Supporting Information

Theoretical investigation of structural and electronic property of $[PW_{12}O_{40}]^{3-}$ on graphene layer

Shizheng Wen, Wei Guan, Jianping Wang, Zhongling Lang, Likai Yan, and Zhongmin Su

Institute of Functional Material Chemistry, Faculty of Chemistry, Northeast Normal University, Changchun 130024, P. R. China, Fax: +86-431-85684009; Tel: +86-431-85099108; E-mail: zmsu@nenu.edu.cn
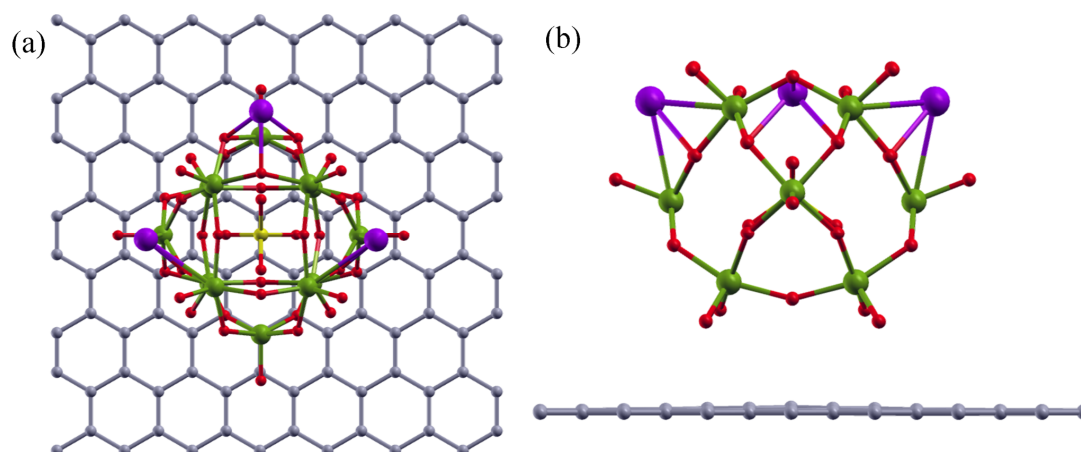
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Due to the charged property of treated system, the charge spurious interactions induced by the periodic boundary conditions may be a trick one. To take full account of this effect, we also checked one of the neutral complexes based on S4-B model which was added three Na cations as counterions to keep electrical neutral of the system (S4-B-Na3). The three Na ions were positioned around the PW_{12} which is farthest to the graphene surface (Figure S1). As there is some uncertainty in determining the position of the Na cations. We just took one of the possible situations which the Na cations were supposed to interact only with the bridging oxygens. Full optimization with the same force convergence was also used for this model. (Due to the same fixed supercell, atoms and charge of our adopted models, we just take this lowest energy configuration as an example for convenient.) The adsorption energy of S4-B-Na3 is -1.76 eV under GGA method which is also confirmed the correction of dipole correction interaction in our model is suitable.

We used the van der Waals density functional (vdW-DF) as proposed by Dion *et al.*[Phys. Rev. Lett. **92**, 246401 (2004)] and recently implemented in the SIESTA code [Phys. Rev. Lett. **103**, 096102 (2009)] to check the adsorption energy (E_a). The vdW-DF is a promising approach for including dispersion in approximate density functional theory exchange-correlation functional. The results of E_a with both GGA and vdW-DF are summarized in Table S1. Here we chose the Group II (S4 series) as an example. It is noted that the implement of calculation van der Waals Force is ineffective at present state. So the structures adopted here are not optimized with vdW-DF, and instead we use the optimized geometries with GGA method. From the results in Table S1, the largest error of E_a between GGA and vdW-DF is within 30 meV.

Table S1. The adsorption energy (E_a) calculated with GGA and vdW-DF method.

	GGA (eV)	vdW-DF (eV)
S4-B	-1.786	-1.767
S4-T	-1.744	-1.739
S4-H	-1.693	-1.663

Figure S1. The final geometries of Na_3-PW_{12} (S4-B-Na3) deposited on graphene layer selected in the calculation (tungsten in green, oxygen in red, phosphorus in yellow and sodium in purple). (a) and (b) with views along $-z$ and y axes directions, respectively.

