Supporting Information

Stacked Homodimers of Substituted Contorted Hexabenzocoronenes and Their Complexes with C_{60} Fullerene

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Table S1. B97-D/TZV(2d,2p) electronic energies (in Hartrees) and interaction energies (in kcal mol^{-1}) for model stacked dimers of C_6H_5X with benzene and a hexagonal face of C_{60}, along with relative interaction energies.

		$C_6H_5X\cdots C_{60}$			$C_6H_5X\cdots C_6H_6$ [a]	
X	C_6H_5X monomer	Dimer	E_{int}	E_{rel} [b]	E_{int}	E_{rel} [b]
H	-232.1495	-2517.2249	-4.7	0.0	-1.8	0.0
BF2	-456.2017	-2741.2783	-5.4	-0.7	-2.8	-1.0
CCH	-308.2631	-2593.3396	-5.4	-0.7	-2.6	-0.8
CF3	-569.1658	-2854.2425	-5.5	-0.8	-3.3	-1.5
CH2OH	-346.6513	-2631.7288	-6.0	-1.3	-2.5	-0.7
CH3	-271.4524	-2556.5294	-5.7	-1.0	-2.4	-0.6
CHO	-345.4480	-2630.5245	-5.4	-0.7	-2.9	-1.1
CN	-324.3587	-2609.4348	-5.2	-0.5	-3.1	-1.3
COCH3	-384.7552	-2669.8327	-6.0	-1.3	-3.0	-1.2
COOCH3	-459.9754	-2745.0528	-6.0	-1.3	-2.9	-1.1
COOH	-420.6913	-2705.7681	-5.6	-0.9	-2.9	-1.1
F	-331.3828	-2616.4586	-5.0	-0.3	-2.4	-0.6
NH2	-287.4955	-2572.5726	-5.8	-1.1	-2.1	-0.3
NHCH3	-326.7851	-2611.8636	-6.6	-1.9	-2.4	-0.6
NHOH	-362.6473	-2647.7246	-5.9	-1.2	-2.5	-0.7
NO	-361.4164	-2646.4927	-5.3	-0.6	-3.1	-1.3
NO2	-436.6239	-2721.7005	-5.4	-0.7	-3.4	-1.6
OCF3	-644.3709	-2929.4485	-6.1	-1.4	-3.1	-1.3
OH	-307.3632	-2592.4397	-5.4	-0.7	-2.1	-0.3
OMe	-346.6473	-2631.7247	-5.9	-1.2	-2.4	-0.6
SCH3	-669.6594	-2954.7376	-6.4	-1.8	-2.7	-0.9
SH	-630.3612	-2915.4380	-5.6	-0.9	-2.5	-0.7
SiF3	-820.7608	-3105.8388	-6.3	-1.6	-3.5	-1.7
SiH3	-522.8380	-2807.9149	-5.7	-1.0	-2.6	-0.8

a. Data from S. E. Wheeler, *J. Am. Chem. Soc.*, 2011, **133**, 10262-10274.
b. Energies relative to X = H.

Table S2. B97-D3M(BJ)/TZVPP[a] electronic energies (in Hartrees) for complexes of C_{60} with c-HBC as function of rotations of C_{60} about the X, Y, and Z-axes.

Degree(°)	X	Y	Z
0	-4129.1395	-4129.1395	-4129.1395
10	-4129.1384	-4129.1385	-4129.1393
20	-4129.1396	-4129.1391	-4129.1383
30	-4129.1390	-4129.1399	-4129.1373
40	-4129.1388	-4129.1401	-4129.1372
50	-4129.1385	-4129.1399	-4129.1384
60	-4129.1399	-4129.1391	-4129.1387
70	-4129.1400	-4129.1390	-4129.1380
80	-4129.1385	-4129.1394	-4129.1376
90	-4129.1397	-4129.1397	-4129.1377
100	-4129.1387	-4129.1393	-4129.1381
110	-4129.1398	-4129.1388	-4129.1388
120	-4129.1373	-4129.1394	-4129.1396
130	-4129.1377	-4129.1393	-4129.1392
140	-4129.1388	-4129.1389	-4129.1381
150	-4129.1381	-4129.1392	-4129.1373
160	-4129.1392	-4129.1395	-4129.1375
170	-4129.1383	-4129.1385	-4129.1385
180	-4129.1395	-4129.1389	-4129.1389
190	-4129.1384	-4129.1386	-4129.1386
200	-4129.1396	-4129.1396	-4129.1376
210	-4129.1390	-4129.1392	-4129.1373
220	-4129.1388	-4129.1389	-4129.1380
230	-4129.1385	-4129.1393	-4129.1390
240	-4129.1399	-4129.1394	-4129.1394
250	-4129.1400	-4129.1388	-4129.1387
260	-4129.1385	-4129.1393	-4129.1383
270	-4129.1397	-4129.1397	-4129.1377
280	-4129.1387	-4129.1394	-4129.1374
290	-4129.1399	-4129.1390	-4129.1382
300	-4129.1373	-4129.1391	-4129.1389
310	-4129.1377	-4129.1399	-4129.1385
320	-4129.1388	-4129.1402	-4129.1373
330	-4129.1381	-4129.1399	-4129.1373
340	-4129.1392	-4129.1391	-4129.1382
350	-4129.1383	-4129.1384	-4129.1392

a: three-body interaction included in the D3 dispersion correction with D3M(BJ), i.e., Becke-Johnson damping with the refitted parameters by Sherrill and coworkers.

Table S3. B97-D3M(BJ)/TZVPP electronic energies for c-HBC monomer, c-HBC···c-HBC homodimer, and c-HBC···C_{60} heterodimer as a function of bowl depth of c-HBC.

Bowl	Monomer	c-HBC···c-HBC Homodimer		c-HBC···C_{60} Heterodimer	
Depth(Å)	E(Hartree)	separation(Å)	E(Hartree)	seperation(Å)	E(Hartree)
0.00	-1843.1202	3.62	-3686.2879	3.17	-4128.8872
0.10	-1843.1274	3.62	-3686.3027	3.17	-4128.8944
0.19	-1843.1476	3.62	-3686.3443	3.17	-4128.9148
0.29	-1843.1791	3.62	-3686.4092	3.16	-4128.9466
0.39	-1843.2185	3.61	-3686.4907	3.15	-4128.9865
0.49	-1843.2609	3.60	-3686.5787	3.15	-4129.0297
0.58	-1843.3004	3.60	-3686.6608	3.15	-4129.0701
0.68	-1843.3322	3.65	-3686.7252	3.14	-4129.1028
0.78	-1843.3536	3.78	-3686.7661	3.13	-4129.1251
0.88	-1843.3644	3.95	-3686.7819	3.13	-4129.1369
0.97	-1843.3662	4.23	-3686.7780	3.12	-4129.1398
1.07	-1843.3602	4.47	-3686.7591	3.12	-4129.1349
1.17	-1843.3482	4.75	-3686.7304	3.12	-4129.1242
1.26	-1843.3315	5.02	-3686.6926	3.13	-4129.1085
1.36	-1843.3108	5.31	-3686.6482	3.15	-4129.0887
1.46	-1843.2864	5.60	-3686.5967	3.19	-4129.0646
1.56	-1843.2581	5.91	-3686.5371	3.25	-4129.0359
1.65	-1843.2256	6.28	-3686.4693	3.42	-4129.0023
1.75	-1843.1885	6.73	-3686.3927	3.60	-4128.9634
1.85	-1843.1460	7.20	-3686.3061	3.74	-4128.9179

Table S4. B97-D3M(BJ)/TZVPP electronic energies (Hartree) for optimized substituted c-HBCs as well as homodimers c-HBC···c-HBC and heterodimers c-HBC···C_{60}.

Substituent	Monomers	*c*-HBC···*c*-HBC Homodimers	*c*-HBC···C_{60} Heterodimers
SCH_3	-7093.8601	-14187.8304	-9379.6686
NH_2	-2507.5979	-5015.2966	-4793.3850
OCH_3	-3217.4567	-6434.9944	-5503.2418
CH_3	-2315.1206	-4630.3207	-4600.9033
CN	-2949.9593	-5899.9771	-5235.7414
SH	-6622.1562	-13244.4332	-8907.9385
C≡CH	-2756.9017	-5513.8981	-5042.6813
OH	-2745.9977	-5492.0820	-5031.7785
F	-3034.1408	-8449.6042	-5319.9179
H	-1843.3662	-3686.7858	-4129.1434
F_{24}	-4224.7909	-6068.3431	-6510.5729
C_{60}	-2285.7448		

Optimized Cartesian Coordinates

Optimized substituted c-HBC monomers, homodimers and c-HBC…C60 heterodimers

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CCH substited_monomer

C	0.717050	3.654808	-0.421706
C	-0.717060	3.654808	-0.421679
C	-1.424208	2.466894	0.000136
C	-2.806705	2.448233	0.421717
C	-3.523684	1.206234	0.421916
C	-2.848411	-0.000001	0.000031
C	-3.523689	-1.206229	-0.421862
C	-2.806709	-2.448229	-0.421692
C	-1.424210	-2.466896	-0.000106
C	-0.717050	-3.654808	0.421706
C	0.717060	-3.654808	0.421679
C	1.424208	-2.466894	-0.000136
C	2.806705	-2.448233	-0.421717
C	3.523684	-1.206234	-0.421916
C	2.848411	0.000001	-0.000031
C	3.523689	1.206229	0.421862
C	2.806709	2.448229	0.421692
C	1.424210	2.466896	0.000106
C	0.719012	1.245374	0.000343
C	-0.719010	1.245372	0.000359
C	-1.437966	0.000000	0.000017
C	-0.719012	-1.245374	-0.000343
C	0.719010	-1.245372	-0.000359
C	1.437966	0.000000	-0.000017
C	3.437286	3.588191	0.964027
C	4.736170	3.561668	1.467515
C	5.452984	2.319603	1.467947
C	4.826249	1.181771	0.964222
C	-1.389156	4.770773	-0.964000
C	-0.717042	5.882284	-1.468005
C	0.716975	5.882276	-1.468054
C	1.389115	4.770765	-0.964083
C	-4.826245	1.181793	0.964274
C	-5.452981	2.319641	1.467961
C	-4.736173	3.561711	1.467478
C	-3.437288	3.588218	0.963992
C	-3.437286	-3.588191	-0.964027
C	-4.736170	-3.561668	-1.467515
C	-5.452984	-2.319603	-1.467947
C	-4.826249	-1.181771	-0.964222
C	1.389156	-4.770773	0.964000
C	0.717042	-5.882284	1.468005
C	-0.716975	-5.882276	1.468054
C	-1.389115	-4.770765	0.964083
C	4.826245	-1.181793	-0.964274
C	5.452981	-2.319641	-1.467961
C	4.736173	-3.561711	-1.467478
C	3.437288	-3.588218	-0.963992
H	2.882259	4.513663	1.050316
H	5.349868	0.238200	1.049992
H	-2.468146	4.752562	-1.049827
H	2.468098	4.752550	-1.049988
H	-5.349867	0.238225	1.050069
H	-2.882266	4.513699	1.050225
H	-2.882259	-4.513663	-1.050316
H	-5.349868	-0.238200	-1.049992
H	2.468146	-4.752562	1.049827
H	-2.468098	-4.752550	1.049988
H	5.349867	-0.238225	-1.050069
H	2.882266	-4.513699	-1.050225
C	-1.456551	6.969255	-2.012283
C	1.456457	6.969241	-2.012384
C	5.308335	4.745614	2.011165
C	6.763913	2.222357	2.012635
C	6.763913	-2.222415	-2.012645
C	5.308348	-4.745679	-2.011070
C	1.456551	-6.969255	2.012283
C	-1.456457	-6.969241	2.012384
C	-5.308335	-4.745614	-2.011165
C	-6.763913	-2.222357	-2.012635
C	-6.763913	2.222415	2.012645
C	-5.308348	4.745679	2.011070
C	5.786544	5.761140	2.466747
C	7.882056	2.127458	2.468995
C	7.882058	-2.127533	-2.469003
C	5.786565	-5.761224	-2.466601
C	2.097519	-7.890435	2.468397
C	-2.097399	-7.890416	2.468544
C	-5.786544	-5.761140	-2.466747
C	-7.882056	-2.127458	-2.468995
C	-7.882058	2.127533	2.469003
C	-5.786565	5.761224	2.466601
C	-2.097519	7.890435	-2.468397
C	2.097399	7.890416	-2.468544

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H      -2.656462        8.704788       -2.871330
H       2.656289        8.704781       -2.871526
H       6.212433        6.652425        2.869469
H       8.866313        2.049835        2.872935
H       8.866319       -2.049929       -2.872939
H       6.212458       -6.652527       -2.869278
H       2.656462       -8.704788        2.871330
H      -2.656289       -8.704781        2.871526
H      -6.212433       -6.652425       -2.869469
H      -8.866313       -2.049835       -2.872935
H      -8.866319        2.049929        2.872939
H      -6.212458        6.652527        2.869278

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CH3 substited_monomer
C      -4.803694       -5.362594        2.046691
C      -3.558901       -4.743037        1.460141
H      -5.649819       -4.669831        1.991684
H      -4.652351       -5.641559        3.098555
H      -5.076478       -6.284228        1.514007
C      -2.328691       -5.453325        1.460719
C      -3.587637       -3.452329        0.957255
C      -2.243937       -6.840658        2.048114
C      -1.196216       -4.832784        0.958562
C      -2.447891       -2.809530        0.415434
H      -4.512262       -2.891771        1.040187
H      -1.222838       -7.231018        1.986622
H      -2.912142       -7.535649        1.521011
H      -2.553619       -6.846527        3.102280
C      -1.209151       -3.524640        0.416120
H      -0.248271       -5.352889        1.042115
C      -2.467466       -1.424592       -0.000338
C       0.000000       -2.849185        0.000338
C      -1.246116       -0.719452       -0.000014
C      -3.657004       -0.715165       -0.416120
C       0.000005       -1.438894        0.000014
C       1.209179       -3.524701       -0.415434
C      -1.246122        0.719443        0.000014
C      -3.657070        0.715171       -0.415434
C      -4.783421       -1.380439       -0.958562
C       1.246122       -0.719443       -0.000014
C       2.447853       -2.809476       -0.416120
C       1.195986       -4.833149       -0.957255
C      -0.000005        1.438894       -0.000014
C      -2.467466        1.424592        0.000338
C      -4.783623        1.380821       -0.957255
C      -5.887064       -0.709957       -1.460719
H      -4.759873       -2.461435       -1.042115
C       1.246116        0.719452        0.000014
C       2.467466       -1.424592       -0.000338
C       3.587205       -3.452345       -0.958562
C       2.328140       -5.453617       -1.460141
H       0.248216       -5.353619       -1.040187
C       0.000000        2.849185       -0.000338
C      -2.447853        2.809476        0.416120
C      -5.887041        0.710580       -1.460141
H      -4.760478        2.461848       -1.040187
C      -7.046152       -1.477022       -2.048114
C       2.467466        1.424592        0.000338
C       3.657070       -0.715171        0.415434
C       3.558373       -4.743369       -1.460719
H       4.511602       -2.891453       -1.042115
C       2.242296       -6.841417       -2.046691
C      -1.209179        3.524701        0.415434
C       1.209151        3.524640       -0.416120
C      -3.587205        3.452345        0.958562
C      -7.045989        1.478824       -2.046691
H      -6.873664       -2.556500       -1.986622
H      -7.206076       -1.211765       -3.102280
H      -7.982134       -1.245835       -1.521011
C       3.657004        0.715165        0.416120
C       2.447891        2.809530       -0.415434
C       4.783623       -1.380821        0.957255
C       4.802215       -5.363635       -2.048114
H       1.219283       -7.227803       -1.991684
H       2.904061       -7.538473       -1.514007
H       2.559558       -6.849833       -3.098555
C      -1.195986        4.833149        0.957255
C       1.196216        4.832784       -0.958562
C      -3.558373        4.743369        1.460719
H      -4.511602        2.891453        1.042115
H      -6.869102        2.557971       -1.991684
H      -7.980540        1.254246       -1.514007
H      -7.211909        1.208275       -3.098555
C       4.783421        1.380439        0.958562
C       3.587637        3.452329       -0.957255
C       5.887041       -0.710580        1.460141
H       4.760478       -2.461848        1.040187
H       5.650826       -4.674518       -1.986622
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H       4.652457       -5.634763       -3.102280
H       5.069992       -6.289813       -1.521011
C      -2.328140        5.453617        1.460141
H      -0.248216        5.353619        1.040187
C       2.328691        5.453325       -1.460719
H       0.248271        5.352889       -1.042115
C      -4.802215        5.363635        2.048114
C       5.887064        0.709957        1.460719
H       4.759873        2.461435        1.042115
C       3.558901        4.743037       -1.460141
H       4.512262        2.891771       -1.040187
C       7.045989       -1.478824        2.046691
C      -2.242296        6.841417        2.046691
C       2.243937        6.840658       -2.048114
H      -5.650826        4.674518        1.986622
H      -5.069992        6.289813        1.521011
H      -4.652457        5.634763        3.102280
C       7.046152        1.477022        2.048114
C       4.803694        5.362594       -2.046691
H       6.869102       -2.557971        1.991684
H       7.211909       -1.208275        3.098555
H       7.980540       -1.254246        1.514007
H      -1.219283        7.227803        1.991684
H      -2.559558        6.849833        3.098555
H      -2.904061        7.538473        1.514007
H       1.222838        7.231018       -1.986622
H       2.553619        6.846527       -3.102280
H       2.912142        7.535649       -1.521011
H       6.873664        2.556500        1.986622
H       7.982134        1.245835        1.521011
H       7.206076        1.211765        3.102280
H       5.649819        4.669831       -1.991684
H       5.076478        6.284228       -1.514007
H       4.652351        5.641559       -3.098555


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CN substited_monomer
C      -0.718846       -1.245057       -0.000275
C      -1.437654       -0.000001        0.000029
C       0.718843       -1.245053       -0.000303
C      -1.423576       -2.465785       -0.000025
C      -0.718843        1.245053        0.000303
C      -2.847202       -0.000002        0.000061
C       1.437654        0.000001       -0.000029
C       1.423573       -2.465780       -0.000078
C      -2.804939       -2.447017       -0.424535
C      -0.716870       -3.652693        0.424615
C       0.718846        1.245057        0.000275
C      -1.423573        2.465780        0.000078
C      -3.521815       -1.205354       -0.424739
C      -3.521808        1.205360        0.424844
C       2.847202        0.000002       -0.000061
C       0.716886       -3.652691        0.424568
C       2.804934       -2.447025       -0.424579
C      -3.428283       -3.588268       -0.974386
C      -1.393550       -4.763173        0.974361
C       1.423576        2.465785        0.000025
C      -2.804934        2.447025        0.424579
C      -0.716886        3.652691       -0.424568
C      -4.821892       -1.174225       -0.974622
C      -4.821890        1.174264        0.974719
C       3.521808       -1.205360       -0.424844
C       3.521815        1.205354        0.424739
C       1.393622       -4.763176        0.974225
C       3.428295       -3.588320       -0.974309
C      -4.720035       -3.548539       -1.486721
H      -2.874778       -4.514492       -1.062200
C      -0.713464       -5.861943        1.486994
H      -2.472417       -4.746727        1.061825
C       0.716870        3.652693       -0.424615
C       2.804939        2.447017        0.424535
C      -3.428295        3.588320        0.974309
C      -1.393622        4.763176       -0.974225
C      -5.433508       -2.312615       -1.487061
H      -5.346983       -0.231649       -1.062039
C      -5.433510        2.312687        1.487083
H      -5.346985        0.231696        1.062185
C       4.821890       -1.174264       -0.974719
C       4.821892        1.174225        0.974622
C       0.713586       -5.861950        1.486915
H       2.472501       -4.746726        1.061560
C       4.720050       -3.548620       -1.486641
H       2.874805       -4.514565       -1.062013
C      -5.286907       -4.732984       -2.051886
C      -1.455902       -6.944744        2.052613
C       1.393550        4.763173       -0.974361
C       3.428283        3.588268        0.974386
C      -4.720050        3.548620        1.486641
H      -2.874805        4.514565        1.062013
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C      -0.713586        5.861950       -1.486915
H      -2.472501        4.746726       -1.061560
C      -6.742362       -2.210965       -2.052951
C      -6.742370        2.211073        2.052964
C       5.433510       -2.312687       -1.487083
H       5.346985       -0.231696       -1.062185
C       5.433508        2.312615        1.487061
H       5.346983        0.231649        1.062039
C       1.456073       -6.944757        2.052458
C       5.286949       -4.733108       -2.051689
N      -5.727322       -5.708301       -2.504987
N      -2.080467       -7.813413        2.506325
C       0.713464        5.861943       -1.486994
H       2.472417        4.746727       -1.061825
C       4.720035        3.548539        1.486721
H       2.874778        4.514492        1.062200
C      -5.286949        4.733108        2.051689
C      -1.456073        6.944757       -2.052458
N      -7.806814       -2.104272       -2.506892
N      -7.806815        2.104398        2.506926
C       6.742370       -2.211073       -2.052964
C       6.742362        2.210965        2.052951
N       2.080674       -7.813442        2.506091
N       5.727379       -5.708456       -2.504706
C       1.455902        6.944744       -2.052613
C       5.286907        4.732984        2.051886
N      -5.727379        5.708456        2.504706
N      -2.080674        7.813442       -2.506091
N       7.806815       -2.104398       -2.506926
N       7.806814        2.104272        2.506892
N       2.080467        7.813413       -2.506325
N       5.727322        5.708301        2.504987

72
F substited_monomer
C      -1.035821        0.998154        0.000111
C      -1.382282       -0.397930       -0.000057
C       0.346533        1.396195        0.000254
C      -2.050907        1.976307        0.000039
C      -0.346533       -1.396195       -0.000255
C      -2.736883       -0.787899        0.000240
C       1.382282        0.397930        0.000057
C       0.686111        2.764355        0.000441
C      -3.376452        1.576538        0.416282
C      -1.700325        3.315629       -0.416398
C       1.035821       -0.998154       -0.000111
C      -0.686111       -2.764355       -0.000441
C      -3.721630        0.185319        0.416590
C      -3.053491       -2.135725       -0.416195
C       2.736883        0.787899       -0.000240
C      -0.322956        3.712281       -0.415918
C       2.021413        3.130432        0.416642
C      -4.300681        2.506144        0.953693
C      -2.663307        4.204361       -0.954863
C       2.050907       -1.976307       -0.000039
C      -2.021413       -3.130432       -0.416643
C       0.322956       -3.712281        0.415918
C      -4.972990       -0.204190        0.954629
C      -4.320608       -2.470958       -0.953916
C       3.053491        2.135725        0.416195
C       3.721630       -0.185319       -0.416589
C       0.019811        4.977501       -0.953426
C       2.310166        4.408861        0.954575
C      -5.518488        2.094462        1.445272
H      -4.044249        3.553535        1.051653
C      -2.297167        5.436790       -1.446025
H      -3.700245        3.908742       -1.053545
C       1.700324       -3.315629        0.416398
C       3.376452       -1.576538       -0.416282
C      -2.310165       -4.408861       -0.954577
C      -0.019812       -4.977501        0.953426
C      -5.857122        0.729188        1.445817
H      -5.235847       -1.249902        1.053366
C      -4.573364       -3.731345       -1.445493
H      -5.099153       -1.724893       -1.051980
C       4.320609        2.470958        0.953915
C       4.972990        0.204191       -0.954628
C      -0.945541        5.826227       -1.445249
H       1.054992        5.279215       -1.051676
C       3.560617        4.707530        1.445837
H       1.536268        5.159738        1.052905
F      -6.374116        2.987533        1.980859
F      -3.221240        6.258381       -1.982316
C       2.663307       -4.204362        0.954864
C       4.300682       -2.506144       -0.953692
C      -3.560617       -4.707529       -1.445838
H      -1.536268       -5.159737       -1.052907
C       0.945540       -5.826227        1.445249
H      -1.054992       -5.279215        1.051676
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F      -7.030797        0.339896        1.981977
F      -5.774693       -4.025514       -1.981039
C       4.573364        3.731345        1.445491
H       5.099153        1.724894        1.051979
C       5.857123       -0.729188       -1.445816
H       5.235847        1.249902       -1.053365
F      -0.599805        7.013767       -1.980748
F       3.810610        5.918725        1.981598
C       2.297166       -5.436790        1.446025
H       3.700244       -3.908742        1.053545
C       5.518488       -2.094463       -1.445271
H       4.044249       -3.553536       -1.051652
F      -3.810610       -5.918724       -1.981600
F       0.599804       -7.013767        1.980748
F       5.774694        4.025515        1.981037
F       7.030798       -0.339897       -1.981975
F       3.221239       -6.258381        1.982317
F       6.374117       -2.987534       -1.980857


72
F24 substited_monomer
C      -0.716492       -1.241104        0.000429
C      -1.432903        0.000000        0.000005
C       0.716492       -1.241103        0.000424
C      -1.419970       -2.459525        0.001338
C      -0.716492        1.241103       -0.000424
C      -2.839720       -0.000001        0.000009
C       1.432903        0.000000       -0.000005
C       1.419970       -2.459524        0.001329
C      -2.773322       -2.433287       -0.507713
C      -0.720499       -3.618097        0.510683
C       0.716492        1.241104       -0.000429
C      -1.419970        2.459524       -0.001329
C      -3.493625       -1.185111       -0.508996
C      -3.493625        1.185111        0.509009
C       2.839720        0.000001       -0.000009
C       0.720503       -3.618099        0.510672
C       2.773323       -2.433288       -0.507716
C      -3.351226       -3.538277       -1.170658
C      -1.388568       -4.671738        1.172623
C       1.419970        2.459525       -0.001338
C      -2.773323        2.433288        0.507716
C      -0.720503        3.618099       -0.510672
C      -4.738904       -1.132784       -1.172846
C      -4.738905        1.132793        1.172859
C       3.493625       -1.185111       -0.509009
C       3.493625        1.185111        0.508996
C       1.388585       -4.671748        1.172583
C       3.351232       -3.538290       -1.170632
C      -4.603881       -3.468350       -1.760049
F      -2.660560       -4.681113       -1.348926
C      -0.701687       -5.722838        1.759587
F      -2.723685       -4.644640        1.351427
C       0.720499        3.618097       -0.510683
C       2.773322        2.433287        0.507713
C      -3.351232        3.538290        1.170632
C      -1.388585        4.671748       -1.172583
C      -5.305056       -2.252722       -1.761507
F      -5.382530        0.037127       -1.352199
C      -5.305060        2.252740        1.761501
F      -5.382533       -0.037115        1.352223
C       4.738905       -1.132793       -1.172859
C       4.738904        1.132784        1.172846
C       0.701714       -5.722845        1.759564
F       2.723709       -4.644664        1.351336
C       4.603889       -3.468371       -1.760021
F       2.660574       -4.681137       -1.348856
F      -5.120600       -4.526634       -2.395794
F      -1.359434       -6.700183        2.394520
C       1.388568        4.671738       -1.172623
C       3.351226        3.538277        1.170658
C      -4.603889        3.468371        1.760021
F      -2.660574        4.681137        1.348856
C      -0.701714        5.722845       -1.759564
F      -2.723709        4.644664       -1.351336
F      -6.478994       -2.170909       -2.398811
F      -6.479001        2.170936        2.398800
C       5.305060       -2.252740       -1.761501
F       5.382533        0.037115       -1.352223
C       5.305056        2.252722        1.761507
F       5.382530       -0.037127        1.352199
F       1.359473       -6.700197        2.394474
F       5.120617       -4.526667       -2.395738
C       0.701687        5.722838       -1.759587
F       2.723685        4.644640       -1.351427
C       4.603881        3.468350        1.760049
F       2.660560        4.681113        1.348926
F      -5.120617        4.526667        2.395738
F      -1.359473        6.700197       -2.394474
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F       6.479001       -2.170936       -2.398800
F       6.478994        2.170909        2.398811
F       1.359434        6.700183       -2.394520
F       5.120600        4.526634        2.395794


96
NH2 substited_monomer
N      -7.145475       -0.370727       -1.966755
C      -5.934947        0.162700       -1.451480
H      -7.103951       -1.382518       -2.022021
H      -7.361211       -0.015051       -2.894438
C      -5.742030        1.572907       -1.426858
C      -4.934461       -0.659990       -0.959403
N      -6.752678        2.449217       -1.850985
C      -4.535909        2.071008       -0.950746
C      -3.724199       -0.168179       -0.416295
H      -5.063592       -1.732680       -1.066520
H      -7.488579        2.049215       -2.412707
H      -6.416056        3.323812       -2.229067
C      -3.513645        1.248117       -0.426053
H      -4.366219        3.140080       -1.025225
C      -2.651182       -1.045042       -0.007509
C      -2.230516        1.774931       -0.015138
C      -1.337552       -0.527399       -0.004282
C      -2.839055       -2.417674        0.401575
C      -1.125976        0.895489       -0.006736
C      -2.008933        3.143013        0.394090
C      -0.212555       -1.424400        0.001573
C      -1.719583       -3.310620        0.413700
C      -4.060213       -2.880298        0.945762
C       0.212552        1.424373       -0.001708
C      -0.677160        3.669812        0.404148
C      -3.039654        3.941951        0.942624
C       1.125961       -0.895508        0.006605
C      -0.421173       -2.821137        0.004043
C      -1.907018       -4.606774        0.945098
C      -4.232311       -4.162238        1.442175
H      -4.884579       -2.181800        1.051951
C       1.337545        0.527368        0.004173
C       0.421195        2.821104       -0.004155
C      -0.476520        4.964686        0.933943
C      -2.828700        5.218975        1.437032
H      -4.031671        3.515182        1.053323
C       2.230493       -1.774945        0.015019
C       0.677183       -3.669825       -0.404339
C      -3.129830       -5.062656        1.421486
H      -1.053710       -5.271869        1.027533
N      -5.481993       -4.593958        1.958679
C       2.651185        1.044989        0.007458
C       1.719643        3.310588       -0.413701
C      -1.511510        5.758036        1.412710
H       0.533902        5.351849        1.013984
N      -3.897129        5.997716        1.952948
C       2.008943       -3.142992       -0.394291
C       3.513586       -1.248168        0.426056
C       0.476566       -4.964667       -0.934218
N      -3.272993       -6.390784        1.850610
H      -6.138206       -3.822956        2.017325
H      -5.397590       -5.003939        2.885133
C       2.839101        2.417626       -0.401568
C       3.724160        0.168122        0.416339
C       1.907144        4.606785       -0.944962
N      -1.259699        7.070815        1.839680
H      -3.698637        6.365621        2.879604
H      -4.751735        5.454528        2.007961
C       3.039676       -3.941816       -0.942965
C       4.535742       -2.071098        0.950890
C       1.511577       -5.757935       -1.413099
H      -0.533842       -5.351866       -1.014258
H      -4.075790       -6.594834        2.425960
H      -2.426657       -6.805312        2.215439
C       4.060300        2.880258       -0.945665
C       4.934349        0.659904        0.959624
C       3.129999        5.062680       -1.421239
H       1.053865        5.271923       -1.027357
H      -0.327229        7.220572        2.199442
H      -1.964395        7.497576        2.421462
C       2.828741       -5.218798       -1.437476
H       4.031648       -3.514943       -1.053737
C       5.741811       -1.573023        1.427158
H       4.365988       -3.140169        1.025349
N       1.259801       -7.070663       -1.840197
C       4.232459        4.162240       -1.441957
H       4.884647        2.181740       -1.051879
C       5.934762       -0.162825        1.451817
H       5.063505        1.732595        1.066750
N       3.273216        6.390857       -1.850219
N       3.897153       -5.997427       -1.953623
N       6.752389       -2.449349        1.851432
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H       1.964627       -7.497492       -2.421760
H       0.327380       -7.220468       -2.200049
N       5.482187        4.593963       -1.958338
N       7.145239        0.370561        1.967222
H       2.426872        6.805429       -2.214991
H       4.075959        6.594893       -2.425653
H       4.751758       -5.454224       -2.008522
H       3.698609       -6.365028       -2.880393
H       6.415615       -3.323986        2.229297
H       7.487986       -2.049418        2.413610
H       5.397868        5.004115       -2.884722
H       6.138355        3.822930       -2.017078
H       7.361043        0.014675        2.894806
H       7.103654        1.382336        2.022729

120
OCH3 substited_monomer
C      -7.456248       -0.976930       -1.976005
O      -7.080282        0.402294       -1.967780
H      -7.465971       -1.386088       -0.955204
H      -6.769238       -1.572668       -2.593595
H      -8.462622       -1.008518       -2.400053
C      -5.852079        0.713983       -1.450540
C      -5.492106        2.091755       -1.464302
C      -4.947220       -0.212214       -0.953968
C      -4.261203        2.473665       -0.972830
O      -6.348320        3.059983       -1.945430
C      -3.689778        0.168868       -0.419046
H      -5.175765       -1.266056       -1.026330
C      -3.335739        1.553430       -0.420218
H      -3.994729        3.518571       -1.076595
C      -6.495356        3.060598       -3.379474
C      -2.711840       -0.810888        0.001075
C      -2.009251        1.950681       -0.005505
H      -7.184933        3.877094       -3.612838
H      -6.910075        2.109999       -3.736036
H      -5.523406        3.246369       -3.859932
C      -1.352951       -0.428091       -0.002042
C      -3.032775       -2.157675        0.419643
C      -0.997699        0.966393       -0.002900
C      -1.652450        3.289516        0.407583
C      -0.322528       -1.431133       -0.000908
C      -2.008721       -3.154925        0.412251
C      -4.302000       -2.489168        0.959451
C       0.387162        1.355475        0.000661
C      -0.276088        3.674277        0.415704
C      -2.615794        4.194304        0.921528
C       1.061580       -1.042333       -0.001523
C      -0.670444       -2.799033       -0.001031
C      -2.316389       -4.427702        0.954906
C      -4.587193       -3.753363        1.452650
H      -5.045909       -1.709067        1.040623
C       1.416910        0.351313       -0.001344
C       0.733065        2.723991        0.006537
C       0.054270        4.938928        0.963634
C      -2.271261        5.448283        1.403203
H      -3.644790        3.870792        0.984513
C       2.072594       -2.027046       -0.003790
C       0.335342       -3.753096       -0.407570
C      -3.563374       -4.743562        1.452938
H      -1.546709       -5.184930        1.041445
O      -5.793337       -4.128816        1.979974
C       2.775027        0.735505       -0.003678
C       2.072487        3.085242       -0.401727
C      -0.896396        5.820788        1.434069
H       1.091977        5.228555        1.076574
O      -3.161296        6.365665        1.888181
C       1.711385       -3.365935       -0.413813
C       3.402153       -1.630607        0.401631
C      -0.000107       -5.023031       -0.940062
O      -3.792418       -6.015878        1.929184
C      -6.836266       -3.152143        1.985788
C       3.094505        2.085933       -0.407990
C       3.756416       -0.245891        0.403412
C       2.375370        4.372756       -0.912904
O      -0.487192        7.050004        1.905604
C      -4.549377        6.015558        1.849926
C       2.670137       -4.269446       -0.937030
C       4.334575       -2.552231        0.940131
C       0.947249       -5.902472       -1.422271
H      -1.037792       -5.321039       -1.029047
C      -3.893627       -6.101502        3.363967
H      -7.058519       -2.811443        0.963897
H      -6.563851       -2.282804        2.601220
H      -7.710133       -3.651631        2.410754
C       4.357153        2.434827       -0.949114
C       5.020712        0.133395        0.921477
C       3.635990        4.703955       -1.386507
H       1.580052        5.101267       -0.979679
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C	-0.601594	7.208162	3.334010
H	-4.871243	5.797957	0.822067
H	-5.084606	6.887062	2.233987
H	-4.753600	5.140829	2.483638
C	2.321196	-5.524168	-1.413376
H	3.697634	-3.944042	-1.012851
C	5.573182	-2.171980	1.413726
H	4.069504	-3.597300	1.045184
O	0.539131	-7.134180	-1.884746
H	-4.067623	-7.156963	3.592417
H	-4.727996	-5.496644	3.740107
H	-2.953765	-5.770836	3.830263
C	4.647188	3.700817	-1.413713
H	5.128471	1.682611	-1.061375
C	5.935919	-0.794444	1.395393
H	5.252980	1.186105	0.993509
O	3.986488	5.935553	-1.865300
H	-0.239895	8.216305	3.556281
H	0.026919	6.466268	3.848502
H	-1.642591	7.105217	3.662814
O	3.206238	-6.438043	-1.912562
O	6.434201	-3.143865	1.877677
C	0.626536	-7.292937	-3.314276
O	5.919118	3.964152	-1.876337
O	7.175007	-0.484036	1.882512
C	2.989853	6.963196	-1.820304
C	4.593659	-6.083357	-1.898008
C	6.626624	-3.135685	3.306299
H	0.266706	-8.303535	-3.528129
H	1.660176	-7.183805	-3.664169
H	-0.016856	-6.555794	-3.817372
C	6.008377	4.144309	-3.303707
C	7.560834	0.894958	1.861404
H	2.636143	7.121599	-0.792143
H	2.132907	6.710393	-2.460639
H	3.479413	7.866264	-2.192174
H	4.933064	-5.866918	-0.875606
H	4.783841	-5.206751	-2.533476
H	5.124691	-6.952455	-2.293181
H	7.312775	-3.959483	3.523507
H	5.668156	-3.306018	3.818537
H	7.064358	-2.188171	3.642574
H	7.063936	4.334334	-3.518923
H	5.401945	4.995599	-3.635264
H	5.682590	3.230194	-3.821727
H	7.531720	1.295294	0.838529
H	8.583112	0.921615	2.245731
H	6.903257	1.498770	2.502745

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OH substited_monomer

C	1.216241	-0.768542	-0.000814
C	1.271460	0.668624	0.000139
C	-0.056474	-1.438509	-0.001658
C	2.409492	-1.522294	-0.002298
C	0.056477	1.438513	0.001562
C	2.519900	1.325109	-0.000061
C	-1.271459	-0.668622	-0.000205
C	-0.112708	-2.848740	-0.005701
C	3.627849	-0.861715	0.413276
C	2.335194	-2.904415	-0.416129
C	-1.216241	0.768545	0.000735
C	0.112710	2.848742	0.005618
C	3.680304	0.569766	0.413020
C	2.555674	2.709089	-0.412909
C	-2.519898	-1.325105	0.000079
C	1.067877	-3.572920	-0.422385
C	-1.347164	-3.478628	0.410546
C	4.723393	-1.579819	0.952028
C	3.455116	-3.590697	-0.947739
C	-2.409487	1.522298	0.002276
C	1.347195	3.478630	-0.410616
C	-1.067852	3.572923	0.422298
C	4.829081	1.197103	0.956443
C	3.723640	3.299518	-0.956698
C	-2.555651	-2.709075	0.412915
C	-3.680337	-0.569764	-0.412958
C	0.992583	-4.881195	-0.959107
C	-1.376084	-4.789186	0.946073
C	5.845288	-0.945829	1.451062
H	4.670728	-2.656775	1.054927
C	3.355649	-4.876226	-1.438919
H	4.407683	-3.077289	-1.035512
C	-2.335182	2.904410	0.416087
C	-3.627877	0.861706	-0.413246
C	1.376101	4.789167	-0.946183
C	-0.992563	4.881217	0.958988
C	5.891078	0.469182	1.453548
H	4.851799	2.278513	1.054689

C	3.724815	4.587065	-1.453561
H	4.627247	2.705217	-1.057105
C	-3.723599	-3.299509	0.956744
C	-4.829140	-1.197110	-0.956305
C	2.104257	-5.539312	-1.449025
H	0.035268	-5.378160	-1.054785
C	-2.533603	-5.352759	1.448213
H	-0.462002	-5.362927	1.035576
O	6.862643	-1.697342	1.980633
O	4.412898	-5.572737	-1.991518
C	-3.455084	3.590698	0.947740
C	-4.723432	1.579813	-0.951955
C	2.533638	5.352736	-1.448305
H	0.462040	5.362932	-1.035704
C	-2.104222	5.539340	1.448912
H	-0.035230	5.378153	1.054645
O	7.015379	1.037557	2.024028
O	4.829586	5.190802	-2.025550
C	-3.724778	-4.587071	1.453550
H	-4.627163	-2.705153	1.057217
C	-5.891156	-0.469188	-1.453393
H	-4.851924	-2.278524	-1.054505
O	1.963814	-6.795330	-1.977394
O	-2.491221	-6.615840	1.977163
H	7.520848	-1.096617	2.356772
H	5.208648	-5.029616	-1.939024
C	-3.355617	4.876236	1.438873
H	-4.407614	3.077234	1.035593
C	-5.845357	0.945816	-1.450932
H	-4.670827	2.656775	-1.054821
O	2.491251	6.615803	-1.977292
O	-1.963783	6.795366	1.977258
H	6.889411	1.992438	2.080043
H	5.549985	4.550579	-2.067775
O	-4.829532	-5.190832	2.025547
O	-7.015466	-1.037577	-2.023829
H	2.826106	-7.086877	-2.304312
H	-3.363860	-6.826084	2.337149
O	-4.412833	5.572746	1.991528
O	-6.862738	1.697342	-1.980441
H	3.363916	6.826088	-2.337187
H	-2.826088	7.086940	2.304120
H	-5.549805	-4.550494	2.068185
H	-6.889735	-1.992520	-2.079303
H	-5.208665	5.029772	1.938753
H	-7.521033	1.096632	-2.356438

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SCH3 substited_monomer

C	-3.982392	-6.038519	-3.833463
S	-4.139498	-6.284272	-2.011899
H	-2.962151	-5.732455	-4.081698
H	-4.706410	-5.296149	-4.179658
H	-4.200337	-7.008841	-4.290846
C	-3.796277	-4.621804	-1.426771
C	-4.777330	-3.588824	-1.474089
C	-2.535252	-4.339410	-0.928141
C	-4.433047	-2.321309	-1.020658
S	-6.380505	-3.984130	-2.143106
C	-2.175791	-3.063355	-0.430974
H	-1.784571	-5.118175	-0.983770
C	-3.161979	-2.028870	-0.474459
H	-5.136059	-1.507496	-1.124085
C	-7.194214	-2.344898	-2.219407
C	-0.824070	-2.740924	-0.036859
C	-2.797955	-0.687597	-0.070712
H	-6.625624	-1.653642	-2.849342
H	-7.329699	-1.915584	-1.221944
H	-8.173816	-2.530295	-2.669142
C	-0.433892	-1.385899	-0.083461
C	0.156342	-3.705963	0.401386
C	-1.429548	-0.348601	-0.080406
C	-3.741620	0.318212	0.362135
C	0.959624	-1.046177	-0.119387
C	1.545658	-3.358672	0.398302
C	-0.214888	-4.938771	0.990813
C	-1.028063	1.033809	-0.065592
C	-3.343375	1.692353	0.374975
C	-5.003354	-0.031073	0.900691
C	1.359312	0.331905	-0.154939
C	1.945941	-2.052688	-0.081203
C	2.472058	-4.262778	0.966448
C	0.708054	-5.828062	1.515269
H	-1.265491	-5.180892	1.096931
C	0.369458	1.371719	-0.082293
C	-2.003751	2.052759	-0.030637
C	-4.244729	2.630732	0.934588
C	-5.892670	0.912450	1.398527
H	-5.250745	-1.080641	0.964395

C	2.727163	0.664539	-0.223216
C	3.280672	-1.716426	-0.533909
C	2.094819	-5.496948	1.482861
H	3.503981	-3.952245	1.034248
S	0.110688	-7.361759	2.232351
C	0.767680	2.724475	-0.022721
C	-1.594912	3.393807	-0.394427
C	-5.493989	2.280603	1.417594
H	-3.932090	3.660609	1.052893
S	-7.496627	0.495810	2.051224
C	3.662638	-0.341970	-0.680001
C	3.107564	1.966110	0.267584
C	4.168539	-2.706109	-1.005240
S	3.259134	-6.675494	2.129313
C	0.263842	-6.976717	4.030346
C	-0.205366	3.732324	-0.366556
C	2.128142	2.999619	0.379017
C	-2.516578	4.349931	-0.879230
S	-6.558689	3.575544	2.061434
C	-7.470248	-1.335497	2.033350
C	4.873658	-0.016103	-1.370866
C	4.396956	2.202316	0.795445
C	5.431081	-2.400078	-1.488209
H	3.851354	-3.740178	-1.029839
C	4.865282	-5.833247	1.871086
H	-0.397881	-6.146007	4.291674
H	1.301054	-6.741051	4.282649
H	-0.048233	-7.881429	4.561715
C	0.172287	5.012920	-0.837588
C	2.511003	4.218070	0.988983
C	-2.133801	5.625692	-1.277801
H	-3.549546	4.051142	-0.978719
C	-6.305047	3.355487	3.875749
H	-6.650060	-1.722127	2.646193
H	-7.390893	-1.725938	1.014327
H	-8.427329	-1.641938	2.464878
C	5.808875	-1.035025	-1.641576
H	5.013163	0.965331	-1.809907
C	4.763844	3.407838	1.373924
H	5.114819	1.390321	0.784304
S	6.491116	-3.794604	-1.879117
H	4.929517	-4.911797	2.458458
H	5.029473	-5.619406	0.810555
H	5.620280	-6.542441	2.222245
C	-0.745783	5.952494	-1.275492
H	1.224059	5.258580	-0.918712
C	3.795776	4.452220	1.461923
H	1.768447	4.993715	1.131627
S	-3.291881	6.864866	-1.813213
H	-5.258595	3.543878	4.131315
H	-6.604306	2.348132	4.176999
H	-6.946770	4.094508	4.365791
S	7.443011	-0.674895	-2.269655
S	6.461684	3.556110	1.940606
C	6.627857	-3.697293	-3.714294
S	-0.138826	7.546840	-1.834608
S	4.110937	6.041507	2.240433
C	-4.901691	6.008915	-1.638211
C	8.008044	0.719634	-1.211233
C	6.244166	3.593673	3.769447
H	7.220596	-2.833629	-4.027395
H	5.629566	-3.662606	-4.159491
H	7.134617	-4.617829	-4.021589
C	-0.278501	7.342965	-3.663420
C	5.210689	6.824249	0.986924
H	-5.068733	5.696082	-0.602925
H	-4.968905	5.147500	-2.310284
H	-5.653169	6.751409	-1.921439
H	7.569827	0.623577	-0.214921
H	7.753709	1.690674	-1.641807
H	9.095180	0.617431	-1.143418
H	5.755485	2.674222	4.104268
H	5.666340	4.474205	4.059568
H	7.253011	3.650711	4.190915
H	-1.314265	7.138155	-3.946564
H	0.382356	6.539688	-4.001526
H	0.040982	8.294906	-4.099368
H	4.681818	6.917313	0.033880
H	6.126892	6.239156	0.873940
H	5.448965	7.819881	1.374884

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SH substited_monomer

C	-0.150053	1.430933	0.001609
C	1.164561	0.844947	0.004017
C	-1.313630	0.585880	-0.002441
C	-0.295444	2.833713	0.007455
C	1.313767	-0.585605	0.002419
C	2.305914	1.673386	0.008525

C	-1.164390	-0.844678	-0.003934
C	-2.602080	1.160360	-0.002287
C	0.837136	3.632438	-0.401735
C	-1.569026	3.380033	0.419753
C	0.150219	-1.430669	-0.001723
C	2.602182	-1.160055	0.002246
C	2.143859	3.048446	-0.408348
C	3.562045	1.091138	0.424943
C	-2.305697	-1.673133	-0.008194
C	-2.728037	2.539653	0.409158
C	-3.712953	0.332240	-0.413345
C	0.684095	4.925745	-0.950423
C	-1.688054	4.682647	0.952686
C	0.295651	-2.833470	-0.007817
C	3.712925	-0.332143	0.413850
C	2.728228	-2.539179	-0.409551
C	3.212457	3.798496	-0.947744
C	4.607459	1.873358	0.963706
C	-3.561960	-1.091021	-0.424045
C	-2.143622	-3.048287	0.408204
C	-3.927949	3.054168	0.950318
C	-4.899459	0.879747	-0.952169
C	1.752995	5.666020	-1.435839
H	-0.313541	5.333064	-1.063713
C	-2.890980	5.191544	1.423777
H	-0.797794	5.294377	1.032491
C	1.569260	-3.379597	-0.420402
C	-0.836936	-3.632345	0.401198
C	4.899036	-0.880032	0.953067
C	3.928190	-3.053449	-0.950785
C	3.053248	5.092934	-1.425018
H	4.185107	3.328749	-1.031902
C	5.791376	1.319571	1.432371
H	4.462602	2.943260	1.053630
C	-4.607532	-1.873657	-0.961748
C	-3.212282	-3.798426	0.947328
C	-4.036980	4.350312	1.433187
H	-4.781233	2.395040	1.055321
C	-5.937218	0.093746	-1.432686
H	-4.982011	1.954957	-1.055482
S	1.408456	7.319217	-2.032470
S	-3.017766	6.857427	2.055166
C	1.688418	-4.682058	-0.953681
C	-0.684039	-4.925958	0.949250
C	5.936668	-0.094427	1.434428
H	4.981343	-1.955310	1.056054
C	4.037373	-4.349473	-1.433925
H	4.781457	-2.394240	-1.055587
S	4.436017	6.029621	-2.062391
S	7.111520	2.342789	2.067606
C	-5.791776	-1.320246	-1.429997
H	-4.462566	-2.943702	-1.050620
C	-3.053193	-5.093076	1.424017
H	-4.184826	-3.328605	1.031971
S	-5.644256	4.880432	2.019200
S	-7.412421	0.931413	-2.006957
H	2.223193	7.286612	-3.110833
H	-1.698289	7.126579	1.973806
C	2.891421	-5.190780	-1.424819
H	0.798185	-5.293750	-1.033773
C	-1.753005	-5.666315	1.434427
H	0.313540	-5.333568	1.062083
S	7.411446	-0.932599	2.009052
S	5.644741	-4.879375	-2.019884
H	5.314877	5.007125	-2.020569
H	6.412784	3.495912	2.021485
S	-7.112259	-2.343917	-2.063795
S	-4.436027	-6.029832	2.061147
H	-5.217802	5.553404	3.111797
H	-7.628737	0.168621	-3.102017
S	3.018370	-6.856475	-2.056661
S	-1.408625	-7.319872	2.030158
H	7.627378	-0.170408	3.104606
H	5.218457	-5.551930	-3.112806
H	-6.413373	-3.496942	-2.017511
H	-5.314774	-5.007217	2.019849
H	1.698919	-7.125785	-1.975386
H	-2.223161	-7.287772	3.108687

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CCH substited_homodimers

C	0.716646	3.652579	-2.373878
C	-0.716583	3.652578	-2.373880
C	-1.424656	2.471529	-1.936890
C	-2.819223	2.456667	-1.559378
C	-3.534115	1.216748	-1.560168
C	-2.849058	0.003110	-1.939753
C	-3.517222	-1.200142	-2.378242
C	-2.801017	-2.441330	-2.376893

C	-1.424665	-2.463781	-1.938957
C	-0.715628	-3.662456	-1.555813
C	0.715700	-3.662458	-1.555829
C	1.424730	-2.463781	-1.938982
C	2.801076	-2.441326	-2.376935
C	3.517281	-1.200138	-2.378286
C	2.849122	0.003111	-1.939784
C	3.534183	1.216746	-1.560197
C	2.819288	2.456663	-1.559385
C	1.424720	2.471529	-1.936892
C	0.719268	1.250282	-1.893287
C	-0.719204	1.250282	-1.893282
C	-1.438790	0.003270	-1.895487
C	-0.719728	-1.242130	-1.896609
C	0.719793	-1.242130	-1.896619
C	1.438854	0.003270	-1.895502
C	3.472116	3.604365	-1.065436
C	4.755572	3.570911	-0.527989
C	5.469833	2.330042	-0.527280
C	4.854065	1.203917	-1.065102
C	-1.386391	4.754855	-2.946223
C	-0.715860	5.858325	-3.465619
C	0.715922	5.858326	-3.465616
C	1.386453	4.754858	-2.946219
C	-4.853989	1.203920	-1.065054
C	-5.469754	2.330048	-0.527237
C	-4.755499	3.570920	-0.527973
C	-3.472050	3.604373	-1.065439
C	-3.421381	-3.573449	-2.946845
C	-4.712672	-3.544607	-3.465513
C	-5.427575	-2.303795	-3.468550
C	-4.806568	-1.170920	-2.951030
C	1.384986	-4.799404	-1.059700
C	0.715902	-5.892578	-0.517516
C	-0.715813	-5.892576	-0.517500
C	-1.384906	-4.799400	-1.059666
C	4.806623	-1.170916	-2.951082
C	5.427628	-2.303791	-3.468604
C	4.712724	-3.544602	-3.465565
C	3.421434	-3.573444	-2.946895
H	2.939334	4.542513	-1.024442
H	5.396128	0.271159	-1.024813
H	-2.463111	4.732773	-3.047178
H	2.463174	4.732778	-3.047169
H	-5.396045	0.271160	-1.024745
H	-2.939273	4.542525	-1.024464
H	-2.864454	-4.495567	-3.045687
H	-5.325226	-0.227140	-3.052725
H	2.463974	-4.805925	-1.022260
H	-2.463892	-4.805915	-1.022201
H	5.325282	-0.227136	-3.052775
H	2.864506	-4.495561	-3.045735
C	-1.456253	6.931465	-4.033995
C	1.456314	6.931469	-4.033986
C	5.297459	4.740984	0.069984
C	6.753597	2.209650	0.070892
C	6.727006	-2.198726	-4.037518
C	5.274564	-4.722836	-4.030448
C	1.460217	-6.945756	0.079889
C	-1.460121	-6.945754	0.079913
C	-5.274513	-4.722838	-4.030405
C	-6.726951	-2.198726	-4.037468
C	-6.753511	2.209656	0.070951
C	-5.297384	4.740996	0.069996
C	0.715628	3.662456	1.555813
C	-0.715700	3.662458	1.555829
C	-1.424730	2.463781	1.938982
C	-2.801076	2.441326	2.376935
C	-3.517281	1.200138	2.378286
C	-2.849122	-0.003111	1.939784
C	-3.534183	-1.216746	1.560197
C	-2.819288	-2.456663	1.559385
C	-1.424720	-2.471529	1.936892
C	-0.716646	-3.652579	2.373878
C	0.716583	-3.652578	2.373880
C	1.424656	-2.471529	1.936890
C	2.819223	-2.456667	1.559378
C	3.534115	-1.216748	1.560168
C	2.849058	-0.003110	1.939753
C	3.517222	1.200142	2.378242
C	2.801017	2.441330	2.376893
C	1.424665	2.463781	1.938957
C	0.719728	1.242130	1.896609
C	-0.719793	1.242130	1.896619
C	-1.438854	-0.003270	1.895502
C	-0.719268	-1.250282	1.893287
C	0.719204	-1.250282	1.893282
C	1.438790	-0.003270	1.895487
C	3.421381	3.573449	2.946845
C	4.712672	3.544607	3.465513

C	5.427575	2.303795	3.468550
C	4.806568	1.170920	2.951030
C	-1.384986	4.799404	1.059700
C	-0.715902	5.892578	0.517516
C	0.715813	5.892576	0.517500
C	1.384906	4.799400	1.059666
C	-4.806623	1.170916	2.951082
C	-5.427628	2.303791	3.468604
C	-4.712724	3.544602	3.465565
C	-3.421434	3.573444	2.946895
C	-3.472116	-3.604365	1.065436
C	-4.755572	-3.570911	0.527989
C	-5.469833	-2.330042	0.527280
C	-4.854065	-1.203917	1.065102
C	1.386391	-4.754855	2.946223
C	0.715860	-5.858325	3.465619
C	-0.715922	-5.858326	3.465616
C	-1.386453	-4.754858	2.946219
C	4.853989	-1.203920	1.065054
C	5.469754	-2.330048	0.527237
C	4.755499	-3.570920	0.527973
C	3.472050	-3.604373	1.065439
H	2.864454	4.495567	3.045687
H	5.325226	0.227140	3.052725
H	-2.463974	4.805925	1.022260
H	2.463892	4.805915	1.022201
H	-5.325282	0.227136	3.052775
H	-2.864506	4.495561	3.045735
H	-2.939334	-4.542513	1.024442
H	-5.396128	-0.271159	1.024813
H	2.463111	-4.732773	3.047178
H	-2.463174	-4.732778	3.047169
H	5.396045	-0.271160	1.024745
H	2.939273	-4.542525	1.024464
C	-1.460217	6.945756	-0.079889
C	1.460121	6.945754	-0.079913
C	5.274513	4.722838	4.030405
C	6.726951	2.198726	4.037468
C	6.753511	-2.209656	-0.070951
C	5.297384	-4.740996	-0.069996
C	1.456253	-6.931465	4.033995
C	-1.456314	-6.931469	4.033986
C	-5.297459	-4.740984	-0.069984
C	-6.753597	-2.209650	-0.070892
C	-6.727006	2.198726	4.037518
C	-5.274564	4.722836	4.030448
C	-5.743628	5.731152	4.511255
C	-2.109759	7.816744	-0.614668
C	2.109661	7.816743	-0.614693
C	5.728089	5.737705	0.606226
C	5.743577	5.731150	4.511222
C	7.833388	2.095895	4.520340
C	7.832090	2.078351	0.605815
C	7.831998	-2.078353	-0.605882
C	5.728010	-5.737718	-0.606240
C	7.833448	-2.095901	-4.520383
C	5.743628	-5.731152	-4.511255
C	2.109759	-7.816744	0.614668
C	-2.109661	-7.816743	0.614693
C	-2.097970	-7.838495	4.517168
C	2.097908	-7.838488	4.517182
C	-5.743577	-5.731150	-4.511222
C	-5.728089	-5.737705	-0.606226
C	-7.833388	-2.095895	-4.520340
C	-7.832090	-2.078351	-0.605815
C	-7.831998	2.078353	0.605882
C	-7.833448	2.095901	4.520383
C	-5.728010	5.737718	0.606240
C	-2.097908	7.838488	-4.517182
C	2.097970	7.838495	-4.517168
H	-2.655739	8.637240	-4.951412
H	2.655803	8.637251	-4.951387
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H	2.668881	8.577922	-1.109442
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H	6.107652	6.601726	1.102445
H	8.803639	2.011277	4.955304
H	8.770362	1.970489	1.100658
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H	6.107563	-6.601742	-1.102462
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CH3 substited_homodimers
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C       3.665491       -0.713602       -1.515859
C       2.457979       -1.423930       -1.872681
C       2.430574       -2.798248       -2.316740
C       1.192616       -3.513001       -2.318109
C      -0.011413       -2.849515       -1.874502
C      -1.230772       -3.540585       -1.520592
C      -2.467000       -2.827927       -1.521899
C      -2.478260       -1.425443       -1.874314
C      -3.654412       -0.714074       -2.319272
C      -3.654283        0.715602       -2.319154
C      -2.477961        1.426682       -1.874194
C      -2.466350        2.829165       -1.521774
C      -1.229988        3.541583       -1.520882
C      -0.010808        2.850211       -1.874838
C       1.193349        3.513373       -2.318575
C       2.431186        2.798400       -2.316996
C       2.458295        1.424113       -1.872783
C       1.236289        0.720640       -1.813727
C       1.236130       -0.720192       -1.813662
C      -0.010084       -1.439692       -1.813624
C      -1.258131       -0.719232       -1.812412
C      -1.257976        0.720215       -1.812411
C      -0.009771        1.440401       -1.813749
C       3.560505        3.427939       -2.895868
C       3.531938        4.712252       -3.411227
C       2.302377        5.420955       -3.415451
C       1.174907        4.804931       -2.900656
C       4.827688       -1.374607       -1.055134
C       5.940095       -0.708883       -0.572140
C       5.940243        0.708325       -0.572132
C       4.827988        1.374284       -1.055156
C       1.173937       -4.804680       -2.899910
C       2.301257       -5.420933       -3.414764
C       3.530918       -4.712395       -3.410846
C       3.559740       -3.428030       -2.895636
C      -3.620372       -3.505901       -1.062944
C      -3.599799       -4.803431       -0.582431
C      -2.371423       -5.510752       -0.580529
C      -1.238001       -4.877307       -1.058646
C      -4.761599        1.378000       -2.903739
C      -5.857892        0.710610       -3.422255
C      -5.857998       -0.708514       -3.422412
C      -4.761812       -1.376178       -2.904019
C      -1.236891        4.878414       -1.059238
C      -2.370062        5.512159       -0.580934
C      -3.598533        4.805004       -0.582231
C      -3.619454        3.507379       -1.062490
H       4.478671        2.862151       -3.000438
H       0.226256        5.317424       -3.007752
H       4.823047       -2.453682       -1.006470
H       4.823549        2.453358       -1.006485
H       0.225199       -5.317062       -3.006778
H       4.477981       -2.862384       -3.000347
H      -4.552914       -2.963073       -1.012307
H      -0.299403       -5.409150       -1.004109
H      -4.730445        2.455842       -3.009579
H      -4.730816       -2.454005       -3.010075
H      -0.298188        5.410122       -1.005143
H      -4.552086        2.964728       -1.011519
C       2.212128        6.799333       -4.022629
H       2.865534        7.508930       -3.495183
H       2.537393        6.796169       -5.071980
H       1.186817        7.181074       -3.978715
C       4.773061        5.324102       -4.012787
H       4.617208        5.589660       -5.067393
H       5.048773        6.253088       -3.493810
H       5.620240        4.633289       -3.951470
C       7.103378        1.476857        0.000856
H       7.231385        1.240949        1.065164
H       8.044172        1.218739       -0.504192
H       6.945442        2.556285       -0.094805
C       7.103094       -1.477663        0.000792
H       8.043915       -1.219776       -0.504327
H       7.231213       -1.241762        1.065083
H       6.944910       -2.557060       -0.094821
C       4.771867       -5.324482       -4.012522
H       5.047445       -6.253527       -3.493582
H       4.615890       -5.589988       -5.067124
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H       2.535531       -6.796309       -5.071261
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H	2.864324	-7.508946	-3.494543
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C	-2.283547	-6.901044	-0.004516
H	-2.530986	-6.888869	1.064948
H	-2.989847	-7.585447	-0.493763
H	-1.273607	-7.309155	-0.117496
C	-4.846977	-5.426118	-0.008261
H	-5.086531	-6.377447	-0.502351
H	-4.712530	-5.640153	1.060121
H	-5.706303	-4.756044	-0.117577
C	-7.006211	-1.476833	-4.028780
H	-7.949706	-1.255291	-3.509733
H	-7.158370	-1.205157	-5.082408
H	-6.829249	-2.555841	-3.971624
C	-7.006017	1.479225	-4.028415
H	-7.158249	1.207805	-5.082098
H	-7.949524	1.257694	-3.509383
H	-6.828905	2.558195	-3.971019
C	-4.845432	5.427995	-0.007787
H	-4.710566	5.642279	1.060485
H	-5.085070	6.379210	-0.502057
H	-5.704870	4.757980	-0.116585
C	-2.281700	6.902623	-0.005401
H	-2.988754	7.586776	-0.493892
H	-2.527691	6.890701	1.064401
H	-1.271974	7.310862	-0.119830
C	3.654412	0.714074	2.319272
C	3.654283	-0.715602	2.319154
C	2.477961	-1.426682	1.874194
C	2.466350	-2.829165	1.521774
C	1.229988	-3.541583	1.520882
C	0.010808	-2.850211	1.874838
C	-1.193349	-3.513373	2.318575
C	-2.431186	-2.798400	2.316996
C	-2.458295	-1.424113	1.872783
C	-3.665651	-0.713532	1.515893
C	-3.665491	0.713602	1.515859
C	-2.457979	1.423930	1.872681
C	-2.430574	2.798248	2.316740
C	-1.192616	3.513001	2.318109
C	0.011413	2.849515	1.874502
C	1.230772	3.540585	1.520592
C	2.467000	2.827927	1.521899
C	2.478260	1.425443	1.874314
C	1.258131	0.719232	1.812412
C	1.257976	-0.720215	1.812411
C	0.009771	-1.440401	1.813749
C	-1.236289	-0.720640	1.813727
C	-1.236130	0.720192	1.813662
C	0.010084	1.439692	1.813624
C	3.620372	3.505901	1.062944
C	3.599799	4.803431	0.582431
C	2.371423	5.510752	0.580529
C	1.238001	4.877307	1.058646
C	4.761599	-1.378000	2.903739
C	5.857892	-0.710610	3.422255
C	5.857998	0.708514	3.422412
C	4.761812	1.376178	2.904019
C	1.236891	-4.878414	1.059238
C	2.370062	-5.512159	0.580934
C	3.598533	-4.805004	0.582231
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C	-3.560505	-3.427939	2.895868
C	-3.531938	-4.712252	3.411227
C	-2.302377	-5.420955	3.415451
C	-1.174907	-4.804931	2.900656
C	-4.827688	1.374607	1.055134
C	-5.940095	0.708883	0.572140
C	-5.940243	-0.708325	0.572132
C	-4.827988	-1.374284	1.055156
C	-1.173937	4.804680	2.899910
C	-2.301257	5.420933	3.414764
C	-3.530918	4.712395	3.410846
C	-3.559740	3.428030	2.895636
H	4.552914	2.963073	1.012307
H	0.299403	5.409150	1.004109
H	4.730445	-2.455842	3.009579
H	4.730816	2.454005	3.010075
H	0.298188	-5.410122	1.005143
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H	-4.478671	-2.862151	3.000438
H	-0.226256	-5.317424	3.007752
H	-4.823047	2.453682	1.006470
H	-4.823549	-2.453358	1.006485
H	-0.225199	5.317062	3.006778
H	-4.477981	2.862384	3.000347
C	2.283547	6.901044	0.004516
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H	2.530986	6.888869	-1.064948
H	1.273607	7.309155	0.117496

