800	0.83944800	2.96230300
Mg	-0.56893400	-5.17128200	4.40774300
Mg	-2.20133300	-2.07927200	4.93762200
Cl	2.52597200	5.50988900	-5.77416900
Cl	2.57367100	2.74494800	-2.97016400
Cl	-0.10656800	3.65494100	-4.95433200
Cl	-0.37074200	0.89836300	-2.58727300
Mg	0.41924700	6.18908700	-4.74353000
Mg	0.09950500	3.36418100	-2.46885900
Cl	0.49818900	2.99048400	0.05026600
Cl	0.26978100	0.16818700	2.37225700
Cl	-2.45468900	1.17706000	0.46740200
Cl	-2.64648900	-1.68915500	2.57620000
Cl	1.89077000	-5.65530500	3.96092600
Cl	-0.74155600	-7.51031600	4.78234800
Cl	4.97956800	-12.24909000	4.37704900
Cl	1.28497600	-10.54032000	4.05827700
Cl	-2.64035500	-4.32092900	5.47652700
Cl	0.71384300	5.78817000	-2.28027200
Cl	-2.24758300	3.92485900	-1.83143500
Mg	-1.65109300	6.45441100	-1.72506700
Cl	-1.87843400	6.08206300	0.66140400
Cl	-2.08386300	3.22457800	3.05579100
Cl	-2.41101600	0.23078000	5.32965600
Cl	-2.07846700	6.44492900	-4.25250200
Mg	-1.75262400	8.96402400	-4.25554000
Cl	0.49877700	8.53940100	-5.05262100
Cl	-1.70588700	8.82644000	-1.83770400
Cl	-3.19526300	10.24979200	-5.36829500

Output coordinates:

Cl	-2.947123	-5.490026	-0.892731
Mg	-0.810413	-4.849900	-0.053536
Mg	-4.251374	-3.593842	-0.113771
Cl	-2.144106	-3.237331	1.420789
Cl	-3.488463	-1.590318	-1.378864
Mg	-1.428888	-1.238310	0.039289

Cl	-0.057930	-2.879359	-1.356824
Cl	1.276203	-4.337351	1.518172
Cl	0.617833	-6.746279	-0.732071
Mg	2.597178	-5.783176	0.088101
Cl	-5.526939	-1.943425	1.415514
Mg	-7.672539	-2.252984	-0.050993
Cl	-6.432364	-4.160381	-0.888304
Mg	2.023215	-2.378267	0.039652
Cl	-2.753304	0.435106	1.370865
Mg	-4.881895	0.064528	0.067554
Mg	-2.023017	2.378525	-0.039147
Mg	5.480965	-3.725796	0.160137
Cl	0.667396	-0.770760	1.378918
Cl	-0.667606	0.770686	-1.378532
Mg	1.428864	1.238070	-0.039330
Cl	3.343641	-4.020128	-1.400609
Cl	4.777178	-5.976439	0.925331
Cl	-6.900293	-0.264423	-1.394106
Mg	-8.275547	1.383170	-0.081730
Cl	-9.847487	-2.739336	-0.845848
Cl	-8.771687	-0.547965	1.552261
Mg	-10.941779	-0.916173	0.294895
Mg	4.251460	3.593806	0.113807
Cl	-4.116352	2.085171	-1.415847
Cl	-3.343445	4.020013	1.401265
Mg	0.810503	4.849886	0.053594
Mg	-5.481173	3.725779	-0.160060
Mg	-2.597191	5.783139	-0.087280
Cl	7.713355	-3.595476	0.943111
Cl	4.116443	-2.085155	1.416590
Cl	6.150650	-1.802032	-1.384816
Cl	2.753456	-0.435225	-1.370183
Mg	8.275561	-1.383340	0.080632
Mg	4.882371	-0.064432	-0.065516
Cl	3.488402	1.590457	1.379285
Cl	0.058049	2.879368	1.357031
Cl	2.143879	3.237284	-1.420670
Cl	-1.276384	4.337559	-1.517835
Cl	-6.151166	1.802454	1.385021
Cl	-7.713266	3.595411	-0.943879
Cl	-12.824802	-1.209132	1.424525
Cl	-10.486462	1.145286	-0.880882
Cl	-4.777313	5.976589	-0.924304
Cl	6.900977	0.264476	1.394245
Cl	5.526576	1.943370	-1.415094
Mg	7.672599	2.253288	0.050488
Cl	6.432489	4.160392	0.888394
Cl	2.947312	5.490024	0.892676
Cl	-0.617639	6.746174	0.732577
Cl	8.771150	0.547917	-1.553036
Mg	10.941657	0.915980	-0.296358
Cl	10.486621	-1.145482	0.879472
Cl	9.847818	2.739273	0.844663
Cl	12.824308	1.209046	-1.426572

Mg₂₅Cl₅₀ (Optimized)

Input Keywords:

#p opt hf/Gen geom=connectivity scfcyc=800

Input coordinates:

Cl	3.89799931	-5.23347148	-4.00835259
Mg	3.79189783	-2.85307206	-3.94660856
Mg	3.61859382	-5.67825430	-1.63042562
Cl	4.19197183	-3.14333102	-1.44303574
Cl	1.29089112	-5.03546632	-1.02313420
Mg	1.80066448	-2.58749357	-0.85981538
Cl	1.46722359	-2.21397590	-3.37980937
Cl	4.36185227	-0.30528072	-3.60086443
Cl	4.14319806	-2.25823403	-6.32639872
Mg	3.91516689	0.05440786	-5.96694728
Cl	4.04604032	-5.85369835	0.89242813
Mg	3.55031732	-8.40014354	0.81626756
Cl	3.78314890	-8.05739754	-1.57631615
Mg	1.92958874	0.26170285	-3.14173740
Cl	2.07249642	-2.89512320	1.61889633
Mg	1.66928775	-5.37071723	1.51640522
Mg	-0.32336987	-2.36638723	2.15874190
Mg	2.26014950	3.14556437	-5.46403019
Cl	2.24778393	-0.10589291	-0.70220664
Cl	-0.61380561	-1.99116779	-0.33803867
Mg	-0.15022392	0.47671143	-0.19251084
Cl	1.56917146	0.61134821	-5.63269088
Cl	4.33337778	2.29971645	-6.52626415
Cl	1.15846284	-7.82014078	1.33641663
Mg	1.44344844	-8.18080673	3.80955196
Cl	3.71307133	-10.76579620	0.95884533
Cl	3.95832082	-8.33788695	3.34486158
Mg	3.74404267	-10.86604440	3.37938085
Mg	-2.10185076	3.54063398	0.47463619
Cl	-0.81814544	-4.81602438	1.97361464
Cl	-0.09649389	-2.69729551	4.64991003
Mg	-2.22782252	0.69254228	2.75838039
Mg	-0.64129640	-5.23496450	4.42176408
Mg	-2.56094958	-2.19214227	5.07906462
Cl	2.44547954	5.49568310	-5.81660854
Cl	2.47512668	2.72842953	-3.03197095
Cl	-0.20411622	3.65059574	-5.03483160
Cl	-0.44426381	0.84049246	-2.66800784
Mg	0.34083289	6.18845540	-4.80602081
Mg	0.02250641	3.31965454	-2.54378144
Cl	0.31294467	2.94477161	-0.04679477
Cl	0.14473100	0.11276150	2.28330843
Cl	-2.54788703	1.05922849	0.31832838
Cl	-2.77553770	-1.77403561	2.64722886
Cl	1.85846407	-5.62611470	4.00063927
Cl	-0.69816285	-7.59104900	4.79016474
Cl	5.23431780	-12.07518628	4.51688225
Cl	1.46997743	-10.53226316	4.14556842
Cl	-2.74629186	-4.54221002	5.43142884
Cl	0.51757560	5.76938379	-2.35811281
Cl	-2.37314117	3.84862192	-2.00388924
Mg	-1.96955203	6.32483390	-1.90078490
Cl	-1.59210941	5.98894449	0.63819513
Cl	-1.76751641	3.16835385	2.99486207
Cl	-4.49291394	4.09653480	1.05823863
Mg	-3.91988887	6.63147936	1.24545775
Mg	-4.09245046	3.80659337	3.56167588
Cl	-1.86893888	0.34217511	5.24875732
Cl	-4.66116025	1.25885595	3.21610761
Cl	-4.63368677	-1.34578596	6.14152009
Mg	-4.21513148	0.89948070	5.58204687

Cl	-2.15941195	6.57936248	-4.38535147
Mg	-1.74568491	9.13374314	-4.19547065
Cl	0.39714673	8.54455004	-5.17433520
Cl	-4.19890081	6.18694663	3.62343249
Cl	-4.44364600	3.21199858	5.94169745
Cl	-4.08640632	9.01056579	1.19056614
Cl	-4.34688571	6.80589976	-1.27763199
Mg	-3.85286459	9.35290643	-1.20196947
Cl	-1.46049545	8.77425291	-1.72197337
Cl	-4.26145842	9.28920752	-3.72943315
Cl	-4.01373842	11.71868960	-1.34545115
Cl	-1.77525649	11.48429716	-4.53602717
Mg	-4.04856547	11.81773318	-3.76614369
Cl	-5.54051959	13.02642938	-4.90170802

Output coordinates:

Cl	5.42020000	5.80911200	-0.96405900
Mg	3.20617300	5.55134800	-0.13299800
Mg	6.38044600	3.72497500	-0.14898500
Cl	4.23855800	3.75054500	1.36949300
Cl	5.29825500	1.86542200	-1.39939600
Mg	3.21808000	1.86356100	0.00973200
Cl	2.12269800	3.72582600	-1.40469200
Cl	1.05948000	5.44662700	1.45160300
Cl	2.11304000	7.65588000	-0.84523200
Mg	0.00000100	7.07498000	0.00002300
Cl	7.34683800	1.90405600	1.40589700
Mg	9.52514500	1.84169300	-0.03495100
Cl	8.62913000	3.92137800	-0.90560700
Mg	0.00003800	3.63180300	0.00014400
Cl	4.23603600	0.00000000	1.37344300
Mg	6.39384200	-0.00006200	0.07298100
Mg	3.21804000	-1.86368000	0.01011000
Mg	-3.20614800	5.55138400	0.13299900
Cl	1.07202200	1.83976800	1.36850700
Cl	2.12805500	0.00002900	-1.36671000
Mg	0.00000900	0.00005700	0.00005700
Cl	-1.05948100	5.44658100	-1.45149800
Cl	-2.11303300	7.65593200	0.84524000
Cl	8.44974500	0.00005200	-1.37402700
Mg	9.52506900	-1.84176600	-0.03537700
Cl	11.76118700	1.96621500	-0.80075200
Cl	10.31115600	0.00021500	1.59645600
Mg	12.52718900	0.00013100	0.37057000
Mg	-3.21806300	-1.86357500	-0.00994400
Cl	5.29823800	-1.86545000	-1.39930300
Cl	4.23851800	-3.75059200	1.36963800
Mg	-0.00008100	-3.63188700	0.00005300
Mg	6.38068300	-3.72506100	-0.14930500
Mg	3.20628300	-5.55132200	-0.13262900
Cl	-5.42016600	5.80917500	0.96408600
Cl	-2.12271300	3.72583400	1.40477400
Cl	-4.23858200	3.75052100	-1.36942500
Cl	-1.07193500	1.83978900	-1.36832300
Mg	-6.38044400	3.72506100	0.14913600
Mg	-3.21808500	1.86354200	-0.00974600
Cl	-2.12801700	-0.00002500	1.36683600
Cl	1.07188000	-1.83972700	1.36844300
Cl	-1.07191300	-1.83973600	-1.36837500
Cl	2.12276800	-3.72591500	-1.40452400
Cl	7.34707400	-1.90458100	1.40573600
Cl	8.62909800	-3.92112700	-0.90677100

Cl	14.41871500	0.00018200	1.52562000
Cl	11.76133500	-1.96638700	-0.80020600
Cl	5.42031500	-5.80923700	-0.96378800
Cl	-5.29823300	1.86545100	1.39949300
Cl	-4.23608100	0.00003900	-1.37321800
Mg	-6.39399500	-0.00004400	-0.07245500
Cl	-5.29832100	-1.86553000	1.39946000
Cl	-2.12282100	-3.72586200	1.40470100
Cl	-4.23838700	-3.75056800	-1.36957600
Mg	-6.38065300	-3.72499000	0.14904900
Mg	-3.20627800	-5.55127500	0.13279500
Cl	1.05931500	-5.44650100	1.45180100
Cl	-1.05934400	-5.44661700	-1.45157800
Cl	2.11316800	-7.65589600	-0.84472700
Mg	-0.00000600	-7.07489600	0.00019700
Cl	-7.34692000	1.90415100	-1.40578100
Mg	-9.52497900	1.84177500	0.03473300
Cl	-8.62904200	3.92127900	0.90600600
Cl	-5.42038500	-5.80917100	0.96376000
Cl	-2.11318900	-7.65580100	0.84515100
Cl	-8.62927300	-3.92127600	0.90597800
Cl	-7.34672100	-1.90432200	-1.40581100
Mg	-9.52523500	-1.84178100	0.03500500
Cl	-8.44996300	0.00000300	1.37402000
Cl	-10.31101400	-0.00018500	-1.59674500
Cl	-11.76139600	-1.96610500	0.80030300
Cl	-11.76122300	1.96653100	0.79978600
Mg	-12.52714600	0.00010800	-0.37103700
Cl	-14.41858900	-0.00003500	-1.52622100

Mg₂₅Cl₅₀ (Frozen)

Input Keywords:

hf/Gen geom=connectivity scfcyc=800 maxdisk=40gb

Input coordinates:

Cl	-17.98247800	-7.95491400	-1.36300000
Cl	-17.98247800	-4.31391400	-1.36300000
Cl	-17.98247800	-0.67291400	-1.36300000
Cl	-17.98247800	2.96808600	-1.36300000
Cl	-17.98247800	6.60908600	-1.36300000
Cl	-15.88047800	-11.59591400	1.36300000
Mg	-16.93147800	-9.77491400	0.00000000
Cl	-15.88047800	-7.95491400	1.36300000
Cl	-14.82947800	-9.77491400	-1.36300000
Mg	-16.93147800	-6.13391400	0.00000000
Cl	-15.88047800	-4.31391400	1.36300000
Cl	-14.82947800	-6.13391400	-1.36300000
Mg	-16.93147800	-2.49291400	0.00000000
Cl	-15.88047800	-0.67291400	1.36300000
Cl	-14.82947800	-2.49291400	-1.36300000
Mg	-16.93147800	1.14808600	0.00000000
Cl	-15.88047800	2.96808600	1.36300000
Cl	-14.82947800	1.14808600	-1.36300000
Mg	-16.93147800	4.78908600	0.00000000
Cl	-14.82947800	4.78908600	-1.36300000
Cl	-12.72747800	-13.41691400	1.36300000
Mg	-13.77847800	-11.59591400	0.00000000
Cl	-12.72747800	-9.77491400	1.36300000
Cl	-11.67547800	-11.59591400	-1.36300000
Mg	-13.77847800	-7.95491400	0.00000000

Cl	-12.72747800	-6.13391400	1.36300000
Cl	-11.67547800	-7.95491400	-1.36300000
Mg	-13.77847800	-4.31391400	0.00000000
Cl	-12.72747800	-2.49291400	1.36300000
Cl	-11.67547800	-4.31391400	-1.36300000
Mg	-13.77847800	-0.67291400	0.00000000
Cl	-12.72747800	1.14808600	1.36300000
Cl	-11.67547800	-0.67291400	-1.36300000
Mg	-13.77847800	2.96808600	0.00000000
Cl	-11.67547800	2.96808600	-1.36300000
Cl	-9.57347800	-15.23691400	1.36300000
Mg	-10.62447800	-13.41691400	0.00000000
Cl	-9.57347800	-11.59591400	1.36300000
Cl	-8.52247800	-13.41691400	-1.36300000
Mg	-10.62447800	-9.77491400	0.00000000
Cl	-9.57347800	-7.95491400	1.36300000
Cl	-8.52247800	-9.77491400	-1.36300000
Mg	-10.62447800	-6.13391400	0.00000000
Cl	-9.57347800	-4.31391400	1.36300000
Cl	-8.52247800	-6.13391400	-1.36300000
Mg	-10.62447800	-2.49291400	0.00000000
Cl	-9.57347800	-0.67291400	1.36300000
Cl	-8.52247800	-2.49291400	-1.36300000
Mg	-10.62447800	1.14808600	0.00000000
Cl	-8.52247800	1.14808600	-1.36300000
Cl	-6.42047800	-17.05791400	1.36300000
Mg	-7.47147800	-15.23691400	0.00000000
Cl	-6.42047800	-13.41691400	1.36300000
Cl	-5.36947800	-15.23691400	-1.36300000
Mg	-7.47147800	-11.59591400	0.00000000
Cl	-6.42047800	-9.77491400	1.36300000
Cl	-5.36947800	-11.59591400	-1.36300000
Mg	-7.47147800	-7.95491400	0.00000000
Cl	-6.42047800	-6.13391400	1.36300000
Cl	-5.36947800	-7.95491400	-1.36300000
Mg	-7.47147800	-4.31391400	0.00000000
Cl	-6.42047800	-2.49291400	1.36300000
Cl	-5.36947800	-4.31391400	-1.36300000
Mg	-7.47147800	-0.67291400	0.00000000
Cl	-5.36947800	-0.67291400	-1.36300000
Cl	-3.26747800	-18.87791400	1.36300000
Mg	-4.31847800	-17.05791400	0.00000000
Cl	-3.26747800	-15.23691400	1.36300000
Mg	-4.31847800	-13.41691400	0.00000000
Cl	-3.26747800	-11.59591400	1.36300000
Mg	-4.31847800	-9.77491400	0.00000000
Cl	-3.26747800	-7.95491400	1.36300000
Mg	-4.31847800	-6.13391400	0.00000000
Cl	-3.26747800	-4.31391400	1.36300000
Mg	-4.31847800	-2.49291400	0.00000000