The DOS is an important way to understand the adsorbate effects on the electronic properties of the interfacial systems. From Figure S2 and S3, in each group the overall TDOS have very similar population. As shown in the text, the energy barrier between each other in the same group is low which means the coexistence of conformation. As discussed above, the POM is physisorption on the graphene layer. It may be more easily separated after catalytic process. It is believed to behavior different from the graphene oxide-POM systems [Li, *et al.* Chem. Commun., 46, 6243 (2010)].
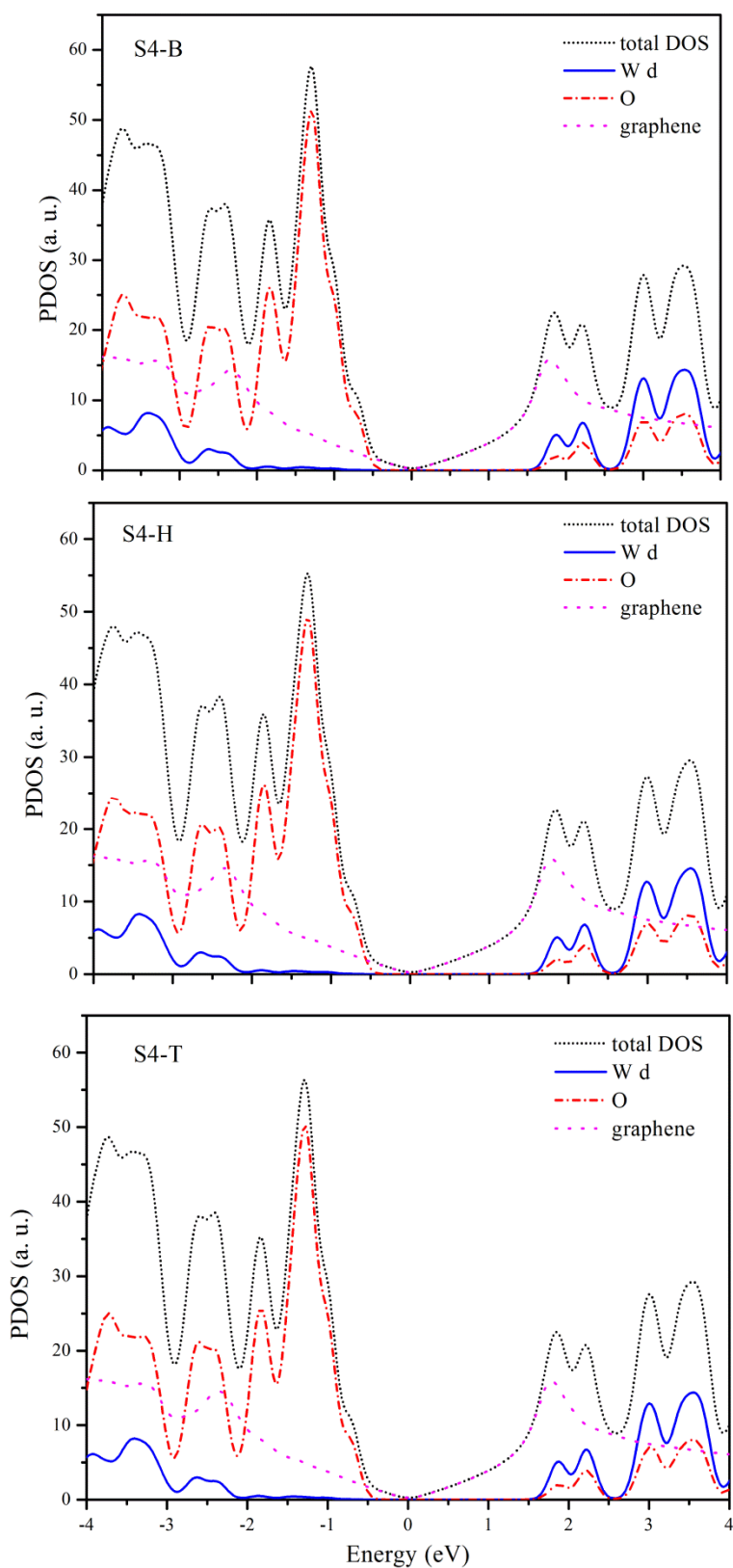
Figure S2. The total and Projected Density of State (TDOS, PDOS) of Group 1 (S4-B, S4-H, and S4-T).
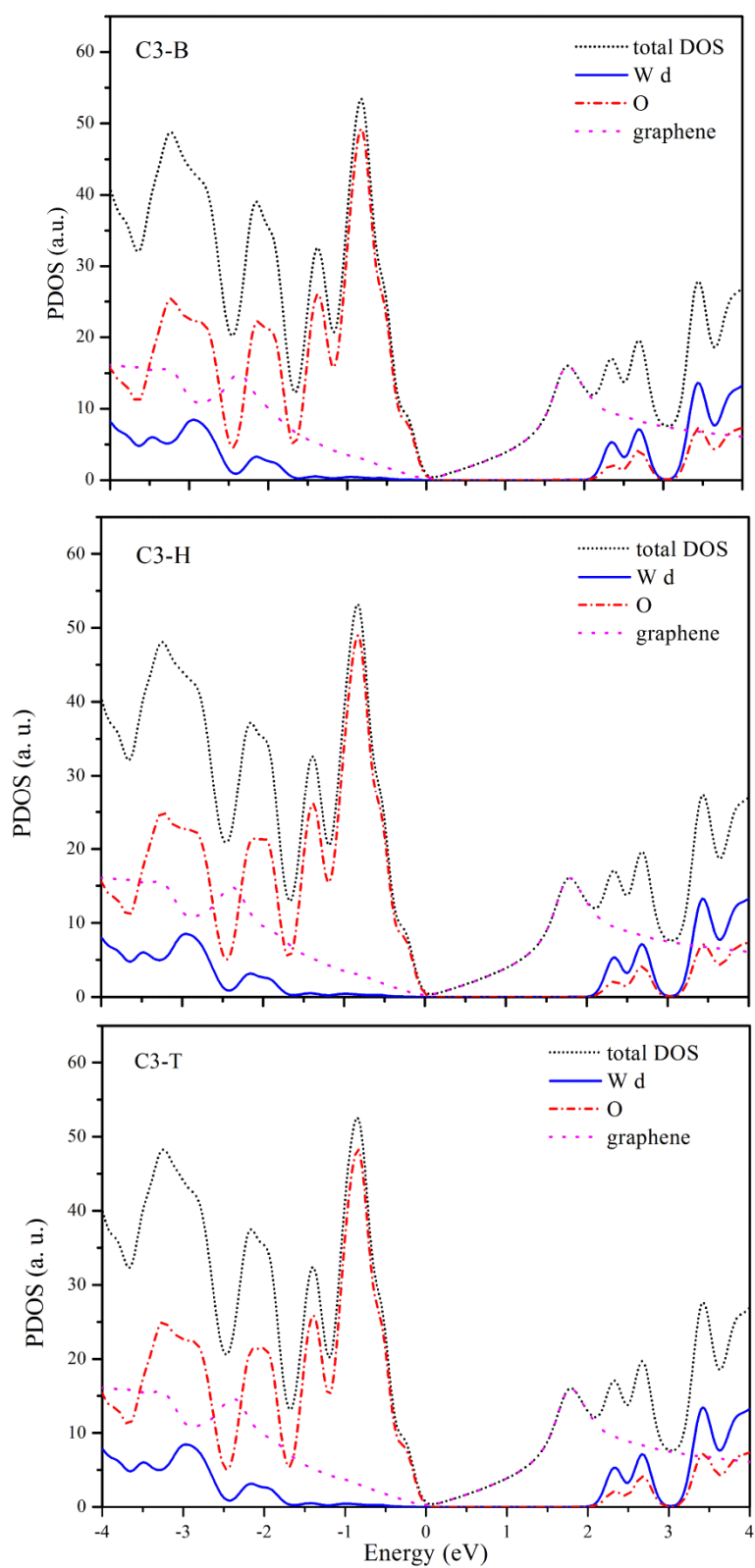
Figure S3. The Projected Density of State (PDOS) of Group 2 (C3-B, C3-H, and C3-T).

Here and followed, the detail Cartesian coordinates of structures discussed in the main text is shown.