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H       5.706303        4.756044        0.117577
C       7.006211        1.476833        4.028780
H       7.158370        1.205157        5.082408
H       7.949706        1.255291        3.509733
H       6.829249        2.555841        3.971624
C       7.006017       -1.479225        4.028415
H       7.949524       -1.257694        3.509383
H       7.158249       -1.207805        5.082098
H       6.828905       -2.558195        3.971019
C       4.845432       -5.427995        0.007787
H       5.085070       -6.379210        0.502057
H       4.710566       -5.642279       -1.060485
H       5.704870       -4.757980        0.116585
C       2.281700       -6.902623        0.005401
H       2.527691       -6.890701       -1.064401
H       2.988754       -7.586776        0.493892
H       1.271974       -7.310862        0.119830
C      -2.212128       -6.799333        4.022629
H      -2.537393       -6.796169        5.071980
H      -2.865534       -7.508930        3.495183
H      -1.186817       -7.181074        3.978715
C      -4.773061       -5.324102        4.012787
H      -5.048773       -6.253088        3.493810
H      -4.617208       -5.589660        5.067393
H      -5.620240       -4.633289        3.951470
C      -7.103378       -1.476857       -0.000856
H      -8.044172       -1.218739        0.504192
H      -7.231385       -1.240949       -1.065164
H      -6.945442       -2.556285        0.094805
C      -7.103094        1.477663       -0.000792
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H      -8.043915        1.219776        0.504327
H      -6.944910        2.557060        0.094821
C      -4.771867        5.324482        4.012522
H      -4.615890        5.589988        5.067124
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H      -5.619186        4.633836        3.951254
C      -2.210717        6.799372        4.021767
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CN substited_homodimers
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C      -0.716528        3.651882       -2.436175
C      -1.422078        2.470439       -1.995301
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C      -2.847923        0.000359       -1.995958
C      -3.517908       -1.201181       -2.437625
C      -2.801323       -2.442155       -2.437133
C      -1.425643       -2.462507       -1.995844
C      -0.715807       -3.657111       -1.603724
C       0.715947       -3.657098       -1.603716
C       1.425776       -2.462490       -1.995788
C       2.801453       -2.442175       -2.437037
C       3.518020       -1.201188       -2.437757
C       2.848071        0.000383       -1.996055
C       3.528612        1.212918       -1.607077
C       2.813181        2.453035       -1.607487
C       1.422187        2.470444       -1.995326
C       0.719111        1.248877       -1.952651
C      -0.718987        1.248874       -1.952636
C      -1.438447        0.002471       -1.953942
C      -0.719436       -1.242645       -1.954755
C       0.719573       -1.242634       -1.954753
C       1.438587        0.002482       -1.953970
C       3.452357        3.598881       -1.090304
C       4.718133        3.547036       -0.520938
C       5.429691        2.312281       -0.519517
C       4.840068        1.191097       -1.088599
C      -1.391845        4.746182       -3.018765
C      -0.712851        5.830552       -3.562035
C       0.712925        5.830560       -3.562033
C       1.391931        4.746197       -3.018764
C      -4.839939        1.191004       -1.088610
C      -5.429604        2.312161       -0.519517
C      -4.718073        3.546933       -0.520901
C      -3.452304        3.598837       -1.090283
C      -3.411223       -3.574498       -3.019093
C      -4.689399       -3.528266       -3.563541
C      -5.402326       -2.293366       -3.564288
C      -4.803338       -1.163259       -3.020102
C       1.389796       -4.781964       -1.084830
C       0.712663       -5.850240       -0.511233
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C	5.402295	-2.293555	-3.564514
C	4.689459	-3.528505	-3.563316
C	3.411344	-3.574653	-3.018729
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H	5.386369	0.260166	-1.054696
H	-2.469036	4.726828	-3.119205
H	2.469122	4.726854	-3.119203
H	-5.386176	0.260034	-1.054726
H	-2.922538	4.539377	-1.056859
H	-2.856099	-4.498080	-3.118194
H	-5.325420	-0.220707	-3.119373
H	2.469383	-4.792731	-1.053726
H	-2.469193	-4.792792	-1.053645
H	5.325372	-0.220809	-3.120105
H	2.856246	-4.498292	-3.117486
C	-1.454555	6.884570	-4.179172
C	1.454619	6.884583	-4.179175
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C	6.688079	2.172911	0.140836
C	6.685387	-2.178127	-4.182891
C	5.231459	-4.697818	-4.180544
C	1.461910	-6.870553	0.149333
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C	-5.231401	-4.697438	-4.181032
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C	-1.425776	2.462490	1.995788
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C	-3.518020	1.201188	2.437757
C	-2.848071	-0.000383	1.996055
C	-3.528612	-1.212918	1.607077
C	-2.813181	-2.453035	1.607487
C	-1.422187	-2.470444	1.995326
C	-0.716625	-3.651886	2.436181
C	0.716528	-3.651882	2.436175
C	1.422078	-2.470439	1.995301
C	2.813079	-2.453016	1.607465
C	3.528474	-1.212885	1.607030
C	2.847923	-0.000359	1.995958
C	3.517908	1.201181	2.437625
C	2.801323	2.442155	2.437133
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C	0.719436	1.242645	1.954755
C	-0.719573	1.242634	1.954753
C	-1.438587	-0.002482	1.953970
C	-0.719111	-1.248877	1.952651
C	0.718987	-1.248874	1.952636
C	1.438447	-0.002471	1.953942
C	3.411223	3.574498	3.019093
C	4.689399	3.528266	3.563541
C	5.402326	2.293366	3.564288
C	4.803338	1.163259	3.020102
C	-1.389796	4.781964	1.084830
C	-0.712663	5.850240	0.511233
C	0.712437	5.850241	0.511190
C	1.389610	4.781979	1.084765
C	-4.803344	1.163349	3.020489
C	-5.402295	2.293555	3.564514
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C	-3.411344	3.574653	3.018729
C	-3.452357	-3.598881	1.090304
C	-4.718133	-3.547036	0.520938
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C	-4.840068	-1.191097	1.088599
C	1.391845	-4.746182	3.018765
C	0.712851	-5.830552	3.562035
C	-0.712925	-5.830560	3.562033
C	-1.391931	-4.746197	3.018764
C	4.839939	-1.191004	1.088610
C	5.429604	-2.312161	0.519517
C	4.718073	-3.546933	0.520901
C	3.452304	-3.598837	1.090283

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H      -2.856246        4.498292        3.117486
H      -2.922533       -4.539390        1.056865
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H       5.386176       -0.260034        1.054726
H       2.922538       -4.539377        1.056859
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C       6.685515        2.177856        4.182450
C       6.687985       -2.172734       -0.140832
C       5.228345       -4.706373       -0.138038
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F substited_homodimers
C       0.720076        3.629207        2.188663
C      -0.720095        3.629210        2.188668
C      -1.419690        2.463123        2.680247
C      -2.765517        2.432300        3.208688
C      -3.485759        1.183757        3.210361
C      -2.839552        0.002765        2.682476
C      -3.500116       -1.185796        2.190802
C      -2.779963       -2.433092        2.190516
C      -1.420150       -2.455972        2.681594
C      -0.720663       -3.606785        3.207944
C       0.720640       -3.606787        3.207932
C       1.420126       -2.455975        2.681586
C       2.779941       -2.433095        2.190515
C       3.500094       -1.185801        2.190798
C       2.839532        0.002762        2.682471
C       3.485744        1.183755        3.210351
C       2.765506        2.432301        3.208659
C       1.419672        2.463121        2.680236
C       0.716591        1.244385        2.659086
C      -0.716610        1.244386        2.659089
C      -1.432842        0.003503        2.659488
C      -0.716260       -1.237841        2.658966
C       0.716239       -1.237842        2.658964
C       1.432822        0.003502        2.659485
C       3.329607        3.528679        3.898355
C       4.574074        3.454279        4.503983
C       5.274734        2.238328        4.506313
C       4.715999        1.123294        3.901872
C      -1.388221        4.702305        1.560779
C      -0.701828        5.761176        0.987691
C       0.701813        5.761174        0.987691
C       1.388205        4.702303        1.560779
C      -4.716022        1.123290        3.901870
C      -5.274754        2.238315        4.506328
C      -4.574081        3.454260        4.504034
C      -3.329610        3.528663        3.898415
C      -3.374765       -3.547284        1.560661
C      -4.634495       -3.481652        0.986305
C      -5.336441       -2.266225        0.987071
C      -4.763034       -1.143114        1.562186
C       1.388185       -4.645593        3.894554
C       0.701712       -5.689330        4.494562
C      -0.701716       -5.689322        4.494583
C      -1.388198       -4.645581        3.894592
C       4.763010       -1.143122        1.562177
C       5.336418       -2.266236        0.987069
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F	2.696503	-4.700511	1.413327
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C	-1.419672	-2.463121	-2.680236
C	-0.720076	-3.629207	-2.188663
C	0.720095	-3.629210	-2.188668
C	1.419690	-2.463123	-2.680247
C	2.765517	-2.432300	-3.208688
C	3.485759	-1.183757	-3.210361
C	2.839552	-0.002765	-2.682476
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C	2.779963	2.433092	-2.190516
C	1.420150	2.455972	-2.681594
C	0.716260	1.237841	-2.658966
C	-0.716239	1.237842	-2.658964
C	-1.432822	-0.003502	-2.659485
C	-0.716591	-1.244385	-2.659086
C	0.716610	-1.244386	-2.659089
C	1.432842	-0.003503	-2.659488
C	3.374765	3.547284	-1.560661
C	4.634495	3.481652	-0.986305
C	5.336441	2.266225	-0.987071
C	4.763034	1.143114	-1.562186
C	-1.388185	4.645593	-3.894554
C	-0.701712	5.689330	-4.494562
C	0.701716	5.689322	-4.494583
C	1.388198	4.645581	-3.894592
C	-4.763010	1.143122	-1.562177
C	-5.336418	2.266236	-0.987069
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C	-4.715999	-1.123294	-3.901872
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C	-0.701813	-5.761174	-0.987691
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C	4.716022	-1.123290	-3.901870
C	5.274754	-2.238315	-4.506328
C	4.574081	-3.454260	-4.504034
C	3.329610	-3.528663	-3.898415
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F	1.359114	6.653954	-5.147832
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F	-5.078449	-4.504968	-5.160693
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F	-5.347671	0.050373	-4.096821
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F       2.630734       -4.663842       -4.091327


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F24 substited_homodimers
C       0.716508        3.637561       -2.299567
C      -0.716437        3.637564       -2.299509
C      -1.425078        2.457373       -1.861078
C      -2.828122        2.445485       -1.510393
C      -3.542856        1.206742       -1.517467
C      -2.849466       -0.010876       -1.873294
C      -3.514132       -1.213297       -2.319746
C      -2.797721       -2.454051       -2.316897
C      -1.424281       -2.478307       -1.870199
C      -0.715137       -3.686475       -1.512523
C       0.715232       -3.686481       -1.512561
C       1.424368       -2.478313       -1.870255
C       2.797805       -2.454055       -2.316961
C       3.514219       -1.213303       -2.319798
C       2.849552       -0.010879       -1.873373
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C       1.425175        2.457376       -1.861143
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C      -1.440007       -0.011092       -1.809076
C      -0.720284       -1.257115       -1.809709
C       0.720375       -1.257117       -1.809733
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C       3.498143        3.606074       -1.056108
C       4.793776        3.557489       -0.598801
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C       4.885499        1.200542       -1.070202
C      -1.392222        4.743352       -2.873944
C      -0.702812        5.822856       -3.374077
C       0.702775        5.822840       -3.374173
C       1.392234        4.743331       -2.874114
C      -4.885376        1.200572       -1.070008
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C       4.806358       -1.179933       -2.901800
C       5.392704       -2.316138       -3.407964
C       4.689906       -3.533599       -3.404580
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H       2.466388        4.738968       -3.002799
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H       2.872013       -4.520213       -3.020315
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C      -2.797805        2.454055        2.316961
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C       0.720284        1.257115        1.809709
C      -0.720375        1.257117        1.809733
C      -1.440097        0.011094        1.809123
C      -0.719779       -1.236914        1.803694
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C	0.719684	-1.236913	1.803666
C	1.440007	0.011092	1.809076
C	3.413599	3.591935	2.895721
C	4.689798	3.533603	3.404547
C	5.392584	2.316136	3.407977
C	4.806246	1.179928	2.901810
C	-1.388647	4.845778	1.060218
C	-0.701619	5.941717	0.594354
C	0.701501	5.941706	0.594309
C	1.388540	4.845757	1.060129
C	-4.806358	1.179933	2.901800
C	-5.392704	2.316138	3.407964
C	-4.689906	3.533599	3.404580
C	-3.413693	3.591934	2.895784
C	-3.498143	-3.606074	1.056108
C	-4.793776	-3.557489	0.598801
C	-5.494892	-2.342062	0.605939
C	-4.885499	-1.200542	1.070202
C	1.392222	-4.743352	2.873944
C	0.702812	-5.822856	3.374077
C	-0.702775	-5.822840	3.374173
C	-1.392234	-4.743331	2.874114
C	4.885376	-1.200572	1.070008
C	5.494740	-2.342111	0.605750
C	4.793624	-3.557537	0.598695
C	3.498011	-3.606100	1.056058
H	2.871917	4.520215	3.020235
H	5.339280	0.247304	3.030878
H	-2.466264	4.875772	1.011120
H	2.466155	4.875725	1.010964
H	-5.339410	0.247310	3.030808
H	-2.872013	4.520213	3.020315
H	-2.985399	-4.553684	0.997684
H	-5.446778	-0.280369	1.019075
H	2.466396	-4.739004	3.002480
H	-2.466388	-4.738968	3.002799
H	5.446663	-0.280411	1.018824
H	2.985249	-4.553704	0.997679
F	-5.380908	-4.665088	0.102154
F	-5.248874	-4.622214	-3.965949
F	-6.613392	-2.257919	-3.972745
F	-6.749444	-2.290423	0.114446
F	-5.248994	4.622207	3.965975
F	-6.613536	2.257924	3.972682
F	-5.380726	4.665156	-0.102055
F	-6.749268	2.290491	-0.114193
F	-1.364875	6.854567	-3.930748
F	1.364784	6.854537	-3.930935
F	1.370377	7.003043	0.100310
F	-1.370510	7.003065	0.100398
F	6.749444	2.290423	-0.114446
F	5.380908	4.665088	-0.102154
F	6.613392	2.257919	3.972745
F	5.248874	4.622214	3.965949
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F	5.248994	-4.622207	-3.965975
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F	1.364875	-6.854567	3.930748
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H substited_homodimers

C	0.716629	3.634579	-2.337889
C	-0.716576	3.634584	-2.337809
C	-1.424842	2.465019	-1.868112
C	-2.829766	2.458082	-1.522260
C	-3.544780	1.219070	-1.523586
C	-2.848083	-0.000046	-1.871418
C	-3.506071	-1.197924	-2.342824
C	-2.789476	-2.438947	-2.341642
C	-1.423136	-2.467838	-1.870217
C	-0.715369	-3.680213	-1.520924
C	0.715447	-3.680218	-1.520947
C	1.423210	-2.467844	-1.870258
C	2.789544	-2.438951	-2.341700
C	3.506143	-1.197930	-2.342873
C	2.848159	-0.000049	-1.871484
C	3.544867	1.219061	-1.523672
C	2.829862	2.458081	-1.522322
C	1.424931	2.465025	-1.868186
C	0.719639	1.246434	-1.793904
C	-0.719551	1.246431	-1.793878
C	-1.440076	-0.001556	-1.795896
C	-0.720453	-1.247545	-1.796236
C	0.720532	-1.247547	-1.796255
C	1.440155	-0.001558	-1.795936

C	3.506575	3.622677	-1.085026
C	4.820239	3.589833	-0.656139
C	5.522035	2.373612	-0.657135
C	4.892195	1.220712	-1.087117
C	-1.388850	4.720144	-2.956741
C	-0.702887	5.784440	-3.511052
C	0.702770	5.784412	-3.511192
C	1.388809	4.720107	-2.956988
C	-4.892094	1.220748	-1.086990
C	-5.521912	2.373669	-0.657029
C	-4.820113	3.589890	-0.656112
C	-3.506459	3.622708	-1.085029
C	-3.392648	-3.564255	-2.960720
C	-4.655913	-3.501621	-3.518412
C	-5.358372	-2.283920	-3.520746
C	-4.781249	-1.157964	-2.964019
C	1.386475	-4.847750	-1.083093
C	0.702056	-5.967943	-0.650097
C	-0.701978	-5.967935	-0.650076
C	-1.386397	-4.847734	-1.083050
C	4.781338	-1.157971	-2.964028
C	5.358464	-2.283924	-3.520756
C	4.655991	-3.501617	-3.518460
C	3.392716	-3.564251	-2.960791
H	2.958136	4.551715	-1.029567
H	5.420257	0.279978	-1.030891
H	-2.465781	4.681637	-3.061931
H	2.465714	4.681575	-3.062406
H	-5.420169	0.280026	-1.030723
H	-2.957998	4.551739	-1.029620
H	-2.821420	-4.478408	-3.063411
H	-5.286436	-0.206023	-3.068896
H	2.465479	-4.837203	-1.031003
H	-2.465399	-4.837166	-1.030928
H	5.286539	-0.206031	-3.068868
H	2.821485	-4.478399	-3.063507
C	0.715369	3.680213	1.520924
C	-0.715447	3.680218	1.520947
C	-1.423210	2.467844	1.870258
C	-2.789544	2.438951	2.341700
C	-3.506143	1.197930	2.342873
C	-2.848159	0.000049	1.871484
C	-3.544867	-1.219061	1.523672
C	-2.829862	-2.458081	1.522322
C	-1.424931	-2.465025	1.868186
C	-0.716629	-3.634579	2.337889
C	0.716576	-3.634584	2.337809
C	1.424842	-2.465019	1.868112
C	2.829766	-2.458082	1.522260
C	3.544780	-1.219070	1.523586
C	2.848083	0.000046	1.871418
C	3.506071	1.197924	2.342824
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C	1.423136	2.467838	1.870217
C	0.720453	1.247545	1.796236
C	-0.720532	1.247547	1.796255
C	-1.440155	0.001558	1.795936
C	-0.719639	-1.246434	1.793904
C	0.719551	-1.246431	1.793878
C	1.440076	0.001556	1.795896
C	3.392648	3.564255	2.960720
C	4.655913	3.501621	3.518412
C	5.358372	2.283920	3.520746
C	4.781249	1.157964	2.964019
C	-1.386475	4.847750	1.083093
C	-0.702056	5.967943	0.650097
C	0.701978	5.967935	0.650076
C	1.386397	4.847734	1.083050
C	-4.781338	1.157971	2.964028
C	-5.358464	2.283924	3.520756
C	-4.655991	3.501617	3.518460
C	-3.392716	3.564251	2.960791
C	-3.506575	-3.622677	1.085026
C	-4.820239	-3.589833	0.656139
C	-5.522035	-2.373612	0.657135
C	-4.892195	-1.220712	1.087117
C	1.388850	-4.720144	2.956741
C	0.702887	-5.784440	3.511052
C	-0.702770	-5.784412	3.511192
C	-1.388809	-4.720107	2.956988
C	4.892094	-1.220748	1.086990
C	5.521912	-2.373669	0.657029
C	4.820113	-3.589890	0.656112
C	3.506459	-3.622708	1.085029
H	2.821420	4.478408	3.063411
H	5.286436	0.206023	3.068896
H	-2.465479	4.837203	1.031003
H	2.465399	4.837166	1.030928
H	-5.286539	0.206031	3.068868
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H      -2.958136       -4.551715        1.029567
H      -5.420257       -0.279978        1.030891
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H      -2.465714       -4.681575        3.062406
H       5.420169       -0.280026        1.030723
H       2.957998       -4.551739        1.029620
H       5.076075        4.378713        4.003987
H       6.326955        2.209655        4.008488
H       6.542755       -2.328184        0.287268
H       5.291954       -4.496102        0.285859
H       5.076153       -4.378704       -4.004042
H       6.327060       -2.209661       -4.008468
H       1.251427       -6.828797       -0.278585
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H      -6.326955       -2.209655       -4.008488
H      -5.292094       -4.496025        0.285856
H      -6.542887       -2.328104        0.287402
H       1.252085       -6.587635        3.995643
H      -1.251899       -6.587583        3.995896
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H       1.251347        6.828782        0.278544
H      -1.252085        6.587635       -3.995643
H       1.251899        6.587583       -3.995896
H      -5.291954        4.496102       -0.285859
H      -6.542755        2.328184       -0.287268
H      -6.327060        2.209661        4.008468
H      -5.076153        4.378704        4.004042
H       6.542887        2.328104       -0.287402
H       5.292094        4.496025       -0.285856

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NH2 substited_homodimers
C      -0.887741        3.642402       -2.299994
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C      -2.327640        1.659085       -1.871164
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C      -2.692037       -2.558272       -2.403270
C      -1.531622       -3.393474       -2.347577
C      -0.268147       -2.830370       -1.940945
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C       2.326103       -1.648492       -1.963919
C       3.584770       -1.044835       -2.337256
C       3.715407        0.380013       -2.310265
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C       1.560370        3.428703       -1.595528
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C      -1.172688        0.845300       -1.901007
C      -1.307506       -0.589222       -1.937787
C      -0.134071       -1.424190       -1.932334
C       1.176523       -0.824247       -1.930270
C       1.307934        0.609973       -1.918632
C       1.719815        4.759954       -1.143124
C       2.891019        5.256436       -0.595144
C       4.024400        4.406327       -0.512807
C       3.901179        3.111996       -0.991647
C      -3.290565        3.816594       -2.681446
C      -3.188389        5.144715       -3.056249
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C      -4.944519       -0.935463       -1.173260
C      -5.960943       -0.219671       -0.563140
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C       1.806183       -5.637505       -0.466235
C       0.738625       -4.918339       -0.989050
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H	-5.597607	-4.456484	-1.061071
H	-6.102905	-5.107645	0.339378
N	-3.514345	-6.169440	-0.131399
H	-4.205716	-6.170436	-0.872480
H	-2.652612	-6.558261	-0.493051
N	0.947765	-7.218048	3.560354
H	1.370199	-7.514769	4.435304
H	-0.053877	-7.361336	3.634110
N	3.651952	-6.274174	3.594763
H	4.467227	-5.778745	3.935864
H	3.418035	-7.031447	4.222937
N	6.572630	-2.854567	0.078268
H	6.150126	-3.779527	0.039447
H	6.953224	-2.622801	-0.835404
N	7.117128	-0.024907	-0.114235
H	7.569096	-0.664751	-0.753617
H	6.993418	0.862531	-0.584641
N	5.817077	4.439362	3.400343
H	5.861333	4.951661	4.277119
H	6.435202	3.638575	3.479723
N	3.681460	6.345448	3.313954
H	2.876053	6.823288	3.700488
H	4.505026	6.546309	3.865188

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C	-2.744846	2.712162	-1.372299
C	-1.627606	3.596324	-1.335456
C	-0.323415	3.096193	-1.699301
C	0.760546	3.930131	-2.156554
C	2.090624	3.410345	-2.183865
C	2.327290	2.055784	-1.740384
C	3.629639	1.534502	-1.395340
C	3.833248	0.124569	-1.352421
C	2.750543	-0.757668	-1.728623
C	2.941787	-2.101716	-2.219752
C	1.824533	-2.989449	-2.292787
C	0.518512	-2.535658	-1.868139
C	-0.605178	-3.416010	-1.638010
C	-1.932038	-2.889948	-1.672720
C	-2.129966	-1.482021	-1.927165
C	-3.373177	-0.916203	-2.399926
C	-3.596092	0.491509	-2.301343
C	-2.551673	1.336015	-1.768106
C	-1.242708	0.807904	-1.708434
C	-0.115711	1.701148	-1.668833
C	1.222395	1.177394	-1.677474
C	1.435597	-0.246814	-1.693217
C	0.310548	-1.142485	-1.750425
C	-1.028921	-0.612471	-1.770036
C	-4.771269	1.032921	-2.883736
C	-5.717995	0.245984	-3.518418
C	-5.462049	-1.143233	-3.671784
C	-4.315672	-1.682233	-3.130497
C	-1.821520	4.918528	-0.868245
C	-3.060224	5.395941	-0.470597
C	-4.183505	4.523262	-0.536286
C	-3.994975	3.221399	-0.950343
C	3.111549	4.196385	-2.777021
C	2.873961	5.463796	-3.284730
C	1.543014	5.964081	-3.285778
C	0.532000	5.195772	-2.750656
C	5.072407	-0.362433	-0.871281
C	6.108692	0.473271	-0.486397
C	5.915955	1.879863	-0.552285
C	4.698439	2.364882	-0.983277

C	2.017707	-4.231901	-2.948316
C	3.233989	-4.631582	-3.458112
C	4.348760	-3.755345	-3.370494
C	4.176747	-2.511498	-2.787719
C	-3.012083	-3.763841	-1.399132
C	-2.836108	-5.112473	-1.136697
C	-1.512730	-5.635110	-1.085682
C	-0.451028	-4.784691	-1.317358
H	-4.899331	2.104406	-2.895873
H	-4.123756	-2.727119	-3.338229
H	-0.957828	5.558392	-0.776795
H	-4.855091	2.570577	-0.916250
H	4.095664	3.767571	-2.891759
H	-0.475639	5.581858	-2.841278
H	5.194981	-1.428708	-0.771942
H	4.553422	3.433478	-0.931279
H	1.179276	-4.890516	-3.131074
H	4.987329	-1.798588	-2.824817
H	-4.007658	-3.353075	-1.354708
H	0.535650	-5.206873	-1.208813
O	3.339040	-5.876336	-4.044051
O	5.525603	-4.206466	-3.911613
O	7.327196	0.042784	-0.034613
O	6.908099	2.786442	-0.245810
O	3.834127	6.278159	-3.822061
O	1.237840	7.220252	-3.769039
O	-3.289471	6.661893	-0.008722
O	-5.464351	4.958776	-0.282197
O	-6.887314	0.715636	-4.053785
O	-6.346349	-1.979462	-4.324145
O	-3.857484	-5.996080	-0.922169
O	-1.253959	-6.973319	-0.910323
C	3.449166	-5.846634	-5.479917
H	2.554022	-5.381974	-5.918784
H	4.345527	-5.299489	-5.797116
H	3.518443	-6.890293	-5.800311
C	-1.602217	-7.540954	0.372372
H	-0.864903	-7.246254	1.126856
H	-2.598514	-7.227625	0.697314
H	-1.577621	-8.625747	0.236629
C	-5.189799	-5.546578	-1.201259
H	-5.824543	-6.430927	-1.105066
H	-5.519307	-4.777953	-0.491911
H	-5.256208	-5.143771	-2.221352
C	-6.407848	-1.785883	-5.750807
H	-6.744912	-0.772416	-5.998806
H	-5.421653	-1.971759	-6.200685
H	-7.128593	-2.519033	-6.124762
C	-7.171626	2.107533	-3.879479
H	-6.434683	2.732073	-4.403793
H	-8.164059	2.263535	-4.308965
H	-7.174653	2.375587	-2.814243
C	-5.772899	5.253889	1.098714
H	-5.918990	4.323061	1.656487
H	-4.980241	5.840438	1.572715
H	-6.702796	5.830067	1.084414
C	-2.172948	7.560659	0.015198
H	-2.565448	8.507905	0.392547
H	-1.374727	7.195190	0.674663
H	-1.764072	7.700563	-0.995310
C	1.317134	7.343217	-5.202942
H	2.330237	7.129120	-5.563606
H	0.599186	6.660762	-5.681033
H	1.051805	8.379206	-5.433256
C	5.184139	5.802782	-3.791871
H	5.299421	4.899263	-4.407213
H	5.792431	6.612325	-4.202106
H	5.497843	5.578181	-2.762829
C	7.373605	2.781794	1.125239
H	6.536474	2.937509	1.812536
H	7.874819	1.844453	1.378038
H	8.076369	3.616982	1.197217
C	7.493413	-1.361001	0.147182
H	8.491364	-1.494294	0.571367
H	6.735374	-1.751223	0.837744
H	7.417692	-1.893836	-0.811873
C	6.617584	-3.286554	-3.953841
H	7.442952	-3.824033	-4.426832
H	6.360833	-2.394170	-4.542141
H	6.909963	-2.971486	-2.941550
C	-2.901316	2.105102	2.320036
C	-1.758896	2.955586	2.410531
C	-0.478782	2.473811	1.935818
C	0.655219	3.328596	1.685883
C	1.973609	2.779269	1.664468
C	2.148523	1.354300	1.868066
C	3.396833	0.738571	2.265882
C	3.563112	-0.677581	2.147557
C	2.465512	-1.489258	1.675165
C	2.591712	-2.886631	1.313215

C	1.451409	-3.735983	1.424762
C	0.174125	-3.168812	1.780943
C	-0.951971	-3.946374	2.239362
C	-2.267425	-3.394553	2.167146
C	-2.438540	-2.038637	1.701363
C	-3.709049	-1.460240	1.331820
C	-3.870786	-0.045044	1.361750
C	-2.759098	0.779349	1.772351
C	-1.463791	0.225340	1.711107
C	-0.310593	1.081654	1.776299
C	1.015349	0.515150	1.743748
C	1.175177	-0.915819	1.675408
C	0.015822	-1.769982	1.685854
C	-1.301661	-1.201351	1.673579
C	-5.096298	0.510482	0.922403
C	-6.152083	-0.271246	0.480549
C	-5.991446	-1.685793	0.448795
C	-4.793406	-2.233134	0.857853
C	-1.891351	4.187379	3.101661
C	-3.090782	4.606696	3.653151
C	-4.211553	3.733922	3.605077
C	-4.096100	2.523768	2.957232
C	3.052371	3.659637	1.393417
C	2.879751	5.019710	1.180631
C	1.561675	5.552892	1.168065
C	0.502542	4.703548	1.394565
C	4.743257	-1.269449	2.670072
C	5.748649	-0.527376	3.265147
C	5.565192	0.872144	3.419724
C	4.412704	1.459332	2.943762
C	1.598939	-5.094777	1.056953
C	2.780134	-5.623933	0.585397
C	3.903404	-4.766724	0.426327
C	3.789458	-3.433324	0.789877
C	-3.344895	-4.146274	2.701458
C	-3.169352	-5.401103	3.262102
C	-1.851178	-5.920222	3.387531
C	-0.789426	-5.188825	2.899430
H	-5.189942	1.584988	0.900916
H	-4.683568	-3.302647	0.761178
H	-1.011704	4.792817	3.258233
H	-4.950507	1.859969	3.001277
H	4.044748	3.250703	1.302546
H	-0.487165	5.125559	1.315899
H	4.822351	-2.346328	2.667649
H	4.272696	2.505717	3.181158
H	0.746295	-5.757416	1.060237
H	4.626673	-2.772494	0.630774
H	-4.326177	-3.698001	2.731584
H	0.201234	-5.588505	3.076098
O	2.844615	-6.967725	0.304507
O	5.027961	-5.342194	-0.097643
O	6.913661	-1.051617	3.764758
O	6.513010	1.664721	4.038378
O	3.896442	5.910832	0.975791
O	1.307466	6.900641	1.032803
O	-3.278122	5.809744	4.280016
O	-5.428418	4.080465	4.157719
O	-7.358360	0.218257	0.063166
O	-7.015244	-2.536070	0.091714
O	-4.183841	-6.183186	3.743677
O	-1.605963	-7.157252	3.944448
C	2.877448	-7.289522	-1.105234
H	1.946103	-6.968006	-1.587863
H	3.731527	-6.821392	-1.602312
H	2.961957	-8.378474	-1.159669
C	-1.814204	-7.225814	5.368358
H	-1.140287	-6.525549	5.883626
H	-2.854896	-6.999528	5.629458
H	-1.572658	-8.252162	5.659772
C	-5.519842	-5.699094	3.569815
H	-6.172917	-6.490581	3.944968
H	-5.685070	-4.775209	4.141958
H	-5.730374	-5.505857	2.508761
C	-7.388965	-2.505952	-1.304309
H	-7.619078	-1.490061	-1.638244
H	-6.580214	-2.913522	-1.920298
H	-8.278215	-3.137218	-1.389361
C	-7.583111	1.624176	0.211152
H	-6.905902	2.209728	-0.423566
H	-8.616987	1.792679	-0.099428
H	-7.448051	1.934148	1.256795
C	-5.443754	4.099745	5.598639
H	-5.202933	3.101514	5.992420
H	-4.733417	4.836398	5.992392
H	-6.462622	4.375025	5.886536
C	-2.178919	6.726827	4.270799
H	-2.551783	7.640944	4.738909
H	-1.328317	6.333315	4.844917
H	-1.852173	6.933798	3.242486

C	1.617877	7.484827	-0.251900
H	2.607746	7.181687	-0.605284
H	0.864725	7.188387	-0.989527
H	1.591185	8.568448	-0.104739
C	5.233344	5.456572	1.220363
H	5.554545	4.722169	0.474375
H	5.863734	6.347204	1.156650
H	5.311368	5.011359	2.221775
C	6.589718	1.486634	5.466334
H	5.625938	1.739262	5.932082
H	6.867041	0.456723	5.721301
H	7.362588	2.176822	5.817414
C	7.033349	-2.476219	3.781341
H	8.002939	-2.688514	4.238142
H	6.227958	-2.933192	4.373185
H	7.003948	-2.889615	2.763120
C	6.142739	-4.489149	-0.338382
H	6.906026	-5.115648	-0.805899
H	5.864148	-3.670570	-1.014256
H	6.525710	-4.067615	0.602797

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C	2.407756	1.210594	1.984525
C	1.689784	2.450069	2.015533
C	0.245145	2.438077	2.037830
C	-0.571445	3.605803	2.297544
C	-1.924856	3.635016	1.823795
C	-2.504583	2.443611	1.255942
C	-3.788538	2.393261	0.592137
C	-4.539861	1.175814	0.620538
C	-3.950239	0.003979	1.228726
C	-4.696220	-1.145628	1.680677
C	-4.004821	-2.379977	1.906211
C	-2.589719	-2.462603	1.631476
C	-1.879405	-3.693807	1.367488
C	-0.449635	-3.677587	1.334688
C	0.256320	-2.490864	1.763289
C	1.584921	-2.512129	2.318089
C	2.294665	-1.282761	2.518300
C	1.682053	-0.035660	2.102299
C	0.292697	-0.025776	1.848233
C	-0.420611	1.223386	1.769789
C	-1.822263	1.225640	1.450654
C	-2.550203	-0.011226	1.397629
C	-1.861076	-1.255114	1.568094
C	-0.428585	-1.263517	1.706385
C	3.509120	-1.322679	3.246312
C	4.063053	-2.503525	3.701763
C	3.369772	-3.710675	3.472539
C	2.156931	-3.705131	2.823995
C	2.432647	3.646554	1.881614
C	3.799009	3.651493	1.700140
C	4.498231	2.426506	1.605838
C	3.800129	1.243782	1.745643
C	-2.701650	4.790945	2.095256
C	-2.201987	5.855294	2.822677
C	-0.889157	5.797961	3.350574
C	-0.113667	4.682948	3.091987
C	-5.763869	1.111644	-0.084249
C	-6.243637	2.187379	-0.808392
C	-5.485693	3.381650	-0.858076
C	-4.293317	3.473595	-0.167592
C	-4.724241	-3.447722	2.495515
C	-6.064135	-3.338798	2.807963
C	-6.753732	-2.125035	2.571649
C	-6.063306	-1.056356	2.034619
C	0.227133	-4.787238	0.782697
C	-0.449248	-5.892692	0.307695
C	-1.855223	-5.938853	0.405936
C	-2.541416	-4.865628	0.935453
H	4.019244	-0.407501	3.515456
H	1.610537	-4.639587	2.751991
H	1.920254	4.594933	1.812838
H	4.346202	0.325548	1.591848
H	-3.749374	4.812626	1.812174
H	0.852657	4.628672	3.577312
H	-6.299715	0.173934	-0.161573
H	-3.699204	4.373334	-0.284985
H	-4.202962	-4.357386	2.777570
H	-6.591200	-0.115477	1.942476
H	1.297584	-4.733801	0.626583
H	-3.618441	-4.879852	0.847626
O	-6.798059	-4.345782	3.405492
O	-8.072699	-1.972801	2.910405
O	-2.576335	-6.966750	-0.171195
O	0.166619	-6.955378	-0.329194
O	3.979400	-4.878882	3.936487
O	5.246408	-2.468697	4.393542

O	5.837448	2.384364	1.331236
O	4.542052	4.796858	1.513400
O	-0.385036	6.800371	4.137777
O	-2.937873	6.982895	3.143184
O	-5.995149	4.392670	-1.655303
O	-7.402497	2.055132	-1.518091
H	-1.941916	-7.557427	-0.605683
H	-6.228941	-5.113968	3.535190
H	-8.381096	-2.795588	3.314327
H	-7.485463	2.832120	-2.090565
H	-5.268469	4.850710	-2.100557
H	-3.853296	6.849199	2.868092
H	-1.085856	7.448307	4.295248
H	3.948177	5.545514	1.349345
H	6.138255	3.285421	1.147120
H	5.437310	-3.359708	4.716775
H	3.313370	-5.576643	3.979667
H	0.909007	-6.612179	-0.850516
C	4.696335	1.145826	-1.680117
C	4.004931	2.380153	-1.905771
C	2.589750	2.462711	-1.631407
C	1.879311	3.693869	-1.367644
C	0.449530	3.677644	-1.335179
C	-0.256285	2.490818	-1.763811
C	-1.584890	2.511953	-2.318556
C	-2.294689	1.282532	-2.518470
C	-1.681929	0.035539	-2.102463
C	-2.407561	-1.210760	-1.984537
C	-1.689566	-2.450228	-2.015732
C	-0.244948	-2.438170	-2.038100
C	0.571669	-3.605840	-2.297933
C	1.925180	-3.634899	-1.824468
C	2.504760	-2.443530	-1.256420
C	3.788611	-2.393261	-0.592442
C	4.539903	-1.175813	-0.620396
C	3.950309	-0.003876	-1.228460
C	2.550312	0.011301	-1.397670
C	1.861159	1.255165	-1.568197
C	0.428691	1.263506	-1.706723
C	-0.292567	0.025727	-1.848522
C	0.420763	-1.223421	-1.770093
C	1.822388	-1.225592	-1.450952
C	5.763787	-1.111796	0.084625
C	6.243389	-2.187696	0.808668
C	5.485300	-3.381891	0.858027
C	4.293138	-3.473744	0.167184
C	4.724463	3.447973	-2.494801
C	6.064451	3.339146	-2.806890
C	6.754046	2.125414	-2.570456
C	6.063528	1.056665	-2.033668
C	-0.227323	4.787362	-0.783422
C	0.448914	5.892888	-0.308363
C	1.854908	5.939057	-0.406267
C	2.541167	4.865757	-0.935545
C	-3.509369	1.322363	-3.246067
C	-4.063669	2.503208	-3.701094
C	-3.370387	3.710400	-3.472087
C	-2.157073	3.704852	-2.824420
C	-2.432447	-3.646724	-1.882033
C	-3.798809	-3.651649	-1.700435
C	-4.497955	-2.426660	-1.605500
C	-3.799865	-1.243932	-1.745364
C	2.702207	-4.790585	-2.096289
C	2.202585	-5.854922	-2.823732
C	0.889571	-5.797881	-3.351167
C	0.113868	-4.683081	-3.092229
H	6.299493	-0.174043	0.162315
H	3.699085	-4.373579	0.284133
H	4.203244	4.357655	-2.776909
H	6.591484	0.115832	-1.941428
H	-1.297809	4.734016	-0.627544
H	3.618143	4.879898	-0.847200
H	-4.019477	0.407139	-3.515097
H	-1.610660	4.639330	-2.752882
H	-1.920219	-4.595201	-1.813215
H	-4.345832	-0.325638	-1.591592
H	3.750050	-4.811873	-1.813608
H	-0.852664	-4.629078	-3.577176
O	-4.541993	-4.796955	-1.514160
O	-5.837008	-2.384502	-1.330239
O	0.385391	-6.800359	-4.138258
O	2.938751	-6.982224	-3.144844
O	5.994348	-4.392982	1.655410
O	7.402104	-2.055668	1.518593
O	8.073120	1.973260	-2.908842
O	6.798479	4.346215	-3.404153
O	2.576016	6.966875	0.170916
O	-0.167217	6.955601	0.328256
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H       1.086227       -7.448239       -4.295870
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H      -5.438546        3.359284       -4.715400
H      -3.314883        5.576779       -3.977845
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H       1.941643        7.557930        0.604935
H       6.229356        5.114383       -3.533934
H       8.381587        2.796075       -3.312652
H       7.484854       -2.832657        2.091103
H       5.267320       -4.851238        2.099820
H       3.853815       -6.848997       -2.868328

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SCH3 substited_homodimers
C       3.775503       -2.266072       -3.078421
C       2.884852       -1.369600       -2.451499
C       3.098278        0.037620       -2.644912
C       4.139084        0.474104       -3.530066
C       5.083657       -0.452623       -4.013783
C       4.863710       -1.843442       -3.821887
C       2.129086        0.942886       -2.059105
C       0.820588        0.473211       -1.830838
C       0.566399       -0.938516       -1.782107
C       1.644470       -1.843496       -1.869176
C      -0.786060       -1.416894       -1.715356
C      -1.040021       -2.800615       -1.816298
C       0.044355       -3.705491       -1.528090
C       1.390617       -3.223758       -1.510507
C      -1.877583       -0.488688       -1.632285
C      -3.208546       -0.955929       -1.679220
C      -3.430973       -2.274315       -2.229253
C      -2.348020       -3.207078       -2.275131
C      -1.614450        0.926403       -1.586927
C      -2.688341        1.835982       -1.514791
C      -3.979766        1.328009       -1.110696
C      -4.259329       -0.066412       -1.241629
C      -0.266509        1.409661       -1.709284
C      -0.018947        2.798177       -1.807992
C      -1.127774        3.660196       -2.142376
C      -2.466721        3.190457       -1.967807
C      -3.534640        4.013562       -2.398785
C      -3.340315        5.268472       -2.958650
C      -2.006118        5.700316       -3.205390
C      -0.951280        4.897109       -2.809455
C      -5.550704       -0.513186       -0.874619
C      -6.559520        0.341361       -0.446451
C      -6.250154        1.712438       -0.229244
C      -4.964276        2.151505       -0.528801
C      -2.561544       -4.427668       -2.960633
C      -3.771535       -4.759845       -3.548938
C      -4.853965       -3.835234       -3.487793
C      -4.647222       -2.612632       -2.864286
C       2.416686       -4.111154       -1.118377
C       2.182558       -5.452925       -0.833225
C       0.839083       -5.928168       -0.832416
C      -0.181470       -5.050163       -1.160195
C       1.339823        3.253214       -1.627552
C       2.407689        2.311191       -1.711100
C       1.676731        4.592582       -1.338898
C       2.981356        5.028265       -1.146023
C       4.029894        4.063481       -1.126164
C       3.712048        2.737839       -1.395435
S       3.201504        6.791919       -0.902951
S       5.769153        4.391258       -0.900201
S      -4.680195        6.344016       -3.419803
S      -1.641711        7.237867       -4.056039
S      -8.225487       -0.326100       -0.315630
S      -7.387817        2.990882        0.279805
S      -3.918298       -6.348957       -4.368881
S      -6.409738       -4.292621       -4.221128
S       3.495967       -6.598331       -0.485846
S       0.400552       -7.638487       -0.527897
S       6.453113        0.173060       -5.010685
S       5.813779       -3.138265       -4.638799
C       4.907174       -2.382996        0.772429
C       3.904298       -1.457407        1.140132
C       4.212286       -0.068206        1.019993
C       5.471973        0.308217        0.496355
C       6.469745       -0.619516        0.216779
C       6.179005       -2.003193        0.377902
C       3.222076        0.901106        1.434851
C       1.871585        0.493940        1.473783
C       1.551909       -0.908490        1.525894
C       2.592603       -1.862342        1.586052
C       0.182968       -1.325149        1.635012
C      -0.118717       -2.688791        1.834207
C       0.931117       -3.546077        2.325337
C       2.296036       -3.145637        2.185033
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C	-0.875130	-0.347918	1.644859
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C	-1.473332	-3.126579	1.605407
C	-0.552387	1.054663	1.634948
C	-1.579770	2.014744	1.755764
C	-2.862537	1.578000	2.258794
C	-3.179002	0.184272	2.279027
C	0.824590	1.473438	1.588292
C	1.149242	2.839379	1.753970
C	0.107311	3.820219	1.564362
C	-1.255778	3.399509	1.491804
C	-2.244693	4.345420	1.143917
C	-1.968326	5.698736	0.988732
C	-0.612846	6.127081	1.087103
C	0.376466	5.191054	1.337522
C	-4.339186	-0.240377	2.972446
C	-5.188572	0.640343	3.624336
C	-4.879646	2.029549	3.597679
C	-3.743213	2.457493	2.936289
C	-1.805363	-4.480161	1.390498
C	-3.097459	-4.921639	1.137902
C	-4.126721	-3.948588	0.984037
C	-3.809489	-2.607199	1.181090
C	3.295403	-3.950535	2.780775
C	3.009810	-5.126836	3.462741
C	1.645846	-5.468493	3.683215
C	0.655114	-4.681422	3.124349
C	2.498252	3.158701	2.166314
C	3.543950	2.203090	1.971422
C	2.800494	4.312992	2.928551
C	4.063841	4.577676	3.432002
C	5.115888	3.647841	3.194711
C	4.826914	2.483244	2.499580
S	4.317122	6.090908	4.362293
S	6.737700	4.021254	3.830218
S	-3.213407	6.930071	0.702172
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S	-6.603018	0.108290	4.573226
S	-5.886049	3.246929	4.452788
S	-3.303407	-6.697107	0.983460
S	-5.848177	-4.264639	0.626617
S	4.271227	-6.202957	4.103624
S	1.158373	-6.879539	4.677168
S	8.119232	-0.167955	-0.284648
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H	5.586721	1.722423	2.413789
H	-3.251729	3.988566	0.995969
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H	-4.512293	-1.301391	3.062792
H	-3.485674	3.504296	3.025780
H	-1.017781	-5.219213	1.402240
H	-4.576308	-1.864632	1.006923
H	4.315568	-3.602233	2.758961
H	-0.371996	-4.918201	3.371719
H	5.660838	1.361329	0.337089
H	4.675600	-3.438408	0.788801
C	7.641534	-3.418426	-1.601574
C	5.808032	-5.428441	3.478792
C	1.539633	-6.255511	6.371001
C	-4.505619	-7.037831	2.333540
C	-5.873938	-5.539763	-0.695693
C	-6.487957	-1.716475	4.467951
C	-5.247541	3.052868	6.172235
C	-4.732779	5.934067	0.510828
C	-0.349436	8.178906	-0.843393
C	4.363154	5.434666	6.086050
C	7.706630	2.547966	3.336634
C	7.905094	1.561278	-0.836548
H	0.888358	5.322885	-1.239059
H	4.494002	1.989296	-1.374579
H	-4.536783	3.619589	-2.336158
H	0.044010	5.208873	-3.097817
H	-5.774596	-1.572226	-0.913596
H	-4.708635	3.173014	-0.287112
H	-1.734622	-5.111966	-3.100869
H	-5.421407	-1.862668	-2.910826
H	3.419048	-3.718481	-1.028798
H	-1.197459	-5.410986	-1.087036
H	4.144634	1.469489	-3.961386
H	3.551132	-3.323279	-3.078464
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C	4.954717	-5.751288	-1.197175
C	0.695717	-7.819237	1.281074
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C	-7.461275	-2.834123	-3.867679
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H	7.152310	1.623535	-1.626721
H	7.626154	2.225426	-0.015152
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H	7.884265	-2.446386	-2.032019
H	5.739492	-3.709138	-6.957701
H	4.148493	-3.085531	-6.421941
H	5.506894	-1.945383	-6.744875
H	8.770558	0.102211	-4.508316
H	7.824702	-0.376111	-3.071048
H	8.086587	-1.555416	-4.398523
H	-1.892203	7.667416	-6.395763
H	-1.419299	5.960867	-6.127956
H	-3.120548	6.483148	-5.856882
H	-7.011818	5.944229	-3.338824
H	-6.158859	4.407275	-3.659491
H	-6.221625	5.074839	-1.995486
H	0.415198	7.643207	-1.410319
H	-1.355171	7.905781	-1.168259
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H	4.360562	8.305967	-2.329099
H	5.215437	6.729647	-2.307928
H	3.721852	6.933561	-3.282853
H	6.853475	5.366986	0.976261
H	5.880411	6.619784	0.128006
H	5.088645	5.421532	1.191615
H	8.724689	2.741006	3.686484
H	7.322497	1.640658	3.813085
H	7.711541	2.423883	2.249537
H	4.535176	6.299420	6.734772
H	3.403473	4.971697	6.332517
H	5.180852	4.718517	6.201159
H	-5.535647	6.658336	0.349376
H	-4.647219	5.288974	-0.366103
H	-4.949848	5.344740	1.406055
H	-5.825464	3.743397	6.794639
H	-5.401958	2.026658	6.516137
H	-4.187427	3.319135	6.207772
H	-9.128259	-1.649593	1.454787
H	-7.380885	-1.962189	1.281162
H	-7.952983	-0.468919	2.110357
H	-7.334059	-2.092312	5.050347
H	-6.576991	-2.059277	3.433597
H	-5.551326	-2.074550	4.906276
H	-8.600732	3.206543	2.310617
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H	-6.784454	-5.347279	-1.270030
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H	-4.630700	-8.125169	2.347432
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H	-5.466287	-6.552115	2.140318
H	1.289162	-7.070551	7.057460
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H	6.613238	-6.108444	3.771187
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H	5.978025	-4.447838	3.934631
H	0.611085	-8.890195	1.488982
H	1.694827	-7.475363	1.555328
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H	5.751556	-6.501013	-1.198749
H	4.742275	-5.438170	-2.223504
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H	-3.956928	-6.749656	-6.726177
H	-4.662313	-5.144276	-6.371988
H	-2.876913	-5.371708	-6.351888
H	-8.450166	-3.093437	-4.256526
H	-7.528302	-2.643665	-2.791962
H	-7.089867	-1.943291	-4.384009

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SH substited_homodimers

C	-1.119020	-3.626959	-1.447767
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C	-2.779666	1.206889	-1.825267
C	-2.882027	2.597389	-1.455453
C	-1.712080	3.416126	-1.440804
C	-0.445106	2.836459	-1.831016
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C	1.974278	2.992654	-2.368760
C	2.132354	1.623189	-1.933676
C	3.407182	1.015406	-1.633316
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C	2.370812	-1.216797	-1.940096
C	2.441518	-2.592732	-2.375886
C	1.272556	-3.414770	-2.303380
C	0.032232	-2.844562	-1.832642
C	-0.082338	-1.438692	-1.795946
C	-1.384488	-0.826038	-1.778075
C	-1.505015	0.606200	-1.778192
C	-0.324785	1.431200	-1.792240
C	0.976937	0.819301	-1.833634
C	1.097897	-0.617295	-1.836816
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C	2.494193	-5.234004	-3.417680
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C	3.590961	-3.117331	-3.009020
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C	-2.089626	-5.671674	-0.485833
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H	-0.940689	5.355768	-0.930412
H	-4.954632	2.519125	-0.899599
H	3.972311	3.207849	-3.145898
H	-0.467195	5.311089	-2.961489
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H	4.418109	2.844139	-1.136936
H	7.330852	1.680053	0.880814
H	5.127531	4.899431	-4.068156
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H	-7.158307	2.244538	-3.816490
H	-7.687583	-1.570708	-4.946283
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C	3.896853	-0.403482	2.261253
C	2.779335	-1.207350	1.825207
C	2.881457	-2.597715	1.454861
C	1.711376	-3.416232	1.439855
C	0.444499	-2.836489	1.830323
C	0.324435	-1.431186	1.791870
C	-0.977162	-0.819018	1.833525
C	-1.097869	0.617604	1.836430
C	0.082545	1.438758	1.795425
C	1.384587	0.825849	1.778176
C	1.504810	-0.606410	1.778072
C	1.825488	-4.736476	0.959003
C	3.016339	-5.270062	0.477233
C	4.169830	-4.439161	0.456077
C	4.080927	-3.152680	0.962209

C	-3.021226	-3.701694	2.998606
C	-2.863955	-4.989301	3.493054
C	-1.578830	-5.589190	3.440400
C	-0.524794	-4.883476	2.881924
C	-4.756591	0.974790	1.234402
C	-5.845387	0.215552	0.830230
C	-5.714491	-1.197504	0.804212
C	-4.522647	-1.771646	1.214294
C	-1.335033	4.711689	2.863675
C	-2.493314	5.235397	3.415156
C	-3.651214	4.419875	3.483347
C	-3.590363	3.118615	3.007792
C	3.509423	3.781846	0.994019
C	3.382270	5.081053	0.523230
C	2.091489	5.670811	0.484826
C	1.007535	4.942673	0.949961
C	5.055852	-0.977739	2.827565
C	6.113543	-0.217714	3.307167
C	5.986841	1.196009	3.318258
C	4.823347	1.775305	2.833814
H	0.939689	-5.355567	0.928780
H	4.954084	-2.519547	0.899127
H	-3.972218	-3.206626	3.147623
H	0.466257	-5.311663	2.959788
H	-4.841247	2.050029	1.191783
H	-4.419082	-2.843501	1.138924
H	-0.432613	5.305421	2.929149
H	-4.440720	2.468750	3.170333
H	4.485861	3.320013	0.954838
H	0.026282	5.387513	0.872862
H	5.107581	-2.054067	2.931671
H	4.695122	2.842102	2.966307
H	7.685996	1.567484	4.950343
H	5.671612	4.966286	0.080577
H	2.533827	7.265673	-1.222046
H	-3.013936	6.710603	5.202823
H	-5.839522	3.926416	4.153522
H	-6.913527	2.256506	0.419197
H	-7.332313	-1.680111	-0.878293
H	-5.127092	-4.897152	4.071954
H	-1.950057	-7.166492	5.184780
H	4.280091	-7.065304	-0.359079
H	5.392261	-5.211670	-1.454588
H	7.157354	-2.246736	3.816926
S	-7.596493	0.975859	-3.945704
S	-7.268876	-2.307319	-3.892787
S	-7.037728	-2.295461	0.290110
S	-7.366828	0.985030	0.311937
S	-4.796177	-5.990432	0.064968
S	-4.217564	-5.878495	4.241164
S	-1.239610	-7.243593	4.036666
S	-1.779913	-7.334943	0.098038
S	2.957317	-6.944553	-0.115513
S	2.463506	-6.930926	-3.990717
S	5.146101	-5.080471	-4.215827
S	5.771774	-4.956813	-0.177609
S	7.366376	-0.984339	-0.310846
S	7.595506	-0.978170	3.947362
S	7.036808	2.295909	-0.287467
S	7.267835	2.305041	3.897295
S	4.217353	5.879836	-4.239334
S	4.798657	5.989533	-0.062724
S	1.238720	7.243419	-4.037890
S	1.782423	7.333802	-0.100097
S	-2.958559	6.944893	0.113073
S	-2.462402	6.932597	3.987356
S	-5.772647	4.956695	0.176231
S	-5.145096	5.082537	4.213873

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CCH substited_heterodimers

C	0.154546	0.397562	0.636644
C	-0.463644	0.862893	1.856987
C	-1.137274	2.085131	1.870457
C	-0.593612	2.438456	-0.513733
C	0.098149	1.167131	-0.523274
C	-1.015462	-0.289909	2.542547
C	-2.407106	2.197710	2.561874
C	-1.268308	2.582107	-1.791101
C	-0.132285	0.530480	-1.802141
C	-0.004154	-1.036836	0.566078
C	-2.536228	3.166280	-1.845085
C	-3.174497	3.629293	-0.625886
C	-2.237562	-0.181027	3.209607
C	-3.264649	3.067962	1.777935
C	-2.947650	1.086401	3.216161
C	-0.980338	1.402544	-2.587508
C	-0.287498	-0.855913	-1.872103
C	-0.221095	-1.654388	-0.664460

C	-0.727005	-1.466634	1.743629	C	3.334376	-2.754564	-2.464928
C	-1.304911	-1.428057	-2.730011	C	3.412454	-1.567887	-3.260250
C	-1.192972	-2.722753	-0.772273	C	3.094833	-0.295662	-2.655419
C	-1.665822	-2.496205	1.640269	C	2.631238	0.855337	-3.389459
C	-1.964864	0.852666	-3.411619	C	2.640131	2.140202	-2.755836
C	-4.366853	0.803088	3.111055	C	3.123466	2.256703	-1.402314
C	-1.866808	-2.582429	-2.049631	C	3.460625	3.511096	-0.769169
C	-1.903543	-3.135469	0.358318	C	3.390999	3.608969	0.655759
C	-2.937253	-2.381486	2.329429	C	2.980490	2.452115	1.418987
C	-3.961961	-2.950232	1.472927	C	2.349347	2.522880	2.712688
C	-6.217448	1.070990	1.501027	C	2.238885	1.334376	3.505309
C	-3.322568	-3.415897	0.255245	C	2.770511	0.094573	2.997288
C	-3.975346	-3.277856	-0.973962	C	2.985099	-1.084512	3.804329
C	-5.291513	-2.668346	-1.031353	C	2.975195	-2.368765	3.174799
C	-3.234347	-2.853354	-2.147821	C	2.747100	-2.450129	1.750040
C	-3.281538	1.460862	-3.468522	C	2.983314	-1.296160	0.976984
C	-6.378761	-0.315856	1.431317	C	3.061943	-1.393808	-0.452553
C	-2.130287	-0.587223	-3.484705	C	3.151074	-0.201432	-1.250406
C	-3.550657	-0.869680	-3.584534	C	3.175717	1.087232	-0.618894
C	-5.520531	-1.186204	2.213952	C	3.106218	1.185632	0.814590
C	-6.288937	1.871321	0.292744	C	3.001496	-0.003868	1.610405
C	-6.519633	1.255972	-0.940876	C	3.281931	-3.503629	3.950867
C	-5.229783	-2.363806	1.416722	C	3.570867	-3.422747	5.312729
C	-5.907649	-2.220977	0.141270	C	3.580109	-2.134822	5.944052
C	-4.091732	-1.980262	-2.929952	C	3.300118	-1.005769	5.175000
C	-5.363491	-1.867359	-2.239755	C	1.610099	-4.759769	-0.987592
C	-6.617767	-0.955001	0.150354	C	0.818898	-5.674374	-0.299281
C	-4.261961	0.396196	-3.575765	C	0.702278	-5.556654	1.125240
C	-5.778141	1.681087	-2.113682	C	1.393585	-4.538005	1.774396
C	-6.686836	-0.183787	-1.013466	C	3.893123	-1.669538	-4.580968
C	-5.486983	0.504272	-2.911008	C	4.275016	-2.885354	-5.146300
C	-6.048046	-0.648518	-2.230842	C	4.203116	-4.074184	-4.346733
C	-5.193742	1.641553	2.356696	C	3.749535	-3.975608	-3.031947
C	-4.631814	2.794220	1.677390	C	1.985485	3.212611	-3.398268
C	-5.308427	2.935759	0.401110	C	1.326712	3.066863	-4.615687
C	-3.217337	-1.246320	3.097937	C	1.321050	1.781184	-5.251743
C	-4.533325	-0.637106	3.037190	C	1.972221	0.719922	-4.630252
C	-1.206041	2.886338	0.662045	C	3.812648	4.802499	1.272958
C	-2.522539	3.493523	0.604126	C	4.269802	5.900128	0.543910
C	-4.594087	3.345432	-0.728349	C	4.336280	5.803391	-0.885419
C	-3.561600	2.594503	-2.699720	C	3.944140	4.614111	-1.499478
C	-4.832959	2.706060	-2.009363	C	1.431688	1.369114	4.663363
C	2.200904	-3.607710	1.085863	C	0.735940	2.507431	5.058103
C	2.303566	-3.714426	-0.339475	C	0.848749	3.698234	4.265750
C	2.927374	-2.647678	-1.082532	C	1.648809	3.676127	3.127372

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H       3.339680       -4.474082        3.472786
H       3.373450       -0.033738        5.647542
H       1.609293       -4.809688       -2.068592
H       1.230454       -4.415995        2.837361
H       4.016594       -0.769812       -5.171562
H       3.762366       -4.868559       -2.418870
H       1.909234        4.167917       -2.895074
H       1.882576       -0.259963       -5.081465
H       3.826191        4.865243        2.354471
H       4.058929        4.531109       -2.573543
H       1.267799        0.458452        5.225034
H       1.651751        4.556427        2.497797
C       3.884388       -4.604389        6.040420
C       3.903469       -1.989589        7.321901
C      -0.123381        2.452835        6.190303
C       0.104380        4.868088        4.582350
C       4.692260        7.075344        1.225421
C       4.824999        6.880061       -1.676734
C       0.612490        4.165899       -5.167625
C       0.602443        1.558857       -6.458876
C       4.761577       -2.922169       -6.482791
C       4.617940       -5.335086       -4.858732
C       0.082131       -6.653702       -1.021267
C      -0.159223       -6.409596        1.868952
C      -0.530640        5.867666        4.837135
H      -1.092448        6.745090        5.066277
C      -0.856294        2.392158        7.152772
H      -1.504488        2.343417        7.998613
C       4.172734       -1.852853        8.495060
H       4.410576       -1.738220        9.528668
C       4.144467       -5.618428        6.649974
H       4.374545       -6.508245        7.191577
C       4.962997       -6.415604       -5.284098
H       5.268431       -7.364288       -5.664569
C       5.168473       -2.940890       -7.623629
H       5.528440       -2.963401       -8.627600
C      -0.013214        1.355279       -7.482020
H      -0.556836        1.181152       -8.383221
C      -0.000735        5.106493       -5.622121
H      -0.541950        5.931837       -6.026967
C       5.233519        7.791524       -2.362189
H       5.594569        8.597573       -2.960501
C       5.044420        8.071837        1.817495
H       5.356325        8.951911        2.333485
C      -0.897564       -7.122099        2.512804
H      -1.548988       -7.753076        3.074494
C      -0.546165       -7.478291       -1.647858
H      -1.101766       -8.206596       -2.194550