Mg₃₆Cl₇₂ (Optimized)

Input Keywords:

#p opt hf/Gen geom=connectivity scfcyc=800

Input coordinates:

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Cl	1.41084000	-1.09899100	7.25347700
Cl	1.27393200	-4.26001000	5.57169100
Cl	1.26586800	-7.38001200	3.75324900

Cl	1.39493900	-10.44708500	1.90388700
Cl	1.71809500	-13.35503700	0.00000000
Cl	1.06564400	5.39142900	7.63640800
Cl	1.43471700	2.08609000	5.53308000
Cl	1.34704800	-1.08980600	3.66428700
Cl	1.29809200	-4.24806800	1.85317100
Cl	1.31718200	-7.36311200	0.00000000
Cl	1.39493900	-10.44708500	-1.90388700
Cl	1.07767700	8.60870700	5.76009100
Cl	1.48244400	5.26889700	3.69348200
Cl	1.39911100	2.09873000	1.85403100
Cl	1.34317800	-1.09048500	0.00000000
Cl	1.29809200	-4.24806800	-1.85317100
Cl	1.26586800	-7.38001200	-3.75324900
Cl	0.88457100	11.81240900	3.89276800
Cl	1.43731000	8.46717900	1.83057300
Cl	1.42582900	5.29359200	0.00000000
Cl	1.39911100	2.09873000	-1.85403100
Cl	1.34704800	-1.08980600	-3.66428700
Cl	1.27393200	-4.26001000	-5.57169100
Cl	0.57927400	14.95505600	1.95013600
Cl	1.31612200	11.63353600	0.00000000
Cl	1.43731000	8.46717900	-1.83057300
Cl	1.48244400	5.26889700	-3.69348200
Cl	1.43471700	2.08609000	-5.53308000
Cl	1.41084000	-1.09899100	-7.25347700
Cl	-1.98412600	17.46704100	0.00000000
Cl	0.57927400	14.95505600	-1.95013600
Cl	0.88457100	11.81240900	-3.89276800
Cl	1.07767700	8.60870700	-5.76009100
Cl	1.06564400	5.39142900	-7.63640800
Cl	0.90629200	2.09479300	-9.47399000
Mg	0.00000000	0.00000000	8.90529000
Mg	-0.19143900	-3.18740300	7.36770300
Mg	-0.25875900	-6.37048800	5.55884700
Mg	-0.19041100	-9.53470700	3.70467700
Mg	0.06117600	-12.66857200	1.83134400
Mg	0.66987500	-15.66306100	0.00000000
Mg	0.19143900	3.18740300	7.36770300
Mg	0.00000000	0.00000000	5.44595300
Mg	-0.03565800	-3.20356700	3.68976300
Mg	-0.06008400	-6.37322200	1.86169800
Mg	0.05170600	-9.52676800	0.00000000
Mg	0.06117600	-12.66857200	-1.83134400
Mg	0.25875900	6.37048800	5.55884700
Mg	0.03565800	3.20356700	3.68976300
Mg	0.00000000	0.00000000	1.82197000
Mg	-0.07291400	-3.19330100	0.00000000
Mg	-0.06008400	-6.37322200	-1.86169800
Mg	-0.19041100	-9.53470700	-3.70467700
Mg	0.19041100	9.53470700	3.70467700
Mg	0.06008400	6.37322200	1.86169800
Mg	0.07291400	3.19330100	0.00000000
Mg	0.00000000	0.00000000	-1.82197000
Mg	-0.03565800	-3.20356700	-3.68976300
Mg	-0.25875900	-6.37048800	-5.55884700
Mg	-0.06117600	12.66857200	1.83134400
Mg	-0.05170600	9.52676800	0.00000000
Mg	0.06008400	6.37322200	-1.86169800
Mg	0.03565800	3.20356700	-3.68976300
Mg	0.00000000	0.00000000	-5.44595300

Mg	-0.19143900	-3.18740300	-7.36770300
Mg	-0.66987500	15.66306100	0.00000000
Mg	-0.06117600	12.66857200	-1.83134400
Mg	0.19041100	9.53470700	-3.70467700
Mg	0.25875900	6.37048800	-5.55884700
Mg	0.19143900	3.18740300	-7.36770300
Mg	0.00000000	0.00000000	-8.90529000
Cl	-0.90629200	-2.09479300	9.47399000
Cl	-1.06564400	-5.39142900	7.63640800
Cl	-1.07767700	-8.60870700	5.76009100
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Cl	-0.57927400	-14.95505600	1.95013600
Cl	1.98412600	-17.46704100	0.00000000
Cl	-1.41084000	1.09899100	7.25347700
Cl	-1.43471700	-2.08609000	5.53308000
Cl	-1.48244400	-5.26889700	3.69348200
Cl	-1.43731000	-8.46717900	1.83057300
Cl	-1.31612200	-11.63353600	0.00000000
Cl	-0.57927400	-14.95505600	-1.95013600
Cl	-1.27393200	4.26001000	5.57169100
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Cl	-1.39911100	-2.09873000	1.85403100
Cl	-1.42582900	-5.29359200	0.00000000
Cl	-1.43731000	-8.46717900	-1.83057300
Cl	-0.88457100	-11.81240900	-3.89276800
Cl	-1.26586800	7.38001200	3.75324900
Cl	-1.29809200	4.24806800	1.85317100
Cl	-1.34317800	1.09048500	0.00000000
Cl	-1.39911100	-2.09873000	-1.85403100
Cl	-1.48244400	-5.26889700	-3.69348200
Cl	-1.07767700	-8.60870700	-5.76009100
Cl	-1.39493900	10.44708500	1.90388700
Cl	-1.31718200	7.36311200	0.00000000
Cl	-1.29809200	4.24806800	-1.85317100
Cl	-1.34704800	1.08980600	-3.66428700
Cl	-1.43471700	-2.08609000	-5.53308000
Cl	-1.06564400	-5.39142900	-7.63640800
Cl	-1.71809500	13.35503700	0.00000000
Cl	-1.39493900	10.44708500	-1.90388700
Cl	-1.26586800	7.38001200	-3.75324900
Cl	-1.27393200	4.26001000	-5.57169100
Cl	-1.41084000	1.09899100	-7.25347700
Cl	-0.90629200	-2.09479300	-9.47399000

Output coordinates:

Cl	5.42020000	5.80911200	-0.96405900
Mg	3.20617300	5.55134800	-0.13299800
Mg	6.38044600	3.72497500	-0.14898500
Cl	4.23855800	3.75054500	1.36949300
Cl	5.29825500	1.86542200	-1.39939600
Mg	3.21808000	1.86356100	0.00973200
Cl	2.12269800	3.72582600	-1.40469200
Cl	1.05948000	5.44662700	1.45160300
Cl	2.11304000	7.65588000	-0.84523200
Mg	0.00000100	7.07498000	0.00002300
Cl	7.34683800	1.90405600	1.40589700
Mg	9.52514500	1.84169300	-0.03495100
Cl	8.62913000	3.92137800	-0.90560700
Mg	0.00003800	3.63180300	0.00014400
Cl	4.23603600	0.00000000	1.37344300
Mg	6.39384200	-0.00006200	0.07298100
Mg	3.21804000	-1.86368000	0.01011000

Mg	-3.20614800	5.55138400	0.13299900
Cl	1.07202200	1.83976800	1.36850700
Cl	2.12805500	0.00002900	-1.36671000
Mg	0.00000900	0.00005700	0.00005700
Cl	-1.05948100	5.44658100	-1.45149800
Cl	-2.11303300	7.65593200	0.84524000
Cl	8.44974500	0.00005200	-1.37402700
Mg	9.52506900	-1.84176600	-0.03537700
Cl	11.76118700	1.96621500	-0.80075200
Cl	10.31115600	0.00021500	1.59645600
Mg	12.52718900	0.00013100	0.37057000
Mg	-3.21806300	-1.86357500	-0.00994400
Cl	5.29823800	-1.86545000	-1.39930300
Cl	4.23851800	-3.75059200	1.36963800
Mg	-0.00008100	-3.63188700	0.00005300
Mg	6.38068300	-3.72506100	-0.14930500
Mg	3.20628300	-5.55132200	-0.13262900
Cl	-5.42016600	5.80917500	0.96408600
Cl	-2.12271300	3.72583400	1.40477400
Cl	-4.23858200	3.75052100	-1.36942500
Cl	-1.07193500	1.83978900	-1.36832300
Mg	-6.38044400	3.72506100	0.14913600
Mg	-3.21808500	1.86354200	-0.00974600
Cl	-2.12801700	-0.00002500	1.36683600
Cl	1.07188000	-1.83972700	1.36844300
Cl	-1.07191300	-1.83973600	-1.36837500
Cl	2.12276800	-3.72591500	-1.40452400
Cl	7.34707400	-1.90458100	1.40573600
Cl	8.62909800	-3.92112700	-0.90677100
Cl	14.41871500	0.00018200	1.52562000
Cl	11.76133500	-1.96638700	-0.80020600
Cl	5.42031500	-5.80923700	-0.96378800
Cl	-5.29823300	1.86545100	1.39949300
Cl	-4.23608100	0.00003900	-1.37321800
Mg	-6.39399500	-0.00004400	-0.07245500
Cl	-5.29832100	-1.86553000	1.39946000
Cl	-2.12282100	-3.72586200	1.40470100
Cl	-4.23838700	-3.75056800	-1.36957600
Mg	-6.38065300	-3.72499000	0.14904900
Mg	-3.20627800	-5.55127500	0.13279500
Cl	1.05931500	-5.44650100	1.45180100
Cl	-1.05934400	-5.44661700	-1.45157800
Cl	2.11316800	-7.65589600	-0.84472700
Mg	-0.00000600	-7.07489600	0.00019700
Cl	-7.34692000	1.90415100	-1.40578100
Mg	-9.52497900	1.84177500	0.03473300
Cl	-8.62904200	3.92127900	0.90600600
Cl	-5.42038500	-5.80917100	0.96376000
Cl	-2.11318900	-7.65580100	0.84515100
Cl	-8.62927300	-3.92127600	0.90597800
Cl	-7.34672100	-1.90432200	-1.40581100
Mg	-9.52523500	-1.84178100	0.03500500
Cl	-8.44996300	0.00000300	1.37402000
Cl	-10.31101400	-0.00018500	-1.59674500
Cl	-11.76139600	-1.96610500	0.80030300
Cl	-11.76122300	1.96653100	0.79978600
Mg	-12.52714600	0.00010800	-0.37103700
Cl	-14.41858900	-0.00003500	-1.52622100

Mg₃₆Cl₇₂ (Frozen)

Input Keywords:

#p hf/Gen geom=connectivity scfcyc=800

Input coordinates:

Cl	-17.98247800	-7.95491400	-1.36300000
Cl	-17.98247800	-4.31391400	-1.36300000
Cl	-17.98247800	-0.67291400	-1.36300000
Cl	-17.98247800	2.96808600	-1.36300000
Cl	-17.98247800	6.60908600	-1.36300000
Cl	-17.98247800	10.25008600	-1.36300000
Cl	-15.88047800	-11.59591400	1.36300000
Mg	-16.93147800	-9.77491400	0.00000000
Cl	-15.88047800	-7.95491400	1.36300000
Cl	-14.82947800	-9.77491400	-1.36300000
Mg	-16.93147800	-6.13391400	0.00000000
Cl	-15.88047800	-4.31391400	1.36300000
Cl	-14.82947800	-6.13391400	-1.36300000
Mg	-16.93147800	-2.49291400	0.00000000
Cl	-15.88047800	-0.67291400	1.36300000
Cl	-14.82947800	-2.49291400	-1.36300000
Mg	-16.93147800	1.14808600	0.00000000
Cl	-15.88047800	2.96808600	1.36300000
Cl	-14.82947800	1.14808600	-1.36300000
Mg	-16.93147800	4.78908600	0.00000000
Cl	-15.88047800	6.60908600	1.36300000
Cl	-14.82947800	4.78908600	-1.36300000
Mg	-16.93147800	8.43008600	0.00000000
Cl	-14.82947800	8.43008600	-1.36300000
Cl	-12.72747800	-13.41691400	1.36300000
Mg	-13.77847800	-11.59591400	0.00000000
Cl	-12.72747800	-9.77491400	1.36300000
Cl	-11.67547800	-11.59591400	-1.36300000
Mg	-13.77847800	-7.95491400	0.00000000
Cl	-12.72747800	-6.13391400	1.36300000
Cl	-11.67547800	-7.95491400	-1.36300000
Mg	-13.77847800	-4.31391400	0.00000000
Cl	-12.72747800	-2.49291400	1.36300000
Cl	-11.67547800	-4.31391400	-1.36300000
Mg	-13.77847800	-0.67291400	0.00000000
Cl	-12.72747800	1.14808600	1.36300000
Cl	-11.67547800	-0.67291400	-1.36300000
Mg	-13.77847800	2.96808600	0.00000000
Cl	-12.72747800	4.78908600	1.36300000
Cl	-11.67547800	2.96808600	-1.36300000
Mg	-13.77847800	6.60908600	0.00000000
Cl	-11.67547800	6.60908600	-1.36300000
Cl	-9.57347800	-15.23691400	1.36300000
Mg	-10.62447800	-13.41691400	0.00000000
Cl	-9.57347800	-11.59591400	1.36300000
Cl	-8.52247800	-13.41691400	-1.36300000
Mg	-10.62447800	-9.77491400	0.00000000
Cl	-9.57347800	-7.95491400	1.36300000
Cl	-8.52247800	-9.77491400	-1.36300000
Mg	-10.62447800	-6.13391400	0.00000000
Cl	-9.57347800	-4.31391400	1.36300000
Cl	-8.52247800	-6.13391400	-1.36300000
Mg	-10.62447800	-2.49291400	0.00000000
Cl	-9.57347800	-0.67291400	1.36300000
Cl	-8.52247800	-2.49291400	-1.36300000
Mg	-10.62447800	1.14808600	0.00000000
Cl	-9.57347800	2.96808600	1.36300000

Cl	-8.52247800	1.14808600	-1.36300000
Mg	-10.62447800	4.78908600	0.00000000
Cl	-8.52247800	4.78908600	-1.36300000
Cl	-6.42047800	-17.05791400	1.36300000
Mg	-7.47147800	-15.23691400	0.00000000
Cl	-6.42047800	-13.41691400	1.36300000
Cl	-5.36947800	-15.23691400	-1.36300000
Mg	-7.47147800	-11.59591400	0.00000000
Cl	-6.42047800	-9.77491400	1.36300000
Cl	-5.36947800	-11.59591400	-1.36300000
Mg	-7.47147800	-7.95491400	0.00000000
Cl	-6.42047800	-6.13391400	1.36300000
Cl	-5.36947800	-7.95491400	-1.36300000
Mg	-7.47147800	-4.31391400	0.00000000
Cl	-6.42047800	-2.49291400	1.36300000
Cl	-5.36947800	-4.31391400	-1.36300000
Mg	-7.47147800	-0.67291400	0.00000000
Cl	-6.42047800	1.14808600	1.36300000
Cl	-5.36947800	-0.67291400	-1.36300000
Mg	-7.47147800	2.96808600	0.00000000
Cl	-5.36947800	2.96808600	-1.36300000
Cl	-3.26747800	-18.87791400	1.36300000
Mg	-4.31847800	-17.05791400	0.00000000
Cl	-3.26747800	-15.23691400	1.36300000
Cl	-2.21647800	-17.05791400	-1.36300000
Mg	-4.31847800	-13.41691400	0.00000000
Cl	-3.26747800	-11.59591400	1.36300000
Cl	-2.21647800	-13.41691400	-1.36300000
Mg	-4.31847800	-9.77491400	0.00000000
Cl	-3.26747800	-7.95491400	1.36300000
Cl	-2.21647800	-9.77491400	-1.36300000
Mg	-4.31847800	-6.13391400	0.00000000
Cl	-3.26747800	-4.31391400	1.36300000
Cl	-2.21647800	-6.13391400	-1.36300000
Mg	-4.31847800	-2.49291400	0.00000000
Cl	-3.26747800	-0.67291400	1.36300000
Cl	-2.21647800	-2.49291400	-1.36300000
Mg	-4.31847800	1.14808600	0.00000000
Cl	-2.21647800	1.14808600	-1.36300000
Cl	-0.11447800	-20.69891400	1.36300000
Mg	-1.16547800	-18.87791400	0.00000000
Cl	-0.11447800	-17.05791400	1.36300000
Mg	-1.16547800	-15.23691400	0.00000000
Cl	-0.11447800	-13.41691400	1.36300000
Mg	-1.16547800	-11.59591400	0.00000000
Cl	-0.11447800	-9.77491400	1.36300000
Mg	-1.16547800	-7.95491400	0.00000000
Cl	-0.11447800	-6.13391400	1.36300000
Mg	-1.16547800	-4.31391400	0.00000000
Cl	-0.11447800	-2.49291400	1.36300000
Mg	-1.16547800	-0.67291400	0.00000000

