

## Supplementary Information

# Aggregation enhancement of coronene molecules by seeding with alkali-metal ions

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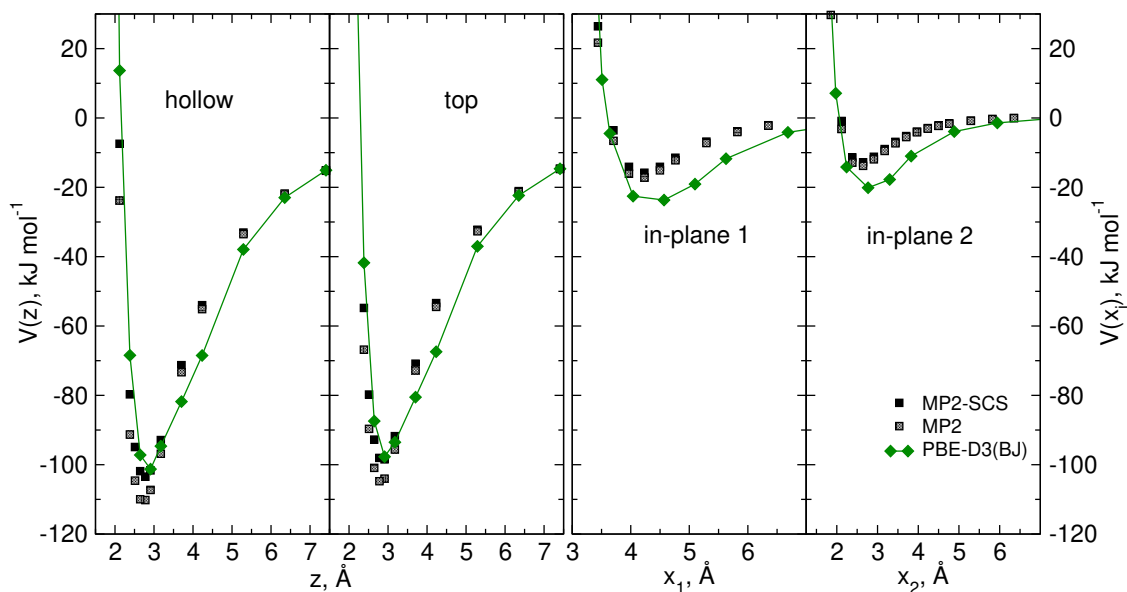


Figure S1: Comparison between PBE-D3(BJ) interaction energies for four different configurations of the coronene- $K^+$  (see Fig. 2 of the main manuscript) with those obtained at the MP2 and MP2-SCS levels.

## Cartesian coordinates and energies of the $K^+Cor_n$ clusters

All coordinates are in Å, while the energies are in  $\text{kJ mol}^{-1}$ .

### Structures in Fig. 3

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$n = 1$ , Energy = -110.18040312

C	1.08059021	2.46690135	2.31601581
C	2.48364498	0.01524169	2.60995759
C	0.62177193	1.49286274	3.24183148
C	2.24093587	2.21511013	1.53717103
C	1.32329931	0.26703292	3.38880237
C	2.94246326	0.98928030	1.68414191
C	0.37906283	3.69273118	2.16904492
C	-0.53857373	1.74465397	4.02067627

C	2.69975415	3.18914873	0.61135536
C	3.18517236	-1.21058813	2.75692847
C	0.86448103	-0.70700569	4.31461804
C	4.10280892	0.73748908	0.90529713
C	-1.24010112	2.97048380	3.87370538
C	1.99822677	4.41497856	0.46438447
C	1.56600841	-1.93283552	4.46158893
C	4.80433630	-0.48834075	1.05226802
C	-0.78128287	3.94452245	2.94788970
C	0.83788108	4.66676983	1.24322925
C	2.72635411	-2.18462679	3.68274415
C	4.34551805	-1.46237941	1.97808370
C	-0.99739186	0.77061543	4.94649177
C	3.86009966	2.93735744	-0.16748926
C	-0.29586448	-0.45521439	5.09346266
C	4.56162704	1.71152761	-0.02051838
H	-1.31977921	4.88547629	2.83507403
H	0.29938473	5.60772367	1.13041357
H	3.26485045	-3.12558063	3.79555983
H	4.88401440	-2.40333325	2.09089937
H	-1.88807981	0.96389180	5.54433748
H	-0.64805602	-1.20289197	5.80412406
H	4.21229120	3.68503502	-0.87815066
H	5.45231499	1.51825125	-0.61836408
H	-2.13078894	3.16376028	4.47155092
H	1.21381706	-2.68051307	5.17225017
H	2.35041813	5.16265612	-0.24627677

H	5.69502412	-0.68161724	0.45442248
K	0.20465800	0.10074000	0.48149700

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n = 2, Energy = -245.07791029

C	-1.46303484	2.61923083	0.27998396
C	-0.33810878	1.71903590	-2.16742078
C	-2.18872734	1.72191644	-0.54742002
C	-0.17487930	3.06644776	-0.11631443
C	-1.62626432	1.27181897	-1.77112239
C	0.38758373	2.61635029	-1.34001680
C	-2.02549787	3.06932830	1.50368633
C	-3.47688288	1.27469951	-0.15112163
C	0.55081320	3.96376215	0.71108955
C	0.22435425	1.26893843	-3.39112315
C	-2.35195682	0.37450458	-2.59852636
C	1.67573926	3.06356721	-1.73631519
C	-4.03934591	1.72479698	1.07258074
C	-0.01164983	4.41385962	1.93479192
C	-1.78949379	-0.07559289	-3.82222873
C	2.23820229	2.61346975	-2.96001756
C	-3.31365343	2.62211139	1.89998477
C	-1.29980539	3.96664271	2.33109036
C	-0.50133823	0.37162402	-4.21852718
C	1.51250981	1.71615534	-3.78742159
C	-4.20257519	0.37738525	-0.97852556
C	1.83896854	4.41097894	0.31479112
C	-3.64011216	-0.07271222	-2.20222793

C	2.40143157	3.96088148	-0.90891125
H	-3.74540320	2.96760873	2.83930556
H	-1.73155516	4.31214004	3.27041115
H	-0.06958846	0.02612668	-5.15784796
H	1.94425958	1.37065800	-4.72674237
H	-5.19137073	0.03409898	-0.67432467
H	-4.19715788	-0.76149586	-2.83734793
H	2.39601426	5.09976259	0.94991112
H	3.39022711	4.30416775	-1.21311214
H	-5.02814128	1.38151086	1.37678173
H	-2.34653929	-0.76437642	-4.45734874
H	0.54539568	5.10264315	2.56991193
H	3.22699766	2.95675587	-3.26421854
C	1.39710721	-2.33818014	-1.11850071
C	1.71671108	-2.22111882	1.70102931
C	2.53912081	-1.70635988	-0.55902938
C	0.41489554	-2.91146974	-0.26820702
C	2.69892275	-1.64782921	0.85073563
C	0.57469748	-2.85293908	1.14155799
C	1.23730527	-2.39671080	-2.52826571
C	3.52133248	-1.13307027	-1.40932307
C	-0.72711806	-3.54329000	-0.82767835
C	1.87651301	-2.16258815	3.11079432
C	3.84093635	-1.01600895	1.41020695
C	-0.40751419	-3.42622868	1.99185167
C	3.36153054	-1.19160094	-2.81908807
C	-0.88692000	-3.60182067	-2.23744335

C	4.00073828	-0.95747829	2.81997196
C	-0.24771226	-3.36769802	3.40161668
C	2.21951693	-1.82342120	-3.37855946
C	0.09529166	-3.02853107	-3.08773710
C	3.01852662	-1.53076789	3.67026571
C	0.89430135	-2.73587775	3.96108807
C	4.66334587	-0.50125013	-0.84985171
C	-1.70932952	-4.11657949	0.02261531
C	4.82314781	-0.44271947	0.55991330
C	-1.54952759	-4.05804883	1.43238032
H	2.09685207	-1.86834967	-4.46070297
H	-0.02737320	-3.07345953	-4.16988061
H	3.14119148	-1.48583942	4.75240922
H	1.01696621	-2.69094929	5.04323158
H	5.41729716	-0.06118975	-1.50254198
H	5.69976397	0.04226938	0.98936666
H	-2.58594568	-4.60156833	-0.40683805
H	-2.30347888	-4.49810920	2.08507059
H	4.11548162	-0.75154068	-3.47177837
H	4.87735424	-0.47248956	3.24942541
H	-1.76353596	-4.08680940	-2.66689680
H	-1.00166333	-3.80775827	4.05430698
K	0.20465800	0.10074000	0.48149700

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n = 3, Energy = -354.65575528

C	3.46280898	-0.17306985	-0.05125487
C	4.48767612	-1.30775666	2.34201334

C	3.41361521	0.56369943	1.16165530
C	4.02443632	-1.47718254	-0.06753093
C	3.92604879	-0.00364397	2.35828940
C	4.53686989	-2.04452594	1.12910317
C	2.95037541	0.39427355	-1.24788897
C	2.85198787	1.86781212	1.17793136
C	4.07363009	-2.21395183	-1.28044109
C	5.00010970	-1.87510006	3.53864744
C	3.87685502	0.73312531	3.57119957
C	5.09849723	-3.34863863	1.11282711
C	2.33955430	2.43515552	-0.01870274
C	3.56119652	-1.64660843	-2.47707520
C	4.38928859	0.16578191	4.76783367
C	5.61093080	-3.91598203	2.30946122
C	2.38874805	1.69838626	-1.23161296
C	2.99956915	-0.34249572	-2.46079919
C	4.95091595	-1.13833080	4.75155766
C	5.56173706	-3.17921277	3.52237143
C	2.80279417	2.60458120	2.39084141
C	4.63525737	-3.51806431	-1.29671704
C	3.31522774	2.03723780	3.58747551
C	5.14769094	-4.08540772	-0.10008293
H	1.99540117	2.13388223	-2.15015599
H	2.60622228	0.09300025	-3.37934222
H	5.34426283	-1.57382677	5.67010070
H	5.95508393	-3.61470874	4.44091447
H	2.37168582	3.60562554	2.40333502

H	3.27746631	2.60278612	4.51851226
H	4.67301879	-4.08361264	-2.22775379
H	5.57879928	-5.08645205	-0.11257655
H	1.90844599	3.43619968	-0.00620930
H	4.35152725	0.73133001	5.69887036
H	3.59895786	-2.21215652	-3.40811188
H	6.04203911	-4.91702619	2.29696777
C	-0.71091506	2.59365311	-2.73240129
C	-0.80929158	4.06720467	-0.30658857
C	-1.42436625	2.07921869	-1.61761669
C	-0.04665213	3.84486330	-2.63427953
C	-1.47355451	2.81599447	-0.40471033
C	-0.09584039	4.58163908	-1.42137317
C	-0.66172680	1.85687732	-3.94530766
C	-2.08862918	0.82800849	-1.71573845
C	0.66679906	4.35929772	-3.74906413
C	-0.85847985	4.80398045	0.90631779
C	-2.18700570	2.30156005	0.71007427
C	0.56842253	5.83284928	-1.32325141
C	-2.03944092	0.09123271	-2.92864481
C	0.71598732	3.62252194	-4.96197050
C	-2.23619397	3.03833584	1.92298063
C	0.51923427	6.56962506	-0.11034505
C	-1.32598973	0.60566710	-4.04342947
C	0.05172439	2.37131171	-5.06009231
C	-1.57193104	4.28954606	2.02110244
C	-0.19421692	6.05519068	1.00443960



C	-2.80208024	0.31357425	-0.60095395
C	1.33106185	5.61050775	-3.65094228
C	-2.85126850	1.05035003	0.61195241
C	1.28187359	6.34728353	-2.43803591
H	-1.28823254	0.04011388	-4.97446318
H	0.08948158	1.80575850	-5.99112602
H	-1.60968822	4.85509928	2.95213615
H	-0.23197410	6.62074389	1.93547331
H	-3.31197226	-0.64686184	-0.67627275
H	-3.39891771	0.65546722	1.46766742
H	1.87871106	6.00539055	-4.50665728
H	1.79176561	7.30771961	-2.36271711
H	-2.54933280	-0.86920323	-3.00396377
H	-2.78384304	2.64345323	2.77869559
H	1.26363639	4.01740454	-5.81768546
H	1.02912616	7.53006100	-0.03502610
C	-2.55197481	-3.02457162	0.60568493
C	-2.65036470	-1.55102576	3.03150057
C	-1.35068436	-2.70908626	1.29399468
C	-3.80246020	-2.60328405	1.13028300
C	-1.39987930	-1.97231333	2.50690250
C	-3.85165515	-1.86651112	2.34319083
C	-2.50277986	-3.76134455	-0.60722289
C	-0.10019896	-3.13037382	0.76939661
C	-5.00375066	-2.91876942	0.44197325
C	-2.69955964	-0.81425283	4.24440840
C	-0.19858885	-1.65682796	3.19521225

C	-5.10214055	-1.44522356	2.86778890
C	-0.05100402	-3.86714675	-0.44351122
C	-4.95455571	-3.65554235	-0.77093457
C	-0.24778379	-0.92005503	4.40812007
C	-5.15133549	-0.70845063	4.08069672
C	-1.25229447	-4.18263215	-1.13182102
C	-3.70407031	-4.07682995	-1.29553269
C	-1.49826919	-0.49876744	4.93271820
C	-3.95004504	-0.39296523	4.76900652
C	1.10109125	-2.81488845	1.45770634
C	-6.25423582	-2.49748186	0.96657134
C	1.05189631	-2.07811552	2.67061416
C	-6.30343076	-1.76070893	2.17947916
H	-1.21453215	-4.74818317	-2.06285585
H	-3.66630800	-4.64238097	-2.22656753
H	-1.53603151	0.06678359	5.86375303
H	-3.98780735	0.17258579	5.70004135
H	2.06097099	-3.13827118	1.05502188
H	1.97401372	-1.83594716	3.19896464
H	-7.17635323	-2.73965022	0.43822087
H	-7.26331049	-1.43732620	2.58216362
H	0.90887548	-4.19052950	-0.84619574
H	0.67433338	-0.67788663	4.93647059
H	-5.87667289	-3.89771075	-1.29928508
H	-6.11121499	-0.38506788	4.48338125
K	0.20465800	0.10074000	0.48149700

n = 4, Energy = -455.75380290

C	2.59074857	3.22586637	-2.00157732
C	-0.06438091	2.22725820	-1.86494385
C	2.06749204	2.45161724	-3.07075502
C	1.78644036	3.50081142	-0.86408287
C	0.73992730	1.95231316	-3.00243829
C	0.45887562	3.00150733	-0.79576614
C	3.91831330	3.72517046	-2.06989405
C	2.87180025	2.17667220	-4.20824946
C	2.30969688	4.27506055	0.20509483
C	-1.39194565	1.72795412	-1.79662711
C	0.21667077	1.17806403	-4.07161599
C	-0.34543259	3.27645237	0.34172830
C	4.19936498	2.67597629	-4.27656620
C	3.63726162	4.77436463	0.13677810
C	-1.11089397	0.67875994	-4.00329926
C	-1.67299733	2.77714829	0.41004504
C	4.72262157	3.45022544	-3.20738850
C	4.44156989	4.49941961	-1.00071635
C	-1.91520223	0.95370497	-2.86580481
C	-2.19625391	2.00289914	-0.65913267
C	2.34854369	1.40242317	-5.27742696
C	1.50538870	4.55000549	1.34258906
C	1.02097895	0.90311909	-5.20911022
C	0.17782397	4.05070140	1.41090580
H	5.74166769	3.83349405	-3.25982880
H	5.46061601	4.88268822	-1.05315666

H	-2.93424835	0.57043635	-2.81336451
H	-3.21530003	1.61963053	-0.60669236
H	2.96593525	1.19137378	-6.15057419
H	0.61932427	0.30880104	-6.02981714
H	1.90704338	5.14432353	2.16329598
H	-0.43956759	4.26175079	2.28405302
H	4.81675657	2.46492702	-5.14971322
H	-1.51254873	0.08444198	-4.82400596
H	4.03891638	5.36868260	0.95748480
H	-2.29038891	2.98819756	1.28319206
C	-3.12327158	0.74873826	2.83215038
C	-3.54173478	-1.15173181	0.76364813
C	-2.18619011	-0.29889346	2.63029357
C	-4.26958465	0.84613494	1.99975606
C	-2.39542171	-1.24912849	1.59604244
C	-4.47881626	-0.10410009	0.96550494
C	-2.91403998	1.69897330	3.86640151
C	-1.03987704	-0.39629014	3.46268789
C	-5.20666613	1.89376666	2.20161287
C	-3.75096638	-2.10196684	-0.27060300
C	-1.45834024	-2.29676021	1.39418564
C	-5.62512933	-0.00670341	0.13311062
C	-0.83064543	0.55394489	4.49693902
C	-4.99743453	2.84400170	3.23586400
C	-1.66757184	-3.24699525	0.35993451
C	-5.83436093	-0.95693844	-0.90114051
C	-1.76772690	1.60157665	4.69879587

C	-3.85112144	2.74660506	4.06825836
C	-2.81388492	-3.14959860	-0.47245985
C	-4.89727947	-2.00457020	-1.10299736
C	-0.10279576	-1.44392175	3.26083102
C	-6.35297900	1.99116324	1.36921861
C	-0.31202737	-2.39415679	2.22657989
C	-6.56221060	1.04092820	0.33496749
H	-1.60711955	2.33098238	5.49269282
H	-3.69051410	3.47601079	4.86215531
H	-2.97449227	-3.87900434	-1.26635681
H	-5.05788681	-2.73397593	-1.89689431
H	0.77712069	-1.51868402	3.89978164
H	0.40728173	-3.19832486	2.07163347
H	-7.07228809	2.79533131	1.52416504
H	-7.44212706	1.11569047	-0.30398313
H	0.04927083	0.47918278	5.13588961
H	-0.94826295	-4.05116325	0.20498798
H	-5.71674341	3.64816971	3.39081053
H	-6.71427720	-0.88217633	-1.54009111
C	2.33973970	-3.61356208	-0.05676081
C	3.21215858	-2.93844308	2.56024113
C	2.38355100	-4.60821941	0.95572990
C	2.73213784	-2.28134524	0.23924946
C	2.81976044	-4.27065991	2.26423087
C	3.16834728	-1.94378574	1.54775043
C	1.90353026	-3.95112158	-1.36526178
C	1.99115286	-5.94043625	0.65971963

C	2.68832653	-1.28668790	-0.77324125
C	3.64836802	-2.60088358	3.86874210
C	2.86357174	-5.26531725	3.27672157
C	3.56074541	-0.61156890	1.84376069
C	1.55494342	-6.27799575	-0.64878134
C	2.25211709	-1.62424740	-2.08174222
C	3.29978118	-4.92775775	4.58522254
C	3.99695486	-0.27400940	3.15226166
C	1.51113210	-5.28333843	-1.66127210
C	1.85971894	-2.95646425	-2.37775254
C	3.69217933	-3.59554090	4.88123286
C	4.04076617	-1.26866673	4.16475242
C	2.03496419	-6.93509336	1.67221027
C	3.08072464	0.04552871	-0.47723092
C	2.47117363	-6.59753386	2.98071124
C	3.51693408	0.38308821	0.83127005
H	1.17629529	-5.54245099	-2.66568476
H	1.52488213	-3.21557681	-3.38216520
H	4.02701614	-3.33642834	5.88564553
H	4.37560298	-1.00955417	5.16916509
H	1.73375714	-7.95771061	1.44499112
H	2.50480343	-7.36103852	3.75790487
H	3.04709484	0.80903337	-1.25442454
H	3.81814113	1.40570546	1.05848920
H	1.25373639	-7.30061279	-0.87600061
H	3.33341103	-5.69126217	5.36241615
H	2.21848725	-0.86074298	-2.85893583

H	4.29816189	0.74860763	3.37948093
C	-2.60792783	-4.26473904	4.14753407
C	-4.76989985	-2.42492591	4.22855319
C	-2.61878866	-3.22406293	5.11359584
C	-3.67805301	-4.38550859	3.22198186
C	-3.69977467	-2.30415636	5.15410540
C	-4.75903902	-3.46560202	3.26249142
C	-1.52694182	-5.18464561	4.10702450
C	-1.54866348	-3.10329339	6.03914805
C	-3.66719218	-5.42618470	2.25592008
C	-5.85088586	-1.50501934	4.26906276
C	-3.71063550	-1.26348025	6.12016718
C	-5.82916420	-3.58637156	2.33693921
C	-0.46767747	-4.02319996	5.99863848
C	-2.58620617	-6.34609127	2.21541052
C	-4.79162151	-0.34357368	6.16067674
C	-6.91015021	-2.66646499	2.37744878
C	-0.45681659	-5.06387611	5.03257671
C	-1.51608094	-6.22532176	3.14096273
C	-5.86174674	-0.46434319	5.23512453
C	-6.92101109	-1.62578884	3.34351055
C	-1.55952441	-2.06261739	7.00520964
C	-4.73731726	-5.54695413	1.33036806
C	-2.64051042	-1.14271082	7.04571920
C	-5.81830327	-4.62704756	1.37087762
H	0.37295432	-5.77000154	5.00148134
H	-0.68631003	-6.93144719	3.10986736

H	-6.69151765	0.24178224	5.26621990
H	-7.75078200	-0.91966341	3.37460592
H	-0.73809023	-1.96991399	7.71566880
H	-2.64884724	-0.34388191	7.78727374
H	-4.72898044	-6.34578304	0.58881352
H	-6.63973745	-4.71975096	0.66041846
H	0.35375666	-3.93049671	6.70909746
H	-4.79995848	0.45525515	6.90223109
H	-2.57786920	-7.14492010	1.47385617
H	-7.73158434	-2.75916825	1.66698980
K	0.20465800	0.10074000	0.48149700

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n = 5, Energy = -556.71294827

C	4.69799884	4.53884889	-1.92052988
C	4.84930333	4.69128206	0.91133710
C	5.40925368	3.54816292	-1.19316618
C	4.06239624	5.60575144	-1.23196008
C	5.48490593	3.62437951	0.22276731
C	4.13804849	5.68196802	0.18397341
C	4.62234660	4.46263230	-3.33646337
C	6.04485628	2.48126037	-1.88173598
C	3.35114140	6.59643740	-1.95932377
C	4.92495558	4.76749864	2.32727059
C	6.19616077	2.63369354	0.95013100
C	3.50244589	6.74887057	0.87254321
C	5.96920404	2.40504379	-3.29766947
C	3.27548916	6.52022081	-3.37525726



C	6.27181302	2.70991013	2.36606449
C	3.57809814	6.82508716	2.28847670
C	5.25794919	3.39572975	-4.02503322
C	3.91109175	5.45331826	-4.06382712
C	5.63621042	3.77681268	3.05463435
C	4.28935298	5.83440119	3.01584045
C	6.75611099	1.49057461	-1.15437229
C	2.71553893	7.66333975	-1.27075398
C	6.83176324	1.56679119	0.26156120
C	2.79119118	7.73955634	0.14517951
H	5.19987810	3.33722547	-5.11191169
H	3.85302066	5.39481398	-5.15070559
H	5.69428151	3.83531696	4.14151282
H	4.34742407	5.89290547	4.10271892
H	7.24400318	0.67161412	-1.68292237
H	7.37772652	0.80633498	0.81988971
H	2.16957565	8.42379596	-1.82908248
H	2.30329899	8.55851683	0.67372960
H	6.45709609	1.58608349	-3.82621962
H	6.81777617	1.94945412	2.92439305
H	2.72952600	7.28067682	-3.93358582
H	3.09020608	7.64404745	2.81702684
C	-3.28834652	-1.95426042	-0.51914793
C	-3.58818463	-0.29466877	1.76590178
C	-3.90932892	-2.46375156	0.65183445
C	-2.81728318	-0.61497345	-0.54760544
C	-4.05924797	-1.63395573	1.79435930

C	-2.96720224	0.21482237	0.59491941
C	-3.13842747	-2.78405624	-1.66167278
C	-4.38039225	-3.80303852	0.68029197
C	-2.19630079	-0.10548231	-1.71858782
C	-3.73810369	0.53512705	2.90842664
C	-4.68023036	-2.14344688	2.96534168
C	-2.49613890	1.55410934	0.56646189
C	-4.23047320	-4.63283435	-0.46223289
C	-2.04638173	-0.93527813	-2.86111267
C	-4.83014942	-1.31365105	4.10786653
C	-2.64605795	2.38390516	1.70898675
C	-3.60949080	-4.12334324	-1.63321531
C	-2.51744507	-2.27456514	-2.83265520
C	-4.35908609	0.02563595	4.07940906
C	-3.26704035	1.87441406	2.87996917
C	-5.00137454	-4.31252949	1.85127422
C	-1.72523755	1.23380448	-1.74704522
C	-5.15129360	-3.48273366	2.99379908
C	-1.87515661	2.06360030	-0.60452036
H	-3.49441209	-4.76029916	-2.51022379
H	-2.40236636	-2.91152105	-3.70966368
H	-4.47416479	0.66259187	4.95641753
H	-3.38211906	2.51136997	3.75697764
H	-5.36296546	-5.34057380	1.87311839
H	-5.62796323	-3.87382199	3.89265182
H	-1.24856792	1.62489280	-2.64589796
H	-1.51356570	3.09164461	-0.62636454

H	-4.59206400	-5.66087852	-0.44038888
H	-5.30681895	-1.70473916	5.00671920
H	-1.56971220	-0.54419003	-3.75996535
H	-2.28446715	3.41194933	1.68714274
C	1.00126855	3.60783011	-2.05177780
C	0.85198127	4.23103663	0.71497598
C	1.66480310	2.78659925	-1.10219797
C	0.26309036	4.74066424	-1.61798074
C	1.59015946	3.09820251	0.28117891
C	0.18844672	5.05226749	-0.23460385
C	1.07591219	3.29622686	-3.43515469
C	2.40298129	1.65376513	-1.53599504
C	-0.40044419	5.56189510	-2.56756056
C	0.77733763	4.54263989	2.09835287
C	2.25369401	2.27697164	1.23075874
C	-0.54973147	6.18510161	0.19919321
C	2.47762493	1.34216187	-2.91937192
C	-0.32580055	5.25029184	-3.95093745
C	2.17905037	2.58857490	2.61413563
C	-0.62437511	6.49670487	1.58257010
C	1.81409038	2.16339272	-3.86895181
C	0.41237764	4.11745771	-4.38473457
C	1.44087217	3.72140903	3.04793275
C	0.03915943	5.67547402	2.53214999
C	3.06651570	0.83253446	-0.58641526
C	-1.13862225	6.69472903	-2.13376345
C	2.99187206	1.14413771	0.79696163

C	-1.21326589	7.00633229	-0.75038656
H	1.87138725	1.92420432	-4.93083965
H	0.46967451	3.87826930	-5.44662241
H	1.38357530	3.96059744	4.10982059
H	-0.01813744	5.91466242	3.59403783
H	3.63314549	-0.03703548	-0.91940034
H	3.50120497	0.51375621	1.52586450
H	-1.64795516	7.32511054	-2.86266633
H	-1.77989568	7.87590222	-0.41740148
H	3.04425459	0.47259211	-3.25235711
H	2.68838314	1.95819360	3.34303851
H	-0.83513333	5.88067315	-4.67984034
H	-1.19100477	7.36627463	1.91555529
C	3.90438947	-1.29094942	3.42895460
C	2.26377494	-2.44274780	1.41715342
C	4.49000894	-1.79431709	2.23728733
C	2.49846273	-1.36348094	3.61472129
C	3.66970168	-2.37021628	1.23138674
C	1.67815547	-1.93938013	2.60882070
C	4.72469673	-0.71505023	4.43485519
C	5.89593568	-1.72178556	2.05152064
C	1.91284325	-0.86011328	4.80638856
C	1.44346768	-3.01864699	0.41125283
C	4.25532116	-2.87358394	0.03971946
C	0.27222873	-2.01191166	2.79458738
C	6.71624294	-1.14588637	3.05742123
C	2.73315051	-0.28421409	5.81228915

C	3.43501390	-3.44948313	-0.96618113
C	-0.54807853	-2.58781085	1.78868679
C	6.13062350	-0.64251868	4.24908855
C	4.13907728	-0.21168254	5.62652251
C	2.02908713	-3.52201468	-0.78041449
C	0.03754091	-3.09117854	0.59701947
C	6.48155497	-2.22515319	0.85985350
C	0.50691670	-0.93264484	4.99215511
C	5.66124771	-2.80105238	-0.14604709
C	-0.31339056	-1.50854403	3.98625452
H	6.76029594	-0.20045524	5.02122347
H	4.76874973	0.23038090	6.39865744
H	1.39941468	-3.96407812	-1.55254941
H	-0.59213153	-3.53324198	-0.17511545
H	7.56075235	-2.16947758	0.71725792
H	6.11077257	-3.18744026	-1.06077768
H	0.05739184	-0.54625696	5.90688571
H	-1.39258794	-1.56421964	4.12885011
H	7.79544017	-1.09021070	2.91482583
H	3.88453854	-3.83587100	-1.88091163
H	2.28362587	0.10217378	6.72701965
H	-1.62727576	-2.64348652	1.93128220
C	-5.16633422	1.73116740	-2.53495785
C	-6.34637450	1.34221856	0.01882821
C	-5.14850935	2.77963657	-1.57746386
C	-5.77417924	0.48822381	-2.21555882
C	-5.73852948	2.58516215	-0.30057083

C	-6.36419938	0.29374939	-0.93866579
C	-4.57631408	1.92564183	-3.81185088
C	-4.54066433	4.02258016	-1.89686289
C	-5.79200412	-0.56024536	-3.17305281
C	-6.93639464	1.14774414	1.29572124
C	-5.72070461	3.63363132	0.65692317
C	-6.97204439	-0.94919420	-0.61926675
C	-3.95064419	4.21705458	-3.17375592
C	-5.20198398	-0.36577093	-4.44994585
C	-6.31072475	3.43915690	1.93381620
C	-7.56206453	-1.14366862	0.65762628
C	-3.96846904	3.16858542	-4.13124997
C	-4.59413894	0.87717266	-4.76934493
C	-6.91856979	2.19621330	2.25321529
C	-7.54423968	-0.09519946	1.61512033
C	-4.52283951	5.07104911	-0.93936896
C	-6.39984907	-1.80318872	-2.85365372
C	-5.11285965	4.87657469	0.33752407
C	-6.98986921	-1.99766315	-1.57676069
H	-3.51556628	3.31786508	-5.11140021
H	-4.14123618	1.02645232	-5.74949517
H	-7.37147255	2.04693364	3.23336553
H	-7.99714244	-0.24447912	2.59527057
H	-4.05625422	6.02513971	-1.18454146
H	-5.09917716	5.68138561	1.07250191
H	-6.41353156	-2.60799965	-3.58863156
H	-7.45645451	-2.95175374	-1.33158818

H	-3.48405893	5.17114497	-3.41892854
H	-6.29704234	4.24396759	2.66879403
H	-5.21566638	-1.17058163	-5.18492368
H	-8.02864979	-2.09775900	0.90279890
K	0.20465800	0.10074000	0.48149700

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n = 6, Energy = -658.57230967

C	5.51931736	2.50365726	3.66247618
C	5.28392966	4.09161536	1.31970405
C	5.99011219	2.00738282	2.41810325
C	4.93082869	3.79391075	3.73546304
C	5.87241834	2.80136187	1.24671719
C	4.81313484	4.58788980	2.56407698
C	5.63701121	1.70967821	4.83386224
C	6.57860087	0.71712933	2.34511638
C	4.46003386	4.29018520	4.97983597
C	5.16623581	4.88559441	0.14831799
C	6.34321317	2.30508743	0.00234426
C	4.22464616	5.87814329	2.63706385
C	6.69629472	-0.07684972	3.51650244
C	4.57772771	3.49620615	6.15122203
C	6.22551932	3.09906648	-1.16904180
C	4.10695231	6.67212234	1.46567779
C	6.22549990	0.41942469	4.76087542
C	5.16621639	2.20595262	6.07823521
C	5.63703064	4.38932001	-1.09605499
C	4.57774713	6.17584794	0.22130481

C	7.04939560	0.22085507	1.10074358
C	3.87154528	5.58043851	5.05282271
C	6.93170175	1.01483412	-0.07064248
C	3.75385143	6.37441756	3.88143665
H	6.31584236	-0.19003807	5.66003791
H	5.25655885	1.59648986	6.97739771
H	5.54668818	4.99878277	-1.99521748
H	4.48740467	6.78531070	-0.67785768
H	7.50112287	-0.76955087	1.04471842
H	7.29308655	0.63389101	-1.02583023
H	3.51016048	5.96138162	6.00801046
H	3.30212416	7.36482350	3.93746181
H	7.14802189	-1.06725551	3.46047746
H	6.58690401	2.71812358	-2.12422947
H	4.21634301	3.87714905	7.10640970
H	3.65522513	7.66252814	1.52170277
C	1.72467538	0.38616063	-3.33910968
C	3.12860033	-1.74821627	-2.09853340
C	3.13578320	0.29438700	-3.46854075
C	1.01553003	-0.58925419	-2.58939048
C	3.83774567	-0.77280144	-2.84825260
C	1.71749251	-1.65644264	-1.96910234
C	1.02271290	1.45334907	-3.95939783
C	3.84492854	1.26980182	-4.21825995
C	-0.39557779	-0.49748057	-2.45995942
C	3.83056280	-2.81540471	-1.47824525
C	5.24885349	-0.86457507	-2.97768366



C	1.00834717	-2.63185746	-1.21938313
C	3.14296606	2.33699027	-4.83854809
C	-1.09754026	0.56970788	-3.08024756
C	5.95081597	-1.93176352	-2.35739552
C	1.71030964	-3.69904591	-0.59909499
C	1.73185821	2.42876394	-4.70911706
C	-0.38839495	1.54512274	-3.82996679
C	5.24167065	-2.90717838	-1.60767629
C	3.12141749	-3.79081958	-0.72852602
C	5.25603615	1.17802811	-4.34769093
C	-1.10472292	-1.47289530	-1.71024030
C	5.95799863	0.11083966	-3.72740278
C	-0.40276045	-2.54008375	-1.08995215
H	1.19302789	3.24794376	-5.18525371
H	-0.92722527	2.36430257	-4.30610344
H	5.78050098	-3.72635821	-1.13153964
H	3.66024782	-4.60999940	-0.25238937
H	5.80038018	1.92676208	-4.92317966
H	7.04117304	0.04039372	-3.82675482
H	-2.18789734	-1.40244936	-1.61088826
H	-0.94710448	-3.28881772	-0.51446342
H	3.68730986	3.08572420	-5.41403677
H	7.03399020	-2.00220959	-2.45674744
H	-2.18071450	0.64015395	-2.98089564
H	1.16596585	-4.44777984	-0.02360631
C	1.96507601	2.47401781	1.83517248
C	1.12952163	2.91914107	4.51272989

C	1.31412672	3.68701408	2.18346137
C	2.19824812	1.48358317	2.82566230
C	0.89634953	3.90957570	3.52224008
C	1.78047093	1.70614480	4.16444100
C	2.38285320	2.25145618	0.49639378
C	1.08095461	4.67744872	1.19297156
C	2.84919741	0.27058691	2.47737341
C	0.71174444	3.14170269	5.85150860
C	0.24540023	5.12257197	3.87052897
C	2.01364303	0.71571016	5.15493082
C	1.49873180	4.45488709	-0.14580715
C	3.26697460	0.04802528	1.13859470
C	-0.17237696	5.34513360	5.20930767
C	1.59586584	0.93827179	6.49370952
C	2.14968111	3.24189081	-0.49409609
C	3.03380251	1.03845991	0.14810483
C	0.06079513	4.35469897	6.19979754
C	0.94491653	2.15126806	6.84199847
C	0.43000540	5.89044477	1.54126051
C	3.08236943	-0.71984752	3.46786316
C	0.01222821	6.11300640	2.88003921
C	2.66459224	-0.49728589	4.80664186
H	2.47036922	3.07105126	-1.52175012
H	3.35449062	0.86762036	-0.87954920
H	-0.25989298	4.52553852	7.22745157
H	0.62422842	2.32210761	7.86965249
H	0.25102116	6.65070806	0.78095489

H	-0.48744418	7.04410925	3.14738773
H	3.58204182	-1.65095038	3.20051464
H	2.84357648	-1.25754918	5.56694748
H	1.31974766	5.21515015	-0.90611276
H	-0.67204928	6.27623625	5.47665631
H	3.76664692	-0.88307738	0.87124606
H	1.77484998	0.17800872	7.25401513
C	-4.35855309	-1.82828006	-0.22986257
C	-2.99442471	0.33424572	1.00635566
C	-4.53000500	-0.50697405	-0.72093768
C	-3.50503699	-2.06832317	0.87932165
C	-3.84794081	0.57428884	-0.10282857
C	-2.82297280	-0.98706028	1.49743077
C	-5.04061728	-2.90954295	-0.84797169
C	-5.38352111	-0.26693094	-1.83012191
C	-3.33358507	-3.38962917	1.37039676
C	-2.31236052	1.41550862	1.62446477
C	-4.01939273	1.89559484	-0.59390367
C	-1.96945669	-1.22710339	2.60661499
C	-6.06558530	-1.34819383	-2.44823102
C	-4.01564926	-4.47089207	0.75228764
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H	6.61784540	1.76526467	-3.31365627
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C	3.65522243	4.89600066	-2.01211217