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CH3 substited_heterodimers
C       1.307742        2.983907        0.452654
C       2.666633        3.451469        0.261203
C       3.628862        3.232780        1.253273
C       1.957138        2.080658        2.656831
C       0.962308        2.308327        1.627431
C       3.011484        3.271915       -1.138528
C       4.970124        2.821395        0.882224
C       1.715763        0.768014        3.232681
C       0.112842        1.137278        1.566322
C       0.813203        2.515526       -0.829635
C       2.793855       -0.042687        3.601709
C       4.153696        0.427616        3.409156
C       4.305104        2.876908       -1.493717
C       5.438272        1.869676        1.873150
C       5.302770        2.648387       -0.464783
C       0.571863        0.186090        2.558169
C      -0.342895        0.681302        0.332492
C       0.004952        1.380448       -0.884763
C       1.864284        2.694745       -1.814510
C      -0.370845       -0.735069        0.043268
C       0.195621        0.393585       -1.926823
C       2.052966        1.739133       -2.819706
C       0.544009       -1.183844        2.279660
C       6.114729        1.516283       -0.872085
C      -0.040572       -0.915471       -1.352968
C       1.197161        0.568724       -2.880944
C       3.395326        1.328324       -3.185742
C       3.367408       -0.094936       -3.475093
C       6.537858       -0.821898       -0.207274
C       2.007943       -0.564631       -3.288282
C       1.776241       -1.829361       -2.735095
C       2.895206       -2.668156       -2.347455
C       0.723820       -2.011468       -1.751731
C       1.661118       -2.025188        2.663563
C       6.060399       -1.275000       -1.440429
C       0.058546       -1.653356        0.996669
C       0.863686       -2.786116        0.589842
C       5.592896       -0.323330       -2.431935
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C	6.176389	-1.520669	1.012002
C	5.350231	-2.647198	0.953687
C	4.446392	-0.905019	-3.105965
C	4.205479	-2.215126	-2.530599
C	1.191625	-2.961425	-0.757723
C	2.533114	-3.368164	-1.126864
C	5.202916	-2.444274	-1.501296
C	1.857744	-3.016046	1.618255
C	4.298142	-2.828609	1.936873
C	4.854415	-3.117658	-0.326681
C	3.151490	-3.411600	1.263016
C	3.495448	-3.590482	-0.135287
C	6.566509	0.600323	0.082150
C	6.221276	0.780393	1.480358
C	5.980679	-0.530620	2.054417
C	4.500849	1.887529	-2.536824
C	5.619587	1.046273	-2.152899
C	3.267431	2.533708	2.472950
C	4.385945	1.690818	2.856414
C	4.966047	-0.703844	3.000676
C	2.765926	-1.465046	3.312486
C	4.108645	-1.873711	2.940958
C	-2.379658	1.840470	-3.233381
C	-2.413353	0.482944	-3.679590
C	-3.021434	-0.521639	-2.840896
C	-3.352908	-1.854803	-3.288812
C	-3.407080	-2.913926	-2.334909
C	-3.127325	-2.625035	-0.946474
C	-2.618553	-3.592610	-0.007408
C	-2.640974	-3.293545	1.390710
C	-3.181375	-2.032959	1.835878
C	-3.513447	-1.736544	3.210842
C	-3.490530	-0.380980	3.652811
C	-3.136539	0.658582	2.712392
C	-2.552367	1.921970	3.089042
C	-2.503031	2.985450	2.134788
C	-3.030610	2.773491	0.810189
C	-3.275445	3.833653	-0.141781
C	-3.240681	3.536261	-1.536095
C	-2.965376	2.182561	-1.960033
C	-3.175752	1.143638	-1.031404
C	-3.200153	-0.221035	-1.475457
C	-3.257511	-1.290204	-0.512094
C	-3.287812	-0.991994	0.892314
C	-3.264385	0.376841	1.338083
C	-3.209292	1.443733	0.377584
C	-3.566168	4.565504	-2.448833
C	-3.899653	5.849059	-2.043615
C	-3.935928	6.144842	-0.654166
C	-3.635649	5.141599	0.254832
C	-1.646732	0.135492	-4.818438
C	-0.846331	1.043436	-5.489129
C	-0.808258	2.392744	-5.041730
C	-1.574220	2.759559	-3.949399
C	-3.823779	-4.190906	-2.775131
C	-4.161268	-4.455686	-4.093776
C	-4.103620	-3.401188	-5.044988
C	-3.714939	-2.138113	-4.625707
C	-1.939504	-4.156560	2.269113
C	-1.228269	-5.259630	1.829895
C	-1.213130	-5.560642	0.440633
C	-1.903677	-4.739243	-0.432434
C	-3.904633	-0.100610	4.974786
C	-4.316802	-1.088860	5.856443
C	-4.340381	-2.439422	5.415512
C	-3.950736	-2.729554	4.116681
C	-1.735208	4.132327	2.455446
C	-1.017183	4.251845	3.632160
C	-1.065571	3.193667	4.580553
C	-1.829569	2.075242	4.298291
H	-3.600046	4.329108	-3.507663
H	-3.724810	5.357100	1.314915
H	-1.595642	-0.906075	-5.114703
H	-1.473180	3.769834	-3.569002
H	-3.928177	-4.984020	-2.041676
H	-3.735463	-1.323453	-5.342530
H	-1.876936	-3.891583	3.318597
H	-1.808863	-4.930409	-1.495465
H	-3.946163	0.934800	5.297720
H	-4.028997	-3.754312	3.767389
H	-1.617223	4.906440	1.705778
H	-1.792140	1.242076	4.991059
C	-0.121524	5.442643	3.860769
H	-0.373866	5.961308	4.795492
H	0.927842	5.128085	3.946916
H	-0.199421	6.156595	3.034608
C	-0.232001	3.252132	5.835810
H	0.836820	3.324759	5.592216
H	-0.480063	4.136048	6.438835
H	-0.384109	2.358599	6.449754

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C      -4.771887       -0.730142        7.249465
H      -5.812272       -1.039259        7.420215
H      -4.164232       -1.242132        8.008259
H      -4.700392        0.348877        7.420189
C      -4.820598       -3.537414        6.332126
H      -4.204926       -3.592570        7.240471
H      -5.852577       -3.357285        6.663523
H      -4.784308       -4.510141        5.831046
C      -0.414582       -6.080431        2.797967
H      -0.711945       -7.137526        2.773554
H       0.652467       -6.045812        2.538541
H      -0.530574       -5.710324        3.821763
C      -0.382979       -6.703865       -0.086538
H       0.679256       -6.561497        0.155934
H      -0.684394       -7.658641        0.365131
H      -0.478715       -6.788126       -1.173756
C      -4.623143       -5.832342       -4.503904
H      -5.631951       -5.799722       -4.937383
H      -3.964868       -6.258271       -5.273777
H      -4.636874       -6.513252       -3.646743
C      -4.499690       -3.642682       -6.480639
H      -3.858878       -4.405324       -6.944412
H      -5.531044       -4.014462       -6.551605
H      -4.422578       -2.723040       -7.069568
C       0.043034        0.588886       -6.618398
H      -0.159037        1.152478       -7.539336
H       1.100793        0.755288       -6.371926
H      -0.097667       -0.476905       -6.824696
C       0.118049        3.387716       -5.693340
H       1.162853        3.056452       -5.616426
H      -0.101536        3.496573       -6.764130
H       0.034473        4.370849       -5.219202
C      -4.258212        6.903760       -3.060940
H      -5.269542        7.296237       -2.887509
H      -3.574369        7.761624       -2.999150
H      -4.213373        6.499983       -4.077553
C      -4.334895        7.517822       -0.171951
H      -3.647281        8.286262       -0.551421
H      -5.337393        7.789254       -0.529904
H      -4.334089        7.564462        0.921846

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CN substited_heterodimers
C      -0.155790       -0.547146        0.444767
C       0.453917       -1.307205        1.512359
C       1.067718       -2.528823        1.227790
C       0.473031       -2.303274       -1.159943
C      -0.154579       -1.033074       -0.862312
C       1.073880       -0.369360        2.429159
C       2.338181       -2.859145        1.845399
C       1.121980       -2.182597       -2.452644
C       0.090096       -0.130968       -1.968799
C       0.077432        0.856157        0.698813
C       2.359570       -2.794203       -2.665944
C       2.989225       -3.554523       -1.601177
C       2.299332       -0.685611        3.020297
C       3.138696       -3.567330        0.863650
C       2.943114       -1.953025        2.721812
C       0.883201       -0.840021       -2.952294
C       0.316842        1.227233       -1.724145
C       0.309377        1.728420       -0.363943
C       0.834304        0.971118        1.927541
C       1.352131        1.933353       -2.453415
C       1.333339        2.747669       -0.249601
C       1.826233        1.950217        2.036052
C       1.886542       -0.161446       -3.650299
C       4.373375       -1.720055        2.651881
C       1.981124        2.873548       -1.541427
C       2.079702        2.854488        0.928150
C       3.098767        1.622671        2.651072
C       4.139191        2.324479        1.922604
C       6.185533       -1.698257        0.977588
C       3.509513        3.085211        0.858679
C       4.136941        3.200414       -0.385260
C       5.419613        2.560296       -0.612214
C       3.360252        3.091440       -1.606161
C       3.169727       -0.800866       -3.876199
C       6.416322       -0.341750        1.222166
C       2.125075        1.247952       -3.396533
C       3.556604        1.479128       -3.465064
C       5.613477        0.365520        2.202526
C       6.200272       -2.202528       -0.382620
C       6.444677       -1.332366       -1.447994
C       5.372416        1.706298        1.701916
C       6.025524        1.827344        0.411767
C       4.162090        2.382415       -2.587192
C       5.435473        2.055459       -1.972526
C       6.671332        0.562117        0.115394
C       4.201044        0.213322       -3.762867
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C	5.667059	-1.442565	-2.668278
C	6.685255	0.075726	-1.194809
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C	6.055750	0.836202	-2.258363
C	5.144424	-2.400309	1.705252
C	4.515743	-3.339237	0.794474
C	5.167875	-3.216479	-0.496181
C	3.330382	0.329617	3.132236
C	4.612402	-0.310769	2.904953
C	1.079077	-3.035686	-0.132227
C	2.361498	-3.675945	-0.357801
C	4.419780	-3.322974	-1.671736
C	3.401253	-2.091683	-3.392959
C	4.673919	-2.419335	-2.778231
C	-1.913034	3.477922	1.765089
C	-2.085076	3.824093	0.385585
C	-2.815911	2.931793	-0.478438
C	-3.289410	3.286453	-1.796251
C	-3.479286	2.252863	-2.766850
C	-3.205038	0.884733	-2.396527
C	-2.849998	-0.152065	-3.332221
C	-2.910612	-1.520911	-2.915576
C	-3.337621	-1.831623	-1.574395
C	-3.734674	-3.148837	-1.134169
C	-3.608355	-3.484018	0.250256
C	-3.076389	-2.498518	1.164214
C	-2.385454	-2.820702	2.386653
C	-2.142769	-1.787160	3.347754
C	-2.613833	-0.451010	3.082890
C	-2.709048	0.587537	4.082566
C	-2.654010	1.955865	3.670288
C	-2.497389	2.259665	2.266613
C	-2.845213	1.264019	1.334080
C	-2.993226	1.600793	-0.052737
C	-3.195348	0.563211	-1.025723
C	-3.271416	-0.808062	-0.610831
C	-3.137499	-1.145171	0.780115
C	-2.912763	-0.111905	1.749616
C	-2.854305	2.964899	4.633780
C	-3.082003	2.664820	5.973377
C	-3.135615	1.299309	6.384949
C	-2.959962	0.294725	5.438289
C	-1.358322	4.918186	-0.133905
C	-0.474462	5.650791	0.646720
C	-0.291270	5.295742	2.016565
C	-1.008653	4.230894	2.545024
C	-4.030127	2.589151	-4.020374
C	-4.376611	3.897621	-4.341486
C	-4.191840	4.928238	-3.371266
C	-3.665807	4.604778	-2.124548
C	-2.354424	-2.510322	-3.755007
C	-1.747122	-2.191348	-4.962606
C	-1.690972	-0.827376	-5.379635
C	-2.242493	0.155508	-4.568723
C	-4.095871	-4.728112	0.696931
C	-4.674375	-5.644682	-0.176381
C	-4.796374	-5.312175	-1.558834
C	-4.337099	-4.077076	-2.006737
C	-1.264598	-2.051529	4.421988
C	-0.630265	-3.277712	4.567331
C	-0.881073	-4.311976	3.615476
C	-1.748127	-4.069612	2.558974
H	-2.881054	4.003155	4.325984
H	-3.069284	-0.736033	5.752964
H	-1.407746	5.144326	-1.191032
H	-0.791923	3.925569	3.560475
H	-4.239428	1.808279	-4.741410
H	-3.593368	5.385356	-1.376945
H	-2.311834	-3.538424	-3.419101
H	-2.108779	1.189500	-4.859488
H	-4.066509	-4.967342	1.753165
H	-4.496604	-3.812749	-3.045089
H	-0.997024	-1.256306	5.105459
H	-1.853626	-4.836777	1.803054
C	-3.300276	3.728948	6.902594
N	-3.473587	4.610759	7.639472
C	-3.409418	0.942923	7.741965
N	-3.629428	0.627993	8.838786
C	0.322722	-3.451814	5.617975
N	1.103416	-3.565392	6.471312
C	-0.192580	-5.562499	3.682565
N	0.366239	-6.581100	3.709933
C	-5.172251	-6.882693	0.336209
N	-5.568427	-7.882475	0.776788
C	-5.420067	-6.205184	-2.484646
N	-5.922209	-6.914291	-3.256406
C	-1.115832	-3.224290	-5.721919
N	-0.597166	-4.078023	-6.315819
C	-1.000494	-0.444647	-6.570824
N	-0.432042	-0.108902	-7.527226

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C      -4.952044        4.176550       -5.620022
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N      -4.880821        7.382850       -3.836103
C       0.303276        6.684662        0.039715
N       0.935387        7.511684       -0.477051
C       0.678612        5.957185        2.831204
N       1.472401        6.468729        3.508591

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F substited_heterodimers
C      -3.395853       -3.474137       -1.380258
C      -3.400296       -2.692601       -2.577816
C      -3.069001       -1.288255       -2.501643
C      -2.551556       -0.520759       -3.608046
C      -2.555221        0.909669       -3.530957
C      -3.072093        1.551102       -2.346920
C      -3.409797        2.954169       -2.268893
C      -3.404044        3.600608       -0.993629
C      -3.052683        2.834454        0.180980
C      -2.510650        3.410023        1.386337
C      -2.473902        2.623942        2.583775
C      -2.994989        1.279146        2.562932
C      -3.302893        0.513400        3.749878
C      -3.312569       -0.914327        3.671860
C      -3.010636       -1.550898        2.409899
C      -2.490559       -2.890681        2.288499
C      -2.517074       -3.541743        1.012122
C      -3.051892       -2.838646       -0.127460
C      -3.172977       -1.437546       -0.044992
C      -3.182205       -0.651245       -1.250699
C      -3.181565        0.781505       -1.172727
C      -3.168463        1.432452        0.110932
C      -3.145637        0.648067        1.313416
C      -3.153514       -0.788238        1.235347
C      -1.848992       -4.783345        0.868118
C      -1.185261       -5.357895        1.925826
C      -1.152069       -4.714315        3.176899
C      -1.789171       -3.508940        3.353734
C      -3.830831       -3.293118       -3.784440
C      -4.225682       -4.612256       -3.815284
C      -4.225887       -5.380004       -2.636259
C      -3.828590       -4.819596       -1.442321
C      -1.875992        1.647884       -4.531296
C      -1.219243        1.010059       -5.557144
C      -1.212944       -0.395291       -5.631194
C      -1.865511       -1.143373       -4.679756
C      -3.842519        4.942802       -0.906830
C      -4.250333        5.626963       -2.030701
C      -4.253866        4.991388       -3.285888
C      -3.850674        3.679289       -3.400810
C      -1.764035        3.122283        3.704420
C      -1.126012        4.339067        3.654272
C      -1.166177        5.113718        2.479958
C      -1.840344        4.658749        1.371696
C      -3.719298       -1.657698        4.804660
C      -4.081313       -1.024145        5.972825
C      -4.071036        0.380595        6.050117
C      -3.699625        1.133546        4.958083
H      -1.768179       -5.263613       -0.098480
H      -1.665634       -3.007125        4.304928
H      -3.910669       -2.712697       -4.695679
H      -3.909850       -5.419217       -0.543854
H      -1.779722        2.723918       -4.461523
H      -1.762710       -2.220158       -4.725538
H      -3.920169        5.440899        0.052008
H      -3.934104        3.200234       -4.368873
H      -1.635698        2.519635        4.594540
H      -1.765071        5.240191        0.461914
H      -3.807817       -2.736387        4.758768
H      -3.774035        2.211782        5.030615
C       1.482183        3.126149       -0.218504
C       2.853235        3.507839       -0.498380
C       3.815370        3.448082        0.514806
C       2.122134        2.636300        2.116862
C       1.125980        2.696037        1.064018
C       3.181387        3.057287       -1.839286
C       5.141771        2.935765        0.225805
C       1.847773        1.463075        2.929033
C       0.242357        1.558954        1.225466
C       0.963821        2.437660       -1.388343
C       2.904394        0.703467        3.441361
C       4.275732        1.087962        3.160768
C       4.459565        2.563130       -2.116205
C       5.589919        2.174916        1.377527
C       5.458241        2.502287       -1.064792
C       0.682865        0.798386        2.378325
C      -0.239578        0.893131        0.100083
C       0.116128        1.340674       -1.229656
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C	2.013505	2.395819	-2.390716
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C	2.166187	1.263699	-3.198629
C	0.614062	-0.598296	2.364264
C	6.234140	1.290296	-1.253358
C	0.006609	-1.001356	-1.254664
C	1.275249	0.128540	-3.037162
C	3.492851	0.750985	-3.484634
C	3.421432	-0.699312	-3.500884
C	6.594539	-0.892136	-0.160287
C	2.050515	-1.085284	-3.225287
C	1.786920	-2.215052	-2.442992
C	2.883607	-3.000081	-1.906586
C	0.738449	-2.174850	-1.439971
C	1.707758	-1.387001	2.898716
C	6.093580	-1.554858	-1.284473
C	0.108028	-1.284894	1.192415
C	0.873805	-2.499287	1.005544
C	5.646021	-0.793625	-2.435943
C	6.222346	-1.337456	1.169883
C	5.363681	-2.429125	1.326755
C	4.477971	-1.456631	-2.985570
C	4.204150	-2.627959	-2.174085
C	1.185661	-2.934941	-0.286051
C	2.511176	-3.444961	-0.574914
C	5.202509	-2.688591	-1.122025
C	1.867186	-2.562793	2.059206
C	4.313801	-2.388840	2.327738
C	4.843790	-3.117092	0.159161
C	3.145789	-3.053778	1.779233
C	3.473011	-3.503306	0.438932
C	6.665686	0.557311	-0.144381
C	6.337357	1.007778	1.195675
C	6.063178	-0.163126	2.007741
C	4.618074	1.388979	-2.954121
C	5.715068	0.602257	-2.421058
C	3.443281	3.003641	1.845282
C	4.540041	2.215994	2.378649
C	5.051525	-0.124017	2.971483
C	2.833288	-0.746469	3.425760
C	4.160612	-1.257703	3.134917
F	-4.694224	6.895451	-1.932103
F	-4.700877	5.663636	-4.364853
F	-0.405597	4.774186	4.706515
F	-0.482124	6.273499	2.432181
F	-4.474397	0.981705	7.186831
F	-4.494328	-1.740781	7.036763
F	-0.439973	-5.261838	4.181113
F	-0.502918	-6.507625	1.757932
F	-4.662834	-6.653986	-2.678669
F	-4.660627	-5.166792	-4.963838
F	-0.523609	1.721026	-6.466136
F	-0.510464	-1.000277	-6.609003

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F24 substited_heterodimers

C	5.382089	1.124628	2.800770
C	5.702448	-0.235655	2.774795
C	4.040128	1.547920	3.155772
C	5.868532	2.005289	1.754836
C	4.692611	-1.225977	3.101944
C	6.520216	-0.767852	1.700676
C	3.697179	2.690059	2.328988
C	3.067922	0.594181	3.472007
C	4.826729	2.972663	1.462573
C	6.656444	1.492417	0.720534
C	3.400028	-0.819299	3.444916
C	4.886643	-2.369381	2.229626
C	6.988713	0.079959	0.692961
C	6.016245	-2.086379	1.363675
C	2.393144	2.839869	1.848195
C	1.716034	0.746758	2.971529
C	4.610669	3.391119	0.146326
C	6.432070	1.927116	-0.645784
C	2.252459	-1.542017	2.928973
C	3.781261	-3.065668	1.731614
C	6.970525	-0.358081	-0.690403
C	5.998803	-2.508281	0.031386
C	1.387451	1.846969	2.173888
C	2.168695	3.275121	0.480396
C	1.212434	-0.573079	2.635965
C	5.428819	2.858303	-0.927434
C	3.257104	3.544774	-0.354763
C	6.626958	0.783649	-1.517832
C	2.439749	-2.643997	2.087824
C	3.763110	-3.504044	0.347414
C	6.484501	-1.627783	-1.015001
C	4.850990	-3.229591	-0.486663

C	0.546354	1.669158	1.006875
C	1.023625	2.552716	-0.039168
C	0.407938	-0.741748	1.508784
C	4.581475	2.682429	-2.092463
C	3.239182	3.106687	-1.738784
C	5.810704	0.613747	-2.639651
C	1.594443	-2.819536	0.920674
C	2.410314	-3.353884	-0.154498
C	5.637235	-1.804654	-2.179802
C	4.627490	-2.795141	-1.853202
C	0.077600	0.397948	0.680638
C	1.007521	2.130082	-1.371811
C	0.599475	-1.883513	0.637607
C	4.769127	1.581005	-2.932717
C	2.133521	2.413557	-2.240192
C	5.306146	-0.704731	-2.976275
C	2.194484	-2.935768	-1.471950
C	3.324035	-2.650304	-2.336897
C	0.061061	-0.038256	-0.697555
C	0.512612	0.809702	-1.707017
C	0.379976	-1.449032	-0.726664
C	3.621435	0.859740	-3.451642
C	2.328453	1.268785	-3.113273
C	3.953139	-0.552903	-3.478292
C	1.154710	-1.966666	-1.764975
C	2.980881	-1.507446	-3.164422
C	1.322865	0.276965	-2.783902
C	1.640033	-1.084463	-2.811067
C	-2.846029	0.346500	1.387861
C	-2.861775	1.363531	0.382369
C	-2.836344	-1.037215	1.010502
C	-2.724087	0.699832	2.743409
C	-2.861617	0.998871	-1.004182
C	-2.756823	2.716714	0.747364
C	-2.838797	-1.400756	-0.372206
C	-2.713232	-2.029508	1.998500
C	-2.131267	1.981574	3.036755
C	-3.140822	-0.288458	3.713625
C	-2.848110	-0.380617	-1.380753
C	-2.751892	1.997948	-1.986767
C	-2.148607	3.006415	2.022984
C	-3.196594	3.689599	-0.228160
C	-2.714571	-2.750063	-0.745837
C	-3.138137	-1.674263	3.334143
C	-2.109176	-3.279655	1.604752
C	-1.335718	2.192186	4.185308
C	-3.695392	0.064160	4.960969
C	-2.724270	-0.738961	-2.734625
C	-3.192393	3.324914	-1.617320
C	-2.140675	1.622048	-3.237829
C	-1.371682	4.168477	2.234775
C	-3.769071	4.923744	0.140122
C	-2.106918	-3.643694	0.210436
C	-3.137911	-3.096998	-2.084383
C	-3.692071	-2.615458	4.225556
C	-1.313843	-4.037372	2.493668
C	-0.615352	3.358831	4.375605
F	-1.132388	1.208634	5.082720
C	-4.190572	-0.889820	5.837192
F	-3.844141	1.356519	5.310212
C	-2.127793	0.231762	-3.618319
C	-3.140467	-2.076296	-3.094850
C	-3.760709	4.218535	-2.547495
C	-1.358035	2.528039	-3.989714
C	-0.634363	4.357574	3.391080
F	-1.206644	5.084718	1.261590
C	-4.281297	5.802390	-0.802585
F	-3.917040	5.255791	1.437165
C	-1.306227	-4.735808	-0.193389
C	-3.689346	-4.355261	-2.400164
C	-4.189263	-2.243779	5.465492
F	-3.837747	-3.905034	3.865345
C	-0.572758	-5.126827	2.069283
F	-1.128004	-3.646514	3.769630
F	0.178432	3.504515	5.442720
F	-4.727945	-0.529366	7.008749
C	-1.332074	-0.150742	-4.721736
C	-3.693718	-2.381176	-4.355153
C	-4.276972	5.446128	-2.160686
F	-3.901375	3.870700	-3.841288
C	-0.618894	2.123131	-5.087746
F	-1.191322	3.803478	-3.590714
F	0.136315	5.441227	3.540269
F	-4.836978	6.960886	-0.427576
C	-0.567868	-5.479054	0.711742
F	-1.120503	-5.020506	-1.496979
C	-4.186322	-4.640092	-3.663150
F	-3.831634	-5.303307	-1.454213
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F	0.216311	-5.790712	2.922125

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C      -0.605496        0.769821       -5.456977
F      -1.134350       -1.448517       -5.022245
C      -4.188347       -3.642550       -4.651025
F      -3.842707       -1.426456       -5.293475
F      -4.828656        6.270559       -3.059284
F       0.155427        2.991565       -5.748474
F       0.223450       -6.474026        0.294485
F      -4.721265       -5.836635       -3.934114
F       0.188476        0.370796       -6.457176
F      -4.725405       -3.903104       -5.848922

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H substited_heterodimers
C      -3.753046       -2.758992       -2.529246
C      -3.760085       -1.603107       -3.372942
C      -3.413838       -0.317586       -2.807255
C      -2.911032        0.796205       -3.576331
C      -2.918008        2.107609       -2.997284
C      -3.424024        2.284122       -1.656682
C      -3.783472        3.564112       -1.085821
C      -3.778561        3.716577        0.336884
C      -3.409355        2.587963        1.163778
C      -2.881905        2.702908        2.501682
C      -2.848294        1.542771        3.343591
C      -3.359162        0.289484        2.840982
C      -3.686611       -0.846096        3.675990
C      -3.693356       -2.154691        3.097161
C      -3.367948       -2.304412        1.695378
C      -2.854232       -3.520248        1.110672
C      -2.873361       -3.676316       -0.314759
C      -3.395576       -2.609576       -1.134410
C      -3.508096       -1.327787       -0.561785
C      -3.516110       -0.165068       -1.411422
C      -3.518744        1.147721       -0.831014
C      -3.509819        1.301290        0.600478
C      -3.491283        0.141544        1.447791
C      -3.495780       -1.174477        0.866050
C      -2.217885       -4.800462       -0.879818
C      -1.582722       -5.741577       -0.092036
C      -1.558038       -5.584744        1.305978
C      -2.174009       -4.492909        1.888133
C      -4.220164       -1.738722       -4.705419
C      -4.639714       -2.959760       -5.204884
C      -4.635727       -4.094987       -4.375129
C      -4.210584       -3.988690       -3.061860
C      -2.262301        3.156831       -3.690412
C      -1.633230        2.941454       -4.902329
C      -1.624117        1.653850       -5.469381
C      -2.245859        0.607280       -4.814344
C      -4.248552        4.932392        0.889754
C      -4.686825        5.970823        0.085789
C      -4.689795        5.821732       -1.312402
C      -4.255660        4.636334       -1.881073
C      -2.158208        1.623997        4.580209
C      -1.544646        2.791996        4.992140
C      -1.583322        3.932694        4.169297
C      -2.230293        3.881187        2.949094
C      -4.130701       -3.243933        3.888998
C      -4.525090       -3.069485        5.204590
C      -4.517223       -1.783812        5.773969
C      -4.116147       -0.696178        5.016921
H      -2.149509       -4.881802       -1.957711
H      -2.074797       -4.336891        2.955530
H      -4.294358       -0.853331       -5.326620
H      -4.279208       -4.850202       -2.407451
H      -2.189543        4.131384       -3.222712
H      -2.162339       -0.394095       -5.219533
H      -4.316790        5.026166        1.967636
H      -4.328790        4.500020       -2.954116
H      -2.051510        0.728865        5.181164
H      -2.174694        4.735450        2.285414
H      -4.208054       -4.224993        3.434135
H      -4.182780        0.300847        5.437286
C       1.114026        2.974819        0.943815
C       2.481659        3.442601        0.822035
C       3.447769        3.028318        1.744952
C       1.764899        1.675858        2.940486
C       0.764837        2.105741        1.982235
C       2.809563        3.511895       -0.590945
C       4.776957        2.665921        1.289633
C       1.501274        0.286018        3.272131
C      -0.111410        0.981947        1.721542
C       0.596767        2.754777       -0.395773
C       2.564780       -0.598975        3.476054
C       3.932520       -0.128019        3.354033
C       4.091199        3.162967       -1.028220
C       5.233887        1.542234        2.086778
C       5.093175        2.732756       -0.070424
C       0.339073       -0.142076        2.518414
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C	-0.590071	0.765582	0.430822
C	-0.241385	1.667681	-0.646009
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C	-0.079447	0.880276	-1.852897
C	1.803397	2.325967	-2.507863
C	0.279595	-1.438633	1.998970
C	5.877441	1.677616	-0.685641
C	-0.334782	-0.506386	-1.519557
C	0.921198	1.203286	-2.769806
C	3.133446	1.962801	-2.959917
C	3.072639	0.616590	-3.501514
C	6.257079	-0.750023	-0.458967
C	1.705002	0.146861	-3.384796
C	1.451769	-1.191753	-3.066070
C	2.556262	-2.108724	-2.850756
C	0.405448	-1.526687	-2.117695
C	1.381840	-2.357597	2.210440
C	5.757713	-0.963608	-1.747155
C	-0.225452	-1.657960	0.658019
C	0.550315	-2.714170	0.043222
C	5.301485	0.160104	-2.544067
C	5.891887	-1.650532	0.618974
C	5.041174	-2.731298	0.368846
C	4.136847	-0.267532	-3.297076
C	3.873858	-1.655612	-2.966028
C	0.861829	-2.649375	-1.317895
C	2.190490	-3.009444	-1.771443
C	4.875432	-2.086002	-2.007506
C	1.547744	-3.146725	1.001380
C	3.993728	-3.065412	1.316049
C	4.523133	-2.952997	-0.968988
C	2.829017	-3.495232	0.563527
C	3.156043	-3.425445	-0.848535
C	6.317612	0.595510	0.081809
C	5.989755	0.526422	1.494033
C	5.726528	-0.861497	1.825847
C	4.256158	2.374178	-2.235019
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C	4.186581	1.209178	3.034564
C	4.716564	-1.182571	2.737717
C	2.504083	-1.944944	2.935308
C	3.834325	-2.305344	2.478784
H	-4.877934	-3.920861	5.780651
H	-4.863825	-1.634988	6.793222
H	-1.015233	-6.292908	1.926297
H	-1.058298	-6.571089	-0.558720
H	-5.009634	-3.028829	-6.224480
H	-5.003427	-5.046915	-4.749036
H	-1.090654	1.469031	-6.397911
H	-1.106402	3.757438	-5.389727
H	-5.070013	6.618213	-1.946594
H	-5.065348	6.883086	0.539262
H	-1.062201	4.838863	4.466118
H	-0.993298	2.811228	5.928378

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NH2 substited_heterodimers

C	1.866208	-1.078937	3.001267
C	3.279775	-0.877559	3.252526
C	4.223900	-1.742146	2.685949
C	2.423858	-3.032995	1.595361
C	1.447740	-2.134174	2.182441
C	3.531813	0.553013	3.285989
C	5.452345	-1.207948	2.127492
C	1.968664	-3.377775	0.258213
C	0.395965	-1.925577	1.209178
C	1.243879	0.229175	2.877681
C	2.894644	-3.517383	-0.782033
C	4.308487	-3.313056	-0.524847
C	4.718204	1.065218	2.748644
C	5.777010	-1.975331	0.939590
C	5.695817	0.168467	2.159908
C	0.712080	-2.694505	0.023260
C	-0.184537	-0.665089	1.082262
C	0.240443	0.428817	1.929729
C	2.273578	1.237761	3.055718
C	-0.466962	-0.127627	-0.226306
C	0.211232	1.642346	1.139409
C	2.246338	2.411132	2.290235
C	0.427905	-2.173269	-1.243964
C	6.271164	0.830180	1.003404
C	-0.234258	1.297994	-0.192841
C	1.188819	2.621698	1.318947
C	3.476823	2.939796	1.731340
C	3.178063	3.478507	0.414980
C	6.286594	0.630288	-1.455956
C	1.763845	3.282719	0.160442

C	1.327485	2.947912	-1.127572
C	2.288298	2.801516	-2.206148
C	0.299214	1.942466	-1.309993
C	1.385448	-2.317653	-2.323015
C	5.687399	1.887910	-1.577020
C	-0.179213	-0.865614	-1.368759
C	0.383071	-0.204051	-2.527902
C	5.362517	2.654273	-0.387733
C	5.848853	-0.465556	-2.300921
C	4.829084	-0.264358	-3.236209
C	4.105048	3.339252	-0.624345
C	3.651881	2.993795	-1.958426
C	0.619122	1.174511	-2.498172
C	1.850192	1.704733	-3.051935
C	4.628841	2.097359	-2.548101
C	1.357016	-1.098634	-3.115950
C	3.799669	-1.271415	-3.418139
C	4.207083	1.041391	-3.362748
C	2.541679	-0.588161	-3.659732
C	2.793070	0.842014	-3.624383
C	6.583972	0.091532	-0.141736
C	6.332155	-1.337317	-0.174664
C	5.877868	-1.681195	-1.508991
C	4.690438	2.280716	1.957695
C	5.650789	2.136231	0.878443
C	3.787873	-2.838273	1.841750
C	4.747553	-2.982325	0.760970
C	4.884037	-2.650156	-1.681463
C	2.597424	-2.978201	-2.097478
C	3.827355	-2.443312	-2.653394
C	-2.270658	2.411646	2.886133
C	-2.374133	3.292900	1.762452
C	-3.051427	2.837049	0.571758
C	-3.429695	3.703818	-0.519726
C	-3.502579	3.159816	-1.838241
C	-3.228014	1.757958	-2.038496
C	-2.733842	1.203988	-3.273833
C	-2.759102	-0.213264	-3.462011
C	-3.283916	-1.058499	-2.420276
C	-3.601719	-2.455991	-2.602402
C	-3.546930	-3.328403	-1.473882
C	-3.165143	-2.794054	-0.186999
C	-2.526827	-3.574864	0.845787
C	-2.409499	-3.027772	2.162723
C	-2.932966	-1.714540	2.437465
C	-3.083845	-1.177279	3.768148
C	-3.048918	0.236767	3.960610
C	-2.855813	1.094810	2.813108
C	-3.144645	0.568489	1.535245
C	-3.231785	1.446934	0.403667
C	-3.336476	0.897554	-0.924662
C	-3.370059	-0.523146	-1.116154
C	-3.301805	-1.404908	0.019890
C	-3.183428	-0.858407	1.342295
C	-3.266769	0.743011	5.258934
C	-3.493088	-0.077418	6.358939
C	-3.565286	-1.486977	6.158337
C	-3.362396	-1.995689	4.884656
C	-1.621593	4.488115	1.777529
C	-0.752801	4.818780	2.808871
C	-0.609131	3.912647	3.901878
C	-1.382000	2.766156	3.928733
C	-3.949108	4.000077	-2.881671
C	-4.287881	5.329788	-2.682910
C	-4.182472	5.882945	-1.372504
C	-3.785867	5.054881	-0.328397
C	-2.036796	-0.747731	-4.556321
C	-1.326696	0.036529	-5.449937
C	-1.344588	1.451905	-5.292199
C	-2.030936	1.992583	-4.212378
C	-3.960078	-4.666874	-1.649100
C	-4.369917	-5.174324	-2.873310
C	-4.379158	-4.315154	-4.010602
C	-4.025671	-2.981080	-3.840906
C	-1.543069	-3.676632	3.075072
C	-0.815222	-4.808772	2.751429
C	-0.983135	-5.391678	1.461900
C	-1.819463	-4.761567	0.549966
H	-3.277599	1.818265	5.408904
H	-3.476823	-3.065421	4.732530
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H	-1.194489	2.050205	4.721891
H	-4.092012	3.574929	-3.871190
H	-3.770802	5.464958	0.676815
H	-1.937671	-1.825075	-4.641413
H	-1.949517	3.061403	-4.046753
H	-4.011532	-5.317027	-0.780167
H	-4.099568	-2.315665	-4.695948
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N       0.328703        4.198920        4.922105
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N      -0.032543        6.014046        2.770458
H       0.738039        6.103715        3.413654
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N      -4.437244        7.238889       -1.142575
H      -4.932472        7.743003       -1.860944
H      -4.758302        7.463642       -0.212003
N      -4.710788        6.153145       -3.755018
H      -4.837500        5.617532       -4.606349
H      -5.577861        6.644150       -3.555405
N      -0.678664        2.285971       -6.195325
H      -0.343495        3.153890       -5.801619
H       0.000887        1.849988       -6.799011
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H       0.390535       -0.207043       -6.508360
H      -0.547797       -1.551262       -6.421307
N      -4.702638       -4.805876       -5.281567
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N       0.102164       -5.383571        3.663333
H       1.020530       -5.517032        3.247134
H       0.216030       -4.800128        4.484833
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N      -3.611810        0.473439        7.640087
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H      -3.989319       -0.120789        8.361273


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OCH3 substited_heterodimers
C      -0.358951       -2.052073       -1.156239
C       0.309915       -3.318652       -1.372452
C       1.011991       -3.543127       -2.560559
C       0.416573       -1.288264       -3.368487
C      -0.309598       -1.056474       -2.135589
C       0.870520       -3.752496       -0.103552
C       2.302776       -4.205483       -2.525971
C       1.064808       -0.044499       -3.749165
C      -0.104725        0.326167       -1.753961
C      -0.208733       -1.702428        0.240520
C       2.339694       -0.068286       -4.323654
C       3.014472       -1.335745       -4.537448
C       2.114508       -4.390901       -0.071173
C       3.154403       -3.581170       -3.521970
C       2.843619       -4.621775       -1.305536
C       0.739225        0.955123       -2.749546
C       0.051398        0.656379       -0.409758
C      -0.000334       -0.373492        0.603123
C       0.543872       -2.751642        0.895591
C       1.029780        1.639252       -0.001703
C       0.948189       -0.034304        1.639554
C       1.471466       -2.425695        1.891827
C       1.696148        1.897664       -2.359821
C       4.256372       -4.427732       -1.034594
C       1.588122        1.211095        1.266275
C       1.674188       -1.041346        2.273100
C       2.761599       -3.087997        1.923640
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C       6.072444       -2.851104       -1.589690
C       3.084592       -0.846537        2.544967
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C       6.211036       -2.512096       -0.240749
C       1.841539        2.249446       -0.959652
C       3.253495        2.440294       -0.686723
C       5.360121       -3.136463        0.755576
C       6.125758       -1.817128       -2.606950
C       6.315964       -0.482518       -2.237382
C       5.033377       -2.136074        1.755006
C       5.681157       -0.894067        1.376568
C       3.794847        2.026922        0.535704
C       5.083066        1.360524        0.567546
C       6.409014       -1.126372        0.142850
C       3.981722        2.206458       -1.920212
C       5.552646        0.566755       -2.886902
C       6.459853       -0.130641       -0.836812
C       5.224537        1.566855       -1.887720
C       5.785537        1.136030       -0.620700
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C	5.077095	-3.827138	-1.994275
C	4.515460	-3.395652	-3.261063
C	5.163265	-2.153630	-3.639885
C	3.077335	-4.053044	0.962053
C	4.400684	-4.075964	0.366114
C	1.065918	-2.509012	-3.577483
C	2.390098	-2.532135	-4.171572
C	4.426749	-1.142986	-4.264629
C	3.335245	0.907214	-3.917822
C	4.625483	0.242839	-3.882236
C	-1.193312	4.100111	-0.532897
C	-1.818783	3.519393	-1.679519
C	-2.771436	2.452100	-1.500103
C	-3.676478	1.995463	-2.529779
C	-4.181242	0.663213	-2.476870
C	-3.759269	-0.203515	-1.399352
C	-3.732425	-1.642718	-1.484140
C	-3.558346	-2.413154	-0.294725
C	-3.464530	-1.738310	0.976705
C	-3.613237	-2.395848	2.255782
C	-3.002548	-1.818313	3.406853
C	-2.235778	-0.601785	3.262836
C	-1.161204	-0.220196	4.143602
C	-0.623686	1.101447	4.066583
C	-1.201657	2.047812	3.143290
C	-0.966372	3.472246	3.193862
C	-1.132022	4.251744	2.011769
C	-1.499290	3.588737	0.779937
C	-2.111928	2.319753	0.871813
C	-2.756190	1.749393	-0.276967
C	-3.251595	0.399537	-0.229344
C	-3.115869	-0.372849	0.972951
C	-2.483567	0.203012	2.129956
C	-1.971033	1.542411	2.075211
C	-1.005351	5.658766	2.096529
C	-0.687683	6.299310	3.286421
C	-0.531493	5.519983	4.469842
C	-0.683536	4.149264	4.404017
C	-1.357769	3.885694	-2.969347
C	-0.326595	4.791754	-3.155103
C	0.296118	5.371767	-2.011833
C	-0.136306	5.019292	-0.751866
C	-5.141486	0.255641	-3.433515
C	-5.583995	1.104471	-4.438777
C	-5.090288	2.441278	-4.482072
C	-4.172555	2.856161	-3.537955
C	-3.284242	-3.799764	-0.411783
C	-3.193851	-4.431713	-1.641538
C	-3.394441	-3.667851	-2.827881
C	-3.648500	-2.317327	-2.728755
C	-3.253016	-2.413705	4.665711
C	-4.032962	-3.544254	4.807800
C	-4.627424	-4.134064	3.654431
C	-4.423288	-3.545889	2.413959
C	0.581425	1.392081	4.754231
C	1.249789	0.436881	5.501729
C	0.701413	-0.876293	5.596644
C	-0.467065	-1.173931	4.930491
H	-1.199478	6.246281	1.210037
H	-0.617810	3.596147	5.333918
H	-1.773908	3.377420	-3.826939
H	0.428780	5.411207	0.084388
H	-5.565055	-0.735472	-3.347428
H	-3.864627	3.895074	-3.565020
H	-3.054562	-4.353995	0.487131
H	-3.695233	-1.760046	-3.656079
H	-2.860212	-1.962618	5.569605
H	-4.926125	-3.942194	1.542182
H	1.030905	2.364494	4.614887
H	-0.795304	-2.205286	4.957877
O	-4.193736	-4.091858	6.060355
O	-5.387760	-5.249961	3.869235
O	-2.881701	-5.749836	-1.817138
O	-3.332403	-4.249207	-4.075442
O	-6.489070	0.760129	-5.402135
O	-5.482771	3.327556	-5.460883
O	0.183298	5.150650	-4.368910
O	1.326834	6.276987	-2.136590
O	-0.524790	7.648643	3.421307
O	-0.204249	6.093474	5.678530
O	2.437903	0.641247	6.139065
O	1.316453	-1.856917	6.341232
C	-5.506872	-3.910509	6.626596
H	-5.727531	-2.838446	6.735189
H	-6.276153	-4.387712	6.007429
H	-5.477741	-4.383048	7.612514
C	2.499183	-2.409272	5.728864
H	2.240639	-2.898848	4.779828
H	3.252667	-1.633489	5.548932
H	2.887433	-3.149355	6.434260

C	3.043173	1.932493	5.997802
H	3.970896	1.887697	6.572491
H	3.263208	2.147259	4.942724
H	2.388645	2.718215	6.399441
C	-1.260067	6.870413	6.279535
H	-1.542389	7.716941	5.642528
H	-2.137861	6.234625	6.466502
H	-0.860625	7.236950	7.229445
C	-0.637861	8.445345	2.236008
H	-1.650673	8.382393	1.813837
H	-0.427310	9.470676	2.548373
H	0.090123	8.124980	1.478009
C	2.585017	5.686225	-2.525123
H	2.932324	4.991809	-1.747909
H	2.495986	5.156264	-3.480721
H	3.290980	6.515611	-2.624556
C	-0.376112	4.518604	-5.526637
H	0.162182	4.936674	-6.380118
H	-0.231344	3.429828	-5.485964
H	-1.449190	4.737963	-5.614016
C	-6.840881	3.795687	-5.335377
H	-7.554280	2.965669	-5.399186
H	-6.970983	4.327535	-4.381428
H	-6.999629	4.486890	-6.168033
C	-6.976370	-0.586968	-5.393231
H	-7.531653	-0.799064	-4.468661
H	-7.642989	-0.665429	-6.255019
H	-6.149030	-1.303501	-5.489968
C	-1.991229	-4.553166	-4.513352
H	-1.402393	-3.629580	-4.601743
H	-1.494755	-5.240375	-3.818213
H	-2.092662	-5.025006	-5.494908
C	-2.553589	-6.505542	-0.647118
H	-2.314203	-7.510935	-1.000730
H	-1.687239	-6.070309	-0.129634
H	-3.405730	-6.546149	0.046734
C	-5.982891	-5.867257	2.724920
H	-6.511346	-6.745758	3.102272
H	-6.690179	-5.186730	2.230023
H	-5.214019	-6.174077	2.001030

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OH substited_heterodimers

C	-3.433002	3.663975	-0.733730
C	-3.404137	3.672957	0.694512
C	-3.066935	2.459150	1.401255
C	-2.502594	2.429053	2.729593
C	-2.484615	1.193433	3.451859
C	-3.025436	0.005790	2.840290
C	-3.330667	-1.206530	3.562164
C	-3.346573	-2.452246	2.862798
C	-3.035128	-2.464250	1.449681
C	-2.503150	-3.610784	0.753277
C	-2.494537	-3.613871	-0.679027
C	-3.029842	-2.485278	-1.396944
C	-3.335582	-2.499685	-2.811720
C	-3.332013	-1.265577	-3.531376
C	-3.038433	-0.037624	-2.829038
C	-2.514233	1.145941	-3.461120
C	-2.555343	2.396573	-2.764815
C	-3.103815	2.439507	-1.431141
C	-3.224238	1.225183	-0.723870
C	-3.205973	1.235596	0.714780
C	-3.177407	-0.003317	1.439298
C	-3.178327	-1.256804	0.733477
C	-3.185208	-1.267972	-0.701111
C	-3.198506	-0.024648	-1.428619
C	-1.872176	3.505982	-3.320935
C	-1.159554	3.410767	-4.499572
C	-1.110949	2.167647	-5.179054
C	-1.778449	1.074155	-4.671172
C	-3.799520	4.852260	1.367759
C	-4.195063	5.981024	0.676939
C	-4.231887	5.973365	-0.739327
C	-3.862268	4.824639	-1.415716
C	-1.740150	1.130210	4.656106
C	-1.037936	2.216550	5.132376
C	-1.060329	3.444253	4.425648
C	-1.783329	3.531386	3.252140
C	-3.760647	-3.615222	3.551781
C	-4.126186	-3.583363	4.885361
C	-4.101929	-2.347265	5.577299
C	-3.720747	-1.192601	4.922410
C	-1.788242	-4.648111	-1.342583
C	-1.126219	-5.636986	-0.647381
C	-1.139979	-5.642690	0.769208
C	-1.818370	-4.644265	1.438825
C	-3.723703	-1.277895	-4.890970
C	-4.088403	-2.447487	-5.528926

C	-4.092448	-3.673327	-4.819102	C	1.702335	-2.458077	2.115952
C	-3.731358	-3.678781	-3.483743	C	0.030347	-1.534970	0.759709
H	-1.811218	4.439265	-2.775757	C	-0.145126	1.285117	0.434321
H	-1.649614	0.113956	-5.161418	C	3.056737	-2.799825	2.160159
H	-3.842831	4.860286	2.453254	C	4.003114	-1.926548	2.831184
H	-3.953677	4.819602	-2.495539	C	2.666045	3.215437	1.467483
H	-1.628865	0.178254	5.166298	C	4.337366	0.474165	3.295875
H	-1.695273	4.445884	2.678857	C	3.706976	2.644858	2.304490
H	-3.851692	-4.557591	3.024896	C	0.947771	-2.646943	0.890523
H	-3.780750	-0.245083	5.451145	C	-0.223602	-0.990692	-0.497539
H	-1.688892	-4.621976	-2.422858	C	-0.308900	0.442667	-0.661981
H	-1.732194	-4.622250	2.517679	C	0.613412	2.509719	0.297005
H	-3.796480	-0.339174	-5.433541	C	0.407060	-1.540508	-1.677509
H	-3.815523	-4.612150	-2.939407	C	0.262862	0.787314	-1.942536
O	-0.371749	-6.624954	-1.245604	C	1.179587	2.841605	-0.938502
O	-0.441626	-6.575918	1.485823	C	1.568681	-3.178624	-0.243614
O	-4.486259	-4.843431	-5.412557	C	4.940340	2.635398	1.540756
O	-4.508027	-2.510287	-6.843854	C	0.713612	-0.439069	-2.571391
O	-0.317341	2.129791	-6.308579	C	0.997287	1.965756	-2.081563
O	-0.461619	4.497491	-4.950256	C	2.527995	3.373545	-0.993814
O	-4.659873	7.062190	-1.449767	C	3.178176	2.826662	-2.171649
O	-4.614518	7.147553	1.284448	C	6.483500	1.021623	0.489193
O	-0.326745	4.521623	4.843331	C	2.231214	1.956524	-2.844715
O	-0.232240	2.181652	6.253407	C	2.672878	0.774302	-3.448823
O	-4.521263	-2.384152	6.893117	C	4.078398	0.417243	-3.398465
O	-4.543121	-4.736144	5.494239	C	1.897609	-0.447060	-3.312938
H	-4.765757	-4.648598	-6.317917	C	2.975316	-3.530855	-0.196840
H	-0.375711	-6.490860	-2.201227	C	6.215266	1.563680	-0.770942
H	0.023734	-7.153230	0.864630	C	1.292488	-2.614799	-1.553596
H	-4.806296	-4.526625	6.401069	C	2.527482	-2.619103	-2.315916
H	-4.539136	-1.485417	7.243384	C	5.288939	2.673037	-0.902011
H	-0.119237	1.264674	6.532051	C	6.577143	-0.417308	0.655175
H	0.199888	4.252815	5.609318	C	6.399623	-1.260921	-0.444945
H	-4.551933	7.044906	2.241782	C	4.532825	2.483396	-2.126639
H	-4.901858	7.759944	-0.825079	C	4.991263	1.256451	-2.751653
H	0.047097	4.233475	-5.729625	C	2.824273	-1.556986	-3.178054
H	-0.217087	1.213302	-6.593288	C	4.172106	-1.021946	-3.231373
H	-4.566095	-1.615169	-7.199222	C	6.031435	0.688343	-1.913844
C	0.126101	0.723931	1.740254	C	3.567991	-3.185539	-1.477200
C	1.062587	1.596613	2.414574	C	5.624068	-2.480368	-0.307890
C	2.061701	1.051244	3.226042	C	6.122000	-0.697590	-1.753583
C	1.244012	-1.228642	2.741321	C	4.867184	-2.670632	-1.531487
C	0.210739	-0.660392	1.900704	C	5.174502	-1.568454	-2.424189
C	1.368164	2.701074	1.522142	C	5.834335	1.567547	1.666996
C	3.410914	1.583996	3.166247	C	5.526553	0.466326	2.560131

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C       5.984938       -0.760140        1.935197
C       3.257049        3.557411        0.185889
C       4.662931        3.199072        0.231824
C       2.154548       -0.388015        3.392081
C       3.561593       -0.744602        3.433990
C       5.237269       -1.933902        2.067637
C       3.705533       -3.346284        0.982380
C       5.052731       -2.810003        0.924881

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SCH3 substited_heterodimers
C       0.483909       -3.535272        5.308233
C       0.484403       -3.995827        3.987924
C      -0.709303       -3.863178        3.173348
C      -1.858968       -3.274482        3.709285
C      -1.859701       -2.797499        5.078995
C      -0.709941       -2.925808        5.864087
C      -2.639617       -2.345376        2.912372
C      -2.240904       -2.038285        1.609970
C      -1.045112       -2.647493        1.057331
C      -0.295650       -3.546741        1.819424
C      -2.311474       -0.668936        1.134290
C      -1.151718       -0.434196        0.301841
C      -0.374147       -1.653664        0.250131
C      -0.508175        0.800852        0.333382
C      -0.994995        1.856457        1.193043
C      -2.109366        1.632989        2.004945
C      -2.779711        0.345599        1.976311
C       0.156233        2.573827        1.707791
C       1.351423        1.962951        1.153968
C       0.936385        0.866328        0.306650
C       1.018896       -1.592016        0.220888
C       1.687052       -0.306984        0.251187
C       2.881716       -0.437236        1.056270
C       3.283200        0.614290        1.884178
C       2.505438        1.838673        1.933391
C      -2.106602        2.106630        3.375836
C      -0.995801        2.791997        3.877115
C       0.156123        3.033228        3.027315
C       1.351292        2.900963        3.841008
C       2.503148        2.314699        3.304914
C      -2.776315        1.114300        4.195504
C      -3.192032        0.024781        3.330621
C      -3.125101       -1.295546        3.789385
C       2.951877       -1.807831        1.528731
C       1.799850       -2.523740        1.007362
C       1.154219       -3.483966        1.794979
C       0.936603        2.578850        5.193851
C      -0.513420        2.513195        5.215735
C      -1.158630        1.557680        6.006367
C      -2.310703        0.844761        5.486349
C      -2.640898       -1.574585        5.128908
C      -2.242379       -0.524985        5.961730
C       3.762658        0.333736        3.223346
C       3.281768        1.384513        4.102064
C       2.881870        1.075718        5.405703
C       1.687556        1.684409        5.962099
C       1.017892        0.691763        6.782064
C      -0.378426        0.629098        6.803599
C      -1.047910       -0.658106        6.775437
C       1.636581       -3.759670        3.136622
C       3.415283       -2.076716        2.819226
C       2.745822       -3.071144        3.637997
C       3.829367       -0.985926        3.682455
C      -0.296299       -1.835461        6.727983
C       1.635618       -2.821206        5.828049
C       2.744665       -2.592931        5.008484
C       3.414106       -1.305020        5.035508
C       2.950659       -0.293602        5.882049
C       1.798525       -0.530912        6.732424
C       1.153645       -1.770884        6.706259
C       0.815162        1.290120       -2.703517
C      -0.539739        1.750703       -2.540996
C      -0.782369        3.102171       -2.209931
C       0.265394        4.060299       -2.479293
C       1.609325        3.603131       -2.614668
C       1.883895        2.187889       -2.509035
C      -1.625168        0.811964       -2.570966
C      -2.927324        1.230405       -2.233689
C      -3.070158        2.463485       -1.500635
C      -2.008683        3.420771       -1.523822
C      -2.135439        4.563387       -0.693963
C      -3.218948        4.766848        0.141530
C      -4.243161        3.778095        0.211269
C      -4.150666        2.663974       -0.611011
C       1.078595       -0.104706       -2.911850
C      -0.010213       -1.042902       -2.940785
C      -1.360882       -0.588230       -2.771780
C      -2.412590       -1.523022       -2.656667
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C	-3.766253	-1.033889	-2.777146
C	-4.028471	0.350134	-2.555714
C	0.267209	-2.423174	-2.992336
C	-0.723184	-3.326458	-2.460007
C	-2.074233	-2.883636	-2.319593
C	-5.341613	0.836073	-2.739397
C	-6.397249	0.005853	-3.100444
C	-6.127134	-1.369465	-3.362847
C	-4.837300	-1.851850	-3.203998
C	2.410344	-0.572847	-2.959736
C	2.640297	-1.906280	-3.466103
C	1.564086	-2.839225	-3.469998
C	-2.981250	-3.740510	-1.647356
C	-2.605176	-4.961487	-1.114182
C	-1.246909	-5.381622	-1.220702
C	-0.346851	-4.563381	-1.887709
C	3.163935	1.640356	-2.132850
C	3.441601	0.264413	-2.397858
C	1.785184	-4.120076	-4.023154
C	3.017148	-4.517582	-4.523136
C	4.096903	-3.577815	-4.526535
C	3.874852	-2.302474	-4.026299
C	4.652678	-0.268975	-1.891696
C	5.549611	0.475432	-1.146970
C	5.244253	1.832386	-0.838300
C	4.071274	2.379738	-1.338854
C	0.004819	5.429661	-2.714402
C	1.007008	6.340429	-3.011120
C	2.357113	5.890474	-3.100407
C	2.620710	4.535164	-2.935434
S	-3.281489	6.267536	1.126039
S	-5.547946	4.001902	1.399475
S	7.055482	-0.317491	-0.573666
S	6.352128	2.721105	0.233785
S	3.311676	-6.142715	-5.190988
S	5.659128	-4.083610	-5.214957
S	-3.849271	-5.966736	-0.297879
S	-0.771388	-6.905673	-0.434559
S	-8.073268	0.580447	-3.270171
S	-7.411623	-2.504390	-3.894806
S	3.623248	7.094597	-3.438086
S	0.559274	8.059753	-3.263184
H	3.622167	4.157260	-3.085672
H	-1.019986	5.782595	-2.710118
H	4.856842	-1.325397	-2.006088
H	3.788728	3.384366	-1.060541
H	0.942480	-4.794749	-4.079731
H	4.657075	-1.560248	-4.101132
H	-3.993815	-3.405194	-1.462648
H	0.699374	-4.829463	-1.914776
H	-5.505819	1.897962	-2.620705
H	-4.643183	-2.886440	-3.462720
H	-1.325315	5.279430	-0.643383
H	-4.883999	1.875326	-0.527680
C	-7.916283	2.371444	-2.921729
C	-7.582028	-2.013890	-5.665296
C	-3.477458	-5.632406	1.477402
C	1.057190	-6.837205	-0.520764
C	1.669450	-6.938193	-5.076924
C	6.769648	-2.700282	-4.765759
C	6.583320	-0.757962	1.153684
C	5.387521	4.227429	0.628493
C	5.131689	6.062513	-3.554050
C	0.658293	8.172609	-5.102328
C	-2.613158	5.649097	2.727629
C	-6.369616	2.363719	1.385734
H	7.466362	-1.226951	1.598810
H	6.319502	0.141652	1.713971
H	5.750038	-1.464565	1.146236
H	5.987946	4.771510	1.362953
H	5.241249	4.855059	-0.256216
H	4.420346	3.960890	1.065613
H	0.423505	9.211516	-5.354744
H	1.667129	7.929099	-5.445830
H	-0.079029	7.505122	-5.557093
H	5.945350	6.763681	-3.759996
H	5.329386	5.542319	-2.611553
H	5.055474	5.339087	-4.371795
H	-2.649907	6.495405	3.420970
H	-3.231824	4.832191	3.106127
H	-1.579280	5.318229	2.599322
H	-7.126457	2.413533	2.173636
H	-6.858524	2.164560	0.426921
H	-5.650742	1.570404	1.613505
H	-8.929555	2.772732	-3.012961
H	-7.545738	2.546029	-1.906755
H	-7.261514	2.861581	-3.648929
H	-8.378359	-2.641036	-6.078463
H	-7.864815	-0.960829	-5.742776
H	-6.645665	-2.204976	-6.197065

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H       7.768623       -3.023810       -5.071319
H       6.502728       -1.786536       -5.305475
H       6.752232       -2.524535       -3.686030
H       1.810040       -7.945527       -5.478477
H       1.332197       -7.002492       -4.037967
H       0.931462       -6.401278       -5.680473
H      -4.135798       -6.292394        2.050990
H      -2.434686       -5.870623        1.698871
H      -3.694217       -4.590058        1.721304
H       1.405454       -7.716896        0.027772
H       1.413211       -6.890334       -1.554363
H       1.433201       -5.928920       -0.039473

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SH substited_heterodimers
C       3.172809       -0.451604        5.174392
C       2.639245        0.682695        5.793413
C       1.448330        0.567645        6.615382
C       0.836116       -0.676626        6.789389
C       1.390741       -1.854055        6.147283
C       2.537031       -1.743792        5.355154
C       0.636749        1.751059        6.397509
C      -0.756922        1.646873        6.361441
C      -1.391906        0.354391        6.541460
C      -0.610748       -0.785319        6.751843
C      -2.542509        0.292999        5.659260
C      -2.869678       -0.905656        5.018933
C      -2.057876       -2.089341        5.236674
C      -0.949828       -2.030183        6.087326
C       0.287114       -2.690300        5.713847
C       0.370438       -3.387238        4.504779
C      -0.780512       -3.449608        3.622655
C      -1.972309       -2.812388        3.981842
C      -2.732547       -2.075633        2.987525
C      -2.270978       -2.003020        1.670927
C      -1.030523       -2.661094        1.300723
C      -0.300851       -3.374770        2.254686
C       1.146177       -3.266744        2.291113
C       1.811813       -2.449487        1.370777
C       1.052627       -1.708627        0.384027
C      -0.339591       -1.811991        0.354349
C      -2.345695       -0.746693        0.947323
C      -1.148220       -0.630789        0.142828
C      -0.535860        0.609679       -0.018524
C       0.905168        0.719302        0.010401
C       1.686712       -0.417441        0.208536
C       1.560954       -3.272983        3.682327
C       2.839660       -0.355447        1.081837
C       2.917831       -1.611972        1.803881
C       2.624177       -2.466532        4.099567
C       3.315657       -1.620518        3.143516
C      -2.880831        0.390257        1.562652
C      -3.360037        0.313116        2.929678
C      -3.286601       -0.896439        3.628544
C       3.170813        0.844696        1.717159
C       3.583328        0.834113        3.107949
C       3.655074       -0.375206        3.807707
C       1.246809        1.968282        0.656433
C       2.358883        2.029271        1.500618
C      -2.244506        1.682441        1.384488
C      -1.092943        1.788363        0.603542
C       0.009345        2.629261        1.028483
C       2.269943        2.750611        2.756424
C       1.076757        3.387349        3.116180
C      -0.075156        3.329339        2.234239
C      -2.331368        2.406177        2.638825
C      -1.267232        3.212512        3.055971
C      -3.019926        1.558445        3.595024
C       3.027073        2.011831        3.750348
C      -2.619115        1.548366        4.934354
C      -1.514842        2.384642        5.367455
C      -0.851001        3.200263        4.445788
C       0.596373        3.308001        4.483308
C       1.325799        2.596705        5.440393
C       2.563858        1.937220        5.067493
C       0.971944        0.951649       -2.994520
C       2.046766        1.855387       -2.873386
C       3.306039        1.348292       -2.386568
C       3.561118       -0.058647       -2.431051
C       2.541961       -0.946401       -2.931971
C       1.220418       -0.461436       -3.013047
C       0.119381       -1.386301       -2.972615
C       0.372211       -2.767109       -2.853980
C       1.681287       -3.250024       -3.228300
C       2.774769       -2.332792       -3.264080
C      -1.230457       -0.897447       -2.925895
C      -2.298281       -1.797477       -2.740560
C      -1.996485       -3.102334       -2.206276
C      -0.653647       -3.591319       -2.263419
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C	-1.480743	0.519206	-2.916244
C	-2.793472	0.990931	-2.715271
C	-3.886935	0.085018	-2.982375
C	-3.638372	-1.320480	-2.996395
C	-4.693104	-2.190577	-3.338952
C	-5.971090	-1.728973	-3.633328
C	-6.212647	-0.328148	-3.643508
C	-5.173973	0.540980	-3.334611
C	-0.334351	-4.769193	-1.552283
C	-1.271517	-5.465956	-0.803442
C	-2.600254	-4.966892	-0.725982
C	-2.931291	-3.812377	-1.419225
C	4.021338	-2.796742	-3.734775
C	4.231245	-4.117080	-4.111349
C	3.147030	-5.034686	-4.055209
C	1.899361	-4.579248	-3.645714
C	4.217175	2.176332	-1.694257
C	5.354242	1.679780	-1.073770
C	5.602873	0.280669	-1.108876
C	4.713237	-0.548227	-1.773775
C	-0.381884	1.442400	-2.941062
C	-0.615216	2.820065	-2.758970
C	0.450918	3.736703	-3.095490
C	1.792332	3.250892	-3.149704
C	0.201514	5.075441	-3.460432
C	1.218310	5.946984	-3.832899
C	2.551282	5.459019	-3.906033
C	2.805410	4.131649	-3.582980
C	-2.961584	2.304250	-2.146658
C	-1.863181	3.220568	-2.157796
C	-4.096805	2.633205	-1.370731
C	-4.187476	3.807918	-0.640887
C	-3.101856	4.726270	-0.665186
C	-1.971579	4.411710	-1.404878
S	-5.684061	4.082820	0.302186
S	-3.194312	6.223172	0.303853
S	-7.301215	-2.853227	-4.026439
S	-7.811377	0.392847	-4.003189
S	-0.825436	-6.928930	0.117178
S	-3.887309	-5.746273	0.243492
S	5.886957	-4.577860	-4.613441
S	3.405767	-6.734608	-4.539169
S	6.467542	2.748220	-0.177408
S	7.015588	-0.485304	-0.320330
S	0.878201	7.651580	-4.246881
S	3.950525	6.475934	-4.367409
H	-4.885720	1.899799	-1.258031
H	-1.110924	5.066455	-1.343881
H	-4.489043	-3.253743	-3.398768
H	-5.347029	1.608110	-3.417943
H	0.697969	-5.096171	-1.526305
H	-3.916784	-3.389347	-1.265738
H	4.831656	-2.087463	-3.859364
H	1.054442	-5.258179	-3.673749
H	3.985694	3.229009	-1.589218
H	4.860024	-1.618431	-1.697092
H	-0.824919	5.424419	-3.477740
H	3.809443	3.746314	-3.721852
H	3.338753	7.174586	-5.350152
H	5.695220	3.849764	-0.277396
H	6.971406	0.227175	0.828247
H	5.538872	-5.372032	-5.650840
H	2.103176	-7.082246	-4.487853
H	0.501253	-6.817853	-0.101299
H	-3.131142	-6.026528	1.329024
H	-6.531981	-3.961354	-4.048402
H	-8.145425	-0.431060	-5.021894
H	-5.088862	4.548127	1.423868
H	-1.901034	6.566760	0.131623
H	-0.464478	7.520777	-4.240774

Optimized structure for monomers, homodimers, and heterodimers for c-HBC with different bowl depth, as shown in Figure 6.