Optimized Cartesian coordinates of PW$_{12}$ using LDA (Cell side 30x30x30 Å)

```
P   -0.000002   0.000638   0.001408
W   -1.686263  -0.974587   2.936952
W    1.686922  -3.092721  -0.059936
W    1.835008   1.058734  -2.811270
W   -1.835153   3.008088  -0.058980
W    1.686267  -0.974580   2.936953
W    1.835148   3.008090  -0.058980
W   -1.835008   1.058737  -2.811270
W   -1.686923  -3.092726  -0.059939
W   -0.000004  -2.119169  -2.813089
W   -3.522116   0.085972  -0.058097
W   -0.000002   1.948028   2.937210
W    3.522121   0.085980  -0.058102
O    0.000004   0.000111   1.563446
O   -0.000012  -1.472181  -0.519408
O    1.276164   0.737133  -0.519023
O   -1.276165   0.737139  -0.519018
O   -2.834630  -1.636381  -0.402520
O    2.832577  -0.164540   1.678656
O   -1.275101  -0.737265  -2.947562
O    1.274682   2.536668   1.677980
O    2.834626  -1.636375  -0.402516
O   -1.274682   2.536665   1.677976
O    1.275097  -0.737267  -2.947560
O   -2.832572  -0.164542   1.678654
O   -0.000001   1.470825  -2.947876
O   -1.559291  -2.372127   1.678466
O   -0.000002   3.272504  -0.402996
O    1.559290  -2.372125   1.678471
O    1.297105   0.749142   3.623659
O   -1.297561  -3.167826  -1.912675
O    3.391475   1.958817   0.205364
O   -3.391584   0.459508  -1.910618
O   -1.297105   0.749137   3.623653
O    3.391586   0.459508  -1.910620
O   -3.391477   1.958815   0.205363
O    1.297558  -3.167818  -1.912670
O    0.000000  -3.915146   0.205377
O   -2.094536   2.706647  -1.912092
O    0.000003  -1.498773   3.624954
O    2.094535   2.706643  -1.912090
O   -2.748682  -1.587694   4.089222
O    2.747888  -4.384711   0.133357
O    2.423956   1.398397  -4.350691
O   -2.421977   4.573771   0.133711
O    2.748685  -1.587693   4.089223
O    2.421976   4.573771   0.133710
O   -2.423956   1.398399  -4.350693
```

```
O    -2.747891   -4.384715    0.133358
O     0.000000   -2.799181   -4.352838
O    -5.171728   -0.187102    0.134345
O    -0.000017    3.174153    4.090613
O     5.171719   -0.187102    0.134346
```

Optimized Cartesian coordinates of PW$_{12}$ using GGA (Cell side 30x30x30 Å)

```
P     0.000010   -0.000500    0.000112
W    -1.742138   -1.005571    3.018486
W     1.741414   -3.180101   -0.057512
W     1.884207    1.083352   -2.898358
W    -1.883410    3.095425   -0.055043
W     1.742137   -1.005573    3.018493
W     1.883395    3.095418   -0.055032
W    -1.884210    1.083343   -2.898366
W    -1.741403   -3.180104   -0.057512
W     0.000008   -2.176971   -2.903875
W    -3.627575    0.080540   -0.054060
W    -0.000014    2.009451    3.019147
W     3.627568    0.080547   -0.054054
O     0.000081    0.000193    1.581518
O     0.000004   -1.490603   -0.528866
O     1.292951    0.743848   -0.526107
O    -1.292948    0.743835   -0.526099
O    -2.967322   -1.713085   -0.398847
O     2.964838   -0.188232    1.750074
O    -1.317732   -0.765479   -3.089833
O     1.316623    2.657213    1.748032
O     2.967329   -1.713082   -0.398846
O    -1.316643    2.657213    1.748023
O     1.317717   -0.765566   -3.089856
O    -2.964847   -0.188233    1.750066
O    -0.000002    1.513990   -3.086321
O    -1.643253   -2.466302    1.746344
O    -0.000012    3.417525   -0.400241
O     1.643254   -2.466288    1.746355
O     1.342222    0.774899    3.716018
O    -1.340346   -3.246506   -1.966759
O     3.482437    2.008543    0.223739
O    -3.482266    0.458199   -1.965292
O    -1.342255    0.774887    3.716036
O     3.482261    0.458208   -1.965284
O    -3.482446    2.008531    0.223739
O     1.340361   -3.246508   -1.966755
O     0.000007   -4.016739    0.227358
O    -2.138696    2.779754   -1.965839
O     0.000000   -1.546277    3.715656
O     2.138681    2.779759   -1.965829
```

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O   -2.808158  -1.623896   4.230649
O    2.804804  -4.530510   0.122707
O    2.519416   1.450840  -4.463173
O   -2.517476   4.693055   0.122707
O    2.808145  -1.623905   4.230680
O    2.517462   4.693053   0.122708
O   -2.519416   1.450836  -4.463176
O   -2.804791  -4.530502   0.122703
O    0.000018  -2.910316  -4.469427
O   -5.328955  -0.166101   0.124464
O   -0.000017   3.244627   4.228373
O    5.328951  -0.166097   0.124469
```

The orthogonal cell is 17.33 × 17.15 × 30.0 Å (for GGA) with 112 carbon atoms plus 53 atoms of PW_{12}.

Optimized Cartesian coordinates of S4-B using GGA

