

Supplementary Information for manuscript:

Supramolecular nanotubes based on halogen bonding interactions: cooperativity and interaction with small guests

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1. Figures S1 and S2

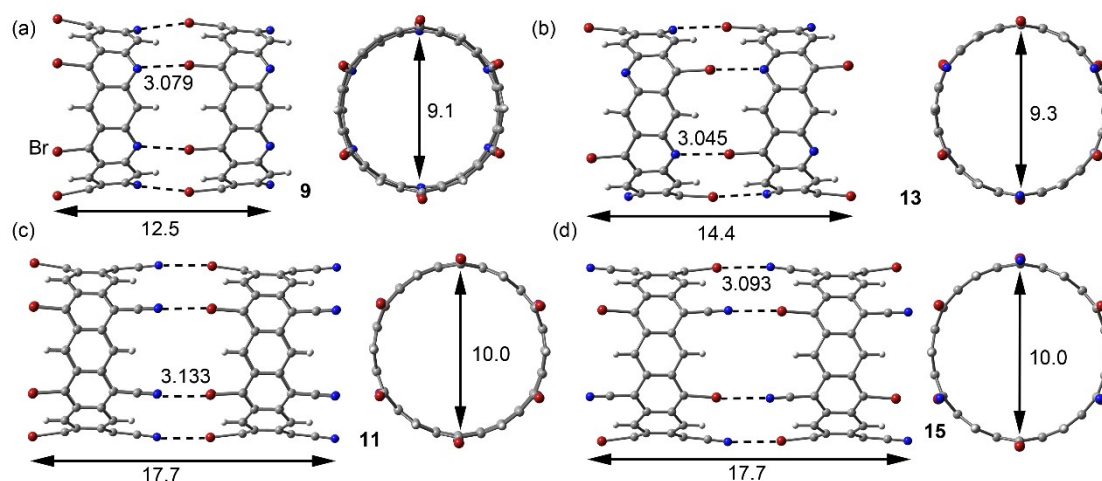


Fig. S1 (a-c) Optimized geometries of bromine dimeric complexes studied in this work. Distances in Å

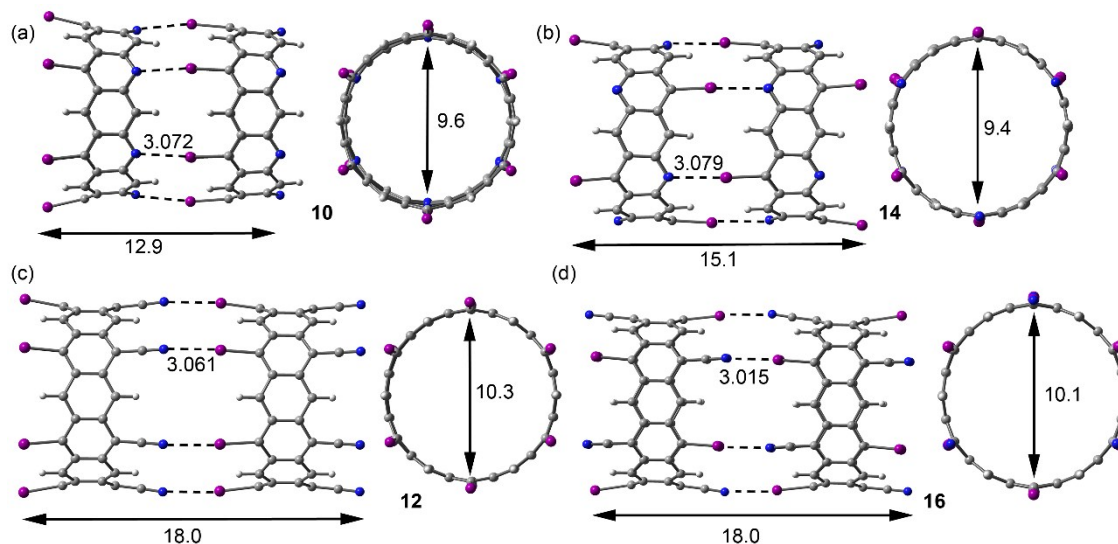


Fig. S2. (a-c) Optimized geometries of iodine dimeric complexes studied in this work. Distances in Å

2. Cartesian Coordinates

9.

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C	-4.7700965	0.0000000	-4.9976665
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C	1.2164493	-4.5431690	-4.3356243
C	2.3850483	-4.1310248	-4.9976665
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H	-2.3655999	-4.0973393	-7.4336693
H	-4.7311999	0.0000000	-7.4336693

H	-2.3655999	4.0973393	-7.4336693
H	2.3655999	4.0973393	-7.4336693
H	4.7311999	0.0000000	-7.4336693
Br	-0.0000000	-5.0230418	-1.6407650
Br	-4.3500818	2.5115209	-1.6407650
Br	4.3500818	2.5115209	-1.6407650
H	2.3810671	4.1241292	-2.4460626
H	4.7621342	0.0000000	-2.4460626
H	2.3810671	-4.1241292	-2.4460626
H	-2.3810671	-4.1241292	-2.4460626
H	-2.3810671	4.1241292	-2.4460626
H	-4.7621342	0.0000000	-2.4460626
H	-4.7320000	0.0000000	2.9863893
H	-2.3660000	4.0980322	2.9863893
H	-2.3660000	-4.0980322	2.9863893
H	2.3660000	4.0980322	2.9863893
H	2.3660000	-4.0980322	2.9863893
H	4.7320000	0.0000000	2.9863893
H	-2.3870211	4.1344419	7.9738509
H	4.7740423	0.0000000	7.9738509
H	-4.7740423	0.0000000	7.9738509
H	2.3870211	-4.1344419	7.9738509
H	2.3870211	4.1344419	7.9738509
H	-2.3870211	-4.1344419	7.9738509
Br	-4.4011856	2.5410257	8.7660131
Br	4.4011856	2.5410257	8.7660131
Br	0.0000000	-5.0820514	8.7660131

C	-4.2461710	2.4515280	2.6522832
C	4.2461710	2.4515280	2.6522832
C	0.0000000	-4.9030559	2.6522832
N	4.3583076	2.5162701	1.4925845
N	0.0000000	-5.0325401	1.4925845
N	-4.3583076	2.5162701	1.4925845
C	4.1422035	-2.3915023	-3.5239961
C	0.0000000	4.7830047	-3.5239961
C	-4.1422035	-2.3915023	-3.5239961
C	-4.1367589	2.3883589	4.0643062
C	4.1367589	2.3883589	4.0643062
C	0.0000000	-4.7767178	4.0643062
C	4.1552047	-2.3990085	6.8836127
C	-4.1552047	-2.3990085	6.8836127
C	0.0000000	4.7980171	6.8836127
C	4.1315622	2.3853585	-6.3574637
C	-4.1315622	2.3853585	-6.3574637
C	0.0000000	-4.7707171	-6.3574637
C	4.2396822	2.4477817	-7.7713702
C	0.0000000	-4.8955634	-7.7713702
C	-4.2396822	2.4477817	-7.7713702
N	-0.0000000	-5.0209757	-8.9320833
N	4.3482925	2.5104878	-8.9320833
N	-4.3482925	2.5104878	-8.9320833
C	0.0000000	4.9030559	2.6522832
C	-4.2461710	-2.4515280	2.6522832
C	4.2461710	-2.4515280	2.6522832