C	1.84837007	5.01669068	-3.67641950
C	1.32041371	7.69183903	-1.09191901
C	3.69981908	6.47695166	-0.12855041
C	0.08611437	6.71833171	-3.45716508
C	3.61062577	3.31504966	-3.89567393
C	4.84492511	4.28855697	-1.53042786
C	1.23122040	4.52993703	-4.85904254
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C	-0.48643864	7.81252905	-2.75622635
C	5.41747813	3.19435963	-2.23136659
C	1.80377341	3.43573968	-5.55998126
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C	0.13071100	8.29928276	-1.57360329
C	4.80032848	2.70760593	-3.41398965
C	2.99347612	2.82829595	-5.07829699
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C	-0.53103512	6.23157804	-4.63978795
C	5.46207461	4.77531064	-0.34780499
C	0.04151789	5.13738070	-5.34072668
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H	-0.30878390	9.13919476	-1.03555880
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C	-7.04929817	0.27842364	3.90598012
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C	-1.58217320	1.24011190	-6.45669195
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H	-6.42138585	-5.50155130	-4.39337018
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H	-5.11611919	-4.97239834	-8.98228901
H	-6.03475261	-4.24551550	-2.31440676
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C	-5.28436227	1.76713858	-7.59357090
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C	0.83544708	7.06229823	-3.16186216

C	-0.27243938	6.77506392	-0.98487253
C	-0.03822941	4.85814534	-2.50795141
C	0.38808161	7.60552632	-1.92850599
C	0.62229157	5.68860774	-3.45158487
C	-1.14611587	4.57091103	-0.33096177
C	-0.71980485	7.31829201	0.24848365
C	-0.25138492	3.48445485	-2.79767412
C	1.49596806	7.89276062	-4.10549563
C	0.60123711	8.97921680	-1.63878328
C	1.06965705	5.14537965	-4.68494105
C	-1.38032584	6.48782961	1.19211711
C	-0.91190590	2.65399245	-1.85404065
C	1.26175810	9.80967920	-2.58241675
C	1.73017803	5.97584204	-5.62857451
C	-1.59348137	5.11413909	0.90239444
C	-1.35927140	3.19722051	-0.62068444
C	1.70912360	9.26645115	-3.81577296
C	1.94333357	7.34953257	-5.33885184
C	-0.50664932	8.69198231	0.53820621
C	0.19598054	2.94122695	-4.03103014
C	0.15387166	9.52244471	-0.40542726
C	0.85650152	3.77168934	-4.97466361
H	-2.10050097	4.47667150	1.62673277
H	-1.86629101	2.55975292	0.10365389
H	2.21614320	9.90391873	-4.54011129
H	2.45035317	7.98700015	-6.06319017
H	-0.85004961	9.10896731	1.48493743

H	0.31749103	10.57689736	-0.18303444
H	0.03236116	1.88677429	-4.25342296
H	1.19990180	3.35470435	-5.92139484
H	-1.72372613	6.90481439	2.13884823
H	1.42537752	10.86413170	-2.36002411
H	-1.07552532	1.59953995	-2.07643329
H	2.07357832	5.55885727	-6.57530563
C	-9.55555230	2.80504229	-8.42593788
C	-8.04180863	3.36506032	-10.76272187
C	-9.09690021	4.12560418	-8.67524621
C	-9.25733255	1.76448942	-9.34502154
C	-8.34002837	4.40561319	-9.84363820
C	-8.50046072	2.04449844	-10.51341354
C	-10.31242413	2.52503327	-7.25754588
C	-9.39511995	5.16615705	-7.75616254
C	-9.71598464	0.44392754	-9.09571322
C	-7.28493679	3.64506934	-11.93111386
C	-7.88137628	5.72617508	-10.09294653
C	-8.20224097	1.00394557	-11.43249721
C	-10.15199179	4.88614803	-6.58777055
C	-10.47285648	0.16391852	-7.92732122
C	-7.12450445	6.00618409	-11.26133852
C	-7.44536914	1.28395458	-12.60088920
C	-10.61064391	3.56558613	-6.33846217
C	-10.77107626	1.20447138	-7.00823751
C	-6.82628467	4.96563124	-12.18042224
C	-6.98671702	2.60451648	-12.85019758

C	-8.93646788	6.48671870	-8.00547093
C	-9.41776488	-0.59662511	-10.01479682
C	-8.17959604	6.76672772	-9.17386293
C	-8.66089305	-0.31661609	-11.18318881
H	-11.19162297	3.35064964	-5.44159793
H	-11.35205531	0.98953489	-6.11137327
H	-6.24530561	5.18056773	-13.07728647
H	-6.40573796	2.81945297	-13.74706181
H	-9.16538305	7.28545303	-7.29997708
H	-7.82753209	7.78039856	-9.36523341
H	-9.76982884	-1.61029595	-9.82342634
H	-8.43197788	-1.11535042	-11.88868267
H	-10.38090700	5.68488212	-5.88227671
H	-6.77244048	7.01985472	-11.45270912
H	-10.82492045	-0.84975211	-7.73595063
H	-7.21645392	0.48522049	-13.30638304
C	-4.18795389	1.77485261	6.54007002
C	-1.36740704	1.55443298	6.78812276
C	-3.34465512	2.75231054	5.94861145
C	-3.62097924	0.68718486	7.25555496
C	-1.93438169	2.64210073	6.07263782
C	-2.21070582	0.57697505	7.37958134
C	-5.59822732	1.88506242	6.41604365
C	-3.91162976	3.83997828	5.23312651
C	-4.46427802	-0.29027307	7.84701354
C	0.04286638	1.44422317	6.91214914
C	-1.09108291	3.61955866	5.48117925

C	-1.64373117	-0.51069269	8.09506628
C	-5.32190319	3.95018809	5.10910013
C	-5.87455145	-0.18006326	7.72298716
C	0.31919051	3.50934885	5.60520562
C	-0.23345774	-0.62090251	8.21909265
C	-6.16520203	2.97273016	5.70055870
C	-6.44152615	0.90760449	7.00750222
C	0.88616522	2.42168110	6.32069057
C	0.60984109	0.35655542	7.62763408
C	-3.06833101	4.81743601	4.64166806
C	-3.89730334	-1.37794061	8.56249835
C	-1.65805759	4.70722620	4.76569443
C	-2.48702992	-1.48815042	8.68652472
H	-7.24773580	3.05732783	5.60535536
H	-7.52405993	0.99220216	6.91229888
H	1.96869899	2.33708343	6.41589391
H	1.69237487	0.27195775	7.72283742
H	-3.50354397	5.65233598	4.09245773
H	-1.01073665	5.45752849	4.31168745
H	-4.54462428	-2.12824291	9.01650533
H	-2.05181696	-2.32305040	9.23573505
H	-5.75711623	4.78508787	4.55988993
H	0.96651148	4.25965093	5.15119877
H	-6.52187241	-0.93036535	8.17699401
H	0.20175530	-1.45580228	8.76830286
C	-12.61954159	0.52427408	0.06351266
C	-12.90228003	2.40341436	2.17407900

C	-12.97091074	0.08140935	1.36612949
C	-12.40954166	1.90670895	-0.18382101
C	-13.11227996	1.02097949	2.42141267
C	-12.55091088	2.84627909	0.87146217
C	-12.47817236	-0.41529606	-0.99177052
C	-13.18091066	-1.30102552	1.61346316
C	-12.05817251	2.34957368	-1.48643785
C	-13.04364925	3.34298449	3.22936218
C	-13.46364911	0.57811476	3.72402951
C	-12.34091095	4.22871395	0.62412850
C	-13.03954144	-2.24059566	0.55817999
C	-11.91680329	1.41000354	-2.54172102
C	-13.60501833	1.51768490	4.77931268
C	-12.48228018	5.16828409	1.67941167
C	-12.68817229	-1.79773097	-0.74443690
C	-12.12680321	0.02756863	-2.29438740
C	-13.39501841	2.90011980	4.53197906
C	-12.83364933	4.72541940	2.98202856
C	-13.53227976	-1.74389007	2.91607985
C	-11.84817264	3.73200837	-1.73377136
C	-13.67364898	-0.80431993	3.97136302
C	-11.98954186	4.67157851	-0.67848819
H	-12.57965648	-2.51895026	-1.55447817
H	-12.01828740	-0.69365066	-3.10442867
H	-13.50353421	3.62133910	5.34202033
H	-12.94216514	5.44663870	3.79206983
H	-13.69347690	-2.80505496	3.10593460

H	-13.94336194	-1.14426545	4.97125913
H	-11.57845967	4.07195388	-2.73366747
H	-11.82834471	5.73274339	-0.86834294
H	-13.20073853	-3.30176041	0.74803454
H	-13.87473124	1.17773960	5.77920868
H	-11.64709037	1.74994884	-3.54161702
H	-12.32108309	6.22944884	1.48955712
C	-6.80120050	5.50881341	-4.90208097
C	-6.30229334	3.28356342	-6.59469836
C	-6.07404512	5.68384319	-6.10914755
C	-7.27890229	4.22115863	-4.54132309
C	-5.82459155	4.57121819	-6.95545624
C	-7.02944871	3.10853364	-5.38763179
C	-7.05065407	6.62143841	-4.05577228
C	-5.59634333	6.97149797	-6.46990543
C	-8.00605766	4.04612885	-3.33425652
C	-6.05283976	2.17093842	-7.44100706
C	-5.09743617	4.74624797	-8.16252282
C	-7.50715051	1.82087886	-5.02687391
C	-5.84579691	8.08412296	-5.62359673
C	-8.25551124	5.15875385	-2.48794782
C	-4.84798259	3.63362297	-9.00883151
C	-7.25769693	0.70825386	-5.87318260
C	-6.57295229	7.90909323	-4.41653012
C	-7.77780946	6.44640867	-2.84870567
C	-5.32568438	2.34596815	-8.64807367
C	-6.53054155	0.88328360	-7.08024921



C	-4.86918807	7.14652760	-7.67697185
C	-8.48375934	2.75847422	-2.97349879
C	-4.61973449	6.03390261	-8.52328055
C	-8.23430576	1.64584922	-3.81980748
H	-6.76443425	8.76315040	-3.76689883
H	-7.96929142	7.30046585	-2.19907438
H	-5.13420242	1.49191098	-9.29770496
H	-6.33905958	0.02922642	-7.72988050
H	-4.50250144	8.13493875	-7.95389167
H	-4.06156588	6.16825648	-9.44983173
H	-9.04192796	2.62412034	-2.04694761
H	-8.60099239	0.65743808	-3.54288766
H	-5.47911040	9.07253401	-5.90051637
H	-4.28981409	3.76797666	-9.93538258
H	-8.81367975	5.02440016	-1.56139676
H	-7.62438343	-0.28015719	-5.59626297
C	-0.32176670	-2.27901337	-1.85159846
C	1.49881750	-4.29054459	-1.01206595
C	0.71921151	-2.70170219	-2.71998696
C	-0.45245281	-2.86209016	-0.56344370
C	1.62950361	-3.70746780	-2.30022071
C	0.45783929	-3.86785576	-0.14367745
C	-1.23205881	-1.27324776	-2.27136471
C	0.84989762	-2.11862541	-4.00814172
C	-1.49343103	-2.43940133	0.30494480
C	2.40910960	-5.29631019	-0.59229970
C	2.67048183	-4.13015663	-3.16860921

C	0.32715318	-4.45093255	1.14447731
C	-0.06039448	-1.11285980	-4.42790798
C	-2.40372313	-1.43363572	-0.11482145
C	3.58077393	-5.13592223	-2.74884296
C	1.23744528	-5.45669815	1.56424357
C	-1.10137273	-0.69017094	-3.55951949
C	-2.27303706	-0.85055890	-1.40297623
C	3.45008786	-5.71899906	-1.46068818
C	2.27842353	-5.87938702	0.69585508
C	1.89087572	-2.54131425	-4.87653002
C	-1.62411703	-3.02247810	1.59309935
C	2.80116783	-3.54707986	-4.45676376
C	-0.71382492	-4.02824371	2.01286560
H	-1.80011804	0.08186037	-3.88173442
H	-2.97178237	-0.07852759	-1.72519116
H	4.14883317	-6.49103037	-1.13847325
H	2.97716884	-6.65141833	1.01807001
H	1.99119114	-2.09374120	-5.86532496
H	3.60022863	-3.87153820	-5.12334374
H	-2.42317784	-2.69801976	2.25967933
H	-0.81414034	-4.47581676	3.00166055
H	0.03992079	-0.66528672	-5.41670273
H	4.37983466	-5.46038063	-3.41542271
H	-3.20278387	-1.10917733	0.55175830
H	1.13713001	-5.90427124	2.55303832
C	-9.58750489	0.94109558	2.93977916
C	-10.22570292	0.07333291	5.56757115

C	-9.71928591	1.88956670	3.98831928
C	-9.77482289	-0.44125687	3.20513503
C	-10.03838492	1.45568536	5.30221527
C	-10.09392190	-0.87513821	4.51903103
C	-9.26840588	1.37497692	1.62588316
C	-9.53196792	3.27191915	3.72296340
C	-9.64304187	-1.38972799	2.15659491
C	-10.54480193	-0.36054843	6.88146714
C	-10.17016594	2.40415648	6.35075539
C	-10.28123990	-2.25749066	4.78438690
C	-9.21286890	3.70580049	2.40906741
C	-9.32394286	-0.95584665	0.84269892
C	-10.48926495	1.97027514	7.66465138
C	-10.60033891	-2.69137200	6.09828290
C	-9.08108787	2.75732939	1.36052723
C	-9.13662485	0.42650582	0.57734299
C	-10.67658296	0.58792267	7.93000731
C	-10.73211994	-1.74290090	7.14682307
C	-9.66374894	4.22039004	4.77150344
C	-9.83035986	-2.77208022	2.42195087
C	-9.98284795	3.78650870	6.08539944
C	-10.14945887	-3.20596155	3.73584686
H	-8.83614568	3.09037913	0.35197331
H	-8.89168266	0.75955556	-0.43121093
H	-10.92152515	0.25487293	8.93856123
H	-10.97706213	-2.07595064	8.15537699
H	-9.51996258	5.28149167	4.56781478

H	-10.08400381	4.51456056	6.89026480
H	-9.72920400	-3.50013207	1.61708550
H	-10.29324523	-4.26706319	3.93953553
H	-9.06908254	4.76690191	2.20537861
H	-10.59042083	2.69832675	8.46951673
H	-9.22278698	-1.68389826	0.03783358
H	-10.74412527	-3.75247342	6.30197169
K	0.20465800	0.10074000	0.48149700

### Structures in Fig. 6

Values in parenthesis are the energies of the structures when the reference is the global minimum (*cf.* Fig. 6).

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n = 2, Energy = -197.977000607820 (47.1)

C	2.64885476	-0.07507234	-1.40134079
C	3.04163470	-0.81860650	1.31131112
C	3.04839924	0.89930192	-0.44878681
C	2.44570025	-1.42121368	-0.99756881
C	3.24478921	0.52753484	0.90753915
C	2.64209022	-1.79298076	0.35875714
C	2.45246478	0.29669475	-2.75766674
C	3.25155374	2.24544327	-0.85255878
C	2.04615577	-2.39558794	-1.95012279
C	3.23802468	-1.19037358	2.66763707
C	3.64433369	1.50190910	1.86009313
C	2.43893572	-3.13912211	0.76252911
C	3.05516377	2.61721035	-2.20888474

C	1.84976580	-2.02382086	-3.30644875
C	3.84072366	1.13014202	3.21641908
C	2.63532569	-3.51088919	2.11885507
C	2.65561928	1.64283610	-3.16143877
C	2.05292030	-0.67767950	-3.71022078
C	3.63756916	-0.21599934	3.62019111
C	3.03487018	-2.53651494	3.07140910
C	3.65109816	3.21981730	0.09999515
C	1.84300133	-3.74172906	-1.54635077
C	3.84748814	2.84805022	1.45632110
C	2.03939130	-4.11349614	-0.19002481
H	2.50486924	1.92820660	-4.20256217
H	1.90217025	-0.39230901	-4.75134417
H	3.78831921	-0.50136983	4.66131450
H	3.18562022	-2.82188544	4.11253250
H	3.80704072	4.25312308	-0.20994251
H	4.15418076	3.59598548	2.18750695
H	1.53630870	-4.48966431	-2.27753662
H	1.88344874	-5.14680192	0.11991284
H	3.21110626	3.65051592	-2.51882250
H	4.14741623	1.87807703	3.94760494
H	1.54307323	-2.77175587	-4.03763461
H	2.47938320	-4.54419476	2.42879283
C	6.21704019	-2.41624618	0.08005912
C	6.22488702	-0.43258560	-1.95233568
C	6.56515787	-1.07652729	0.39686731
C	5.87284593	-2.76413479	-1.25294647

C	6.56908128	-0.08469699	-0.61933009
C	5.87676934	-1.77230450	-2.26914387
C	6.21311677	-3.40807648	1.09625653
C	6.90935213	-0.72863868	1.72987290
C	5.52472825	-4.10385369	-1.56975466
C	6.22881044	0.55924469	-2.96853308
C	6.91719896	1.25502191	-0.30252190
C	5.53257508	-2.12019311	-3.60214946
C	6.90542871	-1.72046897	2.74607030
C	5.52080483	-5.09568398	-0.55355725
C	6.92112238	2.24685220	-1.31871930
C	5.53649850	-1.12836282	-4.61834686
C	6.55731104	-3.06018791	2.42926216
C	5.86499910	-4.74779542	0.77944838
C	6.57692812	1.89896363	-2.65172493
C	5.88461618	0.21135612	-4.30153871
C	7.25746974	0.61108006	2.04668093
C	5.18053406	-4.45174214	-2.90276009
C	7.26139316	1.60291035	1.03048353
C	5.18445747	-3.45991184	-3.91895749
H	6.55429940	-3.82152239	3.20930097
H	5.86198746	-5.50912990	1.55948719
H	6.57993975	2.66029811	-3.43176374
H	5.88762781	0.97269061	-5.08157752
H	7.52167522	0.87812136	3.06990362
H	7.52861027	2.63128621	1.27366732
H	4.91331694	-5.48011800	-3.14594388

H	4.92025199	-3.72695314	-4.94218017
H	7.16963413	-1.45342788	3.76929288
H	7.18833943	3.27522794	-1.07553571
H	5.25358778	-6.12405973	-0.79674084
H	5.27229308	-1.39540391	-5.64156943
K	0.20465800	0.10074000	0.48149700

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n = 3, Energy = -342.650808225643 (12.0)

C	4.60620463	0.85898552	0.09312148
C	6.84874473	2.53630582	0.56557256
C	4.96716159	1.84718314	-0.86059526
C	5.36651772	0.70944806	1.28306376
C	6.08843164	2.68584329	-0.62436972
C	6.48778776	1.54810821	1.51928930
C	3.48493458	0.02032537	-0.14310407
C	4.20684851	1.99672060	-2.05053754
C	5.00556075	-0.27874956	2.23678050
C	7.97001478	3.37496597	0.80179811
C	6.44938861	3.67404090	-1.57808646
C	7.24810085	1.39857074	2.70923159
C	3.08557846	1.15806045	-2.28676309
C	3.88429070	-1.11740971	2.00055496
C	7.57065866	4.51270105	-1.34186092
C	8.36937090	2.23723089	2.94545713
C	2.72462145	0.16986280	-1.33304636
C	3.12397757	-0.96787228	0.81061266
C	8.33097179	4.36316362	-0.15191862

C	8.73032791	3.22542854	1.99174040
C	4.56780551	2.98491810	-3.00425408
C	5.76587380	-0.42828691	3.42672258
C	5.68907556	3.82357826	-2.76802853
C	6.88714385	0.41037324	3.66294812
H	1.86392828	-0.47389743	-1.51437441
H	2.26328441	-1.61163251	0.62928462
H	9.19166495	5.00692385	0.02940943
H	9.59102107	3.86918877	2.17306845
H	3.98418486	3.09970393	-3.91766057
H	5.96614817	4.58212438	-3.50010695
H	5.48880119	-1.18683303	4.15880100
H	7.47076450	0.29558741	4.57635461
H	2.50195780	1.27284613	-3.20016938
H	7.84773135	5.27124710	-2.07393912
H	3.60721801	-1.87595576	2.73263316
H	8.95299156	2.12244521	3.85886342
C	1.06257932	3.84028299	0.66650269
C	1.61970543	2.54638446	3.13247848
C	0.07467318	3.02514074	1.27967854
C	2.32904852	4.00847598	1.28631473
C	0.35323623	2.37819147	2.51266643
C	2.60761157	3.36152671	2.51930262
C	0.78401627	4.48723226	-0.56648521
C	-1.19179602	2.85694775	0.65986650
C	3.31695467	4.82361823	0.67313887
C	1.89826848	1.89943519	4.36546637



C	-0.63466992	1.56304922	3.12584229
C	3.87408077	3.52971970	3.13911466
C	-1.47035907	3.50389702	-0.57312140
C	3.03839162	5.47056750	-0.55984902
C	-0.35610687	0.91609995	4.35883018
C	4.15264382	2.88277043	4.37210256
C	-0.48245294	4.31903930	-1.18629730
C	1.77192241	5.30237454	-1.17966112
C	0.91036234	1.08429291	4.97864228
C	3.16473769	2.06762815	4.98527846
C	-2.17970195	2.04180559	1.27304235
C	4.58342365	4.99181112	1.29295091
C	-1.90113890	1.39485633	2.50603025
C	4.86198670	4.34486185	2.52593881
H	-0.69627950	4.81564118	-2.13274571
H	1.55809585	5.79897642	-2.12610952
H	1.12418890	0.58769103	5.92509069
H	3.37856425	1.57102627	5.93172687
H	-3.15185094	1.91269969	0.79727111
H	-2.65946130	0.76914849	2.97670752
H	5.34174605	5.61751896	0.82227364
H	5.83413569	4.47396776	3.00171005
H	-2.44250785	3.37479124	-1.04889269
H	-1.11442904	0.29039218	4.82950751
H	3.79671379	6.09627527	-1.03052635
H	5.12479260	3.01187621	4.84787385
C	-0.73439172	-1.90194833	-1.87629745

C	-1.77675543	-2.37094632	0.72353299
C	-0.03454932	-2.74389015	-0.97199956
C	-1.95541597	-1.29450551	-1.48068012
C	-0.55573118	-2.97838914	0.32791566
C	-2.47659783	-1.52900450	-0.18076490
C	-0.21320986	-1.66744934	-3.17621267
C	1.18647493	-3.35133297	-1.36761689
C	-2.65525837	-0.45256369	-2.38497801
C	-2.29793729	-2.60544531	2.02344820
C	0.14411122	-3.82033096	1.23221355
C	-3.69762208	-0.92156168	0.21485242
C	1.70765678	-3.11683398	-2.66753210
C	-2.13407651	-0.21806470	-3.68489323
C	-0.37707064	-4.05482995	2.53212877
C	-4.21880393	-1.15606067	1.51476764
C	1.00781441	-2.27489215	-3.57183005
C	-0.91305224	-0.82550751	-4.08051061
C	-1.59809491	-3.44738713	2.92774615
C	-3.51896156	-1.99800249	2.41906559
C	1.88631714	-4.19327465	-0.46331904
C	-3.87628243	0.15487899	-1.98936064
C	1.36513528	-4.42777364	0.83659617
C	-4.39746429	-0.07962000	-0.68944542
H	1.40787652	-2.09488941	-4.56965225
H	-0.51299013	-0.64550477	-5.07833281
H	-1.99815702	-3.62738987	3.92556835
H	-3.91902367	-2.17800523	3.41688778

H	2.82358232	-4.65955123	-0.76699714
H	1.90233831	-5.07405298	1.53074038
H	-4.41348546	0.80115834	-2.68350484
H	-5.33472947	0.38665658	-0.38576732
H	2.64492180	-3.58311041	-2.97121031
H	0.16013218	-4.70110916	3.22627298
H	-2.67127933	0.42821451	-4.37903744
H	-5.15606895	-0.68978423	1.81844584
K	0.20465800	0.10074000	0.48149700

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n = 3, Energy = -333.584116150996 (21.1)

C	-0.56281630	-0.67002053	-2.30873304
C	-3.35774867	-0.20827994	-2.10687121
C	-1.15964849	0.39884572	-3.02825813
C	-1.36345029	-1.50801648	-1.48827703
C	-2.55711467	0.62971601	-2.92732722
C	-2.76091648	-1.27714619	-1.38734611
C	0.83464989	-0.90089082	-2.40966395
C	-0.35901449	1.23684167	-3.84871414
C	-0.76661811	-2.57688273	-0.76875193
C	-4.75521485	0.02259035	-2.00594030
C	-3.15394686	1.69858226	-3.64685232
C	-3.56155047	-2.11514214	-0.56689010
C	1.03845169	1.00597138	-3.94964506
C	0.63084808	-2.80775302	-0.86968285
C	-4.55141304	1.92945255	-3.54592140
C	-4.95901666	-1.88427185	-0.46595919

C	1.63528394	-0.06289488	-3.23011996
C	1.43148213	-1.96975708	-1.69013886
C	-5.35204710	1.09145661	-2.72546539
C	-5.55584891	-0.81540559	-1.18548428
C	-0.95584670	2.30570773	-4.56823909
C	-1.56725208	-3.41487850	0.05170393
C	-2.35331288	2.53657802	-4.46730818
C	-2.96471827	-3.18400820	0.15263484
H	2.70798681	-0.24011221	-3.30759510
H	2.50418500	-2.14697441	-1.76761399
H	-6.42474996	1.26867393	-2.64799025
H	-6.62855177	-0.63818826	-1.10800915
H	-0.34127549	2.94895821	-5.19802581
H	-2.81144466	3.35704586	-5.01961975
H	-1.10912031	-4.23534633	0.60401550
H	-3.57928947	-3.82725869	0.78242156
H	1.65302294	1.64922166	-4.57943163
H	-5.00954490	2.74992021	-4.09823282
H	1.08897993	-3.62822068	-0.31737142
H	-5.57358790	-2.52752214	0.16382738
C	-2.85393079	4.61624350	4.06761682
C	-0.79375044	6.08318806	2.77559125
C	-1.54358416	4.63226335	4.61454930
C	-3.13418725	5.33369593	2.87467156
C	-0.51349398	5.36573563	3.96853652
C	-2.10409708	6.06716821	2.22865877
C	-3.88402097	3.88277122	4.71362961

C	-1.26332770	3.91481093	5.80749457
C	-4.44453389	5.31767607	2.32773908
C	0.23633973	6.81666034	2.12957846
C	0.79685265	5.38175549	4.51546900
C	-2.38435353	6.78462063	1.03571350
C	-2.29341788	3.18133864	6.45350736
C	-5.47462406	4.58420379	2.97375186
C	1.82694283	6.11522777	3.86945621
C	-1.35426336	7.51809292	0.38970072
C	-3.60376455	3.16531876	5.90657490
C	-5.19436765	3.86675133	4.16669716
C	1.54668641	6.83268023	2.67651092
C	-0.04391668	7.53411280	0.93663317
C	0.04701878	3.93083085	6.35442688
C	-4.72479019	6.03512843	1.13479398
C	1.07710896	4.66430313	5.70841409
C	-3.69470002	6.76860071	0.48878119
H	-4.39446754	2.60230133	6.40245793
H	-5.98507063	3.30373390	4.66258019
H	2.33738940	7.39569766	2.18062789
H	0.74678630	8.09713023	0.44075014
H	0.26214526	3.38011028	7.27013847
H	2.08293850	4.67660005	6.12824260
H	-5.73061974	6.02283151	0.71496547
H	-3.90982649	7.31932128	-0.42693040
H	-2.07829160	2.63061811	7.36921880
H	2.83277226	6.12752479	4.28928452

H	-6.48045350	4.57190677	2.55392355
H	-1.56938964	8.06881345	-0.52601073
C	-1.32059601	2.68934393	0.96969147
C	0.51968635	1.87062298	2.97185439
C	-1.75248174	1.85004346	2.03056353
C	0.03143090	3.11928393	0.90990088
C	-0.83234056	1.44068299	3.03164499
C	0.95157208	2.70992345	1.91098234
C	-2.24073719	3.09870441	-0.03138999
C	-3.10450865	1.42010347	2.09035412
C	0.46331663	3.95858440	-0.15097117
C	1.43982753	1.46126251	3.97293585
C	-1.26422629	0.60138252	4.09251704
C	2.30359899	3.13986345	1.85119175
C	-4.02464983	1.82946395	1.08927266
C	-0.45682455	4.36794487	-1.15205263
C	-0.34408511	0.19202204	5.09359850
C	3.22374017	2.73050297	2.85227321
C	-3.59276413	2.66876443	0.02840057
C	-1.80885150	3.93800490	-1.09226208
C	1.00794184	0.62196202	5.03380795
C	2.79185448	1.89120248	3.91314530
C	-3.53639420	0.58080312	3.15122607
C	1.81534337	4.38852427	-0.21076166
C	-2.61625302	0.17144265	4.15230753
C	2.73548455	3.97916379	0.79031980
H	-4.29906965	2.98299182	-0.74003517

H	-2.51515701	4.25223229	-1.86069781
H	1.71424736	0.30773463	5.80224368
H	3.49816000	1.57697509	4.68158103
H	-4.57421777	0.25077872	3.19712168
H	-2.94777099	-0.47280918	4.96663896
H	2.14686133	5.03277610	-1.02509309
H	3.77330811	4.30918820	0.74442419
H	-5.06247325	1.49943968	1.13516813
H	-0.67560287	-0.45222968	5.90792987
H	-0.12530679	5.01219660	-1.96638400
H	4.26156360	3.06052723	2.80637774
K	0.20465800	0.10074000	0.48149700

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n = 3, Energy = -314.581419843304 (40.1)

C	3.53960254	1.37196293	-0.80903850
C	3.51238773	1.23434793	2.02749477
C	4.57313944	0.68218472	-0.12171937
C	2.49245824	1.99293364	-0.07809099
C	4.55953203	0.61337722	1.29654726
C	2.47885083	1.92412614	1.34017564
C	3.55320995	1.44077043	-2.22730513
C	5.62028375	0.06121402	-0.85266688
C	1.45892134	2.68271184	-0.76541012
C	3.49878032	1.16554043	3.44576140
C	5.59306893	-0.07640098	1.98386639
C	1.43170652	2.54509684	2.07112315
C	5.63389116	0.13002152	-2.27093351

C	1.47252875	2.75151934	-2.18367675
C	5.57946152	-0.14520848	3.40213302
C	1.41809911	2.47628934	3.48938978
C	4.60035426	0.81979973	-2.95825270
C	2.51967305	2.13054864	-2.91462432
C	4.53231721	0.47576222	4.13308059
C	2.45163601	1.78651113	4.17670897
C	6.65382045	-0.62856406	-0.16534775
C	0.41177723	3.30368242	-0.03446261
C	6.64021304	-0.69737156	1.25291889
C	0.39816982	3.23487492	1.38380402
H	4.61079938	0.87261675	-4.04692210
H	2.53011818	2.18336566	-4.00329372
H	4.52187209	0.42294520	5.22174999
H	2.44119089	1.73369411	5.26537838
H	7.45761440	-1.10522472	-0.72642721
H	7.43356186	-1.22684925	1.78050895
H	-0.38157160	3.83316011	-0.56205268
H	-0.40562413	3.71153558	1.94488348
H	6.43768491	-0.34663901	-2.83201303
H	6.37281015	-0.67468605	3.92972315
H	0.67918012	3.28099691	-2.71126688
H	0.61430536	2.95294987	4.05046930
C	-0.49384540	-3.18099792	-1.29211774
C	-0.65840690	-3.47369227	1.52796188
C	-1.31494174	-2.30487789	-0.53408438
C	0.24497019	-4.20346513	-0.64011129



C	-1.39722249	-2.45122506	0.87595542
C	0.16268943	-4.34981230	0.76992852
C	-0.41156465	-3.03465075	-2.70215755
C	-2.05375732	-1.28241068	-1.18609084
C	1.06606652	-5.07958517	-1.39814464
C	-0.74068765	-3.62003944	2.93800169
C	-2.21831882	-1.57510503	1.63398878
C	0.90150502	-5.37227951	1.42193498
C	-1.97147657	-1.13606350	-2.59613064
C	1.14834727	-4.93323799	-2.80818445
C	-2.30059957	-1.72145220	3.04402859
C	0.81922427	-5.51862669	2.83197478
C	-1.15038023	-2.01218353	-3.35416406
C	0.40953169	-3.91077078	-3.46019096
C	-1.56178399	-2.74391941	3.69603510
C	-0.00187207	-4.64250666	3.59000820
C	-2.87485351	-0.40629083	-0.42805749
C	1.80488196	-6.10205219	-0.74613818
C	-2.95713426	-0.55263800	0.98198232
C	1.72260120	-6.24839936	0.66390163
H	-1.08722107	-1.89984662	-4.43651851
H	0.47269086	-3.79843387	-4.54254541
H	-1.62494316	-2.85625632	4.77838955
H	-0.06503123	-4.75484357	4.67236265
H	-3.44197257	0.37856084	-0.92854135
H	-3.58741249	0.11987674	1.56385303
H	2.43516019	-6.77456694	-1.32800889

H	2.28972027	-7.03325103	1.16438549
H	-2.53859548	-0.35121202	-3.09661457
H	-2.93087766	-1.04893764	3.62589935
H	1.77862536	-5.60575255	-3.39005521
H	1.38634318	-6.30347817	3.33245871
C	4.48007433	-3.67605429	0.37927486
C	6.11292750	-5.29909315	2.04214433
C	5.48119854	-4.50181360	-0.19715548
C	4.29537670	-3.66181441	1.78713994
C	6.29762513	-5.31333303	0.63427925
C	5.11180329	-4.47333384	2.61857468
C	3.66364774	-2.86453486	-0.45215988
C	5.66589617	-4.51605348	-1.60502057
C	3.29425248	-2.83605510	2.36357029
C	6.92935409	-6.11061257	2.87357907
C	7.29874935	-6.13909234	0.05784891
C	4.92710566	-4.45909395	4.02643976
C	4.84946958	-3.70453406	-2.43645530
C	2.47782589	-2.02453567	1.53213555
C	8.11517593	-6.95061177	0.88928364
C	5.74353225	-5.27061338	4.85787450
C	3.84834533	-2.87877471	-1.86002499
C	2.66252349	-2.03877552	0.12427043
C	7.93047834	-6.93637192	2.29714876
C	6.74465650	-6.09637273	4.28144419
C	6.66702027	-5.34181271	-2.18145072
C	3.10955497	-2.82181530	3.77143518

C	7.48344686	-6.15333214	-1.35001598
C	3.92598156	-3.63333472	4.60286991
H	3.22165171	-2.25584786	-2.49823895
H	2.03582987	-1.41584866	-0.51394352
H	8.55717196	-7.55929877	2.93536272
H	7.37135012	-6.71929958	4.91965815
H	6.80879524	-5.35274334	-3.26213598
H	8.25191551	-6.78718969	-1.79248722
H	2.34108632	-2.18795775	4.21390641
H	3.78420659	-3.62240410	5.68355518
H	4.99124440	-3.71546457	-3.51714041
H	8.88364451	-7.58446927	0.44681263
H	1.70935732	-1.39067817	1.97460656
H	5.60175743	-5.25968287	5.93855961
K	0.20465800	0.10074000	0.48149700

109

n = 3, Energy = -299.655875335568 (55.0)

C	-0.83965166	-2.56852344	1.61828503
C	0.89909277	-2.69796532	-0.62350268
C	0.56666199	-2.60448661	1.81164646
C	-1.37659309	-2.59728121	0.30402974
C	1.43603421	-2.66920755	0.69075261
C	-0.50722088	-2.66200215	-0.81686411
C	-1.70902387	-2.50380249	2.73917888
C	1.10360343	-2.57572884	3.12590175
C	-2.78290674	-2.56131804	0.11066830
C	1.76846499	-2.76268626	-1.74439653