```
C   -0.005502  -0.310838   9.693903
C   -0.005154   2.548217   9.725435
C   -0.004843   3.977817   9.750376
C   -0.004876   6.834886   9.786495
C   -0.004926   8.264389   9.785807
C   -0.004848  11.121528   9.747510
C    1.232744   0.404216   9.704587
C    1.233496   1.833991   9.720912
C    1.233445   4.692162   9.773655
C    1.233914   6.121441   9.795428
C    1.233726   8.978274   9.793666
C    1.233652  10.407608   9.770586
C    2.470823  -0.310695   9.707347
C    2.471318   2.548627   9.740917
C    2.472605   3.978317   9.770287
C    2.472338   6.834978   9.822884
C    2.472244   8.264574   9.821884
C    2.472732  11.121173   9.765868
C    3.708299   0.404927   9.719546
C    3.709009   1.834546   9.736731
C    3.709025   4.691854   9.799532
C    3.709653   6.120586   9.837717
C    3.709682   8.979038   9.835230
C    3.709120  10.407746   9.795108
C    4.945764  -0.310822   9.720601
C    4.945906   2.550612   9.757623
C    4.946655   3.977600   9.789167
C    4.945976   6.835185   9.869747
C    4.946009   8.264384   9.868430
C    4.946635  11.121864   9.782854
C    6.183153   0.405222   9.729610
C    6.183332   1.834742   9.750172
C    6.183720   4.692689   9.827179
C    6.183391   6.120849   9.875969
C    6.183610   8.978888   9.873045
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```
C      6.183542   10.406895    9.822113
C      7.420442   -0.310656    9.725127
C      7.420431    2.549382    9.768773
C      7.420542    3.979236    9.812027
C      7.420622    6.835044    9.910280
C      7.420685    8.264478    9.909275
C      7.420513   11.120177    9.807469
C      8.657867    0.405235    9.727232
C      8.657622    1.834751    9.746784
C      8.657493    4.692733    9.822410
C      8.657802    6.120848    9.871377
C      8.657754    8.978805    9.870076
C      8.657595   10.406983    9.820151
C      9.895242   -0.310865    9.716938
C      9.895287    2.550581    9.750864
C      9.894318    3.977581    9.780053
C      9.895387    6.834999    9.860677
C      9.895213    8.264351    9.860029
C      9.894536   11.121790    9.778037
C     11.132805    0.404849    9.714229
C     11.132306    1.834522    9.729690
C     11.132142    4.691893    9.788638
C     11.131672    6.120548    9.826393
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C     11.132045   10.407552    9.786636
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C     12.368416    3.978288    9.760925
C     12.368886    6.834909    9.812288
C     12.368875    8.264388    9.811323
C     12.368397   11.120930    9.759138
C     13.608384    0.404180    9.699313
C     13.607727    1.833920    9.714823
C     13.607494    4.692088    9.765979
C     13.607175    6.121353    9.787387
C     13.607286    8.978084    9.786108
C     13.607397   10.407355    9.764224
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C     14.845689    6.834829    9.782197
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C     16.084601    4.691863    9.757093
C     16.084650    6.121272    9.774825
C     16.084692    8.978312    9.773632
C     16.084514   10.407748    9.755054
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C     -0.005431   15.410005    9.693058
C      1.233287   13.265704    9.717816
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C    1.232960   14.695481    9.702922
C    2.471245   12.550792    9.736489
C    2.470794   15.410116    9.706426
C    3.709003   13.265052    9.732731
C    3.708350   14.694624    9.717554
C    4.946089   12.548858    9.752610
C    4.945762   15.410222    9.719583
C    6.183589   13.264925    9.746222
C    6.183121   14.694333    9.727869
C    7.420650   12.549999    9.764560
C    7.420451   15.410069    9.724591
C    8.657693   13.264997    9.744732
C    8.657958   14.694422    9.726531
C    9.895252   12.548811    9.749016
C    9.895512   15.410157    9.716730
C   11.132363   13.264993    9.728904
C   11.132962   14.694611    9.714016
C   12.370002   12.550629    9.731815
C   12.370487   15.410131    9.702144
C   13.607834   13.265514    9.714193
C   13.608327   14.695279    9.699363
C   14.846271   12.551107    9.720455
C   14.846425   15.410084    9.690779
C   16.084710   13.265607    9.708429
C   16.084598   14.695514    9.693266
P    7.458590    7.552856   16.150595
W    7.457438    3.927229   16.271662
W   11.085492    7.545035   16.053185
W    7.462143   11.180758   16.269203
W    3.834133    7.557166   16.068226
W    9.206713    5.670861   18.724565
W    5.722835    9.435784   18.728499
W    5.574323    9.303698   13.601037
W    9.332003    5.801844   13.592215
W    9.338085    9.298779   13.597157
W    5.569791    5.807019   13.601026
W    5.715925    5.671762   18.726998
W    9.211348    9.431939   18.719367
O    7.459221    6.263712   17.062362
O    8.741072    7.553012   15.224808
O    7.462381    8.839866   17.064592
O    6.172190    7.556605   15.229725
O    7.452819    5.878981   13.069831
O    9.100851    7.551114   19.193542
O    7.456130    9.223042   13.074182
O    5.822670    7.553615   19.192851
O   10.426265    8.859769   17.325504
O    4.495475    6.238872   17.331392
O    8.768412   10.511201   14.982955
O    6.147477    4.602691   14.987887
O    6.152270   10.514245   14.984990
O    8.761897    4.597736   14.982803
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O      4.502828    8.868935   17.332318
O     10.424284    6.235511   17.327388
O      7.461371    5.406988   19.560786
O      9.584421    7.550162   12.732017
O      7.466738    9.695226   19.562553
O      5.327945    7.555924   12.735837
O      6.112156    4.074972   17.669489
O      8.810622   11.028120   17.664671
O      3.983760    6.222156   14.647518
O     10.927885    8.887030   14.642315
O     10.924263    6.212523   14.639691
O      3.988189    8.893570   14.649574
O      8.804379    4.073711   17.666745
O      6.118768   11.030233   17.667991
O      7.456247    2.234625   15.960692
O     12.781261    7.542832   16.349315
O      7.463089   12.873879   15.961985
O      2.140982    7.561405   16.378191
O     10.265134    5.038875   19.934276
O      4.664834   10.064997   19.939730
O      4.905366   10.366418   12.404625
O      9.996884    4.734178   12.397829
O     10.004541   10.359841   12.398816
O      4.895730    4.742735   12.408788
O      4.658755    5.042041   19.938456
O     10.271653   10.060772   19.928257
```

Optimized Cartesian coordinates of S4-H using GGA