N	-4.3583076	-2.5162701	1.4925845
N	0.0000000	5.0325401	1.4925845
N	4.3583076	-2.5162701	1.4925845
Br	-0.0000000	5.0230418	-1.6407650
Br	-4.3500818	-2.5115209	-1.6407650
Br	4.3500818	-2.5115209	-1.6407650
C	4.2396822	-2.4477817	-7.7713702
C	0.0000000	4.8955634	-7.7713702
C	-4.2396822	-2.4477817	-7.7713702
N	-4.3482925	-2.5104878	-8.9320833
N	4.3482925	-2.5104878	-8.9320833
N	0.0000000	5.0209757	-8.9320833
Br	-0.0000000	5.0820514	8.7660131
Br	4.4011856	-2.5410257	8.7660131
Br	-4.4011856	-2.5410257	8.7660131

12.

C	-4.5721230	-1.2235201	6.2699973
C	-4.7524684	0.0000000	6.9357217
C	-4.5721230	1.2235201	6.2699973
C	-4.1633170	2.4036922	6.9438727
C	-3.3456610	3.3478147	6.2699973
C	-2.3762342	4.1157584	6.9357217
C	-1.2264621	4.5713347	6.2699973
C	1.2264621	4.5713347	6.2699973
C	2.3762342	4.1157584	6.9357217
C	3.3456610	3.3478147	6.2699973

C	4.1633170	2.4036922	6.9438727
C	4.5721230	1.2235201	6.2699973
C	4.7524684	0.0000000	6.9357217
C	4.5721230	-1.2235201	6.2699973
C	3.3456610	-3.3478147	6.2699973
C	2.3762342	-4.1157584	6.9357217
C	1.2264621	-4.5713347	6.2699973
C	0.0000000	-4.8073844	6.9438727
C	-1.2264621	-4.5713347	6.2699973
C	-2.3762342	-4.1157584	6.9357217
C	-3.3456610	-3.3478147	6.2699973
C	-4.5622850	-1.2183686	4.8093069
C	-4.7335091	0.0000000	4.1334192
C	-4.5622850	1.2183686	4.8093069
C	-3.3362806	3.3418704	4.8093069
C	-2.3667546	4.0993391	4.1334192
C	-1.2260044	4.5602390	4.8093069
C	0.0000000	4.7866164	4.1202695
C	1.2260044	4.5602390	4.8093069
C	2.3667546	4.0993391	4.1334192
C	3.3362806	3.3418704	4.8093069
C	4.5622850	1.2183686	4.8093069
C	4.7335091	0.0000000	4.1334192
C	4.5622850	-1.2183686	4.8093069
C	4.1453314	-2.3933082	4.1202695
C	3.3362806	-3.3418704	4.8093069
C	2.3667546	-4.0993391	4.1334192

C	1.2260044	-4.5602390	4.8093069
C	-1.2260044	-4.5602390	4.8093069
C	-2.3667546	-4.0993391	4.1334192
C	-3.3362806	-3.3418704	4.8093069
C	-4.1453314	-2.3933082	4.1202695
C	-4.1401393	2.3903106	-3.6004712
C	-3.3434090	3.3419980	-4.2932101
C	-2.3719072	4.1082638	-3.6300298
C	-1.2225507	4.5664762	-4.2932101
C	1.2225507	4.5664762	-4.2932101
C	2.3719072	4.1082638	-3.6300298
C	3.3434090	3.3419980	-4.2932101
C	4.1401393	2.3903106	-3.6004712
C	4.5659597	1.2244782	-4.2932101
C	4.7438144	0.0000000	-3.6300298
C	4.5659597	-1.2244782	-4.2932101
C	3.3434090	-3.3419980	-4.2932101
C	2.3719072	-4.1082638	-3.6300298
C	1.2225507	-4.5664762	-4.2932101
C	0.0000000	-4.7806211	-3.6004712
C	-1.2225507	-4.5664762	-4.2932101
C	-2.3719072	-4.1082638	-3.6300298
C	-3.3434090	-3.3419980	-4.2932101
C	-4.5659597	-1.2244782	-4.2932101
C	-4.7438144	0.0000000	-3.6300298
C	-4.5659597	1.2244782	-4.2932101
C	-3.3358526	3.3392163	-5.7531012

C	-2.3649069	4.0961388	-6.4302069
C	-1.2239198	4.5585413	-5.7531012
C	0.0000000	4.7707536	-6.4477174
C	1.2239198	4.5585413	-5.7531012
C	2.3649069	4.0961388	-6.4302069
C	3.3358526	3.3392163	-5.7531012
C	4.5597724	1.2193250	-5.7531012
C	4.7298137	0.0000000	-6.4302069
C	4.5597724	-1.2193250	-5.7531012
C	4.1315938	-2.3853768	-6.4477174
C	3.3358526	-3.3392163	-5.7531012
C	2.3649069	-4.0961388	-6.4302069
C	1.2239198	-4.5585413	-5.7531012
C	-1.2239198	-4.5585413	-5.7531012
C	-2.3649069	-4.0961388	-6.4302069
C	-3.3358526	-3.3392163	-5.7531012
C	-4.1315938	-2.3853768	-6.4477174
C	-4.5597724	-1.2193250	-5.7531012
C	-4.7298137	0.0000000	-6.4302069
C	-4.5597724	1.2193250	-5.7531012
H	2.3639915	-4.0945534	-7.5220692
H	-2.3639915	-4.0945534	-7.5220692
H	-4.7279830	0.0000000	-7.5220692
H	-2.3639915	4.0945534	-7.5220692
H	2.3639915	4.0945534	-7.5220692
H	4.7279830	0.0000000	-7.5220692
I	0.0000000	-5.0481975	-1.5030443