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cf0, c-HBC_monomer with bowl depth: 0.00

C	0.000000	1.286711	3.663591
C	0.000000	2.529267	2.946321
C	0.000000	2.545652	1.469931
C	0.000000	3.815788	0.717379
C	0.000000	3.815788	-0.717379
C	0.000000	2.545652	-1.469931
C	0.000000	2.529267	-2.946321
C	0.000000	1.286711	-3.663591
C	0.000000	0.000000	-2.939776
C	0.000000	-1.286711	-3.663591
C	0.000000	-2.529267	-2.946321
C	0.000000	-2.545652	-1.469931

C	0.000000	-3.815788	-0.717379
C	0.000000	-3.815788	0.717379
C	0.000000	-2.545652	1.469931
C	0.000000	-2.529267	2.946321
C	0.000000	-1.286711	3.663591
C	0.000000	0.000000	2.939776
C	0.000000	0.000000	1.491907
C	0.000000	1.291875	0.745960
C	0.000000	1.291875	-0.745960
C	0.000000	0.000000	-1.491907
C	0.000000	-1.291875	-0.745960
C	0.000000	-1.291875	0.745960
C	0.000000	-1.428620	5.090061
C	0.000000	-2.576524	5.841540
C	0.000000	-3.770468	5.152301
C	0.000000	-3.693653	3.782439
C	0.000000	3.693653	3.782439
C	0.000000	3.770468	5.152301
C	0.000000	2.576524	5.841540
C	0.000000	1.428620	5.090061
C	0.000000	5.122138	-1.307584
C	0.000000	6.346950	-0.689314
C	0.000000	6.346950	0.689314
C	0.000000	5.122138	1.307584
C	0.000000	1.428620	-5.090061
C	0.000000	2.576524	-5.841540
C	0.000000	3.770468	-5.152301
C	0.000000	3.693653	-3.782439
C	0.000000	-3.693653	-3.782439
C	0.000000	-3.770468	-5.152301
C	0.000000	-2.576524	-5.841540
C	0.000000	-1.428620	-5.090061
C	0.000000	-5.122138	1.307584
C	0.000000	-6.346950	0.689314
C	0.000000	-6.346950	-0.689314
C	0.000000	-5.122138	-1.307584
H	0.000000	-0.608006	5.742349
H	0.000000	-2.507847	6.926079
H	0.000000	-4.743987	5.635229
H	0.000000	-4.668578	3.397371
H	0.000000	4.668578	3.397371
H	0.000000	4.743987	5.635229
H	0.000000	2.507847	6.926079
H	0.000000	0.608006	5.742349
H	0.000000	5.276702	-2.344489
H	0.000000	7.251868	-1.291014
H	0.000000	7.251868	1.291014
H	0.000000	5.276702	2.344489
H	0.000000	0.608006	-5.742349
H	0.000000	2.507847	-6.926079
H	0.000000	4.743987	-5.635229
H	0.000000	4.668578	-3.397371
H	0.000000	-4.668578	-3.397371
H	0.000000	-4.743987	-5.635229
H	0.000000	-2.507847	-6.926079
H	0.000000	-0.608006	-5.742349
H	0.000000	-5.276702	2.344489
H	0.000000	-7.251868	1.291014
H	0.000000	-7.251868	-1.291014
H	0.000000	-5.276702	-2.344489

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cf1, c-HBC_monomer with bowl depth: 0.10

C	0.044317	3.812762	0.717191
C	0.044317	3.812762	-0.717191
C	0.000000	2.543960	-1.469049
C	-0.044317	2.527769	-2.944025
C	-0.044317	1.285508	-3.661130
C	0.000000	0.000000	-2.937894
C	0.044317	-1.285508	-3.661130
C	0.044317	-2.527769	-2.944025
C	0.000000	-2.543960	-1.469049
C	-0.044317	-3.812762	-0.717191
C	-0.044317	-3.812762	0.717191
C	0.000000	-2.543960	1.469049
C	0.044317	-2.527769	2.944025
C	0.044317	-1.285508	3.661130
C	0.000000	0.000000	2.937894
C	-0.044317	1.285508	3.661130
C	-0.044317	2.527769	2.944025
C	0.000000	2.543960	1.469049
C	0.000000	1.290885	0.745455
C	0.000000	1.290885	-0.745455
C	0.000000	0.000000	-1.491036
C	0.000000	-1.290885	-0.745455
C	0.000000	-1.290885	0.745455
C	0.000000	0.000000	1.491036
C	-0.097238	3.692412	3.777614

C	-0.142885	3.767538	5.146909
C	-0.142885	2.573063	5.836438
C	-0.097238	1.425002	5.086435
C	0.097238	5.116866	-1.308871
C	0.142885	6.340437	-0.689624
C	0.142885	6.340437	0.689624
C	0.097238	5.116866	1.308871
C	-0.097238	1.425002	-5.086435
C	-0.142885	2.573063	-5.836438
C	-0.142885	3.767538	-5.146909
C	-0.097238	3.692412	-3.777614
C	0.097238	-3.692412	-3.777614
C	0.142885	-3.767538	-5.146909
C	0.142885	-2.573063	-5.836438
C	0.097238	-1.425002	-5.086435
C	-0.097238	-5.116866	1.308871
C	-0.142885	-6.340437	0.689624
C	-0.142885	-6.340437	-0.689624
C	-0.097238	-5.116866	-1.308871
C	0.097238	-1.425002	5.086435
C	0.142885	-2.573063	5.836438
C	0.142885	-3.767538	5.146909
C	0.097238	-3.692412	3.777614
H	-0.105484	4.666300	3.388263
H	-0.181387	4.740352	5.629678
H	-0.181387	2.504433	6.920279
H	-0.105484	0.600947	5.735235
H	0.105484	5.266523	-2.346995
H	0.181387	7.244810	-1.290914
H	0.181387	7.244810	1.290914
H	0.105484	5.266523	2.346995
H	-0.105484	0.600947	-5.735235
H	-0.181387	2.504433	-6.920279
H	-0.181387	4.740352	-5.629678
H	-0.105484	4.666300	-3.388263
H	0.105484	-4.666300	-3.388263
H	0.181387	-4.740352	-5.629678
H	0.181387	-2.504433	-6.920279
H	0.105484	-0.600947	-5.735235
H	-0.105484	-5.266523	2.346995
H	-0.181387	-7.244810	1.290914
H	-0.181387	-7.244810	-1.290914
H	-0.105484	-5.266523	-2.346995
H	0.105484	-0.600947	5.735235
H	0.181387	-2.504433	6.920279
H	0.181387	-4.740352	5.629678
H	0.105484	-4.666300	3.388263

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cf2, c-HBC_monomer with bowl depth: 0.19

C	0.088046	3.804764	0.716832
C	0.088046	3.804764	-0.716832
C	0.000000	2.539183	-1.466095
C	-0.088046	2.523187	-2.936748
C	-0.088046	1.281740	-3.653706
C	0.000000	0.000000	-2.932316
C	0.088046	-1.281740	-3.653706
C	0.088046	-2.523187	-2.936748
C	0.000000	-2.539183	-1.466095
C	-0.088046	-3.804764	-0.716832
C	-0.088046	-3.804764	0.716832
C	0.000000	-2.539183	1.466095
C	0.088046	-2.523187	2.936748
C	0.088046	-1.281740	3.653706
C	0.000000	0.000000	2.932316
C	-0.088046	1.281740	3.653706
C	-0.088046	2.523187	2.936748
C	0.000000	2.539183	1.466095
C	0.000000	1.287984	0.743711
C	0.000000	1.287984	-0.743711
C	0.000000	0.000000	-1.487627
C	0.000000	-1.287984	-0.743711
C	0.000000	-1.287984	0.743711
C	0.000000	0.000000	1.487627
C	-0.194476	3.688687	3.761851
C	-0.285142	3.759350	5.129406
C	-0.285142	2.563659	5.820088
C	-0.194476	1.414202	5.075651
C	0.194476	5.102401	-1.313098
C	0.285142	6.322043	-0.690405
C	0.285142	6.322043	0.690405
C	0.194476	5.102401	1.313098
C	-0.194476	1.414202	-5.075651
C	-0.285142	2.563659	-5.820088
C	-0.285142	3.759350	-5.129406
C	-0.194476	3.688687	-3.761851
C	0.194476	-3.688687	-3.761851
C	0.285142	-3.759350	-5.129406

C	0.285142	-2.563659	-5.820088
C	0.194476	-1.414202	-5.075651
C	-0.194476	-5.102401	1.313098
C	-0.285142	-6.322043	0.690405
C	-0.285142	-6.322043	-0.690405
C	-0.194476	-5.102401	-1.313098
C	0.194476	-1.414202	5.075651
C	0.285142	-2.563659	5.820088
C	0.285142	-3.759350	5.129406
C	0.194476	-3.688687	3.761851
H	-0.210967	4.659095	3.359605
H	-0.363000	4.729704	5.612263
H	-0.363000	2.497286	6.901899
H	-0.210967	0.581194	5.715738
H	0.210967	5.240562	-2.354562
H	0.363000	7.225508	-1.289164
H	0.363000	7.225508	1.289164
H	0.210967	5.240562	2.354562
H	-0.210967	0.581194	-5.715738
H	-0.363000	2.497286	-6.901899
H	-0.363000	4.729704	-5.612263
H	-0.210967	4.659095	-3.359605
H	0.210967	-4.659095	-3.359605
H	0.363000	-4.729704	-5.612263
H	0.363000	-2.497286	-6.901899
H	0.210967	-0.581194	-5.715738
H	-0.210967	-5.240562	2.354562
H	-0.363000	-7.225508	1.289164
H	-0.363000	-7.225508	-1.289164
H	-0.210967	-5.240562	-2.354562
H	0.210967	-0.581194	5.715738
H	0.363000	-2.497286	6.901899
H	0.363000	-4.729704	5.612263
H	0.210967	-4.659095	3.359605

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cf3, c-HBC_monomer with bowl depth: 0.29

C	0.131423	3.792003	0.716393
C	0.131423	3.792003	-0.716393
C	0.000000	2.531851	-1.462011
C	-0.131423	2.516662	-2.926378
C	-0.131423	1.275907	-3.642678
C	0.000000	0.000000	-2.923844
C	0.131423	-1.275907	-3.642678
C	0.131423	-2.516662	-2.926378
C	0.000000	-2.531851	-1.462011
C	-0.131423	-3.792003	-0.716393
C	-0.131423	-3.792003	0.716393
C	0.000000	-2.531851	1.462011
C	0.131423	-2.516662	2.926378
C	0.131423	-1.275907	3.642678
C	0.000000	0.000000	2.923844
C	-0.131423	1.275907	3.642678
C	-0.131423	2.516662	2.926378
C	0.000000	2.531851	1.462011
C	0.000000	1.283720	0.741290
C	0.000000	1.283720	-0.741290
C	0.000000	0.000000	-1.482703
C	0.000000	-1.283720	-0.741290
C	0.000000	-1.283720	0.741290
C	0.000000	0.000000	1.482703
C	-0.291714	3.683373	3.738481
C	-0.429388	3.744854	5.103316
C	-0.429388	2.546770	5.795005
C	-0.291714	1.395847	5.058937
C	0.291714	5.078515	-1.320689
C	0.429388	6.291295	-0.691735
C	0.429388	6.291295	0.691735
C	0.291714	5.078515	1.320689
C	-0.291714	1.395847	-5.058937
C	-0.429388	2.546770	-5.795005
C	-0.429388	3.744854	-5.103316
C	-0.291714	3.683373	-3.738481
C	0.291714	-3.683373	-3.738481
C	0.429388	-3.744854	-5.103316
C	0.429388	-2.546770	-5.795005
C	0.291714	-1.395847	-5.058937
C	-0.291714	-5.078515	1.320689
C	-0.429388	-6.291295	0.691735
C	-0.429388	-6.291295	-0.691735
C	-0.291714	-5.078515	-1.320689
C	0.291714	-1.395847	5.058937
C	0.429388	-2.546770	5.795005
C	0.429388	-3.744854	5.103316
C	0.291714	-3.683373	3.738481
H	-0.316451	4.648962	3.317113
H	-0.548619	4.709998	5.588080
H	-0.548619	2.483352	6.873207

```
H      -0.316451        0.548514        5.684672
H       0.316451        5.196754       -2.367565
H       0.548619        7.193567       -1.285493
H       0.548619        7.193567        1.285493
H       0.316451        5.196754        2.367565
H      -0.316451        0.548514       -5.684672
H      -0.548619        2.483352       -6.873207
H      -0.548619        4.709998       -5.588080
H      -0.316451        4.648962       -3.317113
H       0.316451       -4.648962       -3.317113
H       0.548619       -4.709998       -5.588080
H       0.548619       -2.483352       -6.873207
H       0.316451       -0.548514       -5.684672
H      -0.316451       -5.196754        2.367565
H      -0.548619       -7.193567        1.285493
H      -0.548619       -7.193567       -1.285493
H      -0.316451       -5.196754       -2.367565
H       0.316451       -0.548514        5.684672
H       0.548619       -2.483352        6.873207
H       0.548619       -4.709998        5.588080
H       0.316451       -4.648962        3.317113

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cf4, c-HBC_monomer with bowl depth: 0.39

C       0.174607        3.774941        0.715820
C       0.174607        3.774941       -0.715820
C       0.000000        2.521952       -1.456200
C      -0.174607        2.507550       -2.911699
C      -0.174607        1.267834       -3.627567
C       0.000000        0.000000       -2.912336
C       0.174607       -1.267834       -3.627567
C       0.174607       -2.507550       -2.911699
C       0.000000       -2.521952       -1.456200
C      -0.174607       -3.774941       -0.715820
C      -0.174607       -3.774941        0.715820
C       0.000000       -2.521952        1.456200
C       0.174607       -2.507550        2.911699
C       0.174607       -1.267834        3.627567
C       0.000000        0.000000        2.912336
C      -0.174607        1.267834        3.627567
C      -0.174607        2.507550        2.911699
C       0.000000        2.521952        1.456200
C       0.000000        1.277889        0.737918
C       0.000000        1.277889       -0.737918
C       0.000000        0.000000       -1.476059
C       0.000000       -1.277889       -0.737918
C       0.000000       -1.277889        0.737918
C       0.000000        0.000000        1.476059
C      -0.388952        3.675877        3.704804
C      -0.574674        3.725561        5.065499
C      -0.574674        2.524451        5.759085
C      -0.388952        1.370793        5.035972
C       0.388952        5.046055       -1.330728
C       0.574674        6.249242       -0.693480
C       0.574674        6.249242        0.693480
C       0.388952        5.046055        1.330728
C      -0.388952        1.370793       -5.035972
C      -0.574674        2.524451       -5.759085
C      -0.574674        3.725561       -5.065499
C      -0.388952        3.675877       -3.704804
C       0.388952       -3.675877       -3.704804
C       0.574674       -3.725561       -5.065499
C       0.574674       -2.524451       -5.759085
C       0.388952       -1.370793       -5.035972
C      -0.388952       -5.046055        1.330728
C      -0.574674       -6.249242        0.693480
C      -0.574674       -6.249242       -0.693480
C      -0.388952       -5.046055       -1.330728
C       0.388952       -1.370793        5.035972
C       0.574674       -2.524451        5.759085
C       0.574674       -3.725561        5.065499
C       0.388952       -3.675877        3.704804
H      -0.421934        4.634461        3.258073
H      -0.736515        4.684060        5.551155
H      -0.736515        2.466274        6.832014
H      -0.421934        0.504761        5.642821
H       0.421934        5.139011       -2.384193
H       0.736515        7.149255       -1.280464
H       0.736515        7.149255        1.280464
H       0.421934        5.139011        2.384193
H      -0.421934        0.504761       -5.642821
H      -0.736515        2.466274       -6.832014
H      -0.736515        4.684060       -5.551155
H      -0.421934        4.634461       -3.258073
H       0.421934       -4.634461       -3.258073
H       0.736515       -4.684060       -5.551155
H       0.736515       -2.466274       -6.832014
H       0.421934       -0.504761       -5.642821
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H      -0.421934       -5.139011        2.384193
H      -0.736515       -7.149255        1.280464
H      -0.736515       -7.149255       -1.280464
H      -0.421934       -5.139011       -2.384193
H       0.421934       -0.504761        5.642821
H       0.736515       -2.466274        6.832014
H       0.736515       -4.684060        5.551155
H       0.421934       -4.634461        3.258073


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cf5, c-HBC_monomer with bowl depth: 0.49

C       0.217458        3.754460        0.715286
C       0.217458        3.754460       -0.715286
C       0.000000        2.510453       -1.449524
C      -0.217458        2.497371       -2.894357
C      -0.217458        1.258405       -3.609702
C       0.000000        0.000000       -2.899080
C       0.217458       -1.258405       -3.609702
C       0.217458       -2.497371       -2.894357
C       0.000000       -2.510453       -1.449524
C      -0.217458       -3.754460       -0.715286
C      -0.217458       -3.754460        0.715286
C       0.000000       -2.510453        1.449524
C       0.217458       -2.497371        2.894357
C       0.217458       -1.258405        3.609702
C       0.000000        0.000000        2.899080
C      -0.217458        1.258405        3.609702
C      -0.217458        2.497371        2.894357
C       0.000000        2.510453        1.449524
C       0.000000        1.271173        0.734062
C       0.000000        1.271173       -0.734062
C       0.000000        0.000000       -1.468337
C       0.000000       -1.271173       -0.734062
C       0.000000       -1.271173        0.734062
C       0.000000        0.000000        1.468337
C      -0.486190        3.667036        3.664552
C      -0.722272        3.701463        5.019369
C      -0.722272        2.496800        5.714969
C      -0.486190        1.340892        5.007554
C       0.486190        5.005983       -1.343055
C       0.722272        6.196448       -0.695580
C       0.722272        6.196448        0.695580
C       0.486190        5.005983        1.343055
C      -0.486190        1.340892       -5.007554
C      -0.722272        2.496800       -5.714969
C      -0.722272        3.701463       -5.019369
C      -0.486190        3.667036       -3.664552
C       0.486190       -3.667036       -3.664552
C       0.722272       -3.701463       -5.019369
C       0.722272       -2.496800       -5.714969
C       0.486190       -1.340892       -5.007554
C      -0.486190       -5.005983        1.343055
C      -0.722272       -6.196448        0.695580
C      -0.722272       -6.196448       -0.695580
C      -0.486190       -5.005983       -1.343055
C       0.486190       -1.340892        5.007554
C       0.722272       -2.496800        5.714969
C       0.722272       -3.701463        5.019369
C       0.486190       -3.667036        3.664552
H      -0.527418        4.618364        3.191393
H      -0.928725        4.650869        5.505913
H      -0.928725        2.443411        6.780448
H      -0.527418        0.455038        5.593979
H       0.527418        5.070676       -2.403483
H       0.928725        7.092618       -1.274425
H       0.928725        7.092618        1.274425
H       0.527418        5.070676        2.403483
H      -0.527418        0.455038       -5.593979
H      -0.928725        2.443411       -6.780448
H      -0.928725        4.650869       -5.505913
H      -0.527418        4.618364       -3.191393
H       0.527418       -4.618364       -3.191393
H       0.928725       -4.650869       -5.505913
H       0.928725       -2.443411       -6.780448
H       0.527418       -0.455038       -5.593979
H      -0.527418       -5.070676        2.403483
H      -0.928725       -7.092618        1.274425
H      -0.928725       -7.092618       -1.274425
H      -0.527418       -5.070676       -2.403483
H       0.527418       -0.455038        5.593979
H       0.928725       -2.443411        6.780448
H       0.928725       -4.650869        5.505913
H       0.527418       -4.618364        3.191393


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cf6, c-HBC_monomer with bowl depth: 0.58
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C	0.260015	3.733455	0.715092
C	0.260015	3.733455	-0.715092
C	0.000000	2.499105	-1.443015
C	-0.260015	2.486301	-2.876389
C	-0.260015	1.247422	-3.590816
C	0.000000	0.000000	-2.885236
C	0.260015	-1.247422	-3.590816
C	0.260015	-2.486301	-2.876389
C	0.000000	-2.499105	-1.443015
C	-0.260015	-3.733455	-0.715092
C	-0.260015	-3.733455	0.715092
C	0.000000	-2.499105	1.443015
C	0.260015	-2.486301	2.876389
C	0.260015	-1.247422	3.590816
C	0.000000	0.000000	2.885236
C	-0.260015	1.247422	3.590816
C	-0.260015	2.486301	2.876389
C	0.000000	2.499105	1.443015
C	0.000000	1.264792	0.730215
C	0.000000	1.264792	-0.730215
C	0.000000	0.000000	-1.460219
C	0.000000	-1.264792	-0.730215
C	0.000000	-1.264792	0.730215
C	0.000000	0.000000	1.460219
C	-0.583428	3.655344	3.621770
C	-0.872125	3.671540	4.968530
C	-0.872125	2.462701	5.665353
C	-0.583428	1.306031	4.975903
C	0.583428	4.962635	-1.355841
C	0.872125	6.137613	-0.697684
C	0.872125	6.137613	0.697684
C	0.583428	4.962635	1.355841
C	-0.583428	1.306031	-4.975903
C	-0.872125	2.462701	-5.665353
C	-0.872125	3.671540	-4.968530
C	-0.583428	3.655344	-3.621770
C	0.583428	-3.655344	-3.621770
C	0.872125	-3.671540	-4.968530
C	0.872125	-2.462701	-5.665353
C	0.583428	-1.306031	-4.975903
C	-0.583428	-4.962635	1.355841
C	-0.872125	-6.137613	0.697684
C	-0.872125	-6.137613	-0.697684
C	-0.583428	-4.962635	-1.355841
C	0.583428	-1.306031	4.975903
C	0.872125	-2.462701	5.665353
C	0.872125	-3.671540	4.968530
C	0.583428	-3.655344	3.621770
H	-0.632901	4.599951	3.124325
H	-1.124601	4.610131	5.454513
H	-1.124601	2.412493	6.721105
H	-0.632901	0.401276	5.542497
H	0.632901	5.001921	-2.422646
H	1.124601	7.027370	-1.268176
H	1.124601	7.027370	1.268176
H	0.632901	5.001921	2.422646
H	-0.632901	0.401276	-5.542497
H	-1.124601	2.412493	-6.721105
H	-1.124601	4.610131	-5.454513
H	-0.632901	4.599951	-3.124325
H	0.632901	-4.599951	-3.124325
H	1.124601	-4.610131	-5.454513
H	1.124601	-2.412493	-6.721105
H	0.632901	-0.401276	-5.542497
H	-0.632901	-5.001921	2.422646
H	-1.124601	-7.027370	1.268176
H	-1.124601	-7.027370	-1.268176
H	-0.632901	-5.001921	-2.422646
H	0.632901	-0.401276	5.542497
H	1.124601	-2.412493	6.721105
H	1.124601	-4.610131	5.454513
H	0.632901	-4.599951	3.124325

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cf7, c-HBC_monomer with bowl depth: 0.68

C	0.302399	3.712718	0.715184
C	0.302399	3.712718	-0.715184
C	0.000000	2.488680	-1.436815
C	-0.302399	2.475904	-2.857940
C	-0.302399	1.236993	-3.572735
C	0.000000	0.000000	-2.873399
C	0.302399	-1.236993	-3.572735
C	0.302399	-2.475904	-2.857940
C	0.000000	-2.488680	-1.436815
C	-0.302399	-3.712718	-0.715184
C	-0.302399	-3.712718	0.715184
C	0.000000	-2.488680	1.436815
C	0.302399	-2.475904	2.857940

C	0.302399	-1.236993	3.572735
C	0.000000	0.000000	2.873399
C	-0.302399	1.236993	3.572735
C	-0.302399	2.475904	2.857940
C	0.000000	2.488680	1.436815
C	0.000000	1.258800	0.726759
C	0.000000	1.258800	-0.726759
C	0.000000	0.000000	-1.453365
C	0.000000	-1.258800	-0.726759
C	0.000000	-1.258800	0.726759
C	0.000000	0.000000	1.453365
C	-0.680666	3.643188	3.575824
C	-1.021411	3.642613	4.912222
C	-1.021411	2.430751	5.611320
C	-0.680666	1.273887	4.942558
C	0.680666	4.917656	-1.367709
C	1.021411	6.075007	-0.699550
C	1.021411	6.075007	0.699550
C	0.680666	4.917656	1.367709
C	-0.680666	1.273887	-4.942558
C	-1.021411	2.430751	-5.611320
C	-1.021411	3.642613	-4.912222
C	-0.680666	3.643188	-3.575824
C	0.680666	-3.643188	-3.575824
C	1.021411	-3.642613	-4.912222
C	1.021411	-2.430751	-5.611320
C	0.680666	-1.273887	-4.942558
C	-0.680666	-4.917656	1.367709
C	-1.021411	-6.075007	0.699550
C	-1.021411	-6.075007	-0.699550
C	-0.680666	-4.917656	-1.367709
C	0.680666	-1.273887	4.942558
C	1.021411	-2.430751	5.611320
C	1.021411	-3.642613	4.912222
C	0.680666	-3.643188	3.575824
H	-0.738385	4.581226	3.056642
H	-1.318590	4.570250	5.394106
H	-1.318590	2.383365	6.655566
H	-0.738385	0.354480	5.494018
H	0.738385	4.936374	-2.439744
H	1.318590	6.955908	-1.262320
H	1.318590	6.955908	1.262320
H	0.738385	4.936374	2.439744
H	-0.738385	0.354480	-5.494018
H	-1.318590	2.383365	-6.655566
H	-1.318590	4.570250	-5.394106
H	-0.738385	4.581226	-3.056642
H	0.738385	-4.581226	-3.056642
H	1.318590	-4.570250	-5.394106
H	1.318590	-2.383365	-6.655566
H	0.738385	-0.354480	-5.494018
H	-0.738385	-4.936374	2.439744
H	-1.318590	-6.955908	1.262320
H	-1.318590	-6.955908	-1.262320
H	-0.738385	-4.936374	-2.439744
H	0.738385	-0.354480	5.494018
H	1.318590	-2.383365	6.655566
H	1.318590	-4.570250	5.394106
H	0.738385	-4.581226	3.056642

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cf8, c-HBC_monomer with bowl depth: 0.78

C	0.342601	3.693207	0.715499
C	0.342601	3.693207	-0.715499
C	0.000000	2.479858	-1.431690
C	-0.342601	2.466326	-2.840747
C	-0.342601	1.226933	-3.556147
C	0.000000	0.000000	-2.863424
C	0.342601	-1.226933	-3.556147
C	0.342601	-2.466326	-2.840747
C	0.000000	-2.479858	-1.431690
C	-0.342601	-3.693207	-0.715499
C	-0.342601	-3.693207	0.715499
C	0.000000	-2.479858	1.431690
C	0.342601	-2.466326	2.840747
C	0.342601	-1.226933	3.556147
C	0.000000	0.000000	2.863424
C	-0.342601	1.226933	3.556147
C	-0.342601	2.466326	2.840747
C	0.000000	2.479858	1.431690
C	0.000000	1.253749	0.723893
C	0.000000	1.253749	-0.723893
C	0.000000	0.000000	-1.447809
C	0.000000	-1.253749	-0.723893
C	0.000000	-1.253749	0.723893
C	0.000000	0.000000	1.447809
C	-0.777905	3.628540	3.530559
C	-1.177082	3.610388	4.852189

C	-1.177082	2.396154	5.553045
C	-0.777905	1.242804	4.907557
C	0.777905	4.871586	-1.377361
C	1.177082	6.007185	-0.701015
C	1.177082	6.007185	0.701015
C	0.777905	4.871586	1.377361
C	-0.777905	1.242804	-4.907557
C	-1.177082	2.396154	-5.553045
C	-1.177082	3.610388	-4.852189
C	-0.777905	3.628540	-3.530559
C	0.777905	-3.628540	-3.530559
C	1.177082	-3.610388	-4.852189
C	1.177082	-2.396154	-5.553045
C	0.777905	-1.242804	-4.907557
C	-0.777905	-4.871586	1.377361
C	-1.177082	-6.007185	0.701015
C	-1.177082	-6.007185	-0.701015
C	-0.777905	-4.871586	-1.377361
C	0.777905	-1.242804	4.907557
C	1.177082	-2.396154	5.553045
C	1.177082	-3.610388	4.852189
C	0.777905	-3.628540	3.530559
H	-0.843868	4.561236	2.994717
H	-1.523799	4.525678	5.324479
H	-1.523799	2.347226	6.581824
H	-0.843868	0.312211	5.446957
H	0.843868	4.873694	-2.453113
H	1.523799	6.873742	-1.257659
H	1.523799	6.873742	1.257659
H	0.843868	4.873694	2.453113
H	-0.843868	0.312211	-5.446957
H	-1.523799	2.347226	-6.581824
H	-1.523799	4.525678	-5.324479
H	-0.843868	4.561236	-2.994717
H	0.843868	-4.561236	-2.994717
H	1.523799	-4.525678	-5.324479
H	1.523799	-2.347226	-6.581824
H	0.843868	-0.312211	-5.446957
H	-0.843868	-4.873694	2.453113
H	-1.523799	-6.873742	1.257659
H	-1.523799	-6.873742	-1.257659
H	-0.843868	-4.873694	-2.453113
H	0.843868	-0.312211	5.446957
H	1.523799	-2.347226	6.581824
H	1.523799	-4.525678	5.324479
H	0.843868	-4.561236	2.994717

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cf9, c-HBC_monomer with bowl depth: 0.88

C	0.383342	3.674611	0.716164
C	0.383342	3.674611	-0.716164
C	0.000000	2.472708	-1.427494
C	-0.383342	2.457475	-2.824075
C	-0.383342	1.217043	-3.540448
C	0.000000	0.000000	-2.855361
C	0.383342	-1.217043	-3.540448
C	0.383342	-2.457475	-2.824075
C	0.000000	-2.472708	-1.427494
C	-0.383342	-3.674611	-0.716164
C	-0.383342	-3.674611	0.716164
C	0.000000	-2.472708	1.427494
C	0.383342	-2.457475	2.824075
C	0.383342	-1.217043	3.540448
C	0.000000	0.000000	2.855361
C	-0.383342	1.217043	3.540448
C	-0.383342	2.457475	2.824075
C	0.000000	2.472708	1.427494
C	0.000000	1.249661	0.721548
C	0.000000	1.249661	-0.721548
C	0.000000	0.000000	-1.443188
C	0.000000	-1.249661	-0.721548
C	0.000000	-1.249661	0.721548
C	0.000000	0.000000	1.443188
C	-0.875143	3.612157	3.485617
C	-1.326034	3.577647	4.791755
C	-1.326034	2.361565	5.494155
C	-0.875143	1.212964	4.871324
C	0.875143	4.825039	-1.385311
C	1.326034	5.938833	-0.702196
C	1.326034	5.938833	0.702196
C	0.875143	4.825039	1.385311
C	-0.875143	1.212964	-4.871324
C	-1.326034	2.361565	-5.494155
C	-1.326034	3.577647	-4.791755
C	-0.875143	3.612157	-3.485617
C	0.875143	-3.612157	-3.485617
C	1.326034	-3.577647	-4.791755
C	1.326034	-2.361565	-5.494155

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C       0.875143       -1.212964       -4.871324
C      -0.875143       -4.825039        1.385311
C      -1.326034       -5.938833        0.702196
C      -1.326034       -5.938833       -0.702196
C      -0.875143       -4.825039       -1.385311
C       0.875143       -1.212964        4.871324
C       1.326034       -2.361565        5.494155
C       1.326034       -3.577647        4.791755
C       0.875143       -3.612157        3.485617
H      -0.949352        4.539775        2.935734
H      -1.716558        4.481294        5.252371
H      -1.716558        2.309174        6.507044
H      -0.949352        0.273097        5.399982
H       0.949352        4.812830       -2.463693
H       1.716558        6.789700       -1.254227
H       1.716558        6.789700        1.254227
H       0.949352        4.812830        2.463693
H      -0.949352        0.273097       -5.399982
H      -1.716558        2.309174       -6.507044
H      -1.716558        4.481294       -5.252371
H      -0.949352        4.539775       -2.935734
H       0.949352       -4.539775       -2.935734
H       1.716558       -4.481294       -5.252371
H       1.716558       -2.309174       -6.507044
H       0.949352       -0.273097       -5.399982
H      -0.949352       -4.812830        2.463693
H      -1.716558       -6.789700        1.254227
H      -1.716558       -6.789700       -1.254227
H      -0.949352       -4.812830       -2.463693
H       0.949352       -0.273097        5.399982
H       1.716558       -2.309174        6.507044
H       1.716558       -4.481294        5.252371
H       0.949352       -4.539775        2.935734


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cf10, c-HBC_monomer with bowl depth: 0.97

C       0.422503        3.655806        0.716950
C       0.422503        3.655806       -0.716950
C       0.000000        2.466249       -1.423834
C      -0.422503        2.448608       -2.807547
C      -0.422503        1.206820       -3.524503
C       0.000000        0.000000       -2.847667
C       0.422503       -1.206820       -3.524503
C       0.422503       -2.448608       -2.807547
C       0.000000       -2.466249       -1.423834
C      -0.422503       -3.655806       -0.716950
C      -0.422503       -3.655806        0.716950
C       0.000000       -2.466249        1.423834
C       0.422503       -2.448608        2.807547
C       0.422503       -1.206820        3.524503
C       0.000000        0.000000        2.847667
C      -0.422503        1.206820        3.524503
C      -0.422503        2.448608        2.807547
C       0.000000        2.466249        1.423834
C       0.000000        1.246049        0.719408
C       0.000000        1.246049       -0.719408
C       0.000000        0.000000       -1.438745
C       0.000000       -1.246049       -0.719408
C       0.000000       -1.246049        0.719408
C       0.000000        0.000000        1.438745
C      -0.972381        3.592716        3.439074
C      -1.478730        3.539577        4.725616
C      -1.478730        2.321708        5.428703
C      -0.972381        1.181228        4.831145
C       0.972381        4.774679       -1.392136
C       1.478730        5.862372       -0.703121
C       1.478730        5.862372        0.703121
C       0.972381        4.774679        1.392136
C      -0.972381        1.181228       -4.831145
C      -1.478730        2.321708       -5.428703
C      -1.478730        3.539577       -4.725616
C      -0.972381        3.592716       -3.439074
C       0.972381       -3.592716       -3.439074
C       1.478730       -3.539577       -4.725616
C       1.478730       -2.321708       -5.428703
C       0.972381       -1.181228       -4.831145
C      -0.972381       -4.774679        1.392136
C      -1.478730       -5.862372        0.703121
C      -1.478730       -5.862372       -0.703121
C      -0.972381       -4.774679       -1.392136
C       0.972381       -1.181228        4.831145
C       1.478730       -2.321708        5.428703
C       1.478730       -3.539577        4.725616
C       0.972381       -3.592716        3.439074
H      -1.054835        4.514831        2.875927
H      -1.916870        4.429041        5.170770
H      -1.916870        2.262238        6.421544
H      -1.054835        0.232345        5.347771
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H       1.054835        4.747651       -2.472254
H       1.916870        6.692546       -1.250943
H       1.916870        6.692546        1.250943
H       1.054835        4.747651        2.472254
H      -1.054835        0.232345       -5.347771
H      -1.916870        2.262238       -6.421544
H      -1.916870        4.429041       -5.170770
H      -1.054835        4.514831       -2.875927
H       1.054835       -4.514831       -2.875927
H       1.916870       -4.429041       -5.170770
H       1.916870       -2.262238       -6.421544
H       1.054835       -0.232345       -5.347771
H      -1.054835       -4.747651        2.472254
H      -1.916870       -6.692546        1.250943
H      -1.916870       -6.692546       -1.250943
H      -1.054835       -4.747651       -2.472254
H       1.054835       -0.232345        5.347771
H       1.916870       -2.262238        6.421544
H       1.916870       -4.429041        5.170770
H       1.054835       -4.514831        2.875927

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cf11, c-HBC_monomer with bowl depth: 1.07

C       0.461320        3.639058        0.718044
C       0.461320        3.639058       -0.718044
C       0.000000        2.462031       -1.421454
C      -0.461320        2.441192       -2.792638
C      -0.461320        1.197407       -3.510444
C       0.000000        0.000000       -2.842357
C       0.461320       -1.197407       -3.510444
C       0.461320       -2.441192       -2.792638
C       0.000000       -2.462031       -1.421454
C      -0.461320       -3.639058       -0.718044
C      -0.461320       -3.639058        0.718044
C       0.000000       -2.462031        1.421454
C       0.461320       -2.441192        2.792638
C       0.461320       -1.197407        3.510444
C       0.000000        0.000000        2.842357
C      -0.461320        1.197407        3.510444
C      -0.461320        2.441192        2.792638
C       0.000000        2.462031        1.421454
C       0.000000        1.243675        0.717977
C       0.000000        1.243675       -0.717977
C       0.000000        0.000000       -1.435841
C       0.000000       -1.243675       -0.717977
C       0.000000       -1.243675        0.717977
C       0.000000        0.000000        1.435841
C      -1.069619        3.571653        3.394077
C      -1.628344        3.500587        4.659123
C      -1.628344        2.281665        5.362358
C      -1.069619        1.151351        4.790062
C       1.069619        4.724691       -1.396729
C       1.628344        5.785202       -0.703581
C       1.628344        5.785202        0.703581
C       1.069619        4.724691        1.396729
C      -1.069619        1.151351       -4.790062
C      -1.628344        2.281665       -5.362358
C      -1.628344        3.500587       -4.659123
C      -1.069619        3.571653       -3.394077
C       1.069619       -3.571653       -3.394077
C       1.628344       -3.500587       -4.659123
C       1.628344       -2.281665       -5.362358
C       1.069619       -1.151351       -4.790062
C      -1.069619       -4.724691        1.396729
C      -1.628344       -5.785202        0.703581
C      -1.628344       -5.785202       -0.703581
C      -1.069619       -4.724691       -1.396729
C       1.069619       -1.151351        4.790062
C       1.628344       -2.281665        5.362358
C       1.628344       -3.500587        4.659123
C       1.069619       -3.571653        3.394077
H      -1.160319        4.489091        2.821383
H      -2.110820        4.375892        5.086347
H      -2.110820        2.213221        6.333905
H      -1.160319        0.195490        5.296036
H       1.160319        4.685905       -2.477483
H       2.110820        6.592538       -1.248419
H       2.110820        6.592538        1.248419
H       1.160319        4.685905        2.477483
H      -1.160319        0.195490       -5.296036
H      -2.110820        2.213221       -6.333905
H      -2.110820        4.375892       -5.086347
H      -1.160319        4.489091       -2.821383
H       1.160319       -4.489091       -2.821383
H       2.110820       -4.375892       -5.086347
H       2.110820       -2.213221       -6.333905
H       1.160319       -0.195490       -5.296036
H      -1.160319       -4.685905        2.477483
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H      -2.110820       -6.592538        1.248419
H      -2.110820       -6.592538       -1.248419
H      -1.160319       -4.685905       -2.477483
H       1.160319       -0.195490        5.296036
H       2.110820       -2.213221        6.333905
H       2.110820       -4.375892        5.086347
H       1.160319       -4.489091        2.821383


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cf12, c-HBC_monomer with bowl depth: 1.17

C       0.499903        3.622018        0.719085
C       0.499903        3.622018       -0.719085
C       0.000000        2.458433       -1.419277
C      -0.499903        2.433585       -2.777166
C      -0.499903        1.188048       -3.496066
C       0.000000        0.000000       -2.838326
C       0.499903       -1.188048       -3.496066
C       0.499903       -2.433585       -2.777166
C       0.000000       -2.458433       -1.419277
C      -0.499903       -3.622018       -0.719085
C      -0.499903       -3.622018        0.719085
C       0.000000       -2.458433        1.419277
C       0.499903       -2.433585        2.777166
C       0.499903       -1.188048        3.496066
C       0.000000        0.000000        2.838326
C      -0.499903        1.188048        3.496066
C      -0.499903        2.433585        2.777166
C       0.000000        2.458433        1.419277
C       0.000000        1.241653        0.716816
C       0.000000        1.241653       -0.716816
C       0.000000        0.000000       -1.433348
C       0.000000       -1.241653       -0.716816
C       0.000000       -1.241653        0.716816
C       0.000000        0.000000        1.433348
C      -1.166857        3.547605        3.345992
C      -1.781150        3.458236        4.584555
C      -1.781150        2.239210        5.288008
C      -1.166857        1.122428        4.745123
C       1.166857        4.671374       -1.399719
C       1.781150        5.699690       -0.703683
C       1.781150        5.699690        0.703683
C       1.166857        4.671374        1.399719
C      -1.166857        1.122428       -4.745123
C      -1.781150        2.239210       -5.288008
C      -1.781150        3.458236       -4.584555
C      -1.166857        3.547605       -3.345992
C       1.166857       -3.547605       -3.345992
C       1.781150       -3.458236       -4.584555
C       1.781150       -2.239210       -5.288008
C       1.166857       -1.122428       -4.745123
C      -1.166857       -4.671374        1.399719
C      -1.781150       -5.699690        0.703683
C      -1.781150       -5.699690       -0.703683
C      -1.166857       -4.671374       -1.399719
C       1.166857       -1.122428        4.745123
C       1.781150       -2.239210        5.288008
C       1.781150       -3.458236        4.584555
C       1.166857       -3.547605        3.345992
H      -1.265802        4.459676        2.764373
H      -2.310753        4.317751        4.987444
H      -2.310753        2.157766        6.233721
H      -1.265802        0.162013        5.242908
H       1.265802        4.622907       -2.480457
H       2.310753        6.478085       -1.246964
H       2.310753        6.478085        1.246964
H       1.265802        4.622907        2.480457
H      -1.265802        0.162013       -5.242908
H      -2.310753        2.157766       -6.233721
H      -2.310753        4.317751       -4.987444
H      -1.265802        4.459676       -2.764373
H       1.265802       -4.459676       -2.764373
H       2.310753       -4.317751       -4.987444
H       2.310753       -2.157766       -6.233721
H       1.265802       -0.162013       -5.242908
H      -1.265802       -4.622907        2.480457
H      -2.310753       -6.478085        1.246964
H      -2.310753       -6.478085       -1.246964
H      -1.265802       -4.622907       -2.480457
H       1.265802       -0.162013        5.242908
H       2.310753       -2.157766        6.233721
H       2.310753       -4.317751        4.987444
H       1.265802       -4.459676        2.764373


72
cf13, c-HBC_monomer with bowl depth: 1.26

C       0.539256        3.605395        0.720380
```

C	0.539256	3.605395	-0.720380
C	0.000000	2.456228	-1.418051
C	-0.539256	2.426441	-2.762191
C	-0.539256	1.178533	-3.482296
C	0.000000	0.000000	-2.835579
C	0.539256	-1.178533	-3.482296
C	0.539256	-2.426441	-2.762191
C	0.000000	-2.456228	-1.418051
C	-0.539256	-3.605395	-0.720380
C	-0.539256	-3.605395	0.720380
C	0.000000	-2.456228	1.418051
C	0.539256	-2.426441	2.762191
C	0.539256	-1.178533	3.482296
C	0.000000	0.000000	2.835579
C	-0.539256	1.178533	3.482296
C	-0.539256	2.426441	2.762191
C	0.000000	2.456228	1.418051
C	0.000000	1.240315	0.715998
C	0.000000	1.240315	-0.715998
C	0.000000	0.000000	-1.431769
C	0.000000	-1.240315	-0.715998
C	0.000000	-1.240315	0.715998
C	0.000000	0.000000	1.431769
C	-1.264095	3.521268	3.297863
C	-1.930746	3.413542	4.508142
C	-1.930746	2.194654	5.211194
C	-1.264095	1.093371	4.697928
C	1.264095	4.616242	-1.401147
C	1.930746	5.611058	-0.703523
C	1.930746	5.611058	0.703523
C	1.264095	4.616242	1.401147
C	-1.264095	1.093371	-4.697928
C	-1.930746	2.194654	-5.211194
C	-1.930746	3.413542	-4.508142
C	-1.264095	3.521268	-3.297863
C	1.264095	-3.521268	-3.297863
C	1.930746	-3.413542	-4.508142
C	1.930746	-2.194654	-5.211194
C	1.264095	-1.093371	-4.697928
C	-1.264095	-4.616242	1.401147
C	-1.930746	-5.611058	0.703523
C	-1.930746	-5.611058	-0.703523
C	-1.264095	-4.616242	-1.401147
C	1.264095	-1.093371	4.697928
C	1.930746	-2.194654	5.211194
C	1.930746	-3.413542	4.508142
C	1.264095	-3.521268	3.297863
H	-1.371286	4.429087	2.709979
H	-2.503532	4.257091	4.884800
H	-2.503532	2.098110	6.129927
H	-1.371286	0.129289	5.188119
H	1.371286	4.559579	-2.481229
H	2.503532	6.358592	-1.246305
H	2.503532	6.358592	1.246305
H	1.371286	4.559579	2.481229
H	-1.371286	0.129289	-5.188119
H	-2.503532	2.098110	-6.129927
H	-2.503532	4.257091	-4.884800
H	-1.371286	4.429087	-2.709979
H	1.371286	-4.429087	-2.709979
H	2.503532	-4.257091	-4.884800
H	2.503532	-2.098110	-6.129927
H	1.371286	-0.129289	-5.188119
H	-1.371286	-4.559579	2.481229
H	-2.503532	-6.358592	1.246305
H	-2.503532	-6.358592	-1.246305
H	-1.371286	-4.559579	-2.481229
H	1.371286	-0.129289	5.188119
H	2.503532	-2.098110	6.129927
H	2.503532	-4.257091	4.884800
H	1.371286	-4.429087	2.709979

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cf14, c-HBC_monomer with bowl depth: 1.36

C	0.579456	3.587945	0.721714
C	0.579456	3.587945	-0.721714
C	0.000000	2.454289	-1.416911
C	-0.579456	2.418869	-2.746292
C	-0.579456	1.168767	-3.468029
C	0.000000	0.000000	-2.833756
C	0.579456	-1.168767	-3.468029
C	0.579456	-2.418869	-2.746292
C	0.000000	-2.454289	-1.416911
C	-0.579456	-3.587945	-0.721714
C	-0.579456	-3.587945	0.721714
C	0.000000	-2.454289	1.416911
C	0.579456	-2.418869	2.746292
C	0.579456	-1.168767	3.468029

```
C       0.000000        0.000000        2.833756
C      -0.579456        1.168767        3.468029
C      -0.579456        2.418869        2.746292
C       0.000000        2.454289        1.416911
C       0.000000        1.239148        0.715383
C       0.000000        1.239148       -0.715383
C       0.000000        0.000000       -1.430689
C       0.000000       -1.239148       -0.715383
C       0.000000       -1.239148        0.715383
C       0.000000        0.000000        1.430689
C      -1.361333        3.492607        3.245605
C      -2.079166        3.366327        4.424804
C      -2.079166        2.148120        5.127952
C      -1.361333        1.063941        4.647319
C       1.361333        4.557030       -1.402022
C       2.079166        5.515288       -0.703255
C       2.079166        5.515288        0.703255
C       1.361333        4.557030        1.402022
C      -1.361333        1.063941       -4.647319
C      -2.079166        2.148120       -5.127952
C      -2.079166        3.366327       -4.424804
C      -1.361333        3.492607       -3.245605
C       1.361333       -3.492607       -3.245605
C       2.079166       -3.366327       -4.424804
C       2.079166       -2.148120       -5.127952
C       1.361333       -1.063941       -4.647319
C      -1.361333       -4.557030        1.402022
C      -2.079166       -5.515288        0.703255
C      -2.079166       -5.515288       -0.703255
C      -1.361333       -4.557030       -1.402022
C       1.361333       -1.063941        4.647319
C       2.079166       -2.148120        5.127952
C       2.079166       -3.366327        4.424804
C       1.361333       -3.492607        3.245605
H      -1.476769        4.395381        2.650807
H      -2.693746        4.193065        4.771612
H      -2.693746        2.034811        6.017306
H      -1.476769        0.097072        5.130953
H       1.476769        4.492529       -2.481171
H       2.693746        6.228819       -1.246054
H       2.693746        6.228819        1.246054
H       1.476769        4.492529        2.481171
H      -1.476769        0.097072       -5.130953
H      -2.693746        2.034811       -6.017306
H      -2.693746        4.193065       -4.771612
H      -1.476769        4.395381       -2.650807
H       1.476769       -4.395381       -2.650807
H       2.693746       -4.193065       -4.771612
H       2.693746       -2.034811       -6.017306
H       1.476769       -0.097072       -5.130953
H      -1.476769       -4.492529        2.481171
H      -2.693746       -6.228819        1.246054
H      -2.693746       -6.228819       -1.246054
H      -1.476769       -4.492529       -2.481171
H       1.476769       -0.097072        5.130953
H       2.693746       -2.034811        6.017306
H       2.693746       -4.193065        4.771612
H       1.476769       -4.395381        2.650807

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cf15, c-HBC_monomer with bowl depth: 1.46

C       0.620602        3.569082        0.723231
C       0.620602        3.569082       -0.723231
C       0.000000        2.452588       -1.415951
C      -0.620602        2.410719       -2.729199
C      -0.620602        1.157997       -3.452525
C       0.000000        0.000000       -2.831871
C       0.620602       -1.157997       -3.452525
C       0.620602       -2.410719       -2.729199
C       0.000000       -2.452588       -1.415951
C      -0.620602       -3.569082       -0.723231
C      -0.620602       -3.569082        0.723231
C       0.000000       -2.452588        1.415951
C       0.620602       -2.410719        2.729199
C       0.620602       -1.157997        3.452525
C       0.000000        0.000000        2.831871
C      -0.620602        1.157997        3.452525
C      -0.620602        2.410719        2.729199
C       0.000000        2.452588        1.415951
C       0.000000        1.238078        0.714775
C       0.000000        1.238078       -0.714775
C       0.000000        0.000000       -1.429510
C       0.000000       -1.238078       -0.714775
C       0.000000       -1.238078        0.714775
C       0.000000        0.000000        1.429510
C      -1.458571        3.460759        3.189520
C      -2.226120        3.314193        4.334928
C      -2.226120        2.096728        5.037721
```

C	-1.458571	1.031534	4.591870
C	1.458571	4.492509	-1.402615
C	2.226120	5.411118	-0.702854
C	2.226120	5.411118	0.702854
C	1.458571	4.492509	1.402615
C	-1.458571	1.031534	-4.591870
C	-2.226120	2.096728	-5.037721
C	-2.226120	3.314193	-4.334928
C	-1.458571	3.460759	-3.189520
C	1.458571	-3.460759	-3.189520
C	2.226120	-3.314193	-4.334928
C	2.226120	-2.096728	-5.037721
C	1.458571	-1.031534	-4.591870
C	-1.458571	-4.492509	1.402615
C	-2.226120	-5.411118	0.702854
C	-2.226120	-5.411118	-0.702854
C	-1.458571	-4.492509	-1.402615
C	1.458571	-1.031534	4.591870
C	2.226120	-2.096728	5.037721
C	2.226120	-3.314193	4.334928
C	1.458571	-3.460759	3.189520
H	-1.582253	4.358006	2.587502
H	-2.880742	4.122751	4.649816
H	-2.880742	1.964996	5.895406
H	-1.582253	0.061339	5.067512
H	1.582253	4.419424	-2.480657
H	2.880742	6.088115	-1.245627
H	2.880742	6.088115	1.245627
H	1.582253	4.419424	2.480657
H	-1.582253	0.061339	-5.067512
H	-2.880742	1.964996	-5.895406
H	-2.880742	4.122751	-4.649816
H	-1.582253	4.358006	-2.587502
H	1.582253	-4.358006	-2.587502
H	2.880742	-4.122751	-4.649816
H	2.880742	-1.964996	-5.895406
H	1.582253	-0.061339	-5.067512
H	-1.582253	-4.419424	2.480657
H	-2.880742	-6.088115	1.245627
H	-2.880742	-6.088115	-1.245627
H	-1.582253	-4.419424	-2.480657
H	1.582253	-0.061339	5.067512
H	2.880742	-1.964996	5.895406
H	2.880742	-4.122751	4.649816
H	1.582253	-4.358006	2.587502

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cf16, c-HBC_monomer with bowl depth: 1.56

C	0.663197	3.548373	0.724881
C	0.663197	3.548373	-0.724881
C	0.000000	2.451021	-1.415072
C	-0.663197	2.401820	-2.710471
C	-0.663197	1.146238	-3.435471
C	0.000000	0.000000	-2.829997
C	0.663197	-1.146238	-3.435471
C	0.663197	-2.401820	-2.710471
C	0.000000	-2.451021	-1.415072
C	-0.663197	-3.548373	-0.724881
C	-0.663197	-3.548373	0.724881
C	0.000000	-2.451021	1.415072
C	0.663197	-2.401820	2.710471
C	0.663197	-1.146238	3.435471
C	0.000000	0.000000	2.829997
C	-0.663197	1.146238	3.435471
C	-0.663197	2.401820	2.710471
C	0.000000	2.451021	1.415072
C	0.000000	1.237031	0.714145
C	0.000000	1.237031	-0.714145
C	0.000000	0.000000	-1.428285
C	0.000000	-1.237031	-0.714145
C	0.000000	-1.237031	0.714145
C	0.000000	0.000000	1.428285
C	-1.555809	3.426012	3.128997
C	-2.371532	3.257487	4.237712
C	-2.371532	2.040843	4.940019
C	-1.555809	0.996457	4.531565
C	1.555809	4.422578	-1.402917
C	2.371532	5.298345	-0.702392
C	2.371532	5.298345	0.702392
C	1.555809	4.422578	1.402917
C	-1.555809	0.996457	-4.531565
C	-2.371532	2.040843	-4.940019
C	-2.371532	3.257487	-4.237712
C	-1.555809	3.426012	-3.128997
C	1.555809	-3.426012	-3.128997
C	2.371532	-3.257487	-4.237712
C	2.371532	-2.040843	-4.940019
C	1.555809	-0.996457	-4.531565

C	-1.555809	-4.422578	1.402917
C	-2.371532	-5.298345	0.702392
C	-2.371532	-5.298345	-0.702392
C	-1.555809	-4.422578	-1.402917
C	1.555809	-0.996457	4.531565
C	2.371532	-2.040843	4.940019
C	2.371532	-3.257487	4.237712
C	1.555809	-3.426012	3.128997
H	-1.687736	4.317568	2.519766
H	-3.064479	4.046524	4.518207
H	-3.064479	1.889061	5.763585
H	-1.687736	0.022887	4.998685
H	1.687736	4.340592	-2.479633
H	3.064479	5.935917	-1.245330
H	3.064479	5.935917	1.245330
H	1.687736	4.340592	2.479633
H	-1.687736	0.022887	-4.998685
H	-3.064479	1.889061	-5.763585
H	-3.064479	4.046524	-4.518207
H	-1.687736	4.317568	-2.519766
H	1.687736	-4.317568	-2.519766
H	3.064479	-4.046524	-4.518207
H	3.064479	-1.889061	-5.763585
H	1.687736	-0.022887	-4.998685
H	-1.687736	-4.340592	2.479633
H	-3.064479	-5.935917	1.245330
H	-3.064479	-5.935917	-1.245330
H	-1.687736	-4.340592	-2.479633
H	1.687736	-0.022887	4.998685
H	3.064479	-1.889061	5.763585
H	3.064479	-4.046524	4.518207
H	1.687736	-4.317568	2.519766

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cf17, c-HBC_monomer with bowl depth: 1.65

C	0.707284	3.526050	0.726722
C	0.707284	3.526050	-0.726722
C	0.000000	2.449623	-1.414289
C	-0.707284	2.392313	-2.690241
C	-0.707284	1.133530	-3.417063
C	0.000000	0.000000	-2.828353
C	0.707284	-1.133530	-3.417063
C	0.707284	-2.392313	-2.690241
C	0.000000	-2.449623	-1.414289
C	-0.707284	-3.526050	-0.726722
C	-0.707284	-3.526050	0.726722
C	0.000000	-2.449623	1.414289
C	0.707284	-2.392313	2.690241
C	0.707284	-1.133530	3.417063
C	0.000000	0.000000	2.828353
C	-0.707284	1.133530	3.417063
C	-0.707284	2.392313	2.690241
C	0.000000	2.449623	1.414289
C	0.000000	1.236126	0.713630
C	0.000000	1.236126	-0.713630
C	0.000000	0.000000	-1.427240
C	0.000000	-1.236126	-0.713630
C	0.000000	-1.236126	0.713630
C	0.000000	0.000000	1.427240
C	-1.653047	3.388367	3.063883
C	-2.515074	3.196415	4.133221
C	-2.515074	1.980748	4.834944
C	-1.653047	0.958813	4.466397
C	1.653047	4.347304	-1.402829
C	2.515074	5.177398	-0.701821
C	2.515074	5.177398	0.701821
C	1.653047	4.347304	1.402829
C	-1.653047	0.958813	-4.466397
C	-2.515074	1.980748	-4.834944
C	-2.515074	3.196415	-4.133221
C	-1.653047	3.388367	-3.063883
C	1.653047	-3.388367	-3.063883
C	2.515074	-3.196415	-4.133221
C	2.515074	-1.980748	-4.834944
C	1.653047	-0.958813	-4.466397
C	-1.653047	-4.347304	1.402829
C	-2.515074	-5.177398	0.701821
C	-2.515074	-5.177398	-0.701821
C	-1.653047	-4.347304	-1.402829
C	1.653047	-0.958813	4.466397
C	2.515074	-1.980748	4.834944
C	2.515074	-3.196415	4.133221
C	1.653047	-3.388367	3.063883
H	-1.793220	4.274053	2.447458
H	-3.244369	3.964696	4.376635
H	-3.244369	1.807178	5.621946
H	-1.793220	-0.018112	4.924681
H	1.793220	4.256227	-2.478069

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H       3.244369        5.772408       -1.245412
H       3.244369        5.772408        1.245412
H       1.793220        4.256227        2.478069
H      -1.793220       -0.018112       -4.924681
H      -3.244369        1.807178       -5.621946
H      -3.244369        3.964696       -4.376635
H      -1.793220        4.274053       -2.447458
H       1.793220       -4.274053       -2.447458
H       3.244369       -3.964696       -4.376635
H       3.244369       -1.807178       -5.621946
H       1.793220        0.018112       -4.924681
H      -1.793220       -4.256227        2.478069
H      -3.244369       -5.772408        1.245412
H      -3.244369       -5.772408       -1.245412
H      -1.793220       -4.256227       -2.478069
H       1.793220        0.018112        4.924681
H       3.244369       -1.807178        5.621946
H       3.244369       -3.964696        4.376635
H       1.793220       -4.274053        2.447458


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cf18, c-HBC_monomer with bowl depth: 1.75