```
C     -0.005370   -0.311563    9.777830
C     -0.005327    2.547193    9.794226
C     -0.005418    3.976989    9.809496
C     -0.005369    6.834206    9.831841
C     -0.005353    8.263556    9.832499
C     -0.005360   11.120724    9.813031
C      1.232856    0.403278    9.775839
C      1.233138    1.833205    9.783194
C      1.233264    4.691024    9.812108
C      1.233718    6.120642    9.824543
C      1.233569    8.977379    9.827376
C      1.233407   10.407071    9.817244
C      2.471103   -0.311429    9.768911
C      2.471377    2.547538    9.779628
C      2.472329    3.977252    9.794656
C      2.472617    6.834134    9.823833
C      2.472501    8.263761    9.826148
C      2.472340   11.120653    9.804439
C      3.708890    0.403673    9.761164
C      3.709540    1.833618    9.763598
C      3.710729    4.691142    9.788825
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C     3.711151    6.120568    9.810331
C     3.711031    8.977626    9.816970
C     3.710710   10.407013    9.800964
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C     6.184390   10.405877    9.766635
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C     7.421555    6.834491    9.799809
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C     7.421559   11.119845    9.775437
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C     8.658945    1.834202    9.747711
C     8.658863    4.691961    9.781502
C     8.658824    6.121287    9.802526
C     8.658816    8.976695    9.811626
C     8.658922   10.406176    9.797562
C     9.896390   -0.311650    9.748699
C     9.896495    2.549330    9.751133
C     9.896011    3.978039    9.759653
C     9.895928    6.834365    9.801059
C     9.895818    8.263398    9.805110
C     9.895887   11.119940    9.774056
C    11.133749    0.404320    9.750540
C    11.133379    1.833691    9.751813
C    11.133088    4.692226    9.756778
C    11.132336    6.120746    9.780157
C    11.132300    8.977580    9.786857
C    11.133112   10.405745    9.767007
C    12.370875   -0.311574    9.757727
C    12.370456    2.548904    9.763380
C    12.369613    3.977487    9.769025
C    12.368636    6.834301    9.814014
C    12.368593    8.263477    9.816140
C    12.369648   11.120193    9.776628
C    13.608544    0.403453    9.767145
C    13.607821    1.833452    9.772221
C    13.606787    4.691216    9.799096
C    13.606464    6.120555    9.818899
C    13.606602    8.977270    9.820772
C    13.606827   10.406703    9.803001
C    14.846461   -0.311541    9.772713
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C	14.845086	6.833948	9.830597
C	14.845219	8.263517	9.831110
C	14.845204	11.120489	9.805798
C	16.084786	0.403263	9.778586
C	16.084446	1.833134	9.787223
C	16.084374	4.691099	9.816760
C	16.084059	6.120584	9.829000
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C	16.084282	10.406943	9.818670
C	-0.005421	12.550599	9.798222
C	-0.005326	15.409231	9.779017
C	1.233040	13.265028	9.789301
C	1.233114	14.694790	9.779531
C	2.471310	12.550367	9.789657
C	2.471276	15.409364	9.771623
C	3.709543	13.264441	9.775478
C	3.709013	14.694330	9.767830
C	4.946936	12.548842	9.770206
C	4.946527	15.409278	9.756868
C	6.184134	13.264134	9.761048
C	6.183770	14.693614	9.754127
C	7.421318	12.548661	9.765917
C	7.421316	15.409341	9.750922
C	8.658767	13.264015	9.762204
C	8.658876	14.694128	9.754729
C	9.896217	12.548609	9.765408
C	9.896584	15.409229	9.752074
C	11.133240	13.264171	9.761403
C	11.133826	14.693520	9.755734
C	12.370395	12.548730	9.771022
C	12.371071	15.409209	9.759517
C	13.607857	13.264365	9.776122
C	13.608567	14.694296	9.769177
C	14.846281	12.550217	9.790457
C	14.846448	15.409168	9.773279
C	16.084589	13.264930	9.789752
C	16.084711	14.694698	9.780090
P	8.607973	7.560037	16.103413
W	8.603143	3.932093	16.205959
W	12.232992	7.568282	16.020425
W	8.614695	11.175823	16.243896
W	4.981183	7.564175	16.015459
W	10.351882	5.659931	18.664704
W	6.861699	9.430414	18.687545
W	6.723879	9.317393	13.562153
W	10.496954	5.826587	13.552862
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W	6.725729	5.831862	13.546712
W	6.866531	5.665785	18.665561
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O      7.321186    7.567612   15.181262
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O     10.250171    7.541649   19.142064
O      8.609237    9.218053   13.054512
O      6.967923    7.547081   19.135827
O     11.568648    8.869839   17.290879
O      5.651202    6.241053   17.267909
O      9.920099   10.505154   14.961844
O      7.294348    4.621195   14.936679
O      7.305794   10.508672   14.961196
O      9.915023    4.620532   14.939185
O      5.643288    8.873013   17.286381
O     11.560596    6.236406   17.265739
O      8.608315    5.403951   19.511102
O     10.761458    7.572167   12.674304
O      8.606234    9.682466   19.535481
O      6.458481    7.579018   12.674066
O      7.261875    4.069010   17.610600
O      9.955272   11.026439   17.647776
O      5.134759    6.235038   14.590188
O     12.084367    8.903871   14.604482
O     12.083055    6.231615   14.595518
O      5.133236    8.908436   14.603277
O      9.945176    4.066136   17.611389
O      7.266166   11.029831   17.643521
O      8.604549    2.243279   15.873746
O     13.926391    7.564058   16.328959
O      8.615782   12.868248   15.931284
O      3.286650    7.560049   16.318522
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O      5.800397   10.053675   19.898935
O      6.077174   10.414559   12.384169
O     11.140334    4.737399   12.365231
O     11.136480   10.410259   12.381940
O      6.080243    4.748002   12.355981
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O     11.407357   10.044775   19.913509
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Optimized Cartesian coordinates of S4-T using GGA