Mg₄₉Cl₉₈ (Optimized)

Input Keywords:

#p opt hf/gen geom=connectivity scfcyc=800

Input coordinates:

Cl	0.85467100	2.10907200	11.35273100
Cl	1.44337900	-1.07352400	9.13782600
Cl	1.32840100	-4.28447200	7.45682700

Cl	1.30574500	-7.45796800	5.62854300
Cl	1.35556700	-10.59975900	3.77006100
Cl	1.48893600	-13.69514500	1.90115100
Cl	1.78015800	-16.65048200	0.00000000
Cl	1.00394700	5.43169100	9.52999000
Cl	1.41863400	2.12527300	7.43134600
Cl	1.35647900	-1.08906300	5.53817700
Cl	1.32514900	-4.28533200	3.73172000
Cl	1.32475200	-7.44900900	1.87895900
Cl	1.37978200	-10.58780700	0.00000000
Cl	1.48893600	-13.69514500	-1.90115100
Cl	1.03420600	8.65987800	7.66043900
Cl	1.45695300	5.32163800	5.59723000
Cl	1.38813500	2.12681000	3.72316400
Cl	1.35537500	-1.08854400	1.85067800
Cl	1.32208500	-4.27801800	0.00000000
Cl	1.32475200	-7.44900900	-1.87895900
Cl	1.35556700	-10.59975900	-3.77006100
Cl	0.97255200	11.86229800	5.78465800
Cl	1.45055900	8.52228900	3.73294100
Cl	1.41034900	5.33236600	1.87419300
Cl	1.39558500	2.12098200	0.00000000
Cl	1.35537500	-1.08854400	-1.85067800
Cl	1.32514900	-4.28533200	-3.73172000
Cl	1.30574500	-7.45796800	-5.62854300
Cl	0.78553100	15.05088700	3.91223000
Cl	1.37120900	11.71650100	1.85760300
Cl	1.38910500	8.53289000	0.00000000
Cl	1.41034900	5.33236600	-1.87419300
Cl	1.38813500	2.12681000	-3.72316400
Cl	1.35647900	-1.08906300	-5.53817700
Cl	1.32840100	-4.28447200	-7.45682700
Cl	0.56900500	18.17611200	1.96560500
Cl	1.25489500	14.88147600	0.00000000
Cl	1.37120900	11.71650100	-1.85760300
Cl	1.45055900	8.52228900	-3.73294100
Cl	1.45695300	5.32163800	-5.59723000
Cl	1.41863400	2.12527300	-7.43134600
Cl	1.44337900	-1.07352400	-9.13782600
Cl	-1.83640800	20.75969600	0.00000000
Cl	0.56900500	18.17611200	-1.96560500
Cl	0.78553100	15.05088700	-3.91223000
Cl	0.97255200	11.86229800	-5.78465800
Cl	1.03420600	8.65987800	-7.66043900
Cl	1.00394700	5.43169100	-9.52999000
Cl	0.85467100	2.10907200	-11.35273100
Mg	0.00000000	0.00000000	10.76208500
Mg	-0.15691700	-3.21894300	9.25281000
Mg	-0.21985000	-6.41956600	7.44869900
Mg	-0.20327300	-9.60597200	5.59211100
Mg	-0.10054400	-12.77335600	3.72134900
Mg	0.11955200	-15.91123100	1.83832700
Mg	0.62730300	-18.90013500	0.00000000
Mg	0.15691700	3.21894300	9.25281000
Mg	0.00000000	0.00000000	7.32046200
Mg	-0.01584600	-3.23207800	5.57156700
Mg	-0.03227600	-6.42710900	3.74354400
Mg	0.00037500	-9.60548600	1.88157300
Mg	0.12944300	-12.77119400	0.00000000
Mg	0.11955200	-15.91123100	-1.83832700
Mg	0.21985000	6.41956600	7.44869900

Mg	0.01584600	3.23207800	5.57156700
Mg	0.00000000	0.00000000	3.67678800
Mg	-0.04397600	-3.21853800	1.85614500
Mg	-0.05267800	-6.41637900	0.00000000
Mg	0.00037500	-9.60548600	-1.88157300
Mg	-0.10054400	-12.77335600	-3.72134900
Mg	0.20327300	9.60597200	5.59211100
Mg	0.03227600	6.42710900	3.74354400
Mg	0.04397600	3.21853800	1.85614500
Mg	0.00000000	0.00000000	0.00000000
Mg	-0.04397600	-3.21853800	-1.85614500
Mg	-0.03227600	-6.42710900	-3.74354400
Mg	-0.20327300	-9.60597200	-5.59211100
Mg	0.10054400	12.77335600	3.72134900
Mg	-0.00037500	9.60548600	1.88157300
Mg	0.05267800	6.41637900	0.00000000
Mg	0.04397600	3.21853800	-1.85614500
Mg	0.00000000	0.00000000	-3.67678800
Mg	-0.01584600	-3.23207800	-5.57156700
Mg	-0.21985000	-6.41956600	-7.44869900
Mg	-0.11955200	15.91123100	1.83832700
Mg	-0.12944300	12.77119400	0.00000000
Mg	-0.00037500	9.60548600	-1.88157300
Mg	0.03227600	6.42710900	-3.74354400
Mg	0.01584600	3.23207800	-5.57156700
Mg	0.00000000	0.00000000	-7.32046200
Mg	-0.15691700	-3.21894300	-9.25281000
Mg	-0.62730300	18.90013500	0.00000000
Mg	-0.11955200	15.91123100	-1.83832700
Mg	0.10054400	12.77335600	-3.72134900
Mg	0.20327300	9.60597200	-5.59211100
Mg	0.21985000	6.41956600	-7.44869900
Mg	0.15691700	3.21894300	-9.25281000
Mg	0.00000000	0.00000000	-10.76208500
Cl	-0.85467100	-2.10907200	11.35273100
Cl	-1.00394700	-5.43169100	9.52999000
Cl	-1.03420600	-8.65987800	7.66043900
Cl	-0.97255200	-11.86229800	5.78465800
Cl	-0.78553100	-15.05088700	3.91223000
Cl	-0.56900500	-18.17611200	1.96560500
Cl	1.83640800	-20.75969600	0.00000000
Cl	-1.44337900	1.07352400	9.13782600
Cl	-1.41863400	-2.12527300	7.43134600
Cl	-1.45695300	-5.32163800	5.59723000
Cl	-1.45055900	-8.52228900	3.73294100
Cl	-1.37120900	-11.71650100	1.85760300
Cl	-1.25489500	-14.88147600	0.00000000
Cl	-0.56900500	-18.17611200	-1.96560500
Cl	-1.32840100	4.28447200	7.45682700
Cl	-1.35647900	1.08906300	5.53817700
Cl	-1.38813500	-2.12681000	3.72316400
Cl	-1.41034900	-5.33236600	1.87419300
Cl	-1.38910500	-8.53289000	0.00000000
Cl	-1.37120900	-11.71650100	-1.85760300
Cl	-0.78553100	-15.05088700	-3.91223000
Cl	-1.30574500	7.45796800	5.62854300
Cl	-1.32514900	4.28533200	3.73172000
Cl	-1.35537500	1.08854400	1.85067800
Cl	-1.39558500	-2.12098200	0.00000000
Cl	-1.41034900	-5.33236600	-1.87419300
Cl	-1.45055900	-8.52228900	-3.73294100

Cl	-0.97255200	-11.86229800	-5.78465800
Cl	-1.35556700	10.59975900	3.77006100
Cl	-1.32475200	7.44900900	1.87895900
Cl	-1.32208500	4.27801800	0.00000000
Cl	-1.35537500	1.08854400	-1.85067800
Cl	-1.38813500	-2.12681000	-3.72316400
Cl	-1.45695300	-5.32163800	-5.59723000
Cl	-1.03420600	-8.65987800	-7.66043900
Cl	-1.48893600	13.69514500	1.90115100
Cl	-1.37978200	10.58780700	0.00000000
Cl	-1.32475200	7.44900900	-1.87895900
Cl	-1.32514900	4.28533200	-3.73172000
Cl	-1.35647900	1.08906300	-5.53817700
Cl	-1.41863400	-2.12527300	-7.43134600
Cl	-1.00394700	-5.43169100	-9.52999000
Cl	-1.78015800	16.65048200	0.00000000
Cl	-1.48893600	13.69514500	-1.90115100
Cl	-1.35556700	10.59975900	-3.77006100
Cl	-1.30574500	7.45796800	-5.62854300
Cl	-1.32840100	4.28447200	-7.45682700
Cl	-1.44337900	1.07352400	-9.13782600
Cl	-0.85467100	-2.10907200	-11.35273100

Output coordinates:

Cl	0.85043800	2.11077400	9.50106400
Cl	1.44737800	-1.06761700	7.28832800
Cl	1.34480600	-4.26675400	5.60272100
Cl	1.34646100	-7.41555000	3.76919500
Cl	1.43835600	-10.51557100	1.90387300
Cl	1.68652500	-13.47497800	0.00000000
Cl	0.98593300	5.42856400	7.67090400
Cl	1.41294900	2.12481900	5.57761000
Cl	1.36096500	-1.08196100	3.68566700
Cl	1.34229700	-4.26518600	1.86914700
Cl	1.36576800	-7.40853700	0.00000000
Cl	1.43835600	-10.51557100	-1.90387300
Cl	0.99090900	8.64703100	5.79180100
Cl	1.43684900	5.31231700	3.73508300
Cl	1.38318700	2.12590700	1.86475200
Cl	1.36138100	-1.08245500	0.00000000
Cl	1.34229700	-4.26518600	-1.86914700
Cl	1.34646100	-7.41555000	-3.76919500
Cl	0.85293600	11.84139700	3.91508400
Cl	1.39616600	8.50372200	1.86126400
Cl	1.38432300	5.32682600	0.00000000
Cl	1.38318700	2.12590700	-1.86475200
Cl	1.36096500	-1.08196100	-3.68566700
Cl	1.34480600	-4.26675400	-5.60272100
Cl	0.68272200	14.96937500	1.96507900
Cl	1.31992900	11.66455300	0.00000000
Cl	1.39616600	8.50372200	-1.86126400
Cl	1.43684900	5.31231700	-3.73508300
Cl	1.41294900	2.12481900	-5.57761000
Cl	1.44737800	-1.06761700	-7.28832800
Cl	-1.69155000	17.58377800	0.00000000
Cl	0.68272200	14.96937500	-1.96507900
Cl	0.85293600	11.84139700	-3.91508400
Cl	0.99090900	8.64703100	-5.79180100
Cl	0.98593300	5.42856400	-7.67090400
Cl	0.85043800	2.11077400	-9.50106400
Mg	0.00000000	0.00000000	8.91373700
Mg	-0.14642100	-3.21485100	7.39992200

Mg	-0.19172400	-6.40541900	5.58761900
Mg	-0.13713400	-9.57515000	3.72375100
Mg	0.03789500	-12.71624100	1.83987800
Mg	0.50378800	-15.71124400	0.00000000
Mg	0.14642100	3.21485100	7.39992200
Mg	0.00000000	0.00000000	5.47211700
Mg	-0.00421400	-3.22583200	3.71678400
Mg	-0.00448600	-6.41118700	1.87845400
Mg	0.09176100	-9.57891700	0.00000000
Mg	0.03789500	-12.71624100	-1.83987800
Mg	0.19172400	6.40541900	5.58761900
Mg	0.00421400	3.22583200	3.71678400
Mg	0.00000000	0.00000000	1.83098200
Mg	-0.03564600	-3.21440600	0.00000000
Mg	-0.00448600	-6.41118700	-1.87845400
Mg	-0.13713400	-9.57515000	-3.72375100
Mg	0.13713400	9.57515000	3.72375100
Mg	0.00448600	6.41118700	1.87845400
Mg	0.03564600	3.21440600	0.00000000
Mg	0.00000000	0.00000000	-1.83098200
Mg	-0.00421400	-3.22583200	-3.71678400
Mg	-0.19172400	-6.40541900	-5.58761900
Mg	-0.03789500	12.71624100	1.83987800
Mg	-0.09176100	9.57891700	0.00000000
Mg	0.00448600	6.41118700	-1.87845400
Mg	0.00421400	3.22583200	-3.71678400
Mg	0.00000000	0.00000000	-5.47211700
Mg	-0.14642100	-3.21485100	-7.39992200
Mg	-0.50378800	15.71124400	0.00000000
Mg	-0.03789500	12.71624100	-1.83987800
Mg	0.13713400	9.57515000	-3.72375100
Mg	0.19172400	6.40541900	-5.58761900
Mg	0.14642100	3.21485100	-7.39992200
Mg	0.00000000	0.00000000	-8.91373700
Cl	-0.85043800	-2.11077400	9.50106400
Cl	-0.98593300	-5.42856400	7.67090400
Cl	-0.99090900	-8.64703100	5.79180100
Cl	-0.85293600	-11.84139700	3.91508400
Cl	-0.68272200	-14.96937500	1.96507900
Cl	1.69155000	-17.58377800	0.00000000
Cl	-1.44737800	1.06761700	7.28832800
Cl	-1.41294900	-2.12481900	5.57761000
Cl	-1.43684900	-5.31231700	3.73508300
Cl	-1.39616600	-8.50372200	1.86126400
Cl	-1.31992900	-11.66455300	0.00000000
Cl	-0.68272200	-14.96937500	-1.96507900
Cl	-1.34480600	4.26675400	5.60272100
Cl	-1.36096500	1.08196100	3.68566700
Cl	-1.38318700	-2.12590700	1.86475200
Cl	-1.38432300	-5.32682600	0.00000000
Cl	-1.39616600	-8.50372200	-1.86126400
Cl	-0.85293600	-11.84139700	-3.91508400
Cl	-1.34646100	7.41555000	3.76919500
Cl	-1.34229700	4.26518600	1.86914700
Cl	-1.36138100	1.08245500	0.00000000
Cl	-1.38318700	-2.12590700	-1.86475200
Cl	-1.43684900	-5.31231700	-3.73508300
Cl	-0.99090900	-8.64703100	-5.79180100
Cl	-1.43835600	10.51557100	1.90387300
Cl	-1.36576800	7.40853700	0.00000000
Cl	-1.34229700	4.26518600	-1.86914700

Cl	-1.36096500	1.08196100	-3.68566700
Cl	-1.41294900	-2.12481900	-5.57761000
Cl	-0.98593300	-5.42856400	-7.67090400
Cl	-1.68652500	13.47497800	0.00000000
Cl	-1.43835600	10.51557100	-1.90387300
Cl	-1.34646100	7.41555000	-3.76919500
Cl	-1.34480600	4.26675400	-5.60272100
Cl	-1.44737800	1.06761700	-7.28832800
Cl	-0.85043800	-2.11077400	-9.50106400

Mg₄₉Cl₉₈ (Frozen)

Input Keywords:

#p hf/Gen geom=connectivity scfcyc=800

Input coordinates:

Cl	-17.98247800	-7.95491400	-1.36300000
Cl	-17.98247800	-4.31391400	-1.36300000
Cl	-17.98247800	-0.67291400	-1.36300000
Cl	-17.98247800	2.96808600	-1.36300000
Cl	-17.98247800	6.60908600	-1.36300000
Cl	-17.98247800	10.25008600	-1.36300000
Cl	-17.98247800	13.89108600	-1.36300000
Cl	-15.88047800	-11.59591400	1.36300000
Mg	-16.93147800	-9.77491400	0.00000000
Cl	-15.88047800	-7.95491400	1.36300000
Cl	-14.82947800	-9.77491400	-1.36300000
Mg	-16.93147800	-6.13391400	0.00000000
Cl	-15.88047800	-4.31391400	1.36300000
Cl	-14.82947800	-6.13391400	-1.36300000
Mg	-16.93147800	-2.49291400	0.00000000
Cl	-15.88047800	-0.67291400	1.36300000
Cl	-14.82947800	-2.49291400	-1.36300000
Mg	-16.93147800	1.14808600	0.00000000
Cl	-15.88047800	2.96808600	1.36300000
Cl	-14.82947800	1.14808600	-1.36300000
Mg	-16.93147800	4.78908600	0.00000000
Cl	-15.88047800	6.60908600	1.36300000
Cl	-14.82947800	4.78908600	-1.36300000
Mg	-16.93147800	8.43008600	0.00000000
Cl	-15.88047800	10.25008600	1.36300000
Cl	-14.82947800	8.43008600	-1.36300000
Mg	-16.93147800	12.07108600	0.00000000
Cl	-14.82947800	12.07108600	-1.36300000
Cl	-12.72747800	-13.41691400	1.36300000
Mg	-13.77847800	-11.59591400	0.00000000
Cl	-12.72747800	-9.77491400	1.36300000
Cl	-11.67547800	-11.59591400	-1.36300000
Mg	-13.77847800	-7.95491400	0.00000000
Cl	-12.72747800	-6.13391400	1.36300000
Cl	-11.67547800	-7.95491400	-1.36300000
Mg	-13.77847800	-4.31391400	0.00000000
Cl	-12.72747800	-2.49291400	1.36300000
Cl	-11.67547800	-4.31391400	-1.36300000
Mg	-13.77847800	-0.67291400	0.00000000
Cl	-12.72747800	1.14808600	1.36300000
Cl	-11.67547800	-0.67291400	-1.36300000
Mg	-13.77847800	2.96808600	0.00000000
Cl	-12.72747800	4.78908600	1.36300000
Cl	-11.67547800	2.96808600	-1.36300000
Mg	-13.77847800	6.60908600	0.00000000

Cl	-12.72747800	8.43008600	1.36300000
Cl	-11.67547800	6.60908600	-1.36300000
Mg	-13.77847800	10.25008600	0.00000000
Cl	-11.67547800	10.25008600	-1.36300000
Cl	-9.57347800	-15.23691400	1.36300000
Mg	-10.62447800	-13.41691400	0.00000000
Cl	-9.57347800	-11.59591400	1.36300000
Cl	-8.52247800	-13.41691400	-1.36300000
Mg	-10.62447800	-9.77491400	0.00000000
Cl	-9.57347800	-7.95491400	1.36300000
Cl	-8.52247800	-9.77491400	-1.36300000
Mg	-10.62447800	-6.13391400	0.00000000
Cl	-9.57347800	-4.31391400	1.36300000
Cl	-8.52247800	-6.13391400	-1.36300000
Mg	-10.62447800	-2.49291400	0.00000000
Cl	-9.57347800	-0.67291400	1.36300000
Cl	-8.52247800	-2.49291400	-1.36300000
Mg	-10.62447800	1.14808600	0.00000000
Cl	-9.57347800	2.96808600	1.36300000
Cl	-8.52247800	1.14808600	-1.36300000
Mg	-10.62447800	4.78908600	0.00000000
Cl	-9.57347800	6.60908600	1.36300000
Cl	-8.52247800	4.78908600	-1.36300000
Mg	-10.62447800	8.43008600	0.00000000
Cl	-8.52247800	8.43008600	-1.36300000
Cl	-6.42047800	-17.05791400	1.36300000
Mg	-7.47147800	-15.23691400	0.00000000
Cl	-6.42047800	-13.41691400	1.36300000
Cl	-5.36947800	-15.23691400	-1.36300000
Mg	-7.47147800	-11.59591400	0.00000000
Cl	-6.42047800	-9.77491400	1.36300000
Cl	-5.36947800	-11.59591400	-1.36300000
Mg	-7.47147800	-7.95491400	0.00000000
Cl	-6.42047800	-6.13391400	1.36300000
Cl	-5.36947800	-7.95491400	-1.36300000
Mg	-7.47147800	-4.31391400	0.00000000
Cl	-6.42047800	-2.49291400	1.36300000
Cl	-5.36947800	-4.31391400	-1.36300000
Mg	-7.47147800	-0.67291400	0.00000000
Cl	-6.42047800	1.14808600	1.36300000
Cl	-5.36947800	-0.67291400	-1.36300000
Mg	-7.47147800	2.96808600	0.00000000
Cl	-6.42047800	4.78908600	1.36300000
Cl	-5.36947800	2.96808600	-1.36300000
Mg	-7.47147800	6.60908600	0.00000000
Cl	-5.36947800	6.60908600	-1.36300000
Cl	-3.26747800	-18.87791400	1.36300000
Mg	-4.31847800	-17.05791400	0.00000000
Cl	-3.26747800	-15.23691400	1.36300000
Cl	-2.21647800	-17.05791400	-1.36300000
Mg	-4.31847800	-13.41691400	0.00000000
Cl	-3.26747800	-11.59591400	1.36300000
Cl	-2.21647800	-13.41691400	-1.36300000
Mg	-4.31847800	-9.77491400	0.00000000
Cl	-3.26747800	-7.95491400	1.36300000
Cl	-2.21647800	-9.77491400	-1.36300000
Mg	-4.31847800	-6.13391400	0.00000000
Cl	-3.26747800	-4.31391400	1.36300000
Cl	-2.21647800	-6.13391400	-1.36300000
Mg	-4.31847800	-2.49291400	0.00000000
Cl	-3.26747800	-0.67291400	1.36300000

Cl	-2.21647800	-2.49291400	-1.36300000
Mg	-4.31847800	1.14808600	0.00000000
Cl	-3.26747800	2.96808600	1.36300000
Cl	-2.21647800	1.14808600	-1.36300000
Mg	-4.31847800	4.78908600	0.00000000
Cl	-2.21647800	4.78908600	-1.36300000
Cl	-0.11447800	-20.69891400	1.36300000
Mg	-1.16547800	-18.87791400	0.00000000
Cl	-0.11447800	-17.05791400	1.36300000
Cl	0.93652200	-18.87791400	-1.36300000
Mg	-1.16547800	-15.23691400	0.00000000
Cl	-0.11447800	-13.41691400	1.36300000
Cl	0.93652200	-15.23691400	-1.36300000
Mg	-1.16547800	-11.59591400	0.00000000
Cl	-0.11447800	-9.77491400	1.36300000
Cl	0.93652200	-11.59591400	-1.36300000
Mg	-1.16547800	-7.95491400	0.00000000
Cl	-0.11447800	-6.13391400	1.36300000
Cl	0.93652200	-7.95491400	-1.36300000
Mg	-1.16547800	-4.31391400	0.00000000
Cl	-0.11447800	-2.49291400	1.36300000
Cl	0.93652200	-4.31391400	-1.36300000
Mg	-1.16547800	-0.67291400	0.00000000
Cl	-0.11447800	1.14808600	1.36300000
Cl	0.93652200	-0.67291400	-1.36300000
Mg	-1.16547800	2.96808600	0.00000000
Cl	0.93652200	2.96808600	-1.36300000
Cl	3.03852200	-22.51891400	1.36300000
Mg	1.98752200	-20.69891400	0.00000000
Cl	3.03852200	-18.87791400	1.36300000
Mg	1.98752200	-17.05791400	0.00000000
Cl	3.03852200	-15.23691400	1.36300000
Mg	1.98752200	-13.41691400	0.00000000
Cl	3.03852200	-11.59591400	1.36300000
Mg	1.98752200	-9.77491400	0.00000000
Cl	3.03852200	-7.95491400	1.36300000
Mg	1.98752200	-6.13391400	0.00000000
Cl	3.03852200	-4.31391400	1.36300000
Mg	1.98752200	-2.49291400	0.00000000
Cl	3.03852200	-0.67291400	1.36300000
Mg	1.98752200	1.14808600	0.00000000

Mg₆₄Cl_{Mg8} (Frozen)

Input Keywords:

#p hf/Gen geom=connectivity scfcyc=800 MaxDisk=40GB

Input coordinates:

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Cl	-17.98247800	-4.31391400	-1.36300000
Cl	-17.98247800	-0.67291400	-1.36300000
Cl	-17.98247800	2.96808600	-1.36300000
Cl	-17.98247800	6.60908600	-1.36300000
Cl	-17.98247800	10.25008600	-1.36300000
Cl	-17.98247800	13.89108600	-1.36300000
Cl	-17.98247800	17.53208600	-1.36300000
Cl	-15.88047800	-11.59591400	1.36300000
Mg	-16.93147800	-9.77491400	0.00000000
Cl	-15.88047800	-7.95491400	1.36300000
Cl	-14.82947800	-9.77491400	-1.36300000
Mg	-16.93147800	-6.13391400	0.00000000

Cl	-15.88047800	-4.31391400	1.36300000
Cl	-14.82947800	-6.13391400	-1.36300000
Mg	-16.93147800	-2.49291400	0.00000000
Cl	-15.88047800	-0.67291400	1.36300000
Cl	-14.82947800	-2.49291400	-1.36300000
Mg	-16.93147800	1.14808600	0.00000000
Cl	-15.88047800	2.96808600	1.36300000
Cl	-14.82947800	1.14808600	-1.36300000
Mg	-16.93147800	4.78908600	0.00000000
Cl	-15.88047800	6.60908600	1.36300000
Cl	-14.82947800	4.78908600	-1.36300000
Mg	-16.93147800	8.43008600	0.00000000
Cl	-15.88047800	10.25008600	1.36300000
Cl	-14.82947800	8.43008600	-1.36300000
Mg	-16.93147800	12.07108600	0.00000000
Cl	-15.88047800	13.89108600	1.36300000
Cl	-14.82947800	12.07108600	-1.36300000
Mg	-16.93147800	15.71208600	0.00000000
Cl	-14.82947800	15.71208600	-1.36300000
Cl	-12.72747800	-13.41691400	1.36300000
Mg	-13.77847800	-11.59591400	0.00000000
Cl	-12.72747800	-9.77491400	1.36300000
Cl	-11.67547800	-11.59591400	-1.36300000
Mg	-13.77847800	-7.95491400	0.00000000
Cl	-12.72747800	-6.13391400	1.36300000
Cl	-11.67547800	-7.95491400	-1.36300000
Mg	-13.77847800	-4.31391400	0.00000000
Cl	-12.72747800	-2.49291400	1.36300000
Cl	-11.67547800	-4.31391400	-1.36300000
Mg	-13.77847800	-0.67291400	0.00000000
Cl	-12.72747800	1.14808600	1.36300000
Cl	-11.67547800	-0.67291400	-1.36300000
Mg	-13.77847800	2.96808600	0.00000000
Cl	-12.72747800	4.78908600	1.36300000
Cl	-11.67547800	2.96808600	-1.36300000
Mg	-13.77847800	6.60908600	0.00000000
Cl	-12.72747800	8.43008600	1.36300000
Cl	-11.67547800	6.60908600	-1.36300000
Mg	-13.77847800	10.25008600	0.00000000
Cl	-12.72747800	12.07108600	1.36300000
Cl	-11.67547800	10.25008600	-1.36300000
Mg	-13.77847800	13.89108600	0.00000000
Cl	-11.67547800	13.89108600	-1.36300000
Cl	-9.57347800	-15.23691400	1.36300000
Mg	-10.62447800	-13.41691400	0.00000000
Cl	-9.57347800	-11.59591400	1.36300000
Cl	-8.52247800	-13.41691400	-1.36300000
Mg	-10.62447800	-9.77491400	0.00000000
Cl	-9.57347800	-7.95491400	1.36300000
Cl	-8.52247800	-9.77491400	-1.36300000
Mg	-10.62447800	-6.13391400	0.00000000
Cl	-9.57347800	-4.31391400	1.36300000
Cl	-8.52247800	-6.13391400	-1.36300000
Mg	-10.62447800	-2.49291400	0.00000000
Cl	-9.57347800	-0.67291400	1.36300000
Cl	-8.52247800	-2.49291400	-1.36300000
Mg	-10.62447800	1.14808600	0.00000000
Cl	-9.57347800	2.96808600	1.36300000
Cl	-8.52247800	1.14808600	-1.36300000
Mg	-10.62447800	4.78908600	0.00000000
Cl	-9.57347800	6.60908600	1.36300000

Cl	-8.52247800	4.78908600	-1.36300000
Mg	-10.62447800	8.43008600	0.00000000
Cl	-9.57347800	10.25008600	1.36300000
Cl	-8.52247800	8.43008600	-1.36300000
Mg	-10.62447800	12.07108600	0.00000000
Cl	-8.52247800	12.07108600	-1.36300000
Cl	-6.42047800	-17.05791400	1.36300000
Mg	-7.47147800	-15.23691400	0.00000000
Cl	-6.42047800	-13.41691400	1.36300000
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Mg	-7.47147800	-11.59591400	0.00000000
Cl	-6.42047800	-9.77491400	1.36300000
Cl	-5.36947800	-11.59591400	-1.36300000
Mg	-7.47147800	-7.95491400	0.00000000
Cl	-6.42047800	-6.13391400	1.36300000
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Mg	-7.47147800	-4.31391400	0.00000000
Cl	-6.42047800	-2.49291400	1.36300000
Cl	-5.36947800	-4.31391400	-1.36300000
Mg	-7.47147800	-0.67291400	0.00000000
Cl	-6.42047800	1.14808600	1.36300000
Cl	-5.36947800	-0.67291400	-1.36300000
Mg	-7.47147800	2.96808600	0.00000000
Cl	-6.42047800	4.78908600	1.36300000
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Mg	-7.47147800	6.60908600	0.00000000
Cl	-6.42047800	8.43008600	1.36300000
Cl	-5.36947800	6.60908600	-1.36300000
Mg	-7.47147800	10.25008600	0.00000000
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Mg	-4.31847800	-13.41691400	0.00000000
Cl	-3.26747800	-11.59591400	1.36300000
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Mg	-4.31847800	-9.77491400	0.00000000
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Mg	-4.31847800	-6.13391400	0.00000000
Cl	-3.26747800	-4.31391400	1.36300000
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Mg	-4.31847800	-2.49291400	0.00000000
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Mg	-4.31847800	1.14808600	0.00000000
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Mg	-4.31847800	4.78908600	0.00000000
Cl	-3.26747800	6.60908600	1.36300000
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Mg	-4.31847800	8.43008600	0.00000000
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Mg	-1.16547800	-18.87791400	0.00000000
Cl	-0.11447800	-17.05791400	1.36300000
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Mg	-1.16547800	-15.23691400	0.00000000
Cl	-0.11447800	-13.41691400	1.36300000
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Mg	-1.16547800	-11.59591400	0.00000000
Cl	-0.11447800	-9.77491400	1.36300000
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Mg	-1.16547800	-7.95491400	0.00000000
Cl	-0.11447800	-6.13391400	1.36300000
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Mg	-1.16547800	-4.31391400	0.00000000
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Mg	-1.16547800	2.96808600	0.00000000
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Mg	1.98752200	-17.05791400	0.00000000
Cl	3.03852200	-15.23691400	1.36300000
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Mg	1.98752200	-13.41691400	0.00000000
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Mg	1.98752200	-6.13391400	0.00000000
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Mg	1.98752200	-2.49291400	0.00000000
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Mg	1.98752200	1.14808600	0.00000000
Cl	3.03852200	2.96808600	1.36300000
Cl	4.09052200	1.14808600	-1.36300000
Mg	1.98752200	4.78908600	0.00000000
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Cl	6.19252200	-9.77491400	1.36300000
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Mg	5.14152200	-4.31391400	0.00000000
Cl	6.19252200	-2.49291400	1.36300000
Mg	5.14152200	-0.67291400	0.00000000
Cl	6.19252200	1.14808600	1.36300000
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Mg	5.14152200	2.96808600	0.00000000

Mg₈₁Cl₁₆₂ (Frozen)

Input Keywords:

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Mg	-16.93147800	4.78908600	0.00000000
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Mg	-16.93147800	15.71208600	0.00000000
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Mg	-13.77847800	-7.95491400	0.00000000
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Cl	-9.57347800	-11.59591400	1.36300000
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Mg	-10.62447800	-9.77491400	0.00000000
Cl	-9.57347800	-7.95491400	1.36300000
Cl	-8.52247800	-9.77491400	-1.36300000
Mg	-10.62447800	-6.13391400	0.00000000
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Mg	-10.62447800	-2.49291400	0.00000000
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Mg	-10.62447800	1.14808600	0.00000000
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Mg	-10.62447800	15.71208600	0.00000000
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Cl	-6.42047800	-17.05791400	1.36300000
Mg	-7.47147800	-15.23691400	0.00000000
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Mg	-7.47147800	-11.59591400	0.00000000
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Mg	-7.47147800	13.89108600	0.00000000
Cl	-5.36947800	13.89108600	-1.36300000
Cl	-3.26747800	-18.87791400	1.36300000

Mg	-4.31847800	-17.05791400	0.00000000
Cl	-3.26747800	-15.23691400	1.36300000
Cl	-2.21647800	-17.05791400	-1.36300000
Mg	-4.31847800	-13.41691400	0.00000000
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Mg	-4.31847800	-2.49291400	0.00000000
Cl	-3.26747800	-0.67291400	1.36300000
Cl	-2.21647800	-2.49291400	-1.36300000
Mg	-4.31847800	1.14808600	0.00000000
Cl	-3.26747800	2.96808600	1.36300000
Cl	-2.21647800	1.14808600	-1.36300000
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Cl	-2.21647800	12.07108600	-1.36300000
Cl	-0.11447800	-20.69891400	1.36300000
Mg	-1.16547800	-18.87791400	0.00000000
Cl	-0.11447800	-17.05791400	1.36300000
Cl	0.93652200	-18.87791400	-1.36300000
Mg	-1.16547800	-15.23691400	0.00000000
Cl	-0.11447800	-13.41691400	1.36300000
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Mg	-1.16547800	10.25008600	0.00000000
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Mg	1.98752200	-20.69891400	0.00000000
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Mg	1.98752200	8.43008600	0.00000000
Cl	4.09052200	8.43008600	-1.36300000
Cl	6.19252200	-24.33991400	1.36300000
Mg	5.14152200	-22.51891400	0.00000000
Cl	6.19252200	-20.69891400	1.36300000
Cl	7.24352200	-22.51891400	-1.36300000
Mg	5.14152200	-18.87791400	0.00000000
Cl	6.19252200	-17.05791400	1.36300000
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Mg	5.14152200	-15.23691400	0.00000000
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Cl	6.19252200	-9.77491400	1.36300000
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Mg	5.14152200	-4.31391400	0.00000000
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Cl	7.24352200	-4.31391400	-1.36300000
Mg	5.14152200	-0.67291400	0.00000000
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Mg	5.14152200	2.96808600	0.00000000
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Cl	7.24352200	2.96808600	-1.36300000
Mg	5.14152200	6.60908600	0.00000000
Cl	7.24352200	6.60908600	-1.36300000
Cl	9.34552200	-26.15991400	1.36300000
Mg	8.29452200	-24.33991400	0.00000000
Cl	9.34552200	-22.51891400	1.36300000
Mg	8.29452200	-20.69891400	0.00000000
Cl	9.34552200	-18.87791400	1.36300000
Mg	8.29452200	-17.05791400	0.00000000
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Cl	9.34552200	-11.59591400	1.36300000
Mg	8.29452200	-9.77491400	0.00000000
Cl	9.34552200	-7.95491400	1.36300000
Mg	8.29452200	-6.13391400	0.00000000
Cl	9.34552200	-4.31391400	1.36300000
Mg	8.29452200	-2.49291400	0.00000000
Cl	9.34552200	-0.67291400	1.36300000

Mg	8.29452200	1.14808600	0.00000000
Cl	9.34552200	2.96808600	1.36300000
Mg	8.29452200	4.78908600	0.00000000

Mg₁₀₀Cl₂₀₀ (Frozen)

Input Keywords:

#p hf/gen geom=connectivity scfcyc=800 MaxDisk=40GB

Input coordinates:

Cl	-17.98247800	-7.95491400	-1.36300000
Cl	-17.98247800	-4.31391400	-1.36300000
Cl	-17.98247800	-0.67291400	-1.36300000
Cl	-17.98247800	2.96808600	-1.36300000
Cl	-17.98247800	6.60908600	-1.36300000
Cl	-17.98247800	10.25008600	-1.36300000
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Cl	-17.98247800	17.53208600	-1.36300000
Cl	-17.98247800	21.17308600	-1.36300000
Cl	-17.98247800	24.81408600	-1.36300000
Cl	-15.88047800	-11.59591400	1.36300000
Mg	-16.93147800	-9.77491400	0.00000000
Cl	-15.88047800	-7.95491400	1.36300000
Cl	-14.82947800	-9.77491400	-1.36300000
Mg	-16.93147800	-6.13391400	0.00000000
Cl	-15.88047800	-4.31391400	1.36300000
Cl	-14.82947800	-6.13391400	-1.36300000
Mg	-16.93147800	-2.49291400	0.00000000
Cl	-15.88047800	-0.67291400	1.36300000
Cl	-14.82947800	-2.49291400	-1.36300000
Mg	-16.93147800	1.14808600	0.00000000
Cl	-15.88047800	2.96808600	1.36300000
Cl	-14.82947800	1.14808600	-1.36300000
Mg	-16.93147800	4.78908600	0.00000000
Cl	-15.88047800	6.60908600	1.36300000
Cl	-14.82947800	4.78908600	-1.36300000
Mg	-16.93147800	8.43008600	0.00000000
Cl	-15.88047800	10.25008600	1.36300000
Cl	-14.82947800	8.43008600	-1.36300000
Mg	-16.93147800	12.07108600	0.00000000
Cl	-15.88047800	13.89108600	1.36300000
Cl	-14.82947800	12.07108600	-1.36300000
Mg	-16.93147800	15.71208600	0.00000000
Cl	-15.88047800	17.53208600	1.36300000
Cl	-14.82947800	15.71208600	-1.36300000
Mg	-16.93147800	19.35308600	0.00000000
Cl	-15.88047800	21.17308600	1.36300000
Cl	-14.82947800	19.35308600	-1.36300000
Mg	-16.93147800	22.99408600	0.00000000
Cl	-14.82947800	22.99408600	-1.36300000
Cl	-12.72747800	-13.41691400	1.36300000
Mg	-13.77847800	-11.59591400	0.00000000
Cl	-12.72747800	-9.77491400	1.36300000
Cl	-11.67547800	-11.59591400	-1.36300000
Mg	-13.77847800	-7.95491400	0.00000000
Cl	-12.72747800	-6.13391400	1.36300000
Cl	-11.67547800	-7.95491400	-1.36300000
Mg	-13.77847800	-4.31391400	0.00000000
Cl	-12.72747800	-2.49291400	1.36300000
Cl	-11.67547800	-4.31391400	-1.36300000
Mg	-13.77847800	-0.67291400	0.00000000

Cl	-12.72747800	1.14808600	1.36300000
Cl	-11.67547800	-0.67291400	-1.36300000
Mg	-13.77847800	2.96808600	0.00000000
Cl	-12.72747800	4.78908600	1.36300000
Cl	-11.67547800	2.96808600	-1.36300000
Mg	-13.77847800	6.60908600	0.00000000
Cl	-12.72747800	8.43008600	1.36300000
Cl	-11.67547800	6.60908600	-1.36300000
Mg	-13.77847800	10.25008600	0.00000000
Cl	-12.72747800	12.07108600	1.36300000
Cl	-11.67547800	10.25008600	-1.36300000
Mg	-13.77847800	13.89108600	0.00000000
Cl	-12.72747800	15.71208600	1.36300000
Cl	-11.67547800	13.89108600	-1.36300000
Mg	-13.77847800	17.53208600	0.00000000
Cl	-12.72747800	19.35308600	1.36300000
Cl	-11.67547800	17.53208600	-1.36300000
Mg	-13.77847800	21.17308600	0.00000000
Cl	-11.67547800	21.17308600	-1.36300000
Cl	-9.57347800	-15.23691400	1.36300000
Mg	-10.62447800	-13.41691400	0.00000000
Cl	-9.57347800	-11.59591400	1.36300000
Cl	-8.52247800	-13.41691400	-1.36300000
Mg	-10.62447800	-9.77491400	0.00000000
Cl	-9.57347800	-7.95491400	1.36300000
Cl	-8.52247800	-9.77491400	-1.36300000
Mg	-10.62447800	-6.13391400	0.00000000
Cl	-9.57347800	-4.31391400	1.36300000
Cl	-8.52247800	-6.13391400	-1.36300000
Mg	-10.62447800	-2.49291400	0.00000000
Cl	-9.57347800	-0.67291400	1.36300000
Cl	-8.52247800	-2.49291400	-1.36300000
Mg	-10.62447800	1.14808600	0.00000000
Cl	-9.57347800	2.96808600	1.36300000
Cl	-8.52247800	1.14808600	-1.36300000
Mg	-10.62447800	4.78908600	0.00000000
Cl	-9.57347800	6.60908600	1.36300000
Cl	-8.52247800	4.78908600	-1.36300000
Mg	-10.62447800	8.43008600	0.00000000
Cl	-9.57347800	10.25008600	1.36300000
Cl	-8.52247800	8.43008600	-1.36300000
Mg	-10.62447800	12.07108600	0.00000000
Cl	-9.57347800	13.89108600	1.36300000
Cl	-8.52247800	12.07108600	-1.36300000
Mg	-10.62447800	15.71208600	0.00000000
Cl	-9.57347800	17.53208600	1.36300000
Cl	-8.52247800	15.71208600	-1.36300000
Mg	-10.62447800	19.35308600	0.00000000
Cl	-8.52247800	19.35308600	-1.36300000
Cl	-6.42047800	-17.05791400	1.36300000
Mg	-7.47147800	-15.23691400	0.00000000
Cl	-6.42047800	-13.41691400	1.36300000
Cl	-5.36947800	-15.23691400	-1.36300000
Mg	-7.47147800	-11.59591400	0.00000000
Cl	-6.42047800	-9.77491400	1.36300000
Cl	-5.36947800	-11.59591400	-1.36300000
Mg	-7.47147800	-7.95491400	0.00000000
Cl	-6.42047800	-6.13391400	1.36300000
Cl	-5.36947800	-7.95491400	-1.36300000
Mg	-7.47147800	-4.31391400	0.00000000
Cl	-6.42047800	-2.49291400	1.36300000

Cl	-5.36947800	-4.31391400	-1.36300000
Mg	-7.47147800	-0.67291400	0.00000000
Cl	-6.42047800	1.14808600	1.36300000
Cl	-5.36947800	-0.67291400	-1.36300000
Mg	-7.47147800	2.96808600	0.00000000
Cl	-6.42047800	4.78908600	1.36300000
Cl	-5.36947800	2.96808600	-1.36300000
Mg	-7.47147800	6.60908600	0.00000000
Cl	-6.42047800	8.43008600	1.36300000
Cl	-5.36947800	6.60908600	-1.36300000
Mg	-7.47147800	10.25008600	0.00000000
Cl	-6.42047800	12.07108600	1.36300000
Cl	-5.36947800	10.25008600	-1.36300000
Mg	-7.47147800	13.89108600	0.00000000
Cl	-6.42047800	15.71208600	1.36300000
Cl	-5.36947800	13.89108600	-1.36300000
Mg	-7.47147800	17.53208600	0.00000000
Cl	-5.36947800	17.53208600	-1.36300000
Cl	-3.26747800	-18.87791400	1.36300000
Mg	-4.31847800	-17.05791400	0.00000000
Cl	-3.26747800	-15.23691400	1.36300000
Cl	-2.21647800	-17.05791400	-1.36300000
Mg	-4.31847800	-13.41691400	0.00000000
Cl	-3.26747800	-11.59591400	1.36300000
Cl	-2.21647800	-13.41691400	-1.36300000
Mg	-4.31847800	-9.77491400	0.00000000
Cl	-3.26747800	-7.95491400	1.36300000
Cl	-2.21647800	-9.77491400	-1.36300000
Mg	-4.31847800	-6.13391400	0.00000000
Cl	-3.26747800	-4.31391400	1.36300000
Cl	-2.21647800	-6.13391400	-1.36300000
Mg	-4.31847800	-2.49291400	0.00000000
Cl	-3.26747800	-0.67291400	1.36300000
Cl	-2.21647800	-2.49291400	-1.36300000
Mg	-4.31847800	1.14808600	0.00000000
Cl	-3.26747800	2.96808600	1.36300000
Cl	-2.21647800	1.14808600	-1.36300000
Mg	-4.31847800	4.78908600	0.00000000
Cl	-3.26747800	6.60908600	1.36300000
Cl	-2.21647800	4.78908600	-1.36300000
Mg	-4.31847800	8.43008600	0.00000000
Cl	-3.26747800	10.25008600	1.36300000
Cl	-2.21647800	8.43008600	-1.36300000
Mg	-4.31847800	12.07108600	0.00000000
Cl	-3.26747800	13.89108600	1.36300000
Cl	-2.21647800	12.07108600	-1.36300000
Mg	-4.31847800	15.71208600	0.00000000
Cl	-2.21647800	15.71208600	-1.36300000
Cl	-0.11447800	-20.69891400	1.36300000
Mg	-1.16547800	-18.87791400	0.00000000
Cl	-0.11447800	-17.05791400	1.36300000
Cl	0.93652200	-18.87791400	-1.36300000
Mg	-1.16547800	-15.23691400	0.00000000
Cl	-0.11447800	-13.41691400	1.36300000
Cl	0.93652200	-15.23691400	-1.36300000
Mg	-1.16547800	-11.59591400	0.00000000
Cl	-0.11447800	-9.77491400	1.36300000
Cl	0.93652200	-11.59591400	-1.36300000
Mg	-1.16547800	-7.95491400	0.00000000
Cl	-0.11447800	-6.13391400	1.36300000
Cl	0.93652200	-7.95491400	-1.36300000

Mg	-1.16547800	-4.31391400	0.00000000
Cl	-0.11447800	-2.49291400	1.36300000
Cl	0.93652200	-4.31391400	-1.36300000
Mg	-1.16547800	-0.67291400	0.00000000
Cl	-0.11447800	1.14808600	1.36300000
Cl	0.93652200	-0.67291400	-1.36300000
Mg	-1.16547800	2.96808600	0.00000000
Cl	-0.11447800	4.78908600	1.36300000
Cl	0.93652200	2.96808600	-1.36300000
Mg	-1.16547800	6.60908600	0.00000000
Cl	-0.11447800	8.43008600	1.36300000
Cl	0.93652200	6.60908600	-1.36300000
Mg	-1.16547800	10.25008600	0.00000000
Cl	-0.11447800	12.07108600	1.36300000
Cl	0.93652200	10.25008600	-1.36300000
Mg	-1.16547800	13.89108600	0.00000000
Cl	0.93652200	13.89108600	-1.36300000
Cl	3.03852200	-22.51891400	1.36300000
Mg	1.98752200	-20.69891400	0.00000000
Cl	3.03852200	-18.87791400	1.36300000
Cl	4.09052200	-20.69891400	-1.36300000
Mg	1.98752200	-17.05791400	0.00000000
Cl	3.03852200	-15.23691400	1.36300000
Cl	4.09052200	-17.05791400	-1.36300000
Mg	1.98752200	-13.41691400	0.00000000
Cl	3.03852200	-11.59591400	1.36300000
Cl	4.09052200	-13.41691400	-1.36300000
Mg	1.98752200	-9.77491400	0.00000000
Cl	3.03852200	-7.95491400	1.36300000
Cl	4.09052200	-9.77491400	-1.36300000
Mg	1.98752200	-6.13391400	0.00000000
Cl	3.03852200	-4.31391400	1.36300000
Cl	4.09052200	-6.13391400	-1.36300000
Mg	1.98752200	-2.49291400	0.00000000
Cl	3.03852200	-0.67291400	1.36300000
Cl	4.09052200	-2.49291400	-1.36300000
Mg	1.98752200	1.14808600	0.00000000
Cl	3.03852200	2.96808600	1.36300000
Cl	4.09052200	1.14808600	-1.36300000
Mg	1.98752200	4.78908600	0.00000000
Cl	3.03852200	6.60908600	1.36300000
Cl	4.09052200	4.78908600	-1.36300000
Mg	1.98752200	8.43008600	0.00000000
Cl	3.03852200	10.25008600	1.36300000
Cl	4.09052200	8.43008600	-1.36300000
Mg	1.98752200	12.07108600	0.00000000
Cl	4.09052200	12.07108600	-1.36300000
Cl	6.19252200	-24.33991400	1.36300000
Mg	5.14152200	-22.51891400	0.00000000
Cl	6.19252200	-20.69891400	1.36300000
Cl	7.24352200	-22.51891400	-1.36300000
Mg	5.14152200	-18.87791400	0.00000000
Cl	6.19252200	-17.05791400	1.36300000
Cl	7.24352200	-18.87791400	-1.36300000
Mg	5.14152200	-15.23691400	0.00000000
Cl	6.19252200	-13.41691400	1.36300000
Cl	7.24352200	-15.23691400	-1.36300000
Mg	5.14152200	-11.59591400	0.00000000
Cl	6.19252200	-9.77491400	1.36300000
Cl	7.24352200	-11.59591400	-1.36300000
Mg	5.14152200	-7.95491400	0.00000000