C	2.84234786	-2.70517072	0.88411405
C	-1.04416231	-2.69075992	-2.13111940
C	0.23423121	-2.51100789	4.24679560
C	-3.65227896	-2.49659709	1.23156215
C	3.71172007	-2.76989166	-0.23677980
C	-0.17479009	-2.75548087	-3.25201325
C	-1.17208248	-2.47504472	4.05343422
C	-3.11533756	-2.46783932	2.54581749
C	3.17477868	-2.79864944	-1.55103514
C	1.23152359	-2.79144404	-3.05865186
C	2.50991689	-2.61169201	3.31926304
C	-3.31984799	-2.59007581	-1.20358684
C	3.37928910	-2.67641295	2.19836919
C	-2.45047577	-2.65479675	-2.32448069
H	-1.83941745	-2.42536456	4.91383861
H	-3.78267254	-2.41815916	3.40622188
H	3.84211366	-2.84832960	-2.41143953
H	1.89885857	-2.84112420	-3.91905626
H	2.92207621	-2.58961738	4.32809289
H	4.45878348	-2.70401848	2.34679455
H	-4.39934236	-2.56247028	-1.35201220
H	-2.86263510	-2.67687138	-3.33331054
H	0.64639031	-2.48893326	5.25562535
H	4.79121430	-2.79749720	-0.08835464
H	-4.73177318	-2.46899156	1.08313699
H	-0.58694919	-2.77755550	-4.26084300
C	-0.16858334	1.66509884	-2.18767759

C	0.40421253	3.12873530	0.17775530
C	1.17895910	1.91650329	-1.81710338
C	-1.22972785	2.14551263	-1.37553536
C	1.46535704	2.64832152	-0.63438693
C	-0.94332992	2.87733086	-0.19281892
C	-0.45498127	0.93328062	-3.37039403
C	2.24010361	1.43608951	-2.62924561
C	-2.57727029	1.89410818	-1.74610957
C	0.69061046	3.86055353	1.36047174
C	2.81289948	2.89972596	-0.26381272
C	-2.00447443	3.35774464	0.61932331
C	1.95370568	0.70427128	-3.81196205
C	-2.86366822	1.16228995	-2.92882601
C	3.09929741	3.63154419	0.91890372
C	-1.71807649	4.08956287	1.80203976
C	0.60616323	0.45286680	-4.18253631
C	-1.80252373	0.68187614	-3.74096829
C	2.03815291	4.11195801	1.73104600
C	-0.37053404	4.34096734	2.17261402
C	3.58764582	1.68749398	-2.25867135
C	-3.63841457	2.37452194	-0.93396738
C	3.87404376	2.41931220	-1.07595491
C	-3.35201664	3.10634017	0.24874906
H	0.38632257	-0.10888097	-5.09039607
H	-2.02236438	0.12012837	-4.64882805
H	2.25799357	4.67370577	2.63890576
H	-0.15069338	4.90271511	3.08047378

H	4.40218641	1.31872562	-2.88207635
H	4.90842503	2.61229168	-0.79150005
H	-4.67279584	2.18154246	-1.21842225
H	-4.16655723	3.47510852	0.87215406
H	2.76824603	0.33550292	-4.43536705
H	4.13367846	3.82452372	1.20335868
H	-3.89804927	0.96931042	-3.21328097
H	-2.53261684	4.45833123	2.42544476
C	4.11352929	-1.04453417	-6.38053581
C	5.75793362	-2.40058422	-4.50366017
C	3.90227345	-2.42391720	-6.11771740
C	5.14698729	-0.34317617	-5.70491640
C	4.72447562	-3.10194222	-5.17927958
C	5.96918946	-1.02120120	-4.76647858
C	3.29132713	-0.36650915	-7.31897363
C	2.86881545	-3.12527520	-6.79333682
C	5.35824313	1.03620685	-5.96773481
C	6.58013578	-3.07860925	-3.56522235
C	4.51321978	-4.48132525	-4.91646117
C	7.00264746	-0.31984320	-4.09085917
C	2.04661329	-2.44725017	-7.73177464
C	4.53604097	1.71423188	-6.90617263
C	5.33542194	-5.15935027	-3.97802335
C	7.82484962	-0.99786823	-3.15242135
C	2.25786909	-1.06786712	-7.99459309
C	3.50258293	1.01287391	-7.58179208
C	6.36887998	-4.45799230	-3.30240390

C	7.61359382	-2.37725128	-2.88960290
C	2.65755973	-4.50465802	-6.53051837
C	6.39170102	1.73756465	-5.29211544
C	3.47976189	-5.18268305	-5.59208054
C	7.21390318	1.05953962	-4.35367762
H	1.62674211	-0.54741131	-8.71494321
H	2.87145595	1.53332971	-8.30214221
H	7.00000696	-4.97844811	-2.58205378
H	8.24472080	-2.89770708	-2.16925277
H	1.86427148	-5.04302444	-7.04912767
H	3.31760069	-6.24150532	-5.39033965
H	6.55386222	2.79638693	-5.49385634
H	8.00719143	1.59790604	-3.83506831
H	1.25332512	-2.98561636	-8.25038394
H	5.17326089	-6.21817238	-3.77628237
H	4.69820202	2.77305398	-7.10791361
H	8.61813779	-0.45950204	-2.63381204
K	0.20465800	0.10074000	0.48149700

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n = 3, Energy = -274.322678445178 (80.3)

C	2.93571314	-4.16233797	4.36692695
C	4.05458915	-5.13172619	1.94329281
C	2.25152807	-5.15444041	3.61591191
C	4.17933622	-3.65492963	3.90612493
C	2.81096607	-5.63913452	2.40409483
C	4.73877422	-4.13962375	2.69430786
C	2.37627514	-3.67764385	5.57874403

C	1.00790499	-5.66184874	4.07671393
C	4.86352129	-2.66282719	4.65713998
C	4.61402716	-5.61642030	0.73147574
C	2.12678100	-6.63123697	1.65307979
C	5.98239730	-3.63221541	2.23350584
C	0.44846699	-5.17715463	5.28853100
C	4.30408329	-2.17813308	5.86895705
C	2.68621901	-7.11593108	0.44126271
C	6.54183530	-4.11690953	1.02168877
C	1.13265204	-4.18505216	6.03954610
C	3.06046019	-2.68554139	6.32975913
C	3.92984211	-6.60852277	-0.01953936
C	5.85765026	-5.10901199	0.27067367
C	0.32372011	-6.65395104	3.32569891
C	6.10714418	-2.15541900	4.19633793
C	0.88315811	-7.13864515	2.11388184
C	6.66658219	-2.64011312	2.98452086
H	0.70322430	-3.81299825	6.96974367
H	2.63103244	-2.31348748	7.25995669
H	4.35926985	-6.98057668	-0.94973693
H	6.28707800	-5.48106591	-0.65952390
H	-0.63089206	-7.04344058	3.67941316
H	0.35797373	-7.90018865	1.53739842
H	6.63232856	-1.39387551	4.77282135
H	7.62119435	-2.25062357	2.63080661
H	-0.50614501	-5.56664401	5.64224533
H	2.16103484	-7.87747445	-0.13522073



H	4.82926746	-1.41658971	6.44544050
H	7.49644731	-3.72742015	0.66797444
C	0.47571109	-1.87121788	2.85277653
C	2.55501593	-1.84098020	0.91856438
C	1.58873148	-1.00547482	3.02033149
C	0.40234313	-2.72184209	1.71811549
C	2.62838389	-0.99035598	2.05322542
C	1.44199554	-2.70672325	0.75100942
C	-0.56394132	-1.88633671	3.81988260
C	1.66209945	-0.15485061	4.15499252
C	-0.71067726	-3.58758514	1.55056053
C	3.59466834	-1.82586136	-0.04854169
C	3.74140428	-0.12461293	2.22078038
C	1.36862757	-3.55734747	-0.38365161
C	0.62244703	-0.16996945	5.12209860
C	-1.75032967	-3.60270398	2.51766660
C	4.78105669	-0.10949409	1.25367431
C	2.40827999	-3.54222863	-1.35075768
C	-0.49057340	-1.03571250	4.95454367
C	-1.67696175	-2.75207977	3.65232768
C	4.70768877	-0.96011831	0.11901324
C	3.52130042	-2.67648557	-1.18320276
C	2.77511972	0.71089228	4.32254736
C	-0.78404511	-4.43820919	0.41589962
C	3.81477213	0.72601112	3.35544129
C	0.25560730	-4.42309035	-0.55120645
H	-1.28861641	-1.04731781	5.69689971

H	-2.47500476	-2.76368507	4.39468371
H	5.50573178	-0.94851300	-0.62334280
H	4.31934343	-2.66488027	-1.92555879
H	2.83143740	1.36383629	5.19351964
H	4.66913292	1.39056043	3.48405745
H	-1.63840590	-5.10275851	0.28728346
H	0.19928962	-5.07603436	-1.42217873
H	0.67876456	0.48297439	5.99307079
H	5.63541741	0.55505506	1.38229031
H	-2.60469039	-4.26725313	2.38905061
H	2.35196246	-4.19517247	-2.22172987
C	3.40462432	-7.22848609	6.67266073
C	5.89327941	-6.21577020	5.75255101
C	3.96547139	-7.71528092	5.46233787
C	4.08810480	-6.23533331	7.42292873
C	5.20979893	-7.20892298	5.00228301
C	5.33243234	-5.72897537	6.96287387
C	2.16029678	-7.73484404	7.13271559
C	3.28199092	-8.70843370	4.71206986
C	3.52725773	-5.74853848	8.63325160
C	7.13760695	-5.70941225	5.29249615
C	5.77064600	-7.69571781	3.79196014
C	6.01591281	-4.73582259	7.71314187
C	2.03766338	-9.21479165	5.17212473
C	2.28293019	-6.25489643	9.09330646
C	7.01497354	-7.18935986	3.33190528
C	7.26024036	-4.22946464	7.25308701

C	1.47681626	-8.72799684	6.38244761
C	1.59944966	-7.24804923	8.34303848
C	7.69845407	-6.19620706	4.08217326
C	7.82108748	-4.71625945	6.04276413
C	3.84283800	-9.19522839	3.50174719
C	4.21073819	-4.75538584	9.38351941
C	5.08716554	-8.68887045	3.04169233
C	5.45506573	-4.24902790	8.92346455
H	0.52166347	-9.11668004	6.73558830
H	0.64429688	-7.63673242	8.69617916
H	8.65360685	-5.80752387	3.72903258
H	8.77624026	-4.32757625	5.68962344
H	3.31819450	-9.95757813	2.92583718
H	5.51767493	-9.06253695	2.11264159
H	3.78022880	-4.38171934	10.31257014
H	5.97970923	-3.48667816	9.49937456
H	1.51301984	-9.97714127	4.59621493
H	7.44548300	-7.56302620	2.40285471
H	1.85242073	-5.88123009	10.02235702
H	7.78488389	-3.46711502	7.82899681
K	0.20465800	0.10074000	0.48149700

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n = 4, Energy = -431.554716652857 (24.2)

C	0.51094066	-5.15112541	4.11200868
C	2.12467121	-6.31801363	2.08720125
C	1.90227846	-5.33308005	4.32988873
C	-0.07353186	-5.55261488	2.88172491

C	2.70914373	-5.91652416	3.31748502
C	0.73333341	-6.13605899	1.86932120
C	-0.29592461	-4.56768130	5.12441239
C	2.48675098	-4.93159058	5.56017250
C	-1.46486966	-5.37066023	2.66384486
C	2.93153648	-6.90145774	1.07479754
C	4.10048153	-6.09847880	3.53536508
C	0.14886088	-6.53754846	0.63903743
C	1.67988571	-4.34814647	6.57257622
C	-2.27173493	-4.78721612	3.67624857
C	4.90734680	-6.68192291	2.52296136
C	0.95572616	-7.12099257	-0.37336628
C	0.28854788	-4.16619180	6.35469620
C	-1.68726244	-4.38572663	4.90653238
C	4.32287431	-7.08341241	1.29267755
C	2.34706399	-7.30294723	-0.15548627
C	3.87808859	-5.11354524	5.77805242
C	-2.04934199	-5.77214968	1.43356123
C	4.68495386	-5.69698935	4.76564870
C	-1.24247672	-6.35559379	0.42115752
H	-0.33080642	-3.71833684	7.13182296
H	-2.30661674	-3.93787166	5.68365914
H	4.94222861	-7.53126737	0.51555079
H	2.96641829	-7.75080220	-0.93261303
H	4.32673305	-4.80535964	6.72242525
H	5.75295269	-5.83665877	4.93289469
H	-3.11734082	-5.63248027	1.26631524

H	-1.69112118	-6.66377939	-0.52321532
H	2.12852995	-4.03996086	7.51694895
H	5.97534547	-6.82159237	2.69020717
H	-3.33973360	-4.64754666	3.50900276
H	0.50708192	-7.42917817	-1.31773902
C	3.77794560	1.52296957	1.11583894
C	3.05946149	1.11097187	-1.60070998
C	4.61193922	0.74358703	0.27119844
C	2.58470992	2.09635326	0.60220498
C	4.25269717	0.53758818	-1.08707602
C	2.22546787	1.89035441	-0.75606948
C	4.13718765	1.72896842	2.47411339
C	5.80517489	0.17020334	0.78483240
C	1.75071630	2.87573580	1.44684548
C	2.70021944	0.90497303	-2.95898443
C	5.08669079	-0.24179436	-1.93171652
C	1.03223220	2.46373811	-1.26970344
C	6.16441695	0.37620218	2.14310685
C	2.10995835	3.08173465	2.80511993
C	4.72744874	-0.44779321	-3.28999097
C	0.67299014	2.25773926	-2.62797789
C	5.33042334	1.15558473	2.98774741
C	3.30319404	2.50835097	3.31875395
C	3.53421305	0.12559048	-3.80362499
C	1.50698375	1.47835671	-3.47261845
C	6.63916832	-0.60917907	-0.05980807
C	0.55748082	3.44911936	0.93321149

C	6.27992627	-0.81517792	-1.41808253
C	0.19823877	3.24312051	-0.42506297
H	5.60617955	1.31371060	4.03036648
H	3.57895025	2.66647683	4.36137302
H	3.25845684	-0.03253539	-4.84624406
H	1.23122754	1.32023084	-4.51523752
H	7.55510283	-1.04931167	0.33446027
H	6.92010454	-1.41343640	-2.06643338
H	-0.08269745	4.04737785	1.58156234
H	-0.71769574	3.68325311	-0.81933131
H	7.08035128	-0.06393028	2.53737528
H	5.36762680	-1.04605157	-3.93834185
H	1.46978029	3.67999301	3.45347081
H	-0.24294419	2.69787172	-3.02224632
C	5.15418992	-2.49066689	3.44253165
C	3.97187958	-3.24561266	0.97315953
C	5.94898201	-3.08576627	2.42736548
C	3.76824267	-2.27304039	3.22301175
C	5.35782683	-3.46323916	1.19267942
C	3.17708749	-2.65051327	1.98832570
C	5.74534510	-2.11319401	4.67721770
C	7.33492926	-3.30339277	2.64688537
C	2.97345058	-1.67794101	4.23817792
C	3.38072440	-3.62308554	-0.26152653
C	6.15261892	-4.05833854	0.17751326
C	1.79114024	-2.43288677	1.76880580
C	7.92608444	-2.92591989	3.88157143

C	3.56460576	-1.30046812	5.47286398
C	5.56146374	-4.43581142	-1.05717280
C	1.19998506	-2.81035965	0.53411974
C	7.13129238	-2.33082049	4.89673765
C	4.95055304	-1.51809461	5.69238392
C	4.17551646	-4.21818494	-1.27669275
C	1.99477712	-3.40545905	-0.48104647
C	8.12972114	-3.89849208	1.63171928
C	1.58750354	-1.46031458	4.01865795
C	7.53856596	-4.27596496	0.39703323
C	0.99634836	-1.83778747	2.78397189
H	7.58506640	-2.04107019	5.84448958
H	5.40432706	-1.22834431	6.64013585
H	3.72174244	-4.50793523	-2.22444467
H	1.54100310	-3.69520935	-1.42879840
H	9.19358216	-4.06554343	1.80022399
H	8.14865292	-4.73276664	-0.38221410
H	0.97741658	-1.00351290	4.79790528
H	-0.06751266	-1.67073612	2.61546719
H	8.98994527	-3.09297115	4.05007626
H	6.17155046	-4.89261304	-1.83642010
H	2.95451904	-0.84366651	6.25211128
H	0.13612423	-2.64330840	0.36561491
C	-3.05231120	2.34380372	-1.67287579
C	-2.62854664	-0.29805384	-0.72071418
C	-3.08921229	2.07714008	-0.27862729
C	-2.80352782	1.28953858	-2.59104349

C	-2.87733001	0.75621130	0.19745352
C	-2.59164554	-0.03139020	-2.11496268
C	-3.26419348	3.66473250	-2.14895659
C	-3.33799567	3.13140522	0.63954041
C	-2.76662673	1.55620222	-3.98529199
C	-2.41666435	-1.61898262	-0.24463337
C	-2.91423110	0.48954766	1.59170202
C	-2.34286217	-1.08565534	-3.03313038
C	-3.54987795	4.45233400	0.16345961
C	-2.97850901	2.87713100	-4.46137280
C	-2.70234882	-0.83138112	2.06778283
C	-2.13097989	-2.40658412	-2.55704957
C	-3.51297686	4.71899770	-1.23078892
C	-3.22729240	3.93139620	-3.54320512
C	-2.45356544	-1.88564632	1.14961515
C	-2.16788097	-2.67324782	-1.16280105
C	-3.37489673	2.86474150	2.03378869
C	-2.51784339	0.50193715	-4.90345946
C	-3.16301445	1.54381272	2.50986950
C	-2.30596110	-0.81899163	-4.42737866
H	-3.67561889	5.73295002	-1.59623121
H	-3.38993442	4.94534852	-3.90864741
H	-2.29092341	-2.89959864	1.51505744
H	-2.00523895	-3.68720014	-0.79735876
H	-3.56586427	3.67400143	2.73857947
H	-3.19133994	1.33912021	3.58010260
H	-2.48951789	0.70662967	-5.97369257



H	-2.11499357	-1.62825155	-5.13216944
H	-3.74084546	5.26159390	0.86825014
H	-2.73067428	-1.03607377	3.13801573
H	-2.95018356	3.08182364	-5.53160570
H	-1.94001237	-3.21584403	-3.26184011
K	0.20465800	0.10074000	0.48149700

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n = 4, Energy = -421.998077265752 (33.8)

C	-4.50479882	4.76931234	0.49363182
C	-1.99060025	6.08346514	0.62556920
C	-3.79613626	5.06774569	-0.70015836
C	-3.95636210	5.12795539	1.75339069
C	-2.53903698	5.72482209	-0.63418967
C	-2.69926281	5.78503178	1.81935937
C	-5.76189811	4.11223594	0.42766313
C	-4.34457299	4.70910265	-1.95991722
C	-4.66502466	4.82952203	2.94718086
C	-0.73350096	6.74054153	0.69153789
C	-1.83037442	6.02325544	-1.82797984
C	-2.15082608	6.14367483	3.07911824
C	-5.60167228	4.05202625	-2.02588591
C	-5.92212394	4.17244564	2.88121217
C	-0.57327513	6.68033184	-1.76201116
C	-0.89372680	6.80075123	3.14508693
C	-6.31033489	3.75359287	-0.83209574
C	-6.47056072	3.81380256	1.62145331
C	-0.02483835	7.03897491	-0.50225229

C	-0.18506418	7.09918461	1.95129675
C	-3.63591044	5.00753600	-3.15370716
C	-4.11658791	5.18816508	4.20693949
C	-2.37881116	5.66461240	-3.08773847
C	-2.85948863	5.84524147	4.27290818
H	-7.27529134	3.24921735	-0.88273367
H	-7.43551717	3.30942704	1.57081537
H	0.94011810	7.54335043	-0.45161435
H	0.77989227	7.60356013	2.00193469
H	-4.05689359	4.73223956	-4.12070526
H	-1.83483775	5.89369154	-4.00409863
H	-4.66056132	4.95908594	5.12329965
H	-2.43850548	6.12053791	5.23990628
H	-6.02265549	3.77672979	-2.99288377
H	-0.02930168	6.90941101	-2.67837108
H	-6.46609739	3.94336647	3.79757209
H	-0.47274358	7.07604769	4.11208479
C	-0.91472757	2.47578505	-1.10611618
C	-1.10255351	2.55284109	1.72661807
C	-2.05223760	1.92958263	-0.45486053
C	0.12886949	3.06051549	-0.34100471
C	-2.14615057	1.96811065	0.96150660
C	0.03495652	3.09904351	1.07536241
C	-0.82081461	2.43725703	-2.52248330
C	-3.09583467	1.34485219	-1.21997199
C	1.26637952	3.60671791	-0.99226036
C	-1.19646648	2.59136911	3.14298519

C	-3.28366060	1.42190823	1.61276225
C	1.07855358	3.68377395	1.84047388
C	-3.00192170	1.30632417	-2.63633912
C	1.36029248	3.56818989	-2.40862748
C	-3.37757357	1.46043625	3.02912937
C	0.98464062	3.72230197	3.25684100
C	-1.86441167	1.85252658	-3.28759483
C	0.31669543	2.98345944	-3.17373901
C	-2.33397651	2.04516669	3.79424090
C	-0.15286942	3.17609955	3.90809672
C	-4.23334448	0.79864988	-0.56871633
C	2.30997637	4.19144824	-0.22714891
C	-4.32725745	0.83717790	0.84765079
C	2.21606340	4.22997626	1.18921822
H	-1.79232355	1.82295226	-4.37480616
H	0.38878354	2.95388512	-4.26095034
H	-2.40606463	2.07474101	4.88145223
H	-0.22495754	3.20567387	4.99530805
H	-5.03441555	0.34980745	-1.15602024
H	-5.20041665	0.41790980	1.34755833
H	3.18313556	4.61071634	-0.72705644
H	3.01713447	4.67881868	1.77652213
H	-3.80299255	0.85748185	-3.22364308
H	-4.25073255	1.04116826	3.52903698
H	2.23345147	3.98745787	-2.90853509
H	1.78571147	4.17114429	3.84414496
C	-0.65627106	-6.06393579	2.10342138

C	1.00156602	-5.21012520	4.24542587
C	-1.23721840	-5.67511812	3.33943153
C	0.75359482	-6.02584816	1.93841347
C	-0.40829986	-5.24821283	4.41043377
C	1.58251336	-5.59894286	3.00941572
C	-1.48518959	-6.49084108	1.03241913
C	-2.64708428	-5.71320575	3.50443943
C	1.33454217	-6.41466582	0.70240333
C	1.83048456	-4.78321991	5.31642811
C	-0.98924720	-4.85939517	5.64644392
C	2.99237924	-5.56085523	2.84440781
C	-3.47600282	-6.14011105	2.43343719
C	0.50562363	-6.84157111	-0.36859892
C	-0.16032867	-4.43248988	6.71744616
C	3.82129778	-5.13394994	3.91541006
C	-2.89505551	-6.52892873	1.19742699
C	-0.90424229	-6.87965876	-0.20359106
C	1.24953725	-4.39440223	6.55243830
C	3.24035047	-4.74513226	5.15142025
C	-3.22803143	-5.32438812	4.74044944
C	2.74440785	-6.37657816	0.53739556
C	-2.39911289	-4.89748283	5.81145169
C	3.57332639	-5.94967286	1.60839780
H	-3.53133802	-6.85662362	0.37531968
H	-1.54052479	-7.20735365	-1.02569838
H	1.88581976	-4.06670734	7.37454562
H	3.87663298	-4.41743737	5.97352757

H	-4.31025252	-5.35362440	4.86711047
H	-2.84505140	-4.59902418	6.76022012
H	3.19034637	-6.67503681	-0.41137287
H	4.65554748	-5.92043659	1.48173678
H	-4.55822375	-6.16934737	2.56009803
H	-0.60626695	-4.13403124	7.66621451
H	0.95156191	-7.14002975	-1.31736726
H	4.90351871	-5.10471361	3.78874921
C	-2.04206064	-1.77461263	3.76994776
C	-0.82024997	-2.55921600	1.32921513
C	-0.62863608	-1.73614403	3.63898492
C	-2.84457986	-2.20538292	2.68054428
C	-0.01773075	-2.12844572	2.41861860
C	-2.23367453	-2.59768460	1.46017797
C	-2.65296597	-1.38231094	4.99031407
C	0.17388315	-1.30537374	4.72838839
C	-4.25800442	-2.24385152	2.81150712
C	-0.20934464	-2.95151769	0.10884882
C	1.39569381	-2.08997712	2.28765576
C	-3.03619376	-3.02845489	0.37077450
C	-0.43702219	-0.91307205	5.94875470
C	-4.86890975	-1.85154983	4.03187344
C	2.00659914	-2.48227880	1.06728945
C	-2.42528843	-3.42075658	-0.84959182
C	-1.85044677	-0.95154064	6.07971760
C	-4.06639055	-1.42077953	5.12127696
C	1.20407994	-2.91304911	-0.02211408

C	-1.01186384	-3.38228800	-0.98055471
C	1.58730749	-1.26690519	4.59742546
C	-5.06052343	-2.67462176	1.72210374
C	2.19821282	-1.65920687	3.37705914
C	-4.44961810	-3.06692345	0.50173743
H	-2.31938112	-0.65040767	7.01647761
H	-4.53532490	-1.11964656	6.05803698
H	1.67301429	-3.21418208	-0.95887409
H	-0.54292949	-3.68342097	-1.91731472
H	2.20332584	-0.93624346	5.43365777
H	3.28316557	-1.62967815	3.27653134
H	-6.14547618	-2.70415048	1.82263155
H	-5.06563645	-3.39758517	-0.33449488
H	0.17899592	-0.58241036	6.78498697
H	3.09155170	-2.45275014	0.96676150
H	-5.95386231	-1.88107849	4.13240139
H	-3.04130654	-3.75141828	-1.68582409
K	0.20465800	0.10074000	0.48149700

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n = 4, Energy = -409.646162080289 (46.1)

C	2.43227404	-9.26931579	-2.10934854
C	3.18291107	-9.47029787	0.62227181
C	3.76443440	-8.97486734	-1.71558598
C	1.47543219	-9.66425528	-1.13730093
C	4.13975292	-9.07535837	-0.34977580
C	1.85075071	-9.76474632	0.22850925
C	2.05695552	-9.16882475	-3.47515872

C	4.72127624	-8.57992784	-2.68763359
C	0.14327183	-9.95870374	-1.53106349
C	3.55822959	-9.57078891	1.98808199
C	5.47191328	-8.78090992	0.04398676
C	0.89390887	-10.15968582	1.20055686
C	4.34595772	-8.47943680	-4.05344377
C	-0.23204668	-9.85821270	-2.89687367
C	5.84723180	-8.88140096	1.40979694
C	1.26922739	-10.26017685	2.56636704
C	3.01379735	-8.77388525	-4.44720639
C	0.72479514	-9.46327320	-3.86892134
C	4.89038997	-9.27634045	2.38184461
C	2.60138777	-9.96572840	2.96012966
C	6.05343638	-8.28547945	-2.29387097
C	-0.81356979	-10.35364317	-0.55901594
C	6.42875490	-8.38597049	-0.92806079
C	-0.43825127	-10.45413420	0.80679424
H	2.72570075	-8.69674777	-5.49560992
H	0.43669855	-9.38613572	-4.91732488
H	5.17848656	-9.35347794	3.43024815
H	2.88948436	-10.04286589	4.00853319
H	6.78791365	-7.98232164	-3.04002025
H	7.45132879	-8.15995017	-0.62580642
H	-1.83614368	-10.57966348	-0.86127031
H	-1.17272854	-10.75729201	1.55294352
H	5.08043475	-8.17627906	-4.79959305
H	6.86980549	-8.65538071	1.71205142

H	-1.25462037	-10.08423295	-3.19912816
H	0.53475036	-10.56333460	3.31251632
C	-1.31615683	1.10442702	-3.54467220
C	-1.81491199	1.85382275	-0.85111529
C	-2.53696609	0.73637206	-2.91972391
C	-0.34472515	1.84717985	-2.82284203
C	-2.78634367	1.11106992	-1.57294546
C	-0.59410273	2.22187772	-1.47606358
C	-1.06677925	0.72972916	-4.89145066
C	-3.50839778	-0.00638078	-3.64155408
C	0.87608411	2.21523482	-3.44779032
C	-2.06428957	2.22852061	0.49566317
C	-4.00715293	0.74301495	-0.94799717
C	0.37732896	2.96463055	-0.75423341
C	-3.25902020	-0.38107864	-4.98833254
C	1.12546169	1.84053696	-4.79456878
C	-4.25653051	1.11771281	0.39878129
C	0.12795138	3.33932841	0.59254505
C	-2.03821093	-0.01302369	-5.61328088
C	0.15403002	1.09778411	-5.51639900
C	-3.28509884	1.86046566	1.12061151
C	-1.09285789	2.97127346	1.21749339
C	-4.72920683	-0.37443564	-3.01660578
C	1.84751558	2.95798755	-2.72596016
C	-4.97858440	0.00026223	-1.66982733
C	1.59813801	3.33268541	-1.37918171
H	-1.84678730	-0.30064386	-6.64707557



H	0.34545364	0.81016394	-6.55019369
H	-3.47652246	2.14808584	2.15440620
H	-1.28428152	3.25889364	2.25128808
H	-5.47488334	-0.94457695	-3.57068672
H	-5.91568456	-0.28225887	-1.19011347
H	2.78461574	3.24050865	-3.20567402
H	2.34381452	3.90282672	-0.82510077
H	-4.00469649	-0.95121986	-5.54241353
H	-5.19363047	0.83519184	0.87849521
H	2.06256165	2.12305794	-5.27428270
H	0.87362767	3.90946963	1.14662604
C	0.52768543	-2.38814062	-1.23136774
C	1.28174819	-2.58538657	1.49958134
C	-0.42771591	-2.78258225	-0.25770241
C	1.86011814	-2.09232196	-0.83955853
C	-0.05068452	-2.88120522	1.10777213
C	2.23714953	-2.19094494	0.52591601
C	0.15065404	-2.28951764	-2.59684228
C	-1.76014862	-3.07840090	-0.64951163
C	2.81551947	-1.69788033	-1.81322386
C	1.65877958	-2.68400955	2.86505588
C	-1.00608585	-3.27564686	2.08143746
C	3.56958224	-1.89512629	0.91772522
C	-2.13718000	-2.97977793	-2.01498617
C	2.43848809	-1.59925736	-3.17869840
C	-0.62905447	-3.37426983	3.44691200
C	3.94661362	-1.99374926	2.28319977

C	-1.18177869	-2.58533629	-2.98865155
C	1.10605536	-1.89507601	-3.57050767
C	0.70337826	-3.07845118	3.83872127
C	2.99121231	-2.38819090	3.25686515
C	-2.71554973	-3.47284247	0.32415365
C	4.14795197	-1.40206175	-1.42141459
C	-2.33851835	-3.57146544	1.68962819
C	4.52498335	-1.50068472	-0.05594005
H	-1.47119009	-2.50963274	-4.03679745
H	0.81664396	-1.81937246	-4.61865357
H	0.99278966	-3.15415473	4.88686717
H	3.28062371	-2.46389444	4.30501105
H	-3.73833269	-3.69991456	0.02339868
H	-3.07188987	-3.87424109	2.43701923
H	4.88132349	-1.09928610	-2.16880564
H	5.54776631	-1.27361263	0.24481492
H	-3.15996276	-3.20684995	-2.31574125
H	-1.36242576	-3.67704542	4.19430304
H	3.17185938	-1.29648177	-3.92608945
H	4.96939638	-1.76667724	2.58395485
C	1.80337894	-5.60022636	-2.51716347
C	1.13590638	-6.17509074	0.18276446
C	0.48217994	-5.99805854	-2.18165960
C	2.79084166	-5.48982637	-1.50270337
C	0.14844366	-6.28549073	-0.83169564
C	2.45710538	-5.77725856	-0.15273940
C	2.13711522	-5.31279417	-3.86712743

C	-0.50528278	-6.10845853	-3.19611971
C	4.11204065	-5.09199419	-1.83820723
C	0.80217010	-6.46252293	1.53272843
C	-1.17275533	-6.68332291	-0.49619177
C	3.44456810	-5.66685857	0.86172070
C	-0.17154650	-5.82102634	-4.54608367
C	4.44577693	-4.80456200	-3.18817120
C	-1.50649161	-6.97075510	0.85377219
C	3.11083182	-5.95429076	2.21168467
C	1.14965251	-5.42319415	-4.88158759
C	3.45831423	-4.91496198	-4.20263136
C	-0.51902891	-6.86035512	1.86823235
C	1.78963281	-6.35212295	2.54718859
C	-1.82648155	-6.50629066	-2.86061578
C	5.09950315	-4.98159425	-0.82374720
C	-2.16021783	-6.79372285	-1.51065181
C	4.76576687	-5.26902644	0.52621677
H	1.40583035	-5.20255959	-5.91782749
H	3.71449206	-4.69432742	-5.23887125
H	-0.77520674	-7.08098968	2.90447225
H	1.53345497	-6.57275751	3.58342849
H	-2.58446358	-6.59103433	-3.63932112
H	-3.17437772	-7.09910110	-1.25311715
H	6.11366304	-4.67621600	-1.08128186
H	5.52374890	-5.18428277	1.30492212
H	-0.92952829	-5.90576995	-5.32478901
H	-2.52065129	-7.27613331	1.11130698

H	5.45993661	-4.49918379	-3.44570598
H	3.86881361	-5.86954716	2.99039001
K	0.20465800	0.10074000	0.48149700

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C	-2.55193915	0.09832092	1.63228322
C	-2.38102094	2.50661132	2.10145711
C	-3.96031941	1.69426361	0.39995543
C	-1.96853359	1.17186695	2.35584174
C	-3.54783206	0.35951925	0.65434006
C	-3.78940120	4.10255402	0.86912932
C	-1.79761538	3.58015736	2.82501563
C	-4.95621233	1.95546194	-0.57798772
C	-2.13945179	-1.23642345	1.88666785
C	-0.97264067	0.91066862	3.33378489
C	-4.13123762	-0.71402679	-0.06921846
C	-2.21010273	4.91490172	2.57063100
C	-5.36869968	3.29020631	-0.83237236
C	-0.56015332	-0.42407574	3.58816952
C	-3.71875027	-2.04877115	0.18516617
C	-3.20599566	5.17610011	1.59268784
C	-4.78529414	4.36375240	-0.10881384
C	-1.14355886	-1.49762183	2.86461101
C	-2.72285734	-2.30996954	1.16310933
C	-0.80172262	3.31895895	3.80295862
C	-5.53961773	0.88191599	-1.30154608

C	-0.38923526	1.98421458	4.05734325
C	-5.12713038	-0.45282838	-1.04716145
H	-3.52262326	6.20065735	1.39742077
H	-5.10192174	5.38830965	-0.30408091
H	-0.82693126	-2.52217908	3.05987808
H	-2.40622974	-3.33452678	1.35837640
H	-0.35389717	4.14301899	4.35836628
H	0.37521782	1.78371727	4.80801800
H	-6.30407082	1.08241330	-2.05222083
H	-5.57495583	-1.27688843	-1.60256911
H	-1.76227745	5.73896175	3.12603849
H	0.20429963	-0.62457319	4.33884412
H	-6.13315263	3.49070375	-1.58304695
H	-4.16657554	-2.87283118	-0.37024132
C	3.24650928	-0.24225646	0.23380322
C	3.29426644	-0.24121523	3.07340138
C	2.74921386	-1.36132612	0.95267765
C	3.76768328	0.87733381	0.93472787
C	2.77309243	-1.36080550	2.37247673
C	3.79156186	0.87785442	2.35452695
C	3.22263070	-0.24277708	-1.18599586
C	2.22803985	-2.48091639	0.25175300
C	4.26497871	1.99640346	0.21585344
C	3.31814501	-0.24069461	4.49320045
C	2.27579701	-2.47987516	3.09135116
C	4.31273586	1.99744469	3.05545160
C	2.20416127	-2.48143700	-1.16804607

C	4.24110013	1.99588285	-1.20394564
C	2.29967559	-2.47935454	4.51115024
C	4.33661444	1.99796531	4.47525067
C	2.70145670	-1.36236735	-1.88692056
C	3.71992612	0.87629258	-1.90487034
C	2.82084959	-1.35976427	5.21207494
C	3.83931902	0.87889566	5.19412516
C	1.73074453	-3.59998582	0.97062743
C	4.78615261	3.11599352	0.91677809
C	1.75462311	-3.59946521	2.39042651
C	4.81003119	3.11651413	2.33657717
H	2.68312737	-1.36276698	-2.97676628
H	3.70159679	0.87589295	-2.99471606
H	2.83917892	-1.35936464	6.30192066
H	3.85764835	0.87929528	6.28397088
H	1.33068839	-4.45938971	0.43259369
H	1.37289630	-4.45846947	2.94223860
H	5.16787942	3.97499778	0.36496599
H	5.21008733	3.97591802	2.87461091
H	1.80410523	-3.34084067	-1.70607988
H	1.91794888	-3.33835858	5.06296239
H	4.62282684	2.85488689	-1.75575779
H	4.73667048	2.85736898	5.01328448
C	-1.16146819	-4.16035920	-4.03447609
C	-1.05762649	-5.88501059	-1.78050315
C	0.07556484	-4.73050107	-3.63311887
C	-2.34658037	-4.45254303	-3.30884684