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C     -0.006060    8.261237    9.777622
C     -0.006143   11.118711    9.759306
C      1.231635    0.401412    9.724137
C      1.232253    1.831146    9.731697
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C      1.232216   10.404351    9.774042
C      2.469754   -0.313381    9.725739
C      2.470055    2.545562    9.738945
C      2.471457    3.974925    9.755669
C      2.471261    6.831328    9.794695
C      2.471203    8.260884    9.798688
C      2.471219   11.117962    9.776918
C      3.707276    0.402341    9.729798
C      3.708104    1.831913    9.735459
C      3.708406    4.688703    9.768542
C      3.708800    6.117096    9.801729
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C      4.945243   11.118054    9.805194
C      6.181955    0.402652    9.739272
C      6.181854    1.831896    9.748359
C      6.182731    4.689507    9.791154
C      6.183231    6.116501    9.835086
C      6.182813    8.974121    9.846364
C      6.182518   10.402904    9.827315
C      7.419248   -0.313183    9.740692
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C      8.656684    0.402673    9.740443
C      8.656660    1.831820    9.749384
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C      8.656818   10.402964    9.825974
C      9.894106   -0.313668    9.735354
C      9.893893    2.546896    9.745265
C      9.893082    3.974397    9.755362
C      9.893839    6.831628    9.821568
C      9.894146    8.259347    9.824899
C      9.894118   11.117939    9.801835
C     11.131356    0.402140    9.732862
C     11.130473    1.831714    9.738870
C     11.130563    4.688676    9.767501
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C    12.367942    6.831164    9.791597
C    12.368026    8.260673    9.793978
C    12.368029   11.117834    9.772586
C    13.606801    0.401202    9.726667
C    13.606192    1.830998    9.734602
C    13.606203    4.688452    9.763216
C    13.606212    6.117615    9.775991
C    13.606682    8.975000    9.780858
C    13.606867   10.403973    9.770357
C    14.845048   -0.313716    9.722146
C    14.844741    2.544962    9.738926
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C    14.844995    8.261119    9.776106
C    14.844756   11.118462    9.757480
C    16.083399    0.401163    9.722698
C    16.083406    1.830912    9.731346
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C    16.083564    6.117897    9.767918
C    16.083677    8.975412    9.772351
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C     9.894330   15.407572    9.740535
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C    12.369010   15.407328    9.730645
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C    16.083401   14.692723    9.725218
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W	9.339128	5.100199	13.577519
W	9.334302	8.593135	13.589531
W	5.577666	5.095393	13.578809
W	5.719816	4.946050	18.711449
W	9.203108	8.712406	18.718113
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O	5.822222	6.824977	19.179445
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O	8.766578	3.893649	14.963048
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O	3.988864	5.495710	14.630845
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O	10.928867	5.508454	14.624106
O	3.981658	8.171474	14.639901
O	8.809943	3.355396	17.643620
O	6.110420	10.309303	17.670232
O	7.462772	1.523489	15.922839
O	12.777487	6.842203	16.340722
O	7.452694	12.153140	15.960979
O	2.139576	6.823812	16.355749
O	10.269310	4.318953	19.912680
O	4.653083	9.327428	19.933721
O	4.920078	9.670619	12.406132
O	10.004723	4.030988	12.385060
O	9.976934	9.679295	12.398900
O	4.915624	4.022642	12.387757
O	4.662874	4.314890	19.922863

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Optimized Cartesian coordinates of C3-B using GGA

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C   -0.002514   6.783367   9.772572
C   -0.002282   8.212648   9.786520
C   -0.002130   11.069877   9.804470
C   1.235466   0.351375   9.760506
C   1.235555   1.781153   9.751788
C   1.235795   4.639580   9.758228
C   1.236077   6.069097   9.770490
C   1.236389   8.926134   9.802544
C   1.236058   10.355286   9.813280
C   2.473429   -0.363527   9.768683
C   2.473500   2.495897   9.748293
C   2.474010   3.925411   9.753687
C   2.474191   6.782800   9.786692
C   2.474977   8.212408   9.806163
C   2.474991   11.068653   9.831226
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C   3.711432   1.780968   9.745826
C   3.711530   4.640137   9.759837
C   3.711672   6.068705   9.783946
C   3.711742   8.924994   9.831701
C   3.711621   10.353701   9.849177
C   4.948605   -0.363685   9.768364
C   4.948792   2.496104   9.737433
C   4.949652   3.925746   9.745253
C   4.950040   6.783395   9.807164
C   4.949270   8.210709   9.832934
C   4.949110   11.068167   9.865864
C   6.185725   0.351948   9.753734
C   6.185789   1.781271   9.735092
C   6.185898   4.639317   9.751612
C   6.186577   6.067766   9.796095
C   6.186436   8.924754   9.855859
C   6.186398   10.353337   9.872521
C   7.423264   -0.363529   9.764817
C   7.423232   2.498055   9.725953
C   7.423108   3.924868   9.729061
C   7.423647   6.781818   9.819013
C   7.423531   8.210918   9.851187
C   7.423672   11.067793   9.873546
C   8.660809   0.352125   9.751358
C   8.660648   1.781470   9.732402
C   8.660766   4.639576   9.746523
C   8.660535   6.067952   9.790894
C   8.660835   8.924948   9.854320

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C      9.896921     3.926088    9.739955
C      9.897029     6.783709    9.801308
C      9.897976     8.210943    9.826675
C      9.898402    11.068474    9.861877
C     11.135891     0.351728    9.753698
C     11.135306     1.781422    9.740582
C     11.135202     4.640461    9.753629
C     11.135430     6.069011    9.777686
C     11.135745     8.925305    9.823203
C     11.135917    10.354096    9.841863
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C     12.372736     3.925685    9.747988
C     12.372840     6.782995    9.780182
C     12.372235     8.212611    9.799046
C     12.372390    11.068971    9.824954
C     13.611375     0.351674    9.756719
C     13.611140     1.781349    9.747660
C     13.611002     4.639806    9.753717
C     13.610754     6.069093    9.765520
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C     13.611213    10.355453    9.808118
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C     14.849290     6.783438    9.769514
C     14.849262     8.212681    9.783254
C     14.849221    11.069975    9.801820
C     16.087466     0.351422    9.759694
C     16.087481     1.781152    9.752804
C     16.087420     4.639518    9.755103
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C     -0.002560    15.357916    9.780930
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C      1.235515    14.643021    9.793952
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C      2.473636    15.357602    9.789551
C      3.711440    13.212727    9.831200
C      3.711189    14.642339    9.807237
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C      4.948728    15.357722    9.796975
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C      8.660643    13.212871    9.843653
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C    12.373343   12.498608    9.821903
C    12.373476   15.357879    9.785261
C    13.610999   13.213682    9.804832
C    13.611411   14.643208    9.790447
C    14.849367   12.499423    9.801242
C    14.849411   15.358019    9.778876
C    16.087571   13.213847    9.795565
C    16.087570   14.643469    9.785529
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W     9.349506    8.877074   13.927673
W     5.604785   10.769149   16.833243
W     9.226130    6.558915   19.773499
W     9.368870   10.751319   16.865937
W     5.576777    8.848589   13.929408
W     5.711503    4.489298   16.605690
W     7.489896    5.598897   13.826957
W     3.850831    7.757380   16.753624
W     7.456376    9.558943   19.879047
W    11.091478    7.723523   16.716062
O     7.473635    7.601530   18.361725
O     7.468734    6.193619   16.199058
O     8.762723    8.424257   16.277928
O     6.186430    8.429418   16.278223
O     4.501802    5.973811   16.328764
O    10.437243    7.401819   18.523864
O     6.161153    7.016868   13.659932
O     8.792529   10.246975   18.640644
O    10.423575    5.951438   16.327790
O     6.156590   10.255252   18.627812
O     8.790990    7.024019   13.654599
O     4.519527    7.410958   18.535296
O     7.466036    9.288818   13.731061
O     5.821142    5.124616   18.443272
O     7.485142   11.094760   16.515532
O     9.115872    5.124398   18.460828
O     8.810590    8.302959   20.532573
O     6.126986    4.507975   14.700301
O    10.955230    9.645561   17.071336
O     3.997788    8.193417   14.838245
O     6.131120    8.291204   20.533616
O    10.936967    8.185920   14.820855
O     4.004115    9.672591   17.075308
O     8.812973    4.497089   14.715174
O     7.455750    3.638017   16.864057
O     5.348573   10.513752   14.911258
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O      7.479705    5.977596   20.449478
O      9.602154   10.515740   14.924240
O      4.679029    5.871332   20.965821
O     10.259754    3.118007   16.772853
O      9.980983    9.315041   12.366463
O      4.972766   12.354687   17.065040
O     10.287370    5.907572   20.970866
O     10.010462   12.332327   17.108804
O      4.938497    9.287332   12.371273
O      4.642880    3.143069   16.725113
O      7.485981    4.911717   12.230665
O      2.156094    7.507313   16.926878
O      7.455658   10.741085   21.139420
O     12.786136    7.464748   16.876969
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Optimized Cartesian coordinates of C3-H using GGA