Cl	6.19252200	-6.13391400	1.36300000
Cl	7.24352200	-7.95491400	-1.36300000
Mg	5.14152200	-4.31391400	0.00000000
Cl	6.19252200	-2.49291400	1.36300000
Cl	7.24352200	-4.31391400	-1.36300000
Mg	5.14152200	-0.67291400	0.00000000
Cl	6.19252200	1.14808600	1.36300000
Cl	7.24352200	-0.67291400	-1.36300000
Mg	5.14152200	2.96808600	0.00000000
Cl	6.19252200	4.78908600	1.36300000
Cl	7.24352200	2.96808600	-1.36300000
Mg	5.14152200	6.60908600	0.00000000
Cl	6.19252200	8.43008600	1.36300000
Cl	7.24352200	6.60908600	-1.36300000
Mg	5.14152200	10.25008600	0.00000000
Cl	7.24352200	10.25008600	-1.36300000
Cl	9.34552200	-26.15991400	1.36300000
Mg	8.29452200	-24.33991400	0.00000000
Cl	9.34552200	-22.51891400	1.36300000
Cl	10.39652200	-24.33991400	-1.36300000
Mg	8.29452200	-20.69891400	0.00000000
Cl	9.34552200	-18.87791400	1.36300000
Cl	10.39652200	-20.69891400	-1.36300000
Mg	8.29452200	-17.05791400	0.00000000
Cl	9.34552200	-15.23691400	1.36300000
Cl	10.39652200	-17.05791400	-1.36300000
Mg	8.29452200	-13.41691400	0.00000000
Cl	9.34552200	-11.59591400	1.36300000
Cl	10.39652200	-13.41691400	-1.36300000
Mg	8.29452200	-9.77491400	0.00000000
Cl	9.34552200	-7.95491400	1.36300000
Cl	10.39652200	-9.77491400	-1.36300000
Mg	8.29452200	-6.13391400	0.00000000
Cl	9.34552200	-4.31391400	1.36300000
Cl	10.39652200	-6.13391400	-1.36300000
Mg	8.29452200	-2.49291400	0.00000000
Cl	9.34552200	-0.67291400	1.36300000
Cl	10.39652200	-2.49291400	-1.36300000
Mg	8.29452200	1.14808600	0.00000000
Cl	9.34552200	2.96808600	1.36300000
Cl	10.39652200	1.14808600	-1.36300000
Mg	8.29452200	4.78908600	0.00000000
Cl	9.34552200	6.60908600	1.36300000
Cl	10.39652200	4.78908600	-1.36300000
Mg	8.29452200	8.43008600	0.00000000
Cl	10.39652200	8.43008600	-1.36300000
Cl	12.49852200	-27.98091400	1.36300000
Mg	11.44752200	-26.15991400	0.00000000
Cl	12.49852200	-24.33991400	1.36300000
Mg	11.44752200	-22.51891400	0.00000000
Cl	12.49852200	-20.69891400	1.36300000
Mg	11.44752200	-18.87791400	0.00000000
Cl	12.49852200	-17.05791400	1.36300000
Mg	11.44752200	-15.23691400	0.00000000
Cl	12.49852200	-13.41691400	1.36300000
Mg	11.44752200	-11.59591400	0.00000000
Cl	12.49852200	-9.77491400	1.36300000
Mg	11.44752200	-7.95491400	0.00000000
Cl	12.49852200	-6.13391400	1.36300000
Mg	11.44752200	-4.31391400	0.00000000
Cl	12.49852200	-2.49291400	1.36300000

Mg	11.44752200	-0.67291400	0.00000000
Cl	12.49852200	1.14808600	1.36300000
Mg	11.44752200	2.96808600	0.00000000
Cl	12.49852200	4.78908600	1.36300000
Mg	11.44752200	6.60908600	0.00000000

Mg₁₂Cl₂₄ (truncated tetrahedron)

Input keywords:

HF/gen opt iop(2/17=3) freq

Input coordinates:

Mg	1.19675600	1.19675600	-3.98413400
Mg	3.98413400	1.19675600	-1.19675600
Mg	-1.19675600	-1.19675600	-3.98413400
Mg	1.19675600	3.98413400	-1.19675600
Mg	3.98413400	-1.19675600	1.19675600
Mg	-3.98413400	-1.19675600	-1.19675600
Mg	-1.19675600	-3.98413400	-1.19675600
Mg	-1.19675600	3.98413400	1.19675600
Mg	1.19675600	-1.19675600	3.98413400
Mg	1.19675600	-3.98413400	1.19675600
Mg	-3.98413400	1.19675600	1.19675600
Mg	-1.19675600	1.19675600	3.98413400
Cl	3.53888400	3.53888400	-0.82422500
Cl	0.82422500	3.53888400	-3.53888400
Cl	3.53888400	0.82422500	-3.53888400
Cl	-3.53888400	0.82422500	3.53888400
Cl	-3.53888400	3.53888400	0.82422500
Cl	-0.82422500	3.53888400	3.53888400
Cl	0.82422500	-3.53888400	3.53888400
Cl	3.53888400	-0.82422500	3.53888400
Cl	3.53888400	-3.53888400	0.82422500
Cl	-3.53888400	-0.82422500	-3.53888400
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Cl	-0.82422500	-3.53888400	-3.53888400
Cl	5.73400300	0.00000000	0.00000000
Cl	0.00000000	0.00000000	-5.73400300
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Cl	-5.73400300	0.00000000	0.00000000
Cl	0.00000000	0.00000000	5.73400300
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Cl	0.00000000	2.36667600	0.00000000
Cl	2.36667600	0.00000000	0.00000000
Cl	0.00000000	-2.36667600	0.00000000
Cl	0.00000000	0.00000000	-2.36667600
Cl	-2.36667600	0.00000000	0.00000000

Output coordinates:

Mg	1.205412	1.205412	-4.007026
Mg	4.007026	1.205412	-1.205412
Mg	-1.205412	-1.205412	-4.007026
Mg	1.205412	4.007026	-1.205412
Mg	4.007026	-1.205412	1.205412
Mg	-4.007026	-1.205412	-1.205412
Mg	-1.205412	-4.007026	-1.205412
Mg	-1.205412	4.007026	1.205412
Mg	1.205412	-1.205412	4.007026
Mg	1.205412	-4.007026	1.205412
Mg	-4.007026	1.205412	1.205412
Mg	-1.205412	1.205412	4.007026

Cl	3.547223	3.547223	-0.865595
Cl	0.865595	3.547223	-3.547223
Cl	3.547223	0.865595	-3.547223
Cl	-3.547223	0.865595	3.547223
Cl	-3.547223	3.547223	0.865595
Cl	-0.865595	3.547223	3.547223
Cl	0.865595	-3.547223	3.547223
Cl	3.547223	-0.865595	3.547223
Cl	3.547223	-3.547223	0.865595
Cl	-3.547223	-0.865595	-3.547223
Cl	-3.547223	-3.547223	-0.865595
Cl	-0.865595	-3.547223	-3.547223
Cl	5.748275	0.000000	0.000000
Cl	0.000000	0.000000	-5.748275
Cl	0.000000	-5.748275	0.000000
Cl	-5.748275	0.000000	0.000000
Cl	0.000000	0.000000	5.748275
Cl	0.000000	5.748275	0.000000
Cl	0.000000	0.000000	2.416577
Cl	0.000000	2.416577	0.000000
Cl	2.416577	0.000000	0.000000
Cl	0.000000	-2.416577	0.000000
Cl	0.000000	0.000000	-2.416577
Cl	-2.416577	0.000000	0.000000

Mg₂₄Cl₄₈ (truncated octahedron)

Input keywords:

HF/gen opt freq

Input coordinates:

Mg	0.00000000	-2.92007400	5.21101500
Mg	-2.92007400	0.00000000	5.21101500
Mg	0.00000000	-5.21101500	2.92007400
Mg	2.92007400	0.00000000	5.21101500
Mg	-5.21101500	0.00000000	2.92007400
Mg	0.00000000	2.92007400	5.21101500
Mg	2.92007400	-5.21101500	0.00000000
Mg	-2.92007400	-5.21101500	0.00000000
Mg	5.21101500	0.00000000	2.92007400
Mg	-5.21101500	2.92007400	0.00000000
Mg	-5.21101500	-2.92007400	0.00000000
Mg	0.00000000	5.21101500	2.92007400
Mg	0.00000000	-5.21101500	-2.92007400
Mg	5.21101500	-2.92007400	0.00000000
Mg	5.21101500	2.92007400	0.00000000
Mg	-5.21101500	0.00000000	-2.92007400
Mg	-2.92007400	5.21101500	0.00000000
Mg	2.92007400	5.21101500	0.00000000
Mg	0.00000000	-2.92007400	-5.21101500
Mg	5.21101500	0.00000000	-2.92007400
Mg	-2.92007400	0.00000000	-5.21101500
Mg	0.00000000	5.21101500	-2.92007400
Mg	2.92007400	0.00000000	-5.21101500
Mg	0.00000000	2.92007400	-5.21101500
Cl	-1.95032000	-1.95032000	6.15257500
Cl	-1.95032000	-6.15257500	-1.95032000
Cl	-6.15257500	1.95032000	1.95032000
Cl	-1.95032000	6.15257500	1.95032000
Cl	1.95032000	1.95032000	6.15257500
Cl	1.95032000	6.15257500	-1.95032000

Cl	1.95032000	-1.95032000	6.15257500
Cl	6.15257500	-1.95032000	1.95032000
Cl	6.15257500	1.95032000	1.95032000
Cl	1.95032000	6.15257500	1.95032000
Cl	-1.95032000	6.15257500	-1.95032000
Cl	1.95032000	1.95032000	-6.15257500
Cl	-1.95032000	1.95032000	-6.15257500
Cl	-6.15257500	-1.95032000	-1.95032000
Cl	-6.15257500	1.95032000	-1.95032000
Cl	-1.95032000	1.95032000	6.15257500
Cl	-1.95032000	-6.15257500	1.95032000
Cl	1.95032000	-6.15257500	1.95032000
Cl	1.95032000	-6.15257500	-1.95032000
Cl	-1.95032000	-1.95032000	-6.15257500
Cl	1.95032000	-1.95032000	-6.15257500
Cl	6.15257500	1.95032000	-1.95032000
Cl	6.15257500	-1.95032000	-1.95032000
Cl	-6.15257500	-1.95032000	1.95032000
Cl	0.00000000	5.30507300	5.30507300
Cl	5.30507300	5.30507300	0.00000000
Cl	5.30507300	0.00000000	5.30507300
Cl	0.00000000	-5.30507300	5.30507300
Cl	5.30507300	-5.30507300	0.00000000
Cl	5.30507300	0.00000000	-5.30507300
Cl	0.00000000	-5.30507300	-5.30507300
Cl	-5.30507300	-5.30507300	0.00000000
Cl	-5.30507300	0.00000000	-5.30507300
Cl	0.00000000	5.30507300	-5.30507300
Cl	-5.30507300	5.30507300	0.00000000
Cl	-5.30507300	0.00000000	5.30507300
Cl	2.83068500	0.00000000	2.83068500
Cl	0.00000000	-2.83068500	2.83068500
Cl	-2.83068500	0.00000000	2.83068500
Cl	0.00000000	2.83068500	2.83068500
Cl	-2.83068500	0.00000000	-2.83068500
Cl	0.00000000	-2.83068500	-2.83068500
Cl	2.83068500	0.00000000	-2.83068500
Cl	0.00000000	2.83068500	-2.83068500
Cl	2.83068500	2.83068500	0.00000000
Cl	2.83068500	-2.83068500	0.00000000
Cl	-2.83068500	-2.83068500	0.00000000
Cl	-2.83068500	2.83068500	0.00000000

Output coordinates:

Mg	0.000000	-2.935044	5.249232
Mg	-2.935044	0.000000	5.249232
Mg	0.000000	-5.249232	2.935044
Mg	2.935044	0.000000	5.249232
Mg	-5.249232	0.000000	2.935044
Mg	0.000000	2.935044	5.249232
Mg	2.935044	-5.249232	0.000000
Mg	-2.935044	-5.249232	0.000000
Mg	5.249232	0.000000	2.935044
Mg	-5.249232	2.935044	0.000000
Mg	-5.249232	-2.935044	0.000000
Mg	0.000000	5.249232	2.935044
Mg	0.000000	-5.249232	-2.935044
Mg	5.249232	-2.935044	0.000000
Mg	5.249232	2.935044	0.000000
Mg	-5.249232	0.000000	-2.935044
Mg	-2.935044	5.249232	0.000000
Mg	2.935044	5.249232	0.000000

Mg	0.000000	-2.935044	-5.249232
Mg	5.249232	0.000000	-2.935044
Mg	-2.935044	0.000000	-5.249232
Mg	0.000000	5.249232	-2.935044
Mg	2.935044	0.000000	-5.249232
Mg	0.000000	2.935044	-5.249232
Cl	-1.929116	-1.929116	6.191456
Cl	-1.929116	-6.191456	-1.929116
Cl	-6.191456	1.929116	1.929116
Cl	-1.929116	6.191456	1.929116
Cl	1.929116	1.929116	6.191456
Cl	1.929116	6.191456	-1.929116
Cl	1.929116	-1.929116	6.191456
Cl	6.191456	-1.929116	1.929116
Cl	6.191456	1.929116	1.929116
Cl	1.929116	6.191456	1.929116
Cl	-1.929116	6.191456	-1.929116
Cl	1.929116	1.929116	-6.191456
Cl	-1.929116	1.929116	-6.191456
Cl	-6.191456	-1.929116	-1.929116
Cl	-6.191456	1.929116	-1.929116
Cl	-1.929116	1.929116	6.191456
Cl	-1.929116	-6.191456	1.929116
Cl	1.929116	-6.191456	1.929116
Cl	1.929116	-6.191456	-1.929116
Cl	-1.929116	-1.929116	-6.191456
Cl	1.929116	-1.929116	-6.191456
Cl	6.191456	1.929116	-1.929116
Cl	6.191456	-1.929116	-1.929116
Cl	-6.191456	-1.929116	1.929116
Cl	0.000000	5.317455	5.317455
Cl	5.317455	5.317455	0.000000
Cl	5.317455	0.000000	5.317455
Cl	0.000000	-5.317455	5.317455
Cl	5.317455	-5.317455	0.000000
Cl	5.317455	0.000000	-5.317455
Cl	0.000000	-5.317455	-5.317455
Cl	-5.317455	-5.317455	0.000000
Cl	-5.317455	0.000000	-5.317455
Cl	0.000000	5.317455	-5.317455
Cl	-5.317455	5.317455	0.000000
Cl	-5.317455	0.000000	5.317455
Cl	2.873336	0.000000	2.873336
Cl	0.000000	-2.873336	2.873336
Cl	-2.873336	0.000000	2.873336
Cl	0.000000	2.873336	2.873336
Cl	-2.873336	0.000000	-2.873336
Cl	0.000000	-2.873336	-2.873336
Cl	2.873336	0.000000	-2.873336
Cl	0.000000	2.873336	-2.873336
Cl	2.873336	2.873336	0.000000
Cl	2.873336	-2.873336	0.000000
Cl	-2.873336	-2.873336	0.000000
Cl	-2.873336	2.873336	0.000000

Mg₂₄Cl₄₈ (truncated cube)

Input keywords:

HF/gen opt iop(2/17=3) freq

Input coordinates:

Mg	4.44237300	-1.61926700	4.44237300
Mg	4.44237300	-4.44237300	1.61926700
Mg	4.44237300	1.61926700	4.44237300
Mg	1.61926700	-4.44237300	4.44237300
Mg	4.44237300	-4.44237300	-1.61926700
Mg	1.61926700	4.44237300	4.44237300
Mg	4.44237300	4.44237300	1.61926700
Mg	-1.61926700	-4.44237300	4.44237300
Mg	1.61926700	-4.44237300	-4.44237300
Mg	4.44237300	-1.61926700	-4.44237300
Mg	-1.61926700	4.44237300	4.44237300
Mg	4.44237300	4.44237300	-1.61926700
Mg	-4.44237300	-1.61926700	4.44237300
Mg	-4.44237300	-4.44237300	1.61926700
Mg	-1.61926700	-4.44237300	-4.44237300
Mg	4.44237300	1.61926700	-4.44237300
Mg	-4.44237300	1.61926700	4.44237300
Mg	-4.44237300	4.44237300	1.61926700
Mg	1.61926700	4.44237300	-4.44237300
Mg	-4.44237300	-4.44237300	-1.61926700
Mg	-4.44237300	-1.61926700	-4.44237300
Mg	-4.44237300	4.44237300	-1.61926700
Mg	-1.61926700	4.44237300	-4.44237300
Mg	-4.44237300	1.61926700	-4.44237300
Cl	2.99930100	-5.73485600	-2.99930100
Cl	5.73485600	-2.99930100	-2.99930100
Cl	2.99930100	-2.99930100	-5.73485600
Cl	2.99930100	2.99930100	-5.73485600
Cl	5.73485600	2.99930100	-2.99930100
Cl	2.99930100	5.73485600	-2.99930100
Cl	2.99930100	5.73485600	2.99930100
Cl	5.73485600	2.99930100	2.99930100
Cl	2.99930100	2.99930100	5.73485600
Cl	2.99930100	-2.99930100	5.73485600
Cl	5.73485600	-2.99930100	2.99930100
Cl	2.99930100	-5.73485600	2.99930100
Cl	-2.99930100	-5.73485600	-2.99930100
Cl	-2.99930100	-2.99930100	-5.73485600
Cl	-5.73485600	-2.99930100	-2.99930100
Cl	-5.73485600	2.99930100	-2.99930100
Cl	-2.99930100	2.99930100	-5.73485600
Cl	-2.99930100	5.73485600	-2.99930100
Cl	-5.73485600	2.99930100	2.99930100
Cl	-2.99930100	5.73485600	2.99930100
Cl	-2.99930100	2.99930100	5.73485600
Cl	-5.73485600	-2.99930100	2.99930100
Cl	-2.99930100	-5.73485600	2.99930100
Cl	-2.99930100	-2.99930100	5.73485600
Cl	0.00000000	-5.68146200	5.68146200
Cl	5.68146200	-5.68146200	0.00000000
Cl	0.00000000	-5.68146200	-5.68146200
Cl	-5.68146200	-5.68146200	0.00000000
Cl	5.68146200	0.00000000	5.68146200
Cl	-5.68146200	0.00000000	5.68146200
Cl	-5.68146200	0.00000000	-5.68146200
Cl	5.68146200	0.00000000	-5.68146200
Cl	0.00000000	5.68146200	-5.68146200
Cl	-5.68146200	5.68146200	0.00000000
Cl	0.00000000	5.68146200	5.68146200
Cl	5.68146200	5.68146200	0.00000000
Cl	3.20442900	0.00000000	3.20442900

Cl	3.20442900	3.20442900	0.00000000
Cl	3.20442900	0.00000000	-3.20442900
Cl	3.20442900	-3.20442900	0.00000000
Cl	-3.20442900	-3.20442900	0.00000000
Cl	-3.20442900	0.00000000	-3.20442900
Cl	-3.20442900	3.20442900	0.00000000
Cl	-3.20442900	0.00000000	3.20442900
Cl	0.00000000	-3.20442900	3.20442900
Cl	0.00000000	-3.20442900	-3.20442900
Cl	0.00000000	3.20442900	-3.20442900
Cl	0.00000000	3.20442900	3.20442900

Output coordinates:

Mg	4.446965	-1.632734	4.446965
Mg	4.446965	-4.446965	1.632734
Mg	4.446965	1.632734	4.446965
Mg	1.632734	-4.446965	4.446965
Mg	4.446965	-4.446965	-1.632734
Mg	1.632734	4.446965	4.446965
Mg	4.446965	4.446965	1.632734
Mg	-1.632734	-4.446965	4.446965
Mg	1.632734	-4.446965	-4.446965
Mg	4.446965	-1.632734	-4.446965
Mg	-1.632734	4.446965	4.446965
Mg	4.446965	4.446965	-1.632734
Mg	-4.446965	-1.632734	4.446965
Mg	-4.446965	-4.446965	1.632734
Mg	-1.632734	-4.446965	-4.446965
Mg	4.446965	1.632734	-4.446965
Mg	-4.446965	1.632734	4.446965
Mg	-4.446965	4.446965	1.632734
Mg	1.632734	4.446965	-4.446965
Mg	-4.446965	-4.446965	-1.632734
Mg	-4.446965	-1.632734	-4.446965
Mg	-4.446965	4.446965	-1.632734
Mg	-1.632734	4.446965	-4.446965
Mg	-4.446965	1.632734	-4.446965
Cl	3.022525	-5.733469	-3.022525
Cl	5.733469	-3.022525	-3.022525
Cl	3.022525	-3.022525	-5.733469
Cl	3.022525	3.022525	-5.733469
Cl	5.733469	3.022525	-3.022525
Cl	3.022525	5.733469	-3.022525
Cl	3.022525	5.733469	3.022525
Cl	5.733469	3.022525	3.022525
Cl	3.022525	3.022525	5.733469
Cl	3.022525	-3.022525	5.733469
Cl	5.733469	-3.022525	3.022525
Cl	3.022525	-5.733469	3.022525
Cl	-3.022525	-5.733469	-3.022525
Cl	-3.022525	-3.022525	-5.733469
Cl	-5.733469	-3.022525	-3.022525
Cl	-5.733469	3.022525	-3.022525
Cl	-3.022525	3.022525	-5.733469
Cl	-3.022525	5.733469	-3.022525
Cl	-5.733469	3.022525	3.022525
Cl	-3.022525	5.733469	3.022525
Cl	-3.022525	3.022525	5.733469
Cl	-5.733469	-3.022525	3.022525
Cl	-3.022525	-5.733469	3.022525
Cl	-3.022525	-3.022525	5.733469
Cl	0.000000	-5.672853	5.672853

Cl	5.672853	-5.672853	0.000000
Cl	0.000000	-5.672853	-5.672853
Cl	-5.672853	-5.672853	0.000000
Cl	5.672853	0.000000	5.672853
Cl	-5.672853	0.000000	5.672853
Cl	-5.672853	0.000000	-5.672853
Cl	5.672853	0.000000	-5.672853
Cl	0.000000	5.672853	-5.672853
Cl	-5.672853	5.672853	0.000000
Cl	0.000000	5.672853	5.672853
Cl	5.672853	5.672853	0.000000
Cl	3.223380	0.000000	3.223380
Cl	3.223380	3.223380	0.000000
Cl	3.223380	0.000000	-3.223380
Cl	3.223380	-3.223380	0.000000
Cl	-3.223380	-3.223380	0.000000
Cl	-3.223380	0.000000	-3.223380
Cl	-3.223380	3.223380	0.000000
Cl	-3.223380	0.000000	3.223380
Cl	0.000000	-3.223380	3.223380
Cl	0.000000	-3.223380	-3.223380
Cl	0.000000	3.223380	-3.223380
Cl	0.000000	3.223380	3.223380

Mg₄₈Cl₉₆ (truncated cuboctahedron)

Input keywords:

HF/gen opt freq=numer

Input coordinates:

Mg	1.63005900	-7.33020400	-4.48782200
Mg	-1.63005900	-7.33020400	-4.48782200
Mg	1.63005900	-4.48782200	-7.33020400
Mg	4.48782200	-7.33020400	-1.63005900
Mg	-1.63005900	-4.48782200	-7.33020400
Mg	-4.48782200	-7.33020400	-1.63005900
Mg	4.48782200	-1.63005900	-7.33020400
Mg	4.48782200	-7.33020400	1.63005900
Mg	7.33020400	-4.48782200	-1.63005900
Mg	-4.48782200	-1.63005900	-7.33020400
Mg	-4.48782200	-7.33020400	1.63005900
Mg	-7.33020400	-4.48782200	-1.63005900
Mg	4.48782200	1.63005900	-7.33020400
Mg	7.33020400	-1.63005900	-4.48782200
Mg	7.33020400	-4.48782200	1.63005900
Mg	1.63005900	-7.33020400	4.48782200
Mg	-4.48782200	1.63005900	-7.33020400
Mg	-7.33020400	-1.63005900	-4.48782200
Mg	-7.33020400	-4.48782200	1.63005900
Mg	-1.63005900	-7.33020400	4.48782200
Mg	7.33020400	1.63005900	-4.48782200
Mg	1.63005900	4.48782200	-7.33020400
Mg	7.33020400	-1.63005900	4.48782200
Mg	1.63005900	-4.48782200	7.33020400
Mg	-7.33020400	1.63005900	-4.48782200
Mg	-1.63005900	4.48782200	-7.33020400
Mg	-7.33020400	-1.63005900	4.48782200
Mg	-1.63005900	-4.48782200	7.33020400
Mg	7.33020400	4.48782200	-1.63005900
Mg	1.63005900	7.33020400	-4.48782200
Mg	7.33020400	1.63005900	4.48782200

Mg	4.48782200	-1.63005900	7.33020400
Mg	-7.33020400	4.48782200	-1.63005900
Mg	-1.63005900	7.33020400	-4.48782200
Mg	-7.33020400	1.63005900	4.48782200
Mg	-4.48782200	-1.63005900	7.33020400
Mg	7.33020400	4.48782200	1.63005900
Mg	4.48782200	7.33020400	-1.63005900
Mg	4.48782200	1.63005900	7.33020400
Mg	-7.33020400	4.48782200	1.63005900
Mg	-4.48782200	7.33020400	-1.63005900
Mg	-4.48782200	1.63005900	7.33020400
Mg	4.48782200	7.33020400	1.63005900
Mg	1.63005900	4.48782200	7.33020400
Mg	-4.48782200	7.33020400	1.63005900
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Output coordinates:

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Mg₆₀Cl₉₀ (truncated dodecahedron)

Input keywords:

HF/gen opt iop(2/17=5)

Input coordinates:

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Mg	6.00867900	-8.27023700	-4.40245400
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Mg	-4.72057600	-10.04315700	-0.85661300
Mg	-8.09287200	-7.59304100	-0.85661300
Mg	-9.72224600	3.15894900	-4.40245400
Mg	-2.08419300	5.64070300	-9.36596200
Mg	4.72057600	-10.04315700	-0.85661300
Mg	8.09287200	-7.59304100	-0.85661300
Mg	8.09287200	2.62953300	-7.17451100
Mg	4.72057600	3.72525900	-9.36596200
Mg	-2.08419300	-10.89977000	0.85661300
Mg	-9.72224600	-5.35040000	0.85661300
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Mg	-9.72224600	5.35040000	-0.85661300
Mg	0.00000000	8.50934900	-7.17451100
Mg	2.08419300	5.64070300	-9.36596200
Mg	2.08419300	-10.89977000	0.85661300
Mg	9.72224600	-5.35040000	0.85661300
Mg	9.72224600	3.15894900	-4.40245400
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Mg	-9.72224600	-3.15894900	4.40245400
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Mg	9.72224600	5.35040000	-0.85661300
Mg	0.00000000	-8.50934900	7.17451100
Mg	-8.09287200	-2.62953300	7.17451100

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Cl	2.99142200	7.43056400	8.31860600
Cl	6.14248600	5.14118200	8.31860600
Cl	7.99128700	7.68583700	3.22929600
Cl	4.84022200	9.97521900	3.22929600

CI	6.78768700	9.34244900	-0.08392900
CI	10.98270800	3.56849800	0.08392900
CI	10.98270800	1.52081200	-3.22929600
CI	9.77910800	5.22511100	-3.22929600
CI	7.99128700	0.54884000	-8.31860600
CI	6.78768700	4.25313900	-8.31860600
CI	4.84022200	1.57268300	-10.36629300
CI	10.98270800	-1.52081200	3.22929600
CI	10.98270800	-3.56849800	-0.08392900
CI	9.77910800	-5.22511100	3.22929600
CI	4.84022200	-9.97521900	-3.22929600
CI	6.78768700	-9.34244900	0.08392900
CI	7.99128700	-7.68583700	-3.22929600
CI	-4.84022200	9.97521900	3.22929600
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CI	-12.75277700	0.00000000	0.00000000
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CI	-6.37638800	8.77634600	6.70453200
CI	-6.37638800	2.07181400	10.84816000
CI	-10.31721300	-3.35226600	6.70453200
CI	0.00000000	6.70453200	10.84816000
CI	-3.94082500	-5.42408000	10.84816000
CI	-10.31721300	-7.49589400	0.00000000
CI	-10.31721300	3.35226600	-6.70453200
CI	-3.94082500	12.12861200	0.00000000
CI	-6.37638800	-8.77634600	-6.70453200
CI	-3.94082500	-12.12861200	0.00000000
CI	3.94082500	-12.12861200	0.00000000
CI	6.37638800	-8.77634600	-6.70453200
CI	0.00000000	-6.70453200	-10.84816000
CI	10.31721300	-7.49589400	0.00000000
CI	0.00000000	-10.84816000	6.70453200
CI	-6.37638800	-2.07181400	-10.84816000
CI	6.37638800	-2.07181400	-10.84816000
CI	3.94082500	-5.42408000	10.84816000
CI	6.37638800	2.07181400	10.84816000
CI	6.37638800	8.77634600	6.70453200
CI	10.31721300	7.49589400	0.00000000
CI	12.75277700	0.00000000	0.00000000
CI	10.31721300	-3.35226600	6.70453200
CI	10.31721300	3.35226600	-6.70453200
CI	3.94082500	5.42408000	-10.84816000
CI	0.00000000	10.84816000	-6.70453200
CI	3.94082500	12.12861200	0.00000000
CI	-3.94082500	5.42408000	-10.84816000
CI	4.63021900	1.50444900	7.87739900
CI	2.86163300	-3.93869900	7.87739900
CI	-2.86163300	-3.93869900	7.87739900
CI	-4.63021900	1.50444900	7.87739900
CI	0.00000000	4.86850000	7.87739900
CI	7.49185200	-2.43425000	4.86850000
CI	7.49185200	-5.44314900	0.00000000
CI	2.86163300	-8.80720000	0.00000000
CI	0.00000000	-7.87739900	4.86850000
CI	4.63021900	-6.37295000	-4.86850000
CI	0.00000000	-4.86850000	-7.87739900
CI	-4.63021900	-6.37295000	-4.86850000

Cl	-2.86163300	-8.80720000	0.00000000
Cl	-7.49185200	-5.44314900	0.00000000
Cl	-7.49185200	-2.43425000	4.86850000
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Cl	-7.49185200	5.44314900	0.00000000
Cl	-4.63021900	6.37295000	4.86850000
Cl	-2.86163300	8.80720000	0.00000000
Cl	2.86163300	8.80720000	0.00000000
Cl	4.63021900	6.37295000	4.86850000
Cl	7.49185200	5.44314900	0.00000000
Cl	9.26043800	0.00000000	0.00000000
Cl	7.49185200	2.43425000	-4.86850000
Cl	4.63021900	-1.50444900	-7.87739900
Cl	2.86163300	3.93869900	-7.87739900
Cl	-2.86163300	3.93869900	-7.87739900
Cl	-4.63021900	-1.50444900	-7.87739900
Cl	-7.49185200	2.43425000	-4.86850000
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Output coordinates:

Mg	-1.635343	-5.771343	-9.338230
Mg	-4.983525	-3.338747	-9.338230
Mg	1.635343	-5.771343	-9.338230
Mg	-4.983525	-6.859234	-7.162449
Mg	-5.994222	-0.228140	-9.338230
Mg	4.983525	-6.859233	-7.162449
Mg	4.983525	-3.338746	-9.338230
Mg	-5.994222	-8.250339	-4.380238
Mg	-8.063513	2.619994	-7.162449
Mg	-4.715331	3.707884	-9.338230
Mg	5.994223	-8.250339	-4.380238
Mg	5.994222	-0.228139	-9.338230
Mg	-4.715330	-10.010583	-0.859751
Mg	-8.063512	-7.577986	-0.859751
Mg	-9.698856	3.151349	-4.380238
Mg	-2.069291	5.630345	-9.338230
Mg	4.715331	-10.010582	-0.859751
Mg	8.063513	-7.577986	-0.859751
Mg	8.063512	2.619994	-7.162449
Mg	4.715330	3.707885	-9.338230
Mg	-2.069290	-10.870333	0.859751
Mg	-9.698855	-5.327130	0.859751
Mg	-10.977747	1.391105	-0.859751
Mg	-9.698856	5.327129	-0.859751
Mg	-0.000000	8.478479	-7.162449
Mg	2.069290	5.630345	-9.338230
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Mg	9.698855	3.151350	-4.380238
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Mg	-9.698855	-3.151350	4.380238
Mg	-10.977747	-1.391106	0.859751
Mg	-8.063513	7.577986	0.859751
Mg	-0.000000	10.197980	-4.380238
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Mg	10.977747	-1.391105	0.859751
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Mg	9.698855	5.327130	-0.859751
Mg	0.000000	-8.478479	7.162449
Mg	-8.063512	-2.619994	7.162449
Mg	-5.994223	8.250339	4.380238
Mg	-4.715331	10.010582	0.859751