C	0.12748569	-5.59282677	-2.50613240
C	-2.29465952	-5.31486873	-2.18186037
C	-1.21338903	-3.29803351	-5.16146256
C	1.26067702	-4.43831724	-4.35874812
C	-3.58361339	-3.88240117	-3.71020406
C	-1.00570564	-6.74733629	-0.65351669
C	1.36451872	-6.16296863	-2.10477518
C	-3.47977170	-5.60705256	-1.45623112
C	1.20875618	-3.57599155	-5.48573459
C	-3.63553424	-3.02007547	-4.83719053
C	1.41643956	-7.02529433	-0.97778872
C	-3.42785085	-6.46937825	-0.32924466
C	-0.02827685	-3.00584965	-5.88709186
C	-2.45042206	-2.72789161	-5.56281983
C	0.23132739	-7.31747819	-0.25215942
C	-2.19081782	-7.03952015	0.07211261
C	2.49770982	-5.00845908	-3.95739087
C	-4.76872534	-4.17458502	-2.98457484
C	2.54963066	-5.87078478	-2.83040440
C	-4.71680449	-5.03691072	-1.85758837
H	-0.06813159	-2.34392362	-6.75217298
H	-2.49027680	-2.06596558	-6.42790095
H	0.27118212	-7.97940422	0.61292170
H	-2.15096309	-7.70144618	0.93719373
H	3.40740869	-4.78417712	-4.51438801
H	3.49918428	-6.30842892	-2.52232033
H	-5.71827895	-3.73694088	-3.29265892

H	-5.62650337	-5.26119268	-1.30059124
H	2.11845482	-3.35170952	-6.04273174
H	2.36599295	-7.46293848	-0.66970456
H	-4.58508762	-2.58243132	-5.14527468
H	-4.33754949	-6.69366028	0.22775250
C	-1.34656302	4.51646891	-1.86180052
C	-3.45712737	3.66181905	-3.55906045
C	-1.37373539	3.18096333	-2.34355420
C	-2.37467283	5.42464956	-2.22867681
C	-2.42901756	2.75363841	-3.19218416
C	-3.42995500	4.99732463	-3.07730678
C	-0.29128084	4.94379384	-1.01317056
C	-0.34562558	2.27278269	-1.97667791
C	-2.34750046	6.76015513	-1.74692314
C	-4.51240955	3.23449413	-4.40769041
C	-2.45618993	1.41813283	-3.67393783
C	-4.45806481	5.90550528	-3.44418307
C	0.70965660	2.70010761	-1.12804794
C	-1.29221828	7.18748006	-0.89829318
C	-3.51147211	0.99080791	-4.52256779
C	-5.51334699	5.47818035	-4.29281303
C	0.73682901	4.03561321	-0.64629424
C	-0.26410843	6.27929943	-0.53141685
C	-4.53958196	1.89898854	-4.88944412
C	-5.54051940	4.14267476	-4.77456674
C	-0.37279805	0.93727733	-2.45843157
C	-3.37561017	7.66833556	-2.11379944



C	-1.42808022	0.50995240	-3.30706153
C	-4.43089234	7.24101063	-2.96242941
H	1.54686951	4.36363021	0.00511887
H	0.54593208	6.60731643	0.11999625
H	-5.34962247	1.57097153	-5.54085723
H	-6.35055990	3.81465775	-5.42597985
H	0.41638490	0.24015267	-2.17681524
H	-1.44893787	-0.51518930	-3.67685839
H	-3.35475252	8.69347726	-1.74400259
H	-5.22007529	7.93813529	-3.24404573
H	1.49883949	2.00298319	-0.84643157
H	-3.53232990	-0.03433359	-4.89236467
H	-1.27136049	8.21262156	-0.52849630
H	-6.30252988	6.17530477	-4.57442940
K	0.20465800	0.10074000	0.48149700

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C	-3.54827651	-1.81104661	0.83891611
C	-4.56539777	-4.37194349	1.52657231
C	-3.86402008	-2.11003971	2.19069613
C	-3.74109358	-2.79250195	-0.16903580
C	-4.37258070	-3.39048815	2.53452422
C	-4.24965420	-4.07295039	0.17479229
C	-3.03971589	-0.53059817	0.49508802
C	-3.67120301	-1.12858436	3.19864804
C	-3.42535001	-2.49350885	-1.52081582
C	-5.07395840	-5.65239193	1.87040040

C	-4.68832427	-3.68948124	3.88630424
C	-4.44247127	-5.05440573	-0.83315963
C	-3.16264239	0.15186408	2.85481995
C	-2.91678939	-1.21306041	-1.86464392
C	-5.19688490	-4.96992968	4.23013233
C	-4.95103190	-6.33485417	-0.48933153
C	-2.84689880	0.45085723	1.50303992
C	-2.72397230	-0.23160502	-0.85669201
C	-5.38970198	-5.95138508	3.22218043
C	-5.26677548	-6.63384732	0.86244850
C	-3.98694657	-1.42757753	4.55042783
C	-3.61816709	-3.47496413	-2.52876751
C	-4.49550719	-2.70802597	4.89425593
C	-4.12672772	-4.75541257	-2.18493941
H	-2.45652482	1.43373662	1.23911555
H	-2.33359832	0.75127437	-1.12061638
H	-5.78007596	-6.93426447	3.48610480
H	-5.65714946	-7.61672671	1.12637287
H	-3.83893909	-0.67420682	5.32413748
H	-4.73787375	-2.93753476	5.93188998
H	-3.37580054	-3.24545534	-3.56640156
H	-4.27473519	-5.50878328	-2.95864906
H	-3.01463488	0.90523477	3.62852936
H	-5.43925146	-5.19943859	5.26776617
H	-2.67442282	-0.98355150	-2.90227776
H	-5.09903940	-7.08822487	-1.26304094
C	-1.37059232	-6.84991959	0.92997195

C	-1.51246450	-6.06175127	3.65472194
C	-1.69532689	-7.80499384	1.92936212
C	-1.11679384	-5.50076118	1.29295678
C	-1.76626298	-7.41090968	3.29173711
C	-1.18772993	-5.10667701	2.65533177
C	-1.29965622	-7.24400375	-0.43240305
C	-1.94912537	-9.15415225	1.56637729
C	-0.79205926	-4.54568692	0.29356661
C	-1.58340060	-5.66766711	5.01709693
C	-2.09099756	-8.36598393	4.29112728
C	-0.93393145	-3.75751860	3.01831660
C	-1.87818928	-9.54823641	0.20400229
C	-0.72112317	-4.93977108	-1.06880838
C	-2.16193365	-7.97189977	5.65350227
C	-1.00486754	-3.36343444	4.38069159
C	-1.55345470	-8.59316218	-0.79538793
C	-0.97492164	-6.28892951	-1.43179327
C	-1.90813517	-6.62274134	6.01648715
C	-1.32960212	-4.31850868	5.38008181
C	-2.27385989	-10.10922628	2.56576739
C	-0.53826084	-3.19652873	0.65655150
C	-2.34479598	-9.71514212	3.92814239
C	-0.60919693	-2.80244457	2.01892649
H	-1.49900376	-8.89566339	-1.84115460
H	-0.92047070	-6.59143072	-2.47755994
H	-1.96258612	-6.32024014	7.06225382
H	-1.38405306	-4.01600747	6.42584848

H	-2.46867705	-11.14484798	2.28713819
H	-2.59406409	-10.44826258	4.69527997
H	-0.28899272	-2.46340828	-0.11058608
H	-0.41437977	-1.76682288	2.29755570
H	-2.07300638	-10.58385791	-0.07462703
H	-2.41120171	-8.70501999	6.42063984
H	-0.47185511	-4.20665087	-1.83594596
H	-0.81005044	-2.32781295	4.65932091
C	1.66116074	2.42020424	-1.39520851
C	0.15991602	3.40475791	0.80536366
C	0.28282659	2.72230105	-1.55437054
C	2.28887254	2.61038426	-0.13576040
C	-0.46779577	3.21457789	-0.45408445
C	1.53825017	3.10266110	0.96452568
C	2.41178311	1.92792740	-2.49549459
C	-0.34488520	2.53212103	-2.81381865
C	3.66720669	2.30828745	0.02340163
C	-0.59070634	3.89703475	1.90564974
C	-1.84612993	3.51667471	-0.61324648
C	2.16596197	3.29284112	2.22397379
C	0.40573716	2.03984420	-3.91410473
C	4.41782905	1.81601061	-1.07688446
C	-2.59675229	4.00895154	0.48703960
C	1.41533960	3.78511795	3.32425988
C	1.78407135	1.73774736	-3.75494275
C	3.79011729	1.62583057	-2.33633261
C	-1.96904053	4.19913158	1.74648776

C	0.03700542	4.08721479	3.16509790
C	-1.72321916	2.83421784	-2.97298054
C	4.29491829	2.49846748	1.28284960
C	-2.47384152	3.32649467	-1.87269445
C	3.54429593	2.99074431	2.38313568
H	2.36025327	1.35987291	-4.59952850
H	4.36629922	1.24795611	-3.18091837
H	-2.54522245	4.57700604	2.59107351
H	-0.53917651	4.46508924	4.00968365
H	-2.20505433	2.68823458	-3.93974008
H	-3.53185868	3.55838591	-1.99486815
H	5.35293544	2.26657624	1.40502330
H	4.02613109	3.13672757	3.34989523
H	-0.07609778	1.89386090	-4.88086418
H	-3.65476928	4.24084278	0.36486609
H	5.47584605	1.58411937	-0.95471094
H	1.89717455	3.93110125	4.29101933
C	2.51780378	-3.50878945	2.92763483
C	2.48675434	-5.54942982	0.95268614
C	2.65619457	-3.17093089	1.55537405
C	2.36388827	-4.86696819	3.31242127
C	2.64066985	-4.19125108	0.56789970
C	2.34836355	-5.88728837	2.32494693
C	2.53332850	-2.48846926	3.91510918
C	2.81011009	-1.81275216	1.17058761
C	2.22549747	-5.20482674	4.68468206
C	2.47122962	-6.56975000	-0.03478820

C	2.77906065	-3.85339252	-0.80436108
C	2.19444803	-7.24546711	2.70973337
C	2.82563481	-0.79243197	2.15806195
C	2.24102219	-4.18450656	5.67215640
C	2.76353593	-4.87371271	-1.79183543
C	2.17892331	-8.26578730	1.72225902
C	2.68724401	-1.13029048	3.53032278
C	2.39493771	-2.82632778	5.28737001
C	2.60962041	-6.23189149	-1.40704903
C	2.31731411	-7.92792878	0.34999820
C	2.94850085	-1.47489377	-0.20167301
C	2.07158199	-6.56300532	5.06946833
C	2.93297613	-2.49521395	-1.18914735
C	2.05605727	-7.58332550	4.08199398
H	2.69916088	-0.34708700	4.28831361
H	2.40685457	-2.04312429	6.04536084
H	2.59770355	-7.01509497	-2.16503986
H	2.30539724	-8.71113227	-0.40799264
H	3.06664728	-0.43234802	-0.49703729
H	3.03920569	-2.23587178	-2.24250255
H	1.96535243	-6.82234749	6.12282353
H	1.93791084	-8.62587124	4.37735827
H	2.94378120	0.25011365	1.86269788
H	2.86976546	-4.61437074	-2.84519050
H	2.13479266	-4.44384852	6.72551148
H	2.06077691	-9.30833292	2.01762310
K	0.20465800	0.10074000	0.48149700

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C	0.59498356	2.12693459	3.92603024
C	-1.08352369	0.37661108	3.51593090
C	-0.44105869	3.04930537	4.22975459
C	-2.11956594	1.29898186	3.81965526
C	1.30979330	-0.13178333	3.26539404
C	1.95225830	2.54091096	3.97921773
C	-1.40475619	-0.95973606	3.15901906
C	-2.83437569	3.55769979	4.48029145
C	-0.11982619	4.38565252	4.58666643
C	-3.47684068	0.88500550	3.76646777
C	2.98830055	1.61854018	3.67549337
C	-0.36871394	-1.88210684	2.85529471
C	-1.15586844	5.30802330	4.89039079
C	-4.51288293	1.80737628	4.07019212
C	2.66706809	0.28219299	3.31858152
C	0.98856085	-1.46813052	2.90848218
C	-2.51314323	4.89404697	4.83720331
C	-4.19165048	3.14372346	4.42710398
C	2.27349064	3.87725794	4.33612953
C	-2.76203077	-1.37371226	3.10583161
C	1.23744839	4.79962872	4.63985388
C	-3.79807302	-0.45134148	3.40955596
H	3.46233992	-0.42582398	3.08544100

H	1.78383268	-2.17614749	2.67534167
H	-3.30841506	5.60206395	5.07034382
H	-4.98692230	3.85174043	4.66024449
H	3.31534247	4.19502857	4.37695655
H	1.48402831	5.82541640	4.91382145
H	-3.00861069	-2.39949995	2.83186405
H	-4.83992485	-0.76911212	3.36872894
H	4.03015226	1.93631061	3.71632034
H	-0.90928873	6.33381086	5.16435832
H	-0.61529365	-2.90789440	2.58132717
H	-5.55473464	1.48960585	4.02936515
C	0.26565790	2.74830563	-1.25900397
C	-1.18716559	0.79289335	-2.71888966
C	-1.05020157	2.39563317	-0.85833443
C	0.85510562	2.12327196	-2.38961636
C	-1.77661331	1.41792703	-1.58827727
C	0.12869387	1.14556582	-3.11955920
C	0.99206964	3.72601177	-0.52906112
C	-1.63964928	3.02066684	0.27227796
C	2.17096508	2.47594443	-2.79028590
C	-1.91357734	-0.18481279	-3.44883251
C	-3.09247277	1.06525456	-1.18760773
C	0.71814159	0.52053214	-4.25017159
C	-0.91323754	3.99837298	1.00222080
C	2.89737682	3.45365057	-2.06034305
C	-3.81888452	0.08754842	-1.91755058
C	-0.00827015	-0.45717400	-4.98011444



C	0.40262195	4.35104549	0.60155129
C	2.30792913	4.07868428	-0.92973063
C	-3.22943683	-0.53748530	-3.04816300
C	-1.32412965	-0.80984650	-4.57944493
C	-2.95550856	2.66799435	0.67294735
C	2.76041261	1.85091078	-3.92089814
C	-3.68192031	1.69028821	-0.05699549
C	2.03400087	0.87320464	-4.65084098
H	0.96021967	5.10153819	1.16185951
H	2.86552686	4.82917699	-0.36942242
H	-3.78703455	-1.28797800	-3.60847121
H	-1.88172737	-1.56033921	-5.13975314
H	-3.40797201	3.14777375	1.54081187
H	-4.69198153	1.41957482	0.25056075
H	3.77047384	2.12162416	-4.22845438
H	2.48646432	0.39342524	-5.51870550
H	-1.36570077	4.47815240	1.87008520
H	-4.82894559	-0.18316503	-1.60999452
H	3.90743790	3.72436402	-2.36789911
H	0.44419308	-0.93695341	-5.84797883
C	0.69510481	-1.79807644	6.36508880
C	-0.81765325	0.42832985	7.27078057
C	-0.71936730	-1.88863536	6.45150533
C	1.35319789	-0.59431438	6.73151815
C	-1.47574633	-0.77543222	6.90435122
C	0.59681886	0.51888877	7.18436404
C	1.45148384	-2.91127959	5.91224292

C	-1.37746037	-3.09239743	6.08507598
C	2.76767000	-0.50375546	6.64510162
C	-1.57403228	1.54153300	7.72362645
C	-2.89021843	-0.86599114	6.99076775
C	1.25491193	1.72265083	7.55079339
C	-0.62108134	-4.20560058	5.63223010
C	3.52404903	-1.61695861	6.19225574
C	-3.64659746	0.24721201	7.44361363
C	0.49853290	2.83585398	8.00363927
C	0.79339080	-4.11504170	5.54581355
C	2.86595598	-2.82072072	5.82582637
C	-2.98850442	1.45097412	7.81004300
C	-0.91593924	2.74529511	8.09005582
C	-2.79193228	-3.18295622	6.17149254
C	3.42576287	0.70000648	7.01153095
C	-3.54831131	-2.06975308	6.62433842
C	2.66938384	1.81320963	7.46437683
H	1.37399158	-4.96954267	5.19820651
H	3.44655676	-3.67522168	5.47821933
H	-3.56910520	2.30547509	8.15765004
H	-1.49654001	3.59979607	8.43766286
H	-3.29708829	-4.10697084	5.89021928
H	-4.63406817	-2.13926664	6.69067224
H	4.51151973	0.76952004	6.94519713
H	3.17453986	2.73722425	7.74565009
H	-1.12623712	-5.12961512	5.35095685
H	-4.73235415	0.17769862	7.50994749

H	4.60980571	-1.54744522	6.12592188
H	1.00368869	3.75986852	8.28491252
C	2.28848551	-2.75236751	9.62243142
C	0.86167075	-5.08514411	8.85565082
C	0.87640588	-2.79976295	9.76450486
C	2.98715776	-3.87136037	9.09696768
C	0.16299850	-3.96615125	9.38111456
C	2.27375038	-5.03774867	8.71357738
C	3.00189289	-1.58597921	10.00582172
C	0.17773363	-1.68077009	10.28996860
C	4.39923739	-3.82396493	8.95489424
C	0.14826337	-6.25153241	8.47226053
C	-1.24908113	-4.01354669	9.52318800
C	2.97242263	-6.15674153	8.18811364
C	0.89114101	-0.51438179	10.67335890
C	5.11264477	-2.65757663	9.33828454
C	-1.96248851	-5.17993499	9.13979771
C	2.25901525	-7.32312983	7.80472335
C	2.30322067	-0.46698630	10.53128547
C	4.41397255	-1.53858372	9.86374829
C	-1.26381629	-6.29892790	8.61433395
C	0.84693559	-7.37052532	7.94679677
C	-1.23434580	-1.72816563	10.43204198
C	5.09790944	-4.94295768	8.42943057
C	-1.94775318	-2.89455393	10.04865168
C	4.38450206	-6.10934598	8.04604027
H	2.85083617	0.42833989	10.82557801

H	4.96158805	-0.64325753	10.15804083
H	-1.81143179	-7.19425409	8.32004141
H	0.29932010	-8.26585151	7.65250423
H	-1.77065062	-0.86922034	10.83539094
H	-3.03167356	-2.93093493	10.15770807
H	6.18182982	-4.90657669	8.32037418
H	4.92080688	-6.96829128	7.64269131
H	0.35483642	0.34456345	11.07670781
H	-3.04640872	-5.21631614	9.24885402
H	6.19656498	-2.62119548	9.22922823
H	2.79531984	-8.18207507	7.40137443
C	2.33262717	-3.01389711	0.18402165
C	3.21633823	-4.77121891	2.23255146
C	1.51687953	-4.10518242	0.58408691
C	3.59023034	-2.80127269	0.80822129
C	1.95873505	-4.98384332	1.60835181
C	4.03208587	-3.67993359	1.83248619
C	1.89077164	-2.13523621	-0.84024326
C	0.25927635	-4.31780684	-0.04011273
C	4.40597799	-1.70998738	0.40815603
C	3.65819375	-5.64987981	3.25681636
C	1.14298741	-6.07512864	2.00841708
C	5.28968904	-3.46730918	2.45668584
C	-0.18257917	-3.43914594	-1.06437764
C	3.96412246	-0.83132648	-0.61610888
C	1.58484293	-6.95378954	3.03268198
C	5.73154457	-4.34597008	3.48095074

C	0.63316845	-2.34786059	-1.46444294
C	2.70651927	-1.04395086	-1.24030856
C	2.84244613	-6.74116516	3.65688167
C	4.91579694	-5.43725543	3.88101605
C	-0.55647109	-5.40909203	0.35995255
C	5.66358096	-1.49736309	1.03235565
C	-0.11461556	-6.28775293	1.38421746
C	6.10543649	-2.37602399	2.05662055
H	0.29399768	-1.67339556	-2.25067441
H	2.36734850	-0.36948583	-2.02654003
H	3.18161690	-7.41563019	4.44311314
H	5.25496772	-6.11172045	4.66724752
H	-1.52181446	-5.57230376	-0.11918664
H	-0.74078812	-7.12542976	1.69130982
H	6.28975352	-0.65968626	0.72526329
H	7.07077986	-2.21281226	2.53575975
H	-1.14792236	-3.60235751	-1.54351685
H	0.95867060	-7.79146628	3.33977441
H	4.59029480	0.00635026	-0.92320130
H	6.69688776	-4.18275851	3.96008996
K	0.20465800	0.10074000	0.48149700

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n = 5, Energy = -529.520557401478 (27.2)

C	-1.81333729	-2.77400956	-0.63150358
C	-1.77340181	-2.80250331	2.20807258
C	-3.03223577	-2.82431141	0.09524005
C	-0.57447107	-2.73795458	0.06154087

C	-3.01226803	-2.83855829	1.51502813
C	-0.55450333	-2.75220145	1.48132895
C	-1.83330503	-2.75976269	-2.05129166
C	-4.27110199	-2.86036639	-0.59780440
C	0.64442740	-2.68765273	-0.66520276
C	-1.75343407	-2.81675018	3.62786066
C	-4.23116651	-2.88886014	2.24177176
C	0.68436288	-2.71614647	2.17437340
C	-4.29106973	-2.84611952	-2.01759248
C	0.62445966	-2.67340586	-2.08499084
C	-4.21119877	-2.90310701	3.66155984
C	0.70433062	-2.73039335	3.59416148
C	-3.07217125	-2.79581767	-2.74433617
C	-0.61440655	-2.70946084	-2.77803535
C	-2.97233255	-2.86705203	4.35460435
C	-0.51456785	-2.78069520	4.32090517
C	-5.49000022	-2.91066824	0.12893922
C	1.88329338	-2.65159776	0.02784170
C	-5.47003248	-2.92491511	1.54872731
C	1.90326112	-2.66584463	1.44762978
H	-3.08749860	-2.78488169	-3.83417345
H	-0.62973390	-2.69852486	-3.86787263
H	-2.95700520	-2.87798801	5.44444163
H	-0.49924051	-2.79163118	5.41074245
H	-6.44096101	-2.93834424	-0.40304563
H	-6.40566592	-2.96352710	2.10657984
H	2.81892681	-2.61298577	-0.53001084

H	2.85422190	-2.63816862	1.97961464
H	-5.24203027	-2.87379552	-2.54957740
H	-5.14683196	-2.94171899	4.21941244
H	1.56009286	-2.63479388	-2.64284343
H	1.65529117	-2.70271735	4.12614640
C	4.96745170	3.45637862	-2.57016569
C	3.73949353	5.49591353	-1.02161294
C	5.38896367	3.68384247	-1.23338301
C	3.93196064	4.24868223	-3.13267199
C	4.77498459	4.70360992	-0.45910664
C	3.31798156	5.26844969	-2.35839562
C	5.58143078	2.43661117	-3.34444206
C	6.42445472	2.89153886	-0.67087670
C	3.51044867	4.02121838	-4.46945467
C	3.12551445	6.51568099	-0.24733657
C	5.19649656	4.93107377	0.87767604
C	2.28249050	6.06075329	-2.92090193
C	7.03843381	1.87177141	-1.44515308
C	4.12442775	3.00145093	-5.24373105
C	4.58251748	5.95084123	1.65195242
C	1.66851142	7.08052075	-2.14662555
C	6.61692186	1.64430752	-2.78193579
C	5.15991883	2.20914728	-4.68122477
C	3.54702639	6.74314488	1.08944614
C	2.09002337	7.30798464	-0.80984284
C	6.84596656	3.11900276	0.66590579
C	2.47495775	4.81352194	-5.03196080

C	6.23198747	4.13877022	1.44018217
C	1.86097867	5.83328939	-4.25768442
H	7.08821564	0.86152831	-3.37627467
H	5.63121261	1.42636807	-5.27556365
H	3.07573261	7.52592408	1.68378502
H	1.61872959	8.09076384	-0.21550396
H	7.64081539	2.51082601	1.09768886
H	6.55554248	4.31337275	2.46630417
H	2.15140275	4.63891940	-6.05808280
H	1.06612983	6.44146615	-4.68946749
H	7.83328253	1.26359466	-1.01337023
H	4.90607232	6.12544386	2.67807427
H	3.80087291	2.82684830	-6.26985290
H	0.87366270	7.68869749	-2.57840840
C	-5.94844515	0.35851405	2.06688653
C	-3.69222888	0.76919123	3.74212739
C	-4.73956277	0.86302379	1.51873201
C	-6.02921940	0.05934290	3.45266148
C	-3.61145463	1.06836238	2.35635243
C	-4.90111127	0.26468149	4.29028191
C	-7.07655329	0.15317546	1.22926610
C	-4.65878852	1.16219494	0.13295705
C	-7.23810179	-0.44516683	4.00081601
C	-2.56412075	0.97452982	4.57974781
C	-2.40257225	1.57287211	1.80819791
C	-4.98188552	-0.03448966	5.67605687
C	-5.78689665	0.95685635	-0.70466338



C	-8.36620992	-0.65050542	3.16319558
C	-1.27446412	1.77821070	2.64581834
C	-3.85377739	0.17084893	6.51367729
C	-6.99577908	0.45234660	-0.15650889
C	-8.28543572	-0.35133428	1.77742059
C	-1.35523832	1.47903956	4.03159332
C	-2.64489495	0.67535868	5.96552280
C	-3.44990626	1.66670460	-0.41519729
C	-7.31887591	-0.74433790	5.38659077
C	-2.32179812	1.87204318	0.42242314
C	-6.19076778	-0.53899932	6.22421120
H	-7.86172120	0.29472755	-0.79947101
H	-9.15137783	-0.50895333	1.13445846
H	-0.48929620	1.63665861	4.67455545
H	-1.77895284	0.83297773	6.60848493
H	-3.38790346	1.89635008	-1.47892604
H	-1.39385312	2.25930774	0.00165659
H	-8.24682092	-1.13160246	5.80735733
H	-6.25277057	-0.76864480	7.28793996
H	-5.72489403	1.18650175	-1.76839198
H	-0.34651919	2.16547518	2.22505200
H	-9.29415485	-1.03776990	3.58396192
H	-3.91578001	-0.05879647	7.57740590
C	-3.92102005	5.00938979	1.29044184
C	-3.94621221	4.43139501	4.07088909
C	-5.09427130	4.48728421	1.89648421
C	-2.76036488	5.24249798	2.07462309

C	-5.10686737	4.19828683	3.28670784
C	-2.77296096	4.95350059	3.46484671
C	-3.90842397	5.29838718	-0.09978179
C	-6.25492646	4.25417603	1.11230296
C	-1.58711364	5.76460355	1.46858071
C	-3.95880828	4.14239763	5.46111271
C	-6.28011862	3.67618125	3.89275021
C	-1.61230579	5.18660878	4.24902796
C	-6.24233038	4.54317341	-0.27792066
C	-1.57451756	6.05360094	0.07835709
C	-6.29271470	3.38718386	5.28297384
C	-1.62490187	4.89761139	5.63925159
C	-5.06907914	5.06527900	-0.88396309
C	-2.73517273	5.82049276	-0.70582422
C	-5.13205953	3.62029204	6.06715515
C	-2.79815312	4.37550580	6.24529402
C	-7.42817748	3.73207052	1.71834536
C	-0.42645870	5.99771167	2.25276194
C	-7.44077356	3.44307314	3.10856898
C	-0.43905478	5.70871428	3.64298557
H	-5.05941032	5.28711501	-1.95110653
H	-2.72550391	6.04232878	-1.77296765
H	-5.14172835	3.39845603	7.13429858
H	-2.80782194	4.15366979	7.31243746
H	-8.31910302	3.55313534	1.11640337
H	-8.34136792	3.04230192	3.57377055
H	0.47413566	6.39848289	1.78756038

H	0.45187076	5.88764946	4.24492755
H	-7.13325569	4.36423832	-0.87986269
H	-7.19330883	2.98641271	5.74817548
H	-0.67392343	6.45437210	-0.38684456
H	-0.73397656	5.07654649	6.24119361
C	2.87859686	-0.03061497	-3.05985157
C	2.97654813	1.14959862	-0.47855327
C	3.80939161	-0.50397355	-2.09758713
C	1.99677774	1.03285040	-2.73146686
C	3.85836725	0.08613324	-0.80693798
C	2.04575338	1.62295720	-1.44081771
C	2.82962122	-0.62072177	-4.35050072
C	4.69121073	-1.56743893	-2.42597184
C	1.06598299	1.50620898	-3.69373131
C	3.02552377	1.73970542	0.81209588
C	4.78916200	-0.38722534	0.15532647
C	1.16393426	2.68642258	-1.11243300
C	4.64223509	-2.15754573	-3.71662099
C	1.01700735	0.91610218	-4.98438046
C	4.83813764	0.20288146	1.44597562
C	1.21290990	3.27652937	0.17821615
C	3.71144033	-1.68418717	-4.67888549
C	1.89882646	-0.14736322	-5.31276522
C	3.95631853	1.26634686	1.77436038
C	2.14370466	2.80317082	1.14048065
C	5.62200530	-2.04079736	-1.46370745
C	0.18416405	2.56967421	-3.36534654

C	5.67098094	-1.45069056	-0.17305830
C	0.23313969	3.15978101	-2.07469739
H	3.67384636	-2.13715645	-5.66959500
H	1.86123249	-0.60033250	-6.30347473
H	3.99391250	1.71931614	2.76506989
H	2.18129863	3.25614010	2.13119016
H	6.29889469	-2.85711945	-1.71577741
H	6.38546431	-1.81404332	0.56558136
H	-0.53031932	2.93302697	-4.10398620
H	-0.44374970	3.97610309	-1.82262743
H	5.31912430	-2.97386769	-3.96869106
H	5.55262083	-0.16047112	2.18461527
H	0.30252416	1.27945477	-5.72302011
H	0.53602069	4.09285134	0.43028622
K	0.20465800	0.10074000	0.48149700

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n = 5, Energy = -523.823377411255 (32.9)

C	4.07539524	5.08868423	-1.97871668
C	4.42242594	4.75092892	0.81969189
C	3.22723795	5.77531709	-1.07011084
C	5.09706789	4.23317371	-1.48811824
C	3.40075330	5.60643944	0.32909345
C	5.27058324	4.06429606	-0.08891395
C	3.90187989	5.25756188	-3.37792097
C	2.20556530	6.63082761	-1.56070928
C	5.94522519	3.54654084	-2.39672409
C	4.59594129	4.58205127	2.21889618

C	2.55259600	6.29307231	1.23769929
C	6.29225589	3.20878554	0.40168449
C	2.03204995	6.79970526	-2.95991357
C	5.77170984	3.71541849	-3.79592838
C	2.72611135	6.12419466	2.63690358
C	6.46577124	3.03990789	1.80088878
C	2.88020724	6.11307240	-3.86851947
C	4.75003718	4.57092902	-4.28652688
C	3.74778400	5.26868413	3.12750208
C	5.61761395	3.72654075	2.70949468
C	1.35740818	7.31746033	-0.65210348
C	6.96689766	2.69103048	-1.90612560
C	1.53092353	7.14858267	0.74710081
C	7.14041301	2.52215282	-0.50692132
H	2.74701588	6.24270383	-4.94255652
H	4.61684583	4.70056045	-5.36056392
H	3.88097536	5.13905270	4.20153913
H	5.75080530	3.59690932	3.78353172
H	0.57316642	7.97415508	-1.02868962
H	0.87987314	7.67564599	1.44455183
H	7.61794804	2.16396716	-2.60357662
H	7.92465476	1.86545807	-0.13033517
H	1.24780836	7.45639987	-3.33649981
H	2.07506115	6.65125781	3.33435462
H	6.42276004	3.18835534	-4.49337941
H	7.25001282	2.38321328	2.17747502
C	-1.02335396	-2.34440201	-1.18376943

C	-2.02188710	-3.73420373	1.08272175
C	-2.42316034	-2.51112809	-1.01305152
C	-0.12281415	-2.87257679	-0.22124175
C	-2.92242690	-3.20602895	0.12019407
C	-0.62208072	-3.56747765	0.91200384
C	-0.52408740	-1.64950115	-2.31701502
C	-3.32370014	-1.98295331	-1.97557920
C	1.27699222	-2.70585071	-0.39195966
C	-2.52115366	-4.42910459	2.21596734
C	-4.32223328	-3.37275503	0.29091198
C	0.27845909	-4.09565243	1.87453152
C	-2.82443358	-1.28805245	-3.10882479
C	1.77625879	-2.01094985	-1.52520525
C	-4.82149984	-4.06765589	1.42415757
C	-0.22080748	-4.79055329	3.00777711
C	-1.42462718	-1.12132634	-3.27954274
C	0.87571900	-1.48277504	-2.48773298
C	-3.92096006	-4.59583070	2.38668530
C	-1.62061388	-4.95727940	3.17849507
C	-4.72350630	-2.14967942	-1.80486121
C	2.17753180	-3.23402545	0.57056794
C	-5.22277286	-2.84458028	-0.67161562
C	1.67826524	-3.92892632	1.70381353
H	-1.04138737	-0.58791655	-4.14942840
H	1.25895881	-0.94936525	-3.35761863
H	-4.30419987	-5.12924049	3.25657096
H	-2.00385369	-5.49068919	4.04838072

H	-5.41476580	-1.74424946	-2.54370293
H	-6.29727222	-2.97256017	-0.54057159
H	3.25203116	-3.10604557	0.43952392
H	2.36952475	-4.33435628	2.44265526
H	-3.51569284	-0.88262249	-3.84766648
H	-5.89599900	-4.19563584	1.55520172
H	2.85075794	-1.88296990	-1.65624940
H	0.47045178	-5.19598325	3.74661881
C	3.03073406	1.34617038	-0.26735240
C	2.97646994	1.33073556	-3.10679190
C	3.95025273	0.54139258	-0.99069063
C	2.08408333	2.14323077	-0.96373392
C	3.92312067	0.53367517	-2.41041038
C	2.05695127	2.13551336	-2.38345367
C	3.05786612	1.35388779	1.15236735
C	4.89690345	-0.25566781	-0.29430911
C	1.16456467	2.94800856	-0.24039569
C	2.94933788	1.32301815	-4.52651165
C	4.84263933	-0.27110262	-3.13374861
C	1.11030055	2.93257374	-3.07983519
C	4.92403551	-0.24795040	1.12541064
C	1.19169673	2.95572597	1.17932407
C	4.81550727	-0.27882003	-4.55346836
C	1.08316849	2.92485634	-4.49955494
C	4.00451684	0.55682740	1.84874893
C	2.13834745	2.15866558	1.87570564
C	3.86885655	0.51824036	-5.24984994

C	2.00268716	2.12007854	-5.22289323
C	5.81642194	-1.06044545	-1.01764734
C	0.21791412	3.74506879	-0.93677721
C	5.78928988	-1.06816285	-2.43736709
C	0.19078206	3.73735139	-2.35649696
H	4.02534356	0.56275133	2.93853376
H	2.15917417	2.16458951	2.96549047
H	3.84802983	0.51231643	-6.33963477
H	1.98186044	2.11415461	-6.31267806
H	6.54307644	-1.67227355	-0.48310093
H	6.49511766	-1.68591489	-2.99260563
H	-0.48791366	4.36282083	-0.38153867
H	-0.53587244	4.34917949	-2.89104337
H	5.65068983	-0.85977835	1.65995711
H	5.52133487	-0.89657191	-5.10870696
H	0.48586913	3.57347785	1.73456266
H	0.35651417	3.53668429	-5.03410141
C	4.13816266	-2.19565816	5.75214281
C	6.22131847	-2.64417114	3.87467178
C	4.23090200	-3.44247038	5.07889784
C	5.08700122	-1.17310243	5.48665226
C	5.27247990	-3.66672687	4.14016233
C	6.12857913	-1.39735892	4.54791674
C	3.09658475	-1.97140167	6.69087832
C	3.28206343	-4.46502611	5.34438840
C	4.99426188	0.07370979	6.15989722
C	7.26289638	-2.86842763	2.93593626



C	5.36521924	-4.91353909	3.46691736
C	7.07741770	-0.37480319	4.28242619
C	2.24048552	-4.24076962	6.28312391
C	3.95268398	0.29796628	7.09863274
C	6.40679715	-5.13779558	2.52818185
C	8.11899560	-0.59905968	3.34369067
C	2.14774614	-2.99395739	6.95636892
C	3.00384537	-0.72458944	7.36412333
C	7.35563576	-4.11523986	2.26269126
C	8.21173499	-1.84587191	2.67044567
C	3.37480285	-5.71183811	4.67114347
C	5.94310037	1.09626530	5.89440663
C	4.41638076	-5.93609460	3.73240795
C	6.98467827	0.87200881	4.95567111
H	1.34822511	-2.82181685	7.67694755
H	2.20432434	-0.55244890	8.08470196
H	8.15515679	-4.28738039	1.54211262
H	9.01125602	-2.01801245	1.94986703
H	2.64646897	-6.49675773	4.87493552
H	4.48756799	-6.89315477	3.21562129
H	5.87191313	2.05332547	6.41119329
H	7.71301216	1.65692843	4.75187906
H	1.51215168	-5.02568901	6.48691604
H	6.47798451	-6.09485554	2.01139518
H	3.88149662	1.25502624	7.61541940
H	8.84732945	0.18585971	3.13989854
C	-1.10619654	1.94553530	3.64115550