I	-4.3718673	2.5240987	-1.5030443
I	4.3718673	2.5240987	-1.5030443
H	2.3855416	4.1318792	-2.5414626
H	4.7710832	0.0000000	-2.5414626
H	2.3855416	-4.1318792	-2.5414626
H	-2.3855416	-4.1318792	-2.5414626
H	-2.3855416	4.1318792	-2.5414626
H	-4.7710832	0.0000000	-2.5414626
H	-4.7288947	0.0000000	3.0416699
H	-2.3644473	4.0953429	3.0416699
H	-2.3644473	-4.0953429	3.0416699
H	2.3644473	4.0953429	3.0416699
H	2.3644473	-4.0953429	3.0416699
H	4.7288947	0.0000000	3.0416699
H	-2.3895940	4.1388982	8.0245386
H	4.7791880	0.0000000	8.0245386
H	-4.7791880	0.0000000	8.0245386
H	2.3895940	-4.1388982	8.0245386
H	2.3895940	4.1388982	8.0245386
H	-2.3895940	-4.1388982	8.0245386
I	-4.4905859	2.5926410	9.0224255
I	4.4905859	2.5926410	9.0224255
I	0.0000000	-5.1852819	9.0224255
C	-4.2793637	2.4706918	2.7129725
C	4.2793637	2.4706918	2.7129725
C	0.0000000	-4.9413835	2.7129725
N	4.4212256	2.5525958	1.5576196

N	0.0000000	-5.1051915	1.5576196
N	-4.4212256	2.5525958	1.5576196
C	4.1401393	-2.3903106	-3.6004712
C	0.0000000	4.7806211	-3.6004712
C	-4.1401393	-2.3903106	-3.6004712
C	-4.1453314	2.3933082	4.1202695
C	4.1453314	2.3933082	4.1202695
C	0.0000000	-4.7866164	4.1202695
C	4.1633170	-2.4036922	6.9438727
C	-4.1633170	-2.4036922	6.9438727
C	0.0000000	4.8073844	6.9438727
C	4.1315938	2.3853768	-6.4477174
C	-4.1315938	2.3853768	-6.4477174
C	0.0000000	-4.7707536	-6.4477174
C	4.2411372	2.4486217	-7.8614404
C	0.0000000	-4.8972434	-7.8614404
C	-4.2411372	2.4486217	-7.8614404
N	0.0000000	-5.0240244	-9.0220532
N	4.3509328	2.5120122	-9.0220532
N	-4.3509328	2.5120122	-9.0220532
C	0.0000000	4.9413835	2.7129725
C	-4.2793637	-2.4706918	2.7129725
C	4.2793637	-2.4706918	2.7129725
N	-4.4212256	-2.5525958	1.5576196
N	0.0000000	5.1051915	1.5576196
N	4.4212256	-2.5525958	1.5576196
I	0.0000000	5.0481975	-1.5030443

I	-4.3718673	-2.5240987	-1.5030443
I	4.3718673	-2.5240987	-1.5030443
C	4.2411372	-2.4486217	-7.8614404
C	0.0000000	4.8972434	-7.8614404
C	-4.2411372	-2.4486217	-7.8614404
N	-4.3509328	-2.5120122	-9.0220532
N	4.3509328	-2.5120122	-9.0220532
N	0.0000000	5.0240244	-9.0220532
I	0.0000000	5.1852819	9.0224255
I	4.4905859	-2.5926410	9.0224255
I	-4.4905859	-2.5926410	9.0224255

13.

C	-3.2346208	3.3080661	-4.5624034
C	-3.9977930	2.3858760	-5.3067875
C	-4.4774844	1.2169561	-4.6968484
C	-4.6895085	0.0000000	-5.3851718
C	-4.4774844	-1.2169561	-4.6968484
C	-3.9977930	-2.3858760	-5.3067875
C	-3.2346208	-3.3080661	-4.5624034
C	-1.2475589	-4.4552968	-4.5624034
C	-0.0673327	-4.6551283	-5.3067875
C	1.1848273	-4.4860933	-4.6968484
C	2.3447542	-4.0612335	-5.3851718
C	3.2926571	-3.2691371	-4.6968484
C	4.0651257	-2.2692523	-5.3067875
C	4.4821797	-1.1472308	-4.5624034
C	4.4821797	1.1472308	-4.5624034

C	4.0651257	2.2692523	-5.3067875
C	3.2926571	3.2691371	-4.6968484
C	2.3447542	4.0612335	-5.3851718
C	1.1848273	4.4860933	-4.6968484
C	-0.0673327	4.6551283	-5.3067875
C	-1.2475589	4.4552968	-4.5624034
C	-3.2855463	3.2608445	-3.0963665
C	-4.0676338	2.2676393	-2.4874702
C	-4.4922681	1.1496059	-3.2303807
C	-4.4922681	-1.1496059	-3.2303807
C	-4.0676338	-2.2676393	-2.4874702
C	-3.2855463	-3.2608445	-3.0963665
C	-2.3295297	-4.0348638	-2.3973285
C	-1.1812010	-4.4757888	-3.0963665
C	0.0699836	-4.6564938	-2.4874702
C	1.2505462	-4.4652212	-3.2303807
C	3.2417219	-3.3156154	-3.2303807
C	3.9976501	-2.3888545	-2.4874702
C	4.4667473	-1.2149443	-3.0963665
C	4.6590594	0.0000000	-2.3973285
C	4.4667473	1.2149443	-3.0963665
C	3.9976501	2.3888545	-2.4874702
C	3.2417219	3.3156154	-3.2303807
C	1.2505462	4.4652212	-3.2303807
C	0.0699836	4.6564938	-2.4874702
C	-1.1812010	4.4757888	-3.0963665
C	-2.3295297	4.0348638	-2.3973285

C	-4.6591372	0.0000000	2.3972469
C	-4.4668280	-1.2149374	3.0963011
C	-3.9976600	-2.3888558	2.4874668
C	-3.2416944	-3.3155471	3.2304289
C	-1.2505008	-4.4651632	3.2304289
C	-0.0699798	-4.6565030	2.4874668
C	1.1812474	-4.4758552	3.0963011
C	2.3295686	-4.0349312	2.3972469
C	3.2855806	-3.2609178	3.0963011
C	4.0676398	-2.2676472	2.4874668
C	4.4921952	-1.1496162	3.2304289
C	4.4921952	1.1496162	3.2304289
C	4.0676398	2.2676472	2.4874668
C	3.2855806	3.2609178	3.0963011
C	2.3295686	4.0349312	2.3972469
C	1.1812474	4.4758552	3.0963011
C	-0.0699798	4.6565030	2.4874668
C	-1.2505008	4.4651632	3.2304289
C	-3.2416944	3.3155471	3.2304289
C	-3.9976600	2.3888558	2.4874668
C	-4.4668280	1.2149374	3.0963011
C	-4.4824063	-1.1472164	4.5623327
C	-4.0652319	-2.2691623	5.3067563
C	-3.2925539	-3.2689374	4.6968972
C	-2.3445023	-4.0607970	5.3852997
C	-1.1847059	-4.4859041	4.6968972
C	0.0674637	-4.6551752	5.3067563