Mg	-2.069291	10.870333	-0.859751
Mg	2.069290	10.870333	-0.859751
Mg	8.063513	-2.619994	7.162449
Mg	8.063512	7.577986	0.859751
Mg	2.069291	-5.630345	9.338230
Mg	-2.069290	-5.630345	9.338230
Mg	-4.715330	-3.707885	9.338230
Mg	-5.994222	0.228139	9.338230
Mg	-4.983525	6.859233	7.162449
Mg	4.715330	10.010583	0.859751
Mg	4.715331	-3.707884	9.338230
Mg	5.994222	0.228140	9.338230
Mg	5.994222	8.250339	4.380238
Mg	-4.983525	3.338746	9.338230
Mg	-1.635343	5.771343	9.338230
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Mg	4.983525	6.859234	7.162449
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Cl	-6.777293	4.238885	-8.309739
Cl	-7.974500	0.554262	-8.309739
Cl	-2.991391	-4.117297	-10.346548
Cl	-6.125718	-5.135701	-8.309739
Cl	-2.991391	-7.412923	-8.309739
Cl	-4.840172	-9.957553	-3.220481
Cl	-7.974499	-7.680331	-3.220481
Cl	-6.777293	-9.328144	0.075146
Cl	-9.768684	-5.210848	3.220481
Cl	-10.965890	-3.563034	-0.075146
Cl	-10.965890	-1.526225	3.220481
Cl	-10.965891	1.526224	-3.220481
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Cl	-10.965891	3.563033	0.075146
Cl	-1.937121	7.755476	-8.309739
Cl	-0.000000	5.089258	-10.346548
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Cl	2.991391	-4.117296	-10.346548
Cl	2.991391	-7.412923	-8.309739
Cl	6.125719	-5.135701	-8.309739
Cl	0.000001	-11.530220	-0.075146
Cl	-1.937120	-10.900811	3.220481
Cl	1.937121	-10.900811	3.220481
Cl	-6.777293	-4.238886	8.309739
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Cl	-4.840172	-1.572668	10.346548
Cl	-1.937120	-7.755476	8.309739
Cl	0.000000	-5.089258	10.346548
Cl	1.937121	-7.755476	8.309739
Cl	6.777293	-4.238885	8.309739
Cl	7.974500	-0.554262	8.309739
Cl	4.840172	-1.572667	10.346548
Cl	-2.991391	4.117296	10.346548
Cl	-6.125719	5.135701	8.309739
Cl	-2.991391	7.412923	8.309739
Cl	2.991391	4.117297	10.346548
Cl	2.991391	7.412923	8.309739
Cl	6.125718	5.135701	8.309739
Cl	7.974499	7.680331	3.220481
Cl	4.840172	9.957553	3.220481
Cl	6.777293	9.328144	-0.075146
Cl	10.965890	3.563034	0.075146

CI	10.965890	1.526225	-3.220481
CI	9.768684	5.210848	-3.220481
CI	7.974500	0.554263	-8.309739
CI	6.777293	4.238886	-8.309739
CI	4.840172	1.572668	-10.346548
CI	10.965891	-1.526224	3.220481
CI	10.965891	-3.563033	-0.075146
CI	9.768684	-5.210847	3.220481
CI	4.840173	-9.957552	-3.220481
CI	6.777293	-9.328143	0.075146
CI	7.974500	-7.680330	-3.220481
CI	-4.840173	9.957552	3.220481
CI	-7.974500	7.680330	3.220481
CI	-6.777293	9.328143	-0.075146
CI	-1.937121	10.900811	-3.220481
CI	1.937120	10.900811	-3.220481
CI	-0.000001	11.530220	0.075146
CI	-12.706556	-0.000001	0.000000
CI	-10.279820	7.468725	0.000000
CI	-6.353278	8.744536	6.680232
CI	-6.353278	2.064305	10.808842
CI	-10.279819	-3.340116	6.680232
CI	-0.000000	6.680232	10.808842
CI	-3.926541	-5.404421	10.808842
CI	-10.279819	-7.468726	0.000000
CI	-10.279820	3.340115	-6.680232
CI	-3.926542	12.084652	0.000000
CI	-6.353277	-8.744537	-6.680232
CI	-3.926541	-12.084653	0.000000
CI	3.926542	-12.084652	0.000000
CI	6.353278	-8.744536	-6.680232
CI	0.000000	-6.680232	-10.808842
CI	10.279820	-7.468725	0.000000
CI	0.000001	-10.808842	6.680232
CI	-6.353278	-2.064305	-10.808842
CI	6.353278	-2.064305	-10.808842
CI	3.926542	-5.404421	10.808842
CI	6.353278	2.064305	10.808842
CI	6.353277	8.744537	6.680232
CI	10.279819	7.468726	0.000000
CI	12.706556	0.000001	0.000000
CI	10.279820	-3.340115	6.680232
CI	10.279819	3.340116	-6.680232
CI	3.926541	5.404421	-10.808842
CI	-0.000001	10.808842	-6.680232
CI	3.926541	12.084653	0.000000
CI	-3.926542	5.404421	-10.808842
CI	4.622778	1.502032	7.864740
CI	2.857034	-3.932370	7.864740
CI	-2.857034	-3.932370	7.864740
CI	-4.622778	1.502031	7.864740
CI	-0.000000	4.860676	7.864740
CI	7.479812	-2.430338	4.860676
CI	7.479812	-5.434401	0.000000
CI	2.857034	-8.793046	0.000000
CI	0.000000	-7.864740	4.860676
CI	4.622778	-6.362708	-4.860676
CI	0.000000	-4.860676	-7.864740
CI	-4.622778	-6.362708	-4.860676
CI	-2.857033	-8.793046	0.000000
CI	-7.479812	-5.434402	0.000000

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Cl	-9.245556	-0.000000	0.000000
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Cl	4.622778	6.362708	4.860676
Cl	7.479812	5.434402	0.000000
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Cl	7.479812	2.430339	-4.860676
Cl	4.622778	-1.502031	-7.864740
Cl	2.857034	3.932370	-7.864740
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Cl	-4.622778	-1.502032	-7.864740
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Cl	-0.000000	7.864740	-4.860676

Mg₆₀Cl₉₀ (truncated icosahedron)

Input keywords:

HF/gen opt iop(2/17=5)

Input coordinates:

Mg	7.65273100	-6.63409500	1.40596300
Mg	3.94457500	-9.32822800	1.40596300
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Mg	3.70815700	-7.91576500	-5.30494900
Mg	6.38245600	-5.97277200	-5.30494900
Mg	8.67422300	-5.22813200	-1.40596300
Mg	7.65273100	-4.22438800	5.30494900
Mg	3.94457500	-5.42924200	7.71465500
Mg	1.65280800	-8.58358800	5.30494900
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Mg	-2.29176700	-9.86525800	-1.40596300
Mg	0.00000000	-6.71091200	-7.71465500
Mg	0.00000000	-3.89898600	-9.45252100
Mg	3.70815700	-1.20485300	-9.45252100
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Mg	8.67422300	1.08056100	-5.30494900
Mg	10.09061300	-0.86893300	-1.40596300
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Mg	8.67422300	-1.08056100	5.30494900
Mg	2.29176700	-3.15434600	9.45252100
Mg	3.70815700	1.20485300	9.45252100
Mg	6.38245600	2.07378600	7.71465500
Mg	6.38245600	5.97277200	5.30494900
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Mg	7.65273100	6.63409500	-1.40596300
Mg	7.65273100	4.22438800	-5.30494900
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Mg	-7.65273100	4.22438800	-5.30494900
Mg	-8.67422300	1.08056100	-5.30494900
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Mg	-8.67422300	5.22813200	1.40596300
Mg	-3.94457500	9.32822800	-1.40596300
Mg	-1.65280800	8.58358800	-5.30494900
Mg	-3.94457500	5.42924200	-7.71465500
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Mg	-3.70815700	-1.20485300	-9.45252100
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Mg	-6.38245600	5.97277200	5.30494900
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Mg	-2.29176700	9.86525800	1.40596300
Mg	1.65280800	8.58358800	-5.30494900
Mg	3.94457500	9.32822800	-1.40596300
Mg	2.29176700	9.86525800	1.40596300
Mg	3.70815700	7.91576500	5.30494900
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Mg	0.00000000	3.89898600	9.45252100
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Mg	-7.65273100	6.63409500	-1.40596300
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Cl	-9.93193300	3.22708100	1.23919000
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Cl	-2.75069400	7.34791600	-7.00248200
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Cl	2.75069400	9.54929800	-3.44057100
Cl	3.38757800	9.34236200	3.44057100
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Cl	6.13827200	8.44860700	-1.23919000
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Cl	-3.38757800	-1.10069100	9.89473300
Cl	-2.75069400	-7.34791600	7.00248200
Cl	-2.75069400	-9.54929800	3.44057100
Cl	-6.13827200	-8.44860700	1.23919000
Cl	0.00000000	-10.44305300	-1.23919000

CI	-3.38757800	-9.34236200	-3.44057100
CI	-2.09363800	-7.56140700	-7.00248200
CI	2.09363800	-2.88164600	-9.89473300
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CI	6.54435500	-4.32777200	-7.00248200
CI	7.83829500	-0.34543500	-7.00248200
CI	9.93193300	0.33483000	-3.44057100
CI	9.93193300	-0.33483000	3.44057100
CI	7.83829500	0.34543500	7.00248200
CI	6.54435500	4.32777200	7.00248200
CI	3.38757800	-1.10069100	9.89473300
CI	0.00000000	-3.56191000	9.89473300
CI	6.13827200	-4.88669700	7.00248200
CI	2.75069400	-7.34791600	7.00248200
CI	3.38757800	-9.34236200	-3.44057100
CI	2.09363800	-7.56140700	-7.00248200
CI	7.83829500	-6.10872700	-3.44057100
CI	9.93193300	-3.22708100	-1.23919000
CI	6.13827200	-8.44860700	1.23919000
CI	2.75069400	-9.54929800	3.44057100
CI	8.23191100	-5.56696100	3.44057100
CI	5.90935500	-8.13353000	-6.21346400
CI	5.90935500	-1.92006600	-10.05359600
CI	9.56153800	3.10673200	-6.21346400
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CI	9.56153800	-6.94686400	0.00000000
CI	0.00000000	-6.21346400	-10.05359600
CI	-5.90935500	-1.92006600	-10.05359600
CI	-3.65218200	5.02679800	-10.05359600
CI	3.65218200	5.02679800	-10.05359600
CI	-5.90935500	-8.13353000	-6.21346400
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CI	3.65218200	-11.24026200	0.00000000
CI	3.65218200	-5.02679800	10.05359600
CI	9.56153800	-3.10673200	6.21346400
CI	0.00000000	-10.05359600	6.21346400
CI	9.56153800	6.94686400	0.00000000
CI	5.90935500	1.92006600	10.05359600
CI	5.90935500	8.13353000	6.21346400
CI	0.00000000	6.21346400	10.05359600
CI	-5.90935500	8.13353000	6.21346400
CI	-3.65218200	11.24026200	0.00000000
CI	-9.56153800	6.94686400	0.00000000
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CI	-9.56153800	-3.10673200	6.21346400
CI	-11.81871100	0.00000000	0.00000000
CI	-5.90935500	1.92006600	10.05359600
CI	-9.56153800	3.10673200	-6.21346400
CI	3.65218200	11.24026200	0.00000000
CI	-3.65218200	-5.02679800	10.05359600
CI	0.00000000	10.05359600	-6.21346400
CI	2.58966400	-3.56436700	7.12873400
CI	4.19016500	1.36146700	7.12873400
CI	6.77982900	-2.20290000	4.40580000
CI	8.38032900	0.00000000	0.00000000
CI	6.77982900	-4.92583400	0.00000000
CI	4.19016500	-5.76726700	-4.40580000
CI	2.58966400	-7.97016700	0.00000000
CI	-2.58966400	-7.97016700	0.00000000
CI	0.00000000	-7.12873400	4.40580000
CI	-2.58966400	-3.56436700	7.12873400

Cl	-6.77982900	-2.20290000	4.40580000
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Cl	0.00000000	-4.40580000	-7.12873400
Cl	4.19016500	-1.36146700	-7.12873400
Cl	6.77982900	4.92583400	0.00000000
Cl	6.77982900	2.20290000	-4.40580000
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Output coordinates:

Mg	7.394769	-6.434510	1.390039
Mg	3.834473	-9.021217	1.390039
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Mg	6.204308	-5.759419	-5.133556
Mg	8.404692	-5.044471	-1.390039
Mg	7.394769	-4.120890	5.133556
Mg	3.834473	-5.277700	7.447177
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Mg	-2.200385	-9.552164	-1.390039
Mg	-0.000000	-6.523596	-7.447177
Mg	-0.000000	-3.743517	-9.165360
Mg	3.560296	-1.156811	-9.165360
Mg	6.204308	-2.015902	-7.447177
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Mg	9.764604	0.859091	1.390039
Mg	8.404692	-1.012667	5.133556
Mg	2.200384	-3.028569	9.165360
Mg	3.560296	1.156810	9.165360
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Mg	6.204308	5.759419	5.133556
Mg	8.404693	5.044470	1.390039
Mg	7.394770	6.434510	-1.390039
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Mg	3.834474	5.277700	-7.447177
Mg	2.200384	3.028569	-9.165360
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Mg	-7.394769	4.120890	-5.133556
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Mg	-3.834473	9.021217	-1.390039
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Mg	-3.560296	-1.156810	-9.165360
Mg	-6.204308	-2.015902	-7.447177

Mg	-8.404693	-5.044470	-1.390039
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Mg	-7.394770	-4.120889	5.133556
Mg	-8.404692	-1.012667	5.133556
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Mg	-6.204308	5.759419	5.133556
Mg	-3.560296	7.680406	5.133556
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CI	1.909360	-2.628009	-9.990737
CI	3.089410	1.003810	-9.990737
CI	6.790844	-4.214100	-6.818556
CI	7.970894	-0.582281	-6.818556
CI	9.880254	0.038108	-3.570158
CI	9.880254	-0.038109	3.570158
CI	7.970894	0.582280	6.818556
CI	6.790845	4.214099	6.818556
CI	3.089410	-1.003810	9.990737
CI	-0.000000	-3.248398	9.990737
CI	6.106333	-5.156249	6.818556
CI	3.016923	-7.400836	6.818556
CI	3.089409	-9.384904	-3.570158
CI	1.909360	-7.760705	-6.818556
CI	7.970894	-5.838298	-3.570158
CI	9.880254	-3.210290	-1.562538
CI	6.106333	-8.404647	1.562538
CI	3.016923	-9.408456	3.570158
CI	8.015693	-5.776638	3.570158
CI	5.743780	-7.905636	-6.039368
CI	5.743780	-1.866268	-9.771903
CI	9.293632	3.019684	-6.039368
CI	11.487561	-0.000001	0.000000
CI	9.293632	-6.752219	0.000000
CI	-0.000000	-6.039368	-9.771903
CI	-5.743780	-1.866267	-9.771903
CI	-3.549851	4.885952	-9.771903
CI	3.549852	4.885951	-9.771903
CI	-5.743781	-7.905635	-6.039368
CI	-3.549852	-10.925319	0.000000
CI	3.549851	-10.925320	0.000000
CI	3.549851	-4.885952	9.771903
CI	9.293632	-3.019684	6.039368
CI	-0.000000	-9.771903	6.039368
CI	9.293632	6.752218	0.000000
CI	5.743780	1.866267	9.771903
CI	5.743781	7.905635	6.039368
CI	0.000000	6.039368	9.771903
CI	-5.743780	7.905636	6.039368
CI	-3.549851	10.925320	0.000000
CI	-9.293632	6.752219	0.000000
CI	-9.293632	-6.752218	0.000000
CI	-9.293632	-3.019684	6.039368
CI	-11.487561	0.000001	0.000000
CI	-5.743780	1.866268	9.771903
CI	-9.293632	3.019684	-6.039368
CI	3.549852	10.925319	0.000000
CI	-3.549852	-4.885951	9.771903
CI	0.000000	9.771903	-6.039368
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CI	4.012036	1.303589	6.825683
CI	6.491610	-2.109252	4.218504
CI	8.024072	-0.000000	0.000000
CI	6.491610	-4.716431	0.000000
CI	4.012036	-5.522094	-4.218504
CI	2.479574	-7.631346	0.000000
CI	-2.479575	-7.631345	0.000000
CI	-0.000000	-6.825683	4.218504
CI	-2.479575	-3.412841	6.825683
CI	-6.491610	-2.109252	4.218504
CI	-4.012036	1.303590	6.825683

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