C	-1.94427741	4.45152904	2.60037917
C	-1.98529813	1.99345327	2.52702609
C	-0.64613539	3.15061420	4.23489675
C	-2.40433857	3.24645014	2.00663793
C	-1.06517582	4.40361107	3.71450858
C	-0.68715611	0.69253843	4.16154367
C	-2.44535929	0.78837438	1.93328485
C	0.23296620	3.10269622	5.34902616
C	-2.36331785	5.70452591	2.07999101
C	-3.28344016	3.29436812	0.89250852
C	-0.60511467	5.60868996	4.30824983
C	-2.02631885	-0.46462249	2.45367301
C	0.65200663	1.84969936	5.86941432
C	-3.70248059	4.54736498	0.37212036
C	-1.02415511	6.86168683	3.78786167
C	-1.14721725	-0.51254051	3.56780244
C	0.19194550	0.64462041	5.27567310
C	-3.24241945	5.75244393	0.96586158
C	-1.90325671	6.90960485	2.67373224
C	-3.32446075	0.83629246	0.81915560
C	0.69302722	4.30777501	5.94276724
C	-3.74350118	2.08928933	0.29876744
C	0.27398679	5.56077188	5.42237907
H	-0.82555946	-1.47434792	3.96725531
H	0.51360328	-0.31718700	5.67512596
H	-3.56407724	6.71425134	0.56640871
H	-2.22491449	7.87141226	2.27427937

H	-3.67760632	-0.08873296	0.36339642
H	-4.41830457	2.12607142	-0.55644465
H	1.36783062	4.27099292	6.79797933
H	0.62713236	6.48579730	5.87813825
H	-2.37946428	-1.38964785	1.99791402
H	-4.37728387	4.58414724	-0.48309159
H	1.32680991	1.81291710	6.72462627
H	-0.67100968	7.78671219	4.24362066
K	0.20465800	0.10074000	0.48149700

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n = 5, Energy = -497.943021858099 (58.8)

C	-0.60160585	2.89855192	1.38222931
C	0.61859122	1.20951481	3.31196303
C	0.81248913	2.87062434	1.50854447
C	-1.40560229	2.08196093	2.22078101
C	1.42258766	2.02610579	2.47341133
C	-0.79550376	1.23744238	3.18564788
C	-1.21170438	3.74307047	0.41736244
C	1.61648557	3.68721533	0.66999276
C	-2.81969727	2.10988851	2.09446585
C	1.22868975	0.36499625	4.27682990
C	2.83668264	1.99817821	2.59972649
C	-1.59950020	0.42085140	4.02419958
C	1.00638704	4.53173388	-0.29487410
C	-3.42979581	2.95440706	1.12959899
C	3.44678118	1.15365966	3.56459335
C	-0.98940167	-0.42366716	4.98906645

C	-0.40770797	4.55966149	-0.42118930
C	-2.62579939	3.77099808	0.29104724
C	2.64278476	0.33706864	4.40314510
C	0.42469333	-0.45159477	5.11538164
C	3.03058034	3.65928768	0.79630799
C	-3.62369350	1.29329760	2.93301749
C	3.64067887	2.81476912	1.76117485
C	-3.01359497	0.44877905	3.89788435
H	-0.87602302	5.20791866	-1.16182651
H	-3.09411444	4.41925525	-0.44958996
H	3.11109981	-0.31118853	5.14378230
H	0.89300838	-1.09985194	5.85601885
H	3.64773261	4.28610756	0.15263092
H	4.72614624	2.79333177	1.85813507
H	-4.70916087	1.31473495	2.83605727
H	-3.63074724	-0.17804084	4.54156142
H	1.62353907	5.15855373	-0.93855114
H	4.53224836	1.13222219	3.66155368
H	-4.51526299	2.97584453	1.03263866
H	-1.60655370	-1.05048701	5.63274348
C	-0.89417922	-1.77990026	-1.62998663
C	-0.40639925	-2.89469372	0.93612050
C	-1.92824818	-1.80151948	-0.65703541
C	0.38377972	-2.31567777	-1.31988428
C	-1.68435820	-2.35891621	0.62601815
C	0.62766971	-2.87307450	-0.03683072
C	-1.13806921	-1.22250354	-2.91304019

C	-3.20620713	-1.26574197	-0.96713776
C	1.41784869	-2.29405856	-2.29283550
C	-0.16250926	-3.45209044	2.21917406
C	-2.71842716	-2.38053542	1.59896937
C	1.90562866	-3.40885201	0.27327163
C	-3.45009712	-0.70834525	-2.25019132
C	1.17395870	-1.73666183	-3.57588906
C	-2.47453717	-2.93793215	2.88202293
C	2.14951865	-3.96624873	1.55632519
C	-2.41602817	-0.68672601	-3.22314259
C	-0.10400026	-1.20088430	-3.88599146
C	-1.19657821	-3.47370968	3.19212533
C	1.11544970	-3.98786797	2.52927646
C	-4.24027587	-1.28736124	0.00581340
C	2.69580741	-2.82983601	-1.98273309
C	-3.99638588	-1.84475797	1.28886696
C	2.93969740	-3.38723274	-0.69967953
H	-2.60323949	-0.25886516	-4.20802168
H	-0.29121158	-0.77302345	-4.87087055
H	-1.00936689	-3.90157053	4.17700442
H	1.30266102	-4.41572882	3.51415555
H	-5.22124445	-0.87609537	-0.23222292
H	-4.79014313	-1.86135299	2.03570985
H	3.48956465	-2.81324099	-2.72957598
H	3.92066598	-3.79849861	-0.46164321
H	-4.43106549	-0.29707941	-2.48822775
H	-3.26829418	-2.95452725	3.62886581

H	1.96771571	-1.72006673	-4.32273194
H	3.13048702	-4.37751457	1.79436162
C	-0.35169125	6.87273325	7.70459219
C	-2.67272179	7.88735270	6.42047222
C	-1.63801795	6.42310404	8.10408845
C	-0.22587982	7.82967219	6.66303593
C	-2.79853322	6.93041377	7.46202847
C	-1.38639509	8.33698191	6.02097595
C	0.80882402	6.36542352	8.34665217
C	-1.76382938	5.46616510	9.14564471
C	1.06044688	8.27930140	6.26353966
C	-3.83323706	8.39466243	5.77841223
C	-4.08485992	6.48078456	7.86152474
C	-1.26058366	9.29392085	4.97941970
C	-0.60331411	4.95885537	9.78770469
C	2.22096216	7.77199167	6.90559965
C	-5.24537519	6.98809428	7.21946475
C	-2.42109893	9.80123058	4.33735971
C	0.68301264	5.40848456	9.38820845
C	2.09515077	6.81505271	7.94715593
C	-5.11956381	7.94503324	6.17790847
C	-3.70742568	9.35160139	4.73685595
C	-3.05015594	5.01653602	9.54514084
C	1.18625818	9.23624020	5.22198355
C	-4.21067121	5.52384575	8.90308085
C	0.02574291	9.74354993	4.57992357
H	1.57383066	5.01907077	9.88105729

H	2.98596879	6.42563892	8.44000477
H	-6.01038182	8.33444703	5.68505964
H	-4.59824369	9.74101518	4.24400712
H	-3.14672953	4.28198424	10.34464535
H	-5.19806292	5.17870780	9.20973648
H	2.17364988	9.58137816	4.91532792
H	0.12231650	10.47810172	3.78041905
H	-0.69988751	4.22430370	10.58720910
H	-6.23276681	6.64295648	7.52612021
H	3.20835377	8.11712947	6.59894419
H	-2.32452552	10.53578226	3.53785531
C	-1.46515183	3.74235368	5.71695889
C	1.10513488	4.64468007	4.91381954
C	-1.34225868	4.70090327	4.67653588
C	-0.30290163	3.23496728	6.35581222
C	-0.05711532	5.15206646	4.27496621
C	0.98224173	3.68613048	5.95424255
C	-2.75029519	3.29119048	6.11852856
C	-2.50450889	5.20828967	4.03768255
C	-0.42579478	2.27641769	7.39623523
C	2.39027824	5.09584326	4.51224987
C	0.06577783	6.11061606	3.23454321
C	2.14449194	3.17874408	6.59309588
C	-3.78965224	4.75712647	4.43925222
C	-1.71093813	1.82525449	7.79780490
C	1.35092118	6.56177925	2.83297353
C	3.42963529	3.62990728	6.19152621

C	-3.91254545	3.79857686	5.47967525
C	-2.87318839	2.33264087	7.15895158
C	2.51317144	6.05439287	3.47182685
C	3.55252850	4.58845689	5.15110319
C	-2.38161563	6.16683912	2.99725971
C	0.73645533	1.76903144	8.03508840
C	-1.09647228	6.61800231	2.59569004
C	2.02159868	2.22019463	7.63351872
H	-4.89902868	3.45226147	5.78792237
H	-3.85967163	1.98632548	7.46719871
H	3.49965468	6.40070827	3.16357972
H	4.53901173	4.93477228	4.84285606
H	-3.27376551	6.55631182	2.50687223
H	-1.00213881	7.35379045	1.79705540
H	0.64212186	1.03324330	8.83372303
H	2.91374856	1.83072193	8.12390620
H	-4.68180207	5.14659901	3.94886493
H	1.44525480	7.29756726	2.03433904
H	-1.80527175	1.08946648	8.59643939
H	4.32178512	3.24043473	6.68191350
C	-1.69171219	-5.28054212	-2.32856865
C	-2.60232143	-5.94643231	0.27776605
C	-3.02606941	-4.98260829	-1.94499816
C	-0.81265959	-5.91142105	-1.40897179
C	-3.48137403	-5.31555338	-0.64183081
C	-1.26796421	-6.24436614	-0.10580444
C	-1.23640757	-4.94759703	-3.63173600



C	-3.90512200	-4.35172936	-2.86459502
C	0.52169763	-6.20935488	-1.79254228
C	-3.05762605	-6.27937740	1.58093340
C	-4.81573124	-5.01761955	-0.25826032
C	-0.38891161	-6.87524507	0.81379242
C	-3.44981738	-4.01878427	-4.16776237
C	0.97700225	-5.87640979	-3.09570963
C	-5.27103587	-5.35056464	1.04490703
C	-0.84421623	-7.20819016	2.11695977
C	-2.11546014	-4.31671809	-4.55133292
C	0.09794967	-5.24553085	-4.01530655
C	-4.39198329	-5.98144358	1.96450395
C	-2.17857347	-6.91025634	2.50053032
C	-5.23947901	-4.05379562	-2.48102448
C	1.40075001	-6.84023372	-0.87294547
C	-5.69478363	-4.38674071	-1.17785713
C	0.94544539	-7.17317881	0.43022188
H	-1.76596577	-4.06114757	-5.55165147
H	0.44744405	-4.98996033	-5.01562510
H	-4.74147766	-6.23701410	2.96482250
H	-2.52806785	-7.16582686	3.50084887
H	-5.91424481	-3.56952935	-3.18691226
H	-6.71904384	-4.15804499	-0.88342625
H	2.42501023	-7.06892944	-1.16737635
H	1.62021119	-7.65744508	1.13610966
H	-4.12458295	-3.53451808	-4.87365016
H	-6.29529589	-5.12186903	1.33933802

H	2.00126227	-6.10510540	-3.39014062
H	-0.16945067	-7.69245635	2.82284756
K	0.20465800	0.10074000	0.48149700

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n = 5, Energy = -487.611828734242 (69.1)

C	4.37006078	3.83187865	-3.28151889
C	2.33706008	3.06341192	-5.10962353
C	4.52421701	2.65521719	-4.06132897
C	3.19940420	4.62430673	-3.41576113
C	3.50771666	2.27098383	-4.97538129
C	2.18290385	4.24007337	-4.32981344
C	5.38656113	4.21611201	-2.36746657
C	5.69487358	1.86278911	-3.92708674
C	3.04524797	5.80096818	-2.63595105
C	1.32055973	2.67917855	-6.02367584
C	3.66187289	1.09432238	-5.75519137
C	1.01224727	5.03250145	-4.46405568
C	6.71137393	2.24702247	-3.01303442
C	4.06174832	6.18520155	-1.72189873
C	2.64537254	0.71008901	-6.66924369
C	-0.00425308	4.64826809	-5.37810800
C	6.55721775	3.42368394	-2.23322430
C	5.23240494	5.39277348	-1.58765645
C	1.47471591	1.50251708	-6.80348596
C	0.14990311	3.47160662	-6.15791812
C	5.84902969	0.68612785	-4.70689675
C	1.87459152	6.59339608	-2.77019334

C	4.83252934	0.30189448	-5.62094907
C	0.85809117	6.20916271	-3.68424566
H	7.33748910	3.71862362	-1.53159262
H	6.01267630	5.68771316	-0.88602478
H	0.69444456	1.20757740	-7.50511764
H	-0.63036825	3.17666694	-6.85954979
H	6.74763235	0.07785552	-4.60385166
H	4.95086055	-0.60131756	-6.21953573
H	1.75626030	7.49660812	-2.17160669
H	-0.04051149	6.81743505	-3.78729076
H	7.60997651	1.63875035	-2.90998922
H	2.76370358	-0.19312286	-7.26783032
H	3.94341727	7.08841342	-1.12331209
H	-0.90285566	5.25654021	-5.48115319
C	-2.19245048	-4.69320902	6.11913214
C	-3.58992323	-2.56165673	4.86647325
C	-1.56190808	-3.93373216	5.09834260
C	-3.52172925	-4.38690973	6.51359223
C	-2.26064446	-2.86795602	4.47201316
C	-4.22046563	-3.32113359	5.88726278
C	-1.49371410	-5.75898516	6.74546158
C	-0.23262931	-4.24003145	4.70388251
C	-4.15227165	-5.14638658	7.53438176
C	-4.28865961	-1.49588059	4.24014381
C	-1.63010206	-2.10847917	3.45122363
C	-5.54974441	-3.01483430	6.28172287
C	0.46610707	-5.30580759	5.33021196

C	-3.45353528	-6.21216272	8.16071121
C	-2.32883844	-1.04270303	2.82489418
C	-6.24848078	-1.94905816	5.65539343
C	-0.16443530	-6.06528449	6.35100152
C	-2.12425647	-6.51846205	7.76625114
C	-3.65811724	-0.73640370	3.21935425
C	-5.61793841	-1.18958126	4.63460387
C	0.39791290	-3.48055464	3.68309312
C	-5.48155024	-4.84008725	7.92884171
C	-0.30082348	-2.41477850	3.05676367
C	-6.18028661	-3.77431111	7.30251227
H	0.37191865	-6.88338022	6.83177550
H	-1.58790252	-7.33655778	8.24702513
H	-4.19447120	0.08169203	2.73858026
H	-6.15429237	-0.37148553	4.15382989
H	1.41827487	-3.71567171	3.38030329
H	0.18318448	-1.83179975	2.27319981
H	-5.96555819	-5.42306600	8.71240558
H	-7.20064858	-3.53919404	7.60530210
H	1.48646888	-5.54092475	5.02742229
H	-1.84483070	-0.45972428	2.04133043
H	-3.93754301	-6.79514147	8.94427496
H	-7.26884259	-1.71394100	5.95818310
C	1.00085642	0.78235560	-2.61479402
C	1.99661597	2.58474051	-0.65891287
C	2.26374496	0.54684619	-2.00977506
C	0.23584766	1.91905747	-2.24187240

C	2.76162473	1.44803864	-1.03183449
C	0.73372744	2.82024992	-1.26393182
C	0.50297664	-0.11883685	-3.59273459
C	3.02875371	-0.58985568	-2.38269669
C	-1.02704088	2.15456689	-2.84689135
C	2.49449575	3.48593296	0.31902771
C	4.02451327	1.21252922	-0.42681553
C	-0.03128132	3.95695179	-0.89101020
C	2.53087394	-1.49104814	-3.36063726
C	-1.52492065	1.25337444	-3.82483193
C	4.52239305	2.11372167	0.55112504
C	0.46659845	4.85814424	0.08693037
C	1.26798538	-1.25553876	-3.96565626
C	-0.75991192	0.11667253	-4.19775359
C	3.75738431	3.25042358	0.92404670
C	1.72948701	4.62263487	0.69194937
C	4.29164205	-0.82536497	-1.77767775
C	-1.79204944	3.29126862	-2.47396971
C	4.78952183	0.07582749	-0.79973718
C	-1.29416966	4.19246108	-1.49602913
H	0.88581008	-1.94729913	-4.71632892
H	-1.14208722	-0.57508784	-4.94842625
H	4.13955961	3.94218395	1.67471936
H	2.11166231	5.31439524	1.44262203
H	4.87886716	-1.69790380	-2.06393450
H	5.75892228	-0.10495090	-0.33532119
H	-2.76144989	3.47204701	-2.93838570

H	-1.88139476	5.06499991	-1.20977238
H	3.11809882	-2.36358687	-3.64689408
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C	-2.16825881	-3.43143312	0.30129040
C	-3.54343731	-5.16741312	2.07917032
C	-3.52647512	-3.17989017	0.63049347
C	-1.49763175	-4.55096607	0.86102729
C	-4.21406438	-4.04788017	1.51943343
C	-2.18522100	-5.41895607	1.74996725
C	-1.48066956	-2.56344312	-0.58764957
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C	-6.25986994	-4.66432722	2.73757646
C	-2.20218319	-7.40647903	3.19864411
C	-2.15129659	-1.44391013	-1.14738650
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C	-3.56039953	-7.15493611	3.52784722
C	-5.55531830	-1.80881440	0.39995967
C	0.53121143	-5.92204184	1.09156109

C	-6.24290756	-2.67680440	1.28889963
C	-0.15637782	-6.79003184	1.98050105
H	-1.62349923	-0.77763615	-1.82974179
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H	1.57378602	-6.11512766	0.83886295
H	0.35839936	-7.64939172	2.41015828
H	-4.02428988	-0.33300744	-1.24784063
H	-7.30244437	-4.47124157	2.99027467
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H	-1.68740624	-8.26583880	3.62830135
C	0.80769980	-0.37831703	5.38929536
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C	0.24610919	-1.01825840	6.52573326
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C	-3.07795170	0.71838743	6.74817381
C	-1.61069859	-1.29263162	8.11513064
C	-1.95477048	1.99827018	4.47529801
C	2.27495291	-2.38933609	6.75625219

C	1.93088102	0.90156571	3.11641955
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C	-3.24998764	2.36383833	4.92825749
C	2.83654357	-1.74939473	5.61981427
C	2.66450763	-0.10394383	3.79989795
C	-3.63954236	0.07844608	7.88461173
C	-3.81157831	1.72389697	6.06469541
C	0.41814512	-2.66370914	8.34564940
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K	0.20465800	0.10074000	0.48149700

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n = 6, Energy = -635.129273609796 (23.4)

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C	-0.98068086	-1.23612303	4.94788118
C	-2.49707516	-1.38603347	3.01726582
C	-0.77094014	1.95057141	2.96904648
C	0.35827901	0.79582199	5.30507264
C	-2.67450958	0.49600110	1.44384194
C	-2.31964073	-3.26806805	4.59068971
C	-0.41607129	-1.81349773	6.11589426
C	-3.44885988	-2.11331863	2.25466355
C	0.74545415	2.10048186	4.89966183
C	-2.28733443	1.80066096	1.03843113
C	-0.80324644	-3.11815760	6.52130506
C	-3.83603503	-3.41797849	2.66007436
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C	-1.33554969	2.52794617	1.80103338
C	-1.75503118	-3.84544281	5.75870281
C	-3.27142547	-3.99535326	3.82808746
C	0.92288843	0.21844727	6.47308553
C	-3.62629415	-0.23128404	0.68123985
C	0.53571328	-1.08621259	6.87849634
C	-4.01346930	-1.53594391	1.08665066
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H	-1.03835188	3.52941038	1.48983778
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C	-2.37793713	3.86241355	-1.89274840
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C	0.99143149	5.01036918	-0.69093592

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C	-0.85911106	6.53584697	-4.55614495
C	0.87790943	-0.40921183	-6.34268273
C	-1.41136504	0.41635481	-6.69886044
C	2.76334412	5.93157581	-3.76401122
C	0.47406965	6.75714246	-4.12018893
C	3.92135755	1.30153667	-4.95503645
C	-2.94646540	3.77823645	-6.02356950
C	4.29844448	2.56969417	-4.43930216
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H	-1.70081908	-0.55708998	-7.09474097
H	3.05279815	6.90502061	-3.36813069
H	0.76352369	7.73058726	-3.72430840
H	4.65526059	0.49795938	-5.01627472
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H	-3.96982252	3.60836883	-6.35821181
H	-3.30328151	5.84997125	-5.44659694
H	2.94499295	-0.99149361	-5.96796503
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C	-5.09911377	0.73091984	4.46608397
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C	-5.69905640	-0.54573610	4.62923586
C	-5.16898089	3.61508124	2.05952366
C	-2.89451384	0.87297349	7.50489283
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H	-1.90391893	6.01375902	4.80994447
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C	-0.80948777	3.54116759	-9.42097326
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C	3.11105777	-1.64915752	0.31934625
C	4.05860422	-1.99794281	-1.92335399
C	2.04048829	-3.22463400	-1.23659549
C	4.09961190	-1.35652222	-0.65714000
C	2.08149596	-2.58321341	0.02961850
C	2.98803475	-3.57341929	-3.47929573
C	5.04715835	-1.70530751	-2.89984024
C	1.01092649	-4.15868989	-1.52632324
C	3.15206544	-1.00773694	1.58556024

C	5.12917370	-0.42246634	-0.36741225
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C	3.97658888	-3.28078401	-4.45578203
C	1.95847294	-4.50747520	-3.76902354
C	4.18162724	-0.07368102	1.87528804
C	2.16351131	-1.30037221	2.56204654
C	6.07671996	-0.77125174	-2.61011242
C	0.02237255	-4.45132507	-0.54983706
C	6.11772764	-0.12983115	-1.34389843
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H	1.92699522	-4.99983323	-4.74097648
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C	3.23087164	1.89463172	-6.47184967
C	5.29060052	2.92825315	-5.61258016
C	1.86310988	-2.55460297	-4.88114632
C	8.04229613	0.54626114	-2.30333796

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H	4.56120241	-4.67200518	-1.76169076
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H	5.11354796	3.80220112	-6.23945110
H	1.16110635	-3.38828385	-4.89750091
H	0.75339813	-1.37579803	-6.34102949
H	8.92135225	0.50599397	-1.66011236
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H	2.53695425	-4.57927983	-3.24287975
H	1.43727910	0.84881939	-7.13638115
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H	7.13779612	3.70947577	-4.75826211
C	1.57289973	4.42798980	1.07764174
C	0.59441363	2.25236843	2.61869208
C	0.24455850	3.96364812	0.88712543
C	2.41199791	3.80452079	2.03868322
C	-0.24468455	2.87583743	1.65765059
C	1.92275486	2.71671011	2.80920839
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C	-0.59453967	4.58711712	-0.07391606
C	3.74033913	4.26886247	2.22919954
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C	4.22958218	5.35667316	1.45867437
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C	2.27260998	1.00543043	4.54077504
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C	-1.22317067	0.70021602	3.19870096
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H	-7.21869442	-7.17043558	-2.41683921
H	-5.31840352	-8.77468288	-2.75652298
H	-6.07690575	-1.26907286	-8.16104817
H	-0.95141993	-5.59606657	-9.07724704
H	-8.40982330	-5.11436568	-3.05165308
H	-3.28433748	-9.44135939	-3.96785194
C	-2.37738356	-0.46028230	-0.99949706
C	-4.21255655	-0.97810933	1.10516320
C	-3.44698992	0.44045033	-0.75246864
C	-2.22536370	-1.61992845	-0.19419535
C	-4.36457641	0.18153682	0.29986149
C	-3.14295019	-1.87884197	0.85813478
C	-1.45979707	-0.20136879	-2.05182719

C	-3.59900978	1.60009648	-1.55777035
C	-1.15575734	-2.52066109	-0.44122377
C	-5.13014304	-1.23702285	2.15749332
C	-5.43418277	1.08226945	0.54688990
C	-2.99093033	-3.03848812	1.66343649
C	-2.68142329	1.85901000	-2.61010048
C	-0.23817085	-2.26174757	-1.49355389
C	-6.35176926	0.82335594	1.59922003
C	-3.90851682	-3.29740163	2.71576662
C	-1.61181689	0.95827738	-2.85712894
C	-0.39019067	-1.10210141	-2.29885565
C	-6.19974944	-0.33629022	2.40452178
C	-4.97812322	-2.39666901	2.96279508
C	-4.66861602	2.50082892	-1.31074188
C	-1.00373760	-3.68030704	0.36407789
C	-5.58620251	2.24191541	-0.25841175
C	-1.92132409	-3.93922055	1.41640802
H	-0.90747237	1.15702084	-3.66490344
H	0.31415385	-0.90335795	-3.10663014
H	-6.90409397	-0.53503368	3.21229628
H	-5.68246775	-2.59541247	3.77056957
H	-4.78530735	3.39097992	-1.92889606
H	-6.40723845	2.93332292	-0.06879135
H	-0.18270166	-4.37171456	0.17445748
H	-1.80463276	-4.82937156	2.03456219
H	-2.79811446	2.74916082	-3.22825465
H	-7.17280512	1.51476325	1.78884054

H	0.58286501	-2.95315488	-1.68317440
H	-3.79182565	-4.18755245	3.33392078
C	2.83737463	1.21825932	-0.98363218
C	3.16557176	-0.22103310	1.44254248
C	2.80986778	1.90532113	0.25878060
C	3.02898005	-0.18844870	-1.01295763
C	2.97396634	1.18567492	1.47186793
C	3.19307862	-0.90809491	0.20012970
C	2.67327607	1.93790553	-2.19671951
C	2.61826235	3.31202915	0.28810605
C	3.05648691	-0.87551051	-2.25537041
C	3.32967032	-0.94067931	2.65562981
C	2.94645948	1.87273673	2.71428071
C	3.38468404	-2.31480293	0.17080425
C	2.45416379	4.03167536	-0.92498128
C	2.89238835	-0.15586430	-3.46845774
C	3.11055805	1.15309052	3.92736804
C	3.54878260	-3.03444914	1.38389158
C	2.48167064	3.34461358	-2.16739412
C	2.70078292	1.25084375	-3.43913234
C	3.30216347	-0.25361753	3.89804264
C	3.52127575	-2.34738736	2.62630441
C	2.59075552	3.99909076	1.53051870
C	3.24809231	-2.28221833	-2.28469574
C	2.75485408	3.27944455	2.74360603
C	3.41219087	-3.00186454	-1.07160841
H	2.35570766	3.89701804	-3.09856674

H	2.57481994	1.80324821	-4.37030497
H	3.42812645	-0.80602199	4.82921527
H	3.64723873	-2.89979182	3.55747704
H	2.44367811	5.07888786	1.55302910
H	2.73373966	3.80683713	3.69728916
H	3.26920673	-2.80961091	-3.23837886
H	3.55926829	-4.08166164	-1.09411881
H	2.30708639	5.11147229	-0.90247106
H	3.08944365	1.68048287	4.88105109
H	2.91350274	-0.68325665	-4.42214080
H	3.69586000	-4.11424607	1.36138135
C	-2.61341199	1.70859004	3.58900341
C	-5.25127238	1.97801765	4.60620586
C	-3.42955818	2.79165389	3.16795926
C	-3.11619599	0.76024000	4.51864878
C	-4.74848837	2.92636769	3.67656049
C	-4.43512619	0.89495380	5.02725001
C	-1.29448179	1.57387623	3.08040218
C	-2.92677417	3.74000393	2.23831389
C	-2.30004980	-0.32282385	4.93969293
C	-6.57020258	2.11273146	5.11480709
C	-5.56463456	4.00943154	3.25551634
C	-4.93791020	-0.05339624	5.95689538
C	-1.60784398	3.60529012	1.72971266
C	-0.98111961	-0.45753766	4.43109170
C	-6.88356476	4.14414535	3.76411757
C	-6.25684039	0.08131757	6.46549661

C	-0.79169773	2.52222627	2.15075679
C	-0.47833555	0.49081238	3.50144631
C	-7.38634882	3.19579531	4.69376296
C	-7.07298664	1.16438142	6.04445248
C	-3.74292033	4.82306758	1.81726987
C	-2.80283384	-1.27117370	5.86933817
C	-5.06185053	4.95778139	2.32587110
C	-4.12176404	-1.13645989	6.37793940
H	0.22072047	2.41881920	1.76035164
H	0.53408265	0.38740531	3.11104116
H	-8.39876702	3.29920238	5.08416811
H	-8.08540484	1.26778849	6.43485763
H	-3.35698048	5.55102649	1.10366878
H	-5.68832898	5.78914738	2.00267520
H	-2.17635538	-2.10253969	6.19253407
H	-4.50770389	-1.86441880	7.09154049
H	-1.22190404	4.33324883	1.01611168
H	-7.51004324	4.97551115	3.44092182
H	-0.35464113	-1.28890346	4.75428745
H	-6.64278033	-0.64664114	7.17909759
C	6.54425925	0.48989034	-1.61789227
C	6.70142448	0.45222009	1.21750533
C	6.74925217	-0.73780446	-0.93441333
C	6.41784895	1.69875001	-0.88367241
C	6.82783479	-0.75663959	0.48328547
C	6.49643156	1.67991489	0.53402639
C	6.46567663	0.50872547	-3.03559107

C	6.87566247	-1.94666413	-1.66863319
C	6.21285603	2.92644481	-1.56715135
C	6.78000710	0.43338496	2.63520413
C	7.03282771	-1.98433438	1.16676441
C	6.37002126	2.88877456	1.26824625
C	6.79707986	-1.92782900	-3.08633199
C	6.13427341	2.94527994	-2.98485015
C	7.11141032	-2.00316951	2.58446321
C	6.44860388	2.86993943	2.68594505
C	6.59208693	-0.70013421	-3.76981099
C	6.26068371	1.73642027	-3.71907007
C	6.98500002	-0.79430984	3.31868313
C	6.65359680	1.64224463	3.36942405
C	7.08065536	-3.17435869	-0.98515425
C	6.08644576	4.13530425	-0.83293149
C	7.15923798	-3.19319382	0.43254455
C	6.16502837	4.11646912	0.58476731
H	6.53176648	-0.68567626	-4.85804452
H	6.20036326	1.75087821	-4.80730360
H	7.04532048	-0.80876779	4.40691666
H	6.71391725	1.62778668	4.45765758
H	7.17768863	-4.10228628	-1.54874558
H	7.31659171	-4.13557936	0.95718687
H	5.92909202	5.07768979	-1.35757381
H	6.06799510	5.04439671	1.14835864
H	6.89411309	-2.85575636	-3.64992338
H	7.26876403	-2.94555481	3.10910559

H	5.97691970	3.88766524	-3.50949253
H	6.35157064	3.79786678	3.24953644
C	-2.87962982	-2.35547136	-4.48183858
C	-4.81540491	-2.81293561	-2.45474688
C	-2.77768287	-3.50044856	-3.64815154
C	-3.94946431	-1.43922627	-4.30197977
C	-3.74557041	-3.72918069	-2.63460569
C	-4.91735185	-1.66795840	-3.28843392
C	-1.91174228	-2.12673923	-5.49538444
C	-1.70784838	-4.41669365	-3.82801035
C	-4.05141126	-0.29424907	-5.13566682
C	-5.78329245	-3.04166774	-1.44120102
C	-3.64362347	-4.87415790	-1.80091864
C	-5.98718634	-0.75171332	-3.10857511
C	-0.73996084	-4.18796152	-4.84155620
C	-3.08352372	-0.06551694	-6.14921267
C	-4.61151101	-5.10289003	-0.78737279
C	-6.95507389	-0.98044545	-2.09502926
C	-0.84190775	-3.04298430	-5.67524329
C	-2.01368919	-0.98176201	-6.32907152
C	-5.68134554	-4.18664496	-0.60751394
C	-6.85312698	-2.12542267	-1.26134217
C	-1.60590155	-5.56167065	-2.99432337
C	-5.12124564	0.62199582	-4.95580794
C	-2.57378909	-5.79040278	-1.98077752
C	-6.08913318	0.39326369	-3.94226209
H	-0.09895185	-2.86740824	-6.45324676



H	-1.27073329	-0.80618595	-7.10707499
H	-6.42430143	-4.36222102	0.17048953
H	-7.59608287	-2.30099873	-0.48333870
H	-0.78469050	-6.26498562	-3.13238401
H	-2.49553401	-6.66929383	-1.34083460
H	-5.19950071	1.50088686	-5.59575086
H	-6.91034423	1.09657865	-3.80420145
H	0.08125014	-4.89127627	-4.97961694
H	-4.53325609	-5.98178088	-0.14742989
H	-3.16177864	0.81337392	-6.78915557
H	-7.77628486	-0.27713070	-1.95696851
K	0.20465800	0.10074000	0.48149700

## Cartesian coordinates and energies of the Cs<sup>+</sup>Cor<sub>n</sub> clusters

All coordinates are in Å, while the energies are in kJ mol<sup>-1</sup>.