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C     -0.002758   -0.312984    9.821568
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C     -0.002565    6.833187    9.814407
C     -0.002522    8.262466    9.812515
C     -0.002484   11.119683    9.812560
C      1.235334    0.401832    9.819681
C      1.235754    1.831620    9.821257
C      1.235799    4.690002    9.819203
C      1.236087    6.119429    9.814372
C      1.236212    8.976365    9.809827
C      1.236081   10.405742    9.810279
C      2.473569   -0.313010    9.815753
C      2.473785    2.546115    9.817002
C      2.474342    3.975741    9.816766
C      2.474460    6.833241    9.807647
C      2.474926    8.262453    9.804701
C      2.474889   11.119189    9.807745
C      3.711316    0.402233    9.810874
C      3.711792    1.831778    9.810652
C      3.712349    4.690412    9.810786
C      3.712847    6.119585    9.806082
C      3.713688    8.975678    9.795813
C      3.712568   10.404903    9.799649
C      4.949222   -0.312629    9.807881
C      4.949449    2.546805    9.804203
C      4.950406    3.976082    9.804650
C      4.950655    6.834289    9.798279
C      4.950666    8.262233    9.781919
C      4.950783   11.118428    9.795080
C      6.186704    0.403012    9.803202
C      6.187240    1.832524    9.799651
C      6.188287    4.690754    9.797426
C      6.187685    6.119549    9.801227
C      6.187988    8.976106    9.769959
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C      6.187294   10.404437    9.780481
C      7.424094   -0.312662    9.801664
C      7.424436    2.548420    9.790854
C      7.424851    3.976333    9.779993
C      7.425073    6.833776    9.800032
C      7.424732    8.261990    9.788331
C      7.424070   11.118321    9.796516
C      8.661441    0.403377    9.798794
C      8.661511    1.832560    9.793032
C      8.661727    4.691346    9.770286
C      8.661819    6.119550    9.788547
C      8.661901    8.975600    9.799077
C      8.661852   10.404519    9.800187
C      9.898650   -0.312711    9.802988
C      9.898530    2.548348    9.792743
C      9.898193    3.976587    9.782805
C      9.898323    6.833920    9.799506
C      9.898817    8.261941    9.787075
C      9.899455   11.118364    9.797120
C     11.136009    0.403001    9.805806
C     11.135559    1.832531    9.802415
C     11.135024    4.690919    9.799463
C     11.135850    6.119774    9.801823
C     11.135731    8.976303    9.769602
C     11.136265   10.404493    9.780466
C     12.373505   -0.312609    9.811096
C     12.373431    2.546892    9.807671
C     12.372725    3.976189    9.807622
C     12.372795    6.834434    9.800609
C     12.372759    8.262699    9.783957
C     12.372509   11.118688    9.795364
C     13.611363    0.402323    9.814309
C     13.610993    1.831833    9.814278
C     13.610713    4.690564    9.813995
C     13.610391    6.119827    9.809429
C     13.609865    8.976177    9.797282
C     13.610842   10.405270    9.800167
C     14.849185   -0.312944    9.818601
C     14.849017    2.546108    9.819808
C     14.848728    3.975867    9.819684
C     14.848843    6.833453    9.810669
C     14.848609    8.262665    9.807119
C     14.848523   11.119480    9.808808
C     16.087427    0.401859    9.821500
C     16.087103    1.831598    9.822927
C     16.087275    4.690036    9.820902
C     16.087129    6.119464    9.816172
C     16.087224    8.976530    9.811075
C     16.087373   10.405914    9.811205
C     -0.002541   12.549264    9.814515
C     -0.002695   15.408062    9.819129
C      1.235870   13.263761    9.814355
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C     1.235572   14.693395    9.816943
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C     3.711985   13.263336    9.810275
C     3.711530   14.693027    9.812492
C     4.949455   12.547798    9.803418
C     4.949089   15.408224    9.809260
C     6.186759   13.263410    9.803235
C     6.186502   14.693011    9.805859
C     7.424058   12.547724    9.802066
C     7.423964   15.408467    9.804209
C     8.661511   13.263225    9.804683
C     8.661468   14.692840    9.805150
C     9.898984   12.547714    9.802706
C     9.898883   15.408410    9.805420
C    11.136185   13.263460    9.804731
C    11.136333   14.692990    9.807951
C    12.373553   12.548084    9.804732
C    12.373681   15.408327    9.811976
C    13.611028   13.263513    9.811990
C    13.611323   14.693194    9.814927
C    14.849350   12.549219    9.812379
C    14.849158   15.408038    9.817881
C    16.087399   13.263845    9.815292
C    16.087386   14.693501    9.818096
P     8.602307    7.570683   16.771772
W     6.860607    6.576537   19.802054
W    10.351482    4.391801   16.731907
W    10.490096    8.647256   13.883268
W     6.719239   10.667723   16.726811
W    10.345203    6.566777   19.802020
W    10.483838   10.672585   16.716559
W     6.718388    8.654620   13.881583
W     6.864181    4.385861   16.741591
W     8.597591    5.383929   13.889928
W     4.978943    7.645386   16.725164
W     8.612099    9.590545   19.795195
W    12.229792    7.653729   16.732835
O     8.605968    7.575245   18.351412
O     8.605280    6.081087   16.243152
O     9.887450    8.317915   16.236135
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O     5.643145    5.856054   16.390162
O    11.564472    7.384161   18.532654
O     7.287823    6.805040   13.667252
O     9.924430   10.235993   18.524173
O    11.567391    5.861000   16.388293
O     7.289931   10.234989   18.526873
O     9.912712    6.801446   13.672151
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O    12.079818   9.580052  16.992409
O     5.134109   8.020060  14.809208
O     7.267821   8.354852  20.492603
O    12.074838   8.018988  14.811852
O     5.127223   9.576077  16.993959
O     9.945227   4.332267  14.816400
O     8.607420   3.556496  17.009071
O     6.479839  10.343193  14.806238
O     8.603631   6.032540  20.498957
O    10.732130  10.342896  14.800906
O     5.800672   5.966670  21.022112
O    11.417331   3.049870  16.911541
O    11.147500   9.018685  12.317376
O     6.082778  12.259287  16.901346
O    11.405816   5.957179  21.021860
O    11.121227  12.263918  16.886798
O     6.054096   9.029746  12.318876
O     5.802197   3.041111  16.923723
O     8.598188   4.622796  12.326355
O     3.284231   7.394523  16.902007
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Optimized Cartesian coordinates of C3-T using GGA