C	1.2476846	-4.4554860	4.5623327
C	3.2347217	-3.3082695	4.5623327
C	3.9977681	-2.3860129	5.3067563
C	4.4772598	-1.2169666	4.6968972
C	4.6890045	0.0000000	5.3852997
C	4.4772598	1.2169666	4.6968972
C	3.9977681	2.3860129	5.3067563
C	3.2347217	3.3082695	4.5623327
C	1.2476846	4.4554860	4.5623327
C	0.0674637	4.6551752	5.3067563
C	-1.1847059	4.4859041	4.6968972
C	-2.3445023	4.0607970	5.3852997
C	-3.2925539	3.2689374	4.6968972
C	-4.0652319	2.2691623	5.3067563
C	-4.4824063	1.1472164	4.5623327
Br	4.9015201	0.0000000	7.2766490
Br	-2.4507601	4.2448409	7.2766490
Br	-2.4507601	-4.2448409	7.2766490
H	3.9405798	2.4581609	6.3923554
H	0.1585399	4.6417226	6.3923554
H	-4.0991196	2.1835618	6.3923554
H	-4.0991196	-2.1835618	6.3923554
H	0.1585399	-4.6417226	6.3923554
H	3.9405798	-2.4581609	6.3923554
N	-4.6549062	0.0000000	5.2485152
N	2.3274531	4.0312670	5.2485152
N	2.3274531	-4.0312670	5.2485152

N	4.6761536	0.0000000	2.5507565
N	-2.3380768	4.0496678	2.5507565
N	-2.3380768	-4.0496678	2.5507565
Br	2.3903953	4.1402861	0.4924334
Br	-4.7807906	0.0000000	0.4924334
Br	2.3903953	-4.1402861	0.4924334
H	-0.1577435	-4.6442570	1.4019645
H	4.1009163	-2.1855186	1.4019645
H	4.1009163	2.1855186	1.4019645
H	-0.1577435	4.6442570	1.4019645
H	-3.9431728	-2.4587384	1.4019645
H	-3.9431728	2.4587384	1.4019645
Br	-2.3903905	-4.1402778	-0.4925214
Br	-2.3903905	4.1402778	-0.4925214
Br	4.7807810	0.0000000	-0.4925214
N	2.3381179	4.0497389	-2.5506840
N	-4.6762357	0.0000000	-2.5506840
N	2.3381179	-4.0497389	-2.5506840
H	-4.1008857	2.1855458	-1.4019635
H	-4.1008857	-2.1855458	-1.4019635
H	0.1577047	4.6442441	-1.4019635
H	0.1577047	-4.6442441	-1.4019635
H	3.9431810	2.4586983	-1.4019635
H	3.9431810	-2.4586983	-1.4019635
H	-3.9405785	-2.4580234	-6.3923849
H	4.0990000	-2.1836294	-6.3923849
H	-3.9405785	2.4580234	-6.3923849

H	4.0990000	2.1836294	-6.3923849
H	-0.1584215	-4.6416528	-6.3923849
H	-0.1584215	4.6416528	-6.3923849
Br	-4.9029178	0.0000000	-7.2763871
Br	2.4514589	-4.2460514	-7.2763871
Br	2.4514589	4.2460514	-7.2763871
N	-2.3272613	-4.0309349	-5.2486040
N	4.6545227	0.0000000	-5.2486040
N	-2.3272613	4.0309349	-5.2486040

14.

C	-3.31027610	-3.23424771	-4.68975615
C	-2.38814130	-3.99763721	-5.43423625
C	-1.21507690	-4.47750401	-4.83253534
C	0.00000000	-4.69690961	-5.52530544
C	1.21507690	-4.47750401	-4.83253534
C	2.38814130	-3.99763721	-5.43423625
C	3.31027610	-3.23424771	-4.68975615
C	4.45607873	-1.24965934	-4.68975615
C	4.65612603	-0.06937243	-5.43423625
C	4.48517067	1.18646454	-4.83253534
C	4.06764304	2.34845481	-5.52530544
C	3.27009377	3.29103947	-4.83253534
C	2.26798473	4.06700964	-5.43423625
C	1.14580263	4.48390705	-4.68975615
C	-1.14580263	4.48390705	-4.68975615

C	-2.26798473	4.06700964	-5.43423625
C	-3.27009377	3.29103947	-4.83253534
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C	-4.48517067	1.18646454	-4.83253534
C	-4.65612603	-0.06937243	-5.43423625
C	-4.45607873	-1.24965934	-4.68975615
C	-3.26471160	-3.28396851	-3.22324465
C	-2.27093420	-4.07289770	-2.62418825
C	-1.15055450	-4.49398971	-3.36435144
C	1.15055450	-4.49398971	-3.36435144
C	2.27093420	-4.07289770	-2.62418825
C	3.26471160	-3.28396851	-3.22324465
C	4.03645508	-2.33044843	-2.51354635
C	4.47635595	-1.18533893	-3.22324465
C	4.66269998	0.06976214	-2.62418825
C	4.46718650	1.25058543	-3.36435144
C	3.31663200	3.24340428	-3.36435144
C	2.39176578	4.00313556	-2.62418825
C	1.21164435	4.46930743	-3.22324465
C	-0.00000000	4.66089686	-2.51354635
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C	-3.31663200	3.24340428	-3.36435144
C	-4.46718650	1.25058543	-3.36435144
C	-4.66269998	0.06976214	-2.62418825
C	-4.47635595	-1.18533893	-3.22324465
C	-4.03645508	-2.33044843	-2.51354635

C	0.00000000	-4.66102019	2.51354596
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C	2.39171260	-4.00313799	2.62417615
C	3.31654950	-3.24336599	3.36433385
C	4.46711209	-1.25053313	3.36433385
C	4.66267549	-0.06971488	2.62417615
C	4.47642249	1.18538918	3.22324376
C	4.03656189	2.33051009	2.51354596
C	3.26478839	3.28400100	3.22324376
C	2.27096289	4.07285286	2.62417615
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C	-2.39171260	-4.00313799	2.62417615
C	-1.21163410	-4.46939019	3.22324376
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I	-4.33198328	-2.50107171	7.61521373
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H	-2.46496510	3.93940352	6.52008103
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H	-2.17914098	-4.10442416	6.52008103
H	2.17914098	-4.10442416	6.52008103
H	4.64410608	0.16502063	6.52008103
H	2.46496510	3.93940352	6.52008103
N	0.00000000	-4.65706628	5.37743276
N	-4.03313771	2.32853314	5.37743276
N	4.03313771	2.32853314	5.37743276