### Structures in Fig. 4

37

n = 1, Energy = -100.80474063

C	-0.04434214	2.82057654	-1.58029288
C	-2.43755961	1.31314768	-1.32384041
C	-0.97788431	3.13883651	-0.55872072
C	-0.30740871	1.74860214	-2.47363881
C	-2.17449305	2.38512208	-0.43049449
C	-1.50401744	0.99488771	-2.34541257
C	1.15226659	3.57429097	-1.70851912
C	-0.71481775	4.21081091	0.33462520
C	0.62613347	1.43034217	-3.49521097

C	-3.63416835	0.55943325	-1.19561417
C	-3.10803522	2.70338205	0.59107768
C	-1.76708401	-0.07708670	-3.23875850
C	0.48179099	4.96452534	0.20639897
C	1.82274220	2.18405660	-3.62343721
C	-4.30464396	1.94966762	0.71930391
C	-2.96369274	-0.83080113	-3.11053226
C	1.41533321	4.64626540	-0.81517320
C	2.08580882	3.25603103	-2.73009129
C	-4.56771057	0.87769319	-0.17404201
C	-3.89723496	-0.51254119	-2.08896009
C	-1.64835986	4.52907075	1.35619718
C	0.36306684	0.35836790	-4.38855671
C	-2.84496859	3.77535632	1.48442341
C	-0.83354190	-0.39534653	-4.26033047
H	2.33385677	5.22482082	-0.91360038
H	3.00433238	3.83458645	-2.82851846
H	-5.48623413	0.29913777	-0.07561483
H	-4.81575853	-1.09109660	-1.99053292
H	-1.44642848	5.35192441	2.04193461
H	-3.56156088	4.01965450	2.26858804
H	1.07965912	0.11406972	-5.17272133
H	-1.03547328	-1.21820019	-4.94606791
H	0.68372248	5.78737890	0.89213621
H	-5.02123623	2.19396564	1.50346836
H	2.53933447	1.93975858	-4.40760165
H	-3.16562424	-1.65365469	-3.79626950

Cs        0.20465800        0.10074000        0.48149700

73

n = 2, Energy = -221.03922978

C	1.66255312	3.25166074	0.64345716
C	2.08710405	1.73838665	-1.72199365
C	0.75165515	3.35824868	-0.44065721
C	2.78572656	2.38843576	0.54484613
C	0.96393061	2.60161163	-1.62338261
C	2.99800202	1.63179871	-0.63787928
C	1.45027766	4.00829778	1.82618257
C	-0.37151829	4.22147366	-0.34204617
C	3.69662453	2.28184782	1.62896050
C	2.29937951	0.98174960	-2.90471905
C	0.05303264	2.70819957	-2.70749699
C	4.12117546	0.76857373	-0.73649031
C	-0.58379375	4.97811071	0.84067923
C	3.48434907	3.03848486	2.81168591
C	0.26530811	1.95156252	-3.89022239
C	4.33345092	0.01193668	-1.91921572
C	0.32710421	4.87152280	1.92479366
C	2.36117562	3.90170988	2.91029699
C	1.38848155	1.08833751	-3.98883348
C	3.42255296	0.11852459	-3.00333014
C	-1.28241606	4.32806150	-1.42616045
C	4.81979777	1.41862293	1.53034937
C	-1.07014060	3.57142446	-2.60888586
C	5.03207324	0.66198588	0.34762397

H	0.16416038	5.45232163	2.83266030
H	2.19823179	4.48250871	3.81816363
H	1.55142539	0.50753868	-4.89670012
H	3.58549679	-0.46227424	-3.91119678
H	-2.14457040	4.99067792	-1.35046607
H	-1.76935109	3.65324198	-3.44105822
H	5.51900826	1.33680541	2.36252174
H	5.89422758	-0.00063053	0.27192959
H	-1.44594790	5.64072706	0.91637375
H	-0.43390218	2.03337992	-4.72239471
H	4.18355935	2.95666747	3.64385823
H	5.19560508	-0.65067967	-1.99491024
C	-1.72550022	-1.76067756	2.45392184
C	-0.52014968	0.38670175	3.86866270
C	-2.39254661	-0.51082217	2.55041372
C	-0.45577855	-1.93684329	3.06480039
C	-1.78987135	0.56286749	3.25778415
C	0.14689672	-0.86315364	3.77217082
C	-2.32817548	-2.83436722	1.74655141
C	-3.66226828	-0.33465644	1.93953517
C	0.21126785	-3.18669868	2.96830852
C	0.08252558	1.46039141	4.57603312
C	-2.45691775	1.81272288	3.35427602
C	1.41661838	-1.03931937	4.38304937
C	-4.26494355	-1.40834609	1.23216474
C	-0.39140742	-4.26038834	2.26093809
C	-1.85424248	2.88641253	4.06164645

C	2.01929365	0.03437029	5.09041980
C	-3.59789717	-2.65820153	1.13567283
C	-1.66112911	-4.08422265	1.65005951
C	-0.58452079	2.71024685	4.67252503
C	1.35224728	1.28422572	5.18691170
C	-4.32931449	0.91519882	2.03602710
C	1.48098933	-3.36286428	3.57918702
C	-3.72663922	1.98888847	2.74339752
C	2.08366459	-2.28917462	4.28655744
H	-4.06051408	-3.48237172	0.59269134
H	-2.12374602	-4.90839284	1.10707801
H	-0.12190388	3.53441704	5.21550653
H	1.81486418	2.10839591	5.72989320
H	-5.30396008	1.05042465	1.56711324
H	-4.23866786	2.94828459	2.81746523
H	1.99301796	-4.32226040	3.50511931
H	3.05831019	-2.42440046	4.75547130
H	-5.23958898	-1.27312044	0.76325091
H	-2.36627090	3.84580856	4.13571424
H	0.12062100	-5.21978437	2.18687030
H	2.99393908	-0.10085537	5.55933363
Cs	0.20465800	0.10074000	0.48149700

109

n = 3, Energy = -343.42551181

C	3.32069301	2.59064486	-0.31251013
C	2.81907547	2.66213190	2.48192523
C	3.05421033	3.82884442	0.32955599

C	3.33636692	1.38818882	0.44264143
C	2.80340156	3.86458794	1.72677367
C	3.08555815	1.42393234	1.83985911
C	3.57150177	2.55490133	-1.70972780
C	3.03853641	5.03130046	-0.42559557
C	3.60284960	0.14998925	-0.19942469
C	2.56826671	2.69787542	3.87914291
C	2.53691888	5.10278750	2.36883979
C	3.10123206	0.22147630	2.59501067
C	3.28934518	4.99555694	-1.82281324
C	3.85365836	0.11424573	-1.59664237
C	2.28611012	5.13853103	3.76605747
C	2.85042330	0.25721982	3.99222835
C	3.55582787	3.75735737	-2.46487942
C	3.83798446	1.31670177	-2.35179398
C	2.30178402	3.93607499	4.52120909
C	2.58394061	1.49541939	4.63429453
C	2.77205376	6.26949978	0.21647056
C	3.61852348	-1.05246655	0.55572686
C	2.52124500	6.30524331	1.61368824
C	3.36771471	-1.01672303	1.95294454
H	3.74835008	3.72992044	-3.53739153
H	4.03050667	1.28926484	-3.42430609
H	2.10926180	3.96351192	5.59372120
H	2.39141840	1.52285631	5.70680664
H	2.76002237	7.19251191	-0.36318806
H	2.31669137	7.25569236	2.10654184

H	3.82307710	-2.00291560	0.06287326
H	3.37974610	-1.93973515	2.53260317
H	3.27731383	5.91856882	-2.40247192
H	2.08155651	6.08897985	4.25891114
H	4.05821197	-0.83620309	-2.08949603
H	2.86245465	-0.66579206	4.57188703
C	1.01704281	-3.34443601	-1.52107009
C	1.04294405	-3.90998643	1.26192854
C	-0.12067248	-3.04635055	-0.72536345
C	2.16770872	-3.92529668	-0.92527741
C	-0.10772186	-3.32912576	0.66613586
C	2.18065934	-4.20807189	0.46622190
C	1.00409219	-3.06166081	-2.91256940
C	-1.27133840	-2.46548989	-1.32115613
C	3.30542401	-4.22338214	-1.72098405
C	1.05589467	-4.19276163	2.65342785
C	-1.24543715	-3.03104030	1.46184249
C	3.33132526	-4.78893256	1.06201458
C	-1.28428902	-2.18271468	-2.71265545
C	3.29247339	-3.94060694	-3.11248336
C	-1.23248653	-3.31381551	2.85334181
C	3.34427588	-5.07170776	2.45351390
C	-0.14657373	-2.48080013	-3.50836214
C	2.14180748	-3.35974626	-3.70827610
C	-0.08182062	-3.89467618	3.44913455
C	2.20656059	-4.77362231	3.24922059
C	-2.40905347	-2.16740451	-0.52544952

C	4.45608971	-4.80424272	-1.12519135
C	-2.39610285	-2.45017972	0.86604980
C	4.46904033	-5.08701793	0.26630797
H	-0.15651470	-2.26374030	-4.57648480
H	2.13186651	-3.14268642	-4.77639876
H	-0.07187965	-4.11173602	4.51725721
H	2.21650156	-4.99068214	4.31734325
H	-3.29231119	-1.72153255	-0.98278336
H	-3.26941960	-2.22136761	1.47683873
H	5.32940646	-5.03305483	-1.73598028
H	5.35229805	-5.53288989	0.72364181
H	-2.16754652	-1.73684279	-3.16998937
H	-2.10580307	-3.08500350	3.46413078
H	4.16578993	-4.16941895	-3.72327234
H	4.22753338	-5.51757965	2.91084782
C	-4.11429875	0.86544318	-1.19285845
C	-2.68299865	1.90566843	1.02860750
C	-3.00902810	1.73182654	-1.40299354
C	-4.50391934	0.51917244	0.12800961
C	-2.29337805	2.25193916	-0.29226056
C	-3.78826930	1.03928507	1.23874259
C	-4.82994879	0.34533056	-2.30359143
C	-2.61940750	2.07809727	-2.72386161
C	-5.60918999	-0.34721092	0.33814470
C	-1.96734860	2.42578105	2.13934048
C	-1.18810741	3.11832252	-0.50239565
C	-4.17788989	0.69301433	2.55961065



C	-3.33505755	1.55798465	-3.83459458
C	-6.32484003	-0.86732354	-0.77258828
C	-0.47245736	3.63843514	0.60833733
C	-3.46223984	1.21312695	3.67034363
C	-4.44032823	0.69160127	-3.62445954
C	-5.93521947	-0.52105282	-2.09345639
C	-0.86207793	3.29216443	1.92920544
C	-2.35696917	2.07951034	3.46020859
C	-1.51413701	2.94448052	-2.93399655
C	-5.99881044	-0.69348153	1.65901261
C	-0.79848696	3.46459314	-1.82326357
C	-5.28316039	-0.17336891	2.76974559
H	-4.98966521	0.29235991	-4.47706439
H	-6.48455645	-0.92029419	-2.94606124
H	-0.31274095	3.69140579	2.78181029
H	-1.80763219	2.47875170	4.31281344
H	-1.21506200	3.21027992	-3.94790240
H	0.04992509	4.12963395	-1.98456448
H	-6.84722249	-1.35852234	1.82031353
H	-5.58223540	-0.43916831	3.78365145
H	-3.03598272	1.82378391	-4.84850034
H	0.37595457	4.30347585	0.44703661
H	-7.17325197	-1.53236425	-0.61128756
H	-3.76131468	0.94732769	4.68424938
Cs	0.20465800	0.10074000	0.48149700

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n = 4, Energy = -440.50483286

C	3.17619218	-1.56967809	0.46197163
C	2.05382790	-3.86138886	1.70855083
C	3.52341999	-1.89136434	1.80075873
C	2.26778223	-2.39384723	-0.25352586
C	2.96223785	-3.03721973	2.42404832
C	1.70660008	-3.53970261	0.36976373
C	3.73737432	-0.42382271	-0.16131796
C	4.43182995	-1.06719521	2.51625622
C	1.92055441	-2.07216098	-1.59231296
C	1.49264576	-5.00724425	2.33184042
C	3.30946567	-3.35890598	3.76283542
C	0.79819013	-4.36387175	-0.34573376
C	4.99301209	0.07866018	1.89296663
C	2.48173656	-0.92630560	-2.21560255
C	2.74828352	-4.50476136	4.38612501
C	0.23700799	-5.50972713	0.27755583
C	4.64578430	0.40034647	0.55417951
C	3.39014653	-0.10213641	-1.50010508
C	1.83987355	-5.32893054	3.67062754
C	0.58423578	-5.83141343	1.61634295
C	4.77905764	-1.38888151	3.85504312
C	1.01214458	-2.89633007	-2.30781025
C	4.21787550	-2.53473689	4.47833271
C	0.45096244	-4.04218545	-1.68452066
H	5.07655085	1.27991148	0.07573893
H	3.82091309	0.77742859	-1.97854566
H	1.40910699	-6.20849555	4.14906812

H	0.15346922	-6.71097843	2.09478354
H	5.47635830	-0.75624459	4.40426309
H	4.48440956	-2.78166507	5.50599332
H	0.74561052	-2.64940188	-3.33547086
H	-0.24633822	-4.67482237	-2.23374063
H	5.69031265	0.71129709	2.44218638
H	3.01481744	-4.75168964	5.41378545
H	2.21520264	-0.67937732	-3.24326299
H	-0.46029257	-6.14236405	-0.27166392
C	-1.64160909	4.55734476	-4.49731327
C	-3.39108371	5.00843435	-2.30609072
C	-2.86007823	3.83451694	-4.40112077
C	-1.29787727	5.50571737	-3.49789449
C	-3.73481553	4.06006173	-3.30550950
C	-2.17261458	5.73126216	-2.40228321
C	-0.76687178	4.33179996	-5.59292454
C	-3.20381005	2.88614433	-5.40053955
C	-0.07940814	6.22854519	-3.59408698
C	-4.26582102	5.23397914	-1.21047944
C	-4.95328467	3.33723392	-3.20931700
C	-1.82888275	6.67963478	-1.40286443
C	-2.32907274	2.66059953	-6.49615083
C	0.79532917	6.00300039	-4.68969826
C	-5.82802197	3.56277871	-2.11370573
C	-2.70362006	6.90517957	-0.30725316
C	-1.11060357	3.38342734	-6.59234337
C	0.45159739	5.05462777	-5.68911708

C	-5.48429019	4.51115134	-1.11428690
C	-3.92208923	6.18235176	-0.21106062
C	-4.42227903	2.16331667	-5.30434697
C	0.26432354	7.17691764	-2.59466829
C	-5.29701634	2.38886147	-4.20873570
C	-0.61041377	7.40246243	-1.49905702
H	-0.43915032	3.21029789	-7.43334071
H	1.12305064	4.88149832	-6.53011443
H	-6.15574344	4.68428078	-0.27328956
H	-4.59354248	6.35548121	0.62993673
H	-4.68612956	1.43534044	-6.07150652
H	-6.23232019	1.83401470	-4.13489780
H	1.19962739	7.73176440	-2.66850618
H	-0.34656325	8.13043866	-0.73189747
H	-2.59292308	1.93262345	-7.26331033
H	-6.76332571	3.00793212	-2.03986770
H	1.73063291	6.55784698	-4.76353628
H	-2.43976972	7.63315565	0.45990635
C	-1.95518219	-0.18333667	3.13018876
C	-3.20801963	2.36507401	3.09017774
C	-1.23464298	0.96860771	3.54279931
C	-3.30214013	-0.06107571	2.69757270
C	-1.86106169	2.24281305	3.52279379
C	-3.92855885	1.21312963	2.67756719
C	-1.32876348	-1.45754201	3.15019427
C	0.11231496	0.84634675	3.97541536
C	-4.02267935	-1.21302009	2.28496216

C	-3.83443835	3.63927935	3.07017222
C	-1.14052247	3.39475743	3.93540434
C	-5.27551678	1.33539059	2.24495113
C	0.73873368	-0.42785859	3.99542088
C	-3.39626063	-2.48722543	2.30496767
C	-1.76694119	4.66896277	3.91539882
C	-5.90193550	2.60959593	2.22494562
C	0.01819449	-1.57980303	3.58281033
C	-2.04930267	-2.60948644	2.73758373
C	-3.11389915	4.79122378	3.48278277
C	-5.18139631	3.76154036	2.63755617
C	0.83285398	1.99829102	4.38802583
C	-5.36963708	-1.09075903	1.85234619
C	0.20643526	3.27249636	4.36802031
C	-5.99605580	0.18344631	1.83234067
H	0.49903700	-2.55789018	3.59816668
H	-1.56846015	-3.58757359	2.75294008
H	-3.59474167	5.76931093	3.46742642
H	-5.66223882	4.73962751	2.62219982
H	1.86678657	1.90444283	4.72010438
H	0.75952529	4.15673543	4.68474252
H	-5.92272711	-1.97499809	1.53562397
H	-7.02998840	0.27729451	1.50026212
H	1.77266610	-0.52170694	4.32749935
H	-1.21385139	5.55320178	4.23212095
H	-3.94935043	-3.37146444	1.98824555
H	-6.93586792	2.70344428	1.89286715

C	1.28351982	1.87406708	-3.84862016
C	-1.06181137	1.60620552	-2.26961057
C	1.11823141	2.66738309	-2.68254576
C	0.27614264	0.94682028	-4.22518977
C	-0.05443419	2.53345232	-1.89304096
C	-0.89652296	0.81288950	-3.43568497
C	2.45618542	2.00799785	-4.63812495
C	2.12560859	3.59462989	-2.30597615
C	0.44143105	0.15350426	-5.39126417
C	-2.23447697	1.47227474	-1.48010578
C	-0.21972261	3.32676833	-0.72696656
C	-1.90390014	-0.11435729	-3.81225458
C	3.29827419	3.72856067	-3.09548094
C	1.61409665	0.28743504	-6.18076896
C	-1.39238821	3.19283756	0.06253823
C	-3.07656574	-0.24828807	-3.02274979
C	3.46356265	2.93524465	-4.26155538
C	2.62147388	1.21468184	-5.80419939
C	-2.39976544	2.26559076	-0.31403134
C	-3.24185420	0.54502794	-1.85667535
C	1.96032009	4.38794574	-1.13990190
C	-0.56594605	-0.77374237	-5.76783363
C	0.78765449	4.25401496	-0.35039710
C	-1.73861164	-0.90767314	-4.97832883
H	4.36370733	3.03805067	-4.86758368
H	3.52161856	1.31748785	-6.41022769
H	-3.29991011	2.16278474	0.29199696

H	-4.14199888	0.44222193	-1.25064705
H	2.73358855	5.09970567	-0.85084490
H	0.66077818	4.86296887	0.54468826
H	-0.43906973	-1.38269627	-6.66291899
H	-2.51188010	-1.61943308	-5.26738583
H	4.07154261	4.44032044	-2.80642413
H	-1.51926465	3.80179129	0.95762348
H	1.74097310	-0.32151870	-7.07585421
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Cs	0.20465800	0.10074000	0.48149700

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C	1.82671704	1.46141067	-3.21005047
C	-0.86338816	2.32290245	-2.91548941
C	0.80994873	0.52044586	-2.89833378
C	2.51520107	3.77408619	-3.68620333
C	-0.17490414	4.63557797	-3.39164227
C	3.17176964	1.03066478	-3.35733100
C	-1.55187219	0.01022693	-2.43933656
C	-2.20844076	2.75364834	-2.76820888
C	1.13823302	-0.85126484	-2.73389762
C	0.84186417	5.57654278	-3.70335896
C	4.18853796	1.97162960	-3.66904770
C	-3.22520908	1.81268353	-2.45649219

C	0.12146470	-1.79222966	-2.42218093
C	2.18691682	5.14579693	-3.85063950
C	3.86025371	3.34334034	-3.83348387
C	-2.89692483	0.44097278	-2.29205602
C	-1.22358794	-1.36148381	-2.27490038
C	-1.51995658	5.06632368	-3.24436174
C	3.50005377	-0.34104575	-3.19289484
C	-2.53672489	4.12535887	-2.93264504
C	2.48328546	-1.28201056	-2.88117815
H	2.96739387	5.86808679	-4.08991498
H	4.64073076	4.06563019	-4.07275935
H	-3.67740188	-0.28131707	-2.05278054
H	-2.00406499	-2.08377366	-2.03562491
H	-1.77194949	6.11925663	-3.37058387
H	-3.56919493	4.45600189	-2.81959167
H	4.53252381	-0.67168876	-3.30594821
H	2.73527837	-2.33494351	-2.75495602
H	0.58987147	6.62947560	-3.82958110
H	-4.25767900	2.14332633	-2.34343880
H	5.22100788	1.64098679	-3.78210108
H	0.37345741	-2.84516248	-2.29595878
C	-2.11312102	-0.51607801	-5.85788492
C	0.68504899	-0.48537355	-6.34255116
C	-1.46471555	0.70068167	-6.19768824
C	-1.36244148	-1.71748546	-5.76041472
C	-0.06563055	0.71603391	-6.44002136
C	0.03664352	-1.70213323	-6.00274784



C	-3.51220602	-0.53143024	-5.61555179
C	-2.21539509	1.90208913	-6.29515843
C	-2.01084694	-2.93424515	-5.42061140
C	2.08413399	-0.47002132	-6.58488429
C	0.58277492	1.93279359	-6.77982468
C	0.78732306	-2.90354069	-5.90527765
C	-3.61448009	1.88673690	-6.05282531
C	-3.40993195	-2.94959738	-5.17827828
C	1.98185992	1.94814582	-7.02215781
C	2.18640806	-2.88818845	-6.14761077
C	-4.26288561	0.66997721	-5.71302198
C	-4.16061154	-1.74818993	-5.27574846
C	2.73253952	0.74673837	-6.92468762
C	2.83481359	-1.67142877	-6.48741410
C	-1.56698961	3.11884858	-6.63496171
C	-1.26016742	-4.13565237	-5.32314124
C	-0.16790461	3.13420081	-6.87729484
C	0.13891759	-4.12030014	-5.56547437
H	-5.33683109	0.65819275	-5.52700572
H	-5.23455702	-1.75997439	-5.08973220
H	3.80648499	0.75852283	-7.11070388
H	3.90875907	-1.65964431	-6.67343036
H	-2.14321549	4.04105580	-6.70978040
H	0.32981511	4.06819250	-7.13812980
H	-1.75788713	-5.06964405	-5.06230628
H	0.71514346	-5.04250736	-5.49065568
H	-4.19070602	2.80894388	-6.12764394

H	2.47957971	2.88213727	-7.28299274
H	-3.90765173	-3.88358883	-4.91744334
H	2.76263399	-3.81039544	-6.07279214
C	2.19216472	2.03973093	2.39903101
C	0.65977726	2.01031938	4.78995617
C	2.67513630	1.35168833	3.54346795
C	0.94299941	2.71306775	2.45005665
C	1.90894257	1.33698256	4.73893053
C	0.17680568	2.69836198	3.64551923
C	2.95835845	2.05443670	1.20356843
C	3.92430162	0.67835151	3.49244231
C	0.46002783	3.40111035	1.30561971
C	-0.10641647	1.99561361	5.98541875
C	2.39191416	0.64893996	5.88336747
C	-1.07235964	3.37169880	3.69654487
C	4.69049535	0.69305728	2.29697973
C	1.22622156	3.41581612	0.11015713
C	1.62572042	0.63423419	7.07883005
C	-1.83855337	3.35699303	4.89200745
C	4.20752380	1.38109988	1.15254274
C	2.47538690	2.74247930	0.05913144
C	0.37655508	1.30757101	7.12985574
C	-1.35558182	2.66895043	6.03644444
C	4.40727303	-0.00969096	4.63687914
C	-0.78913732	4.07444704	1.35664545
C	3.64107930	-0.02439673	5.83234172
C	-1.55533105	4.05974127	2.55210804

H	4.79565840	1.39238811	0.23489897
H	3.06352150	2.75376753	-0.85851233
H	-0.21157952	1.29628278	8.04749951
H	-1.94371641	2.65766220	6.95408821
H	5.36613945	-0.52654815	4.59771159
H	4.01181106	-0.55254216	6.71081804
H	-1.15986908	4.60259247	0.47816914
H	-2.51419747	4.57659846	2.59127559
H	5.64936163	0.17620022	2.25781202
H	1.99645198	0.10608889	7.95730631
H	0.85549000	3.94396142	-0.76831913
H	-2.79741965	3.87385009	4.93117516
C	4.40018898	4.73379088	3.28927306
C	2.27771962	6.26074917	2.18061544
C	3.28656694	5.09111188	4.09461009
C	4.45257634	5.13994903	1.92960722
C	2.22533226	5.85459102	3.54028128
C	3.39134166	5.90342817	1.37527841
C	5.46142366	3.97031174	3.84360187
C	3.23417958	4.68495373	5.45427593
C	5.56619838	4.78262803	1.12427019
C	1.21648494	7.02422831	1.62628663
C	1.11171022	6.21191201	4.34561831
C	3.44372902	6.30958632	0.01561257
C	4.29541426	3.92147459	6.00860474
C	6.62743306	4.01914889	1.67859900
C	0.05047554	6.97539116	3.79128950

C	2.38249434	7.07306546	-0.53871625
C	5.40903635	3.56415357	5.20326774
C	6.57504575	3.61299072	3.03826486
C	0.10286285	7.38154933	2.43162363
C	1.26887225	7.43038648	0.26662076
C	2.12055765	5.04227473	6.25961275
C	5.61858563	5.18878618	-0.23539544
C	1.05932297	5.80575387	5.70528394
C	4.55735095	5.95226532	-0.78972426
H	6.22364603	2.97810270	5.62877363
H	7.38965543	3.02693985	3.46377076
H	-0.71174683	7.96760019	2.00611774
H	0.45426257	8.01643734	-0.15888514
H	2.08034480	4.73050543	7.30330001
H	0.20450035	6.08003550	6.32346526
H	6.47340825	4.91450455	-0.85357676
H	4.59756380	6.26403462	-1.83341151
H	4.25520157	3.60970526	7.05229182
H	-0.80434702	7.24967282	4.40947058
H	7.48225562	3.74486723	1.06041792
H	2.42270703	7.38483478	-1.58240332
C	-2.85229073	-3.29438382	0.23283809
C	-0.37594810	-3.09112524	1.60834259
C	-1.74372033	-4.07937077	-0.18100638
C	-2.72268981	-2.40776758	1.33443481
C	-0.50554901	-3.97774147	0.50674587
C	-1.48451849	-2.30613829	2.02218706

C	-4.09046205	-3.39601311	-0.45491416
C	-1.87332125	-4.96598700	-1.28260310
C	-3.83126021	-1.62278064	1.74827928
C	0.86222322	-2.98949594	2.29609484
C	0.60302139	-4.76272842	0.09290140
C	-1.35491758	-1.41952206	3.12378377
C	-3.11149256	-5.06761629	-1.97035534
C	-5.06943153	-1.72440993	1.06052703
C	1.84119270	-4.66109913	0.78065365
C	-0.11674626	-1.31789276	3.81153602
C	-4.22006302	-4.28262935	-1.55651090
C	-5.19903250	-2.61102617	-0.04106972
C	1.97079367	-3.77448288	1.88225040
C	0.99182419	-2.10287970	3.39769158
C	-0.76475094	-5.75097378	-1.69644742
C	-3.70165920	-0.73616457	2.84987585
C	0.47342037	-5.64934449	-1.00869517
C	-2.46348788	-0.63453527	3.53762810
H	-5.17049025	-4.36064057	-2.08443338
H	-6.14945973	-2.68903739	-0.56899219
H	2.92122090	-3.69647167	2.41017287
H	1.94225142	-2.02486849	3.92561406
H	-0.86423333	-6.43154547	-2.54203934
H	1.32436532	-6.25190495	-1.32636456
H	-4.55260415	-0.13360410	3.16754524
H	-2.36400549	0.04603641	4.38322002
H	-3.21097510	-5.74818782	-2.81594715

H	2.69213761	-5.26365942	0.46298444
H	-5.92037643	-1.12184964	1.37819624
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Cs	0.20465800	0.10074000	0.48149700

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C	1.01630035	-3.24161499	-5.43277281
C	3.22359064	-1.45538678	-5.37931352
C	0.87305024	-1.92073877	-5.93393695
C	2.26319562	-3.66937710	-4.90487902
C	1.97669538	-1.02762467	-5.90720731
C	3.36684076	-2.77626300	-4.87814938
C	-0.08734479	-4.13472909	-5.45950245
C	-0.37384503	-1.49297665	-6.46183074
C	2.40644574	-4.99025332	-4.40371488
C	4.32723579	-0.56227268	-5.35258388
C	1.83344526	0.29325155	-6.40837145
C	4.61373603	-3.20402512	-4.35025559
C	-1.47749017	-2.38609076	-6.48856038
C	1.30280059	-5.88336742	-4.43044452
C	2.93709041	1.18636565	-6.38164181
C	5.71738117	-2.31091102	-4.32352595
C	-1.33424010	-3.70696701	-5.98739624
C	0.05590528	-5.45560534	-4.95833831
C	4.18398572	0.75860357	-5.85374802
C	5.57413110	-0.99003476	-4.82469009
C	-0.51709501	-0.17210061	-6.96299478

C	3.65334087	-5.41801527	-3.87582119
C	0.58655013	0.72101350	-6.93626514
C	4.75698601	-4.52490117	-3.84909155
H	-2.18140429	-4.39252639	-6.00791406
H	-0.79125891	-6.14116473	-4.97885613
H	5.03114991	1.44416295	-5.83323020
H	6.42129529	-0.30447538	-4.80417227
H	-1.47421892	0.15625205	-7.36820906
H	0.47659050	1.73492561	-7.32096159
H	3.76330049	-6.43192738	-3.49112474
H	5.71410992	-4.85325382	-3.44387727
H	-2.43461399	-2.05773831	-6.89377456
H	2.82713096	2.20027763	-6.76633816
H	1.41276004	-6.89727941	-4.04574817
H	6.67450499	-2.63926347	-3.91831177
C	0.79447082	-0.64666448	3.74688713
C	-0.05915395	1.77555763	4.95922548
C	-0.37589612	-0.62904019	4.55083408
C	1.53802537	0.54682228	3.54910936
C	-0.80270850	0.58207087	5.15700326
C	1.11121298	1.75793334	4.15527854
C	1.22128321	-1.85777554	3.14071796
C	-1.11945067	-1.82252696	4.74861185
C	2.70839230	0.52919799	2.74516241
C	-0.48596634	2.98666869	5.56539466
C	-1.97307544	0.59969516	5.96095021
C	1.85476753	2.95142011	3.95750076

C	-0.69263828	-3.03363802	4.14244268
C	3.13520469	-0.68191306	2.13899323
C	-2.39988783	1.81080622	6.56711938
C	1.42795514	4.16253117	4.56366994
C	0.47772868	-3.05126236	3.33849570
C	2.39165016	-1.87539988	2.33677098
C	-1.65633330	3.00429303	6.36934163
C	0.25758819	4.18015551	5.36761691
C	-2.28981742	-1.80490255	5.55255871
C	3.45194667	1.72268465	2.54738473
C	-2.71662980	-0.59379149	6.15872788
C	3.02513428	2.93379570	3.15355391
H	0.80535225	-3.98091798	2.87319685
H	2.71927374	-2.80505551	1.87147213
H	-1.98395687	3.93394866	6.83464049
H	-0.07003539	5.10981113	5.83291577
H	-2.86057414	-2.72102979	5.70437406
H	-3.61501014	-0.58026301	6.77584214
H	4.35032700	1.70915616	1.93027047
H	3.59589100	3.84992294	3.00173855
H	-1.26339480	-3.94976519	4.29425791
H	-3.29826800	1.82433487	7.18423357
H	4.03358486	-0.69544172	1.52187904
H	1.99871166	5.07865834	4.41185470
C	4.76550941	-0.78384252	5.30805718
C	2.46929287	-1.66606947	6.72744603
C	4.35200988	-2.13926648	5.21726025



C	4.03090067	0.13046798	6.10854854
C	3.20390160	-2.58037996	5.92695468
C	2.88279240	-0.31064550	6.81824296
C	5.91361768	-0.34272904	4.59836276
C	5.08661861	-3.05357697	4.41676890
C	4.44440021	1.48589194	6.19934546
C	1.32118459	-2.10718294	7.43714046
C	2.79040207	-3.93580392	5.83615775
C	2.14818366	0.60366499	7.61873431
C	6.23472689	-2.61246350	3.70707448
C	5.59250848	1.92700542	5.48965104
C	1.64229380	-4.37691740	6.54585217
C	1.00007539	0.16255151	8.32842874
C	6.64822647	-1.25703951	3.79787138
C	6.32711726	1.01269495	4.68915966
C	0.90768501	-3.46260693	7.34634356
C	0.58657581	-1.19287247	8.23763184
C	4.67311905	-4.40900072	4.32597206
C	3.70979150	2.40020221	6.99983673
C	3.52501078	-4.85011420	5.03566648
C	2.56168323	1.95908874	7.70953116
H	7.52952080	-0.91843834	3.25310597
H	7.20841160	1.35129612	4.14439425
H	0.02639068	-3.80120810	7.89110897
H	-0.29471853	-1.53147364	8.78239725
H	5.23700889	-5.11083068	3.71151034
H	3.20760619	-5.89054537	4.96597023

H	4.02719609	3.44063338	7.06953298
H	1.99779338	2.66091870	8.32399288
H	6.79861675	-3.31429322	3.09261281
H	1.32488913	-5.41734837	6.47615604
H	5.90991315	2.96743639	5.55934718
H	0.43618553	0.86438124	8.94289040
C	-5.25219872	4.04878449	0.20910027
C	-6.30594857	1.90396402	1.74368683
C	-5.06765705	4.02522522	1.61686069
C	-5.96361531	2.99993352	-0.43136688
C	-5.59453198	2.95281498	2.38415397
C	-6.49049024	1.92752329	0.33592640
C	-4.72532379	5.12119472	-0.55819301
C	-4.35624046	5.07407618	2.25732784
C	-6.14815697	3.02349279	-1.83912730
C	-6.83282350	0.83155378	2.51098010
C	-5.40999032	2.92925571	3.79191440
C	-7.20190683	0.87867233	-0.30454074
C	-3.82936553	6.14648642	1.49003456
C	-5.62128204	4.09590303	-2.60642058
C	-5.93686525	1.85684548	4.55920767
C	-7.72878176	-0.19373791	0.46275253
C	-4.01390717	6.17004573	0.08227410
C	-4.90986543	5.14475404	-1.96595347
C	-6.64828186	0.80799447	3.91874056
C	-7.54424012	-0.21729723	1.87051299
C	-4.17169888	5.05051681	3.66508806

C	-6.85957348	1.97464193	-2.47959425
C	-4.69857381	3.97810658	4.43238134
C	-7.38644841	0.90223170	-1.71230097
H	-3.60947503	6.99323383	-0.50670451
H	-4.50543328	5.96794214	-2.55493208
H	-7.05271401	-0.01519363	4.50771918
H	-7.94867226	-1.04048532	2.45949161
H	-3.62561145	5.85562078	4.15671431
H	-4.55691857	3.96002236	5.51298627
H	-7.00122872	1.99272614	-3.56019918
H	-7.93253584	0.09712772	-2.20392722
H	-3.28327817	6.95159034	1.98166058
H	-5.79521011	1.83876112	5.63981244
H	-5.76293718	4.11398739	-3.68702534
H	-8.27486912	-0.99884183	-0.02887349
C	2.83646456	-0.65003245	-1.86863231
C	2.86535570	-3.31003885	-0.87408179
C	1.67406444	-1.45914066	-1.97144265
C	4.01331024	-1.17092744	-1.26854672
C	1.68851002	-2.78914386	-1.47416739
C	4.02775581	-2.50093064	-0.77127146
C	2.82201898	0.67997076	-2.36590757
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C	5.17571035	-0.36181923	-1.16573639
C	2.87980127	-4.64004205	-0.37680653
C	0.52610991	-3.59825207	-1.57697772
C	5.20460150	-3.02182564	-0.17118587

C	0.48277319	0.39175754	-3.06880350
C	5.16126478	0.96818397	-1.66301165
C	0.54055548	-4.92825527	-1.07970246
C	5.21904707	-4.35182884	0.32608939
C	1.64517330	1.20086581	-2.96599319
C	3.98441909	1.48907902	-2.26309726
C	1.71740116	-5.44915032	-0.47961685
C	4.05664696	-5.16093710	0.22327908
C	-0.66518112	-1.74735384	-2.67433850
C	6.35255581	-0.88271425	-0.56565086
C	-0.65073555	-3.07735705	-2.17706325
C	6.36700138	-2.21271746	-0.06837560
H	1.63408480	2.22178371	-3.34770446
H	3.97333059	2.50999692	-2.64480853
H	1.72848967	-6.47006822	-0.09790558
H	4.06773546	-6.18185501	0.60499035
H	-1.56853459	-1.34751189	-3.13496763
H	-1.54300051	-3.69843311	-2.25598105
H	7.24482077	-0.26163819	-0.48673305
H	7.27035485	-2.61255941	0.39225352
H	-0.42058005	0.79159958	-3.52943257
H	-0.35170926	-5.54933136	-1.15862018
H	6.05352951	1.58926006	-1.58409393
H	6.12240031	-4.75167087	0.78671847
C	-3.12000994	1.19617539	-2.80631347
C	-2.90924014	1.08193504	0.02354956
C	-3.68814590	0.10607833	-2.09546185

C	-2.44648908	2.22915226	-2.10223357
C	-3.58276100	0.04895816	-0.68053033
C	-2.34110418	2.17203209	-0.68730206
C	-3.22539483	1.25329556	-4.22124498
C	-4.36166676	-0.92689855	-2.79954174
C	-1.87835312	3.31924932	-2.81308519
C	-2.80385525	1.02481486	1.43848107
C	-4.15089696	-1.04113889	0.03032128
C	-1.66758333	3.20500897	0.01677784
C	-4.46705165	-0.86977837	-4.21447326
C	-1.98373801	3.37636949	-4.22801670
C	-4.04551207	-1.09825907	1.44525280
C	-1.56219843	3.14788880	1.43170935
C	-3.89891569	0.22031868	-4.92532493
C	-2.65725888	2.34339261	-4.93209666
C	-3.37199121	-0.06528219	2.14933275
C	-2.13033439	2.05779174	2.14256103
C	-4.92980260	-2.01699539	-2.08869013
C	-1.20483238	4.35222599	-2.10900529
C	-4.82441770	-2.07411557	-0.67375861
C	-1.09944749	4.29510582	-0.69407378
H	-3.97980973	0.26416445	-6.01143428
H	-2.73815291	2.38723838	-6.01820600
H	-3.29109717	-0.10912796	3.23544210
H	-2.04944035	2.01394598	3.22867038
H	-5.44680105	-2.80991434	-2.62914585
H	-5.26052211	-2.91088029	-0.12810487

H	-0.76872797	5.18899071	-2.65465903
H	-0.58244903	5.08802477	-0.15361805
H	-4.98404999	-1.66269712	-4.75492904
H	-4.48161635	-1.93502359	1.99090659
H	-1.54763373	4.21313401	-4.77367050
H	-1.04520009	3.94080754	1.97216514
Cs	0.20465800	0.10074000	0.48149700

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C	-6.03188870	1.87441555	-1.33413208
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C	-5.52401120	3.16486474	-1.02884302
C	-6.49784082	1.49362178	1.05062882
C	-5.50304852	3.61969245	0.31618196
C	-6.05285139	1.41958784	-2.67915706
C	-7.02668100	-0.25165512	-0.59968522
C	-5.03709639	4.00048623	-2.06857894
C	-5.96900064	3.23889868	2.70094286
C	-6.98475563	0.65800030	2.09036474
C	-4.99517102	4.91014165	0.62147102
C	-7.04764369	-0.70648283	-1.94471020
C	-5.05805908	3.54565852	-3.41360392
C	-6.96379294	1.11282801	3.43538972
C	-4.97420833	5.36496936	1.96649600
C	-6.56072888	0.12913863	-2.98444618
C	-5.56593658	2.25520931	-3.71889304