C       0.752765        3.501082        0.728644
C       0.752765        3.501082       -0.728644
C       0.000000        2.447960       -1.413350
C      -0.752765        2.381569       -2.667681
C      -0.752765        1.119528       -3.396516
C       0.000000        0.000000       -2.826541
C       0.752765       -1.119528       -3.396516
C       0.752765       -2.381569       -2.667681
C       0.000000       -2.447960       -1.413350
C      -0.752765       -3.501082       -0.728644
C      -0.752765       -3.501082        0.728644
C       0.000000       -2.447960        1.413350
C       0.752765       -2.381569        2.667681
C       0.752765       -1.119528        3.396516
C       0.000000        0.000000        2.826541
C      -0.752765        1.119528        3.396516
C      -0.752765        2.381569        2.667681
C       0.000000        2.447960        1.413350
C       0.000000        1.235025        0.713005
C       0.000000        1.235025       -0.713005
C       0.000000        0.000000       -1.426088
C       0.000000       -1.235025       -0.713005
C       0.000000       -1.235025        0.713005
C       0.000000        0.000000        1.426088
C      -1.750285        3.347062        2.992094
C      -2.658037        3.129327        4.017716
C      -2.658037        1.914795        4.718975
C      -1.750285        0.917733        4.394870
C       1.750285        4.264732       -1.402594
C       2.658037        5.044185       -0.701206
C       2.658037        5.044185        0.701206
C       1.750285        4.264732        1.402594
C      -1.750285        0.917733       -4.394870
C      -2.658037        1.914795       -4.718975
C      -2.658037        3.129327       -4.017716
C      -1.750285        3.347062       -2.992094
C       1.750285       -3.347062       -2.992094
C       2.658037       -3.129327       -4.017716
C       2.658037       -1.914795       -4.718975
C       1.750285       -0.917733       -4.394870
C      -1.750285       -4.264732        1.402594
C      -2.658037       -5.044185        0.701206
C      -2.658037       -5.044185       -0.701206
C      -1.750285       -4.264732       -1.402594
C       1.750285       -0.917733        4.394870
C       2.658037       -1.914795        4.718975
C       2.658037       -3.129327        4.017716
C       1.750285       -3.347062        2.992094
H      -1.898704        4.226359        2.367978
H      -3.422397        3.874962        4.220731
H      -3.422397        1.717728        5.466177
H      -1.898704       -0.062538        4.843992
H       1.898704        4.163946       -2.476168
H       3.422397        5.592771       -1.245483
H       3.422397        5.592771        1.245483
H       1.898704        4.163946        2.476168
H      -1.898704       -0.062538       -4.843992
H      -3.422397        1.717728       -5.466177
H      -3.422397        3.874962       -4.220731
H      -1.898704        4.226359       -2.367978
H       1.898704       -4.226359       -2.367978
H       3.422397       -3.874962       -4.220731
H       3.422397       -1.717728       -5.466177
H       1.898704        0.062538       -4.843992
H      -1.898704       -4.163946        2.476168
H      -3.422397       -5.592771        1.245483
```

```
H      -3.422397       -5.592771       -1.245483
H      -1.898704       -4.163946       -2.476168
H       1.898704        0.062538        4.843992
H       3.422397       -1.717728        5.466177
H       3.422397       -3.874962        4.220731
H       1.898704       -4.226359        2.367978

72
cf19, c-HBC_monomer with bowl depth: 1.85

C       0.800475        3.474066        0.730828
C       0.800475        3.474066       -0.730828
C       0.000000        2.446588       -1.412595
C      -0.800475        2.370016       -2.643255
C      -0.800475        1.104298       -3.374397
C       0.000000        0.000000       -2.825215
C       0.800475       -1.104298       -3.374397
C       0.800475       -2.370016       -2.643255
C       0.000000       -2.446588       -1.412595
C      -0.800475       -3.474066       -0.730828
C      -0.800475       -3.474066        0.730828
C       0.000000       -2.446588        1.412595
C       0.800475       -2.370016        2.643255
C       0.800475       -1.104298        3.374397
C       0.000000        0.000000        2.825215
C      -0.800475        1.104298        3.374397
C      -0.800475        2.370016        2.643255
C       0.000000        2.446588        1.412595
C       0.000000        1.234134        0.712570
C       0.000000        1.234134       -0.712570
C       0.000000        0.000000       -1.425323
C       0.000000       -1.234134       -0.712570
C       0.000000       -1.234134        0.712570
C       0.000000        0.000000        1.425323
C      -1.847523        3.302839        2.915573
C      -2.797487        3.058707        3.895940
C      -2.797487        1.845568        4.596708
C      -1.847523        0.874334        4.318615
C       1.847523        4.176656       -1.402166
C       2.797487        4.903568       -0.700466
C       2.797487        4.903568        0.700466
C       1.847523        4.176656        1.402166
C      -1.847523        0.874334       -4.318615
C      -2.797487        1.845568       -4.596708
C      -2.797487        3.058707       -3.895940
C      -1.847523        3.302839       -2.915573
C       1.847523       -3.302839       -2.915573
C       2.797487       -3.058707       -3.895940
C       2.797487       -1.845568       -4.596708
C       1.847523       -0.874334       -4.318615
C      -1.847523       -4.176656        1.402166
C      -2.797487       -4.903568        0.700466
C      -2.797487       -4.903568       -0.700466
C      -1.847523       -4.176656       -1.402166
C       1.847523       -0.874334        4.318615
C       2.797487       -1.845568        4.596708
C       2.797487       -3.058707        3.895940
C       1.847523       -3.302839        2.915573
H      -2.004187        4.176071        2.284404
H      -3.593216        3.781412        4.057410
H      -3.593216        1.624338        5.303387
H      -2.004187       -0.108782        4.759505
H       2.004187        4.066741       -2.474038
H       3.593216        5.404700       -1.245628
H       3.593216        5.404700        1.245628
H       2.004187        4.066741        2.474038
H      -2.004187       -0.108782       -4.759505
H      -3.593216        1.624338       -5.303387
H      -3.593216        3.781412       -4.057410
H      -2.004187        4.176071       -2.284404
H       2.004187       -4.176071       -2.284404
H       3.593216       -3.781412       -4.057410
H       3.593216       -1.624338       -5.303387
H       2.004187        0.108782       -4.759505
H      -2.004187       -4.066741        2.474038
H      -3.593216       -5.404700        1.245628
H      -3.593216       -5.404700       -1.245628
H      -2.004187       -4.066741       -2.474038
H       2.004187        0.108782        4.759505
H       3.593216       -1.624338        5.303387
H       3.593216       -3.781412        4.057410
H       2.004187       -4.176071        2.284404

144
cf0, c-HBC_homodimers with bowl depth: 0.00

C       3.663591        1.286711        1.810000
C       2.946321        2.529267        1.810000
```

C	1.469931	2.545652	1.810000
C	0.717379	3.815788	1.810000
C	-0.717379	3.815788	1.810000
C	-1.469931	2.545652	1.810000
C	-2.946321	2.529267	1.810000
C	-3.663591	1.286711	1.810000
C	-2.939776	0.000000	1.810000
C	-3.663591	-1.286711	1.810000
C	-2.946321	-2.529267	1.810000
C	-1.469931	-2.545652	1.810000
C	-0.717379	-3.815788	1.810000
C	0.717379	-3.815788	1.810000
C	1.469931	-2.545652	1.810000
C	2.946321	-2.529267	1.810000
C	3.663591	-1.286711	1.810000
C	2.939776	0.000000	1.810000
C	1.491907	0.000000	1.810000
C	0.745960	1.291875	1.810000
C	-0.745960	1.291875	1.810000
C	-1.491907	0.000000	1.810000
C	-0.745960	-1.291875	1.810000
C	0.745960	-1.291875	1.810000
C	5.090061	-1.428620	1.810000
C	5.841540	-2.576524	1.810000
C	5.152301	-3.770468	1.810000
C	3.782439	-3.693653	1.810000
C	3.782439	3.693653	1.810000
C	5.152301	3.770468	1.810000
C	5.841540	2.576524	1.810000
C	5.090061	1.428620	1.810000
C	-1.307584	5.122138	1.810000
C	-0.689314	6.346950	1.810000
C	0.689314	6.346950	1.810000
C	1.307584	5.122138	1.810000
C	-5.090061	1.428620	1.810000
C	-5.841540	2.576524	1.810000
C	-5.152301	3.770468	1.810000
C	-3.782439	3.693653	1.810000
C	-3.782439	-3.693653	1.810000
C	-5.152301	-3.770468	1.810000
C	-5.841540	-2.576524	1.810000
C	-5.090061	-1.428620	1.810000
C	1.307584	-5.122138	1.810000
C	0.689314	-6.346950	1.810000
C	-0.689314	-6.346950	1.810000
C	-1.307584	-5.122138	1.810000
H	5.742349	-0.608006	1.810000
H	6.926079	-2.507847	1.810000
H	5.635229	-4.743987	1.810000
H	3.397371	-4.668578	1.810000
H	3.397371	4.668578	1.810000
H	5.635229	4.743987	1.810000
H	6.926079	2.507847	1.810000
H	5.742349	0.608006	1.810000
H	-2.344489	5.276702	1.810000
H	-1.291014	7.251868	1.810000
H	1.291014	7.251868	1.810000
H	2.344489	5.276702	1.810000
H	-5.742349	0.608006	1.810000
H	-6.926079	2.507847	1.810000
H	-5.635229	4.743987	1.810000
H	-3.397371	4.668578	1.810000
H	-3.397371	-4.668578	1.810000
H	-5.635229	-4.743987	1.810000
H	-6.926079	-2.507847	1.810000
H	-5.742349	-0.608006	1.810000
H	2.344489	-5.276702	1.810000
H	1.291014	-7.251868	1.810000
H	-1.291014	-7.251868	1.810000
H	-2.344489	-5.276702	1.810000
C	3.663591	1.286711	-1.810000
C	2.946321	2.529267	-1.810000
C	1.469931	2.545652	-1.810000
C	0.717379	3.815788	-1.810000
C	-0.717379	3.815788	-1.810000
C	-1.469931	2.545652	-1.810000
C	-2.946321	2.529267	-1.810000
C	-3.663591	1.286711	-1.810000
C	-2.939776	0.000000	-1.810000
C	-3.663591	-1.286711	-1.810000
C	-2.946321	-2.529267	-1.810000
C	-1.469931	-2.545652	-1.810000
C	-0.717379	-3.815788	-1.810000
C	0.717379	-3.815788	-1.810000
C	1.469931	-2.545652	-1.810000
C	2.946321	-2.529267	-1.810000
C	3.663591	-1.286711	-1.810000
C	2.939776	0.000000	-1.810000
C	1.491907	0.000000	-1.810000
C	0.745960	1.291875	-1.810000

C	-0.745960	1.291875	-1.810000
C	-1.491907	0.000000	-1.810000
C	-0.745960	-1.291875	-1.810000
C	0.745960	-1.291875	-1.810000
C	5.090061	-1.428620	-1.810000
C	5.841540	-2.576524	-1.810000
C	5.152301	-3.770468	-1.810000
C	3.782439	-3.693653	-1.810000
C	3.782439	3.693653	-1.810000
C	5.152301	3.770468	-1.810000
C	5.841540	2.576524	-1.810000
C	5.090061	1.428620	-1.810000
C	-1.307584	5.122138	-1.810000
C	-0.689314	6.346950	-1.810000
C	0.689314	6.346950	-1.810000
C	1.307584	5.122138	-1.810000
C	-5.090061	1.428620	-1.810000
C	-5.841540	2.576524	-1.810000
C	-5.152301	3.770468	-1.810000
C	-3.782439	3.693653	-1.810000
C	-3.782439	-3.693653	-1.810000
C	-5.152301	-3.770468	-1.810000
C	-5.841540	-2.576524	-1.810000
C	-5.090061	-1.428620	-1.810000
C	1.307584	-5.122138	-1.810000
C	0.689314	-6.346950	-1.810000
C	-0.689314	-6.346950	-1.810000
C	-1.307584	-5.122138	-1.810000
H	5.742349	-0.608006	-1.810000
H	6.926079	-2.507847	-1.810000
H	5.635229	-4.743987	-1.810000
H	3.397371	-4.668578	-1.810000
H	3.397371	4.668578	-1.810000
H	5.635229	4.743987	-1.810000
H	6.926079	2.507847	-1.810000
H	5.742349	0.608006	-1.810000
H	-2.344489	5.276702	-1.810000
H	-1.291014	7.251868	-1.810000
H	1.291014	7.251868	-1.810000
H	2.344489	5.276702	-1.810000
H	-5.742349	0.608006	-1.810000
H	-6.926079	2.507847	-1.810000
H	-5.635229	4.743987	-1.810000
H	-3.397371	4.668578	-1.810000
H	-3.397371	-4.668578	-1.810000
H	-5.635229	-4.743987	-1.810000
H	-6.926079	-2.507847	-1.810000
H	-5.742349	-0.608006	-1.810000
H	2.344489	-5.276702	-1.810000
H	1.291014	-7.251868	-1.810000
H	-1.291014	-7.251868	-1.810000
H	-2.344489	-5.276702	-1.810000

144

cf1, c-HBC_homodimers with bowl depth: 0.10

C	1.854317	3.812762	0.717191
C	1.854317	3.812762	-0.717191
C	1.810000	2.543960	-1.469049
C	1.765683	2.527769	-2.944025
C	1.765683	1.285508	-3.661130
C	1.810000	0.000000	-2.937894
C	1.854317	-1.285508	-3.661130
C	1.854317	-2.527769	-2.944025
C	1.810000	-2.543960	-1.469049
C	1.765683	-3.812762	-0.717191
C	1.765683	-3.812762	0.717191
C	1.810000	-2.543960	1.469049
C	1.854317	-2.527769	2.944025
C	1.854317	-1.285508	3.661130
C	1.810000	0.000000	2.937894
C	1.765683	1.285508	3.661130
C	1.765683	2.527769	2.944025
C	1.810000	2.543960	1.469049
C	1.810000	1.290885	0.745455
C	1.810000	1.290885	-0.745455
C	1.810000	0.000000	-1.491036
C	1.810000	-1.290885	-0.745455
C	1.810000	-1.290885	0.745455
C	1.810000	0.000000	1.491036
C	1.712762	3.692412	3.777614
C	1.667115	3.767538	5.146909
C	1.667115	2.573063	5.836438
C	1.712762	1.425002	5.086435
C	1.907238	5.116866	-1.308871
C	1.952885	6.340437	-0.689624
C	1.952885	6.340437	0.689624
C	1.907238	5.116866	1.308871
C	1.712762	1.425002	-5.086435

C	1.667115	2.573063	-5.836438
C	1.667115	3.767538	-5.146909
C	1.712762	3.692412	-3.777614
C	1.907238	-3.692412	-3.777614
C	1.952885	-3.767538	-5.146909
C	1.952885	-2.573063	-5.836438
C	1.907238	-1.425002	-5.086435
C	1.712762	-5.116866	1.308871
C	1.667115	-6.340437	0.689624
C	1.667115	-6.340437	-0.689624
C	1.712762	-5.116866	-1.308871
C	1.907238	-1.425002	5.086435
C	1.952885	-2.573063	5.836438
C	1.952885	-3.767538	5.146909
C	1.907238	-3.692412	3.777614
H	1.704516	4.666300	3.388263
H	1.628613	4.740352	5.629678
H	1.628613	2.504433	6.920279
H	1.704516	0.600947	5.735235
H	1.915484	5.266523	-2.346995
H	1.991387	7.244810	-1.290914
H	1.991387	7.244810	1.290914
H	1.915484	5.266523	2.346995
H	1.704516	0.600947	-5.735235
H	1.628613	2.504433	-6.920279
H	1.628613	4.740352	-5.629678
H	1.704516	4.666300	-3.388263
H	1.915484	-4.666300	-3.388263
H	1.991387	-4.740352	-5.629678
H	1.991387	-2.504433	-6.920279
H	1.915484	-0.600947	-5.735235
H	1.704516	-5.266523	2.346995
H	1.628613	-7.244810	1.290914
H	1.628613	-7.244810	-1.290914
H	1.704516	-5.266523	-2.346995
H	1.915484	-0.600947	5.735235
H	1.991387	-2.504433	6.920279
H	1.991387	-4.740352	5.629678
H	1.915484	-4.666300	3.388263
C	-1.765683	3.812762	0.717191
C	-1.765683	3.812762	-0.717191
C	-1.810000	2.543960	-1.469049
C	-1.854317	2.527769	-2.944025
C	-1.854317	1.285508	-3.661130
C	-1.810000	0.000000	-2.937894
C	-1.765683	-1.285508	-3.661130
C	-1.765683	-2.527769	-2.944025
C	-1.810000	-2.543960	-1.469049
C	-1.854317	-3.812762	-0.717191
C	-1.854317	-3.812762	0.717191
C	-1.810000	-2.543960	1.469049
C	-1.765683	-2.527769	2.944025
C	-1.765683	-1.285508	3.661130
C	-1.810000	0.000000	2.937894
C	-1.854317	1.285508	3.661130
C	-1.854317	2.527769	2.944025
C	-1.810000	2.543960	1.469049
C	-1.810000	1.290885	0.745455
C	-1.810000	1.290885	-0.745455
C	-1.810000	0.000000	-1.491036
C	-1.810000	-1.290885	-0.745455
C	-1.810000	-1.290885	0.745455
C	-1.810000	0.000000	1.491036
C	-1.907238	3.692412	3.777614
C	-1.952885	3.767538	5.146909
C	-1.952885	2.573063	5.836438
C	-1.907238	1.425002	5.086435
C	-1.712762	5.116866	-1.308871
C	-1.667115	6.340437	-0.689624
C	-1.667115	6.340437	0.689624
C	-1.712762	5.116866	1.308871
C	-1.907238	1.425002	-5.086435
C	-1.952885	2.573063	-5.836438
C	-1.952885	3.767538	-5.146909
C	-1.907238	3.692412	-3.777614
C	-1.712762	-3.692412	-3.777614
C	-1.667115	-3.767538	-5.146909
C	-1.667115	-2.573063	-5.836438
C	-1.712762	-1.425002	-5.086435
C	-1.907238	-5.116866	1.308871
C	-1.952885	-6.340437	0.689624
C	-1.952885	-6.340437	-0.689624
C	-1.907238	-5.116866	-1.308871
C	-1.712762	-1.425002	5.086435
C	-1.667115	-2.573063	5.836438
C	-1.667115	-3.767538	5.146909
C	-1.712762	-3.692412	3.777614
H	-1.915484	4.666300	3.388263
H	-1.991387	4.740352	5.629678
H	-1.991387	2.504433	6.920279

```
H      -1.915484        0.600947        5.735235
H      -1.704516        5.266523       -2.346995
H      -1.628613        7.244810       -1.290914
H      -1.628613        7.244810        1.290914
H      -1.704516        5.266523        2.346995
H      -1.915484        0.600947       -5.735235
H      -1.991387        2.504433       -6.920279
H      -1.991387        4.740352       -5.629678
H      -1.915484        4.666300       -3.388263
H      -1.704516       -4.666300       -3.388263
H      -1.628613       -4.740352       -5.629678
H      -1.628613       -2.504433       -6.920279
H      -1.704516       -0.600947       -5.735235
H      -1.915484       -5.266523        2.346995
H      -1.991387       -7.244810        1.290914
H      -1.991387       -7.244810       -1.290914
H      -1.915484       -5.266523       -2.346995
H      -1.704516       -0.600947        5.735235
H      -1.628613       -2.504433        6.920279
H      -1.628613       -4.740352        5.629678
H      -1.704516       -4.666300        3.388263


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cf2, c-HBC_homodimers with bowl depth: 0.19

C       1.898046        3.804764        0.716832
C       1.898046        3.804764       -0.716832
C       1.810000        2.539183       -1.466095
C       1.721954        2.523187       -2.936748
C       1.721954        1.281740       -3.653706
C       1.810000        0.000000       -2.932316
C       1.898046       -1.281740       -3.653706
C       1.898046       -2.523187       -2.936748
C       1.810000       -2.539183       -1.466095
C       1.721954       -3.804764       -0.716832
C       1.721954       -3.804764        0.716832
C       1.810000       -2.539183        1.466095
C       1.898046       -2.523187        2.936748
C       1.898046       -1.281740        3.653706
C       1.810000        0.000000        2.932316
C       1.721954        1.281740        3.653706
C       1.721954        2.523187        2.936748
C       1.810000        2.539183        1.466095
C       1.810000        1.287984        0.743711
C       1.810000        1.287984       -0.743711
C       1.810000        0.000000       -1.487627
C       1.810000       -1.287984       -0.743711
C       1.810000       -1.287984        0.743711
C       1.810000        0.000000        1.487627
C       1.615524        3.688687        3.761851
C       1.524858        3.759350        5.129406
C       1.524858        2.563659        5.820088
C       1.615524        1.414202        5.075651
C       2.004476        5.102401       -1.313098
C       2.095142        6.322043       -0.690405
C       2.095142        6.322043        0.690405
C       2.004476        5.102401        1.313098
C       1.615524        1.414202       -5.075651
C       1.524858        2.563659       -5.820088
C       1.524858        3.759350       -5.129406
C       1.615524        3.688687       -3.761851
C       2.004476       -3.688687       -3.761851
C       2.095142       -3.759350       -5.129406
C       2.095142       -2.563659       -5.820088
C       2.004476       -1.414202       -5.075651
C       1.615524       -5.102401        1.313098
C       1.524858       -6.322043        0.690405
C       1.524858       -6.322043       -0.690405
C       1.615524       -5.102401       -1.313098
C       2.004476       -1.414202        5.075651
C       2.095142       -2.563659        5.820088
C       2.095142       -3.759350        5.129406
C       2.004476       -3.688687        3.761851
H       1.599033        4.659095        3.359605
H       1.447000        4.729704        5.612263
H       1.447000        2.497286        6.901899
H       1.599033        0.581194        5.715738
H       2.020967        5.240562       -2.354562
H       2.173000        7.225508       -1.289164
H       2.173000        7.225508        1.289164
H       2.020967        5.240562        2.354562
H       1.599033        0.581194       -5.715738
H       1.447000        2.497286       -6.901899
H       1.447000        4.729704       -5.612263
H       1.599033        4.659095       -3.359605
H       2.020967       -4.659095       -3.359605
H       2.173000       -4.729704       -5.612263
H       2.173000       -2.497286       -6.901899
H       2.020967       -0.581194       -5.715738
```

H	1.599033	-5.240562	2.354562
H	1.447000	-7.225508	1.289164
H	1.447000	-7.225508	-1.289164
H	1.599033	-5.240562	-2.354562
H	2.020967	-0.581194	5.715738
H	2.173000	-2.497286	6.901899
H	2.173000	-4.729704	5.612263
H	2.020967	-4.659095	3.359605
C	-1.721954	3.804764	0.716832
C	-1.721954	3.804764	-0.716832
C	-1.810000	2.539183	-1.466095
C	-1.898046	2.523187	-2.936748
C	-1.898046	1.281740	-3.653706
C	-1.810000	0.000000	-2.932316
C	-1.721954	-1.281740	-3.653706
C	-1.721954	-2.523187	-2.936748
C	-1.810000	-2.539183	-1.466095
C	-1.898046	-3.804764	-0.716832
C	-1.898046	-3.804764	0.716832
C	-1.810000	-2.539183	1.466095
C	-1.721954	-2.523187	2.936748
C	-1.721954	-1.281740	3.653706
C	-1.810000	0.000000	2.932316
C	-1.898046	1.281740	3.653706
C	-1.898046	2.523187	2.936748
C	-1.810000	2.539183	1.466095
C	-1.810000	1.287984	0.743711
C	-1.810000	1.287984	-0.743711
C	-1.810000	0.000000	-1.487627
C	-1.810000	-1.287984	-0.743711
C	-1.810000	-1.287984	0.743711
C	-1.810000	0.000000	1.487627
C	-2.004476	3.688687	3.761851
C	-2.095142	3.759350	5.129406
C	-2.095142	2.563659	5.820088
C	-2.004476	1.414202	5.075651
C	-1.615524	5.102401	-1.313098
C	-1.524858	6.322043	-0.690405
C	-1.524858	6.322043	0.690405
C	-1.615524	5.102401	1.313098
C	-2.004476	1.414202	-5.075651
C	-2.095142	2.563659	-5.820088
C	-2.095142	3.759350	-5.129406
C	-2.004476	3.688687	-3.761851
C	-1.615524	-3.688687	-3.761851
C	-1.524858	-3.759350	-5.129406
C	-1.524858	-2.563659	-5.820088
C	-1.615524	-1.414202	-5.075651
C	-2.004476	-5.102401	1.313098
C	-2.095142	-6.322043	0.690405
C	-2.095142	-6.322043	-0.690405
C	-2.004476	-5.102401	-1.313098
C	-1.615524	-1.414202	5.075651
C	-1.524858	-2.563659	5.820088
C	-1.524858	-3.759350	5.129406
C	-1.615524	-3.688687	3.761851
H	-2.020967	4.659095	3.359605
H	-2.173000	4.729704	5.612263
H	-2.173000	2.497286	6.901899
H	-2.020967	0.581194	5.715738
H	-1.599033	5.240562	-2.354562
H	-1.447000	7.225508	-1.289164
H	-1.447000	7.225508	1.289164
H	-1.599033	5.240562	2.354562
H	-2.020967	0.581194	-5.715738
H	-2.173000	2.497286	-6.901899
H	-2.173000	4.729704	-5.612263
H	-2.020967	4.659095	-3.359605
H	-1.599033	-4.659095	-3.359605
H	-1.447000	-4.729704	-5.612263
H	-1.447000	-2.497286	-6.901899
H	-1.599033	-0.581194	-5.715738
H	-2.020967	-5.240562	2.354562
H	-2.173000	-7.225508	1.289164
H	-2.173000	-7.225508	-1.289164
H	-2.020967	-5.240562	-2.354562
H	-1.599033	-0.581194	5.715738
H	-1.447000	-2.497286	6.901899
H	-1.447000	-4.729704	5.612263
H	-1.599033	-4.659095	3.359605

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cf3, c-HBC_homodimers with bowl depth: 0.29

C	1.941423	3.792003	0.716393
C	1.941423	3.792003	-0.716393
C	1.810000	2.531851	-1.462011
C	1.678577	2.516662	-2.926378
C	1.678577	1.275907	-3.642678

C	1.810000	0.000000	-2.923844
C	1.941423	-1.275907	-3.642678
C	1.941423	-2.516662	-2.926378
C	1.810000	-2.531851	-1.462011
C	1.678577	-3.792003	-0.716393
C	1.678577	-3.792003	0.716393
C	1.810000	-2.531851	1.462011
C	1.941423	-2.516662	2.926378
C	1.941423	-1.275907	3.642678
C	1.810000	0.000000	2.923844
C	1.678577	1.275907	3.642678
C	1.678577	2.516662	2.926378
C	1.810000	2.531851	1.462011
C	1.810000	1.283720	0.741290
C	1.810000	1.283720	-0.741290
C	1.810000	0.000000	-1.482703
C	1.810000	-1.283720	-0.741290
C	1.810000	-1.283720	0.741290
C	1.810000	0.000000	1.482703
C	1.518286	3.683373	3.738481
C	1.380612	3.744854	5.103316
C	1.380612	2.546770	5.795005
C	1.518286	1.395847	5.058937
C	2.101714	5.078515	-1.320689
C	2.239388	6.291295	-0.691735
C	2.239388	6.291295	0.691735
C	2.101714	5.078515	1.320689
C	1.518286	1.395847	-5.058937
C	1.380612	2.546770	-5.795005
C	1.380612	3.744854	-5.103316
C	1.518286	3.683373	-3.738481
C	2.101714	-3.683373	-3.738481
C	2.239388	-3.744854	-5.103316
C	2.239388	-2.546770	-5.795005
C	2.101714	-1.395847	-5.058937
C	1.518286	-5.078515	1.320689
C	1.380612	-6.291295	0.691735
C	1.380612	-6.291295	-0.691735
C	1.518286	-5.078515	-1.320689
C	2.101714	-1.395847	5.058937
C	2.239388	-2.546770	5.795005
C	2.239388	-3.744854	5.103316
C	2.101714	-3.683373	3.738481
H	1.493549	4.648962	3.317113
H	1.261381	4.709998	5.588080
H	1.261381	2.483352	6.873207
H	1.493549	0.548514	5.684672
H	2.126451	5.196754	-2.367565
H	2.358619	7.193567	-1.285493
H	2.358619	7.193567	1.285493
H	2.126451	5.196754	2.367565
H	1.493549	0.548514	-5.684672
H	1.261381	2.483352	-6.873207
H	1.261381	4.709998	-5.588080
H	1.493549	4.648962	-3.317113
H	2.126451	-4.648962	-3.317113
H	2.358619	-4.709998	-5.588080
H	2.358619	-2.483352	-6.873207
H	2.126451	-0.548514	-5.684672
H	1.493549	-5.196754	2.367565
H	1.261381	-7.193567	1.285493
H	1.261381	-7.193567	-1.285493
H	1.493549	-5.196754	-2.367565
H	2.126451	-0.548514	5.684672
H	2.358619	-2.483352	6.873207
H	2.358619	-4.709998	5.588080
H	2.126451	-4.648962	3.317113
C	-1.678577	3.792003	0.716393
C	-1.678577	3.792003	-0.716393
C	-1.810000	2.531851	-1.462011
C	-1.941423	2.516662	-2.926378
C	-1.941423	1.275907	-3.642678
C	-1.810000	0.000000	-2.923844
C	-1.678577	-1.275907	-3.642678
C	-1.678577	-2.516662	-2.926378
C	-1.810000	-2.531851	-1.462011
C	-1.941423	-3.792003	-0.716393
C	-1.941423	-3.792003	0.716393
C	-1.810000	-2.531851	1.462011
C	-1.678577	-2.516662	2.926378
C	-1.678577	-1.275907	3.642678
C	-1.810000	0.000000	2.923844
C	-1.941423	1.275907	3.642678
C	-1.941423	2.516662	2.926378
C	-1.810000	2.531851	1.462011
C	-1.810000	1.283720	0.741290
C	-1.810000	1.283720	-0.741290
C	-1.810000	0.000000	-1.482703
C	-1.810000	-1.283720	-0.741290
C	-1.810000	-1.283720	0.741290

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C      -1.810000        0.000000        1.482703
C      -2.101714        3.683373        3.738481
C      -2.239388        3.744854        5.103316
C      -2.239388        2.546770        5.795005
C      -2.101714        1.395847        5.058937
C      -1.518286        5.078515       -1.320689
C      -1.380612        6.291295       -0.691735
C      -1.380612        6.291295        0.691735
C      -1.518286        5.078515        1.320689
C      -2.101714        1.395847       -5.058937
C      -2.239388        2.546770       -5.795005
C      -2.239388        3.744854       -5.103316
C      -2.101714        3.683373       -3.738481
C      -1.518286       -3.683373       -3.738481
C      -1.380612       -3.744854       -5.103316
C      -1.380612       -2.546770       -5.795005
C      -1.518286       -1.395847       -5.058937
C      -2.101714       -5.078515        1.320689
C      -2.239388       -6.291295        0.691735
C      -2.239388       -6.291295       -0.691735
C      -2.101714       -5.078515       -1.320689
C      -1.518286       -1.395847        5.058937
C      -1.380612       -2.546770        5.795005
C      -1.380612       -3.744854        5.103316
C      -1.518286       -3.683373        3.738481
H      -2.126451        4.648962        3.317113
H      -2.358619        4.709998        5.588080
H      -2.358619        2.483352        6.873207
H      -2.126451        0.548514        5.684672
H      -1.493549        5.196754       -2.367565
H      -1.261381        7.193567       -1.285493
H      -1.261381        7.193567        1.285493
H      -1.493549        5.196754        2.367565
H      -2.126451        0.548514       -5.684672
H      -2.358619        2.483352       -6.873207
H      -2.358619        4.709998       -5.588080
H      -2.126451        4.648962       -3.317113
H      -1.493549       -4.648962       -3.317113
H      -1.261381       -4.709998       -5.588080
H      -1.261381       -2.483352       -6.873207
H      -1.493549       -0.548514       -5.684672
H      -2.126451       -5.196754        2.367565
H      -2.358619       -7.193567        1.285493
H      -2.358619       -7.193567       -1.285493
H      -2.126451       -5.196754       -2.367565
H      -1.493549       -0.548514        5.684672
H      -1.261381       -2.483352        6.873207
H      -1.261381       -4.709998        5.588080
H      -1.493549       -4.648962        3.317113

144
cf4, c-HBC_homodimers with bowl depth: 0.39

C       1.979607        3.774941        0.715820
C       1.979607        3.774941       -0.715820
C       1.805000        2.521952       -1.456200
C       1.630393        2.507550       -2.911699
C       1.630393        1.267834       -3.627567
C       1.805000        0.000000       -2.912336
C       1.979607       -1.267834       -3.627567
C       1.979607       -2.507550       -2.911699
C       1.805000       -2.521952       -1.456200
C       1.630393       -3.774941       -0.715820
C       1.630393       -3.774941        0.715820
C       1.805000       -2.521952        1.456200
C       1.979607       -2.507550        2.911699
C       1.979607       -1.267834        3.627567
C       1.805000        0.000000        2.912336
C       1.630393        1.267834        3.627567
C       1.630393        2.507550        2.911699
C       1.805000        2.521952        1.456200
C       1.805000        1.277889        0.737918
C       1.805000        1.277889       -0.737918
C       1.805000        0.000000       -1.476059
C       1.805000       -1.277889       -0.737918
C       1.805000       -1.277889        0.737918
C       1.805000        0.000000        1.476059
C       1.416048        3.675877        3.704804
C       1.230326        3.725561        5.065499
C       1.230326        2.524451        5.759085
C       1.416048        1.370793        5.035972
C       2.193952        5.046055       -1.330728
C       2.379674        6.249242       -0.693480
C       2.379674        6.249242        0.693480
C       2.193952        5.046055        1.330728
C       1.416048        1.370793       -5.035972
C       1.230326        2.524451       -5.759085
C       1.230326        3.725561       -5.065499
C       1.416048        3.675877       -3.704804
```

C	2.193952	-3.675877	-3.704804
C	2.379674	-3.725561	-5.065499
C	2.379674	-2.524451	-5.759085
C	2.193952	-1.370793	-5.035972
C	1.416048	-5.046055	1.330728
C	1.230326	-6.249242	0.693480
C	1.230326	-6.249242	-0.693480
C	1.416048	-5.046055	-1.330728
C	2.193952	-1.370793	5.035972
C	2.379674	-2.524451	5.759085
C	2.379674	-3.725561	5.065499
C	2.193952	-3.675877	3.704804
H	1.383066	4.634461	3.258073
H	1.068485	4.684060	5.551155
H	1.068485	2.466274	6.832014
H	1.383066	0.504761	5.642821
H	2.226934	5.139011	-2.384193
H	2.541515	7.149255	-1.280464
H	2.541515	7.149255	1.280464
H	2.226934	5.139011	2.384193
H	1.383066	0.504761	-5.642821
H	1.068485	2.466274	-6.832014
H	1.068485	4.684060	-5.551155
H	1.383066	4.634461	-3.258073
H	2.226934	-4.634461	-3.258073
H	2.541515	-4.684060	-5.551155
H	2.541515	-2.466274	-6.832014
H	2.226934	-0.504761	-5.642821
H	1.383066	-5.139011	2.384193
H	1.068485	-7.149255	1.280464
H	1.068485	-7.149255	-1.280464
H	1.383066	-5.139011	-2.384193
H	2.226934	-0.504761	5.642821
H	2.541515	-2.466274	6.832014
H	2.541515	-4.684060	5.551155
H	2.226934	-4.634461	3.258073
C	-1.630393	3.774941	0.715820
C	-1.630393	3.774941	-0.715820
C	-1.805000	2.521952	-1.456200
C	-1.979607	2.507550	-2.911699
C	-1.979607	1.267834	-3.627567
C	-1.805000	0.000000	-2.912336
C	-1.630393	-1.267834	-3.627567
C	-1.630393	-2.507550	-2.911699
C	-1.805000	-2.521952	-1.456200
C	-1.979607	-3.774941	-0.715820
C	-1.979607	-3.774941	0.715820
C	-1.805000	-2.521952	1.456200
C	-1.630393	-2.507550	2.911699
C	-1.630393	-1.267834	3.627567
C	-1.805000	0.000000	2.912336
C	-1.979607	1.267834	3.627567
C	-1.979607	2.507550	2.911699
C	-1.805000	2.521952	1.456200
C	-1.805000	1.277889	0.737918
C	-1.805000	1.277889	-0.737918
C	-1.805000	0.000000	-1.476059
C	-1.805000	-1.277889	-0.737918
C	-1.805000	-1.277889	0.737918
C	-1.805000	0.000000	1.476059
C	-2.193952	3.675877	3.704804
C	-2.379674	3.725561	5.065499
C	-2.379674	2.524451	5.759085
C	-2.193952	1.370793	5.035972
C	-1.416048	5.046055	-1.330728
C	-1.230326	6.249242	-0.693480
C	-1.230326	6.249242	0.693480
C	-1.416048	5.046055	1.330728
C	-2.193952	1.370793	-5.035972
C	-2.379674	2.524451	-5.759085
C	-2.379674	3.725561	-5.065499
C	-2.193952	3.675877	-3.704804
C	-1.416048	-3.675877	-3.704804
C	-1.230326	-3.725561	-5.065499
C	-1.230326	-2.524451	-5.759085
C	-1.416048	-1.370793	-5.035972
C	-2.193952	-5.046055	1.330728
C	-2.379674	-6.249242	0.693480
C	-2.379674	-6.249242	-0.693480
C	-2.193952	-5.046055	-1.330728
C	-1.416048	-1.370793	5.035972
C	-1.230326	-2.524451	5.759085
C	-1.230326	-3.725561	5.065499
C	-1.416048	-3.675877	3.704804
H	-2.226934	4.634461	3.258073
H	-2.541515	4.684060	5.551155
H	-2.541515	2.466274	6.832014
H	-2.226934	0.504761	5.642821
H	-1.383066	5.139011	-2.384193
H	-1.068485	7.149255	-1.280464

```
H      -1.068485        7.149255        1.280464
H      -1.383066        5.139011        2.384193
H      -2.226934        0.504761       -5.642821
H      -2.541515        2.466274       -6.832014
H      -2.541515        4.684060       -5.551155
H      -2.226934        4.634461       -3.258073
H      -1.383066       -4.634461       -3.258073
H      -1.068485       -4.684060       -5.551155
H      -1.068485       -2.466274       -6.832014
H      -1.383066       -0.504761       -5.642821
H      -2.226934       -5.139011        2.384193
H      -2.541515       -7.149255        1.280464
H      -2.541515       -7.149255       -1.280464
H      -2.226934       -5.139011       -2.384193
H      -1.383066       -0.504761        5.642821
H      -1.068485       -2.466274        6.832014
H      -1.068485       -4.684060        5.551155
H      -1.383066       -4.634461        3.258073


144
cf5, c-HBC_homodimers with bowl depth: 0.49
C       2.017458        3.754460        0.715286
C       2.017458        3.754460       -0.715286
C       1.800000        2.510453       -1.449524
C       1.582542        2.497371       -2.894357
C       1.582542        1.258405       -3.609702
C       1.800000        0.000000       -2.899080
C       2.017458       -1.258405       -3.609702
C       2.017458       -2.497371       -2.894357
C       1.800000       -2.510453       -1.449524
C       1.582542       -3.754460       -0.715286
C       1.582542       -3.754460        0.715286
C       1.800000       -2.510453        1.449524
C       2.017458       -2.497371        2.894357
C       2.017458       -1.258405        3.609702
C       1.800000        0.000000        2.899080
C       1.582542        1.258405        3.609702
C       1.582542        2.497371        2.894357
C       1.800000        2.510453        1.449524
C       1.800000        1.271173        0.734062
C       1.800000        1.271173       -0.734062
C       1.800000        0.000000       -1.468337
C       1.800000       -1.271173       -0.734062
C       1.800000       -1.271173        0.734062
C       1.800000        0.000000        1.468337
C       1.313810        3.667036        3.664552
C       1.077728        3.701463        5.019369
C       1.077728        2.496800        5.714969
C       1.313810        1.340892        5.007554
C       2.286190        5.005983       -1.343055
C       2.522272        6.196448       -0.695580
C       2.522272        6.196448        0.695580
C       2.286190        5.005983        1.343055
C       1.313810        1.340892       -5.007554
C       1.077728        2.496800       -5.714969
C       1.077728        3.701463       -5.019369
C       1.313810        3.667036       -3.664552
C       2.286190       -3.667036       -3.664552
C       2.522272       -3.701463       -5.019369
C       2.522272       -2.496800       -5.714969
C       2.286190       -1.340892       -5.007554
C       1.313810       -5.005983        1.343055
C       1.077728       -6.196448        0.695580
C       1.077728       -6.196448       -0.695580
C       1.313810       -5.005983       -1.343055
C       2.286190       -1.340892        5.007554
C       2.522272       -2.496800        5.714969
C       2.522272       -3.701463        5.019369
C       2.286190       -3.667036        3.664552
H       1.272582        4.618364        3.191393
H       0.871275        4.650869        5.505913
H       0.871275        2.443411        6.780448
H       1.272582        0.455038        5.593979
H       2.327418        5.070676       -2.403483
H       2.728725        7.092618       -1.274425
H       2.728725        7.092618        1.274425
H       2.327418        5.070676        2.403483
H       1.272582        0.455038       -5.593979
H       0.871275        2.443411       -6.780448
H       0.871275        4.650869       -5.505913
H       1.272582        4.618364       -3.191393
H       2.327418       -4.618364       -3.191393
H       2.728725       -4.650869       -5.505913
H       2.728725       -2.443411       -6.780448
H       2.327418       -0.455038       -5.593979
H       1.272582       -5.070676        2.403483
H       0.871275       -7.092618        1.274425
H       0.871275       -7.092618       -1.274425
```

```
H       1.272582       -5.070676       -2.403483
H       2.327418       -0.455038        5.593979
H       2.728725       -2.443411        6.780448
H       2.728725       -4.650869        5.505913
H       2.327418       -4.618364        3.191393
C      -1.582542        3.754460        0.715286
C      -1.582542        3.754460       -0.715286
C      -1.800000        2.510453       -1.449524
C      -2.017458        2.497371       -2.894357
C      -2.017458        1.258405       -3.609702
C      -1.800000        0.000000       -2.899080
C      -1.582542       -1.258405       -3.609702
C      -1.582542       -2.497371       -2.894357
C      -1.800000       -2.510453       -1.449524
C      -2.017458       -3.754460       -0.715286
C      -2.017458       -3.754460        0.715286
C      -1.800000       -2.510453        1.449524
C      -1.582542       -2.497371        2.894357
C      -1.582542       -1.258405        3.609702
C      -1.800000        0.000000        2.899080
C      -2.017458        1.258405        3.609702
C      -2.017458        2.497371        2.894357
C      -1.800000        2.510453        1.449524
C      -1.800000        1.271173        0.734062
C      -1.800000        1.271173       -0.734062
C      -1.800000        0.000000       -1.468337
C      -1.800000       -1.271173       -0.734062
C      -1.800000       -1.271173        0.734062
C      -1.800000        0.000000        1.468337
C      -2.286190        3.667036        3.664552
C      -2.522272        3.701463        5.019369
C      -2.522272        2.496800        5.714969
C      -2.286190        1.340892        5.007554
C      -1.313810        5.005983       -1.343055
C      -1.077728        6.196448       -0.695580
C      -1.077728        6.196448        0.695580
C      -1.313810        5.005983        1.343055
C      -2.286190        1.340892       -5.007554
C      -2.522272        2.496800       -5.714969
C      -2.522272        3.701463       -5.019369
C      -2.286190        3.667036       -3.664552
C      -1.313810       -3.667036       -3.664552
C      -1.077728       -3.701463       -5.019369
C      -1.077728       -2.496800       -5.714969
C      -1.313810       -1.340892       -5.007554
C      -2.286190       -5.005983        1.343055
C      -2.522272       -6.196448        0.695580
C      -2.522272       -6.196448       -0.695580
C      -2.286190       -5.005983       -1.343055
C      -1.313810       -1.340892        5.007554
C      -1.077728       -2.496800        5.714969
C      -1.077728       -3.701463        5.019369
C      -1.313810       -3.667036        3.664552
H      -2.327418        4.618364        3.191393
H      -2.728725        4.650869        5.505913
H      -2.728725        2.443411        6.780448
H      -2.327418        0.455038        5.593979
H      -1.272582        5.070676       -2.403483
H      -0.871275        7.092618       -1.274425
H      -0.871275        7.092618        1.274425
H      -1.272582        5.070676        2.403483
H      -2.327418        0.455038       -5.593979
H      -2.728725        2.443411       -6.780448
H      -2.728725        4.650869       -5.505913
H      -2.327418        4.618364       -3.191393
H      -1.272582       -4.618364       -3.191393
H      -0.871275       -4.650869       -5.505913
H      -0.871275       -2.443411       -6.780448
H      -1.272582       -0.455038       -5.593979
H      -2.327418       -5.070676        2.403483
H      -2.728725       -7.092618        1.274425
H      -2.728725       -7.092618       -1.274425
H      -2.327418       -5.070676       -2.403483
H      -1.272582       -0.455038        5.593979
H      -0.871275       -2.443411        6.780448
H      -0.871275       -4.650869        5.505913
H      -1.272582       -4.618364        3.191393
```

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144
cf6, c-HBC_homodimers with bowl depth: 0.58
C       2.060015        3.733455        0.715092
C       2.060015        3.733455       -0.715092
C       1.800000        2.499105       -1.443015
C       1.539985        2.486301       -2.876389
C       1.539985        1.247422       -3.590816
C       1.800000        0.000000       -2.885236
C       2.060015       -1.247422       -3.590816
C       2.060015       -2.486301       -2.876389
```

C	1.800000	-2.499105	-1.443015
C	1.539985	-3.733455	-0.715092
C	1.539985	-3.733455	0.715092
C	1.800000	-2.499105	1.443015
C	2.060015	-2.486301	2.876389
C	2.060015	-1.247422	3.590816
C	1.800000	0.000000	2.885236
C	1.539985	1.247422	3.590816
C	1.539985	2.486301	2.876389
C	1.800000	2.499105	1.443015
C	1.800000	1.264792	0.730215
C	1.800000	1.264792	-0.730215
C	1.800000	0.000000	-1.460219
C	1.800000	-1.264792	-0.730215
C	1.800000	-1.264792	0.730215
C	1.800000	0.000000	1.460219
C	1.216572	3.655344	3.621770
C	0.927875	3.671540	4.968530
C	0.927875	2.462701	5.665353
C	1.216572	1.306031	4.975903
C	2.383428	4.962635	-1.355841
C	2.672125	6.137613	-0.697684
C	2.672125	6.137613	0.697684
C	2.383428	4.962635	1.355841
C	1.216572	1.306031	-4.975903
C	0.927875	2.462701	-5.665353
C	0.927875	3.671540	-4.968530
C	1.216572	3.655344	-3.621770
C	2.383428	-3.655344	-3.621770
C	2.672125	-3.671540	-4.968530
C	2.672125	-2.462701	-5.665353
C	2.383428	-1.306031	-4.975903
C	1.216572	-4.962635	1.355841
C	0.927875	-6.137613	0.697684
C	0.927875	-6.137613	-0.697684
C	1.216572	-4.962635	-1.355841
C	2.383428	-1.306031	4.975903
C	2.672125	-2.462701	5.665353
C	2.672125	-3.671540	4.968530
C	2.383428	-3.655344	3.621770
H	1.167099	4.599951	3.124325
H	0.675399	4.610131	5.454513
H	0.675399	2.412493	6.721105
H	1.167099	0.401276	5.542497
H	2.432901	5.001921	-2.422646
H	2.924601	7.027370	-1.268176
H	2.924601	7.027370	1.268176
H	2.432901	5.001921	2.422646
H	1.167099	0.401276	-5.542497
H	0.675399	2.412493	-6.721105
H	0.675399	4.610131	-5.454513
H	1.167099	4.599951	-3.124325
H	2.432901	-4.599951	-3.124325
H	2.924601	-4.610131	-5.454513
H	2.924601	-2.412493	-6.721105
H	2.432901	-0.401276	-5.542497
H	1.167099	-5.001921	2.422646
H	0.675399	-7.027370	1.268176
H	0.675399	-7.027370	-1.268176
H	1.167099	-5.001921	-2.422646
H	2.432901	-0.401276	5.542497
H	2.924601	-2.412493	6.721105
H	2.924601	-4.610131	5.454513
H	2.432901	-4.599951	3.124325
C	-1.539985	3.733455	0.715092
C	-1.539985	3.733455	-0.715092
C	-1.800000	2.499105	-1.443015
C	-2.060015	2.486301	-2.876389
C	-2.060015	1.247422	-3.590816
C	-1.800000	0.000000	-2.885236
C	-1.539985	-1.247422	-3.590816
C	-1.539985	-2.486301	-2.876389
C	-1.800000	-2.499105	-1.443015
C	-2.060015	-3.733455	-0.715092
C	-2.060015	-3.733455	0.715092
C	-1.800000	-2.499105	1.443015
C	-1.539985	-2.486301	2.876389
C	-1.539985	-1.247422	3.590816
C	-1.800000	0.000000	2.885236
C	-2.060015	1.247422	3.590816
C	-2.060015	2.486301	2.876389
C	-1.800000	2.499105	1.443015
C	-1.800000	1.264792	0.730215
C	-1.800000	1.264792	-0.730215
C	-1.800000	0.000000	-1.460219
C	-1.800000	-1.264792	-0.730215
C	-1.800000	-1.264792	0.730215
C	-1.800000	0.000000	1.460219
C	-2.383428	3.655344	3.621770
C	-2.672125	3.671540	4.968530

C	-2.672125	2.462701	5.665353
C	-2.383428	1.306031	4.975903
C	-1.216572	4.962635	-1.355841
C	-0.927875	6.137613	-0.697684
C	-0.927875	6.137613	0.697684
C	-1.216572	4.962635	1.355841
C	-2.383428	1.306031	-4.975903
C	-2.672125	2.462701	-5.665353
C	-2.672125	3.671540	-4.968530
C	-2.383428	3.655344	-3.621770
C	-1.216572	-3.655344	-3.621770
C	-0.927875	-3.671540	-4.968530
C	-0.927875	-2.462701	-5.665353
C	-1.216572	-1.306031	-4.975903
C	-2.383428	-4.962635	1.355841
C	-2.672125	-6.137613	0.697684
C	-2.672125	-6.137613	-0.697684
C	-2.383428	-4.962635	-1.355841
C	-1.216572	-1.306031	4.975903
C	-0.927875	-2.462701	5.665353
C	-0.927875	-3.671540	4.968530
C	-1.216572	-3.655344	3.621770
H	-2.432901	4.599951	3.124325
H	-2.924601	4.610131	5.454513
H	-2.924601	2.412493	6.721105
H	-2.432901	0.401276	5.542497
H	-1.167099	5.001921	-2.422646
H	-0.675399	7.027370	-1.268176
H	-0.675399	7.027370	1.268176
H	-1.167099	5.001921	2.422646
H	-2.432901	0.401276	-5.542497
H	-2.924601	2.412493	-6.721105
H	-2.924601	4.610131	-5.454513
H	-2.432901	4.599951	-3.124325
H	-1.167099	-4.599951	-3.124325
H	-0.675399	-4.610131	-5.454513
H	-0.675399	-2.412493	-6.721105
H	-1.167099	-0.401276	-5.542497
H	-2.432901	-5.001921	2.422646
H	-2.924601	-7.027370	1.268176
H	-2.924601	-7.027370	-1.268176
H	-2.432901	-5.001921	-2.422646
H	-1.167099	-0.401276	5.542497
H	-0.675399	-2.412493	6.721105
H	-0.675399	-4.610131	5.454513
H	-1.167099	-4.599951	3.124325

144

cf7, c-HBC_homodimers with bowl depth: 0.68

C	2.127399	3.712718	0.715184
C	2.127399	3.712718	-0.715184
C	1.825000	2.488680	-1.436815
C	1.522601	2.475904	-2.857940
C	1.522601	1.236993	-3.572735
C	1.825000	0.000000	-2.873399
C	2.127399	-1.236993	-3.572735
C	2.127399	-2.475904	-2.857940
C	1.825000	-2.488680	-1.436815
C	1.522601	-3.712718	-0.715184
C	1.522601	-3.712718	0.715184
C	1.825000	-2.488680	1.436815
C	2.127399	-2.475904	2.857940
C	2.127399	-1.236993	3.572735
C	1.825000	0.000000	2.873399
C	1.522601	1.236993	3.572735
C	1.522601	2.475904	2.857940
C	1.825000	2.488680	1.436815
C	1.825000	1.258800	0.726759
C	1.825000	1.258800	-0.726759
C	1.825000	0.000000	-1.453365
C	1.825000	-1.258800	-0.726759
C	1.825000	-1.258800	0.726759
C	1.825000	0.000000	1.453365
C	1.144334	3.643188	3.575824
C	0.803589	3.642613	4.912222
C	0.803589	2.430751	5.611320
C	1.144334	1.273887	4.942558
C	2.505666	4.917656	-1.367709
C	2.846411	6.075007	-0.699550
C	2.846411	6.075007	0.699550
C	2.505666	4.917656	1.367709
C	1.144334	1.273887	-4.942558
C	0.803589	2.430751	-5.611320
C	0.803589	3.642613	-4.912222
C	1.144334	3.643188	-3.575824
C	2.505666	-3.643188	-3.575824
C	2.846411	-3.642613	-4.912222
C	2.846411	-2.430751	-5.611320

C	2.505666	-1.273887	-4.942558
C	1.144334	-4.917656	1.367709
C	0.803589	-6.075007	0.699550
C	0.803589	-6.075007	-0.699550
C	1.144334	-4.917656	-1.367709
C	2.505666	-1.273887	4.942558
C	2.846411	-2.430751	5.611320
C	2.846411	-3.642613	4.912222
C	2.505666	-3.643188	3.575824
H	1.086615	4.581226	3.056642
H	0.506410	4.570250	5.394106
H	0.506410	2.383365	6.655566
H	1.086615	0.354480	5.494018
H	2.563385	4.936374	-2.439744
H	3.143590	6.955908	-1.262320
H	3.143590	6.955908	1.262320
H	2.563385	4.936374	2.439744
H	1.086615	0.354480	-5.494018
H	0.506410	2.383365	-6.655566
H	0.506410	4.570250	-5.394106
H	1.086615	4.581226	-3.056642
H	2.563385	-4.581226	-3.056642
H	3.143590	-4.570250	-5.394106
H	3.143590	-2.383365	-6.655566
H	2.563385	-0.354480	-5.494018
H	1.086615	-4.936374	2.439744
H	0.506410	-6.955908	1.262320
H	0.506410	-6.955908	-1.262320
H	1.086615	-4.936374	-2.439744
H	2.563385	-0.354480	5.494018
H	3.143590	-2.383365	6.655566
H	3.143590	-4.570250	5.394106
H	2.563385	-4.581226	3.056642
C	-1.522601	3.712718	0.715184
C	-1.522601	3.712718	-0.715184
C	-1.825000	2.488680	-1.436815
C	-2.127399	2.475904	-2.857940
C	-2.127399	1.236993	-3.572735
C	-1.825000	0.000000	-2.873399
C	-1.522601	-1.236993	-3.572735
C	-1.522601	-2.475904	-2.857940
C	-1.825000	-2.488680	-1.436815
C	-2.127399	-3.712718	-0.715184
C	-2.127399	-3.712718	0.715184
C	-1.825000	-2.488680	1.436815
C	-1.522601	-2.475904	2.857940
C	-1.522601	-1.236993	3.572735
C	-1.825000	0.000000	2.873399
C	-2.127399	1.236993	3.572735
C	-2.127399	2.475904	2.857940
C	-1.825000	2.488680	1.436815
C	-1.825000	1.258800	0.726759
C	-1.825000	1.258800	-0.726759
C	-1.825000	0.000000	-1.453365
C	-1.825000	-1.258800	-0.726759
C	-1.825000	-1.258800	0.726759
C	-1.825000	0.000000	1.453365
C	-2.505666	3.643188	3.575824
C	-2.846411	3.642613	4.912222
C	-2.846411	2.430751	5.611320
C	-2.505666	1.273887	4.942558
C	-1.144334	4.917656	-1.367709
C	-0.803589	6.075007	-0.699550
C	-0.803589	6.075007	0.699550
C	-1.144334	4.917656	1.367709
C	-2.505666	1.273887	-4.942558
C	-2.846411	2.430751	-5.611320
C	-2.846411	3.642613	-4.912222
C	-2.505666	3.643188	-3.575824
C	-1.144334	-3.643188	-3.575824
C	-0.803589	-3.642613	-4.912222
C	-0.803589	-2.430751	-5.611320
C	-1.144334	-1.273887	-4.942558
C	-2.505666	-4.917656	1.367709
C	-2.846411	-6.075007	0.699550
C	-2.846411	-6.075007	-0.699550
C	-2.505666	-4.917656	-1.367709
C	-1.144334	-1.273887	4.942558
C	-0.803589	-2.430751	5.611320
C	-0.803589	-3.642613	4.912222
C	-1.144334	-3.643188	3.575824
H	-2.563385	4.581226	3.056642
H	-3.143590	4.570250	5.394106
H	-3.143590	2.383365	6.655566
H	-2.563385	0.354480	5.494018
H	-1.086615	4.936374	-2.439744
H	-0.506410	6.955908	-1.262320
H	-0.506410	6.955908	1.262320
H	-1.086615	4.936374	2.439744
H	-2.563385	0.354480	-5.494018

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H      -3.143590        2.383365       -6.655566
H      -3.143590        4.570250       -5.394106
H      -2.563385        4.581226       -3.056642
H      -1.086615       -4.581226       -3.056642
H      -0.506410       -4.570250       -5.394106
H      -0.506410       -2.383365       -6.655566
H      -1.086615       -0.354480       -5.494018
H      -2.563385       -4.936374        2.439744
H      -3.143590       -6.955908        1.262320
H      -3.143590       -6.955908       -1.262320
H      -2.563385       -4.936374       -2.439744
H      -1.086615       -0.354480        5.494018
H      -0.506410       -2.383365        6.655566
H      -0.506410       -4.570250        5.394106
H      -1.086615       -4.581226        3.056642
```