N	0.00000000	4.68462861	2.68544523
N	-4.05700739	-2.34231431	2.68544523
N	4.05700739	-2.34231431	2.68544523
I	-4.15538789	2.39911432	0.39176784
I	0.00000000	-4.79822864	0.39176784
I	4.15538789	2.39911432	0.39176784
H	4.65961700	-0.15586759	1.53804564
H	2.19482321	4.11328049	1.53804564
H	-2.19482321	4.11328049	1.53804564
H	-4.65961700	-0.15586759	1.53804564
H	2.46479379	-3.95741290	1.53804564
H	-2.46479379	-3.95741290	1.53804564
I	4.15523591	-2.39902657	-0.39177285
I	-4.15523591	-2.39902657	-0.39177285
I	-0.00000000	4.79805315	-0.39177285
N	-4.05717571	2.34241149	-2.68547666
N	0.00000000	-4.68482297	-2.68547666
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H	-2.19479610	-4.11333580	-1.53805775
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H	-4.65965135	0.15591872	-1.53805775
H	4.65965135	0.15591872	-1.53805775
H	-2.46485525	3.95741708	-1.53805775
H	2.46485525	3.95741708	-1.53805775
H	2.46491750	-3.93935632	-6.52009385
H	2.17912389	4.10435933	-6.52009385
H	-2.46491750	-3.93935632	-6.52009385

H	-2.17912389	4.10435933	-6.52009385
H	4.64404139	-0.16500302	-6.52009385
H	-4.64404139	-0.16500302	-6.52009385
I	0.00000000	-5.00242492	-7.61518654
I	4.33222706	2.50121246	-7.61518654
I	-4.33222706	2.50121246	-7.61518654
N	4.03298502	-2.32844498	-5.37743715
N	-0.00000000	4.65688997	-5.37743715
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15.

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C	3.3408080	3.3468042	5.9319346
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C	4.5688215	1.2198225	5.9319346
C	4.7396699	-0.0090330	6.5926567
C	4.5615686	-1.2183479	5.9033190
C	3.3359045	-3.3412604	5.9033190
C	2.3776578	-4.1001580	6.5926567
C	1.2280135	-4.5666267	5.9319346
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C	-1.2256641	4.5596083	5.9033190
C	1.2267388	4.5588657	4.4451172
C	2.3799011	4.0985783	3.7848970
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C	3.3347241	-3.3418198	4.4451172
C	2.3595224	-4.1103439	3.7848970
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C	-4.1340956	-2.3868212	3.7632391
C	-4.5614629	-1.2170459	4.4451172
C	-4.7394235	0.0117656	3.7848970
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C	4.1340956	2.3868212	-3.7632391
C	4.5614629	1.2170459	-4.4451172
C	4.7394235	-0.0117656	-3.7848970
C	4.5687559	-1.2217446	-4.4733888
C	3.3424398	-3.3457863	-4.4733888
C	2.3799011	-4.0985783	-3.7848970
C	1.2267388	-4.5588657	-4.4451172
C	-0.0000000	-4.7736424	-3.7632391
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C	-3.3424398	-3.3457863	-4.4733888
C	-4.5687559	-1.2217446	-4.4733888
C	-4.7394235	-0.0117656	-3.7848970
C	-4.5614629	1.2170459	-4.4451172
C	-4.1340956	2.3868212	-3.7632391
C	-3.3347241	3.3418198	-4.4451172
C	-2.3595224	4.1103439	-3.7848970
C	-1.2263161	4.5675309	-4.4733888
C	1.2263161	4.5675309	-4.4733888
C	2.3595224	4.1103439	-3.7848970
C	3.3347241	3.3418198	-4.4451172
C	4.5615686	1.2183479	-5.9033190
C	4.7396699	0.0090330	-6.5926567
C	4.5688215	-1.2198225	-5.9319346
C	4.1500483	-2.3960315	-6.6047750
C	3.3408080	-3.3468042	-5.9319346
C	2.3620121	-4.1091910	-6.5926567

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C	-1.2256641	-4.5596083	-5.9033190
C	-2.3620121	-4.1091910	-6.5926567
C	-3.3408080	-3.3468042	-5.9319346
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H	4.7521770	0.0265061	-7.6822728
H	2.3531336	-4.1287591	-7.6822728
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Br	-4.3270362	2.4982155	-1.8787440
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Br	0.0000000	-4.9964310	-1.8787440

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H	-2.3995241	-4.1019746	-2.6952080
H	-4.7521763	-0.0270615	-2.6952080
H	-2.3526522	4.1290361	-2.6952080
H	4.7521763	-0.0270615	-2.6952080
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C	0.0000000	4.7881153	-3.7847777
C	4.1466294	2.3940576	3.7847777
C	0.0000000	-4.7881153	3.7847777
C	-4.1466294	2.3940576	3.7847777
C	4.2172213	-2.4348138	8.0118972
C	-0.0000000	4.8696277	8.0118972
C	-4.2172213	-2.4348138	8.0118972
C	-4.1301874	-2.3845648	6.5953843
C	0.0000000	4.7691296	6.5953843
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16.

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C	4.7410094	-0.0141703	6.6579823
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C	3.3370333	-3.3404986	5.9619907
C	2.3827766	-4.0987494	6.6579823
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C	3.3290330	-3.3357899	4.5027035
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C	-1.2252416	-4.5766381	4.5521823
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C	4.5533953	1.2151322	-4.5027035
C	4.7413134	-0.0206412	-3.8577602
C	4.5761057	-1.2272287	-4.5521823

C	3.3508640	-3.3494094	-4.5521823
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C	1.2243623	-4.5509221	-4.5027035
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C	-2.3885325	-4.0957772	-3.8577602
C	-3.3508640	-3.3494094	-4.5521823
C	-4.5761057	-1.2272287	-4.5521823
C	-4.7413134	-0.0206412	-3.8577602
C	-4.5533953	1.2151322	-4.5027035
C	-4.1194628	2.3783730	-3.8084918
C	-3.3290330	3.3357899	-4.5027035
C	-2.3527809	4.1164184	-3.8577602
C	-1.2252416	4.5766381	-4.5521823
C	1.2252416	4.5766381	-4.5521823
C	2.3527809	4.1164184	-3.8577602
C	3.3290330	3.3357899	-4.5027035
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C	4.1525830	-2.3974949	-6.6913961
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C	-1.2244400	-4.5602049	-5.9619907
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C	-2.3827766	4.0987494	-6.6579823
C	-1.2264184	4.5676496	-6.0115477
C	0.0000000	4.7949899	-6.6913961
C	1.2264184	4.5676496	-6.0115477
C	2.3827766	4.0987494	-6.6579823
C	3.3370333	3.3404986	-5.9619907
I	-4.4456820	-2.5667157	-8.7726767
I	0.0000000	5.1334315	-8.7726767
I	4.4456820	-2.5667157	-8.7726767
H	-4.7557759	0.0419891	-7.7480876
H	-2.4142515	4.0976282	-7.7480876
H	2.4142515	4.0976282	-7.7480876
H	4.7557759	0.0419891	-7.7480876
H	2.3415243	-4.1396172	-7.7480876
H	-2.3415243	-4.1396172	-7.7480876
I	-4.3332220	2.5017869	-1.7084379
I	4.3332220	2.5017869	-1.7084379
I	0.0000000	-5.0035738	-1.7084379
H	2.4183076	-4.0963174	-2.7676683
H	-2.4183076	-4.0963174	-2.7676683
H	-4.7566687	-0.0461571	-2.7676683
H	-2.3383611	4.1424745	-2.7676683