C	-6.45591545	2.40327722	3.74067884
C	-5.46112314	4.52934789	3.00623198
C	-7.51359572	-1.08727640	0.44005063
C	-4.52921900	5.29093521	-1.76328981
C	-7.49263303	-0.63244869	1.78507561
C	-4.50825631	5.74576292	-0.41826483
H	-6.57681996	-0.21998966	-4.01689488
H	-5.58202765	1.90608101	-4.75134174
H	-6.43982437	2.75240552	4.77312754
H	-5.44503207	4.87847619	4.03868068
H	-7.90344538	-2.07783256	0.20570902
H	-7.86639162	-1.27387651	2.58318282
H	-4.15546041	5.93236304	-2.56139702
H	-4.11840664	6.73631908	-0.18392323
H	-7.43749326	-1.69703881	-2.17905193
H	-7.33755143	0.47140041	4.23349692
H	-4.68430059	4.18708612	-4.21171112
H	-4.58435876	6.35552533	2.20083773
C	0.61621501	-6.66008093	-0.19694912
C	2.58250595	-5.68874736	-2.00133560
C	1.96628598	-6.53388723	0.22469481
C	0.24928951	-6.30060785	-1.52078630
C	2.94943145	-6.04822045	-0.67749843
C	1.23243498	-5.81494106	-2.42297954
C	-0.36693046	-7.14574771	0.70524412
C	2.33321148	-6.89336031	1.54853198
C	-1.10078146	-6.42680155	-1.94243023

C	3.56565142	-5.20308058	-2.90352884
C	4.29950242	-5.92202675	-0.25585450
C	0.86550948	-5.45546798	-3.74681671
C	1.35006601	-7.37902709	2.45072522
C	-2.08392693	-6.91246833	-1.04023699
C	5.28264789	-5.43635996	-1.15804774
C	1.84865495	-4.96980120	-4.64900995
C	-0.00000500	-7.50522081	2.02908133
C	-1.71700147	-7.27194143	0.28360022
C	4.91572243	-5.07688686	-2.48188495
C	3.19872596	-4.84360748	-4.22736605
C	3.68328228	-6.76716658	1.97017574
C	-1.46770679	-6.06732849	-3.26626723
C	4.66642775	-6.28149980	1.06798250
C	-0.48456132	-5.58166171	-4.16846047
H	-0.75467296	-7.87802135	2.72160991
H	-2.47166943	-7.64474197	0.97612880
H	5.67039039	-4.70408632	-3.17441353
H	3.95339392	-4.47080694	-4.91989464
H	3.96493641	-7.04310017	2.98636070
H	5.70274992	-6.18463281	1.39163881
H	-2.50402896	-6.16419548	-3.58992354
H	-0.76621545	-5.30572812	-5.18464543
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H	3.44177795	-3.08832816	-1.01217742
H	-4.72818229	-0.22880197	-5.16458159
H	-5.41527372	-1.16193073	-2.93808748
H	3.53651715	-1.10768837	-5.38367493
H	1.68328649	-3.62453368	0.62164983
H	-2.96969083	0.30740356	-6.79840885
H	-4.82292149	-2.20944175	-0.79308408
C	8.28267139	4.76291179	9.19686604
C	8.30977395	6.95430097	7.39057747
C	9.24876159	4.81433892	8.15743107
C	7.33013247	5.80717925	9.33315672
C	9.26231287	5.91003351	7.25428679
C	7.34368375	6.90287384	8.43001244
C	8.26912011	3.66721719	10.10001033
C	10.20130051	3.77007146	8.02114039
C	6.36404227	5.75575211	10.37259169
C	8.32332522	8.04999556	6.48743318
C	10.22840307	5.96146065	6.21485182
C	6.39114482	7.94714130	8.56630312



C	10.18774924	2.67437687	8.92428468
C	6.35049099	4.66005752	11.27573598
C	10.24195435	7.05715524	5.31170753
C	6.40469610	9.04283589	7.66315883
C	9.22165904	2.62294969	9.96371968
C	7.30302991	3.61579001	11.13944533
C	9.28941542	8.10142274	5.44799818
C	7.37078630	9.09426307	6.62372383
C	11.16739053	3.82149869	6.98170554
C	5.41150353	6.80001948	10.50888226
C	11.18094181	4.91719328	6.07856125
C	5.42505481	7.89571407	9.60573797
H	9.21125700	1.78188839	10.65697829
H	7.29262788	2.77472871	11.83270394
H	9.29981746	8.94248405	4.75473957
H	7.38118834	9.93532437	5.93046522
H	11.89856485	3.01991304	6.87708802
H	11.92251816	4.95666903	5.28068505
H	4.66992718	6.76054373	11.30675846
H	4.69388049	8.69729972	9.71035549
H	10.91892337	1.87279127	8.81966731
H	10.98353052	7.09663112	4.51383141
H	5.60891482	4.62058163	12.07361210
H	5.67352197	9.84442149	7.76777620
C	2.26787031	4.76170918	-3.81976771
C	3.95180956	5.44691824	-1.63792522
C	3.57357648	4.21077419	-3.73031321

C	1.80413376	5.65524869	-2.81830098
C	4.41554611	4.55337872	-2.63939196
C	2.64610339	5.99785322	-1.72737973
C	1.42590068	4.41910465	-4.91068896
C	4.03731303	3.31723467	-4.73177994
C	0.49842759	6.20618368	-2.90775548
C	4.79377919	5.78952277	-0.54700398
C	5.72125228	4.00244373	-2.54993745
C	2.18236684	6.89139274	-0.72591299
C	3.19534340	2.97463014	-5.82270119
C	-0.34354204	5.86357915	-3.99867673
C	6.56322191	4.34504826	-1.45901621
C	3.02433647	7.23399727	0.36500825
C	1.88963719	3.52556512	-5.91215574
C	0.12019447	4.97003962	-5.00014351
C	6.09948540	5.23858779	-0.45754943
C	4.33004268	6.68306230	0.45446280
C	5.34301903	2.76629983	-4.64232535
C	0.03469122	7.09972305	-1.90628883
C	6.18498866	3.10890436	-3.55140410
C	0.87666084	7.44232758	-0.81536759
H	1.24333660	3.26257996	-6.74955300
H	-0.52610612	4.70705446	-5.83754077
H	6.74578599	5.50157295	0.37984783
H	4.97634327	6.94604745	1.29186006
H	5.69898586	2.08041380	-5.41105692
H	7.18725616	2.68600351	-3.48273833

H	-0.96757629	7.52262390	-1.97495461
H	0.52069401	8.12821361	-0.04663602
H	3.55131003	2.28874424	-6.59143272
H	7.56548927	3.92214757	-1.39035030
H	-1.34580940	6.28647984	-4.06734264
H	2.66836984	7.91988317	1.13373978
Cs	0.20465800	0.10074000	0.48149700

**Structures in Fig. 7** Values in parenthesis are the energies of the structures when the reference is the global minimum (*cf.* Fig. 7).

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n = 2, Energy = -187.969101870334 (33.1)

C	2.55720023	2.49344583	-0.03607747
C	2.10431405	1.83144311	2.68830246
C	1.58248352	3.20276784	0.71438219
C	3.30547385	1.45312246	0.57565283
C	1.35604043	2.87176648	2.07657216
C	3.07903075	1.12212110	1.93784280
C	2.78364332	2.82444719	-1.39826744
C	0.83420991	4.24309121	0.10265189
C	4.28019055	0.74380045	-0.17480683
C	1.87787096	1.50044175	4.05049243
C	0.38132373	3.58108849	2.82703182
C	3.82730437	0.08179773	2.54957310
C	1.06065300	4.57409257	-1.25953808
C	4.50663364	1.07480181	-1.53699680
C	0.15488064	3.25008713	4.18922179
C	3.60086128	-0.24920363	3.91176307

C	2.03536972	3.86477057	-2.00999780
C	3.75836004	2.11512519	-2.14872716
C	0.90315424	2.20976374	4.80095215
C	2.62614456	0.46011837	4.66222279
C	-0.14050663	4.95241304	0.85311154
C	5.02846400	-0.29652275	0.43692348
C	-0.36694972	4.62141169	2.21530151
C	4.80202091	-0.62752411	1.79911345
H	2.20918870	4.11884907	-3.05562244
H	3.93217902	2.36920369	-3.19435180
H	0.72933526	1.95568525	5.84657679
H	2.45232558	0.20603987	5.70784743
H	-0.71488573	5.75097120	0.38354389
H	-1.11514783	5.16589132	2.79135861
H	5.77666211	-0.84100238	-0.13913362
H	5.37640001	-1.42608226	2.26868110
H	0.48627407	5.37265056	-1.72910580
H	-0.59331731	3.79456657	4.76527894
H	5.25483159	0.53032236	-2.11305395
H	4.17524021	-1.04776163	4.38133079
C	5.39185674	3.45527891	3.58359606
C	4.78966520	5.03911204	1.30446520
C	6.08530412	3.23682263	2.36383885
C	4.39731359	4.46565175	3.66378784
C	5.78420835	4.02873920	1.22427342
C	4.09621782	5.25756831	2.52422241
C	5.69295251	2.66336234	4.72316149

C	7.07984727	2.22644979	2.28364706
C	3.70386621	4.68410802	4.88354506
C	4.48856944	5.83102860	0.16489977
C	6.47765574	3.81028292	0.00451620
C	3.10167467	6.26794115	2.60441420
C	7.38094304	1.43453323	3.42321249
C	4.00496198	3.89219146	6.02311049
C	6.17655997	4.60219949	-1.13504923
C	2.80057890	7.05985772	1.46484877
C	6.68749567	1.65298947	4.64296975
C	4.99950514	2.88181858	5.94291875
C	5.18201680	5.61257236	-1.05485749
C	3.49402627	6.84140148	0.24509151
C	7.77329449	2.00799363	1.06388997
C	2.70932323	5.69448074	4.96373672
C	7.47219872	2.79991020	-0.07567546
C	2.40822746	6.48639731	3.82417129
H	6.91861847	1.04510988	5.51770656
H	5.23062794	2.27393900	6.81765555
H	4.95089401	6.22045195	-1.92959429
H	3.26290348	7.44928106	-0.62964530
H	8.53671149	1.23242568	1.00233428
H	8.00449290	2.63222190	-1.01196804
H	2.17702905	5.86216904	5.90002930
H	1.64481046	7.26196526	3.88572698
H	8.14435989	0.65896536	3.36165698
H	6.70885397	4.43451134	-2.07134174

H	3.47266798	4.05987960	6.95940300
H	2.03716206	7.83542558	1.52640428
Cs	0.20465800	0.10074000	0.48149700

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n = 3, Energy = -308.777741759207 (34.6)

C	1.68060746	2.86442580	-0.65160748
C	-0.19229348	1.74971290	-2.47239212
C	2.10377739	1.89951230	-1.60358921
C	0.32098705	3.27198285	-0.61001807
C	1.16732693	1.34215585	-2.51398153
C	-0.61546342	2.71462640	-1.52041039
C	2.61705793	3.42178225	0.25878485
C	3.46339780	1.49195525	-1.64517862
C	-0.10218289	4.23689635	0.34196366
C	-1.12874395	1.19235645	-3.38278445
C	1.59049686	0.37724235	-3.46596326
C	-1.97508383	3.12218345	-1.47882098
C	4.39984827	2.04931170	-0.73478629
C	0.83426758	4.79425280	1.25235599
C	0.65404639	-0.18011410	-4.37635559
C	-2.91153429	2.56482699	-2.38921331
C	3.97667837	3.01422522	0.21719548
C	2.19388803	4.38669577	1.21076662
C	-0.70557405	0.22744292	-4.33476622
C	-2.48836440	1.59991347	-3.34119508
C	3.88656757	0.52704188	-2.59716025
C	-1.46180312	4.64445326	0.38355298

C	2.95011710	-0.03031457	-3.50755258
C	-2.39825359	4.08709681	-0.52683935
H	4.69550299	3.44205516	0.91601772
H	2.91271265	4.81452570	1.90958886
H	-1.42439867	-0.20038701	-5.03358846
H	-3.20718902	1.17208354	-4.04001732
H	4.93021994	0.21419876	-2.62908453
H	3.27494477	-0.77098767	-4.23829918
H	-1.78663080	5.38512637	1.11429958
H	-3.44190596	4.39993994	-0.49491507
H	5.44350051	1.73646873	-0.76671044
H	0.97887386	-0.92078710	-5.10710213
H	0.50944012	5.53492579	1.98310253
H	-3.95518654	2.87766997	-2.35728916
C	1.91774233	3.90470329	-4.93255572
C	-0.14018485	5.48954626	-3.78416206
C	2.21499509	4.78470276	-3.85847853
C	0.59152598	3.81712531	-5.43243608
C	1.18603150	5.57712424	-3.28428170
C	-0.43743760	4.60954680	-4.85823925
C	2.94670592	3.11228181	-5.50675255
C	3.54121144	4.87228074	-3.35859816
C	0.29427323	2.93712585	-6.50651328
C	-1.16914843	6.28196775	-3.20996523
C	1.48328426	6.45712371	-2.21020450
C	-1.76365395	4.52196882	-5.35811961
C	4.57017502	4.07985925	-3.93279500

C	1.32323682	2.14470437	-7.08071011
C	0.45432067	7.24954519	-1.63600767
C	-2.79261754	5.31439031	-4.78392278
C	4.27292231	3.19985975	-5.00687221
C	2.64945320	2.23228231	-6.58082977
C	-0.87189572	7.16196725	-2.13588801
C	-2.49536482	6.19438981	-3.70984557
C	3.83846404	5.75228011	-2.28452112
C	-1.03194296	2.84954797	-7.00639349
C	2.80950045	6.54470159	-1.71032429
C	-2.06090655	3.64196945	-6.43219666
H	5.06276052	2.59159259	-5.44762891
H	3.43929141	1.62401514	-7.02158647
H	-1.66173393	7.77023442	-1.69513131
H	-3.28520303	6.80265697	-3.26908886
H	4.85647526	5.81950548	-1.90081009
H	3.03767338	7.22019419	-0.88585651
H	-1.26011589	2.17405536	-7.83086127
H	-3.07891778	3.57474408	-6.81590769
H	5.58818614	4.14708449	-3.54908414
H	0.68249340	7.92503774	-0.81154002
H	1.09506409	1.46921182	-7.90517776
H	-3.81062865	5.24716507	-5.16763364
C	-2.59147805	-1.82848192	-0.30350286
C	-1.00091524	-2.64848548	1.90178706
C	-1.51510036	-2.73316719	-0.50188565
C	-2.87257432	-1.33379843	0.99752489



C	-0.71981896	-3.14316897	0.60075931
C	-2.07729292	-1.74380021	2.10016985
C	-3.38675945	-1.41848015	-1.40614782
C	-1.23400409	-3.22785068	-1.80291340
C	-3.94895201	-0.42911317	1.19590768
C	-0.20563383	-3.05848725	3.00443202
C	0.35655872	-4.04785423	0.40237652
C	-2.35838919	-1.24911672	3.40119760
C	-2.02928549	-2.81784890	-2.90555836
C	-4.74423341	-0.01911139	0.09326272
C	1.15184013	-4.45785601	1.50502148
C	-1.56310779	-1.65911850	4.50384256
C	-3.10566321	-1.91316362	-2.70717562
C	-4.46313717	-0.51379486	-1.20776508
C	0.87074389	-3.96317254	2.80604927
C	-0.48673007	-2.56380378	4.30545981
C	-0.15762654	-4.13253581	-2.00129605
C	-4.23004815	0.06557019	2.49693528
C	0.63765487	-4.54253758	-0.89865109
C	-3.43476675	-0.34443159	3.59958024
H	-3.71612567	-1.59844396	-3.55357206
H	-5.07359963	-0.19907521	-2.05416152
H	1.48120634	-4.27789219	3.65244571
H	0.12373239	-2.87852344	5.15185625
H	0.05814458	-4.51225769	-2.99997236
H	1.46388851	-5.23697916	-1.05093087
H	-5.05628180	0.76001176	2.64921506

H	-3.65053787	0.03529029	4.59825656
H	-1.81351454	-3.19757063	-3.90423458
H	1.97807368	-5.15229746	1.35274189
H	-5.57046696	0.67533006	0.24554231
H	-1.77887874	-1.27939677	5.50251877
Cs	0.20465800	0.10074000	0.48149700

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n = 3, Energy = -285.528940533242 (57.9)

C	3.77997520	1.39313950	-0.75862050
C	3.74260982	1.25270436	2.07765898
C	4.74516226	0.60836082	-0.07383116
C	2.79610545	2.10770061	-0.02527010
C	4.72647957	0.53814325	1.34430858
C	2.77742276	2.03748304	1.39286964
C	3.79865789	1.46335706	-2.17676024
C	5.72903201	-0.10620029	-0.80718156
C	1.83091839	2.89247929	-0.71005944
C	3.72392713	1.18248679	3.49579873
C	5.69166663	-0.24663543	2.02909792
C	1.79355301	2.75204415	2.12622004
C	5.74771470	-0.03598273	-2.22532130
C	1.84960108	2.96269685	-2.12819918
C	5.67298394	-0.31685300	3.44723767
C	1.77487032	2.68182658	3.54435979
C	4.78252764	0.74879596	-2.91011070
C	2.83347083	2.24813575	-2.86154964
C	4.68911419	0.39770811	4.18058813

C	2.74005738	1.89704790	4.22914919
C	6.69421888	-0.89097883	-0.12239221
C	0.84704883	3.60704025	0.02329096
C	6.67553619	-0.96119640	1.29574753
C	0.82836614	3.53682269	1.44143070
H	4.79686858	0.80269535	-3.99868271
H	2.84781177	2.30203514	-3.95012165
H	4.67477325	0.34380871	5.26916013
H	2.72571645	1.84314850	5.31772119
H	7.44944292	-1.43948002	-0.68531615
H	7.41641929	-1.56359699	1.82139572
H	0.10616573	4.20944085	-0.50235723
H	0.07314210	4.08532388	2.00435463
H	6.50293855	-0.58448377	-2.78824529
H	6.41386685	-0.91925345	3.97288592
H	1.10871817	3.56509731	-2.65384743
H	1.01964647	3.23032763	4.10728378
C	-0.54015289	-3.46619512	-1.16571700
C	-0.64079489	-3.67779408	1.66460040
C	-1.42638691	-2.64180946	-0.42316895
C	0.29576013	-4.39638027	-0.49310634
C	-1.47670791	-2.74760893	0.99198975
C	0.24543913	-4.50217975	0.92205235
C	-0.48983189	-3.36039565	-2.58087570
C	-2.26229993	-1.71162431	-1.09577961
C	1.18199416	-5.22076594	-1.23565439
C	-0.69111589	-3.78359355	3.07975910

C	-2.36294194	-1.92322326	1.73453779
C	1.08135215	-5.43236489	1.59466301
C	-2.21197893	-1.60582483	-2.51093831
C	1.23231516	-5.11496646	-2.65081309
C	-2.41326294	-2.02902274	3.14969649
C	1.03103115	-5.53816437	3.00982171
C	-1.32574491	-2.43021050	-3.25348641
C	0.39640214	-4.18478131	-3.32342380
C	-1.57734992	-2.95920789	3.82230721
C	0.14479713	-4.71377870	3.75236981
C	-3.14853379	-0.88723881	-0.35323157
C	2.01790701	-6.15095092	-0.56304373
C	-3.19885479	-0.99303829	1.06192713
C	1.96758601	-6.25675039	0.85211497
H	-1.28711822	-2.34899823	-4.33977015
H	0.43502882	-4.10356904	-4.40970754
H	-1.61597660	-3.04042016	4.90859094
H	0.10617044	-4.79499097	4.83865355
H	-3.79018540	-0.17322338	-0.86953132
H	-3.87913309	-0.36023514	1.63191123
H	2.69818531	-6.78375407	-1.13302783
H	2.60923762	-6.97076582	1.36841473
H	-2.85363037	-0.89180957	-3.02723813
H	-3.09354107	-1.39621976	3.71968065
H	1.91259329	-5.74776944	-3.22079724
H	1.67268259	-6.25217963	3.52612153
C	4.72405836	-3.90302729	0.31262010

C	6.39534527	-5.52502264	1.93789875
C	5.71070358	-4.72999041	-0.28659880
C	4.57305660	-3.88706185	1.72447832
C	6.54634703	-5.54098809	0.52604053
C	5.40870005	-4.69805952	2.53711765
C	3.88841491	-3.09202962	-0.50001923
C	5.86170535	-4.74595586	-1.69845703
C	3.58641138	-3.06009873	2.32369722
C	7.23098872	-6.33602031	2.75053808
C	7.53299225	-6.36795121	-0.07317837
C	5.25769828	-4.68209407	3.94897588
C	5.02606189	-3.93495819	-2.51109635
C	2.75076793	-2.24910105	1.51105790
C	8.36863570	-7.17894888	0.73946095
C	6.09334174	-5.49309175	4.76161520
C	4.03941664	-3.10799503	-1.91187749
C	2.90176966	-2.26506647	0.09919964
C	8.21763397	-7.16298347	2.15131921
C	7.07998699	-6.32005490	4.16239634
C	6.84835045	-5.57291890	-2.29767573
C	3.43540972	-3.04413336	3.73555525
C	7.68399391	-6.38391657	-1.48503640
C	4.27105318	-3.85513103	4.54819458
H	3.39797205	-2.48546868	-2.53566398
H	2.26032507	-1.64254011	-0.52458686
H	8.85907856	-7.78550982	2.77510571
H	7.72143158	-6.94258125	4.78618283

H	6.96426028	-5.58517408	-3.38142615
H	8.44134840	-7.01869817	-1.94500027
H	2.67805523	-2.40935176	4.19551912
H	4.15514335	-3.84287585	5.63194500
H	5.14197158	-3.94721325	-3.59484661
H	9.12599012	-7.81373043	0.27949732
H	1.99341351	-1.61431950	1.97102153
H	5.97743205	-5.48083668	5.84536547
Cs	0.20465800	0.10074000	0.48149700

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n = 3, Energy = -275.898000220350 (67.5)

C	-0.90922538	-2.98638317	1.38654735
C	0.87928456	-2.95981585	-0.81938235
C	0.49256966	-3.03254203	1.60844843
C	-1.41676546	-2.92694065	0.06168142
C	1.38682463	-3.01925837	0.50548358
C	-0.52251048	-2.91365699	-1.04128343
C	-1.80348036	-2.99966683	2.48951221
C	1.00010973	-3.09198455	2.93331437
C	-2.81856050	-2.88078179	-0.16021966
C	1.77353953	-2.94653219	-1.92234720
C	2.78861968	-3.06541723	0.72738466
C	-1.03005056	-2.85421447	-2.36614936
C	0.10585476	-3.10526821	4.03627922
C	-3.71281547	-2.89406545	0.94274520
C	3.68287465	-3.05213357	-0.37558019
C	-0.13579558	-2.84093081	-3.46911422

C	-1.29594032	-3.05910935	3.81437819
C	-3.20527544	-2.95350797	2.26761117
C	3.17533461	-2.99269105	-1.70044617
C	1.26599950	-2.88708967	-3.24721318
C	2.40190459	-3.13814340	3.15521530
C	-3.32610039	-2.82133928	-1.48508544
C	3.29615956	-3.12485974	2.05225044
C	-2.43184542	-2.80805562	-2.58805029
H	-1.98237544	-3.06930597	4.66102018
H	-3.89171056	-2.96370459	3.11425317
H	3.86176974	-2.98249444	-2.54708816
H	1.95243462	-2.87689306	-4.09385518
H	2.79149526	-3.18377182	4.17218994
H	4.37218543	-3.16029154	2.22258300
H	-4.40212626	-2.78590748	-1.65541799
H	-2.82143609	-2.76242721	-3.60502493
H	0.49544521	-3.15089662	5.05325376
H	4.75890037	-3.08756536	-0.20524784
H	-4.78884120	-2.85863366	0.77241284
H	-0.52538603	-2.79530240	-4.48608875
C	-0.12583583	1.71423444	-2.51030991
C	0.22543413	3.39397577	-0.24741840
C	1.18201400	2.06471600	-2.08241792
C	-1.25805069	2.20362355	-1.80675614
C	1.35764899	2.90458666	-0.95097216
C	-1.08241571	3.04349421	-0.67531039
C	-0.30147082	0.87436378	-3.64175567

C	2.31422886	1.57532689	-2.78597168
C	-2.56590053	1.85314199	-2.23464813
C	0.40106912	4.23384643	0.88402736
C	2.66549883	3.25506822	-0.52308017
C	-2.21463056	3.53288332	0.02824338
C	2.13859387	0.73545623	-3.91741744
C	-2.74153551	1.01327133	-3.36609389
C	2.84113381	4.09493888	0.60836558
C	-2.03899558	4.37275398	1.15968914
C	0.83074403	0.38497464	-4.34530948
C	-1.60932066	0.52388219	-4.06964770
C	1.70891896	4.58432802	1.31191940
C	-0.73114573	4.72323557	1.58758117
C	3.62207846	1.92580846	-2.35807967
C	-3.69811515	2.34253109	-1.53109439
C	3.79771344	2.76567912	-1.22663391
C	-3.52248016	3.18240175	-0.39964864
H	0.69592563	-0.25971479	-5.21381357
H	-1.74413906	-0.12080724	-4.93815180
H	1.84373736	5.22901744	2.18042349
H	-0.59632733	5.36792499	2.45608527
H	4.49117305	1.55015060	-2.89813154
H	4.80162645	3.03471076	-0.89818159
H	-4.70202815	2.07349945	-1.85954671
H	-4.39157475	3.55805961	0.14040323
H	3.00768822	0.35979834	-4.45746933
H	3.84504658	4.36397056	0.93681798



H	-3.74544829	0.74423965	-3.69454628
H	-2.90808992	4.74841186	1.69974103
C	4.19152563	-1.04720956	-6.50806673
C	5.76546850	-2.54342614	-4.67786475
C	3.91760064	-2.42440304	-6.29663518
C	5.25242204	-0.41812437	-5.80439728
C	4.70457208	-3.17251133	-5.38153419
C	6.03939348	-1.16623266	-4.88929629
C	3.40455419	-0.29910127	-7.42316772
C	2.85670422	-3.05348823	-7.00030463
C	5.52634703	0.95906911	-6.01582883
C	6.55243994	-3.29153443	-3.76276376
C	4.43064710	-4.54970481	-5.17010265
C	7.10028990	-0.53714746	-4.18562685
C	2.06973279	-2.30537994	-7.91540562
C	4.73937559	1.70717740	-6.93092982
C	5.21761854	-5.29781310	-4.25500166
C	7.88726134	-1.28525575	-3.27052586
C	2.34365774	-0.92818643	-8.12683720
C	3.67847914	1.07809225	-7.63459930
C	6.27851499	-4.66872794	-3.55133217
C	7.61333639	-2.66244927	-3.05909427
C	2.58277937	-4.43068151	-6.78887303
C	6.58724332	1.58815411	-5.31215943
C	3.36975081	-5.17878980	-5.87377204
C	7.37421475	0.84004582	-4.39705844
H	1.73957406	-0.35393431	-8.82927384

H	3.07439546	1.65234436	-8.33703594
H	6.88259867	-5.24298005	-2.84889553
H	8.21742007	-3.23670138	-2.35665763
H	1.76842923	-4.91357091	-7.32901370
H	3.15948442	-6.23593137	-5.71147600
H	6.79750971	2.64529568	-5.47445548
H	8.18856489	1.32293522	-3.85691777
H	1.25538275	-2.78826911	-8.45554628
H	5.00735231	-6.35495450	-4.09270552
H	4.94964182	2.76431881	-7.09322595
H	8.70161138	-0.80236658	-2.73038519
Cs	0.20465800	0.10074000	0.48149700

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n = 3, Energy = -264.182820224709 (79.2)

C	3.09597211	-4.40071011	4.53047385
C	4.21841999	-5.37257039	2.10948275
C	2.41299170	-5.39372400	3.77956689
C	4.34017646	-3.89362636	4.07088525
C	2.97421564	-5.87965414	2.56907135
C	4.90140040	-4.37955650	2.86038970
C	2.53474818	-3.91477998	5.74096940
C	1.16878735	-5.90080775	4.23915549
C	5.02315688	-2.90061248	4.82179220
C	4.77964392	-5.85850052	0.89898720
C	2.29123522	-6.87266802	1.81816439
C	6.14560475	-3.87247275	2.40080110
C	0.60756341	-5.41487761	5.44965104

C	4.46193294	-2.41468234	6.03228775
C	2.85245916	-7.35859816	0.60766885
C	6.70682869	-4.35840288	1.19030555
C	1.29054380	-4.42186371	6.20055804
C	3.21772857	-2.92176607	6.49187640
C	4.09666353	-6.85151443	0.14808020
C	6.02384830	-5.35141679	0.43939855
C	0.48580712	-6.89382149	3.48824857
C	6.26736104	-2.39352887	4.36220357
C	1.04703106	-7.37975163	2.27775302
C	6.82858498	-2.87945901	3.15170803
H	0.85974517	-4.04886101	7.12974120
H	2.78692993	-2.54876338	7.42105956
H	4.52746217	-7.22451712	-0.78110296
H	6.45464693	-5.72441948	-0.48978461
H	-0.46925124	-7.28306188	3.84103138
H	0.52277138	-8.14199475	1.70135257
H	6.79162072	-1.63128575	4.93860402
H	7.78364334	-2.49021862	2.79892521
H	-0.34749478	-5.80411784	5.80243393
H	2.32819969	-8.12084116	0.03126838
H	4.98619241	-1.65243934	6.60868822
H	7.66188688	-3.96916266	0.83752266
C	0.62689351	-2.10129650	3.03327834
C	2.70911880	-2.07311531	1.10217939
C	1.73955028	-1.23521106	3.20147764
C	0.55534939	-2.95329134	1.89952956

C	2.78066292	-1.22112047	2.23592817
C	1.59646203	-2.93920075	0.93398008
C	-0.41421914	-2.11538710	3.99882781
C	1.81109440	-0.38321622	4.33522643
C	-0.55730738	-3.81937678	1.73133025
C	3.75023145	-2.05902472	0.13662991
C	3.89331969	-0.35503503	2.40412748
C	1.52491791	-3.79119559	-0.19976870
C	0.76998175	-0.39730681	5.30077590
C	-1.59842003	-3.83346738	2.69687972
C	4.93443234	-0.34094443	1.43857800
C	2.56603056	-3.77710500	-1.16531818
C	-0.34267506	-1.26339225	5.13257664
C	-1.52687595	-2.98147253	3.83062855
C	4.86288826	-1.19293928	0.30482918
C	3.67868737	-2.91101956	-0.99711891
C	2.92375105	0.48286905	4.50342561
C	-0.62885139	-4.67137146	0.59758159
C	3.96486370	0.49695965	3.53787613
C	0.41226126	-4.65728087	-0.36796788
H	-1.14183896	-1.27420827	5.87373782
H	-2.32603984	-2.99228855	4.57178973
H	5.66205216	-1.18212326	-0.43633200
H	4.47785127	-2.90020354	-1.73828009
H	2.97866874	1.13686516	5.37369763
H	4.81894537	1.16177178	3.66698690
H	-1.48293306	-5.33618359	0.46847083

H	0.35734357	-5.31127697	-1.23823991
H	0.82489928	0.25668913	6.17104784
H	5.78851394	0.32386753	1.56768860
H	-2.45250163	-4.49827934	2.56776913
H	2.51111303	-4.43110094	-2.03559012
C	3.56113259	-7.46372284	6.84206824
C	6.05094248	-6.45163543	5.92439439
C	4.12376372	-7.95173860	5.63306579
C	4.24340640	-6.46966338	7.59223376
C	5.36866866	-7.44569489	5.17422887
C	5.48831135	-5.96361968	7.13339684
C	2.31622764	-7.96976655	7.30090516
C	3.44148990	-8.94579806	4.88290027
C	3.68077527	-5.98164763	8.80123620
C	7.29584742	-5.94559172	5.46555747
C	5.93129980	-7.93371064	3.96522643
C	6.17058516	-4.96956022	7.88356236
C	2.19658496	-9.45184176	5.34173720
C	2.43587032	-6.48769133	9.26007313
C	7.17620474	-7.42766694	3.50638950
C	7.41549010	-4.46351651	7.42472544
C	1.63395377	-8.96382603	6.55073966
C	1.75359646	-7.48175081	8.50990762
C	7.85847861	-6.43360746	4.25655501
C	7.97812129	-4.95153224	6.21572297
C	4.00412105	-9.43381367	3.67389802
C	4.36304907	-4.98758831	9.55140154

C	5.24902599	-8.92776996	3.21506110
C	5.60795402	-4.48154460	9.09256461
H	0.67835777	-9.35226801	6.90294545
H	0.79800045	-7.87019280	8.86211341
H	8.81407461	-6.04516547	3.90434922
H	8.93371729	-4.56309026	5.86351718
H	3.48040379	-10.19685938	3.09806667
H	5.68090484	-9.30237365	2.28702392
H	3.93117022	-4.61298462	10.47943871
H	6.13167127	-3.71849889	9.66839596
H	1.67286766	-10.21488735	4.76590606
H	7.60808366	-7.80227046	2.57835250
H	2.00399141	-6.11308781	10.18811013
H	7.93920740	-3.70047092	8.00055657
Cs	0.20465800	0.10074000	0.48149700

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n = 4, Energy = -411.752879859596 (28.8)

C	0.24325607	-5.28608870	4.37850086
C	1.84770955	-6.46628180	2.35403234
C	1.64358944	-5.42146852	4.57121525
C	-0.35485056	-5.74080542	3.17355221
C	2.44581618	-6.01156508	3.55898099
C	0.44737619	-6.33090197	2.16131796
C	-0.55897067	-4.69599214	5.39073512
C	2.24169607	-4.96675180	5.77616390
C	-1.75518392	-5.60542559	2.98083783
C	2.64993629	-7.05637835	1.34179809

C	3.84614955	-6.14694491	3.75169538
C	-0.15073044	-6.78561870	0.95636931
C	1.43946933	-4.37665525	6.78839815
C	-2.55741067	-5.01532904	3.99307208
C	4.64837629	-6.73704146	2.73946112
C	0.65149630	-7.37571525	-0.05586495
C	0.03913592	-4.24127540	6.59568381
C	-1.95930407	-4.56061229	5.19802077
C	4.05026970	-7.19175821	1.53451243
C	2.05182970	-7.51109510	0.13684940
C	3.64202924	-5.10213166	5.96887815
C	-2.35329036	-6.06014228	1.77588932
C	4.44425598	-5.69222821	4.95664389
C	-1.55106362	-6.65023884	0.76365506
H	-0.57665781	-3.78831398	7.37268049
H	-2.57509781	-4.10765087	5.97501745
H	4.66606343	-7.64471962	0.75751575
H	2.66762344	-7.96405652	-0.64014728
H	4.10113932	-4.75308852	6.89380360
H	5.51915986	-5.79614653	5.10457257
H	-3.42819424	-5.95622396	1.62796063
H	-2.01017369	-6.99928198	-0.16127039
H	1.89857918	-4.02761211	7.71332351
H	5.72328001	-6.84095983	2.88738962
H	-3.63231438	-4.91141066	3.84514358
H	0.19238645	-7.72475839	-0.98079030
C	3.29898708	2.07505729	1.22119893

C	2.41152496	1.76577659	-1.45879285
C	3.96491434	1.17025614	0.35270837
C	2.18932877	2.82521809	0.74969359
C	3.52118328	1.01561579	-0.98728752
C	1.74559771	2.67057774	-0.59030230
C	3.74271815	2.22969765	2.56119482
C	5.07457265	0.42009534	0.82421370
C	1.52340152	3.73001924	1.61818415
C	1.96779390	1.61113623	-2.79878874
C	4.18711053	0.11081464	-1.85577808
C	0.63593940	3.42073854	-1.06180763
C	5.51830371	0.57473570	2.16420959
C	1.96713258	3.88465959	2.95818004
C	3.74337947	-0.04382571	-3.19577397
C	0.19220833	3.26609818	-2.40180352
C	4.85237648	1.47953685	3.03270021
C	3.07679091	3.13449880	3.42968543
C	2.63372114	0.70633508	-3.66727936
C	0.85813557	2.36129703	-3.27029413
C	5.74049973	-0.48470565	-0.04427681
C	0.41374337	4.48017988	1.14667878
C	5.29676867	-0.63934600	-1.38427270
C	-0.02998769	4.32553953	-0.19331711
H	5.19298692	1.59823965	4.06128855
H	3.41740136	3.25320160	4.45827377
H	2.29311069	0.58763228	-4.69586770
H	0.51752512	2.24259422	-4.29888248