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C    -0.008847   6.834902   9.809283
C    -0.008943   8.264291   9.806324
C    -0.009040  11.121778   9.812435
C     1.228679   0.404149   9.826748
C     1.229247   1.833856   9.826611
C     1.229375   4.692051   9.818188
C     1.229977   6.121476   9.810619
C     1.230000   8.978247   9.803678
C     1.229415  10.407628   9.806071
C     2.466737  -0.310557   9.820473
C     2.467198   2.548313   9.821050
C     2.467689   3.977861   9.819401
C     2.467981   6.835275   9.805080
C     2.468602   8.264387   9.797862
C     2.467615  11.121201   9.803999
C     3.704387   0.404603   9.814000
C     3.705254   1.834102   9.814902
C     3.705614   4.692436   9.815514
C     3.706072   6.121834   9.808275
C     3.705804   8.977698   9.783539
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C      4.942696    6.835148   9.800239
C      4.942702    8.263612   9.779350
C      4.942122   11.121074   9.793872
C      6.179391    0.405441   9.799631
C      6.180327    1.835008   9.798133
C      6.179890    4.692655   9.806587
C      6.179129    6.121043   9.822672
C      6.179526    8.977773   9.791355
C      6.179014   10.405889   9.791851
C      7.416516   -0.310354   9.796538
C      7.416403    2.549436   9.786521
C      7.416487    3.978446   9.788700
C      7.416574    6.835393   9.825395
C      7.416636    8.263850   9.811374
C      7.416685   11.120599   9.792391
C      8.653703    0.405410   9.799869
C      8.652576    1.835059   9.798548
C      8.653260    4.692769   9.802715
C      8.654133    6.120963   9.816955
C      8.653810    8.977528   9.784851
C      8.654281   10.405714   9.786825
C      9.891016   -0.310409   9.805620
C      9.890669    2.548836   9.807621
C      9.889669    3.978069   9.808332
C      9.890613    6.834986   9.789248
C      9.890579    8.263373   9.766978
C      9.891331   11.120894   9.786126
C     11.128850    0.404499   9.813853
C     11.127894    1.834190   9.814641
C     11.127592    4.692347   9.810257
C     11.127292    6.121599   9.798592
C     11.127791    8.977808   9.769529
C     11.128407   10.405603   9.783152
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C     12.365998    2.548227   9.820427
C     12.365504    3.977801   9.816845
C     12.365359    6.835332   9.796007
C     12.364792    8.264384   9.786752
C     12.365830   11.121244   9.796036
C     13.604529    0.403989   9.826830
C     13.603899    1.833774   9.826572
C     13.603834    4.692092   9.815684
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C     13.603346    8.978370   9.796106
C     13.604014   10.407628   9.799285
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C     14.842158    3.977635   9.822180
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C    14.842015    6.834971    9.806319
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C    16.080693    1.833779    9.830813
C    16.080718    4.691873    9.819289
C    16.080676    6.121259    9.811782
C    16.080859    8.978509    9.805340
C    16.080856   10.407740    9.809182
C    -0.009282   12.551302    9.819379
C    -0.009377   15.410358    9.828754
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C     1.228844   14.695674    9.823566
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C     2.466538   15.410487    9.818931
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C     3.704210   14.695414    9.810467
C     4.941779   12.550114    9.798703
C     4.941637   15.410809    9.803895
C     6.179269   13.265745    9.797143
C     6.178944   14.695239    9.798320
C     7.416581   12.550012    9.794354
C     7.416519   15.410701    9.796859
C     8.654108   13.265658    9.794692
C     8.654004   14.695188    9.797176
C     9.891512   12.549924    9.793456
C     9.891524   15.410626    9.802870
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C    12.366638   12.550780    9.806087
C    12.366669   15.410357    9.818116
C    13.604514   13.265862    9.816521
C    13.604438   14.695557    9.822728
C    14.842746   12.551317    9.817697
C    14.842594   15.410130    9.828592
C    16.080876   13.266046    9.823166
C    16.080841   14.695811    9.828185
P     7.467370    6.809852   16.765591
W     5.739370    5.810790   19.807071
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W     9.338305    7.887301   13.865036
W     5.584488    9.909570   16.708158
W     9.223932    5.829115   19.793065
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W     5.567707    7.873172   13.879082
W     5.718735    3.629006   16.740495
W     7.465596    4.612471   13.890333
W     3.840699    6.890192   16.743140
W     7.468347    8.839892   19.784209
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O     7.466007    5.319173   16.240736
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O      6.139025    7.597853   20.490293
O     10.926605    7.251294   14.788781
O      3.991561    8.818511   16.997224
O      8.807068    3.565991   14.820598
O      7.464586    2.797161   17.012534
O      5.334536    9.572606   14.796605
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O      4.681513    5.204038   21.030707
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O      4.947464   11.501539   16.873808
O     10.290573    5.224273   21.009440
O      9.984595   11.500314   16.865935
O      4.888527    8.239522   12.320712
O      4.655686    2.285445   16.924279
O      7.460026    3.841997   12.331330
O      2.146425    6.641688   16.929602
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O     12.788836    6.637179   16.865889
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