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cf8, c-HBC_homodimers with bowl depth: 0.78
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```
C       2.232601        3.693207        0.715499
C       2.232601        3.693207       -0.715499
C       1.890000        2.479858       -1.431690
C       1.547399        2.466326       -2.840747
C       1.547399        1.226933       -3.556147
C       1.890000        0.000000       -2.863424
C       2.232601       -1.226933       -3.556147
C       2.232601       -2.466326       -2.840747
C       1.890000       -2.479858       -1.431690
C       1.547399       -3.693207       -0.715499
C       1.547399       -3.693207        0.715499
C       1.890000       -2.479858        1.431690
C       2.232601       -2.466326        2.840747
C       2.232601       -1.226933        3.556147
C       1.890000        0.000000        2.863424
C       1.547399        1.226933        3.556147
C       1.547399        2.466326        2.840747
C       1.890000        2.479858        1.431690
C       1.890000        1.253749        0.723893
C       1.890000        1.253749       -0.723893
C       1.890000        0.000000       -1.447809
C       1.890000       -1.253749       -0.723893
C       1.890000       -1.253749        0.723893
C       1.890000        0.000000        1.447809
C       1.112095        3.628540        3.530559
C       0.712918        3.610388        4.852189
C       0.712918        2.396154        5.553045
C       1.112095        1.242804        4.907557
C       2.667905        4.871586       -1.377361
C       3.067082        6.007185       -0.701015
C       3.067082        6.007185        0.701015
C       2.667905        4.871586        1.377361
C       1.112095        1.242804       -4.907557
C       0.712918        2.396154       -5.553045
C       0.712918        3.610388       -4.852189
C       1.112095        3.628540       -3.530559
C       2.667905       -3.628540       -3.530559
C       3.067082       -3.610388       -4.852189
C       3.067082       -2.396154       -5.553045
C       2.667905       -1.242804       -4.907557
C       1.112095       -4.871586        1.377361
C       0.712918       -6.007185        0.701015
C       0.712918       -6.007185       -0.701015
C       1.112095       -4.871586       -1.377361
C       2.667905       -1.242804        4.907557
C       3.067082       -2.396154        5.553045
C       3.067082       -3.610388        4.852189
C       2.667905       -3.628540        3.530559
H       1.046132        4.561236        2.994717
H       0.366201        4.525678        5.324479
H       0.366201        2.347226        6.581824
H       1.046132        0.312211        5.446957
H       2.733868        4.873694       -2.453113
H       3.413799        6.873742       -1.257659
H       3.413799        6.873742        1.257659
H       2.733868        4.873694        2.453113
H       1.046132        0.312211       -5.446957
H       0.366201        2.347226       -6.581824
H       0.366201        4.525678       -5.324479
H       1.046132        4.561236       -2.994717
H       2.733868       -4.561236       -2.994717
H       3.413799       -4.525678       -5.324479
H       3.413799       -2.347226       -6.581824
H       2.733868       -0.312211       -5.446957
H       1.046132       -4.873694        2.453113
H       0.366201       -6.873742        1.257659
H       0.366201       -6.873742       -1.257659
H       1.046132       -4.873694       -2.453113
H       2.733868       -0.312211        5.446957
H       3.413799       -2.347226        6.581824
```

H	3.413799	-4.525678	5.324479
H	2.733868	-4.561236	2.994717
C	-1.547399	3.693207	0.715499
C	-1.547399	3.693207	-0.715499
C	-1.890000	2.479858	-1.431690
C	-2.232601	2.466326	-2.840747
C	-2.232601	1.226933	-3.556147
C	-1.890000	0.000000	-2.863424
C	-1.547399	-1.226933	-3.556147
C	-1.547399	-2.466326	-2.840747
C	-1.890000	-2.479858	-1.431690
C	-2.232601	-3.693207	-0.715499
C	-2.232601	-3.693207	0.715499
C	-1.890000	-2.479858	1.431690
C	-1.547399	-2.466326	2.840747
C	-1.547399	-1.226933	3.556147
C	-1.890000	0.000000	2.863424
C	-2.232601	1.226933	3.556147
C	-2.232601	2.466326	2.840747
C	-1.890000	2.479858	1.431690
C	-1.890000	1.253749	0.723893
C	-1.890000	1.253749	-0.723893
C	-1.890000	0.000000	-1.447809
C	-1.890000	-1.253749	-0.723893
C	-1.890000	-1.253749	0.723893
C	-1.890000	0.000000	1.447809
C	-2.667905	3.628540	3.530559
C	-3.067082	3.610388	4.852189
C	-3.067082	2.396154	5.553045
C	-2.667905	1.242804	4.907557
C	-1.112095	4.871586	-1.377361
C	-0.712918	6.007185	-0.701015
C	-0.712918	6.007185	0.701015
C	-1.112095	4.871586	1.377361
C	-2.667905	1.242804	-4.907557
C	-3.067082	2.396154	-5.553045
C	-3.067082	3.610388	-4.852189
C	-2.667905	3.628540	-3.530559
C	-1.112095	-3.628540	-3.530559
C	-0.712918	-3.610388	-4.852189
C	-0.712918	-2.396154	-5.553045
C	-1.112095	-1.242804	-4.907557
C	-2.667905	-4.871586	1.377361
C	-3.067082	-6.007185	0.701015
C	-3.067082	-6.007185	-0.701015
C	-2.667905	-4.871586	-1.377361
C	-1.112095	-1.242804	4.907557
C	-0.712918	-2.396154	5.553045
C	-0.712918	-3.610388	4.852189
C	-1.112095	-3.628540	3.530559
H	-2.733868	4.561236	2.994717
H	-3.413799	4.525678	5.324479
H	-3.413799	2.347226	6.581824
H	-2.733868	0.312211	5.446957
H	-1.046132	4.873694	-2.453113
H	-0.366201	6.873742	-1.257659
H	-0.366201	6.873742	1.257659
H	-1.046132	4.873694	2.453113
H	-2.733868	0.312211	-5.446957
H	-3.413799	2.347226	-6.581824
H	-3.413799	4.525678	-5.324479
H	-2.733868	4.561236	-2.994717
H	-1.046132	-4.561236	-2.994717
H	-0.366201	-4.525678	-5.324479
H	-0.366201	-2.347226	-6.581824
H	-1.046132	-0.312211	-5.446957
H	-2.733868	-4.873694	2.453113
H	-3.413799	-6.873742	1.257659
H	-3.413799	-6.873742	-1.257659
H	-2.733868	-4.873694	-2.453113
H	-1.046132	-0.312211	5.446957
H	-0.366201	-2.347226	6.581824
H	-0.366201	-4.525678	5.324479
H	-1.046132	-4.561236	2.994717

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cf9, c-HBC_homodimers with bowl depth: 0.88

C	2.358342	3.674611	0.716164
C	2.358342	3.674611	-0.716164
C	1.975000	2.472708	-1.427494
C	1.591658	2.457475	-2.824075
C	1.591658	1.217043	-3.540448
C	1.975000	0.000000	-2.855361
C	2.358342	-1.217043	-3.540448
C	2.358342	-2.457475	-2.824075
C	1.975000	-2.472708	-1.427494
C	1.591658	-3.674611	-0.716164
C	1.591658	-3.674611	0.716164

C	1.975000	-2.472708	1.427494
C	2.358342	-2.457475	2.824075
C	2.358342	-1.217043	3.540448
C	1.975000	0.000000	2.855361
C	1.591658	1.217043	3.540448
C	1.591658	2.457475	2.824075
C	1.975000	2.472708	1.427494
C	1.975000	1.249661	0.721548
C	1.975000	1.249661	-0.721548
C	1.975000	0.000000	-1.443188
C	1.975000	-1.249661	-0.721548
C	1.975000	-1.249661	0.721548
C	1.975000	0.000000	1.443188
C	1.099857	3.612157	3.485617
C	0.648966	3.577647	4.791755
C	0.648966	2.361565	5.494155
C	1.099857	1.212964	4.871324
C	2.850143	4.825039	-1.385311
C	3.301034	5.938833	-0.702196
C	3.301034	5.938833	0.702196
C	2.850143	4.825039	1.385311
C	1.099857	1.212964	-4.871324
C	0.648966	2.361565	-5.494155
C	0.648966	3.577647	-4.791755
C	1.099857	3.612157	-3.485617
C	2.850143	-3.612157	-3.485617
C	3.301034	-3.577647	-4.791755
C	3.301034	-2.361565	-5.494155
C	2.850143	-1.212964	-4.871324
C	1.099857	-4.825039	1.385311
C	0.648966	-5.938833	0.702196
C	0.648966	-5.938833	-0.702196
C	1.099857	-4.825039	-1.385311
C	2.850143	-1.212964	4.871324
C	3.301034	-2.361565	5.494155
C	3.301034	-3.577647	4.791755
C	2.850143	-3.612157	3.485617
H	1.025648	4.539775	2.935734
H	0.258442	4.481294	5.252371
H	0.258442	2.309174	6.507044
H	1.025648	0.273097	5.399982
H	2.924352	4.812830	-2.463693
H	3.691558	6.789700	-1.254227
H	3.691558	6.789700	1.254227
H	2.924352	4.812830	2.463693
H	1.025648	0.273097	-5.399982
H	0.258442	2.309174	-6.507044
H	0.258442	4.481294	-5.252371
H	1.025648	4.539775	-2.935734
H	2.924352	-4.539775	-2.935734
H	3.691558	-4.481294	-5.252371
H	3.691558	-2.309174	-6.507044
H	2.924352	-0.273097	-5.399982
H	1.025648	-4.812830	2.463693
H	0.258442	-6.789700	1.254227
H	0.258442	-6.789700	-1.254227
H	1.025648	-4.812830	-2.463693
H	2.924352	-0.273097	5.399982
H	3.691558	-2.309174	6.507044
H	3.691558	-4.481294	5.252371
H	2.924352	-4.539775	2.935734
C	-1.591658	3.674611	0.716164
C	-1.591658	3.674611	-0.716164
C	-1.975000	2.472708	-1.427494
C	-2.358342	2.457475	-2.824075
C	-2.358342	1.217043	-3.540448
C	-1.975000	0.000000	-2.855361
C	-1.591658	-1.217043	-3.540448
C	-1.591658	-2.457475	-2.824075
C	-1.975000	-2.472708	-1.427494
C	-2.358342	-3.674611	-0.716164
C	-2.358342	-3.674611	0.716164
C	-1.975000	-2.472708	1.427494
C	-1.591658	-2.457475	2.824075
C	-1.591658	-1.217043	3.540448
C	-1.975000	0.000000	2.855361
C	-2.358342	1.217043	3.540448
C	-2.358342	2.457475	2.824075
C	-1.975000	2.472708	1.427494
C	-1.975000	1.249661	0.721548
C	-1.975000	1.249661	-0.721548
C	-1.975000	0.000000	-1.443188
C	-1.975000	-1.249661	-0.721548
C	-1.975000	-1.249661	0.721548
C	-1.975000	0.000000	1.443188
C	-2.850143	3.612157	3.485617
C	-3.301034	3.577647	4.791755
C	-3.301034	2.361565	5.494155
C	-2.850143	1.212964	4.871324
C	-1.099857	4.825039	-1.385311

C	-0.648966	5.938833	-0.702196
C	-0.648966	5.938833	0.702196
C	-1.099857	4.825039	1.385311
C	-2.850143	1.212964	-4.871324
C	-3.301034	2.361565	-5.494155
C	-3.301034	3.577647	-4.791755
C	-2.850143	3.612157	-3.485617
C	-1.099857	-3.612157	-3.485617
C	-0.648966	-3.577647	-4.791755
C	-0.648966	-2.361565	-5.494155
C	-1.099857	-1.212964	-4.871324
C	-2.850143	-4.825039	1.385311
C	-3.301034	-5.938833	0.702196
C	-3.301034	-5.938833	-0.702196
C	-2.850143	-4.825039	-1.385311
C	-1.099857	-1.212964	4.871324
C	-0.648966	-2.361565	5.494155
C	-0.648966	-3.577647	4.791755
C	-1.099857	-3.612157	3.485617
H	-2.924352	4.539775	2.935734
H	-3.691558	4.481294	5.252371
H	-3.691558	2.309174	6.507044
H	-2.924352	0.273097	5.399982
H	-1.025648	4.812830	-2.463693
H	-0.258442	6.789700	-1.254227
H	-0.258442	6.789700	1.254227
H	-1.025648	4.812830	2.463693
H	-2.924352	0.273097	-5.399982
H	-3.691558	2.309174	-6.507044
H	-3.691558	4.481294	-5.252371
H	-2.924352	4.539775	-2.935734
H	-1.025648	-4.539775	-2.935734
H	-0.258442	-4.481294	-5.252371
H	-0.258442	-2.309174	-6.507044
H	-1.025648	-0.273097	-5.399982
H	-2.924352	-4.812830	2.463693
H	-3.691558	-6.789700	1.254227
H	-3.691558	-6.789700	-1.254227
H	-2.924352	-4.812830	-2.463693
H	-1.025648	-0.273097	5.399982
H	-0.258442	-2.309174	6.507044
H	-0.258442	-4.481294	5.252371
H	-1.025648	-4.539775	2.935734

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cf10, c-HBC_homodimers with bowl depth: 0.97

C	2.537503	3.655806	0.716950
C	2.537503	3.655806	-0.716950
C	2.115000	2.466249	-1.423834
C	1.692497	2.448608	-2.807547
C	1.692497	1.206820	-3.524503
C	2.115000	0.000000	-2.847667
C	2.537503	-1.206820	-3.524503
C	2.537503	-2.448608	-2.807547
C	2.115000	-2.466249	-1.423834
C	1.692497	-3.655806	-0.716950
C	1.692497	-3.655806	0.716950
C	2.115000	-2.466249	1.423834
C	2.537503	-2.448608	2.807547
C	2.537503	-1.206820	3.524503
C	2.115000	0.000000	2.847667
C	1.692497	1.206820	3.524503
C	1.692497	2.448608	2.807547
C	2.115000	2.466249	1.423834
C	2.115000	1.246049	0.719408
C	2.115000	1.246049	-0.719408
C	2.115000	0.000000	-1.438745
C	2.115000	-1.246049	-0.719408
C	2.115000	-1.246049	0.719408
C	2.115000	0.000000	1.438745
C	1.142619	3.592716	3.439074
C	0.636270	3.539577	4.725616
C	0.636270	2.321708	5.428703
C	1.142619	1.181228	4.831145
C	3.087381	4.774679	-1.392136
C	3.593730	5.862372	-0.703121
C	3.593730	5.862372	0.703121
C	3.087381	4.774679	1.392136
C	1.142619	1.181228	-4.831145
C	0.636270	2.321708	-5.428703
C	0.636270	3.539577	-4.725616
C	1.142619	3.592716	-3.439074
C	3.087381	-3.592716	-3.439074
C	3.593730	-3.539577	-4.725616
C	3.593730	-2.321708	-5.428703
C	3.087381	-1.181228	-4.831145
C	1.142619	-4.774679	1.392136
C	0.636270	-5.862372	0.703121

C	0.636270	-5.862372	-0.703121
C	1.142619	-4.774679	-1.392136
C	3.087381	-1.181228	4.831145
C	3.593730	-2.321708	5.428703
C	3.593730	-3.539577	4.725616
C	3.087381	-3.592716	3.439074
H	1.060165	4.514831	2.875927
H	0.198130	4.429041	5.170770
H	0.198130	2.262238	6.421544
H	1.060165	0.232345	5.347771
H	3.169835	4.747651	-2.472254
H	4.031870	6.692546	-1.250943
H	4.031870	6.692546	1.250943
H	3.169835	4.747651	2.472254
H	1.060165	0.232345	-5.347771
H	0.198130	2.262238	-6.421544
H	0.198130	4.429041	-5.170770
H	1.060165	4.514831	-2.875927
H	3.169835	-4.514831	-2.875927
H	4.031870	-4.429041	-5.170770
H	4.031870	-2.262238	-6.421544
H	3.169835	-0.232345	-5.347771
H	1.060165	-4.747651	2.472254
H	0.198130	-6.692546	1.250943
H	0.198130	-6.692546	-1.250943
H	1.060165	-4.747651	-2.472254
H	3.169835	-0.232345	5.347771
H	4.031870	-2.262238	6.421544
H	4.031870	-4.429041	5.170770
H	3.169835	-4.514831	2.875927
C	-1.692497	3.655806	0.716950
C	-1.692497	3.655806	-0.716950
C	-2.115000	2.466249	-1.423834
C	-2.537503	2.448608	-2.807547
C	-2.537503	1.206820	-3.524503
C	-2.115000	0.000000	-2.847667
C	-1.692497	-1.206820	-3.524503
C	-1.692497	-2.448608	-2.807547
C	-2.115000	-2.466249	-1.423834
C	-2.537503	-3.655806	-0.716950
C	-2.537503	-3.655806	0.716950
C	-2.115000	-2.466249	1.423834
C	-1.692497	-2.448608	2.807547
C	-1.692497	-1.206820	3.524503
C	-2.115000	0.000000	2.847667
C	-2.537503	1.206820	3.524503
C	-2.537503	2.448608	2.807547
C	-2.115000	2.466249	1.423834
C	-2.115000	1.246049	0.719408
C	-2.115000	1.246049	-0.719408
C	-2.115000	0.000000	-1.438745
C	-2.115000	-1.246049	-0.719408
C	-2.115000	-1.246049	0.719408
C	-2.115000	0.000000	1.438745
C	-3.087381	3.592716	3.439074
C	-3.593730	3.539577	4.725616
C	-3.593730	2.321708	5.428703
C	-3.087381	1.181228	4.831145
C	-1.142619	4.774679	-1.392136
C	-0.636270	5.862372	-0.703121
C	-0.636270	5.862372	0.703121
C	-1.142619	4.774679	1.392136
C	-3.087381	1.181228	-4.831145
C	-3.593730	2.321708	-5.428703
C	-3.593730	3.539577	-4.725616
C	-3.087381	3.592716	-3.439074
C	-1.142619	-3.592716	-3.439074
C	-0.636270	-3.539577	-4.725616
C	-0.636270	-2.321708	-5.428703
C	-1.142619	-1.181228	-4.831145
C	-3.087381	-4.774679	1.392136
C	-3.593730	-5.862372	0.703121
C	-3.593730	-5.862372	-0.703121
C	-3.087381	-4.774679	-1.392136
C	-1.142619	-1.181228	4.831145
C	-0.636270	-2.321708	5.428703
C	-0.636270	-3.539577	4.725616
C	-1.142619	-3.592716	3.439074
H	-3.169835	4.514831	2.875927
H	-4.031870	4.429041	5.170770
H	-4.031870	2.262238	6.421544
H	-3.169835	0.232345	5.347771
H	-1.060165	4.747651	-2.472254
H	-0.198130	6.692546	-1.250943
H	-0.198130	6.692546	1.250943
H	-1.060165	4.747651	2.472254
H	-3.169835	0.232345	-5.347771
H	-4.031870	2.262238	-6.421544
H	-4.031870	4.429041	-5.170770
H	-3.169835	4.514831	-2.875927

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H      -1.060165       -4.514831       -2.875927
H      -0.198130       -4.429041       -5.170770
H      -0.198130       -2.262238       -6.421544
H      -1.060165       -0.232345       -5.347771
H      -3.169835       -4.747651        2.472254
H      -4.031870       -6.692546        1.250943
H      -4.031870       -6.692546       -1.250943
H      -3.169835       -4.747651       -2.472254
H      -1.060165       -0.232345        5.347771
H      -0.198130       -2.262238        6.421544
H      -0.198130       -4.429041        5.170770
H      -1.060165       -4.514831        2.875927


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cf11, c-HBC_homodimers with bowl depth: 1.07

C       2.696320        3.639058        0.718044
C       2.696320        3.639058       -0.718044
C       2.235000        2.462031       -1.421454
C       1.773680        2.441192       -2.792638
C       1.773680        1.197407       -3.510444
C       2.235000        0.000000       -2.842357
C       2.696320       -1.197407       -3.510444
C       2.696320       -2.441192       -2.792638
C       2.235000       -2.462031       -1.421454
C       1.773680       -3.639058       -0.718044
C       1.773680       -3.639058        0.718044
C       2.235000       -2.462031        1.421454
C       2.696320       -2.441192        2.792638
C       2.696320       -1.197407        3.510444
C       2.235000        0.000000        2.842357
C       1.773680        1.197407        3.510444
C       1.773680        2.441192        2.792638
C       2.235000        2.462031        1.421454
C       2.235000        1.243675        0.717977
C       2.235000        1.243675       -0.717977
C       2.235000        0.000000       -1.435841
C       2.235000       -1.243675       -0.717977
C       2.235000       -1.243675        0.717977
C       2.235000        0.000000        1.435841
C       1.165381        3.571653        3.394077
C       0.606656        3.500587        4.659123
C       0.606656        2.281665        5.362358
C       1.165381        1.151351        4.790062
C       3.304619        4.724691       -1.396729
C       3.863344        5.785202       -0.703581
C       3.863344        5.785202        0.703581
C       3.304619        4.724691        1.396729
C       1.165381        1.151351       -4.790062
C       0.606656        2.281665       -5.362358
C       0.606656        3.500587       -4.659123
C       1.165381        3.571653       -3.394077
C       3.304619       -3.571653       -3.394077
C       3.863344       -3.500587       -4.659123
C       3.863344       -2.281665       -5.362358
C       3.304619       -1.151351       -4.790062
C       1.165381       -4.724691        1.396729
C       0.606656       -5.785202        0.703581
C       0.606656       -5.785202       -0.703581
C       1.165381       -4.724691       -1.396729
C       3.304619       -1.151351        4.790062
C       3.863344       -2.281665        5.362358
C       3.863344       -3.500587        4.659123
C       3.304619       -3.571653        3.394077
H       1.074681        4.489091        2.821383
H       0.124180        4.375892        5.086347
H       0.124180        2.213221        6.333905
H       1.074681        0.195490        5.296036
H       3.395319        4.685905       -2.477483
H       4.345820        6.592538       -1.248419
H       4.345820        6.592538        1.248419
H       3.395319        4.685905        2.477483
H       1.074681        0.195490       -5.296036
H       0.124180        2.213221       -6.333905
H       0.124180        4.375892       -5.086347
H       1.074681        4.489091       -2.821383
H       3.395319       -4.489091       -2.821383
H       4.345820       -4.375892       -5.086347
H       4.345820       -2.213221       -6.333905
H       3.395319       -0.195490       -5.296036
H       1.074681       -4.685905        2.477483
H       0.124180       -6.592538        1.248419
H       0.124180       -6.592538       -1.248419
H       1.074681       -4.685905       -2.477483
H       3.395319       -0.195490        5.296036
H       4.345820       -2.213221        6.333905
H       4.345820       -4.375892        5.086347
H       3.395319       -4.489091        2.821383
C      -1.773680        3.639058        0.718044
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C	-1.773680	3.639058	-0.718044
C	-2.235000	2.462031	-1.421454
C	-2.696320	2.441192	-2.792638
C	-2.696320	1.197407	-3.510444
C	-2.235000	0.000000	-2.842357
C	-1.773680	-1.197407	-3.510444
C	-1.773680	-2.441192	-2.792638
C	-2.235000	-2.462031	-1.421454
C	-2.696320	-3.639058	-0.718044
C	-2.696320	-3.639058	0.718044
C	-2.235000	-2.462031	1.421454
C	-1.773680	-2.441192	2.792638
C	-1.773680	-1.197407	3.510444
C	-2.235000	0.000000	2.842357
C	-2.696320	1.197407	3.510444
C	-2.696320	2.441192	2.792638
C	-2.235000	2.462031	1.421454
C	-2.235000	1.243675	0.717977
C	-2.235000	1.243675	-0.717977
C	-2.235000	0.000000	-1.435841
C	-2.235000	-1.243675	-0.717977
C	-2.235000	-1.243675	0.717977
C	-2.235000	0.000000	1.435841
C	-3.304619	3.571653	3.394077
C	-3.863344	3.500587	4.659123
C	-3.863344	2.281665	5.362358
C	-3.304619	1.151351	4.790062
C	-1.165381	4.724691	-1.396729
C	-0.606656	5.785202	-0.703581
C	-0.606656	5.785202	0.703581
C	-1.165381	4.724691	1.396729
C	-3.304619	1.151351	-4.790062
C	-3.863344	2.281665	-5.362358
C	-3.863344	3.500587	-4.659123
C	-3.304619	3.571653	-3.394077
C	-1.165381	-3.571653	-3.394077
C	-0.606656	-3.500587	-4.659123
C	-0.606656	-2.281665	-5.362358
C	-1.165381	-1.151351	-4.790062
C	-3.304619	-4.724691	1.396729
C	-3.863344	-5.785202	0.703581
C	-3.863344	-5.785202	-0.703581
C	-3.304619	-4.724691	-1.396729
C	-1.165381	-1.151351	4.790062
C	-0.606656	-2.281665	5.362358
C	-0.606656	-3.500587	4.659123
C	-1.165381	-3.571653	3.394077
H	-3.395319	4.489091	2.821383
H	-4.345820	4.375892	5.086347
H	-4.345820	2.213221	6.333905
H	-3.395319	0.195490	5.296036
H	-1.074681	4.685905	-2.477483
H	-0.124180	6.592538	-1.248419
H	-0.124180	6.592538	1.248419
H	-1.074681	4.685905	2.477483
H	-3.395319	0.195490	-5.296036
H	-4.345820	2.213221	-6.333905
H	-4.345820	4.375892	-5.086347
H	-3.395319	4.489091	-2.821383
H	-1.074681	-4.489091	-2.821383
H	-0.124180	-4.375892	-5.086347
H	-0.124180	-2.213221	-6.333905
H	-1.074681	-0.195490	-5.296036
H	-3.395319	-4.685905	2.477483
H	-4.345820	-6.592538	1.248419
H	-4.345820	-6.592538	-1.248419
H	-3.395319	-4.685905	-2.477483
H	-1.074681	-0.195490	5.296036
H	-0.124180	-2.213221	6.333905
H	-0.124180	-4.375892	5.086347
H	-1.074681	-4.489091	2.821383

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cf12, c-HBC_homodimers with bowl depth: 1.17

C	2.874903	3.622018	0.719085
C	2.874903	3.622018	-0.719085
C	2.375000	2.458433	-1.419277
C	1.875097	2.433585	-2.777166
C	1.875097	1.188048	-3.496066
C	2.375000	0.000000	-2.838326
C	2.874903	-1.188048	-3.496066
C	2.874903	-2.433585	-2.777166
C	2.375000	-2.458433	-1.419277
C	1.875097	-3.622018	-0.719085
C	1.875097	-3.622018	0.719085
C	2.375000	-2.458433	1.419277
C	2.874903	-2.433585	2.777166
C	2.874903	-1.188048	3.496066

C	2.375000	0.000000	2.838326
C	1.875097	1.188048	3.496066
C	1.875097	2.433585	2.777166
C	2.375000	2.458433	1.419277
C	2.375000	1.241653	0.716816
C	2.375000	1.241653	-0.716816
C	2.375000	0.000000	-1.433348
C	2.375000	-1.241653	-0.716816
C	2.375000	-1.241653	0.716816
C	2.375000	0.000000	1.433348
C	1.208143	3.547605	3.345992
C	0.593850	3.458236	4.584555
C	0.593850	2.239210	5.288008
C	1.208143	1.122428	4.745123
C	3.541857	4.671374	-1.399719
C	4.156150	5.699690	-0.703683
C	4.156150	5.699690	0.703683
C	3.541857	4.671374	1.399719
C	1.208143	1.122428	-4.745123
C	0.593850	2.239210	-5.288008
C	0.593850	3.458236	-4.584555
C	1.208143	3.547605	-3.345992
C	3.541857	-3.547605	-3.345992
C	4.156150	-3.458236	-4.584555
C	4.156150	-2.239210	-5.288008
C	3.541857	-1.122428	-4.745123
C	1.208143	-4.671374	1.399719
C	0.593850	-5.699690	0.703683
C	0.593850	-5.699690	-0.703683
C	1.208143	-4.671374	-1.399719
C	3.541857	-1.122428	4.745123
C	4.156150	-2.239210	5.288008
C	4.156150	-3.458236	4.584555
C	3.541857	-3.547605	3.345992
H	1.109198	4.459676	2.764373
H	0.064247	4.317751	4.987444
H	0.064247	2.157766	6.233721
H	1.109198	0.162013	5.242908
H	3.640802	4.622907	-2.480457
H	4.685753	6.478085	-1.246964
H	4.685753	6.478085	1.246964
H	3.640802	4.622907	2.480457
H	1.109198	0.162013	-5.242908
H	0.064247	2.157766	-6.233721
H	0.064247	4.317751	-4.987444
H	1.109198	4.459676	-2.764373
H	3.640802	-4.459676	-2.764373
H	4.685753	-4.317751	-4.987444
H	4.685753	-2.157766	-6.233721
H	3.640802	-0.162013	-5.242908
H	1.109198	-4.622907	2.480457
H	0.064247	-6.478085	1.246964
H	0.064247	-6.478085	-1.246964
H	1.109198	-4.622907	-2.480457
H	3.640802	-0.162013	5.242908
H	4.685753	-2.157766	6.233721
H	4.685753	-4.317751	4.987444
H	3.640802	-4.459676	2.764373
C	-1.875097	3.622018	0.719085
C	-1.875097	3.622018	-0.719085
C	-2.375000	2.458433	-1.419277
C	-2.874903	2.433585	-2.777166
C	-2.874903	1.188048	-3.496066
C	-2.375000	0.000000	-2.838326
C	-1.875097	-1.188048	-3.496066
C	-1.875097	-2.433585	-2.777166
C	-2.375000	-2.458433	-1.419277
C	-2.874903	-3.622018	-0.719085
C	-2.874903	-3.622018	0.719085
C	-2.375000	-2.458433	1.419277
C	-1.875097	-2.433585	2.777166
C	-1.875097	-1.188048	3.496066
C	-2.375000	0.000000	2.838326
C	-2.874903	1.188048	3.496066
C	-2.874903	2.433585	2.777166
C	-2.375000	2.458433	1.419277
C	-2.375000	1.241653	0.716816
C	-2.375000	1.241653	-0.716816
C	-2.375000	0.000000	-1.433348
C	-2.375000	-1.241653	-0.716816
C	-2.375000	-1.241653	0.716816
C	-2.375000	0.000000	1.433348
C	-3.541857	3.547605	3.345992
C	-4.156150	3.458236	4.584555
C	-4.156150	2.239210	5.288008
C	-3.541857	1.122428	4.745123
C	-1.208143	4.671374	-1.399719
C	-0.593850	5.699690	-0.703683
C	-0.593850	5.699690	0.703683
C	-1.208143	4.671374	1.399719

C	-3.541857	1.122428	-4.745123
C	-4.156150	2.239210	-5.288008
C	-4.156150	3.458236	-4.584555
C	-3.541857	3.547605	-3.345992
C	-1.208143	-3.547605	-3.345992
C	-0.593850	-3.458236	-4.584555
C	-0.593850	-2.239210	-5.288008
C	-1.208143	-1.122428	-4.745123
C	-3.541857	-4.671374	1.399719
C	-4.156150	-5.699690	0.703683
C	-4.156150	-5.699690	-0.703683
C	-3.541857	-4.671374	-1.399719
C	-1.208143	-1.122428	4.745123
C	-0.593850	-2.239210	5.288008
C	-0.593850	-3.458236	4.584555
C	-1.208143	-3.547605	3.345992
H	-3.640802	4.459676	2.764373
H	-4.685753	4.317751	4.987444
H	-4.685753	2.157766	6.233721
H	-3.640802	0.162013	5.242908
H	-1.109198	4.622907	-2.480457
H	-0.064247	6.478085	-1.246964
H	-0.064247	6.478085	1.246964
H	-1.109198	4.622907	2.480457
H	-3.640802	0.162013	-5.242908
H	-4.685753	2.157766	-6.233721
H	-4.685753	4.317751	-4.987444
H	-3.640802	4.459676	-2.764373
H	-1.109198	-4.459676	-2.764373
H	-0.064247	-4.317751	-4.987444
H	-0.064247	-2.157766	-6.233721
H	-1.109198	-0.162013	-5.242908
H	-3.640802	-4.622907	2.480457
H	-4.685753	-6.478085	1.246964
H	-4.685753	-6.478085	-1.246964
H	-3.640802	-4.622907	-2.480457
H	-1.109198	-0.162013	5.242908
H	-0.064247	-2.157766	6.233721
H	-0.064247	-4.317751	4.987444
H	-1.109198	-4.459676	2.764373

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cf13, c-HBC_homodimers with bowl depth: 1.26

C	3.049256	3.605395	0.720380
C	3.049256	3.605395	-0.720380
C	2.510000	2.456228	-1.418051
C	1.970744	2.426441	-2.762191
C	1.970744	1.178533	-3.482296
C	2.510000	0.000000	-2.835579
C	3.049256	-1.178533	-3.482296
C	3.049256	-2.426441	-2.762191
C	2.510000	-2.456228	-1.418051
C	1.970744	-3.605395	-0.720380
C	1.970744	-3.605395	0.720380
C	2.510000	-2.456228	1.418051
C	3.049256	-2.426441	2.762191
C	3.049256	-1.178533	3.482296
C	2.510000	0.000000	2.835579
C	1.970744	1.178533	3.482296
C	1.970744	2.426441	2.762191
C	2.510000	2.456228	1.418051
C	2.510000	1.240315	0.715998
C	2.510000	1.240315	-0.715998
C	2.510000	0.000000	-1.431769
C	2.510000	-1.240315	-0.715998
C	2.510000	-1.240315	0.715998
C	2.510000	0.000000	1.431769
C	1.245905	3.521268	3.297863
C	0.579254	3.413542	4.508142
C	0.579254	2.194654	5.211194
C	1.245905	1.093371	4.697928
C	3.774095	4.616242	-1.401147
C	4.440746	5.611058	-0.703523
C	4.440746	5.611058	0.703523
C	3.774095	4.616242	1.401147
C	1.245905	1.093371	-4.697928
C	0.579254	2.194654	-5.211194
C	0.579254	3.413542	-4.508142
C	1.245905	3.521268	-3.297863
C	3.774095	-3.521268	-3.297863
C	4.440746	-3.413542	-4.508142
C	4.440746	-2.194654	-5.211194
C	3.774095	-1.093371	-4.697928
C	1.245905	-4.616242	1.401147
C	0.579254	-5.611058	0.703523
C	0.579254	-5.611058	-0.703523
C	1.245905	-4.616242	-1.401147
C	3.774095	-1.093371	4.697928

C	4.440746	-2.194654	5.211194
C	4.440746	-3.413542	4.508142
C	3.774095	-3.521268	3.297863
H	1.138714	4.429087	2.709979
H	0.006468	4.257091	4.884800
H	0.006468	2.098110	6.129927
H	1.138714	0.129289	5.188119
H	3.881286	4.559579	-2.481229
H	5.013532	6.358592	-1.246305
H	5.013532	6.358592	1.246305
H	3.881286	4.559579	2.481229
H	1.138714	0.129289	-5.188119
H	0.006468	2.098110	-6.129927
H	0.006468	4.257091	-4.884800
H	1.138714	4.429087	-2.709979
H	3.881286	-4.429087	-2.709979
H	5.013532	-4.257091	-4.884800
H	5.013532	-2.098110	-6.129927
H	3.881286	-0.129289	-5.188119
H	1.138714	-4.559579	2.481229
H	0.006468	-6.358592	1.246305
H	0.006468	-6.358592	-1.246305
H	1.138714	-4.559579	-2.481229
H	3.881286	-0.129289	5.188119
H	5.013532	-2.098110	6.129927
H	5.013532	-4.257091	4.884800
H	3.881286	-4.429087	2.709979
C	-1.970744	3.605395	0.720380
C	-1.970744	3.605395	-0.720380
C	-2.510000	2.456228	-1.418051
C	-3.049256	2.426441	-2.762191
C	-3.049256	1.178533	-3.482296
C	-2.510000	0.000000	-2.835579
C	-1.970744	-1.178533	-3.482296
C	-1.970744	-2.426441	-2.762191
C	-2.510000	-2.456228	-1.418051
C	-3.049256	-3.605395	-0.720380
C	-3.049256	-3.605395	0.720380
C	-2.510000	-2.456228	1.418051
C	-1.970744	-2.426441	2.762191
C	-1.970744	-1.178533	3.482296
C	-2.510000	0.000000	2.835579
C	-3.049256	1.178533	3.482296
C	-3.049256	2.426441	2.762191
C	-2.510000	2.456228	1.418051
C	-2.510000	1.240315	0.715998
C	-2.510000	1.240315	-0.715998
C	-2.510000	0.000000	-1.431769
C	-2.510000	-1.240315	-0.715998
C	-2.510000	-1.240315	0.715998
C	-2.510000	0.000000	1.431769
C	-3.774095	3.521268	3.297863
C	-4.440746	3.413542	4.508142
C	-4.440746	2.194654	5.211194
C	-3.774095	1.093371	4.697928
C	-1.245905	4.616242	-1.401147
C	-0.579254	5.611058	-0.703523
C	-0.579254	5.611058	0.703523
C	-1.245905	4.616242	1.401147
C	-3.774095	1.093371	-4.697928
C	-4.440746	2.194654	-5.211194
C	-4.440746	3.413542	-4.508142
C	-3.774095	3.521268	-3.297863
C	-1.245905	-3.521268	-3.297863
C	-0.579254	-3.413542	-4.508142
C	-0.579254	-2.194654	-5.211194
C	-1.245905	-1.093371	-4.697928
C	-3.774095	-4.616242	1.401147
C	-4.440746	-5.611058	0.703523
C	-4.440746	-5.611058	-0.703523
C	-3.774095	-4.616242	-1.401147
C	-1.245905	-1.093371	4.697928
C	-0.579254	-2.194654	5.211194
C	-0.579254	-3.413542	4.508142
C	-1.245905	-3.521268	3.297863
H	-3.881286	4.429087	2.709979
H	-5.013532	4.257091	4.884800
H	-5.013532	2.098110	6.129927
H	-3.881286	0.129289	5.188119
H	-1.138714	4.559579	-2.481229
H	-0.006468	6.358592	-1.246305
H	-0.006468	6.358592	1.246305
H	-1.138714	4.559579	2.481229
H	-3.881286	0.129289	-5.188119
H	-5.013532	2.098110	-6.129927
H	-5.013532	4.257091	-4.884800
H	-3.881286	4.429087	-2.709979
H	-1.138714	-4.429087	-2.709979
H	-0.006468	-4.257091	-4.884800
H	-0.006468	-2.098110	-6.129927

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H      -1.138714       -0.129289       -5.188119
H      -3.881286       -4.559579        2.481229
H      -5.013532       -6.358592        1.246305
H      -5.013532       -6.358592       -1.246305
H      -3.881286       -4.559579       -2.481229
H      -1.138714       -0.129289        5.188119
H      -0.006468       -2.098110        6.129927
H      -0.006468       -4.257091        4.884800
H      -1.138714       -4.429087        2.709979

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cf14, c-HBC_homodimers with bowl depth: 1.36

C       3.234456        3.587945        0.721714
C       3.234456        3.587945       -0.721714
C       2.655000        2.454289       -1.416911
C       2.075544        2.418869       -2.746292
C       2.075544        1.168767       -3.468029
C       2.655000        0.000000       -2.833756
C       3.234456       -1.168767       -3.468029
C       3.234456       -2.418869       -2.746292
C       2.655000       -2.454289       -1.416911
C       2.075544       -3.587945       -0.721714
C       2.075544       -3.587945        0.721714
C       2.655000       -2.454289        1.416911
C       3.234456       -2.418869        2.746292
C       3.234456       -1.168767        3.468029
C       2.655000        0.000000        2.833756
C       2.075544        1.168767        3.468029
C       2.075544        2.418869        2.746292
C       2.655000        2.454289        1.416911
C       2.655000        1.239148        0.715383
C       2.655000        1.239148       -0.715383
C       2.655000        0.000000       -1.430689
C       2.655000       -1.239148       -0.715383
C       2.655000       -1.239148        0.715383
C       2.655000        0.000000        1.430689
C       1.293667        3.492607        3.245605
C       0.575834        3.366327        4.424804
C       0.575834        2.148120        5.127952
C       1.293667        1.063941        4.647319
C       4.016333        4.557030       -1.402022
C       4.734166        5.515288       -0.703255
C       4.734166        5.515288        0.703255
C       4.016333        4.557030        1.402022
C       1.293667        1.063941       -4.647319
C       0.575834        2.148120       -5.127952
C       0.575834        3.366327       -4.424804
C       1.293667        3.492607       -3.245605
C       4.016333       -3.492607       -3.245605
C       4.734166       -3.366327       -4.424804
C       4.734166       -2.148120       -5.127952
C       4.016333       -1.063941       -4.647319
C       1.293667       -4.557030        1.402022
C       0.575834       -5.515288        0.703255
C       0.575834       -5.515288       -0.703255
C       1.293667       -4.557030       -1.402022
C       4.016333       -1.063941        4.647319
C       4.734166       -2.148120        5.127952
C       4.734166       -3.366327        4.424804
C       4.016333       -3.492607        3.245605
H       1.178231        4.395381        2.650807
H      -0.038746        4.193065        4.771612
H      -0.038746        2.034811        6.017306
H       1.178231        0.097072        5.130953
H       4.131769        4.492529       -2.481171
H       5.348746        6.228819       -1.246054
H       5.348746        6.228819        1.246054
H       4.131769        4.492529        2.481171
H       1.178231        0.097072       -5.130953
H      -0.038746        2.034811       -6.017306
H      -0.038746        4.193065       -4.771612
H       1.178231        4.395381       -2.650807
H       4.131769       -4.395381       -2.650807
H       5.348746       -4.193065       -4.771612
H       5.348746       -2.034811       -6.017306
H       4.131769       -0.097072       -5.130953
H       1.178231       -4.492529        2.481171
H      -0.038746       -6.228819        1.246054
H      -0.038746       -6.228819       -1.246054
H       1.178231       -4.492529       -2.481171
H       4.131769       -0.097072        5.130953
H       5.348746       -2.034811        6.017306
H       5.348746       -4.193065        4.771612
H       4.131769       -4.395381        2.650807
C      -2.075544        3.587945        0.721714
C      -2.075544        3.587945       -0.721714
C      -2.655000        2.454289       -1.416911
C      -3.234456        2.418869       -2.746292
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C	-3.234456	1.168767	-3.468029
C	-2.655000	0.000000	-2.833756
C	-2.075544	-1.168767	-3.468029
C	-2.075544	-2.418869	-2.746292
C	-2.655000	-2.454289	-1.416911
C	-3.234456	-3.587945	-0.721714
C	-3.234456	-3.587945	0.721714
C	-2.655000	-2.454289	1.416911
C	-2.075544	-2.418869	2.746292
C	-2.075544	-1.168767	3.468029
C	-2.655000	0.000000	2.833756
C	-3.234456	1.168767	3.468029
C	-3.234456	2.418869	2.746292
C	-2.655000	2.454289	1.416911
C	-2.655000	1.239148	0.715383
C	-2.655000	1.239148	-0.715383
C	-2.655000	0.000000	-1.430689
C	-2.655000	-1.239148	-0.715383
C	-2.655000	-1.239148	0.715383
C	-2.655000	0.000000	1.430689
C	-4.016333	3.492607	3.245605
C	-4.734166	3.366327	4.424804
C	-4.734166	2.148120	5.127952
C	-4.016333	1.063941	4.647319
C	-1.293667	4.557030	-1.402022
C	-0.575834	5.515288	-0.703255
C	-0.575834	5.515288	0.703255
C	-1.293667	4.557030	1.402022
C	-4.016333	1.063941	-4.647319
C	-4.734166	2.148120	-5.127952
C	-4.734166	3.366327	-4.424804
C	-4.016333	3.492607	-3.245605
C	-1.293667	-3.492607	-3.245605
C	-0.575834	-3.366327	-4.424804
C	-0.575834	-2.148120	-5.127952
C	-1.293667	-1.063941	-4.647319
C	-4.016333	-4.557030	1.402022
C	-4.734166	-5.515288	0.703255
C	-4.734166	-5.515288	-0.703255
C	-4.016333	-4.557030	-1.402022
C	-1.293667	-1.063941	4.647319
C	-0.575834	-2.148120	5.127952
C	-0.575834	-3.366327	4.424804
C	-1.293667	-3.492607	3.245605
H	-4.131769	4.395381	2.650807
H	-5.348746	4.193065	4.771612
H	-5.348746	2.034811	6.017306
H	-4.131769	0.097072	5.130953
H	-1.178231	4.492529	-2.481171
H	0.038746	6.228819	-1.246054
H	0.038746	6.228819	1.246054
H	-1.178231	4.492529	2.481171
H	-4.131769	0.097072	-5.130953
H	-5.348746	2.034811	-6.017306
H	-5.348746	4.193065	-4.771612
H	-4.131769	4.395381	-2.650807
H	-1.178231	-4.395381	-2.650807
H	0.038746	-4.193065	-4.771612
H	0.038746	-2.034811	-6.017306
H	-1.178231	-0.097072	-5.130953
H	-4.131769	-4.492529	2.481171
H	-5.348746	-6.228819	1.246054
H	-5.348746	-6.228819	-1.246054
H	-4.131769	-4.492529	-2.481171
H	-1.178231	-0.097072	5.130953
H	0.038746	-2.034811	6.017306
H	0.038746	-4.193065	4.771612
H	-1.178231	-4.395381	2.650807

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cf15, c-HBC_homodimers with bowl depth: 1.46

C	3.420602	3.569082	0.723231
C	3.420602	3.569082	-0.723231
C	2.800000	2.452588	-1.415951
C	2.179398	2.410719	-2.729199
C	2.179398	1.157997	-3.452525
C	2.800000	0.000000	-2.831871
C	3.420602	-1.157997	-3.452525
C	3.420602	-2.410719	-2.729199
C	2.800000	-2.452588	-1.415951
C	2.179398	-3.569082	-0.723231
C	2.179398	-3.569082	0.723231
C	2.800000	-2.452588	1.415951
C	3.420602	-2.410719	2.729199
C	3.420602	-1.157997	3.452525
C	2.800000	0.000000	2.831871
C	2.179398	1.157997	3.452525
C	2.179398	2.410719	2.729199

C	2.800000	2.452588	1.415951
C	2.800000	1.238078	0.714775
C	2.800000	1.238078	-0.714775
C	2.800000	0.000000	-1.429510
C	2.800000	-1.238078	-0.714775
C	2.800000	-1.238078	0.714775
C	2.800000	0.000000	1.429510
C	1.341429	3.460759	3.189520
C	0.573880	3.314193	4.334928
C	0.573880	2.096728	5.037721
C	1.341429	1.031534	4.591870
C	4.258571	4.492509	-1.402615
C	5.026120	5.411118	-0.702854
C	5.026120	5.411118	0.702854
C	4.258571	4.492509	1.402615
C	1.341429	1.031534	-4.591870
C	0.573880	2.096728	-5.037721
C	0.573880	3.314193	-4.334928
C	1.341429	3.460759	-3.189520
C	4.258571	-3.460759	-3.189520
C	5.026120	-3.314193	-4.334928
C	5.026120	-2.096728	-5.037721
C	4.258571	-1.031534	-4.591870
C	1.341429	-4.492509	1.402615
C	0.573880	-5.411118	0.702854
C	0.573880	-5.411118	-0.702854
C	1.341429	-4.492509	-1.402615
C	4.258571	-1.031534	4.591870
C	5.026120	-2.096728	5.037721
C	5.026120	-3.314193	4.334928
C	4.258571	-3.460759	3.189520
H	1.217747	4.358006	2.587502
H	-0.080742	4.122751	4.649816
H	-0.080742	1.964996	5.895406
H	1.217747	0.061339	5.067512
H	4.382253	4.419424	-2.480657
H	5.680742	6.088115	-1.245627
H	5.680742	6.088115	1.245627
H	4.382253	4.419424	2.480657
H	1.217747	0.061339	-5.067512
H	-0.080742	1.964996	-5.895406
H	-0.080742	4.122751	-4.649816
H	1.217747	4.358006	-2.587502
H	4.382253	-4.358006	-2.587502
H	5.680742	-4.122751	-4.649816
H	5.680742	-1.964996	-5.895406
H	4.382253	-0.061339	-5.067512
H	1.217747	-4.419424	2.480657
H	-0.080742	-6.088115	1.245627
H	-0.080742	-6.088115	-1.245627
H	1.217747	-4.419424	-2.480657
H	4.382253	-0.061339	5.067512
H	5.680742	-1.964996	5.895406
H	5.680742	-4.122751	4.649816
H	4.382253	-4.358006	2.587502
C	-2.179398	3.569082	0.723231
C	-2.179398	3.569082	-0.723231
C	-2.800000	2.452588	-1.415951
C	-3.420602	2.410719	-2.729199
C	-3.420602	1.157997	-3.452525
C	-2.800000	0.000000	-2.831871
C	-2.179398	-1.157997	-3.452525
C	-2.179398	-2.410719	-2.729199
C	-2.800000	-2.452588	-1.415951
C	-3.420602	-3.569082	-0.723231
C	-3.420602	-3.569082	0.723231
C	-2.800000	-2.452588	1.415951
C	-2.179398	-2.410719	2.729199
C	-2.179398	-1.157997	3.452525
C	-2.800000	0.000000	2.831871
C	-3.420602	1.157997	3.452525
C	-3.420602	2.410719	2.729199
C	-2.800000	2.452588	1.415951
C	-2.800000	1.238078	0.714775
C	-2.800000	1.238078	-0.714775
C	-2.800000	0.000000	-1.429510
C	-2.800000	-1.238078	-0.714775
C	-2.800000	-1.238078	0.714775
C	-2.800000	0.000000	1.429510
C	-4.258571	3.460759	3.189520
C	-5.026120	3.314193	4.334928
C	-5.026120	2.096728	5.037721
C	-4.258571	1.031534	4.591870
C	-1.341429	4.492509	-1.402615
C	-0.573880	5.411118	-0.702854
C	-0.573880	5.411118	0.702854
C	-1.341429	4.492509	1.402615
C	-4.258571	1.031534	-4.591870
C	-5.026120	2.096728	-5.037721
C	-5.026120	3.314193	-4.334928

```
C      -4.258571        3.460759       -3.189520
C      -1.341429       -3.460759       -3.189520
C      -0.573880       -3.314193       -4.334928
C      -0.573880       -2.096728       -5.037721
C      -1.341429       -1.031534       -4.591870
C      -4.258571       -4.492509        1.402615
C      -5.026120       -5.411118        0.702854
C      -5.026120       -5.411118       -0.702854
C      -4.258571       -4.492509       -1.402615
C      -1.341429       -1.031534        4.591870
C      -0.573880       -2.096728        5.037721
C      -0.573880       -3.314193        4.334928
C      -1.341429       -3.460759        3.189520
H      -4.382253        4.358006        2.587502
H      -5.680742        4.122751        4.649816
H      -5.680742        1.964996        5.895406
H      -4.382253        0.061339        5.067512
H      -1.217747        4.419424       -2.480657
H       0.080742        6.088115       -1.245627
H       0.080742        6.088115        1.245627
H      -1.217747        4.419424        2.480657
H      -4.382253        0.061339       -5.067512
H      -5.680742        1.964996       -5.895406
H      -5.680742        4.122751       -4.649816
H      -4.382253        4.358006       -2.587502
H      -1.217747       -4.358006       -2.587502
H       0.080742       -4.122751       -4.649816
H       0.080742       -1.964996       -5.895406
H      -1.217747       -0.061339       -5.067512
H      -4.382253       -4.419424        2.480657
H      -5.680742       -6.088115        1.245627
H      -5.680742       -6.088115       -1.245627
H      -4.382253       -4.419424       -2.480657
H      -1.217747       -0.061339        5.067512
H       0.080742       -1.964996        5.895406
H       0.080742       -4.122751        4.649816
H      -1.217747       -4.358006        2.587502


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cf16, c-HBC_homodimers with bowl depth: 1.56

C       3.618197        3.548373        0.724881
C       3.618197        3.548373       -0.724881
C       2.955000        2.451021       -1.415072
C       2.291803        2.401820       -2.710471
C       2.291803        1.146238       -3.435471
C       2.955000        0.000000       -2.829997
C       3.618197       -1.146238       -3.435471
C       3.618197       -2.401820       -2.710471
C       2.955000       -2.451021       -1.415072
C       2.291803       -3.548373       -0.724881
C       2.291803       -3.548373        0.724881
C       2.955000       -2.451021        1.415072
C       3.618197       -2.401820        2.710471
C       3.618197       -1.146238        3.435471
C       2.955000        0.000000        2.829997
C       2.291803        1.146238        3.435471
C       2.291803        2.401820        2.710471
C       2.955000        2.451021        1.415072
C       2.955000        1.237031        0.714145
C       2.955000        1.237031       -0.714145
C       2.955000        0.000000       -1.428285
C       2.955000       -1.237031       -0.714145
C       2.955000       -1.237031        0.714145
C       2.955000        0.000000        1.428285
C       1.399191        3.426012        3.128997
C       0.583468        3.257487        4.237712
C       0.583468        2.040843        4.940019
C       1.399191        0.996457        4.531565
C       4.510809        4.422578       -1.402917
C       5.326532        5.298345       -0.702392
C       5.326532        5.298345        0.702392
C       4.510809        4.422578        1.402917
C       1.399191        0.996457       -4.531565
C       0.583468        2.040843       -4.940019
C       0.583468        3.257487       -4.237712
C       1.399191        3.426012       -3.128997
C       4.510809       -3.426012       -3.128997
C       5.326532       -3.257487       -4.237712
C       5.326532       -2.040843       -4.940019
C       4.510809       -0.996457       -4.531565
C       1.399191       -4.422578        1.402917
C       0.583468       -5.298345        0.702392
C       0.583468       -5.298345       -0.702392
C       1.399191       -4.422578       -1.402917
C       4.510809       -0.996457        4.531565
C       5.326532       -2.040843        4.940019
C       5.326532       -3.257487        4.237712
C       4.510809       -3.426012        3.128997
```

H	1.267264	4.317568	2.519766
H	-0.109479	4.046524	4.518207
H	-0.109479	1.889061	5.763585
H	1.267264	0.022887	4.998685
H	4.642736	4.340592	-2.479633
H	6.019479	5.935917	-1.245330
H	6.019479	5.935917	1.245330
H	4.642736	4.340592	2.479633
H	1.267264	0.022887	-4.998685
H	-0.109479	1.889061	-5.763585
H	-0.109479	4.046524	-4.518207
H	1.267264	4.317568	-2.519766
H	4.642736	-4.317568	-2.519766
H	6.019479	-4.046524	-4.518207
H	6.019479	-1.889061	-5.763585
H	4.642736	-0.022887	-4.998685
H	1.267264	-4.340592	2.479633
H	-0.109479	-5.935917	1.245330
H	-0.109479	-5.935917	-1.245330
H	1.267264	-4.340592	-2.479633
H	4.642736	-0.022887	4.998685
H	6.019479	-1.889061	5.763585
H	6.019479	-4.046524	4.518207
H	4.642736	-4.317568	2.519766
C	-2.291803	3.548373	0.724881
C	-2.291803	3.548373	-0.724881
C	-2.955000	2.451021	-1.415072
C	-3.618197	2.401820	-2.710471
C	-3.618197	1.146238	-3.435471
C	-2.955000	0.000000	-2.829997
C	-2.291803	-1.146238	-3.435471
C	-2.291803	-2.401820	-2.710471
C	-2.955000	-2.451021	-1.415072
C	-3.618197	-3.548373	-0.724881
C	-3.618197	-3.548373	0.724881
C	-2.955000	-2.451021	1.415072
C	-2.291803	-2.401820	2.710471
C	-2.291803	-1.146238	3.435471
C	-2.955000	0.000000	2.829997
C	-3.618197	1.146238	3.435471
C	-3.618197	2.401820	2.710471
C	-2.955000	2.451021	1.415072
C	-2.955000	1.237031	0.714145
C	-2.955000	1.237031	-0.714145
C	-2.955000	0.000000	-1.428285
C	-2.955000	-1.237031	-0.714145
C	-2.955000	-1.237031	0.714145
C	-2.955000	0.000000	1.428285
C	-4.510809	3.426012	3.128997
C	-5.326532	3.257487	4.237712
C	-5.326532	2.040843	4.940019
C	-4.510809	0.996457	4.531565
C	-1.399191	4.422578	-1.402917
C	-0.583468	5.298345	-0.702392
C	-0.583468	5.298345	0.702392
C	-1.399191	4.422578	1.402917
C	-4.510809	0.996457	-4.531565
C	-5.326532	2.040843	-4.940019
C	-5.326532	3.257487	-4.237712
C	-4.510809	3.426012	-3.128997
C	-1.399191	-3.426012	-3.128997
C	-0.583468	-3.257487	-4.237712
C	-0.583468	-2.040843	-4.940019
C	-1.399191	-0.996457	-4.531565
C	-4.510809	-4.422578	1.402917
C	-5.326532	-5.298345	0.702392
C	-5.326532	-5.298345	-0.702392
C	-4.510809	-4.422578	-1.402917
C	-1.399191	-0.996457	4.531565
C	-0.583468	-2.040843	4.940019
C	-0.583468	-3.257487	4.237712
C	-1.399191	-3.426012	3.128997
H	-4.642736	4.317568	2.519766
H	-6.019479	4.046524	4.518207
H	-6.019479	1.889061	5.763585
H	-4.642736	0.022887	4.998685
H	-1.267264	4.340592	-2.479633
H	0.109479	5.935917	-1.245330
H	0.109479	5.935917	1.245330
H	-1.267264	4.340592	2.479633
H	-4.642736	0.022887	-4.998685
H	-6.019479	1.889061	-5.763585
H	-6.019479	4.046524	-4.518207
H	-4.642736	4.317568	-2.519766
H	-1.267264	-4.317568	-2.519766
H	0.109479	-4.046524	-4.518207
H	0.109479	-1.889061	-5.763585
H	-1.267264	-0.022887	-4.998685
H	-4.642736	-4.340592	2.479633
H	-6.019479	-5.935917	1.245330

```
H      -6.019479       -5.935917       -1.245330
H      -4.642736       -4.340592       -2.479633
H      -1.267264       -0.022887        4.998685
H       0.109479       -1.889061        5.763585
H       0.109479       -4.046524        4.518207
H      -1.267264       -4.317568        2.519766

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cf17, c-HBC_homodimers with bowl depth: 1.65

C       3.847284        3.526050        0.726722
C       3.847284        3.526050       -0.726722
C       3.140000        2.449623       -1.414289
C       2.432716        2.392313       -2.690241
C       2.432716        1.133530       -3.417063
C       3.140000        0.000000       -2.828353
C       3.847284       -1.133530       -3.417063
C       3.847284       -2.392313       -2.690241
C       3.140000       -2.449623       -1.414289
C       2.432716       -3.526050       -0.726722
C       2.432716       -3.526050        0.726722
C       3.140000       -2.449623        1.414289
C       3.847284       -2.392313        2.690241
C       3.847284       -1.133530        3.417063
C       3.140000        0.000000        2.828353
C       2.432716        1.133530        3.417063
C       2.432716        2.392313        2.690241
C       3.140000        2.449623        1.414289
C       3.140000        1.236126        0.713630
C       3.140000        1.236126       -0.713630
C       3.140000        0.000000       -1.427240
C       3.140000       -1.236126       -0.713630
C       3.140000       -1.236126        0.713630
C       3.140000        0.000000        1.427240
C       1.486953        3.388367        3.063883
C       0.624926        3.196415        4.133221
C       0.624926        1.980748        4.834944
C       1.486953        0.958813        4.466397
C       4.793047        4.347304       -1.402829
C       5.655074        5.177398       -0.701821
C       5.655074        5.177398        0.701821
C       4.793047        4.347304        1.402829
C       1.486953        0.958813       -4.466397
C       0.624926        1.980748       -4.834944
C       0.624926        3.196415       -4.133221
C       1.486953        3.388367       -3.063883
C       4.793047       -3.388367       -3.063883
C       5.655074       -3.196415       -4.133221
C       5.655074       -1.980748       -4.834944
C       4.793047       -0.958813       -4.466397
C       1.486953       -4.347304        1.402829
C       0.624926       -5.177398        0.701821
C       0.624926       -5.177398       -0.701821
C       1.486953       -4.347304       -1.402829
C       4.793047       -0.958813        4.466397
C       5.655074       -1.980748        4.834944
C       5.655074       -3.196415        4.133221
C       4.793047       -3.388367        3.063883
H       1.346780        4.274053        2.447458
H      -0.104369        3.964696        4.376635
H      -0.104369        1.807178        5.621946
H       1.346780       -0.018112        4.924681
H       4.933220        4.256227       -2.478069
H       6.384369        5.772408       -1.245412
H       6.384369        5.772408        1.245412
H       4.933220        4.256227        2.478069
H       1.346780       -0.018112       -4.924681
H      -0.104369        1.807178       -5.621946
H      -0.104369        3.964696       -4.376635
H       1.346780        4.274053       -2.447458
H       4.933220       -4.274053       -2.447458
H       6.384369       -3.964696       -4.376635
H       6.384369       -1.807178       -5.621946
H       4.933220        0.018112       -4.924681
H       1.346780       -4.256227        2.478069
H      -0.104369       -5.772408        1.245412
H      -0.104369       -5.772408       -1.245412
H       1.346780       -4.256227       -2.478069
H       4.933220        0.018112        4.924681
H       6.384369       -1.807178        5.621946
H       6.384369       -3.964696        4.376635
H       4.933220       -4.274053        2.447458
C      -2.432716        3.526050        0.726722
C      -2.432716        3.526050       -0.726722
C      -3.140000        2.449623       -1.414289
C      -3.847284        2.392313       -2.690241
C      -3.847284        1.133530       -3.417063
C      -3.140000        0.000000       -2.828353
C      -2.432716       -1.133530       -3.417063
```

C	-2.432716	-2.392313	-2.690241
C	-3.140000	-2.449623	-1.414289
C	-3.847284	-3.526050	-0.726722
C	-3.847284	-3.526050	0.726722
C	-3.140000	-2.449623	1.414289
C	-2.432716	-2.392313	2.690241
C	-2.432716	-1.133530	3.417063
C	-3.140000	0.000000	2.828353
C	-3.847284	1.133530	3.417063
C	-3.847284	2.392313	2.690241
C	-3.140000	2.449623	1.414289
C	-3.140000	1.236126	0.713630
C	-3.140000	1.236126	-0.713630
C	-3.140000	0.000000	-1.427240
C	-3.140000	-1.236126	-0.713630
C	-3.140000	-1.236126	0.713630
C	-3.140000	0.000000	1.427240
C	-4.793047	3.388367	3.063883
C	-5.655074	3.196415	4.133221
C	-5.655074	1.980748	4.834944
C	-4.793047	0.958813	4.466397
C	-1.486953	4.347304	-1.402829
C	-0.624926	5.177398	-0.701821
C	-0.624926	5.177398	0.701821
C	-1.486953	4.347304	1.402829
C	-4.793047	0.958813	-4.466397
C	-5.655074	1.980748	-4.834944
C	-5.655074	3.196415	-4.133221
C	-4.793047	3.388367	-3.063883
C	-1.486953	-3.388367	-3.063883
C	-0.624926	-3.196415	-4.133221
C	-0.624926	-1.980748	-4.834944
C	-1.486953	-0.958813	-4.466397
C	-4.793047	-4.347304	1.402829
C	-5.655074	-5.177398	0.701821
C	-5.655074	-5.177398	-0.701821
C	-4.793047	-4.347304	-1.402829
C	-1.486953	-0.958813	4.466397
C	-0.624926	-1.980748	4.834944
C	-0.624926	-3.196415	4.133221
C	-1.486953	-3.388367	3.063883
H	-4.933220	4.274053	2.447458
H	-6.384369	3.964696	4.376635
H	-6.384369	1.807178	5.621946
H	-4.933220	-0.018112	4.924681
H	-1.346780	4.256227	-2.478069
H	0.104369	5.772408	-1.245412
H	0.104369	5.772408	1.245412
H	-1.346780	4.256227	2.478069
H	-4.933220	-0.018112	-4.924681
H	-6.384369	1.807178	-5.621946
H	-6.384369	3.964696	-4.376635
H	-4.933220	4.274053	-2.447458
H	-1.346780	-4.274053	-2.447458
H	0.104369	-3.964696	-4.376635
H	0.104369	-1.807178	-5.621946
H	-1.346780	0.018112	-4.924681
H	-4.933220	-4.256227	2.478069
H	-6.384369	-5.772408	1.245412
H	-6.384369	-5.772408	-1.245412
H	-4.933220	-4.256227	-2.478069
H	-1.346780	0.018112	4.924681
H	0.104369	-1.807178	5.621946
H	0.104369	-3.964696	4.376635
H	-1.346780	-4.274053	2.447458

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cf18, c-HBC_homodimers with bowl depth: 1.75

C	4.117765	3.501082	0.728644
C	4.117765	3.501082	-0.728644
C	3.365000	2.447960	-1.413350
C	2.612235	2.381569	-2.667681
C	2.612235	1.119528	-3.396516
C	3.365000	0.000000	-2.826541
C	4.117765	-1.119528	-3.396516
C	4.117765	-2.381569	-2.667681
C	3.365000	-2.447960	-1.413350
C	2.612235	-3.501082	-0.728644
C	2.612235	-3.501082	0.728644
C	3.365000	-2.447960	1.413350
C	4.117765	-2.381569	2.667681
C	4.117765	-1.119528	3.396516
C	3.365000	0.000000	2.826541
C	2.612235	1.119528	3.396516
C	2.612235	2.381569	2.667681
C	3.365000	2.447960	1.413350
C	3.365000	1.235025	0.713005
C	3.365000	1.235025	-0.713005

C	3.365000	0.000000	-1.426088
C	3.365000	-1.235025	-0.713005
C	3.365000	-1.235025	0.713005
C	3.365000	0.000000	1.426088
C	1.614715	3.347062	2.992094
C	0.706963	3.129327	4.017716
C	0.706963	1.914795	4.718975
C	1.614715	0.917733	4.394870
C	5.115285	4.264732	-1.402594
C	6.023037	5.044185	-0.701206
C	6.023037	5.044185	0.701206
C	5.115285	4.264732	1.402594
C	1.614715	0.917733	-4.394870
C	0.706963	1.914795	-4.718975
C	0.706963	3.129327	-4.017716
C	1.614715	3.347062	-2.992094
C	5.115285	-3.347062	-2.992094
C	6.023037	-3.129327	-4.017716
C	6.023037	-1.914795	-4.718975
C	5.115285	-0.917733	-4.394870
C	1.614715	-4.264732	1.402594
C	0.706963	-5.044185	0.701206
C	0.706963	-5.044185	-0.701206
C	1.614715	-4.264732	-1.402594
C	5.115285	-0.917733	4.394870
C	6.023037	-1.914795	4.718975
C	6.023037	-3.129327	4.017716
C	5.115285	-3.347062	2.992094
H	1.466296	4.226359	2.367978
H	-0.057397	3.874962	4.220731
H	-0.057397	1.717728	5.466177
H	1.466296	-0.062538	4.843992
H	5.263704	4.163946	-2.476168
H	6.787397	5.592771	-1.245483
H	6.787397	5.592771	1.245483
H	5.263704	4.163946	2.476168
H	1.466296	-0.062538	-4.843992
H	-0.057397	1.717728	-5.466177
H	-0.057397	3.874962	-4.220731
H	1.466296	4.226359	-2.367978
H	5.263704	-4.226359	-2.367978
H	6.787397	-3.874962	-4.220731
H	6.787397	-1.717728	-5.466177
H	5.263704	0.062538	-4.843992
H	1.466296	-4.163946	2.476168
H	-0.057397	-5.592771	1.245483
H	-0.057397	-5.592771	-1.245483
H	1.466296	-4.163946	-2.476168
H	5.263704	0.062538	4.843992
H	6.787397	-1.717728	5.466177
H	6.787397	-3.874962	4.220731
H	5.263704	-4.226359	2.367978
C	-2.612235	3.501082	0.728644
C	-2.612235	3.501082	-0.728644
C	-3.365000	2.447960	-1.413350
C	-4.117765	2.381569	-2.667681
C	-4.117765	1.119528	-3.396516
C	-3.365000	0.000000	-2.826541
C	-2.612235	-1.119528	-3.396516
C	-2.612235	-2.381569	-2.667681
C	-3.365000	-2.447960	-1.413350
C	-4.117765	-3.501082	-0.728644
C	-4.117765	-3.501082	0.728644
C	-3.365000	-2.447960	1.413350
C	-2.612235	-2.381569	2.667681
C	-2.612235	-1.119528	3.396516
C	-3.365000	0.000000	2.826541
C	-4.117765	1.119528	3.396516
C	-4.117765	2.381569	2.667681
C	-3.365000	2.447960	1.413350
C	-3.365000	1.235025	0.713005
C	-3.365000	1.235025	-0.713005
C	-3.365000	0.000000	-1.426088
C	-3.365000	-1.235025	-0.713005
C	-3.365000	-1.235025	0.713005
C	-3.365000	0.000000	1.426088
C	-5.115285	3.347062	2.992094
C	-6.023037	3.129327	4.017716
C	-6.023037	1.914795	4.718975
C	-5.115285	0.917733	4.394870
C	-1.614715	4.264732	-1.402594
C	-0.706963	5.044185	-0.701206
C	-0.706963	5.044185	0.701206
C	-1.614715	4.264732	1.402594
C	-5.115285	0.917733	-4.394870
C	-6.023037	1.914795	-4.718975
C	-6.023037	3.129327	-4.017716
C	-5.115285	3.347062	-2.992094
C	-1.614715	-3.347062	-2.992094
C	-0.706963	-3.129327	-4.017716