H	4.7566687	-0.0461571	-2.7676683
H	2.3383611	4.1424745	-2.7676683
I	4.3332220	-2.5017869	1.7084379
I	0.0000000	5.0035738	1.7084379
I	-4.3332220	-2.5017869	1.7084379
H	2.4183076	4.0963174	2.7676683
H	4.7566687	0.0461571	2.7676683
H	-2.4183076	4.0963174	2.7676683
H	2.3383611	-4.1424745	2.7676683
H	-4.7566687	0.0461571	2.7676683
H	-2.3383611	-4.1424745	2.7676683
H	4.7557759	-0.0419891	7.7480876
H	-2.4142515	-4.0976282	7.7480876
H	2.3415243	4.1396172	7.7480876
H	-4.7557759	-0.0419891	7.7480876
H	2.4142515	-4.0976282	7.7480876
H	-2.3415243	4.1396172	7.7480876
I	4.4456820	2.5667157	8.7726767
I	0.0000000	-5.1334315	8.7726767
I	-4.4456820	2.5667157	8.7726767
C	4.3058987	-2.4860118	-2.4589086
C	-4.3058987	-2.4860118	-2.4589086
C	0.0000000	4.9720236	-2.4589086
C	4.3058987	2.4860118	2.4589086
C	0.0000000	-4.9720236	2.4589086
C	-4.3058987	2.4860118	2.4589086
N	-4.4483215	-2.5682396	-1.3039372

N	0.0000000	5.1364793	-1.3039372
N	4.4483215	-2.5682396	-1.3039372
N	0.0000000	-5.1364793	1.3039372
N	-4.4483215	2.5682396	1.3039372
N	4.4483215	2.5682396	1.3039372
C	-4.1662202	-2.4053683	-3.8662639
C	4.1662202	-2.4053683	-3.8662639
C	0.0000000	4.8107367	-3.8662639
C	4.1662202	2.4053683	3.8662639
C	0.0000000	-4.8107367	3.8662639
C	-4.1662202	2.4053683	3.8662639
C	4.2293279	-2.4418036	8.0693237
C	0.0000000	4.8836072	8.0693237
C	-4.2293279	-2.4418036	8.0693237
C	-4.1348670	-2.3872666	6.6533379
C	0.0000000	4.7745331	6.6533379
C	4.1348670	-2.3872666	6.6533379
C	0.0000000	-4.7745331	-6.6533379
C	4.1348670	2.3872666	-6.6533379
C	-4.1348670	2.3872666	-6.6533379
C	0.0000000	-4.8836072	-8.0693237
C	-4.2293279	2.4418036	-8.0693237
C	4.2293279	2.4418036	-8.0693237
N	-4.3127689	2.4899783	-9.2330350
N	0.0000000	-4.9799566	-9.2330350
N	4.3127689	2.4899783	-9.2330350
N	-4.3127689	-2.4899783	9.2330350

N	0.0000000	4.9799566	9.2330350
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17.

C	-2.3866297	4.1337639	6.6297721
C	-3.3220228	3.3253376	7.3149589
C	-4.1283413	2.3834990	6.6571828
C	-4.5408382	1.2142873	7.3149589
C	-4.5408382	-1.2142873	7.3149589
C	-4.1283413	-2.3834990	6.6571828
C	-3.3220228	-3.3253376	7.3149589
C	-2.3866297	-4.1337639	6.6297721
C	-1.2188155	-4.5396249	7.3149589
C	-0.0000000	-4.7669979	6.6571828
C	1.2188155	-4.5396249	7.3149589
C	3.3220228	-3.3253376	7.3149589
C	4.1283413	-2.3834990	6.6571828
C	4.5408382	-1.2142873	7.3149589
C	4.7732594	0.0000000	6.6297721
C	4.5408382	1.2142873	7.3149589
C	4.1283413	2.3834990	6.6571828
C	3.3220228	3.3253376	7.3149589
C	1.2188155	4.5396249	7.3149589
C	-0.0000000	4.7669979	6.6571828
C	-1.2188155	4.5396249	7.3149589
C	-3.2078926	3.2597556	8.7783245
C	-3.9390271	2.2741984	9.4685878

C	-4.4269774	1.1482387	8.7783245
C	-4.4269774	-1.1482387	8.7783245
C	-3.9390271	-2.2741984	9.4685878
C	-3.2078926	-3.2597556	8.7783245
C	-1.2190849	-4.4079943	8.7783245
C	0.0000000	-4.5483967	9.4685878
C	1.2190849	-4.4079943	8.7783245
C	3.2078926	-3.2597556	8.7783245
C	3.9390271	-2.2741984	9.4685878
C	4.4269774	-1.1482387	8.7783245
C	4.4269774	1.1482387	8.7783245
C	3.9390271	2.2741984	9.4685878
C	3.2078926	3.2597556	8.7783245
C	1.2190849	4.4079943	8.7783245
C	0.0000000	4.5483967	9.4685878
C	-1.2190849	4.4079943	8.7783245
H	3.8287889	-2.2105523	10.5504991
H	3.8287889	2.2105523	10.5504991
H	0.0000000	4.4211046	10.5504991
H	-3.8287889	2.2105523	10.5504991
H	-3.8287889	-2.2105523	10.5504991
H	0.0000000	-4.4211046	10.5504991
N	-2.2696584	3.9311637	9.4768945
N	4.5393169	0.0000000	9.4768945
N	-2.2696584	-3.9311637	9.4768945
Br	4.9573534	-0.0000000	4.7263892
Br	-2.4786767	4.2931940	4.7263892

Br	-2.4786767	-4.2931940	4.7263892
H	-4.2139320	-2.4329148	5.5733134
H	-0.0000000	-4.8658295	5.5733134
H	4.2139320	-2.4329148	5.5733134
H	4.2139320	2.4329148	5.5733134
H	-4.2139320	2.4329148	5.5733134
H	-0.0000000	4.8658295	5.5733134
Br	2.4786767	-4.2931940	4.7263892
Br	-4.9573534	0.0000000	4.7263892
Br	2.4786767	4.2931940	4.7263892
C	2.3866297	4.1337639	6.6297721
C	-4.7732594	0.0000000	6.6297721
C	2.3866297	-4.1337639	6.6297721
N	2.2696584	-3.9311637	9.4768945
N	2.2696584	3.9311637	9.4768945
N	-4.5393169	0.0000000	9.4768945
C	1.2179768	4.5432742	-8.1905500
C	-0.0000000	4.7693457	-8.8529525
C	-1.2179768	4.5432742	-8.1905500
C	-2.4044361	4.1646055	-8.8581343
C	-3.3256025	3.3264360	-8.1905500
C	-4.1303745	2.3846728	-8.8529525
C	-4.5435793	1.2168382	-8.1905500
C	-4.5435793	-1.2168382	-8.1905500
C	-4.1303745	-2.3846728	-8.8529525
C	-3.3256025	-3.3264360	-8.1905500
C	-2.4044361	-4.1646055	-8.8581343

C	-1.2179768	-4.5432742	-8.1905500
C	-0.0000000	-4.7693457	-8.8529525
C	1.2179768	-4.5432742	-8.1905500
C	3.3256025	-3.3264360	-8.1905500
C	4.1303745	-2.3846728	-8.8529525
C	4.5435793	-1.2168382	-8.1905500
C	4.8088722	0.0000000	-8.8581343
C	4.5435793	1.2168382	-8.1905500
C	4.1303745	2.3846728	-8.8529525
C	3.3256025	3.3264360	-8.1905500
C	1.2167563	4.4089628	-6.7267645
C	0.0000000	4.5491090	-6.0356199
C	-1.2167563	4.4089628	-6.7267645
C	-3.2098957	3.2582233	-6.7267645
C	-3.9396440	2.2745545	-6.0356199
C	-4.4266519	1.1507396	-6.7267645
C	-4.4266519	-1.1507396	-6.7267645
C	-3.9396440	-2.2745545	-6.0356199
C	-3.2098957	-3.2582233	-6.7267645
C	-1.2167563	-4.4089628	-6.7267645
C	0.0000000	-4.5491090	-6.0356199
C	1.2167563	-4.4089628	-6.7267645
C	3.2098957	-3.2582233	-6.7267645
C	3.9396440	-2.2745545	-6.0356199
C	4.4266519	-1.1507396	-6.7267645
C	4.4266519	1.1507396	-6.7267645
C	3.9396440	2.2745545	-6.0356199

C	3.2098957	3.2582233	-6.7267645
C	-2.3860640	4.1327840	-1.1243311
C	-3.3218801	3.3246769	-0.4393543
C	-4.1255138	2.3818665	-1.0979187
C	-4.5401947	1.2144941	-0.4393543
C	-4.5401947	-1.2144941	-0.4393543
C	-4.1255138	-2.3818665	-1.0979187
C	-3.3218801	-3.3246769	-0.4393543
C	-2.3860640	-4.1327840	-1.1243311
C	-1.2183146	-4.5391710	-0.4393543
C	-0.0000000	-4.7637330	-1.0979187
C	1.2183146	-4.5391710	-0.4393543
C	3.3218801	-3.3246769	-0.4393543
C	4.1255138	-2.3818665	-1.0979187
C	4.5401947	-1.2144941	-0.4393543
C	4.7721279	0.0000000	-1.1243311
C	4.5401947	1.2144941	-0.4393543
C	4.1255138	2.3818665	-1.0979187
C	3.3218801	3.3246769	-0.4393543
C	1.2183146	4.5391710	-0.4393543
C	0.0000000	4.7637330	-1.0979187
C	-1.2183146	4.5391710	-0.4393543
C	-3.2141161	3.2630859	1.0238912
C	-3.9463779	2.2784424	1.7144688
C	-4.4329733	1.1519632	1.0238912
C	-4.4329733	-1.1519632	1.0238912
C	-3.9463779	-2.2784424	1.7144688

C	-3.2141161	-3.2630859	1.0238912
C	-1.2188573	-4.4150491	1.0238912
C	-0.0000000	-4.5568847	1.7144688
C	1.2188573	-4.4150491	1.0238912
C	3.2141161	-3.2630859	1.0238912
C	3.9463779	-2.2784424	1.7144688
C	4.4329733	-1.1519632	1.0238912
C	4.4329733	1.1519632	1.0238912
C	3.9463779	2.2784424	1.7144688
C	3.2141161	3.2630859	1.0238912
C	1.2188573	4.4150491	1.0238912
C	-0.0000000	4.5568847	1.7144688
C	-1.2188573	4.4150491	1.0238912
H	3.8362527	-2.2148615	2.7967736
H	3.8362527	2.2148615	2.7967736
H	0.0000000	4.4297230	2.7967736
H	-3.8362527	2.2148615	2.7967736
H	-3.8362527	-2.2148615	2.7967736
H	0.0000000	-4.4297230	2.7967736
N	-2.2802158	3.9494495	1.7153191
N	4.5604315	0.0000000	1.7153191
N	-2.2802158	-3.9494495	1.7153191
Br	4.9565642	0.0000000	-3.0270902
Br	-2.4782821	4.2925105	-3.0270902
Br	-2.4782821	-4.2925105	-3.0270902
H	-4.2095684	-2.4303954	-2.1818673
H	-0.0000000	-4.8607909	-2.1818673

H	4.2095684	-2.4303954	-2.1818673
H	4.2095684	2.4303954	-2.1818673
H	-4.2095684	2.4303954	-2.1818673
H	-0.0000000	4.8607909	-2.1818673
N	4.5579117	0.0000000	-6.0356761
N	-2.2789558	3.9472673	-6.0356761
N	-2.2789558	-3.9472673	-6.0356761
H	0.0000000	4.4212414	-4.9535002
H	-3.8289073	2.2106207	-4.9535002
H	3.8289073	2.2106207	-4.9535002
H	-3.8289073	-2.2106207	-4.9535002
H	3.8289073	-2.2106207	-4.9535002
H	0.0000000	-4.4212414	-4.9535002
H	-4.2145154	2.4332516	-9.9377497
H	0.0000000	-4.8665031	-9.9377497
H	0.0000000	4.8665031	-9.9377497
H	4.2145154	-2.4332516	-9.9377497
H	-4.2145154	-2.4332516	-9.9377497
H	4.2145154	2.4332516	-9.9377497
Br	-2.5959413	4.4963022	-10.7253719
Br	-2.5959413	-4.4963022	-10.7253719
Br	5.1918825	0.0000000	-10.7253719
Br	2.5959413	4.4963022	-10.7253719
Br	-5.1918825	0.0000000	-10.7253719
Br	2.5959413	-4.4963022	-10.7253719
N	2.2789558	3.9472673	-6.0356761
N	-4.5579117	-0.0000000	-6.0356761

N	2.2789558	-3.9472673	-6.0356761
C	2.4044361	4.1646055	-8.8581343
C	-4.8088722	0.0000000	-8.8581343
C	2.4044361	-4.1646055	-8.8581343
Br	2.4782821	-4.2925105	-3.0270902
Br	-4.9565642	0.0000000	-3.0270902
Br	2.4782821	4.2925105	-3.0270902
C	2.3860640	4.1327840	-1.1243311
C	-4.7721279	0.0000000	-1.1243311
C	2.3860640	-4.1327840	-1.1243311
N	2.2802158	-3.9494495	1.7153191
N	2.2802158	3.9494495	1.7153191
N	-4.5604315	0.0000000	1.7153191

18.