```
C      -0.706963       -1.914795       -4.718975
C      -1.614715       -0.917733       -4.394870
C      -5.115285       -4.264732        1.402594
C      -6.023037       -5.044185        0.701206
C      -6.023037       -5.044185       -0.701206
C      -5.115285       -4.264732       -1.402594
C      -1.614715       -0.917733        4.394870
C      -0.706963       -1.914795        4.718975
C      -0.706963       -3.129327        4.017716
C      -1.614715       -3.347062        2.992094
H      -5.263704        4.226359        2.367978
H      -6.787397        3.874962        4.220731
H      -6.787397        1.717728        5.466177
H      -5.263704       -0.062538        4.843992
H      -1.466296        4.163946       -2.476168
H       0.057397        5.592771       -1.245483
H       0.057397        5.592771        1.245483
H      -1.466296        4.163946        2.476168
H      -5.263704       -0.062538       -4.843992
H      -6.787397        1.717728       -5.466177
H      -6.787397        3.874962       -4.220731
H      -5.263704        4.226359       -2.367978
H      -1.466296       -4.226359       -2.367978
H       0.057397       -3.874962       -4.220731
H       0.057397       -1.717728       -5.466177
H      -1.466296        0.062538       -4.843992
H      -5.263704       -4.163946        2.476168
H      -6.787397       -5.592771        1.245483
H      -6.787397       -5.592771       -1.245483
H      -5.263704       -4.163946       -2.476168
H      -1.466296        0.062538        4.843992
H       0.057397       -1.717728        5.466177
H       0.057397       -3.874962        4.220731
H      -1.466296       -4.226359        2.367978

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cf19, c-HBC_homodimers with bowl depth: 1.85

C       4.395475        3.474066        0.730828
C       4.395475        3.474066       -0.730828
C       3.595000        2.446588       -1.412595
C       2.794525        2.370016       -2.643255
C       2.794525        1.104298       -3.374397
C       3.595000        0.000000       -2.825215
C       4.395475       -1.104298       -3.374397
C       4.395475       -2.370016       -2.643255
C       3.595000       -2.446588       -1.412595
C       2.794525       -3.474066       -0.730828
C       2.794525       -3.474066        0.730828
C       3.595000       -2.446588        1.412595
C       4.395475       -2.370016        2.643255
C       4.395475       -1.104298        3.374397
C       3.595000        0.000000        2.825215
C       2.794525        1.104298        3.374397
C       2.794525        2.370016        2.643255
C       3.595000        2.446588        1.412595
C       3.595000        1.234134        0.712570
C       3.595000        1.234134       -0.712570
C       3.595000        0.000000       -1.425323
C       3.595000       -1.234134       -0.712570
C       3.595000       -1.234134        0.712570
C       3.595000        0.000000        1.425323
C       1.747477        3.302839        2.915573
C       0.797513        3.058707        3.895940
C       0.797513        1.845568        4.596708
C       1.747477        0.874334        4.318615
C       5.442523        4.176656       -1.402166
C       6.392487        4.903568       -0.700466
C       6.392487        4.903568        0.700466
C       5.442523        4.176656        1.402166
C       1.747477        0.874334       -4.318615
C       0.797513        1.845568       -4.596708
C       0.797513        3.058707       -3.895940
C       1.747477        3.302839       -2.915573
C       5.442523       -3.302839       -2.915573
C       6.392487       -3.058707       -3.895940
C       6.392487       -1.845568       -4.596708
C       5.442523       -0.874334       -4.318615
C       1.747477       -4.176656        1.402166
C       0.797513       -4.903568        0.700466
C       0.797513       -4.903568       -0.700466
C       1.747477       -4.176656       -1.402166
C       5.442523       -0.874334        4.318615
C       6.392487       -1.845568        4.596708
C       6.392487       -3.058707        3.895940
C       5.442523       -3.302839        2.915573
H       1.590813        4.176071        2.284404
H       0.001784        3.781412        4.057410
H       0.001784        1.624338        5.303387
```

H	1.590813	-0.108782	4.759505
H	5.599187	4.066741	-2.474038
H	7.188216	5.404700	-1.245628
H	7.188216	5.404700	1.245628
H	5.599187	4.066741	2.474038
H	1.590813	-0.108782	-4.759505
H	0.001784	1.624338	-5.303387
H	0.001784	3.781412	-4.057410
H	1.590813	4.176071	-2.284404
H	5.599187	-4.176071	-2.284404
H	7.188216	-3.781412	-4.057410
H	7.188216	-1.624338	-5.303387
H	5.599187	0.108782	-4.759505
H	1.590813	-4.066741	2.474038
H	0.001784	-5.404700	1.245628
H	0.001784	-5.404700	-1.245628
H	1.590813	-4.066741	-2.474038
H	5.599187	0.108782	4.759505
H	7.188216	-1.624338	5.303387
H	7.188216	-3.781412	4.057410
H	5.599187	-4.176071	2.284404
C	-2.794525	3.474066	0.730828
C	-2.794525	3.474066	-0.730828
C	-3.595000	2.446588	-1.412595
C	-4.395475	2.370016	-2.643255
C	-4.395475	1.104298	-3.374397
C	-3.595000	0.000000	-2.825215
C	-2.794525	-1.104298	-3.374397
C	-2.794525	-2.370016	-2.643255
C	-3.595000	-2.446588	-1.412595
C	-4.395475	-3.474066	-0.730828
C	-4.395475	-3.474066	0.730828
C	-3.595000	-2.446588	1.412595
C	-2.794525	-2.370016	2.643255
C	-2.794525	-1.104298	3.374397
C	-3.595000	0.000000	2.825215
C	-4.395475	1.104298	3.374397
C	-4.395475	2.370016	2.643255
C	-3.595000	2.446588	1.412595
C	-3.595000	1.234134	0.712570
C	-3.595000	1.234134	-0.712570
C	-3.595000	0.000000	-1.425323
C	-3.595000	-1.234134	-0.712570
C	-3.595000	-1.234134	0.712570
C	-3.595000	0.000000	1.425323
C	-5.442523	3.302839	2.915573
C	-6.392487	3.058707	3.895940
C	-6.392487	1.845568	4.596708
C	-5.442523	0.874334	4.318615
C	-1.747477	4.176656	-1.402166
C	-0.797513	4.903568	-0.700466
C	-0.797513	4.903568	0.700466
C	-1.747477	4.176656	1.402166
C	-5.442523	0.874334	-4.318615
C	-6.392487	1.845568	-4.596708
C	-6.392487	3.058707	-3.895940
C	-5.442523	3.302839	-2.915573
C	-1.747477	-3.302839	-2.915573
C	-0.797513	-3.058707	-3.895940
C	-0.797513	-1.845568	-4.596708
C	-1.747477	-0.874334	-4.318615
C	-5.442523	-4.176656	1.402166
C	-6.392487	-4.903568	0.700466
C	-6.392487	-4.903568	-0.700466
C	-5.442523	-4.176656	-1.402166
C	-1.747477	-0.874334	4.318615
C	-0.797513	-1.845568	4.596708
C	-0.797513	-3.058707	3.895940
C	-1.747477	-3.302839	2.915573
H	-5.599187	4.176071	2.284404
H	-7.188216	3.781412	4.057410
H	-7.188216	1.624338	5.303387
H	-5.599187	-0.108782	4.759505
H	-1.590813	4.066741	-2.474038
H	-0.001784	5.404700	-1.245628
H	-0.001784	5.404700	1.245628
H	-1.590813	4.066741	2.474038
H	-5.599187	-0.108782	-4.759505
H	-7.188216	1.624338	-5.303387
H	-7.188216	3.781412	-4.057410
H	-5.599187	4.176071	-2.284404
H	-1.590813	-4.176071	-2.284404
H	-0.001784	-3.781412	-4.057410
H	-0.001784	-1.624338	-5.303387
H	-1.590813	0.108782	-4.759505
H	-5.599187	-4.066741	2.474038
H	-7.188216	-5.404700	1.245628
H	-7.188216	-5.404700	-1.245628
H	-5.599187	-4.066741	-2.474038
H	-1.590813	0.108782	4.759505

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H      -0.001784       -1.624338        5.303387
H      -0.001784       -3.781412        4.057410
H      -1.590813       -4.176071        2.284404

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cf0, c-HBC_heterodimers_with_C60 with bowl depth: 0.00

C      -0.269240        0.718135       -1.230444
C       0.568222        1.159988       -2.330292
C       1.375221        2.292536       -2.183610
C       0.568427        2.600024        0.128733
C      -0.269335        1.424655       -0.023848
C       1.085966       -0.018272       -3.000988
C       2.731463        2.289083       -2.700815
C       1.086006        2.608733        1.484901
C      -0.268619        0.706622        1.237068
C      -0.269325       -0.733154       -1.221641
C       2.392235        3.042057        1.731763
C       3.230468        3.483160        0.631904
C       2.392322       -0.021279       -3.498980
C       3.569704        3.020898       -1.768870
C       3.230173        1.153742       -3.346015
C       0.568250        1.438325        2.169818
C      -0.269042       -0.691675        1.245722
C      -0.269653       -1.425017       -0.006548
C       0.568124       -1.188392       -2.316152
C       0.568410       -1.411794        2.187050
C       0.568519       -2.598209        0.160394
C       1.375275       -2.318916       -2.155591
C       1.376380        0.744176        3.074937
C       4.585496        0.706618       -3.083609
C       1.085976       -2.590659        1.516599
C       1.376379       -3.035719       -0.893348
C       2.731541       -2.321882       -2.673037
C       3.569828       -3.042059       -1.731997
C       6.231105        0.691673       -1.245955
C       2.731595       -3.483161       -0.632137
C       3.230615       -3.475366        0.674266
C       4.585898       -3.024850        0.930084
C       2.392359       -3.020900        1.768636
C       2.731854        1.194302        3.331522
C       6.230682       -0.706624       -1.237302
C       1.376567       -0.706619        3.083375
C       2.731890       -1.153744        3.345782
C       5.393814       -1.438326       -2.170051
C       6.231716        1.425016        0.006314
C       6.231389        0.733153        1.221408
C       4.876058       -2.608734       -1.485134
C       5.393636       -2.600026       -0.128966
C       3.230601       -2.289085        2.700581
C       4.586843       -2.292538        2.183377
C       6.231398       -1.424657        0.023614
C       3.569742        0.021278        3.498747
C       5.393940        1.188390        2.315919
C       6.231304       -0.718137        1.230211
C       4.876097        0.018271        3.000755
C       5.393842       -1.159989        2.330059
C       5.393654        1.411792       -2.187283
C       4.876088        2.590658       -1.516832
C       5.393545        2.598208       -0.160627
C       3.230209       -1.194303       -3.331755
C       4.585683       -0.744177       -3.075171
C       1.376166        3.024849       -0.930317
C       2.731448        3.475365       -0.674499
C       4.585685        3.035718        0.893115
C       3.230523        2.321880        2.672804
C       4.586789        2.318914        2.155358
C      -3.439702       -3.671358       -1.264243
C      -3.439751       -2.961668       -2.511144
C      -3.439752       -1.485405       -2.536519
C      -3.439801       -0.740602       -3.811214
C      -3.439801        0.694130       -3.819951
C      -3.439752        1.454402       -2.554422
C      -3.439751        2.930865       -2.547028
C      -3.439703        3.655688       -1.308863
C      -3.439652        2.939722       -0.017768
C      -3.439602        3.671359        1.264512
C      -3.439553        2.961669        2.511413
C      -3.439553        1.485407        2.536788
C      -3.439503        0.740603        3.811483
C      -3.439503       -0.694128        3.820220
C      -3.439553       -1.454401        2.554691
C      -3.439553       -2.930863        2.547297
C      -3.439602       -3.655687        1.309132
C      -3.439652       -2.939721        0.018037
C      -3.439652       -1.491879        0.009220
C      -3.439703       -0.753812       -1.287174
C      -3.439703        0.738080       -1.296259
C      -3.439652        1.491880       -0.008951
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C	-3.439602	0.753814	1.287443
C	-3.439602	-0.738078	1.296528
C	-3.439596	-5.081266	1.459725
C	-3.439551	-5.825741	2.612184
C	-3.439505	-5.129244	3.801908
C	-3.439508	-3.759875	3.716753
C	-3.439797	-3.804861	-3.670416
C	-3.439800	-5.175165	-3.738888
C	-3.439753	-5.857121	-2.540769
C	-3.439708	-5.098666	-1.397462
C	-3.439853	1.276369	-5.129871
C	-3.439900	0.650651	-6.350895
C	-3.439900	-0.727951	-6.342500
C	-3.439853	-1.338751	-5.113946
C	-3.439708	5.081268	-1.459456
C	-3.439753	5.825742	-2.611915
C	-3.439800	5.129245	-3.801639
C	-3.439797	3.759877	-3.716484
C	-3.439508	3.804863	3.670685
C	-3.439505	5.175167	3.739157
C	-3.439551	5.857123	2.541038
C	-3.439596	5.098667	1.397731
C	-3.439452	-1.276367	5.130140
C	-3.439404	-0.650650	6.351165
C	-3.439404	0.727953	6.342769
C	-3.439452	1.338753	5.114215
H	-3.439628	-5.738539	0.643098
H	-3.439554	-6.910678	2.550112
H	-3.439466	-5.606235	4.778350
H	-3.439469	-3.368877	4.689315
H	-3.439835	-3.425737	-4.647668
H	-3.439838	-5.664013	-4.709448
H	-3.439750	-6.941222	-2.465489
H	-3.439676	-5.745944	-0.572891
H	-3.439859	2.312313	-5.290747
H	-3.439936	1.246830	-7.259461
H	-3.439936	-1.335151	-7.243737
H	-3.439859	-2.376578	-5.262192
H	-3.439676	5.738541	-0.642829
H	-3.439750	6.910679	-2.549843
H	-3.439838	5.606236	-4.778081
H	-3.439835	3.368879	-4.689046
H	-3.439470	3.425739	4.647937
H	-3.439467	5.664014	4.709717
H	-3.439554	6.941223	2.465758
H	-3.439628	5.745946	0.573160
H	-3.439446	-2.312312	5.291016
H	-3.439368	-1.246828	7.259730
H	-3.439368	1.335152	7.244006
H	-3.439446	2.376580	5.262462

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cf1, c-HBC_heterodimers_with_C60 with bowl depth: 0.10

C	-0.269241	0.720307	-1.229174
C	0.568220	1.164100	-2.328241
C	1.375219	2.296388	-2.179560
C	0.568428	2.599793	0.133323
C	-0.269335	1.424695	-0.021332
C	1.085964	-0.012974	-3.001016
C	2.731461	2.293848	-2.696771
C	1.086007	2.606107	1.489503
C	-0.268618	0.704437	1.238314
C	-0.269326	-0.730996	-1.222934
C	2.392237	3.038995	1.737130
C	3.230469	3.482039	0.638050
C	2.392319	-0.015101	-3.499014
C	3.569703	3.024016	-1.763536
C	3.230171	1.159648	-3.343975
C	0.568252	1.434492	2.172354
C	-0.269041	-0.693873	1.244499
C	-0.269653	-1.425004	-0.009063
C	0.568122	-1.184301	-2.318247
C	0.568412	-1.415653	2.184553
C	0.568519	-2.598489	0.155806
C	1.375273	-2.315106	-2.159683
C	1.376383	0.738746	3.076245
C	4.585494	0.712061	-3.082360
C	1.085977	-2.593333	1.512022
C	1.376379	-3.034138	-0.898707
C	2.731539	-2.317159	-2.677134
C	3.569827	-3.038996	-1.737367
C	6.231104	0.693872	-1.244736
C	2.731595	-3.482040	-0.638288
C	3.230616	-3.476551	0.668127
C	4.585898	-3.026488	0.924739
C	2.392361	-3.024017	1.763298
C	2.731857	1.188418	3.333623
C	6.230681	-0.704438	-1.238552

C	1.376570	-0.712062	3.082122
C	2.731893	-1.159649	3.343738
C	5.393812	-1.434493	-2.172591
C	6.231716	1.425003	0.008826
C	6.231390	0.730995	1.222696
C	4.876057	-2.606108	-1.489741
C	5.393636	-2.599794	-0.133560
C	3.230603	-2.293849	2.696533
C	4.586844	-2.296389	2.179323
C	6.231398	-1.424696	0.021094
C	3.569744	0.015100	3.498776
C	5.393941	1.184300	2.318010
C	6.231305	-0.720308	1.228937
C	4.876099	0.012973	3.000779
C	5.393843	-1.164101	2.328004
C	5.393652	1.415652	-2.184791
C	4.876087	2.593332	-1.512259
C	5.393545	2.598488	-0.156044
C	3.230207	-1.188419	-3.333861
C	4.585681	-0.738747	-3.076483
C	1.376165	3.026487	-0.924976
C	2.731448	3.476550	-0.668364
C	4.585685	3.034137	0.898470
C	3.230525	2.317158	2.676897
C	4.586790	2.315105	2.159446
C	-3.395487	0.700698	-3.815692
C	-3.395487	-0.733671	-3.809490
C	-3.439754	-1.480035	-2.537447
C	-3.484070	-2.954927	-2.514876
C	-3.484020	-3.666654	-1.269526
C	-3.439652	-2.937866	0.012841
C	-3.395284	-3.655536	1.301463
C	-3.395234	-2.933066	2.540611
C	-3.439551	-1.458034	2.550426
C	-3.483817	-0.700697	3.815966
C	-3.483817	0.733672	3.809764
C	-3.439551	1.480036	2.537721
C	-3.395234	2.954929	2.515150
C	-3.395284	3.666655	1.269800
C	-3.439652	2.937867	-0.012567
C	-3.484020	3.655538	-1.301188
C	-3.484070	2.933068	-2.540337
C	-3.439754	1.458035	-2.550152
C	-3.439704	0.739867	-1.293959
C	-3.439704	-0.751029	-1.287512
C	-3.439652	-1.491021	0.006585
C	-3.439601	-0.739865	1.294233
C	-3.439601	0.751031	1.287787
C	-3.439652	1.491023	-0.006310
C	-3.537037	3.761613	-3.708572
C	-3.582687	5.130570	-3.789616
C	-3.582640	5.825258	-2.598134
C	-3.536947	5.080226	-1.446842
C	-3.342618	-1.330984	-5.111025
C	-3.297020	-0.717034	-6.337264
C	-3.297020	0.662201	-6.343228
C	-3.342618	1.286733	-5.122345
C	-3.536947	-5.092549	-1.402853
C	-3.582640	-5.847509	-2.547659
C	-3.582687	-5.163152	-3.745104
C	-3.537037	-3.793545	-3.675902
C	-3.342267	-3.761612	3.708846
C	-3.296617	-5.130569	3.789890
C	-3.296665	-5.825257	2.598408
C	-3.342357	-5.080225	1.447116
C	-3.536686	1.330985	5.111299
C	-3.582284	0.717035	6.337538
C	-3.582284	-0.662200	6.343503
C	-3.536686	-1.286732	5.122619
C	-3.342357	5.092550	1.403127
C	-3.296665	5.847510	2.547933
C	-3.296617	5.163153	3.745378
C	-3.342267	3.793546	3.676176
H	-3.545322	3.368054	-4.680766
H	-3.621228	5.609128	-4.764507
H	-3.621139	6.909385	-2.534190
H	-3.545160	5.732583	-0.625600
H	-3.334378	-2.369746	-5.256192
H	-3.258554	-1.322229	-7.239030
H	-3.258554	1.259575	-7.250195
H	-3.334378	2.324200	-5.276490
H	-3.545160	-5.737779	-0.576000
H	-3.621139	-6.931043	-2.474341
H	-3.621228	-5.650123	-4.715820
H	-3.545322	-3.408409	-4.651464
H	-3.333982	-3.368053	4.681041
H	-3.258076	-5.609127	4.764781
H	-3.258165	-6.909384	2.534464
H	-3.334144	-5.732582	0.625874
H	-3.544926	2.369747	5.256466

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H      -3.620750        1.322230        7.239304
H      -3.620750       -1.259574        7.250469
H      -3.544926       -2.324199        5.276764
H      -3.334144        5.737781        0.576274
H      -3.258165        6.931044        2.474615
H      -3.258076        5.650124        4.716094
H      -3.333982        3.408410        4.651738

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cf2, c-HBC_heterodimers_with_C60 with bowl depth: 0.19

C      -0.269244        0.676479       -1.253829
C       0.568215        1.081208       -2.367875
C       1.375214        2.218037       -2.259248
C       0.568428        2.602878        0.041488
C      -0.269335        1.423055       -0.071598
C       1.085957       -0.118876       -2.998691
C       2.731455        2.197246       -2.776051
C       1.086010        2.657050        1.396600
C      -0.268615        0.747700        1.212683
C      -0.269329       -0.773700       -1.196373
C       2.392241        3.098408        1.628792
C       3.230470        3.502387        0.514759
C       2.392311       -0.138577       -3.496307
C       3.569699        2.959895       -1.869168
C       3.230163        1.040912       -3.382826
C       0.568257        1.510264        2.120374
C      -0.269038       -0.649521        1.268212
C      -0.269653       -1.424436        0.041233
C       0.568117       -1.265377       -2.275009
C       0.568417       -1.337675        2.233152
C       0.568519       -2.591371        0.247412
C       1.375268       -2.389883       -2.076637
C       1.376390        0.846851        3.048255
C       4.585487        0.602836       -3.105580
C       1.085980       -2.538356        1.602600
C       1.376376       -3.063964       -0.791071
C       2.731533       -2.410196       -2.593697
C       3.569823       -3.098417       -1.629043
C       6.231102        0.649511       -1.268463
C       2.731593       -3.502397       -0.515010
C       3.230617       -3.450807        0.790396
C       4.585900       -2.991967        1.030961
C       2.392365       -2.959905        1.868916
C       2.731865        1.305326        3.289599
C       6.230679       -0.747710       -1.212934
C       1.376577       -0.602846        3.105329
C       2.731901       -1.040921        3.382574
C       5.393807       -1.510274       -2.120625
C       6.231716        1.424426       -0.041484
C       6.231393        0.773690        1.196122
C       4.876054       -2.657060       -1.396851
C       5.393636       -2.602888       -0.041739
C       3.230609       -2.197256        2.775799
C       4.586849       -2.218047        2.258997
C       6.231399       -1.423065        0.071347
C       3.569752        0.138568        3.496055
C       5.393947        1.265367        2.274758
C       6.231308       -0.676488        1.253578
C       4.876106        0.118866        2.998440
C       5.393849       -1.081218        2.367624
C       5.393647        1.337665       -2.233403
C       4.876084        2.538346       -1.602851
C       5.393545        2.591361       -0.247663
C       3.230199       -1.305336       -3.289851
C       4.585674       -0.846861       -3.048506
C       1.376163        2.991957       -1.031213
C       2.731446        3.450797       -0.790647
C       4.585687        3.063954        0.790820
C       3.230531        2.410186        2.593446
C       4.586795        2.389873        2.076386
C      -3.351767        0.565558       -3.830032
C      -3.351767       -0.866980       -3.773241
C      -3.439759       -1.565522       -2.478969
C      -3.527804       -3.034387       -2.404726
C      -3.527752       -3.701605       -1.135853
C      -3.439652       -2.930009        0.116302
C      -3.351552       -3.600060        1.425608
C      -3.351500       -2.834487        2.637680
C      -3.439545       -1.364355        2.595411
C      -3.527538       -0.565547        3.830322
C      -3.527538        0.866992        3.773531
C      -3.439545        1.565534        2.479259
C      -3.351500        3.034399        2.405016
C      -3.351552        3.701617        1.136142
C      -3.439652        2.930020       -0.116012
C      -3.527752        3.600071       -1.425318
C      -3.527805        2.834499       -2.637390
C      -3.439759        1.364366       -2.595121
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C	-3.439706	0.692113	-1.316288
C	-3.439706	-0.794142	-1.257368
C	-3.439652	-1.486454	0.059074
C	-3.439598	-0.692101	1.316578
C	-3.439598	0.794153	1.257658
C	-3.439652	1.486465	-0.058784
C	-3.634284	3.612786	-3.834655
C	-3.724953	4.976469	-3.959431
C	-3.724902	5.713973	-2.792039
C	-3.634188	5.015653	-1.613999
C	-3.245391	-1.514181	-5.046244
C	-3.154777	-0.940290	-6.289599
C	-3.154777	0.439436	-6.344297
C	-3.245391	1.109953	-5.150275
C	-3.634188	-5.127681	-1.211879
C	-3.724902	-5.917067	-2.330941
C	-3.724953	-5.274291	-3.553053
C	-3.634284	-3.905011	-3.536622
C	-3.245021	-3.612775	3.834945
C	-3.154352	-4.976457	3.959721
C	-3.154402	-5.713961	2.792328
C	-3.245116	-5.015642	1.614288
C	-3.633913	1.514193	5.046534
C	-3.724528	0.940302	6.289889
C	-3.724528	-0.439424	6.344587
C	-3.633913	-1.109942	5.150564
C	-3.245117	5.127693	1.212169
C	-3.154402	5.917078	2.331231
C	-3.154352	5.274303	3.553343
C	-3.245021	3.905022	3.536912
H	-3.650816	3.172415	-4.788367
H	-3.802852	5.420509	-4.948148
H	-3.802757	6.797564	-2.768568
H	-3.650644	5.688235	-0.806999
H	-3.228906	-2.560301	-5.143042
H	-3.076957	-1.574368	-7.168640
H	-3.076957	1.001936	-7.270774
H	-3.228906	2.145127	-5.329583
H	-3.650644	-5.734268	-0.354169
H	-3.802757	-6.995399	-2.221764
H	-3.802852	-5.795207	-4.503515
H	-3.650816	-3.541521	-4.522202
H	-3.228489	-3.172404	4.788657
H	-3.076453	-5.420497	4.948438
H	-3.076547	-6.797553	2.768858
H	-3.228661	-5.688224	0.807289
H	-3.650398	2.560312	5.143332
H	-3.802348	1.574380	7.168930
H	-3.802348	-1.001925	7.271064
H	-3.650398	-2.145116	5.329873
H	-3.228661	5.734280	0.354459
H	-3.076547	6.995411	2.222053
H	-3.076453	5.795219	4.503805
H	-3.228489	3.541532	4.522492

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cf3, c-HBC_heterodimers_with_C60 with bowl depth: 0.29

C	-0.273886	0.719883	-1.229422
C	0.563573	1.163298	-2.328643
C	1.370573	2.295637	-2.180354
C	0.563785	2.599839	0.132426
C	-0.273978	1.424688	-0.021822
C	1.081316	-0.014008	-3.001013
C	2.726813	2.292919	-2.697566
C	1.081366	2.606620	1.488604
C	-0.273258	0.704864	1.238072
C	-0.273971	-0.731417	-1.222681
C	2.387597	3.039593	1.736078
C	3.225827	3.482258	0.636845
C	2.387670	-0.016307	-3.499012
C	3.565057	3.023409	-1.764584
C	3.225522	1.158496	-3.344381
C	0.563613	1.435240	2.171858
C	-0.273681	-0.693444	1.244738
C	-0.274296	-1.425007	-0.008572
C	0.563475	-1.185099	-2.317840
C	0.563773	-1.414900	2.185040
C	0.563876	-2.598435	0.156701
C	1.370627	-2.315851	-2.158888
C	1.371745	0.739806	3.075988
C	4.580846	0.710999	-3.082613
C	1.081337	-2.592812	1.512914
C	1.371734	-3.034447	-0.897664
C	2.726891	-2.318081	-2.676340
C	3.565181	-3.039595	-1.736326
C	6.226459	0.693443	-1.244986
C	2.726951	-3.482259	-0.637093
C	3.225974	-3.476321	0.669319

C	4.581257	-3.026169	0.925774
C	2.387721	-3.023410	1.764336
C	2.727220	1.189567	3.333209
C	6.226036	-0.704865	-1.238320
C	1.371932	-0.711000	3.082365
C	2.727256	-1.158497	3.344133
C	5.389165	-1.435242	-2.172106
C	6.227074	1.425005	0.008324
C	6.226749	0.731416	1.222433
C	4.871412	-2.606621	-1.488851
C	5.388993	-2.599840	-0.132674
C	3.225965	-2.292920	2.697318
C	4.582205	-2.295638	2.180106
C	6.226756	-1.424689	0.021574
C	3.565108	0.016306	3.498765
C	5.389303	1.185098	2.317592
C	6.226664	-0.719884	1.229174
C	4.871462	0.014007	3.000765
C	5.389205	-1.163299	2.328395
C	5.389005	1.414899	-2.185288
C	4.871441	2.592811	-1.513162
C	5.388902	2.598434	-0.156949
C	3.225558	-1.189568	-3.333457
C	4.581033	-0.739807	-3.076236
C	1.371521	3.026168	-0.926022
C	2.726804	3.476320	-0.669567
C	4.581044	3.034446	0.897416
C	3.225887	2.318080	2.676092
C	4.582151	2.315849	2.158640
C	-3.303030	0.698682	-3.795169
C	-3.303030	-0.734088	-3.788479
C	-3.434400	-1.473815	-2.524855
C	-3.565823	-2.938095	-2.502824
C	-3.565771	-3.648595	-1.258738
C	-3.434295	-2.923811	0.013794
C	-3.302819	-3.636681	1.293037
C	-3.302767	-2.914596	2.530435
C	-3.434190	-1.450174	2.538792
C	-3.565560	-0.698681	3.795455
C	-3.565560	0.734090	3.788766
C	-3.434190	1.473816	2.525141
C	-3.302767	2.938096	2.503110
C	-3.302819	3.648596	1.259024
C	-3.434295	2.923813	-0.013508
C	-3.565771	3.636682	-1.292751
C	-3.565823	2.914597	-2.530149
C	-3.434400	1.450175	-2.538506
C	-3.434348	0.735289	-1.287024
C	-3.434348	-0.747275	-1.280102
C	-3.434295	-1.482686	0.007065
C	-3.434242	-0.735288	1.287310
C	-3.434242	0.747276	1.280388
C	-3.434295	1.482687	-0.006779
C	-3.726162	3.721244	-3.700632
C	-3.863839	5.085777	-3.768478
C	-3.863789	5.783052	-2.573637
C	-3.726067	5.052366	-1.419295
C	-3.142793	-1.344384	-5.072163
C	-3.005169	-0.721099	-6.287872
C	-3.005169	0.662356	-6.294331
C	-3.142793	1.296965	-5.084495
C	-3.726067	-5.065398	-1.372058
C	-3.863789	-5.806831	-2.519526
C	-3.863839	-5.120743	-3.720826
C	-3.726162	-3.755636	-3.665724
C	-3.142428	-3.721243	3.700918
C	-3.004751	-5.085776	3.768764
C	-3.004801	-5.783051	2.573923
C	-3.142523	-5.052364	1.419582
C	-3.725797	1.344386	5.072449
C	-3.863421	0.721101	6.288158
C	-3.863421	-0.662354	6.294617
C	-3.725797	-1.296964	5.084781
C	-3.142523	5.065399	1.372344
C	-3.004801	5.806833	2.519812
C	-3.004751	5.120745	3.721112
C	-3.142428	3.755638	3.666010
H	-3.750940	3.295373	-4.664242
H	-3.983110	5.566030	-4.735870
H	-3.983017	6.861539	-2.515248
H	-3.750769	5.682050	-0.574892
H	-3.118060	-2.391801	-5.185514
H	-2.885976	-1.319063	-7.187367
H	-2.885976	1.251895	-7.199370
H	-3.118060	2.343278	-5.207621
H	-3.750769	-5.687170	-0.521812
H	-3.983017	-6.884725	-2.451070
H	-3.983110	-5.610008	-4.683692
H	-3.750940	-3.338781	-4.633268
H	-3.117650	-3.295371	4.664528

H	-2.885480	-5.566029	4.736156
H	-2.885573	-6.861537	2.515534
H	-3.117821	-5.682049	0.575178
H	-3.750530	2.391802	5.185800
H	-3.982614	1.319065	7.187653
H	-3.982614	-1.251893	7.199656
H	-3.750530	-2.343276	5.207907
H	-3.117821	5.687171	0.522098
H	-2.885573	6.884727	2.451356
H	-2.885480	5.610009	4.683978
H	-3.117650	3.338782	4.633554

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cf4, c-HBC_heterodimers_with_C60 with bowl depth: 0.39

C	-0.278532	0.716037	-1.231665
C	0.558924	1.156014	-2.332269
C	1.365923	2.288811	-2.187521
C	0.559143	2.600240	0.124298
C	-0.278621	1.424612	-0.026274
C	1.076664	-0.023387	-3.000958
C	2.722162	2.284477	-2.704727
C	1.076728	2.611260	1.480447
C	-0.277898	0.708730	1.235864
C	-0.278617	-0.735235	-1.220388
C	2.382959	3.045004	1.726563
C	3.221186	3.484232	0.625949
C	2.383017	-0.027243	-3.498951
C	3.560409	3.017879	-1.774035
C	3.220869	1.148037	-3.347994
C	0.558976	1.442021	2.167361
C	-0.278321	-0.689551	1.246901
C	-0.278939	-1.425026	-0.004117
C	0.558826	-1.192338	-2.314126
C	0.559136	-1.408064	2.189450
C	0.559234	-2.597932	0.164819
C	1.365977	-2.322587	-2.151643
C	1.367111	0.749416	3.073657
C	4.576194	0.701361	-3.084833
C	1.076698	-2.588071	1.521007
C	1.367089	-3.037238	-0.888180
C	2.722240	-2.326435	-2.669090
C	3.560533	-3.045006	-1.726828
C	6.221813	0.689549	-1.247165
C	2.722306	-3.484234	-0.626214
C	3.221333	-3.474212	0.680171
C	4.576617	-3.023261	0.935214
C	2.383083	-3.017881	1.773770
C	2.722587	1.199978	3.329467
C	6.221390	-0.708732	-1.236129
C	1.367298	-0.701363	3.084568
C	2.722623	-1.148040	3.347729
C	5.384516	-1.442023	-2.167626
C	6.222431	1.425024	0.003852
C	6.222110	0.735233	1.220123
C	4.866764	-2.611262	-1.480712
C	5.384350	-2.600242	-0.124563
C	3.221330	-2.284479	2.704462
C	4.577569	-2.288813	2.187257
C	6.222113	-1.424615	0.026009
C	3.560475	0.027241	3.498686
C	5.384667	1.192336	2.313861
C	6.222025	-0.716039	1.231400
C	4.866828	0.023385	3.000693
C	5.384569	-1.156016	2.332004
C	5.384356	1.408062	-2.189715
C	4.866794	2.588069	-1.521272
C	5.384259	2.597930	-0.165084
C	3.220905	-1.199980	-3.329732
C	4.576381	-0.749418	-3.073922
C	1.366875	3.023259	-0.935479
C	2.722159	3.474210	-0.680436
C	4.576404	3.037236	0.887915
C	3.221252	2.326433	2.668825
C	4.577515	2.322585	2.151378
C	-3.254499	0.686377	-3.780260
C	-3.254499	-0.745219	-3.769102
C	-3.429050	-1.475811	-2.510373
C	-3.603657	-2.931153	-2.484619
C	-3.603601	-3.637337	-1.239362
C	-3.428938	-2.912246	0.022852
C	-3.254274	-3.617574	1.296214
C	-3.254219	-2.892066	2.530313
C	-3.428825	-1.436498	2.533378
C	-3.603377	-0.686375	3.780566
C	-3.603377	0.745222	3.769408
C	-3.428825	1.475813	2.510678
C	-3.254219	2.931156	2.484925
C	-3.254274	3.637339	1.239667

C	-3.428938	2.912249	-0.022546
C	-3.603601	3.617576	-1.295908
C	-3.603657	2.892068	-2.530007
C	-3.429050	1.436501	-2.533072
C	-3.428995	0.727937	-1.283449
C	-3.428995	-0.747854	-1.271946
C	-3.428938	-1.476013	0.011657
C	-3.428881	-0.727935	1.283754
C	-3.428881	0.747857	1.272252
C	-3.428938	1.476015	-0.011352
C	-3.818054	3.676043	-3.704471
C	-4.003778	5.036309	-3.764750
C	-4.003724	5.739236	-2.569082
C	-3.817951	5.025136	-1.409832
C	-3.040211	-1.370016	-5.035395
C	-2.854542	-0.742165	-6.243520
C	-2.854542	0.644753	-6.254330
C	-3.040211	1.291359	-5.056138
C	-3.817951	-5.046502	-1.331331
C	-4.003724	-5.778584	-2.479309
C	-4.003778	-5.094381	-3.685789
C	-3.818054	-3.733340	-3.646720
C	-3.039822	-3.676041	3.704776
C	-2.854098	-5.036307	3.765056
C	-2.854151	-5.739233	2.569388
C	-3.039925	-5.025134	1.410137
C	-3.817665	1.370018	5.035700
C	-4.003333	0.742167	6.243826
C	-4.003333	-0.644751	6.254636
C	-3.817665	-1.291357	5.056444
C	-3.039925	5.046504	1.331636
C	-2.854151	5.778587	2.479615
C	-2.854098	5.094383	3.686094
C	-3.039822	3.733342	3.647025
H	-3.851078	3.221854	-4.659542
H	-4.165662	5.514480	-4.726998
H	-4.165563	6.812586	-2.519262
H	-3.850894	5.638717	-0.548554
H	-3.007233	-2.424173	-5.120138
H	-2.692741	-1.336146	-7.138938
H	-2.692741	1.224704	-7.158898
H	-3.007233	2.344068	-5.157303
H	-3.850894	-5.646582	-0.460594
H	-4.165563	-6.851027	-2.412765
H	-4.165662	-5.587493	-4.640466
H	-3.851078	-3.294094	-4.608755
H	-3.006797	-3.221852	4.659848
H	-2.692214	-5.514478	4.727304
H	-2.692313	-6.812583	2.519568
H	-3.006981	-5.638714	0.548860
H	-3.850643	2.424176	5.120444
H	-4.165134	1.336148	7.139243
H	-4.165134	-1.224702	7.159203
H	-3.850643	-2.344066	5.157609
H	-3.006981	5.646585	0.460899
H	-2.692313	6.851030	2.413070
H	-2.692214	5.587495	4.640772
H	-3.006797	3.294096	4.609061

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cf5, c-HBC_heterodimers_with_C60 with bowl depth: 0.49

C	-0.278550	0.717842	-1.230610
C	0.558890	1.159432	-2.330580
C	1.365892	2.292015	-2.184183
C	0.559145	2.600055	0.128102
C	-0.278621	1.424650	-0.024181
C	1.076622	-0.018988	-3.001004
C	2.722124	2.288439	-2.701414
C	1.076749	2.609087	1.484258
C	-0.277880	0.706917	1.236906
C	-0.278635	-0.733445	-1.221461
C	2.382984	3.042470	1.730991
C	3.221196	3.483310	0.631010
C	2.382967	-0.022113	-3.499021
C	3.560384	3.020476	-1.769660
C	3.220822	1.152944	-3.346353
C	0.559007	1.438842	2.169464
C	-0.278303	-0.691378	1.245892
C	-0.278939	-1.425019	-0.006202
C	0.558792	-1.188944	-2.315880
C	0.559167	-1.411272	2.187376
C	0.559236	-2.598171	0.161003
C	1.365946	-2.319430	-2.155065
C	1.367155	0.744909	3.074733
C	4.576150	0.705882	-3.083867
C	1.076719	-2.590298	1.517196
C	1.367075	-3.035933	-0.892651
C	2.722202	-2.322519	-2.672537

C	3.560508	-3.042472	-1.731341
C	6.221795	0.691376	-1.246242
C	2.722297	-3.483312	-0.631360
C	3.221343	-3.475206	0.675031
C	4.576630	-3.024629	0.930715
C	2.383108	-3.020478	1.769310
C	2.722635	1.195096	3.331184
C	6.221372	-0.706920	-1.237256
C	1.367342	-0.705884	3.083517
C	2.722671	-1.152946	3.346004
C	5.384485	-1.438845	-2.169814
C	6.222431	1.425017	0.005852
C	6.222127	0.733443	1.221111
C	4.866743	-2.609089	-1.484608
C	5.384348	-2.600057	-0.128452
C	3.221368	-2.288441	2.701064
C	4.577600	-2.292017	2.183833
C	6.222113	-1.424652	0.023832
C	3.560525	0.022111	3.498672
C	5.384700	1.188942	2.315530
C	6.222042	-0.717844	1.230260
C	4.866871	0.018986	3.000654
C	5.384602	-1.159434	2.330230
C	5.384325	1.411270	-2.187725
C	4.866773	2.590296	-1.517545
C	5.384257	2.598169	-0.161353
C	3.220858	-1.195098	-3.331534
C	4.576337	-0.744911	-3.075083
C	1.366862	3.024627	-0.931065
C	2.722150	3.475204	-0.675381
C	4.576417	3.035930	0.892301
C	3.221290	2.322517	2.672187
C	4.577546	2.319428	2.154715
C	-3.211701	0.691514	-3.758722
C	-3.211701	-0.739029	-3.749669
C	-3.429086	-1.465380	-2.501028
C	-3.646543	-2.910101	-2.478791
C	-3.646470	-3.617592	-1.235323
C	-3.428938	-2.899021	0.018547
C	-3.211406	-3.601665	1.281411
C	-3.211333	-2.878494	2.515826
C	-3.428790	-1.433607	2.519777
C	-3.646175	-0.691512	3.759126
C	-3.646175	0.739032	3.750073
C	-3.428790	1.465383	2.501432
C	-3.211333	2.910104	2.479194
C	-3.211406	3.617594	1.235726
C	-3.428938	2.899023	-0.018144
C	-3.646470	3.601668	-1.281008
C	-3.646543	2.878497	-2.515422
C	-3.429086	1.433610	-2.519374
C	-3.429013	0.726004	-1.275591
C	-3.429013	-0.742090	-1.266301
C	-3.428938	-1.468306	0.009494
C	-3.428863	-0.726002	1.275995
C	-3.428863	0.742093	1.266704
C	-3.428938	1.468309	-0.009090
C	-3.915344	3.641275	-3.689922
C	-4.151428	4.995847	-3.732907
C	-4.151357	5.699056	-2.532670
C	-3.915207	4.998970	-1.372323
C	-2.943042	-1.374705	-4.997211
C	-2.707031	-0.734777	-6.191763
C	-2.707031	0.656355	-6.200566
C	-2.943042	1.311351	-5.014209
C	-3.915207	-5.015938	-1.308947
C	-4.151357	-5.730653	-2.460341
C	-4.151428	-5.042690	-3.669382
C	-3.915344	-3.687682	-3.643543
C	-2.942532	-3.641272	3.690325
C	-2.706448	-4.995844	3.733311
C	-2.706519	-5.699054	2.533074
C	-2.942669	-4.998967	1.372727
C	-3.914833	1.374708	4.997614
C	-4.150845	0.734779	6.192167
C	-4.150845	-0.656353	6.200970
C	-3.914833	-1.311348	5.014612
C	-2.942669	5.015940	1.309350
C	-2.706519	5.730655	2.460745
C	-2.706448	5.042693	3.669785
C	-2.942532	3.687685	3.643946
H	-3.956628	3.162105	-4.638234
H	-4.357937	5.476373	-4.685361
H	-4.357807	6.764852	-2.486013
H	-3.956383	5.590989	-0.490195
H	-2.901818	-2.435521	-5.055194
H	-2.500630	-1.319281	-7.084264
H	-2.500630	1.229518	-7.100393
H	-2.901818	2.371348	-5.085613
H	-3.956383	-5.596745	-0.419397

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H      -4.357807       -6.795773       -2.400198
H      -4.357937       -5.535232       -4.615678
H      -3.956628       -3.220553       -4.597843
H      -2.901248       -3.162103        4.638638
H      -2.499939       -5.476371        4.685765
H      -2.500069       -6.764849        2.486416
H      -2.901493       -5.590986        0.490599
H      -3.956057        2.435524        5.055598
H      -4.357245        1.319284        7.084668
H      -4.357245       -1.229515        7.100797
H      -3.956057       -2.371346        5.086017
H      -2.901493        5.596748        0.419801
H      -2.500069        6.795775        2.400602
H      -2.499939        5.535235        4.616081
H      -2.901248        3.220556        4.598247


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cf6, c-HBC_heterodimers_with_C60 with bowl depth: 0.58

C      -0.278483        0.722830       -1.227702
C       0.559018        1.168880       -2.325825
C       1.366011        2.300860       -2.174789
C       0.559137        2.599514        0.138683
C      -0.278620        1.424736       -0.018415
C       1.076786       -0.006809       -3.000998
C       2.722271        2.299383       -2.691955
C       1.076667        2.603042        1.494893
C      -0.277948        0.701892        1.239749
C      -0.278568       -0.728482       -1.224442
C       2.382888        3.035420        1.743455
C       3.221160        3.480721        0.645318
C       2.383159       -0.007913       -3.498952
C       3.560480        3.027633       -1.757192
C       3.221005        1.166515       -3.341470
C       0.558888        1.430027        2.175316
C      -0.278371       -0.696428        1.243061
C      -0.278938       -1.424982       -0.012000
C       0.558920       -1.179536       -2.320655
C       0.559048       -1.420137        2.181661
C       0.559228       -2.598803        0.150488
C       1.366065       -2.310665       -2.164385
C       1.366986        0.732425        3.077806
C       4.576319        0.718392       -3.080726
C       1.076637       -2.596433        1.506730
C       1.367126       -3.032285       -0.904889
C       2.722349       -2.311654       -2.681790
C       3.560604       -3.035420       -1.743478
C       6.221863        0.696428       -1.243085
C       2.722333       -3.480721       -0.645341
C       3.221307       -3.477916        0.661100
C       4.576580       -3.028380        0.918684
C       2.383012       -3.027633        1.757169
C       2.722452        1.181568        3.336156
C       6.221440       -0.701892       -1.239773
C       1.367173       -0.718392        3.080702
C       2.722488       -1.166515        3.341447
C       5.384604       -1.430027       -2.175340
C       6.222430        1.424982        0.011976
C       6.222060        0.728482        1.224419
C       4.866825       -2.603042       -1.494917
C       5.384356       -2.599514       -0.138707
C       3.221221       -2.299383        2.691932
C       4.577481       -2.300860        2.174765
C       6.222112       -1.424736        0.018391
C       3.560333        0.007913        3.498928
C       5.384572        1.179536        2.320631
C       6.221975       -0.722830        1.227678
C       4.866706        0.006809        3.000974
C       5.384474       -1.168881        2.325801
C       5.384444        1.420137       -2.181685
C       4.866855        2.596433       -1.506754
C       5.384265        2.598803       -0.150512
C       3.221041       -1.181568       -3.336179
C       4.576506       -0.732425       -3.077830
C       1.366912        3.028380       -0.918708
C       2.722186        3.477916       -0.661123
C       4.576367        3.032285        0.904865
C       3.221143        2.311654        2.681767
C       4.577427        2.310665        2.164361
C      -3.168938        0.706615       -3.735056
C      -3.168938       -0.723565       -3.731809
C      -3.428948       -1.448684       -2.495809
C      -3.688963       -2.882025       -2.479751
C      -3.688958       -3.593638       -1.239253
C      -3.428938       -2.885229        0.006563
C      -3.168918       -3.587975        1.255582
C      -3.168913       -2.870738        2.492837
C      -3.428928       -1.437338        2.502388
C      -3.688938       -0.706615        3.735083
```

C	-3.688938	0.723565	3.731837
C	-3.428928	1.448684	2.495837
C	-3.168913	2.882025	2.479778
C	-3.168918	3.593638	1.239280
C	-3.428938	2.885229	-0.006536
C	-3.688958	3.587975	-1.255555
C	-3.688963	2.870738	-2.492809
C	-3.428948	1.437338	-2.502360
C	-3.428943	0.727342	-1.266433
C	-3.428943	-0.733084	-1.263117
C	-3.428938	-1.460215	0.003328
C	-3.428933	-0.727342	1.266460
C	-3.428933	0.733084	1.263145
C	-3.428938	1.460215	-0.003301
C	-4.012381	3.613463	-3.663540
C	-4.301078	4.960183	-3.682792
C	-4.301073	5.659748	-2.475538
C	-4.012371	4.972926	-1.317307
C	-2.845530	-1.367102	-4.959533
C	-2.556837	-0.711614	-6.136003
C	-2.556837	0.683750	-6.139171
C	-2.845530	1.344573	-4.965689
C	-4.012371	-4.978855	-1.294716
C	-4.301073	-5.670929	-2.449817
C	-4.301078	-4.976851	-3.660235
C	-4.012380	-3.630058	-3.647097
C	-2.845495	-3.613463	3.663567
C	-2.556798	-4.960183	3.682819
C	-2.556803	-5.659748	2.475565
C	-2.845505	-4.972926	1.317334
C	-4.012346	1.367102	4.959561
C	-4.301038	0.711614	6.136031
C	-4.301038	-0.683750	6.139198
C	-4.012346	-1.344573	4.965716
C	-2.845505	4.978855	1.294744
C	-2.556803	5.670929	2.449845
C	-2.556798	4.976851	3.660262
C	-2.845495	3.630058	3.647125
H	-4.061857	3.113875	-4.607015
H	-4.553557	5.444034	-4.622482
H	-4.553549	6.715611	-2.427725
H	-4.061841	5.541572	-0.413840
H	-2.796057	-2.433994	-4.996398
H	-2.304365	-1.284125	-7.024464
H	-2.304365	1.252221	-7.030221
H	-2.796057	2.411286	-5.007396
H	-4.061840	-5.543394	-0.388677
H	-4.553548	-6.726564	-2.397212
H	-4.553557	-5.464964	-4.597719
H	-4.061857	-3.134759	-4.592831
H	-2.796018	-3.113875	4.607042
H	-2.304318	-5.444034	4.622510
H	-2.304327	-6.715611	2.427753
H	-2.796035	-5.541572	0.413867
H	-4.061819	2.433994	4.996425
H	-4.553511	1.284125	7.024491
H	-4.553511	-1.252221	7.030249
H	-4.061819	-2.411286	5.007424
H	-2.796035	5.543394	0.388705
H	-2.304327	6.726564	2.397239
H	-2.304318	5.464964	4.597747
H	-2.796018	3.134759	4.592858

132
cf7, c-HBC_heterodimers_with_C60 with bowl depth: 0.68

C	-0.283142	0.720048	-1.229332
C	0.554344	1.163610	-2.328473
C	1.361340	2.295929	-2.180012
C	0.554496	2.599821	0.132789
C	-0.283263	1.424691	-0.021638
C	1.072103	-0.013605	-3.000989
C	2.717593	2.293281	-2.697192
C	1.072044	2.606421	1.488980
C	-0.282574	0.704698	1.238160
C	-0.283227	-0.731253	-1.222786
C	2.378269	3.039361	1.736544
C	3.216526	3.482173	0.637390
C	2.378469	-0.015837	-3.498956
C	3.555814	3.023646	-1.764092
C	3.216317	1.158945	-3.344147
C	0.554274	1.434949	2.172065
C	-0.282997	-0.693611	1.244639
C	-0.283581	-1.425005	-0.008769
C	0.554246	-1.184788	-2.317985
C	0.554434	-1.415193	2.184864
C	0.554587	-2.598456	0.156366
C	1.361394	-2.315561	-2.159165
C	1.362385	0.739394	3.076121

C	4.571635	0.711413	-3.082406
C	1.072014	-2.593015	1.512592
C	1.362470	-3.034326	-0.898037
C	2.717671	-2.317722	-2.676585
C	3.555938	-3.039361	-1.736647
C	6.217204	0.693611	-1.244742
C	2.717681	-3.482174	-0.637494
C	3.216673	-3.476410	0.668931
C	4.571949	-3.026292	0.925479
C	2.378393	-3.023646	1.763989
C	2.717853	1.189120	3.333435
C	6.216781	-0.704698	-1.238263
C	1.362572	-0.711413	3.082303
C	2.717889	-1.158945	3.344043
C	5.379932	-1.434950	-2.172168
C	6.217788	1.425005	0.008666
C	6.217434	0.731253	1.222683
C	4.862162	-2.606421	-1.489083
C	5.379711	-2.599821	-0.132892
C	3.216614	-2.293281	2.697089
C	4.572867	-2.295930	2.179909
C	6.217470	-1.424691	0.021535
C	3.555737	0.015837	3.498853
C	5.379961	1.184788	2.317882
C	6.217349	-0.720048	1.229229
C	4.862103	0.013605	3.000886
C	5.379863	-1.163611	2.328370
C	5.379772	1.415193	-2.184967
C	4.862192	2.593014	-1.512695
C	5.379620	2.598455	-0.156469
C	3.216353	-1.189120	-3.333538
C	4.571822	-0.739394	-3.076224
C	1.362257	3.026292	-0.925582
C	2.717534	3.476410	-0.669034
C	4.571736	3.034326	0.897934
C	3.216536	2.317722	2.676482
C	4.572813	2.315560	2.159062
C	-3.121246	0.698341	-3.715869
C	-3.121246	-0.732012	-3.709383
C	-3.423624	-1.448085	-2.482080
C	-3.726023	-2.869138	-2.462854
C	-3.726001	-3.578307	-1.220715
C	-3.423581	-2.873369	0.013089
C	-3.121160	-3.567089	1.253235
C	-3.121139	-2.846683	2.488892
C	-3.423537	-1.425515	2.495229
C	-3.725915	-0.698341	3.715988
C	-3.725915	0.732013	3.709501
C	-3.423537	1.448086	2.482199
C	-3.121139	2.869138	2.462973
C	-3.121160	3.578308	1.220834
C	-3.423581	2.873370	-0.012970
C	-3.726001	3.567089	-1.253116
C	-3.726023	2.846684	-2.488773
C	-3.423624	1.425515	-2.495110
C	-3.423603	0.721044	-1.262023
C	-3.423603	-0.732459	-1.255432
C	-3.423581	-1.453350	0.006650
C	-3.423559	-0.721043	1.262142
C	-3.423559	0.732460	1.255551
C	-3.423581	1.453350	-0.006531
C	-4.104310	3.559267	-3.659294
C	-4.445055	4.895654	-3.664773
C	-4.445034	5.600240	-2.456094
C	-4.104269	4.936731	-1.296215
C	-2.743000	-1.389994	-4.911356
C	-2.402275	-0.727090	-6.071731
C	-2.402275	0.671995	-6.078075
C	-2.743000	1.345396	-4.923760
C	-4.104269	-4.948283	-1.251390
C	-4.445034	-5.622284	-2.405204
C	-4.445055	-4.928689	-3.620223
C	-4.104310	-3.592307	-3.626864
C	-2.742851	-3.559267	3.659413
C	-2.402106	-4.895654	3.664892
C	-2.402127	-5.600240	2.456213
C	-2.742893	-4.936730	1.296334
C	-4.104161	1.389995	4.911475
C	-4.444886	0.727091	6.071850
C	-4.444886	-0.671995	6.078194
C	-4.104161	-1.345395	4.923879
C	-2.742893	4.948284	1.251509
C	-2.402128	5.622285	2.405323
C	-2.402106	4.928689	3.620342
C	-2.742851	3.592308	3.626983
H	-4.162045	3.035837	-4.594967
H	-4.742250	5.373327	-4.594581
H	-4.742212	6.644690	-2.413438
H	-4.161972	5.492354	-0.379317
H	-2.685281	-2.462103	-4.925213

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H      -2.105112       -1.293849       -6.950076
H      -2.105112        1.230765       -6.961524
H      -2.685281        2.417335       -4.947340
H      -4.161972       -5.495569       -0.329491
H      -4.742212       -6.666305       -2.353078
H      -4.742250       -5.414774       -4.545661
H      -4.162045       -3.077384       -4.567246
H      -2.685116       -3.035836        4.595086
H      -2.104911       -5.373326        4.594700
H      -2.104949       -6.644690        2.413557
H      -2.685190       -5.492354        0.379436
H      -4.161880        2.462104        4.925332
H      -4.742050        1.293850        6.950195
H      -4.742050       -1.230765        6.961643
H      -4.161880       -2.417334        4.947459
H      -2.685190        5.495569        0.329610
H      -2.104949        6.666305        2.353197
H      -2.104911        5.414775        4.545780
H      -2.685116        3.077385        4.567365

132
cf8, c-HBC_heterodimers_with_C60 with bowl depth: 0.78

C      -0.287796        0.716863       -1.231189
C       0.549680        1.157578       -2.331483
C       1.356677        2.290277       -2.185962
C       0.549854        2.600156        0.126052
C      -0.287906        1.424630       -0.025324
C       1.067433       -0.021375       -3.000953
C       2.712925        2.286290       -2.703145
C       1.067415        2.610267        1.482217
C      -0.287206        0.707901        1.236334
C      -0.287881       -0.734417       -1.220886
C       2.373642        3.043847        1.728647
C       3.211889        3.483812        0.628343
C       2.373795       -0.024897       -3.498925
C       3.551155        3.019068       -1.771947
C       3.211644        1.150282       -3.347165
C       0.549651        1.440568        2.168337
C      -0.287629       -0.690386        1.246433
C      -0.288224       -1.425023       -0.005077
C       0.549582       -1.190786       -2.314915
C       0.549811       -1.409531        2.188516
C       0.549945       -2.598042        0.163088
C       1.356731       -2.321143       -2.153174
C       1.357770        0.747356        3.074184
C       4.566964        0.703429       -3.084279
C       1.067385       -2.589090        1.519291
C       1.357819       -3.036641       -0.890190
C       2.713003       -2.324645       -2.670600
C       3.551279       -3.043848       -1.728805
C       6.212549        0.690385       -1.246591
C       2.713032       -3.483813       -0.628500
C       3.212036       -3.474667        0.677900
C       4.567315       -3.023886        0.933270
C       2.373766       -3.019069        1.771790
C       2.713241        1.197747        3.330320
C       6.212126       -0.707902       -1.236491
C       1.357957       -0.703430        3.084122
C       2.713277       -1.150283        3.347008
C       5.375270       -1.440569       -2.168494
C       6.213145        1.425022        0.004920
C       6.212802        0.734416        1.220728
C       4.857506       -2.610268       -1.482374
C       5.375067       -2.600157       -0.126209
C       3.211996       -2.286291        2.702988
C       4.568244       -2.290278        2.185805
C       6.212827       -1.424631        0.025166
C       3.551126        0.024896        3.498768
C       5.375339        1.190785        2.314757
C       6.212717       -0.716864        1.231032
C       4.857488        0.021374        3.000796
C       5.375241       -1.157579        2.331326
C       5.375110        1.409530       -2.188673
C       4.857536        2.589089       -1.519448
C       5.374976        2.598041       -0.163245
C       3.211680       -1.197748       -3.330477
C       4.567151       -0.747357       -3.074341
C       1.357606        3.023885       -0.933427
C       2.712885        3.474666       -0.678058
C       4.567102        3.036640        0.890033
C       3.211918        2.324643        2.670442
C       4.568190        2.321142        2.153017
C      -3.075721        0.689172       -3.698129
C      -3.075721       -0.741790       -3.687935
C      -3.418289       -1.449319       -2.469505
C      -3.760890       -2.858244       -2.445927
C      -3.760857       -3.564796       -1.201469
C      -3.418224       -2.863351        0.020489
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C	-3.075590	-3.547316	1.252316
C	-3.075557	-2.823105	2.486582
C	-3.418158	-1.413987	2.490085
C	-3.760727	-0.689171	3.698310
C	-3.760727	0.741791	3.688116
C	-3.418158	1.449320	2.469687
C	-3.075557	2.858245	2.446108
C	-3.075590	3.564798	1.201651
C	-3.418224	2.863352	-0.020307
C	-3.760857	3.547317	-1.252135
C	-3.760890	2.823106	-2.486400
C	-3.418289	1.413989	-2.489903
C	-3.418257	0.714944	-1.258783
C	-3.418257	-0.732805	-1.248470
C	-3.418224	-1.447772	0.010404
C	-3.418190	-0.714943	1.258965
C	-3.418190	0.732807	1.248651
C	-3.418224	1.447773	-0.010223
C	-4.196225	3.504622	-3.653487
C	-4.595401	4.826347	-3.644740
C	-4.595369	5.535835	-2.435530
C	-4.196162	4.898580	-1.277621
C	-2.640448	-1.412029	-4.861580
C	-2.241301	-0.743790	-6.001979
C	-2.241301	0.658204	-6.011967
C	-2.640448	1.342623	-4.881204
C	-4.196162	-4.916285	-1.207701
C	-4.595369	-5.569973	-2.356413
C	-4.595401	-4.877784	-3.575609
C	-4.196225	-3.556317	-3.603186
C	-2.640222	-3.504620	3.653669
C	-2.241046	-4.826346	3.644921
C	-2.241078	-5.535834	2.435711
C	-2.640286	-4.898579	1.277802
C	-4.195999	1.412031	4.861762
C	-4.595146	0.743791	6.002161
C	-4.595146	-0.658203	6.012148
C	-4.195999	-1.342622	4.881386
C	-2.640286	4.916286	1.207883
C	-2.241078	5.569974	2.356594
C	-2.241046	4.877786	3.575790
C	-2.640222	3.556319	3.603367
H	-4.262213	2.962149	-4.582341
H	-4.942143	5.292105	-4.563362
H	-4.942085	6.564937	-2.393922
H	-4.262100	5.444595	-0.350893
H	-2.574485	-2.487769	-4.856027
H	-1.894607	-1.306593	-6.864558
H	-1.894607	1.208661	-6.882477
H	-2.574485	2.418332	-4.890977
H	-4.262100	-5.449042	-0.273288
H	-4.942085	-6.598377	-2.300148
H	-4.942143	-5.356583	-4.487502
H	-4.262213	-3.027133	-4.539674
H	-2.574235	-2.962148	4.582522
H	-1.894304	-5.292104	4.563543
H	-1.894362	-6.564936	2.394104
H	-2.574347	-5.444594	0.351074
H	-4.261962	2.487770	4.856208
H	-4.941840	1.306594	6.864740
H	-4.941840	-1.208660	6.882658
H	-4.261962	-2.418331	4.891159
H	-2.574347	5.449043	0.273469
H	-1.894362	6.598378	2.300330
H	-1.894305	5.356584	4.487683
H	-2.574235	3.027134	4.539855

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cf9, c-HBC_heterodimers_with_C60 with bowl depth: 0.88

C	-0.287811	0.699837	-1.240942
C	0.549652	1.125356	-2.347212
C	1.356651	2.259952	-2.217314
C	0.549856	2.601645	0.090221
C	-0.287906	1.424146	-0.044939
C	1.067397	-0.062706	-3.000387
C	2.712893	2.248842	-2.734410
C	1.067433	2.630434	1.446112
C	-0.287191	0.724862	1.226470
C	-0.287896	-0.751162	-1.210651
C	2.373662	3.067366	1.686533
C	3.211896	3.492134	0.580263
C	2.373753	-0.073086	-3.498279
C	3.551134	2.994376	-1.813403
C	3.211604	1.104072	-3.362729
C	0.549677	1.470296	2.148284
C	-0.287614	-0.673154	1.255827
C	-0.288224	-1.424958	0.014554
C	0.549554	-1.222556	-2.298301