C	4.5709786	1.2207768	11.3942218
C	4.7491861	0.0000000	12.0664375
C	4.5709786	-1.2207768	11.3942218
C	4.1550710	-2.3989313	12.0636942
C	3.3427130	-3.3481952	11.3942218
C	2.3745930	-4.1129158	12.0664375
C	1.2282656	-4.5689720	11.3942218
C	-1.2282656	-4.5689720	11.3942218
C	-2.3745930	-4.1129158	12.0664375
C	-3.3427130	-3.3481952	11.3942218
C	-4.1550710	-2.3989313	12.0636942
C	-4.5709786	-1.2207768	11.3942218

C	-4.7491861	-0.0000000	12.0664375
C	-4.5709786	1.2207768	11.3942218
C	-3.3427130	3.3481952	11.3942218
C	-2.3745930	4.1129158	12.0664375
C	-1.2282656	4.5689720	11.3942218
C	0.0000000	4.7978627	12.0636942
C	1.2282656	4.5689720	11.3942218
C	2.3745930	4.1129158	12.0664375
C	3.3427130	3.3481952	11.3942218
C	4.5621680	1.2177995	9.9345520
C	4.7354947	0.0000000	9.2583410
C	4.5621680	-1.2177995	9.9345520
C	3.3357294	-3.3420536	9.9345520
C	2.3677473	-4.1010587	9.2583410
C	1.2264387	-4.5598532	9.9345520
C	-0.0000000	-4.7791277	9.2449677
C	-1.2264387	-4.5598532	9.9345520
C	-2.3677473	-4.1010587	9.2583410
C	-3.3357294	-3.3420536	9.9345520
C	-4.5621680	-1.2177995	9.9345520
C	-4.7354947	0.0000000	9.2583410
C	-4.5621680	1.2177995	9.9345520
C	-4.1388460	2.3895638	9.2449677
C	-3.3357294	3.3420536	9.9345520
C	-2.3677473	4.1010587	9.2583410
C	-1.2264387	4.5598532	9.9345520
C	1.2264387	4.5598532	9.9345520

C	2.3677473	4.1010587	9.2583410
C	3.3357294	3.3420536	9.9345520
C	4.1388460	2.3895638	9.2449677
H	4.7326472	0.0000000	8.1668365
H	2.3663236	-4.0985927	8.1668365
H	2.3663236	4.0985927	8.1668365
H	-2.3663236	-4.0985927	8.1668365
H	-2.3663236	4.0985927	8.1668365
H	-4.7326472	0.0000000	8.1668365
H	2.3865525	-4.1336302	13.1540266
H	-4.7731050	0.0000000	13.1540266
H	4.7731050	0.0000000	13.1540266
H	-2.3865525	4.1336302	13.1540266
H	-2.3865525	-4.1336302	13.1540266
H	2.3865525	4.1336302	13.1540266
Br	4.3997262	-2.5401831	13.9464788
Br	-4.3997262	-2.5401831	13.9464788
Br	0.0000000	5.0803662	13.9464788
C	4.2499623	-2.4537169	7.8333638
C	-4.2499623	-2.4537169	7.8333638
C	-0.0000000	4.9074338	7.8333638
N	-4.3636675	-2.5193646	6.6738066
N	0.0000000	5.0387292	6.6738066
N	4.3636675	-2.5193646	6.6738066
C	4.1388460	-2.3895638	9.2449677
C	-4.1388460	-2.3895638	9.2449677
C	-0.0000000	4.7791277	9.2449677

C	-4.1550710	2.3989313	12.0636942
C	4.1550710	2.3989313	12.0636942
C	0.0000000	-4.7978627	12.0636942
C	0.0000000	-4.9074338	7.8333638
C	4.2499623	2.4537169	7.8333638
C	-4.2499623	2.4537169	7.8333638
N	4.3636675	2.5193646	6.6738066
N	0.0000000	-5.0387292	6.6738066
N	-4.3636675	2.5193646	6.6738066
Br	-0.0000000	-5.0803662	13.9464788
Br	-4.3997262	2.5401831	13.9464788
Br	4.3997262	2.5401831	13.9464788
C	4.5664381	1.2210263	0.9991319
C	4.7381433	0.0000000	1.6710668
C	4.5664381	-1.2210263	0.9991319
C	4.1417810	-2.3912584	1.6810614
C	3.3406588	-3.3441383	0.9991319
C	2.3690716	-4.1033525	1.6710668
C	1.2257793	-4.5651645	0.9991319
C	-1.2257793	-4.5651645	0.9991319
C	-2.3690716	-4.1033525	1.6710668
C	-3.3406588	-3.3441383	0.9991319
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C	-4.7381433	0.0000000	1.6710668
C	-4.5664381	1.2210263	0.9991319
C	-3.3406588	3.3441383	0.9991319

C	-2.3690716	4.1033525	1.6710668
C	-1.2257793	4.5651645	0.9991319
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22.

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23.

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C	3.2363432	3.3110600	-8.4540461
C	1.1812506	4.4739062	-6.9876386
C	-0.0705698	4.6511415	-6.3792609
C	-1.2501598	4.4642902	-7.1255507
C	-3.2411088	3.3148153	-7.1255507
C	-3.9927218	2.3866860	-6.3792609
C	-4.4651417	1.2139600	-6.9876386
C	-4.6556770	0.0000000	-6.2835199
C	-4.4651417	-1.2139600	-6.9876386
C	-3.9927218	-2.3866860	-6.3792609
C	-3.2411088	-3.3148153	-7.1255507
C	-1.2501598	-4.4642902	-7.1255507
C	-0.0705698	-4.6511415	-6.3792609
C	1.1812506	-4.4739062	-6.9876386
C	2.3278385	-4.0319346	-6.2835199
C	3.2838911	-3.2599462	-6.9876386
C	4.0632916	-2.2644555	-6.3792609
C	4.4912686	-1.1494749	-7.1255507
C	4.4912686	1.1494749	-7.1255507
C	4.0632916	2.2644555	-6.3792609
C	3.2838911	3.2599462	-6.9876386
C	2.3278385	4.0319346	-6.2835199
C	-2.3278902	4.0320241	-1.4999806

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C	-4.4812204	-1.1478750	-0.6748532
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24.

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C	0.0124567	-4.7141406	-1.4163695
C	-1.2125523	-4.5365653	-0.7517850
C	-2.3891608	-4.1381478	-1.4271305
C	-4.7681935	0.0000000	-8.9065834
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C	-0.0176276	4.7280729	-8.9266260

C	1.2110270	4.5414186	-9.5865472
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C	4.0890523	2.3764381	-11.7570819
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25.

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