C	0.549837	-1.379255	2.207715
C	0.549947	-2.595550	0.198849
C	1.356705	-2.350579	-2.121017
C	1.357806	0.789625	3.063583
C	4.566927	0.660882	-3.093729
C	1.067403	-2.567919	1.554794
C	1.357809	-3.048614	-0.848298
C	2.712971	-2.361207	-2.638361
C	3.551258	-3.067371	-1.686760
C	6.212535	0.673149	-1.256054
C	2.713024	-3.492139	-0.580490
C	3.212043	-3.465001	0.725655
C	4.567325	-3.010747	0.974775
C	2.373787	-2.994380	1.813176
C	2.713280	1.243501	3.313476
C	6.212112	-0.724867	-1.226697
C	1.357993	-0.660886	3.093502
C	2.713316	-1.104076	3.362502
C	5.375244	-1.470301	-2.148511
C	6.213145	1.424953	-0.014781
C	6.212816	0.751158	1.210424
C	4.857488	-2.630439	-1.446339
C	5.375065	-2.601650	-0.090448
C	3.212027	-2.248846	2.734183
C	4.568270	-2.259957	2.217087
C	6.212827	-1.424151	0.044712
C	3.551168	0.073081	3.498052
C	5.375366	1.222552	2.298074
C	6.212731	-0.699842	1.240715
C	4.857523	0.062701	3.000160
C	5.375268	-1.125361	2.346985
C	5.375084	1.379251	-2.207942
C	4.857518	2.567914	-1.555021
C	5.374974	2.595545	-0.199076
C	3.211640	-1.243506	-3.313703
C	4.567114	-0.789630	-3.063810
C	1.357595	3.010742	-0.975002
C	2.712877	3.464997	-0.725882
C	4.567112	3.048610	0.848071
C	3.211949	2.361202	2.638134
C	4.568216	2.350575	2.120790
C	-3.035022	0.639227	-3.688657
C	-3.035022	-0.792789	-3.658728
C	-3.418318	-1.478849	-2.442209
C	-3.801660	-2.874806	-2.397782
C	-3.801612	-3.565103	-1.142652
C	-3.418224	-2.854735	0.059796
C	-3.034835	-3.514242	1.290874
C	-3.034787	-2.772105	2.516066
C	-3.418129	-1.375511	2.502128
C	-3.801425	-0.639221	3.688919
C	-3.801425	0.792794	3.658990
C	-3.418129	1.478854	2.442471
C	-3.034787	2.874811	2.398044
C	-3.034835	3.565108	1.142913
C	-3.418224	2.854740	-0.059534
C	-3.801612	3.514247	-1.290612
C	-3.801660	2.772111	-2.515804
C	-3.418318	1.375516	-2.501866
C	-3.418271	0.695281	-1.264334
C	-3.418271	-0.747500	-1.234180
C	-3.418224	-1.442870	0.030287
C	-3.418176	-0.695275	1.264596
C	-3.418176	0.747506	1.234442
C	-3.418224	1.442876	-0.030025
C	-4.293505	3.409381	-3.684038
C	-4.744395	4.715955	-3.676811
C	-4.744348	5.443613	-2.475672
C	-4.293413	4.844918	-1.314324
C	-2.543265	-1.485829	-4.794941
C	-2.092417	-0.826137	-5.922783
C	-2.092417	0.577948	-5.952129
C	-2.543265	1.284188	-4.852835
C	-4.293413	-4.895603	-1.110745
C	-4.744348	-5.542298	-2.246064
C	-4.744395	-4.865462	-3.476557
C	-4.293505	-3.560331	-3.538369
C	-2.542942	-3.409375	3.684300
C	-2.092052	-4.715950	3.677073
C	-2.092099	-5.443607	2.475934
C	-2.543034	-4.844913	1.314586
C	-4.293182	1.485834	4.795203
C	-4.744030	0.826142	5.923045
C	-4.744030	-0.577943	5.952391
C	-4.293182	-1.284183	4.853097
C	-2.543034	4.895608	1.111007
C	-2.092099	5.542304	2.246325
C	-2.092053	4.865468	3.476819
C	-2.542942	3.560336	3.538631
H	-4.367750	2.840235	-4.599961

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H      -5.134953        5.157589       -4.589871
H      -5.134870        6.457376       -2.444442
H      -4.367586        5.393100       -0.385706
H      -2.469056       -2.563720       -4.760204
H      -1.701926       -1.395827       -6.761944
H      -1.701926        1.112079       -6.814360
H      -2.469056        2.362590       -4.863165
H      -4.367586       -5.404506       -0.160034
H      -5.134870       -6.553871       -2.172504
H      -5.134953       -5.344860       -4.370367
H      -4.367750       -3.029951       -4.477272
H      -2.468698       -2.840229        4.600223
H      -1.701494       -5.157583        4.590133
H      -1.701577       -6.457370        2.444704
H      -2.468861       -5.393094        0.385968
H      -4.367391        2.563726        4.760466
H      -5.134521        1.395833        6.762206
H      -5.134521       -1.112074        6.814622
H      -4.367391       -2.362584        4.863427
H      -2.468861        5.404511        0.160296
H      -1.701577        6.553876        2.172766
H      -1.701494        5.344865        4.370629
H      -2.468698        3.029957        4.477534

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cf10, c-HBC_heterodimers_with_C60 with bowl depth: 0.97

C      -0.292423        0.717982       -1.230541
C       0.545067        1.159697       -2.330423
C       1.352062        2.292263       -2.183861
C       0.545210        2.600040        0.128423
C      -0.292549        1.424652       -0.024032
C       1.062828       -0.018647       -3.000958
C       2.708317        2.288746       -2.701031
C       1.062753        2.608919        1.484603
C      -0.291864        0.706777        1.236974
C      -0.292508       -0.733307       -1.221556
C       2.368977        3.042274        1.731444
C       3.207238        3.483239        0.631551
C       2.369197       -0.021716       -3.498916
C       3.546535        3.020678       -1.769156
C       3.207044        1.153325       -3.346077
C       0.544980        1.438596        2.169653
C      -0.292287       -0.691519        1.245802
C      -0.292867       -1.425018       -0.006376
C       0.544969       -1.188681       -2.315989
C       0.545140       -1.411520        2.187241
C       0.545301       -2.598189        0.160733
C       1.352116       -2.319185       -2.155266
C       1.353088        0.744561        3.074880
C       4.562360        0.706233       -3.083580
C       1.062723       -2.590470        1.516951
C       1.353188       -3.035831       -0.892933
C       2.708395       -2.322216       -2.672677
C       3.546659       -3.042275       -1.731525
C       6.207923        0.691519       -1.245883
C       2.708398       -3.483240       -0.631632
C       3.207385       -3.475282        0.674783
C       4.562660       -3.024733        0.930579
C       2.369101       -3.020678        1.769075
C       2.708555        1.194719        3.331442
C       6.207500       -0.706777       -1.237055
C       1.353275       -0.706234        3.083499
C       2.708591       -1.153325        3.345996
C       5.370655       -1.438597       -2.169734
C       6.208502        1.425018        0.006295
C       6.208143        0.733306        1.221475
C       4.852882       -2.608919       -1.484684
C       5.370426       -2.600041       -0.128504
C       3.207318       -2.288747        2.700950
C       4.563573       -2.292264        2.183780
C       6.208184       -1.424653        0.023951
C       3.546439        0.021715        3.498835
C       5.370666        1.188681        2.315908
C       6.208058       -0.717982        1.230460
C       4.852807        0.018647        3.000877
C       5.370568       -1.159697        2.330341
C       5.370495        1.411520       -2.187322
C       4.852912        2.590469       -1.517032
C       5.370335        2.598189       -0.160814
C       3.207080       -1.194719       -3.331524
C       4.562547       -0.744561       -3.074961
C       1.352975        3.024733       -0.930660
C       2.708251        3.475281       -0.674864
C       4.562447        3.035830        0.892852
C       3.207240        2.322215        2.672596
C       4.563519        2.319185        2.155185
C      -2.990414        0.694217       -3.660150
C      -2.990414       -0.739655       -3.651239
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C	-3.412900	-1.439133	-2.457306
C	-3.835403	-2.822710	-2.431060
C	-3.835386	-3.531935	-1.184841
C	-3.412866	-2.847612	0.017744
C	-2.990347	-3.516935	1.228741
C	-2.990330	-2.792275	2.466050
C	-3.412833	-1.408479	2.475097
C	-3.835319	-0.694216	3.660244
C	-3.835319	0.739656	3.651332
C	-3.412833	1.439134	2.457400
C	-2.990330	2.822710	2.431154
C	-2.990347	3.531935	1.184934
C	-3.412866	2.847612	-0.017650
C	-3.835386	3.516935	-1.228648
C	-3.835403	2.792276	-2.465956
C	-3.412900	1.408480	-2.475003
C	-3.412884	0.711651	-1.250449
C	-3.412884	-0.727138	-1.241507
C	-3.412866	-1.438717	0.008988
C	-3.412849	-0.711650	1.250543
C	-3.412849	0.727138	1.241601
C	-3.412866	1.438717	-0.008895
C	-4.385297	3.416681	-3.613959
C	-4.891645	4.703528	-3.568810
C	-4.891628	5.414170	-2.355334
C	-4.385264	4.823711	-1.211169
C	-2.440551	-1.421782	-4.765902
C	-1.934217	-0.739540	-5.857863
C	-1.934217	0.666675	-5.866602
C	-2.440551	1.362436	-4.783205
C	-4.385264	-4.838392	-1.151121
C	-4.891628	-5.443026	-2.287859
C	-4.891645	-4.747522	-3.510074
C	-4.385297	-3.461335	-3.571214
C	-2.440436	-3.416680	3.614053
C	-1.934088	-4.703527	3.568903
C	-1.934105	-5.414169	2.355427
C	-2.440469	-4.823711	1.211262
C	-4.385182	1.421782	4.765995
C	-4.891516	0.739540	5.857956
C	-4.891516	-0.666675	5.866695
C	-4.385182	-1.362436	4.783299
C	-2.440469	4.838393	1.151215
C	-1.934105	5.443027	2.287952
C	-1.934088	4.747522	3.510167
C	-2.440436	3.461335	3.571307
H	-4.467763	2.847814	-4.532555
H	-5.329797	5.143146	-4.461017
H	-5.329767	6.407361	-2.302029
H	-4.467705	5.346224	-0.265514
H	-2.358096	-2.501711	-4.732163
H	-1.496088	-1.292510	-6.684622
H	-1.496088	1.209327	-6.700170
H	-2.358097	2.442702	-4.762891
H	-4.467705	-5.349111	-0.199045
H	-5.329767	-6.435479	-2.222214
H	-5.329797	-5.198195	-4.396748
H	-4.467763	-2.903929	-4.496810
H	-2.357970	-2.847813	4.532649
H	-1.495936	-5.143145	4.461110
H	-1.495965	-6.407361	2.302122
H	-2.358028	-5.346224	0.265607
H	-4.467636	2.501712	4.732256
H	-5.329645	1.292511	6.684716
H	-5.329645	-1.209327	6.700264
H	-4.467636	-2.442701	4.762985
H	-2.358028	5.349112	0.199138
H	-1.495965	6.435479	2.222307
H	-1.495936	5.198195	4.396842
H	-2.357970	2.903930	4.496903

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cf11, c-HBC_heterodimers_with_C60 with bowl depth: 1.07

C	-0.292383	-0.720969	1.228803
C	0.545143	-1.165354	2.327581
C	1.352133	-2.297562	2.178242
C	0.545205	-2.599721	-0.134756
C	-0.292548	-1.424706	0.020581
C	1.062927	0.011357	3.000959
C	2.708405	-2.295301	2.695374
C	1.062704	-2.605305	-1.490971
C	-0.291905	-0.703770	-1.238677
C	-0.292468	0.730337	1.223344
C	2.368919	-3.038059	-1.738908
C	3.207216	-3.481695	-0.640116
C	2.369312	0.013216	3.498881
C	3.546592	-3.024967	1.761696
C	3.207154	-1.161450	3.343160

C	0.544909	-1.433322	-2.173159
C	-0.292328	0.694544	-1.244108
C	-0.292866	1.424998	0.009847
C	0.545045	1.183051	2.318852
C	0.545069	1.416829	-2.183823
C	0.545296	2.598572	-0.154439
C	1.352187	2.313942	2.160849
C	1.352987	-0.737089	-3.076724
C	4.562462	-0.713723	3.081705
C	1.062674	2.594147	-1.510688
C	1.353218	3.033653	0.900261
C	2.708483	2.315716	2.678221
C	3.546716	3.038059	1.738794
C	6.207963	-0.694544	1.243995
C	2.708419	3.481695	0.640003
C	3.207363	3.476910	-0.666444
C	4.562630	3.026984	-0.923378
C	2.369043	3.024966	-1.761810
C	2.708446	-1.186623	-3.334424
C	6.207540	0.703769	1.238564
C	1.353174	0.713722	-3.081819
C	2.708482	1.161450	-3.343273
C	5.370726	1.433321	2.173046
C	6.208501	-1.424999	-0.009961
C	6.208103	-0.730338	-1.223457
C	4.852931	2.605304	1.490857
C	5.370430	2.599720	0.134643
C	3.207230	2.295301	-2.695487
C	4.563502	2.297561	-2.178355
C	6.208183	1.424706	-0.020694
C	3.546323	-0.013216	-3.498994
C	5.370590	-1.183052	-2.318965
C	6.208018	0.720968	-1.228916
C	4.852708	-0.011357	-3.001073
C	5.370492	1.165354	-2.327694
C	5.370566	-1.416830	2.183710
C	4.852961	-2.594147	1.510575
C	5.370339	-2.598572	0.154326
C	3.207190	1.186622	3.334311
C	4.562649	0.737088	3.076610
C	1.353005	-3.026985	0.923265
C	2.708272	-3.476911	0.666330
C	4.562417	-3.033653	-0.900374
C	3.207152	-2.315716	-2.678335
C	4.563448	-2.313943	-2.160963
C	-2.951477	-0.704263	3.641807
C	-2.951477	0.731814	3.636370
C	-3.412819	1.430764	2.456698
C	-3.874140	2.801859	2.430678
C	-3.874163	3.514952	1.184184
C	-3.412866	2.842337	-0.010694
C	-2.951569	3.505886	-1.210630
C	-2.951593	2.783377	-2.451689
C	-3.412914	1.412124	-2.467329
C	-3.874256	0.704264	-3.641676
C	-3.874256	-0.731814	-3.636240
C	-3.412914	-1.430763	-2.456567
C	-2.951593	-2.801859	-2.430547
C	-2.951569	-3.514951	-1.184053
C	-3.412866	-2.842336	0.010825
C	-3.874163	-3.505886	1.210761
C	-3.874140	-2.783377	2.451820
C	-3.412819	-1.412124	2.467460
C	-3.412843	-0.713264	1.246449
C	-3.412843	0.722680	1.241014
C	-3.412866	1.435831	-0.005370
C	-3.412890	0.713264	-1.246318
C	-3.412890	-0.722679	-1.240883
C	-3.412866	-1.435830	0.005501
C	-4.482417	-3.380532	3.584561
C	-5.041143	-4.645838	3.518295
C	-5.041167	-5.353682	2.302044
C	-4.482463	-4.785669	1.169561
C	-2.343157	1.414604	4.719415
C	-1.784411	0.725475	5.782531
C	-1.784411	-0.681676	5.787858
C	-2.343157	-1.378834	4.729989
C	-4.482463	4.794386	1.133296
C	-5.041167	5.370957	2.261447
C	-5.041143	4.672341	3.483022
C	-4.482417	3.407573	3.558865
C	-2.343316	3.380533	-3.584430
C	-1.784590	4.645839	-3.518164
C	-1.784566	5.353683	-2.301913
C	-2.343269	4.785670	-1.169430
C	-4.482576	-1.414604	-4.719284
C	-5.041321	-0.725475	-5.782401
C	-5.041321	0.681677	-5.787727
C	-4.482576	1.378834	-4.729858
C	-2.343270	-4.794386	-1.133165

C	-1.784566	-5.370956	-2.261316
C	-1.784590	-4.672341	-3.482891
C	-2.343316	-3.407573	-3.558734
H	-4.573099	-2.804369	4.499827
H	-5.523603	-5.069746	4.395220
H	-5.523644	-6.325481	2.237288
H	-4.573182	-5.295258	0.215624
H	-2.252458	2.495204	4.676536
H	-1.301920	1.273366	6.587790
H	-1.301920	-1.223454	6.597242
H	-2.252458	-2.459727	4.695293
H	-4.573182	5.296738	0.175529
H	-5.523644	6.342238	2.189335
H	-5.523602	5.102876	4.356713
H	-4.573099	2.838356	4.478466
H	-2.252633	2.804370	-4.499696
H	-1.302130	5.069746	-4.395090
H	-1.302089	6.325482	-2.237157
H	-2.252551	5.295258	-0.215493
H	-4.573275	-2.495203	-4.676405
H	-5.523813	-1.273365	-6.587659
H	-5.523813	1.223455	-6.597111
H	-4.573275	2.459728	-4.695162
H	-2.252551	-5.296738	-0.175398
H	-1.302089	-6.342237	-2.189204
H	-1.302130	-5.102875	-4.356582
H	-2.252634	-2.838356	-4.478336

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cf12, c-HBC_heterodimers_with_C60 with bowl depth: 1.17

C	-0.292393	-0.718384	1.230313
C	0.545124	-1.160458	2.330030
C	1.352115	-2.292977	2.183079
C	0.545206	-2.599998	-0.129286
C	-0.292548	-1.424660	0.023574
C	1.062902	0.017666	3.000937
C	2.708383	-2.289629	2.700216
C	1.062716	-2.608433	-1.485481
C	-0.291895	-0.706373	-1.237197
C	-0.292478	0.732907	1.221803
C	2.368933	-3.041708	-1.732497
C	3.207221	-3.483033	-0.632769
C	2.369283	0.020572	3.498865
C	3.546578	-3.021256	1.768081
C	3.207126	-1.154419	3.345621
C	0.544927	-1.437887	-2.170137
C	-0.292318	0.691926	-1.245568
C	-0.292866	1.425016	0.006849
C	0.545026	1.187924	2.316364
C	0.545087	1.412235	-2.186793
C	0.545297	2.598242	-0.159898
C	1.352169	2.318480	2.155991
C	1.353012	-0.743556	-3.075156
C	4.562436	-0.707242	3.083237
C	1.062686	2.590965	-1.516130
C	1.353211	3.035539	0.893892
C	2.708461	2.321342	2.673369
C	3.546702	3.041708	1.732432
C	6.207953	-0.691927	1.245503
C	2.708414	3.483033	0.632704
C	3.207368	3.475501	-0.673726
C	4.562638	3.025036	-0.929703
C	2.369057	3.021256	-1.768146
C	2.708473	-1.193630	-3.331900
C	6.207530	0.706372	1.237132
C	1.353199	0.707241	-3.083301
C	2.708509	1.154418	-3.345686
C	5.370708	1.437887	2.170072
C	6.208501	-1.425016	-0.006914
C	6.208113	-0.732908	-1.221868
C	4.852919	2.608433	1.485417
C	5.370429	2.599998	0.129221
C	3.207252	2.289629	-2.700281
C	4.563520	2.292977	-2.183144
C	6.208183	1.424659	-0.023639
C	3.546352	-0.020572	-3.498929
C	5.370609	-1.187924	-2.316429
C	6.208028	0.718383	-1.230378
C	4.852733	-0.017667	-3.001002
C	5.370511	1.160458	-2.330095
C	5.370548	-1.412235	2.186728
C	4.852949	-2.590966	1.516065
C	5.370338	-2.598242	0.159833
C	3.207162	1.193630	3.331835
C	4.562623	0.743555	3.075091
C	1.352998	-3.025037	0.929638
C	2.708267	-3.475502	0.673661
C	4.562425	-3.035539	-0.893957

C	3.207174	-2.321342	-2.673434
C	4.563466	-2.318481	-2.156056
C	-2.912924	-0.697747	3.626221
C	-2.912924	0.740399	3.617753
C	-3.412839	1.433727	2.450071
C	-3.912743	2.791447	2.417234
C	-3.912756	3.503001	1.167486
C	-3.412866	2.838277	-0.016674
C	-2.912976	3.489011	-1.208580
C	-2.912990	2.762790	-2.449862
C	-3.412893	1.404778	-2.466709
C	-3.912809	0.697747	-3.626146
C	-3.912809	-0.740398	-3.617678
C	-3.412893	-1.433727	-2.449997
C	-2.912990	-2.791446	-2.417159
C	-2.912976	-3.503000	-1.167411
C	-3.412866	-2.838277	0.016749
C	-3.912756	-3.489010	1.208655
C	-3.912743	-2.762789	2.449937
C	-3.412839	-1.404777	2.466784
C	-3.412853	-0.709493	1.245889
C	-3.412853	0.724114	1.237448
C	-3.412866	1.433323	-0.008402
C	-3.412880	0.709493	-1.245815
C	-3.412880	-0.724114	-1.237374
C	-3.412866	-1.433323	0.008477
C	-4.579685	-3.325046	3.567294
C	-5.193979	-4.564114	3.485226
C	-5.193992	-5.274732	2.270363
C	-4.579711	-4.738432	1.150397
C	-2.245958	1.427199	4.663076
C	-1.631654	0.737230	5.695466
C	-1.631654	-0.670112	5.703752
C	-2.245958	-1.372190	4.679559
C	-4.579711	4.751650	1.094520
C	-5.193992	5.301101	2.208093
C	-5.193978	4.604837	3.431240
C	-4.579685	3.366822	3.527893
C	-2.246048	3.325046	-3.567219
C	-1.631754	4.564114	-3.485151
C	-1.631741	5.274732	-2.270288
C	-2.246022	4.738432	-1.150322
C	-4.579775	-1.427199	-4.663002
C	-5.194079	-0.737229	-5.695391
C	-5.194079	0.670112	-5.703677
C	-4.579775	1.372191	-4.679484
C	-2.246022	-4.751649	-1.094445
C	-1.631741	-5.301100	-2.208018
C	-1.631754	-4.604837	-3.431165
C	-2.246048	-3.366822	-3.527818
H	-4.678620	-2.738067	4.475926
H	-5.723572	-4.961935	4.347104
H	-5.723596	-6.220908	2.194494
H	-4.678667	-5.241863	0.192931
H	-2.147014	2.507633	4.608246
H	-1.102042	1.285084	6.470643
H	-1.102042	-1.208800	6.485327
H	-2.147014	-2.453195	4.637455
H	-4.678667	5.243771	0.131192
H	-5.723596	6.246318	2.121088
H	-5.723572	5.012780	4.288374
H	-4.678620	2.790583	4.443374
H	-2.147113	2.738067	-4.475851
H	-1.102161	4.961935	-4.347029
H	-1.102137	6.220908	-2.194420
H	-2.147066	5.241863	-0.192856
H	-4.678719	-2.507633	-4.608171
H	-5.723690	-1.285084	-6.470568
H	-5.723690	1.208801	-6.485252
H	-4.678719	2.453195	-4.637380
H	-2.147066	-5.243771	-0.131117
H	-1.102137	-6.246317	-2.121013
H	-1.102161	-5.012780	-4.288299
H	-2.147113	-2.790583	-4.443299

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cf13, c-HBC_heterodimers_with_C60 with bowl depth: 1.26

C	-0.287734	-0.719484	1.229674
C	0.549798	-1.162542	2.328984
C	1.356788	-2.294929	2.181009
C	0.549847	-2.599882	-0.131619
C	-0.287905	-1.424680	0.022303
C	1.067586	0.014982	3.000937
C	2.713062	-2.292044	2.698130
C	1.067339	-2.607104	-1.487828
C	-0.287269	-0.705266	-1.237825
C	-0.287819	0.731814	1.222462
C	2.373552	-3.040158	-1.735249

C	3.211855	-3.482466	-0.635927
C	2.373973	0.017443	3.498849
C	3.551244	-3.022837	1.765330
C	3.211814	-1.157411	3.344543
C	0.549540	-1.435946	-2.171429
C	-0.287692	0.693040	-1.244945
C	-0.288223	1.425009	0.008127
C	0.549700	1.185852	2.317418
C	0.549700	1.414190	-2.185536
C	0.549938	2.598384	-0.157581
C	1.356842	2.316551	2.158045
C	1.357613	-0.740805	-3.075838
C	4.567121	-0.709999	3.082541
C	1.067309	2.592320	-1.513827
C	1.357866	3.034738	0.896588
C	2.713140	2.318949	2.675407
C	3.551368	3.040157	1.735104
C	6.212613	-0.693041	1.244800
C	2.713065	3.482465	0.635782
C	3.212002	3.476102	-0.670661
C	4.567268	3.025866	-0.927059
C	2.373677	3.022836	-1.765476
C	2.713071	-1.190650	-3.333003
C	6.212190	0.705265	1.237679
C	1.357800	0.709999	-3.082686
C	2.713107	1.157410	-3.344689
C	5.375381	1.435945	2.171284
C	6.213144	-1.425010	-0.008273
C	6.212739	-0.731815	-1.222607
C	4.857582	2.607103	1.487683
C	5.375074	2.599881	0.131473
C	3.211859	2.292043	-2.698276
C	4.568133	2.294928	-2.181154
C	6.212826	1.424680	-0.022449
C	3.550948	-0.017443	-3.498995
C	5.375220	-1.185853	-2.317563
C	6.212654	0.719483	-1.229819
C	4.857335	-0.014983	-3.001083
C	5.375122	1.162541	-2.329129
C	5.375221	-1.414191	2.185391
C	4.857612	-2.592321	1.513681
C	5.374983	-2.598384	0.157436
C	3.211850	1.190649	3.332857
C	4.567308	0.740805	3.075693
C	1.357653	-3.025867	0.926914
C	2.712918	-3.476103	0.670516
C	4.567055	-3.034739	-0.896733
C	3.211781	-2.318950	-2.675552
C	4.568079	-2.316552	-2.158190
C	-2.878879	-0.702367	3.609018
C	-2.878879	0.738375	3.601823
C	-3.418163	1.430299	2.449200
C	-3.957420	2.774273	2.412715
C	-3.957451	3.488138	1.161227
C	-3.418224	2.835544	-0.014076
C	-2.878996	3.476368	-1.195837
C	-2.879027	2.750041	-2.440133
C	-3.418284	1.405769	-2.463195
C	-3.957568	0.702368	-3.608850
C	-3.957568	-0.738374	-3.601656
C	-3.418284	-1.430298	-2.449033
C	-2.879027	-2.774273	-2.412547
C	-2.878996	-3.488137	-1.161059
C	-3.418224	-2.835543	0.014243
C	-3.957451	-3.476367	1.196004
C	-3.957420	-2.750040	2.440301
C	-3.418163	-1.405768	2.463362
C	-3.418193	-0.709795	1.243959
C	-3.418193	0.722183	1.236808
C	-3.418224	1.431752	-0.007066
C	-3.418254	0.709796	-1.243791
C	-3.418254	-0.722182	-1.236640
C	-3.418224	-1.431751	0.007233
C	-4.682232	-3.280238	3.537807
C	-5.348886	-4.491040	3.436142
C	-5.348916	-5.200169	2.220780
C	-4.682292	-4.692409	1.116931
C	-2.154015	1.424181	4.609241
C	-1.487340	0.731533	5.607511
C	-1.487340	-0.675495	5.614538
C	-2.154015	-1.378078	4.623234
C	-4.682292	4.703330	1.070013
C	-5.348916	5.222089	2.168736
C	-5.348886	4.525132	3.391119
C	-4.682232	3.315406	3.504871
C	-2.154215	3.280239	-3.537639
C	-1.487561	4.491041	-3.435974
C	-1.487531	5.200170	-2.220612
C	-2.154155	4.692410	-1.116764
C	-4.682432	-1.424180	-4.609073

C	-5.349107	-0.731532	-5.607344
C	-5.349107	0.675496	-5.614370
C	-4.682432	1.378079	-4.623066
C	-2.154155	-4.703329	-1.069846
C	-1.487531	-5.222088	-2.168568
C	-1.487561	-4.525131	-3.390952
C	-2.154215	-3.315405	-3.504703
H	-4.789401	-2.687828	4.442681
H	-5.921651	-4.863481	4.281575
H	-5.921704	-6.119373	2.128839
H	-4.789506	-5.187408	0.155312
H	-2.046826	2.503967	4.547182
H	-0.914536	1.278041	6.352312
H	-0.914536	-1.214538	6.364759
H	-2.046826	-2.458430	4.571962
H	-4.789506	5.188701	0.103498
H	-5.921704	6.140328	2.067619
H	-5.921651	4.905998	4.232791
H	-4.789401	2.732062	4.415617
H	-2.047046	2.687829	-4.442514
H	-0.914796	4.863482	-4.281408
H	-0.914743	6.119374	-2.128671
H	-2.046941	5.187409	-0.155144
H	-4.789621	-2.503966	-4.547015
H	-5.921911	-1.278040	-6.352144
H	-5.921911	1.214539	-6.364591
H	-4.789621	2.458431	-4.571795
H	-2.046941	-5.188700	-0.103330
H	-0.914743	-6.140327	-2.067452
H	-0.914796	-4.905997	-4.232623
H	-2.047046	-2.732062	-4.415449

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cf14, c-HBC_heterodimers_with_C60 with bowl depth: 1.36

C	-0.278492	0.713893	-1.232918
C	0.559001	1.151954	-2.334258
C	1.365995	2.285001	-2.191456
C	0.559138	2.600452	0.119792
C	-0.278620	1.424565	-0.028762
C	1.076764	-0.028609	-3.000877
C	2.722251	2.279767	-2.708608
C	1.076678	2.613833	1.475936
C	-0.277939	0.710879	1.234620
C	-0.278577	-0.737358	-1.219116
C	2.382901	3.048005	1.721341
C	3.221165	3.485317	0.619992
C	2.383133	-0.033331	-3.498820
C	3.560467	3.014788	-1.779166
C	3.220980	1.142211	-3.349880
C	0.558904	1.445791	2.164867
C	-0.278362	-0.687380	1.248089
C	-0.278938	-1.425031	-0.001646
C	0.558903	-1.196363	-2.312029
C	0.559064	-1.404252	2.191916
C	0.559229	-2.597641	0.169359
C	1.366049	-2.326327	-2.147553
C	1.367009	0.754764	3.072394
C	4.576296	0.695993	-3.085897
C	1.076648	-2.585420	1.525544
C	1.367119	-3.038778	-0.882848
C	2.722329	-2.331075	-2.664947
C	3.560591	-3.048006	-1.721409
C	6.221854	0.687379	-1.248158
C	2.722328	-3.485317	-0.620060
C	3.221312	-3.473022	0.686323
C	4.576587	-3.021627	0.940625
C	2.383025	-3.014789	1.779098
C	2.722476	1.205771	3.327464
C	6.221431	-0.710880	-1.234688
C	1.367196	-0.695994	3.085829
C	2.722512	-1.142211	3.349812
C	5.384588	-1.445791	-2.164935
C	6.222430	1.425031	0.001578
C	6.222069	0.737357	1.219048
C	4.866814	-2.613833	-1.476004
C	5.384355	-2.600453	-0.119860
C	3.221241	-2.279768	2.708540
C	4.577497	-2.285002	2.191388
C	6.222112	-1.424565	0.028694
C	3.560359	0.033330	3.498752
C	5.384590	1.196362	2.311961
C	6.221984	-0.713893	1.232850
C	4.866728	0.028608	3.000809
C	5.384492	-1.151955	2.334190
C	5.384428	1.404251	-2.191984
C	4.866844	2.585419	-1.525612
C	5.384263	2.597641	-0.169427
C	3.221016	-1.205772	-3.327532

C	4.576483	-0.754765	-3.072462
C	1.366906	3.021627	-0.940693
C	2.722181	3.473022	-0.686391
C	4.576374	3.038778	0.882780
C	3.221163	2.331074	2.664879
C	4.577443	2.326326	2.147485
C	-2.849523	0.687474	-3.594630
C	-2.849523	-0.755889	-3.580868
C	-3.428966	-1.440246	-2.440629
C	-4.008422	-2.769229	-2.392530
C	-4.008407	-3.479014	-1.135603
C	-3.428938	-2.833627	0.027057
C	-2.849468	-3.456728	1.201811
C	-2.849454	-2.723105	2.444975
C	-3.428910	-1.393447	2.467726
C	-4.008353	-0.687473	3.594709
C	-4.008353	0.755890	3.580947
C	-3.428910	1.440246	2.440708
C	-2.849454	2.769229	2.392608
C	-2.849468	3.479015	1.135682
C	-3.428938	2.833628	-0.026978
C	-4.008407	3.456729	-1.201733
C	-4.008422	2.723106	-2.444897
C	-3.428966	1.393447	-2.467647
C	-3.428952	0.703537	-1.245873
C	-3.428952	-0.727164	-1.232232
C	-3.428938	-1.430624	0.013680
C	-3.428924	-0.703536	1.245951
C	-3.428924	0.727165	1.232310
C	-3.428938	1.430624	-0.013601
C	-4.790311	3.212159	-3.523337
C	-5.508142	4.392508	-3.408298
C	-5.508128	5.107239	-2.196850
C	-4.790283	4.636965	-1.108146
C	-2.067657	-1.445405	-4.543432
C	-1.349835	-0.755806	-5.508317
C	-1.349835	0.650640	-5.521727
C	-2.067657	1.358511	-4.570166
C	-4.790283	-4.657251	-1.019530
C	-5.508128	-5.148199	-2.099069
C	-5.508142	-4.456697	-3.323924
C	-4.790311	-3.278756	-3.461449
C	-2.067565	-3.212158	3.523416
C	-1.349733	-4.392508	3.408376
C	-1.349747	-5.107238	2.196928
C	-2.067593	-4.636964	1.108224
C	-4.790219	1.445406	4.543511
C	-5.508041	0.755807	5.508395
C	-5.508041	-0.650639	5.521805
C	-4.790219	-1.358510	4.570245
C	-2.067593	4.657252	1.019608
C	-1.349747	5.148200	2.099147
C	-1.349733	4.456698	3.324003
C	-2.067565	3.278757	3.461528
H	-4.905757	2.608781	-4.420398
H	-6.122732	4.731418	-4.238298
H	-6.122707	5.997633	-2.092018
H	-4.905708	5.129795	-0.145931
H	-1.952220	-2.523890	-4.468647
H	-0.735263	-1.305384	-6.216647
H	-0.735263	1.186611	-6.240408
H	-1.952220	2.438226	-4.515958
H	-4.905708	-5.131645	-0.048092
H	-6.122707	-6.036432	-1.977279
H	-6.122732	-4.811372	-4.147311
H	-4.905757	-2.692592	-4.369852
H	-1.952119	-2.608780	4.420477
H	-0.735144	-4.731418	4.238376
H	-0.735169	-5.997632	2.092097
H	-1.952168	-5.129794	0.146009
H	-4.905655	2.523891	4.468725
H	-6.122613	1.305384	6.216726
H	-6.122613	-1.186610	6.240486
H	-4.905655	-2.438225	4.516037
H	-1.952168	5.131645	0.048171
H	-0.735169	6.036433	1.977357
H	-0.735144	4.811372	4.147390
H	-1.952119	2.692593	4.369930

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cf15, c-HBC_heterodimers_with_C60 with bowl depth: 1.46

C	-0.259931	0.714805	-1.232387
C	0.577551	1.153682	-2.333410
C	1.384548	2.286623	-2.189776
C	0.577710	2.600363	0.121712
C	-0.260049	1.424585	-0.027705
C	1.095309	-0.026387	-3.000907
C	2.740799	2.281772	-2.706944

C	1.095263	2.612739	1.477861
C	-0.259356	0.709965	1.235148
C	-0.260016	-0.736455	-1.219660
C	2.401488	3.046730	1.723576
C	3.239742	3.484856	0.622543
C	2.401674	-0.030740	-3.498865
C	3.579023	3.016104	-1.776965
C	3.239522	1.144690	-3.349062
C	0.577495	1.444188	2.165931
C	-0.259779	-0.688304	1.247582
C	-0.260367	-1.425030	-0.002699
C	0.577453	-1.194650	-2.312920
C	0.577655	-1.405874	2.190870
C	0.577802	-2.597766	0.167430
C	1.384602	-2.324736	-2.149287
C	1.385608	0.752489	3.072939
C	4.594840	0.698278	-3.085422
C	1.095233	-2.586549	1.523619
C	1.385682	-3.038124	-0.885110
C	2.740877	-2.329101	-2.666697
C	3.579147	-3.046731	-1.723697
C	6.240414	0.688303	-1.247704
C	2.740893	-3.484857	-0.622665
C	3.239889	-3.473530	0.683722
C	4.595166	-3.022323	0.938347
C	2.401612	-3.016105	1.776844
C	2.741077	1.203307	3.328331
C	6.239991	-0.709966	-1.235269
C	1.385795	-0.698279	3.085301
C	2.741113	-1.144691	3.348941
C	5.403140	-1.444189	-2.166053
C	6.241002	1.425029	0.002578
C	6.240651	0.736454	1.219538
C	4.885372	-2.612740	-1.477982
C	5.402925	-2.600364	-0.121833
C	3.239836	-2.281773	2.706822
C	4.596088	-2.286624	2.189654
C	6.240684	-1.424586	0.027584
C	3.578962	0.030739	3.498743
C	5.403182	1.194649	2.312798
C	6.240566	-0.714806	1.232266
C	4.885326	0.026386	3.000786
C	5.403084	-1.153683	2.333289
C	5.402980	1.405873	-2.190991
C	4.885402	2.586548	-1.523741
C	5.402834	2.597765	-0.167551
C	3.239558	-1.203308	-3.328453
C	4.595027	-0.752490	-3.073061
C	1.385469	3.022322	-0.938468
C	2.740746	3.473529	-0.683843
C	4.594953	3.038123	0.884988
C	3.239758	2.329100	2.666576
C	4.596034	2.324735	2.149166
C	-2.829837	0.691818	-3.575247
C	-2.829837	-0.754588	-3.562527
C	-3.450416	-1.437463	-2.439972
C	-4.071017	-2.750292	-2.386543
C	-4.070992	-3.462574	-1.127509
C	-3.450366	-2.831761	0.024973
C	-2.829741	-3.442208	1.188370
C	-2.829716	-2.707894	2.434683
C	-3.450317	-1.394328	2.465015
C	-4.070896	-0.691817	3.575387
C	-4.070896	0.754589	3.562667
C	-3.450317	1.437464	2.440112
C	-2.829716	2.750293	2.386683
C	-2.829741	3.462575	1.127649
C	-3.450366	2.831762	-0.024833
C	-4.070992	3.442209	-1.188230
C	-4.071017	2.707895	-2.434543
C	-3.450416	1.394329	-2.464875
C	-3.450392	0.703861	-1.244246
C	-3.450392	-0.725634	-1.231675
C	-3.450366	-1.429454	0.012641
C	-3.450341	-0.703859	1.244386
C	-3.450341	0.725635	1.231815
C	-3.450366	1.429455	-0.012501
C	-4.909008	3.158964	-3.488573
C	-5.676554	4.305617	-3.352070
C	-5.676529	5.019089	-2.140832
C	-4.908958	4.582622	-1.071774
C	-1.991887	-1.442066	-4.479961
C	-1.224356	-0.750411	-5.404703
C	-1.224356	0.655243	-5.417065
C	-1.991887	1.363055	-4.504629
C	-4.908958	-4.600763	-0.991015
C	-5.676529	-5.055963	-2.052231
C	-5.676554	-4.363904	-3.275829
C	-4.909008	-3.219829	-3.432478
C	-1.991725	-3.158963	3.488713

C	-1.224179	-4.305616	3.352210
C	-1.224204	-5.019088	2.140972
C	-1.991774	-4.582621	1.071914
C	-4.908846	1.442068	4.480101
C	-5.676377	0.750412	5.404843
C	-5.676377	-0.655242	5.417205
C	-4.908846	-1.363054	4.504769
C	-1.991775	4.600764	0.991155
C	-1.224204	5.055965	2.052371
C	-1.224179	4.363905	3.275969
C	-1.991725	3.219830	3.432618
H	-5.032708	2.549080	-4.380489
H	-6.331192	4.613383	-4.163353
H	-6.331148	5.877899	-2.016634
H	-5.032621	5.066778	-0.105797
H	-1.868203	-2.519424	-4.397401
H	-0.569748	-1.299116	-6.076914
H	-0.569748	1.192041	-6.098822
H	-1.868203	2.441698	-4.441030
H	-5.032621	-5.067855	-0.016672
H	-6.331148	-5.912457	-1.912949
H	-6.331192	-4.685890	-4.081574
H	-5.032708	-2.625724	-4.334982
H	-1.868025	-2.549078	4.380629
H	-0.569541	-4.613382	4.163493
H	-0.569585	-5.877898	2.016774
H	-1.868112	-5.066776	0.105937
H	-5.032530	2.519425	4.397541
H	-6.330985	1.299117	6.077054
H	-6.330985	-1.192040	6.098962
H	-5.032530	-2.441697	4.441170
H	-1.868112	5.067856	0.016812
H	-0.569585	5.912458	1.913089
H	-0.569541	4.685891	4.081714
H	-1.868025	2.625726	4.335122

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cf16, c-HBC_heterodimers_with_C60 with bowl depth: 1.56

C	-0.232076	0.716509	-1.231398
C	0.605405	1.156908	-2.331814
C	1.412402	2.289649	-2.186614
C	0.605568	2.600192	0.125307
C	-0.232192	1.424622	-0.025735
C	1.123162	-0.022237	-3.000943
C	2.768652	2.285514	-2.703790
C	1.123122	2.610693	1.481471
C	-0.231497	0.708256	1.236128
C	-0.232161	-0.734767	-1.220677
C	2.429348	3.044343	1.727784
C	3.267600	3.483992	0.627357
C	2.429526	-0.025901	-3.498908
C	3.606878	3.018559	-1.772798
C	3.267374	1.149321	-3.347481
C	0.605355	1.441191	2.167925
C	-0.231920	-0.690028	1.246629
C	-0.232510	-1.425025	-0.004671
C	0.605307	-1.191450	-2.314571
C	0.605515	-1.408903	2.188922
C	0.605659	-2.597995	0.163836
C	1.412456	-2.321761	-2.152503
C	1.413470	0.748238	3.073975
C	4.622693	0.702544	-3.084460
C	1.123092	-2.588653	1.520038
C	1.413538	-3.036897	-0.889313
C	2.768730	-2.325411	-2.669920
C	3.607002	-3.044344	-1.727915
C	6.268270	0.690028	-1.246760
C	2.768750	-3.483993	-0.627488
C	3.267747	-3.474472	0.678912
C	4.623025	-3.023618	0.934159
C	2.429472	-3.018560	1.772667
C	2.768939	1.198703	3.329988
C	6.267847	-0.708257	-1.236259
C	1.413657	-0.702545	3.084329
C	2.768975	-1.149322	3.347350
C	5.430994	-1.441192	-2.168056
C	6.268859	1.425024	0.004539
C	6.268510	0.734766	1.220546
C	4.913227	-2.610693	-1.481602
C	5.430782	-2.600193	-0.125438
C	3.267697	-2.285515	2.703659
C	4.623948	-2.289650	2.186483
C	6.268541	-1.424623	0.025604
C	3.606824	0.025900	3.498777
C	5.431042	1.191450	2.314440
C	6.268425	-0.716510	1.231267
C	4.913188	0.022236	3.000812
C	5.430944	-1.156909	2.331683

C	5.430834	1.408902	-2.189053
C	4.913257	2.588652	-1.520169
C	5.430691	2.597994	-0.163967
C	3.267410	-1.198704	-3.330119
C	4.622880	-0.748239	-3.074106
C	1.413325	3.023617	-0.934290
C	2.768603	3.474471	-0.679043
C	4.622811	3.036896	0.889182
C	3.267619	2.325410	2.669789
C	4.623894	2.321761	2.152372
C	-2.819389	0.698565	-3.553586
C	-2.819389	-0.751157	-3.542842
C	-3.482563	-1.433197	-2.440391
C	-4.145758	-2.728195	-2.381577
C	-4.145731	-3.443871	-1.120657
C	-3.482509	-2.829919	0.021048
C	-2.819287	-3.426882	1.171727
C	-2.819260	-2.692597	2.421902
C	-3.482456	-1.396869	2.461516
C	-4.145629	-0.698564	3.553738
C	-4.145629	0.751158	3.542994
C	-3.482456	1.433198	2.440543
C	-2.819260	2.728196	2.381729
C	-2.819287	3.443872	1.120808
C	-3.482509	2.829920	-0.020897
C	-4.145731	3.426883	-1.171576
C	-4.145758	2.692598	-2.421751
C	-3.482563	1.396870	-2.461365
C	-3.482536	0.704959	-1.242214
C	-3.482536	-0.723292	-1.231629
C	-3.482509	-1.428245	0.010660
C	-3.482482	-0.704957	1.242365
C	-3.482482	0.723293	1.231780
C	-3.482509	1.428246	-0.010509
C	-5.038393	3.103522	-3.448997
C	-5.854112	4.213456	-3.288675
C	-5.854086	4.924760	-2.077269
C	-5.038340	4.524057	-1.029903
C	-1.926796	-1.435653	-4.412018
C	-1.111092	-0.741637	-5.292970
C	-1.111092	0.663108	-5.303381
C	-1.926796	1.370104	-4.432811
C	-5.038340	-4.538824	-0.962738
C	-5.854086	-4.955007	-2.004050
C	-5.854112	-4.261735	-3.225866
C	-5.038393	-3.154300	-3.402620
C	-1.926626	-3.103521	3.449148
C	-1.110907	-4.213455	3.288826
C	-1.110933	-4.924759	2.077420
C	-1.926679	-4.524056	1.030054
C	-5.038222	1.435654	4.412169
C	-5.853926	0.741638	5.293121
C	-5.853926	-0.663107	5.303532
C	-5.038222	-1.370103	4.432963
C	-1.926679	4.538825	0.962889
C	-1.110933	4.955008	2.004202
C	-1.110907	4.261736	3.226017
C	-1.926626	3.154301	3.402771
H	-5.170339	2.487701	-4.336011
H	-6.547076	4.488096	-4.079754
H	-6.547029	5.749428	-1.931580
H	-5.170246	4.998379	-0.059818
H	-1.794868	-2.511732	-4.322058
H	-0.418159	-1.289285	-5.926516
H	-0.418159	1.201306	-5.944974
H	-1.794868	2.447398	-4.358810
H	-5.170246	-4.998717	0.014270
H	-6.547029	-5.777425	-1.846154
H	-6.547076	-4.548070	-4.012787
H	-5.170339	-2.551693	-4.298664
H	-1.794680	-2.487700	4.336162
H	-0.417942	-4.488095	4.079905
H	-0.417989	-5.749427	1.931731
H	-1.794773	-4.998378	0.059969
H	-5.170151	2.511733	4.322209
H	-6.546859	1.289287	5.926667
H	-6.546859	-1.201305	5.945125
H	-5.170151	-2.447397	4.358961
H	-1.794773	4.998718	-0.014119
H	-0.417989	5.777426	1.846306
H	-0.417942	4.548071	4.012939
H	-1.794680	2.551694	4.298815

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cf17, c-HBC_heterodimers_with_C60 with bowl depth: 1.65

C	-0.153141	0.716568	-1.231366
C	0.684346	1.157020	-2.331757
C	1.491341	2.289754	-2.186498

C	0.684496	2.600186	0.125433
C	-0.153263	1.424624	-0.025670
C	1.202106	-0.022093	-3.000940
C	2.847595	2.285643	-2.703667
C	1.202043	2.610622	1.481601
C	-0.152575	0.708197	1.236160
C	-0.153226	-0.734709	-1.220715
C	2.508267	3.044260	1.727941
C	3.346525	3.483962	0.627540
C	2.508472	-0.025734	-3.498898
C	3.685815	3.018644	-1.772636
C	3.346320	1.149482	-3.347411
C	0.684272	1.441087	2.167996
C	-0.152998	-0.690088	1.246593
C	-0.153581	-1.425025	-0.004741
C	0.684248	-1.191340	-2.314626
C	0.684432	-1.409008	2.188856
C	0.684587	-2.598003	0.163713
C	1.491395	-2.321658	-2.152608
C	1.492382	0.748091	3.074017
C	4.701637	0.702692	-3.084404
C	1.202013	-2.588726	1.519919
C	1.492471	-3.036854	-0.889453
C	2.847673	-2.325283	-2.670019
C	3.685939	-3.044261	-1.728043
C	6.347205	0.690087	-1.246696
C	2.847682	-3.483963	-0.627642
C	3.346672	-3.474505	0.678762
C	4.701948	-3.023663	0.934037
C	2.508391	-3.018645	1.772534
C	2.847850	1.198543	3.330058
C	6.346782	-0.708198	-1.236262
C	1.492569	-0.702693	3.084302
C	2.847886	-1.149482	3.347308
C	5.509934	-1.441088	-2.168098
C	6.347788	1.425024	0.004639
C	6.347433	0.734708	1.220613
C	4.992163	-2.610622	-1.481703
C	5.509711	-2.600187	-0.125536
C	3.346612	-2.285644	2.703565
C	4.702865	-2.289755	2.186396
C	6.347470	-1.424624	0.025567
C	3.685734	0.025733	3.498795
C	5.509959	1.191339	2.314524
C	6.347348	-0.716569	1.231264
C	4.992101	0.022092	3.000837
C	5.509861	-1.157021	2.331654
C	5.509774	1.409007	-2.188959
C	4.992193	2.588725	-1.520021
C	5.509620	2.598002	-0.163815
C	3.346356	-1.198544	-3.330161
C	4.701824	-0.748092	-3.074119
C	1.492258	3.023662	-0.934139
C	2.847534	3.474504	-0.678864
C	4.701735	3.036854	0.889350
C	3.346534	2.325282	2.669916
C	4.702811	2.321658	2.152506
C	-2.866355	0.700741	-3.531258
C	-2.866355	-0.752664	-3.520556
C	-3.573621	-1.432287	-2.439084
C	-4.280904	-2.707782	-2.372369
C	-4.280883	-3.425316	-1.108269
C	-3.573581	-2.828276	0.020884
C	-2.866278	-3.408624	1.158706
C	-2.866257	-2.672553	2.412103
C	-3.573540	-1.396214	2.460029
C	-4.280806	-0.700740	3.531376
C	-4.280806	0.752665	3.520674
C	-3.573540	1.432287	2.439202
C	-2.866257	2.707783	2.372488
C	-2.866278	3.425317	1.108387
C	-3.573581	2.828277	-0.020766
C	-4.280883	3.408625	-1.158588
C	-4.280904	2.672554	-2.411985
C	-3.573621	1.396215	-2.459911
C	-3.573601	0.704510	-1.241288
C	-3.573601	-0.722712	-1.230779
C	-3.573581	-1.427201	0.010568
C	-3.573560	-0.704509	1.241406
C	-3.573560	0.722713	1.230897
C	-3.573581	1.427202	-0.010450
C	-5.226684	3.038852	-3.410748
C	-6.088708	4.109575	-3.226660
C	-6.088687	4.820230	-2.016193
C	-5.226644	4.459217	-0.991586
C	-1.920606	-1.434800	-4.336826
C	-1.058592	-0.739923	-5.172073
C	-1.058592	0.663681	-5.182408
C	-1.920606	1.370782	-4.357483
C	-5.226644	-4.473335	-0.925815

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C      -6.088687       -4.849396       -1.944995
C      -6.088708       -4.156643       -3.165795
C      -5.226684       -3.088748       -3.365630
C      -1.920478       -3.038852        3.410866
C      -1.058454       -4.109574        3.226778
C      -1.058474       -4.820229        2.016311
C      -1.920518       -4.459216        0.991704
C      -5.226556        1.434800        4.336944
C      -6.088569        0.739923        5.172191
C      -6.088569       -0.663681        5.182526
C      -5.226556       -1.370782        4.357601
C      -1.920518        4.473336        0.925933
C      -1.058474        4.849397        1.945113
C      -1.058454        4.156644        3.165913
C      -1.920478        3.088748        3.365748
H      -5.366871        2.415923       -4.291869
H      -6.818015        4.347326       -3.996701
H      -6.817980        5.608488       -1.848410
H      -5.366800        4.924681       -0.018060
H      -1.780431       -2.509340       -4.237836
H      -0.329307       -1.287880       -5.763076
H      -0.329307        1.202877       -5.781416
H      -1.780431        2.446664       -4.274328
H      -5.366800       -4.924414        0.054460
H      -6.817980       -5.635099       -1.765623
H      -6.818015       -4.405707       -3.932251
H      -5.366871       -2.478860       -4.255828
H      -1.780290       -2.415922        4.291987
H      -0.329146       -4.347325        3.996819
H      -0.329182       -5.608487        1.848528
H      -1.780361       -4.924681        0.018178
H      -5.366730        2.509341        4.237955
H      -6.817854        1.287881        5.763194
H      -6.817854       -1.202876        5.781534
H      -5.366730       -2.446663        4.274446
H      -1.780361        4.924414       -0.054342
H      -0.329182        5.635100        1.765741
H      -0.329146        4.405708        3.932369
H      -1.780290        2.478861        4.255946


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cf18, c-HBC_heterodimers_with_C60 with bowl depth: 1.75

C      -0.069573        0.712394       -1.233786
C       0.767910        1.149117       -2.335665
C       1.574906        2.282337       -2.194245
C       0.768068        2.600596        0.116624
C      -0.069692        1.424529       -0.030495
C       1.285668       -0.032255       -3.000853
C       2.931158        2.276475       -2.711402
C       1.285619        2.615624        1.472747
C      -0.069000        0.712379        1.233753
C      -0.069658       -0.738838       -1.218221
C       2.591844        3.050094        1.717613
C       3.430098        3.486067        0.615727
C       2.592033       -0.037582       -3.498800
C       3.769382        3.012624       -1.782860
C       3.429882        1.138140       -3.351295
C       0.767850        1.448420        2.163100
C      -0.069423       -0.685863        1.248922
C      -0.070010       -1.425032        0.000083
C       0.767812       -1.199171       -2.310583
C       0.768010       -1.401588        2.193611
C       0.768159       -2.597434        0.172506
C       1.574960       -2.328934       -2.144740
C       1.575963        0.758496        3.071460
C       4.785200        0.692243       -3.086782
C       1.285589       -2.583565        1.528671
C       1.576040       -3.039849       -0.879170
C       2.931236       -2.334311       -2.662140
C       3.769506       -3.050095       -1.717737
C       6.430772        0.685862       -1.249046
C       2.931251       -3.486068       -0.615851
C       3.430245       -3.472186        0.690511
C       4.785523       -3.020483        0.944254
C       2.591968       -3.012625        1.782736
C       2.931432        1.209813        3.325971
C       6.430349       -0.712380       -1.233877
C       1.576150       -0.692245        3.086657
C       2.931468       -1.138141        3.351171
C       5.593499       -1.448421       -2.163224
C       6.431359        1.425031       -0.000207
C       6.431008        0.738837        1.218097
C       5.075730       -2.615625       -1.472871
C       5.593282       -2.600597       -0.116748
C       3.430191       -2.276476        2.711277
C       4.786443       -2.282338        2.194121
C       6.431041       -1.424530        0.030370
C       3.769316        0.037580        3.498676
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C	5.593537	1.199169	2.310458
C	6.430923	-0.712396	1.233662
C	5.075681	0.032254	3.000729
C	5.593439	-1.149119	2.335541
C	5.593339	1.401587	-2.193735
C	5.075760	2.583563	-1.528795
C	5.593191	2.597432	-0.172630
C	3.429918	-1.209814	-3.326095
C	4.785387	-0.758497	-3.071584
C	1.575827	3.020481	-0.944378
C	2.931104	3.472185	-0.690636
C	4.785309	3.039847	0.879046
C	3.430113	2.334310	2.662015
C	4.786389	2.328933	2.144616
C	-2.917313	0.690969	-3.508655
C	-2.917313	-0.766234	-3.492991
C	-3.670057	-1.439581	-2.432555
C	-4.422821	-2.693125	-2.352670
C	-4.422796	-3.408353	-1.082868
C	-3.670009	-2.826377	0.030454
C	-2.917222	-3.384285	1.156029
C	-2.917198	-2.641927	2.410163
C	-3.669962	-1.386955	2.463082
C	-4.422706	-0.690968	3.508798
C	-4.422706	0.766236	3.493134
C	-3.669962	1.439582	2.432698
C	-2.917198	2.693127	2.352814
C	-2.917222	3.408354	1.083011
C	-3.670009	2.826378	-0.030311
C	-4.422796	3.384287	-1.155886
C	-4.422821	2.641928	-2.410020
C	-3.670057	1.386956	-2.462939
C	-3.670033	0.699689	-1.242546
C	-3.670033	-0.726238	-1.227218
C	-3.670009	-1.426005	0.015401
C	-3.669985	-0.699688	1.242689
C	-3.669985	0.726240	1.227361
C	-3.670009	1.426006	-0.015257
C	-5.420360	2.955945	-3.378925
C	-6.328107	3.983848	-3.172209
C	-6.328084	4.698122	-1.965285
C	-5.420312	4.384753	-0.964815
C	-1.919808	-1.448354	-4.249372
C	-1.012071	-0.755385	-5.036337
C	-1.012071	0.646946	-5.051411
C	-1.919808	1.356672	-4.279525
C	-5.420312	-4.404480	-0.870334
C	-6.328084	-4.739283	-1.863837
C	-6.328107	-4.051120	-3.085836
C	-5.420360	-3.027897	-3.314601
C	-1.919659	-2.955943	3.379068
C	-1.011911	-3.983847	3.172352
C	-1.011935	-4.698120	1.965428
C	-1.919706	-4.384751	0.964958
C	-5.420211	1.448356	4.249515
C	-6.327948	0.755387	5.036480
C	-6.327948	-0.646944	5.051554
C	-5.420211	-1.356670	4.279668
C	-1.919706	4.404481	0.870477
C	-1.011935	4.739285	1.863980
C	-1.011911	4.051121	3.085980
C	-1.919659	3.027899	3.314744
H	-5.568796	2.322413	-4.251459
H	-7.092482	4.178837	-3.919968
H	-7.092440	5.447399	-1.776246
H	-5.568712	4.844386	0.010575
H	-1.771387	-2.520783	-4.137055
H	-0.247721	-1.305528	-5.579055
H	-0.247721	1.185295	-5.605831
H	-1.771387	2.431267	-4.190287
H	-5.568712	-4.843039	0.114711
H	-7.092440	-5.484324	-1.658735
H	-7.092482	-4.262138	-3.829231
H	-5.568796	-2.413269	-4.200553
H	-1.771223	-2.322412	4.251603
H	-0.247537	-4.178835	3.920111
H	-0.247579	-5.447397	1.776389
H	-1.771306	-4.844384	-0.010432
H	-5.568632	2.520784	4.137198
H	-7.092297	1.305529	5.579199
H	-7.092297	-1.185293	5.605974
H	-5.568632	-2.431266	4.190430
H	-1.771307	4.843040	-0.114568
H	-0.247579	5.484325	1.658878
H	-0.247537	4.262139	3.829374
H	-1.771223	2.413271	4.200696

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cf19, c-HBC_heterodimers_with_C60 with bowl depth: 1.85

C	-0.004589	0.704967	-1.238047
C	0.832880	1.135060	-2.342541
C	1.639878	2.269109	-2.207945
C	0.833069	2.601250	0.100981
C	-0.004692	1.424320	-0.039056
C	1.350629	-0.050289	-3.000624
C	2.996123	2.260138	-2.725074
C	1.350639	2.624427	1.456982
C	-0.003984	0.719780	1.229449
C	-0.004674	-0.746146	-1.213760
C	2.656867	3.060361	1.699216
C	3.495107	3.489703	0.594719
C	2.656988	-0.058608	-3.498547
C	3.834359	3.001854	-1.800984
C	3.494838	1.117978	-3.358122
C	0.832879	1.461393	2.154344
C	-0.004407	-0.678345	1.253020
C	-0.005010	-1.425006	0.008646
C	0.832782	-1.213035	-2.303346
C	0.833039	-1.388380	2.201983
C	0.833160	-2.596350	0.188100
C	1.639932	-2.341782	-2.130728
C	1.641003	0.776940	3.066823
C	4.850159	0.673679	-3.090951
C	1.350609	-2.574331	1.544151
C	1.641028	-3.045078	-0.860908
C	2.996201	-2.350268	-2.648103
C	3.834483	-3.060364	-1.699428
C	6.495756	0.678341	-1.253231
C	2.996242	-3.489707	-0.594930
C	3.495254	-3.467975	0.711319
C	4.850534	-3.014755	0.962325
C	2.656991	-3.001858	1.800773
C	2.996476	1.229778	3.318600
C	6.495333	-0.719784	-1.229660
C	1.641190	-0.673682	3.090739
C	2.996512	-1.117982	3.357910
C	5.658471	-1.461397	-2.154556
C	6.496359	1.425003	-0.008857
C	6.496024	0.746143	1.213549
C	5.140711	-2.624430	-1.457194
C	5.658280	-2.601253	-0.101192
C	3.495226	-2.260142	2.724863
C	4.851471	-2.269112	2.207733
C	6.496041	-1.424323	0.038845
C	3.834362	0.058605	3.498335
C	5.658567	1.213032	2.303135
C	6.495939	-0.704970	1.237835
C	5.140721	0.050285	3.000412
C	5.658469	-1.135063	2.342329
C	5.658311	1.388376	-2.202194
C	5.140741	2.574328	-1.544362
C	5.658189	2.596347	-0.188312
C	3.494874	-1.229782	-3.318811
C	4.850346	-0.776944	-3.067035
C	1.640815	3.014751	-0.962536
C	2.996095	3.467971	-0.711530
C	4.850321	3.045074	0.860697
C	3.495148	2.350265	2.647892
C	4.851417	2.341778	2.130516
C	-2.944647	0.672508	-3.485730
C	-2.944647	-0.788943	-3.461235
C	-3.745089	-1.453395	-2.422450
C	-4.545562	-2.682598	-2.325239
C	-4.545520	-3.392427	-1.047446
C	-3.745009	-2.824816	0.047467
C	-2.944498	-3.355416	1.160788
C	-2.944457	-2.603165	2.414075
C	-3.744930	-1.371394	2.470039
C	-4.545371	-0.672504	3.485974
C	-4.545371	0.788947	3.461479
C	-3.744930	1.453399	2.422694
C	-2.944457	2.682603	2.325483
C	-2.944498	3.392431	1.047690
C	-3.745009	2.824820	-0.047223
C	-4.545520	3.355420	-1.160544
C	-4.545562	2.603169	-2.413831
C	-3.745089	1.371398	-2.469795
C	-3.745050	0.691790	-1.245780
C	-3.745049	-0.733150	-1.221897
C	-3.745009	-1.425121	0.024008
C	-3.744969	-0.691786	1.246024
C	-3.744969	0.733154	1.222141
C	-3.745009	1.425125	-0.023764
C	-5.592640	2.859817	-3.351053
C	-6.542596	3.844138	-3.123353
C	-6.542556	4.565138	-1.922128
C	-5.592561	4.303359	-0.946401
C	-1.897622	-1.471961	-4.152510

C	-0.947682	-0.782542	-4.891110
C	-0.947682	0.618193	-4.914587
C	-1.897622	1.331977	-4.199505
C	-5.592561	-4.332658	-0.801657
C	-6.542556	-4.626987	-1.768063
C	-6.542596	-3.946648	-2.992775
C	-5.592640	-2.970510	-3.253333
C	-1.897379	-2.859813	3.351297
C	-0.947423	-3.844134	3.123597
C	-0.947462	-4.565134	1.922372
C	-1.897458	-4.303355	0.946645
C	-5.592396	1.471965	4.152754
C	-6.542336	0.782546	4.891354
C	-6.542336	-0.618189	4.914831
C	-5.592396	-1.331973	4.199749
C	-1.897458	4.332662	0.801901
C	-0.947462	4.626991	1.768307
C	-0.947423	3.946652	2.993020
C	-1.897379	2.970514	3.253577
H	-5.749332	2.214103	-4.213580
H	-7.338349	3.993475	-3.848637
H	-7.338278	5.275425	-1.712746
H	-5.749193	4.760663	0.029193
H	-1.740955	-2.541841	-4.024653
H	-0.151969	-1.336026	-5.383062
H	-0.151969	1.154880	-5.424811
H	-1.740955	2.405540	-4.107574
H	-5.749193	-4.757011	0.188715
H	-7.338278	-5.329859	-1.534996
H	-7.338348	-4.120206	-3.712647
H	-5.749332	-2.354063	-4.137015
H	-1.740686	-2.214099	4.213824
H	-0.151670	-3.993471	3.848881
H	-0.151740	-5.275421	1.712990
H	-1.740826	-4.760659	-0.028949
H	-5.749064	2.541845	4.024897
H	-7.338049	1.336030	5.383306
H	-7.338049	-1.154876	5.425055
H	-5.749064	-2.405536	4.107818
H	-1.740826	4.757015	-0.188471
H	-0.151740	5.329863	1.535240
H	-0.151670	4.120210	3.712891
H	-1.740686	2.354067	4.137259