H	6.59227979	-1.06053336	0.31765335
H	5.80793824	-1.33387653	-2.05093100
H	-0.09742620	5.17471041	1.81333707
H	-0.88176774	4.90136724	-0.55524728
H	6.37008361	-0.00109185	2.52613985
H	4.25454885	-0.73835609	-3.86243227
H	1.45596320	4.57918997	3.62483835
H	-0.65957157	3.84192573	-2.76373378
C	4.83516623	-2.44822002	3.50387508
C	3.60352746	-3.38035953	1.12064589
C	5.62527868	-3.02782403	2.47616813
C	3.42923439	-2.33468577	3.33996743
C	5.00945930	-3.49389379	1.28455353
C	2.81341501	-2.80075552	2.14835284
C	5.45098561	-1.98215027	4.69548968
C	7.03121052	-3.14135829	2.64007578
C	2.63912194	-1.75508175	4.36767438
C	2.98770808	-3.84642928	-0.07096871
C	5.79957176	-4.07349780	0.25684658
C	1.40748317	-2.68722126	1.98444519
C	7.64702990	-2.67528854	3.83169038
C	3.25494132	-1.28901200	5.55928898
C	5.18375237	-4.53956755	-0.93476801
C	0.79166379	-3.15329101	0.79283059
C	6.85691747	-2.09568451	4.85939738
C	4.66087318	-1.40254624	5.72319668
C	3.77782051	-4.42603331	-1.09867571

C	1.58177622	-3.73289505	-0.23487641
C	7.82132276	-3.72096223	1.61236892
C	1.23319031	-1.64154756	4.20376665
C	7.20550338	-4.18703199	0.42075432
C	0.61737093	-2.10761732	3.01215205
H	7.32962388	-1.73792676	5.77408742
H	5.13357958	-1.04478849	6.63788672
H	3.30511411	-4.78379106	-2.01336575
H	1.10906981	-4.09065280	-1.14956645
H	8.90052406	-3.80811179	1.73818534
H	7.81199822	-4.63193933	-0.36811939
H	0.62669547	-1.19664022	4.99264036
H	-0.46183037	-2.02046777	2.88633562
H	8.72623101	-2.76243800	3.95750694
H	5.79024698	-4.98447485	-1.72364169
H	2.64844671	-0.84410471	6.34816266
H	-0.28753732	-3.06614155	0.66701403
C	-3.30567001	2.34475303	-1.05751230
C	-2.97680391	-0.37517624	-0.30956083
C	-3.35106522	1.97470765	0.31267227
C	-3.09584174	1.35483378	-2.05372114
C	-3.18663218	0.61474301	0.68664801
C	-2.93140869	-0.00513086	-1.67974541
C	-3.47010305	3.70471766	-1.43148804
C	-3.56089349	2.96462690	1.30888111
C	-3.05044652	1.72487916	-3.42390572
C	-2.81237087	-1.73514087	0.06441490

C	-3.23202740	0.24469763	2.05683258
C	-2.72158043	-0.99505011	-2.67595425
C	-3.72532654	4.32459153	0.93490537
C	-3.21487957	3.08484379	-3.79788145
C	-3.06759435	-1.11526700	2.43080831
C	-2.55714738	-2.35501474	-2.30197851
C	-3.67993133	4.69463697	-0.43527921
C	-3.42470784	4.07476310	-2.80167263
C	-2.85776608	-2.10518631	1.43459949
C	-2.60254259	-2.72506018	-0.93179392
C	-3.60628868	2.59458146	2.67906545
C	-2.84061828	0.73495996	-4.42011433
C	-3.44185564	1.23461682	3.05304119
C	-2.67618524	-0.62500467	-4.04613859
H	-3.80615105	5.73855343	-0.72234508
H	-3.55092757	5.11867956	-3.08873850
H	-2.73154635	-3.14910277	1.72166536
H	-2.47632287	-3.76897664	-0.64472805
H	-3.76735406	3.35444911	3.44376106
H	-3.47670127	0.95056790	4.10480269
H	-2.80577265	1.01900889	-5.47187583
H	-2.51511986	-1.38487232	-4.81083419
H	-3.88639189	5.08445918	1.69960073
H	-3.10243995	-1.39931604	3.48256960
H	-3.18003397	3.36889283	-4.84964274
H	-2.39608203	-3.11488239	-3.06667387
Cs	0.20465800	0.10074000	0.48149700

n = 4, Energy = -406.046837565924 (34.4)

C	-2.53701818	0.16084824	2.75451255
C	-2.27533786	-2.60274643	3.35423534
C	-2.18955159	-0.25076022	4.06837918
C	-2.75364461	-0.80934064	1.74050731
C	-2.05871143	-1.63255756	4.36824057
C	-2.62280445	-2.19113797	2.04036871
C	-2.66785835	1.54264557	2.45465115
C	-1.97292516	0.71942865	5.08238441
C	-3.10111121	-0.39773218	0.42664069
C	-2.14449769	-3.98454377	3.65409673
C	-1.71124483	-2.04416602	5.68210720
C	-2.83943088	-3.16132685	1.02636348
C	-2.10376533	2.10122599	4.78252301
C	-3.23195137	0.98406516	0.12677929
C	-1.58040467	-3.42596335	5.98196860
C	-2.70859072	-4.54312418	1.32622487
C	-2.45123192	2.51283450	3.46865637
C	-3.01532495	1.95425409	1.14078451
C	-1.79703110	-4.39615228	4.96796338
C	-2.36112412	-4.95473270	2.64009151
C	-1.62545862	0.30782014	6.39625081
C	-3.31773758	-1.36792100	-0.58736432
C	-1.49461846	-1.07397720	6.69611221
C	-3.18689742	-2.74971833	-0.28750293
H	-2.55166557	3.57350987	3.23848109

H	-3.11575859	3.01492946	0.91060923
H	-1.69659745	-5.45682765	5.19813866
H	-2.26069048	-6.01540807	2.87026680
H	-1.45917494	1.05254264	7.17460703
H	-1.22790112	-1.38993018	7.70464373
H	-3.58445492	-1.05196802	-1.59589585
H	-3.35318111	-3.49444083	-1.06585914
H	-1.93748170	2.84594849	5.56087899
H	-1.31368738	-3.74191645	6.99049991
H	-3.49866866	1.30001825	-0.88175202
H	-2.87487434	-5.28784669	0.54786890
C	4.22371081	-1.10975026	0.11184158
C	3.73473016	0.31564127	2.51907161
C	3.20771976	-1.54729359	1.00218876
C	4.99521154	0.04048883	0.42510942
C	2.96322944	-0.83459782	2.20580377
C	4.75072121	0.75318460	1.62872443
C	4.46820114	-1.82244602	-1.09177344
C	2.43621904	-2.69753268	0.68892092
C	6.01120259	0.47803216	-0.46523776
C	3.49023984	1.02833704	3.72268663
C	1.94723839	-1.27214115	3.09615095
C	5.52222194	1.90342369	1.94199227
C	2.68070936	-3.41022844	-0.51469409
C	6.25569291	-0.23466360	-1.66885278
C	1.70274806	-0.55944538	4.29976597
C	5.27773161	2.61611946	3.14560728

C	3.69670042	-2.97268515	-1.40504132
C	5.48419220	-1.38490273	-1.98212067
C	2.47424878	0.59079374	4.61303385
C	4.26174055	2.17857616	4.03595451
C	1.42022816	-3.13507585	1.57926804
C	6.78270314	1.62827110	-0.15196987
C	1.17573783	-2.42238009	2.78288306
C	6.53821282	2.34096686	1.05164515
H	3.88437256	-3.51975440	-2.32894295
H	5.67186434	-1.93197198	-2.90602229
H	2.28657663	1.13786300	5.53693548
H	4.07406841	2.72564542	4.95985614
H	0.82801979	-4.01800594	1.33880188
H	0.39585730	-2.75824086	3.46631862
H	7.56258367	1.96413187	-0.83540543
H	7.13042118	3.22389695	1.29211131
H	2.08850118	-4.29315841	-0.75516036
H	0.92286769	-0.89530597	4.98320152
H	7.03557328	0.10119698	-2.35228833
H	5.86993980	3.49904942	3.38607355
C	0.03500405	-4.11159403	-4.98020406
C	-1.55551719	-5.58946421	-3.14942788
C	0.64978907	-5.01797417	-4.07637083
C	-1.37504160	-3.94414899	-4.96864920
C	-0.14547155	-5.75690925	-3.16098274
C	-2.17030222	-4.68308408	-4.05326111
C	0.83026467	-3.37265895	-5.89559216

C	2.05983472	-5.18541921	-4.08792570
C	-1.98982662	-3.03776886	-5.87248243
C	-2.35077781	-6.32839930	-2.23403978
C	0.46931348	-6.66328938	-2.25714951
C	-3.58034786	-4.51563904	-4.04170624
C	2.85509534	-4.44648412	-5.00331379
C	-1.19456600	-2.29883377	-6.78787052
C	-0.32594714	-7.40222447	-1.34176142
C	-4.37560848	-5.25457412	-3.12631815
C	2.24031034	-3.54010396	-5.90714706
C	0.21547968	-2.46627878	-6.79942542
C	-1.73599282	-7.23477946	-1.33020651
C	-3.76082349	-6.16095429	-2.22248488
C	2.67461954	-6.09179924	-3.18409255
C	-3.39987207	-2.87032392	-5.86092748
C	1.87935892	-6.83073432	-2.26870446
C	-4.19513269	-3.60925901	-4.94553939
H	2.85075685	-2.97289325	-6.60980408
H	0.82592618	-1.89906808	-7.50208245
H	-2.34643932	-7.80199017	-0.62754949
H	-4.37126999	-6.72816499	-1.51982786
H	3.75697862	-6.22033102	-3.19296212
H	2.35127143	-7.52647688	-1.57491692
H	-3.87178458	-2.17458137	-6.55471501
H	-5.27749177	-3.48072722	-4.93666982
H	3.93745425	-4.57501577	-5.01218348
H	0.14596514	-8.09796695	-0.64797393

H	-1.66647828	-1.60309129	-7.48165801
H	-5.45796740	-5.12604247	-3.11744846
C	0.13655672	3.86058747	-0.98169799
C	-1.56078403	2.32493386	-2.66288860
C	0.63503887	2.69302355	-1.61786630
C	-1.21059580	4.26032459	-1.18612498
C	-0.21363151	1.92519675	-2.45846160
C	-2.05926618	3.49249778	-2.02672029
C	0.98522710	4.62841428	-0.14110269
C	1.98219139	2.29328643	-1.41343931
C	-1.70907794	5.42788851	-0.54995667
C	-2.40945441	1.55710706	-3.50348390
C	0.28485063	0.75763282	-3.09462991
C	-3.40641870	3.89223490	-2.23114728
C	2.83086177	3.06111324	-0.57284400
C	-0.86040756	6.19571531	0.29063863
C	-0.56381975	-0.01019398	-3.93522522
C	-4.25508908	3.12440810	-3.07174258
C	2.33237966	4.22867719	0.06332434
C	0.48674499	5.79597823	0.49506566
C	-1.91097230	0.38954310	-4.13965225
C	-3.75660697	1.95684414	-3.70791093
C	2.48067335	1.12572267	-2.04960758
C	-3.05623029	5.82762547	-0.75438371
C	1.63200298	0.35789586	-2.89020288
C	-3.90490066	5.05979867	-1.59497901
H	2.98382379	4.81806535	0.70857000



H	1.13818913	6.38536638	1.14031132
H	-2.56241644	-0.19984505	-4.78489791
H	-4.40805110	1.36745599	-4.35315659
H	3.51475531	0.81888216	-1.89268826
H	2.01464073	-0.53833286	-3.37852929
H	-3.43886804	6.72385420	-0.26605729
H	-4.93898262	5.36663918	-1.75189833
H	3.86494358	2.75427292	-0.41592461
H	-0.18118221	-0.90642258	-4.42355163
H	-1.24304510	7.09194392	0.77896504
H	-5.28917089	3.43124842	-3.22866198
Cs	0.20465800	0.10074000	0.48149700

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n = 4, Energy = -396.292075573918 (44.2)

C	1.22201762	0.02268593	-2.70869487
C	2.95117371	-1.32218811	-0.90122909
C	2.27237639	0.73297531	-2.06944883
C	1.03623689	-1.36004048	-2.44420803
C	3.13695444	0.06053829	-1.16571594
C	1.90081494	-2.03247750	-1.54047514
C	0.35743957	0.69512294	-3.61242776
C	2.45815712	2.11570172	-2.33393567
C	-0.01412189	-2.07032986	-3.08345407
C	3.81575176	-1.99462513	0.00250380
C	4.18731322	0.77082768	-0.52646989
C	1.71503421	-3.41520390	-1.27598830
C	1.59357907	2.78813873	-3.23766856

C	-0.87869993	-1.39789285	-3.98718696
C	5.05189126	0.09839066	0.37726300
C	2.57961226	-4.08764092	-0.37225541
C	0.54322026	2.07784938	-3.87691464
C	-0.69291924	-0.01516641	-4.25167384
C	4.86611057	-1.28433577	0.64174988
C	3.62997107	-3.37735156	0.26699068
C	3.50851578	2.82599090	-1.69468966
C	-0.19990249	-3.45305606	-2.81896719
C	4.37309382	2.15355388	-0.79095677
C	0.66467555	-4.12549308	-1.91523431
H	-0.12043469	2.59401579	-4.57062507
H	-1.35657419	0.50100000	-4.94538427
H	5.52976552	-1.80050219	1.33546030
H	4.29362602	-3.89351798	0.96070110
H	3.65112214	3.88737957	-1.89771126
H	5.17935521	2.69877608	-0.30026787
H	-1.00616388	-3.99827826	-3.30965610
H	0.52206919	-5.18688176	-1.71221271
H	1.73618528	3.84952723	-3.44069023
H	5.85815256	0.64361263	0.86795190
H	-1.68496123	-1.94311482	-4.47787587
H	2.43700605	-5.14902942	-0.16923374
C	-2.85668430	-2.16623500	5.98842172
C	-2.72505078	-4.69071751	4.69410329
C	-3.88927870	-2.56212690	5.09768130
C	-1.75827315	-3.03258436	6.23200292

C	-3.82346194	-3.82436815	4.45052208
C	-1.69245639	-4.29482561	5.58484371
C	-2.92250106	-0.90399375	6.63558093
C	-4.98768985	-1.69577754	4.85410009
C	-0.72567875	-2.63669246	7.12274334
C	-2.65923402	-5.95295876	4.04694408
C	-4.85605633	-4.22026005	3.55978166
C	-0.59404523	-5.16117497	5.82842492
C	-5.05350661	-0.43353629	5.50125931
C	-0.79149551	-1.37445121	7.76990256
C	-4.79023957	-5.48250131	2.91262245
C	-0.52822847	-6.42341622	5.18126570
C	-4.02091222	-0.03764434	6.39199975
C	-1.88990667	-0.50810180	7.52632138
C	-3.69182841	-6.34885072	3.15620363
C	-1.56082286	-6.81930817	4.29052525
C	-6.02028404	-2.09166949	3.96335978
C	0.37273220	-3.50304177	7.36632444
C	-5.95446728	-3.35391074	3.31620057
C	0.43854896	-4.76528302	6.71916523
H	-4.07143353	0.93125911	6.88876279
H	-1.94042798	0.46080165	8.02308442
H	-3.64130710	-7.31775417	2.65944059
H	-1.51030155	-7.78821162	3.79376222
H	-6.86343072	-1.42665479	3.77638545
H	-6.74709264	-3.65779961	2.63246314
H	1.16535755	-3.19915291	8.05006187

H	1.28169563	-5.43029772	6.90613956
H	-5.89665308	0.23147841	5.31428511
H	-5.58286472	-5.78639027	2.22888511
H	0.00112964	-1.07056224	8.45363990
H	0.31491800	-7.08843092	5.36823990
C	-0.71662933	-0.31601869	3.66328925
C	-1.83352324	-2.23248305	1.88978655
C	-0.04518050	-1.54573820	3.43232069
C	-1.94652511	-0.04453136	3.00750646
C	-0.60362746	-2.50397038	2.54556934
C	-2.50497207	-1.00276354	2.12075511
C	-0.15818237	0.64221349	4.55004061
C	1.18471528	-1.81722553	4.08810349
C	-2.61797394	1.18518815	3.23847502
C	-2.39197020	-3.19071523	1.00303519
C	0.06782137	-3.73368989	2.31460078
C	-3.73486785	-0.73127621	1.46497231
C	1.74316223	-0.85899335	4.97485484
C	-2.05952698	2.14342033	4.12522637
C	-0.49062559	-4.69192207	1.42784943
C	-4.29331480	-1.68950839	0.57822096
C	1.07171343	0.37072620	5.20582344
C	-0.82963118	1.87193304	4.78100920
C	-1.72052139	-4.42043478	0.77206660
C	-3.62186600	-2.91922794	0.34725236
C	1.85616392	-3.04694489	3.85713489
C	-3.84786954	1.45667534	2.58269227

C	1.29771696	-4.00517707	2.97038353
C	-4.40631649	0.49844315	1.69594091
H	1.50038044	1.10627059	5.88649874
H	-0.40096417	2.60747743	5.46168450
H	-2.14918840	-5.15597917	0.09139129
H	-4.05053301	-3.65477233	-0.33342294
H	2.80023894	-3.25534013	4.36051749
H	1.81312493	-4.94911678	2.79309076
H	-4.36327750	2.40061504	2.75998504
H	-5.35039151	0.70683839	1.19255831
H	2.68723709	-1.06738840	5.47823744
H	0.02478217	-5.63586167	1.25055658
H	-2.57493474	3.08735993	4.30251922
H	-5.23738966	-1.48111334	0.07483836
C	4.31613939	-1.38981737	-4.50902957
C	3.94285911	-4.15340693	-3.97159670
C	5.18035583	-2.06004423	-3.60331108
C	3.26528281	-2.10138530	-5.14603163
C	4.99371569	-3.44183901	-3.33459465
C	3.07864268	-3.48318008	-4.87731520
C	4.50277953	-0.00802259	-4.77774601
C	6.23121241	-1.34847630	-2.96630903
C	2.40106638	-1.43115844	-6.05175012
C	3.75621898	-5.53520171	-3.70288027
C	5.85793213	-4.11206586	-2.42887616
C	2.02778610	-4.19474800	-5.51431725
C	6.41785255	0.03331848	-3.23502546

C	2.58770651	-0.04936366	-6.32046656
C	5.67129199	-5.49386064	-2.16015972
C	1.84114596	-5.57654278	-5.24560082
C	5.55363611	0.70354539	-4.14074396
C	3.63856310	0.66220432	-5.68346451
C	4.62043541	-6.20542863	-2.79716177
C	2.70536239	-6.24676970	-4.33988231
C	7.09542866	-2.01870316	-2.06059068
C	1.35020998	-2.14272636	-6.68875203
C	6.90878852	-3.40049794	-1.79187425
C	1.16356985	-3.52452114	-6.42003559
H	5.69690213	1.76421880	-4.34701220
H	3.78182911	1.72287773	-5.88973275
H	4.47716939	-7.26610203	-2.59089353
H	2.56209638	-7.30744310	-4.13361407
H	7.90207217	-1.47249958	-1.57162426
H	7.57216600	-3.91496789	-1.09663957
H	0.68683251	-1.62825642	-7.38398671
H	0.35692634	-4.07072472	-6.90900201
H	7.22449588	0.57952211	-2.74605920
H	6.33466928	-6.00833065	-1.46492518
H	1.92432923	0.46510634	-7.01570110
H	1.03450263	-6.12274642	-5.73456708
Cs	0.20465800	0.10074000	0.48149700

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n = 4, Energy = -386.500172487918 (54.0)

C	-3.60639401	-1.61434381	0.72560210
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C	-4.38771032	-4.24398511	1.46053813
C	-3.87760590	-1.92051434	2.08541966
C	-3.72584027	-2.62299393	-0.26674744
C	-4.26826406	-3.23533499	2.45288767
C	-4.11649842	-3.93781457	0.10072058
C	-3.21573585	-0.29952316	0.35813409
C	-3.75815964	-0.91186423	3.07776920
C	-3.45462837	-2.31682339	-1.62656500
C	-4.77836848	-5.55880576	1.82800615
C	-4.53947595	-3.54150553	3.81270523
C	-4.23594468	-4.94646469	-0.89162897
C	-3.36750149	0.40295642	2.71030118
C	-3.06397022	-1.00200274	-1.99403301
C	-4.93013411	-4.85632618	4.18017325
C	-4.62660284	-6.26128534	-0.52416095
C	-3.09628957	0.70912701	1.35048361
C	-2.94452394	0.00664743	-1.00168349
C	-5.04958039	-5.86497635	3.18782372
C	-4.89781475	-6.56745593	0.83565662
C	-4.02937152	-1.21803483	4.43758653
C	-3.57407465	-3.32547344	-2.61891431
C	-4.42002968	-2.53285548	4.80505454
C	-3.96473280	-4.64029409	-2.25144630
H	-2.79641819	1.71839070	1.06841311
H	-2.64465255	1.01591112	-1.28375399
H	-5.34945177	-6.87424004	3.46989423
H	-5.19768614	-7.57671962	1.11772713

H	-3.93768390	-0.44378926	5.19931971
H	-4.62821347	-2.76787371	5.84885826
H	-3.36589085	-3.09045521	-3.66271803
H	-4.05642043	-5.41453966	-3.01317948
H	-3.27581383	1.17720198	3.47203412
H	-5.13831791	-5.09134453	5.22397675
H	-2.85578642	-0.76698439	-3.03783652
H	-4.71829050	-7.03553090	-1.28589389
C	-1.31383719	-7.12203369	1.04016627
C	-1.48605231	-6.31701885	3.75823407
C	-1.62127434	-8.07679395	2.04531070
C	-1.09250760	-5.76476602	1.39405573
C	-1.70738190	-7.67428653	3.40434460
C	-1.17861516	-5.36225860	2.75308964
C	-1.22772964	-7.52454111	-0.31886763
C	-1.84260393	-9.43406162	1.69142124
C	-0.78507046	-4.81000576	0.38891130
C	-1.57215986	-5.91451144	5.11726797
C	-2.01481904	-8.62904678	4.40948904
C	-0.95728557	-4.00499093	3.10697910
C	-1.75649637	-9.83656904	0.33238733
C	-0.69896290	-5.21251318	-0.97012260
C	-2.10092660	-8.22653936	5.76852294
C	-1.04339313	-3.60248351	4.46601300
C	-1.44905922	-8.88180880	-0.67275716
C	-0.92029249	-6.56978087	-1.32401213
C	-1.87959701	-6.86927167	6.12241246



C	-1.35083028	-4.55724375	5.47115749
C	-2.15004102	-10.38882165	2.69656561
C	-0.56374092	-3.45273832	0.74280083
C	-2.23614858	-9.98631423	4.05559951
C	-0.64984848	-3.05023090	2.10183473
H	-1.38296258	-9.19077575	-1.71595919
H	-0.85419584	-6.87874782	-2.36721415
H	-1.94569366	-6.56030473	7.16561449
H	-1.41692692	-4.24827680	6.51435952
H	-2.31993488	-11.43066806	2.42491805
H	-2.47213909	-10.71919366	4.82715410
H	-0.32775041	-2.71985889	-0.02875376
H	-0.47995462	-2.00838449	2.37348228
H	-1.92639018	-10.87841524	0.06073966
H	-2.33691706	-8.95941855	6.54007752
H	-0.46297244	-4.47963399	-1.74167718
H	-0.87349932	-2.56063730	4.73766068
C	1.77551668	2.63609979	-1.44262270
C	0.72370336	3.56417941	1.02678137
C	0.41514429	3.03371632	-1.35494070
C	2.60998241	2.70252307	-0.29560266
C	-0.11076237	3.49775613	-0.12023867
C	2.08407575	3.16656288	0.93909937
C	2.30142334	2.17205998	-2.67732474
C	-0.41932144	2.96729305	-2.50196074
C	3.97035480	2.30490653	-0.38328466
C	0.19779670	4.02821922	2.26148341

C	-1.47113476	3.89537266	-0.03255667
C	2.91854148	3.23298615	2.08611941
C	0.10658522	2.50325324	-3.73666278
C	4.49626146	1.84086673	-1.61798670
C	-1.99704142	4.35941247	1.20214537
C	2.39263482	3.69702596	3.32082145
C	1.46695763	2.10563669	-3.82434483
C	3.66179575	1.77444343	-2.76500679
C	-1.16257571	4.42583577	2.34916546
C	1.03226241	4.09464251	3.40850350
C	-1.77969361	3.36490955	-2.41427865
C	4.80482031	2.37132984	0.76373528
C	-2.30560027	3.82894935	-1.17957661
C	4.27891365	2.83536965	1.99843732
H	1.87064653	1.74943713	-4.77210902
H	4.06548465	1.41824388	-3.71277098
H	-1.56626461	4.78203532	3.29692965
H	0.62857351	4.45084207	4.35626769
H	-2.42023428	3.31392267	-3.29473776
H	-3.34982988	4.13416207	-1.11227143
H	5.84904992	2.06611713	0.69643010
H	4.91945432	2.88635653	2.87889643
H	-0.53395521	2.45226631	-4.61712185
H	-3.04127084	4.66462517	1.26945070
H	5.54049088	1.53565403	-1.68529203
H	3.03317525	3.74801289	4.20128052
C	2.65157983	-3.43434003	2.91054055

C	2.56288960	-5.52058973	0.98562607
C	2.83297636	-3.13817409	1.53366688
C	2.42583819	-4.77363081	3.32495699
C	2.78863125	-4.18129894	0.57120964
C	2.38149308	-5.81675566	2.36249975
C	2.69592494	-2.39121518	3.87299779
C	3.05871800	-1.79888331	1.11925044
C	2.24444166	-5.06979675	4.70183066
C	2.51854449	-6.56371458	0.02316883
C	2.97002777	-3.88513301	-0.80566404
C	2.15575143	-7.15604645	2.77691618
C	3.10306311	-0.75575846	2.08170768
C	2.28878677	-4.02667190	5.66428790
C	2.92568266	-4.92825786	-1.76812128
C	2.11140632	-8.19917130	1.81445894
C	2.92166659	-1.05192435	3.45858139
C	2.51452842	-2.68738107	5.24987150
C	2.69994102	-6.26754869	-1.35370488
C	2.29280285	-7.90300541	0.43758523
C	3.24011449	-1.50271753	-0.25762306
C	2.01870006	-6.40908737	5.11624692
C	3.19576938	-2.54584238	-1.22008030
C	1.97435494	-7.45221222	4.15378968
H	2.95570614	-0.25121588	4.19736896
H	2.54856797	-1.88667260	5.98865907
H	2.66590146	-7.06825716	-2.09249244
H	2.25876329	-8.70371388	-0.30120233

H	3.41339506	-0.47467029	-0.57573150
H	3.33501039	-2.31850370	-2.27697638
H	1.87945904	-6.63642605	6.17314300
H	1.80107437	-8.48025946	4.47189812
H	3.27634365	0.27228867	1.76359946
H	3.06492363	-4.70091938	-2.82501722
H	2.14954580	-4.25401037	6.72118385
H	1.93812578	-9.22721842	2.13256717
Cs	0.20465800	0.10074000	0.48149700

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n = 4, Energy = -384.955205062682 (55.5)

C	8.36691795	6.74557643	1.39463527
C	6.19046468	8.07724347	2.64175739
C	7.52433840	7.59692300	0.63196313
C	8.12127086	6.56006338	2.78086847
C	6.43611176	8.26275652	1.25552419
C	7.03304422	7.22589690	3.40442953
C	9.45514458	6.07974291	0.77107421
C	7.76998548	7.78243605	-0.75427007
C	8.96385041	5.70871681	3.54354062
C	5.10223804	8.74307699	3.26531845
C	5.59353221	9.11410309	0.49285205
C	6.78739714	7.04038385	4.79066274
C	8.85821212	7.11660254	-1.37783113
C	10.05207704	5.04288329	2.91997956
C	4.50530558	9.77993661	1.11641311
C	5.69917050	7.70621737	5.41422380

C	9.70079171	6.26525594	-0.61515902
C	10.29772417	5.22839631	1.53374633
C	4.25965845	9.59442359	2.50264634
C	4.85659091	8.55756396	4.65155168
C	6.92740599	8.63378252	-1.51694201
C	8.71820326	5.52320386	4.92977361
C	5.83917936	9.29961604	-0.89338095
C	7.62997663	6.18903738	5.55333467
H	10.53612057	5.75415840	-1.09380798
H	11.13305303	4.71729878	1.05509737
H	3.42432959	10.10552112	2.98129529
H	4.02126206	9.06866150	5.13020064
H	7.11596608	8.77618341	-2.58102252
H	5.19241050	9.95311452	-1.47881245
H	9.36497212	4.86970538	5.51520512
H	7.44141654	6.04663649	6.61741519
H	9.04677231	7.25900330	-2.44191147
H	3.85853673	10.43343502	0.53098184
H	10.69884589	4.38938488	3.50541083
H	5.51061031	7.56381660	6.47830413
C	2.28996722	2.63160829	-0.24367378
C	1.77950802	2.26378716	2.52575550
C	1.19751573	3.29823580	0.37159654
C	3.12718912	1.78107021	0.52577054
C	0.94228613	3.11432524	1.75631118
C	2.87195952	1.59715965	1.91048518
C	2.54519682	2.81551885	-1.62838842

C	0.36029384	4.14877388	-0.39784778
C	4.21964061	1.11444270	-0.08949979
C	1.52427842	2.07987660	3.91047014
C	-0.15016537	3.78095275	2.37158150
C	3.70918141	0.74662157	2.67992949
C	0.61552344	4.33268444	-1.78256242
C	4.47487021	1.29835326	-1.47421443
C	-0.40539497	3.59704219	3.75629614
C	3.45395181	0.56271101	4.06464413
C	1.70797494	3.66605693	-2.39783280
C	3.63764833	2.14889134	-2.24365880
C	0.43182692	2.74650410	4.52574052
C	2.36150030	1.22933851	4.67991451
C	-0.73215747	4.81540124	0.21742256
C	5.05686232	0.26390477	0.67994452
C	-0.98738707	4.63149068	1.60213720
C	4.80163271	0.07999420	2.06465916
H	1.90389061	3.80722771	-3.46074750
H	3.83356400	2.29006212	-3.30657351
H	0.23591125	2.60533332	5.58865522
H	2.16558463	1.08816773	5.74282922
H	-1.37481378	5.46827912	-0.37320727
H	-1.82595907	5.14319777	2.07442219
H	5.89543432	-0.24780232	0.20765953
H	5.44428903	-0.57288368	2.65528899
H	-0.02713268	4.98556218	-2.37319229
H	-1.24396679	4.10874912	4.22858121

H	5.31344204	0.78664632	-1.94649949
H	4.09660792	-0.09016674	4.65527401
C	-0.07607366	-3.09032323	-0.49517490
C	0.46404979	-2.84605508	2.28226983
C	1.26370467	-3.12949273	-0.02628275
C	-1.14579026	-2.92901964	0.42465531
C	1.53376639	-3.00735866	1.36243962
C	-0.87572854	-2.80688557	1.81337768
C	-0.34613538	-3.21245730	-1.88389727
C	2.33342127	-3.29079632	-0.94611296
C	-2.48556859	-2.88985013	-0.04423685
C	0.73411151	-2.72392101	3.67099220
C	2.87354472	-3.04652817	1.83133178
C	-1.94544514	-2.64558199	2.73320789
C	2.06335955	-3.41293039	-2.33483532
C	-2.75563032	-3.01198421	-1.43295921
C	3.14360645	-2.92439410	3.22005414
C	-1.67538342	-2.52344792	4.12193025
C	0.72358121	-3.37376089	-2.80372754
C	-1.68591372	-3.17328779	-2.35278948
C	2.07388986	-2.76309051	4.13988441
C	-0.33560508	-2.56261742	4.59082247
C	3.67319937	-3.32996581	-0.47722076
C	-3.55528496	-2.72854657	0.87559332
C	3.94326110	-3.20783173	0.91150161
C	-3.28522324	-2.60641250	2.26431569
H	0.51628032	-3.46751168	-3.86971860

H	-1.89321462	-3.26703859	-3.41878054
H	2.28119075	-2.66933971	5.20587547
H	-0.12830419	-2.46886662	5.65681353
H	4.49431995	-3.45378336	-1.18328766
H	4.97168259	-3.23789847	1.27142589
H	-4.58370646	-2.69847983	0.51566904
H	-4.10634382	-2.48259495	2.97038259
H	2.88447989	-3.53674792	-3.04090224
H	4.17202772	-2.95446081	3.57997852
H	-3.78405159	-2.98191749	-1.79288359
H	-2.49650375	-2.39963038	4.82799717
C	4.09801677	5.25241611	1.90831458
C	5.77438986	3.54643671	3.43965618
C	5.18720144	4.58451096	1.28865375
C	3.84701865	5.06733156	3.29364621
C	6.02538798	3.73152126	2.05432454
C	4.68520519	4.21434186	4.05931701
C	3.25983022	6.10540581	1.14264379
C	5.43819956	4.76959551	-0.09667788
C	2.75783398	5.73523670	3.91330705
C	6.61257641	2.69344702	4.20532697
C	7.11457265	3.06361612	1.43466371
C	4.43420707	4.02925731	5.44464864
C	4.60001302	5.62258521	-0.86234868
C	1.91964743	6.58822640	3.14763625
C	7.95275920	2.21062642	2.20033451
C	5.27239362	3.17626761	6.21031944



C	3.51082831	6.29049039	-0.24268788
C	2.17064552	6.77331099	1.76230459
C	7.70176111	2.02554183	3.58566617
C	6.36157832	2.50836243	5.59065863
C	6.52738410	4.10169041	-0.71633852
C	2.50683599	5.55015211	5.29863849
C	7.36557065	3.24870072	0.04933227
C	3.34502253	4.69716241	6.06430928
H	2.86743163	6.94525006	-0.83042106
H	1.52724884	7.42807065	1.17457140
H	8.34515780	1.37078217	4.17339936
H	7.00497500	1.85360276	6.17839182
H	6.72005171	4.24376236	-1.77972698
H	8.20163500	2.73601292	-0.42632294
H	1.67077163	6.06283990	5.77429369
H	3.15235493	4.55509046	7.12769774
H	4.79268046	5.76465724	-1.92573698
H	8.78882346	1.69793864	1.72467952
H	1.08358317	7.10091418	3.62329123
H	5.07972618	3.03419558	7.27370774
Cs	0.20465800	0.10074000	0.48149700

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n = 5, Energy = -517.944067561807 (19.5)

C	5.26941055	4.35163907	-1.50910878
C	5.03252050	4.64933995	1.30529290
C	5.97899498	3.48049585	-0.64077734
C	4.44138110	5.37163274	-0.97023939

C	5.86054995	3.62934629	0.76642350
C	4.32293608	5.52048318	0.43696145
C	5.38785558	4.20278863	-2.91630962
C	6.80702443	2.46050218	-1.17964673
C	3.73179668	6.24277597	-1.83857084
C	4.91407547	4.79819039	2.71249373
C	6.57013437	2.75820306	1.63475495
C	3.49490663	6.54047685	0.97583084
C	6.92546945	2.31165174	-2.58684757
C	3.85024171	6.09392553	-3.24577167
C	6.45168934	2.90705350	3.04195579
C	3.37646160	6.68932729	2.38303168
C	6.21588504	3.18279496	-3.45517907
C	4.67827117	5.07393186	-3.78464113
C	5.62365988	3.92704717	3.58082524
C	4.08604601	5.81818407	3.25136318
C	7.51660870	1.58935913	-0.31131531
C	2.90376738	7.26276946	-1.29970141
C	7.39816367	1.73820957	1.09588553
C	2.78532235	7.41161990	0.10749943
H	6.30680411	3.06853653	-4.53535431
H	4.76919023	4.95967342	-4.86481636
H	5.53274082	4.04130560	4.66100048
H	3.99512695	5.93244250	4.33153842
H	8.15220883	0.80640617	-0.72495451
H	7.94284473	1.06951505	1.76242168
H	2.35908633	7.93146398	-1.96623757

H	2.14972222	8.19457286	0.52113863
H	7.56106944	1.52869895	-3.00048686
H	6.99637024	2.23835917	3.70849197
H	3.30556081	6.76261986	-3.91230786
H	2.74086161	7.47228008	2.79667097
C	7.84332738	6.87221674	1.45957602
C	9.50314328	4.82297123	0.40543963
C	7.97175449	6.71522759	0.05413625
C	8.54480822	6.00458313	2.33794760
C	8.80166244	5.69060484	-0.47293195
C	9.37471617	4.97996037	1.81087940
C	7.01341943	7.89683949	1.98664422
C	7.27027365	7.58286120	-0.82423533
C	8.41638111	6.16157227	3.74338738
C	10.33305123	3.79834847	-0.12162857
C	8.93008955	5.53361569	-1.87837172
C	10.07619701	4.11232676	2.68925098
C	6.44036571	8.60748396	-0.29716713
C	7.58647316	7.18619503	4.27045557
C	9.75999750	4.50899293	-2.40543992
C	10.90610495	3.08770401	2.16218279
C	6.31193856	8.76447315	1.10827266
C	6.88499229	8.05382868	3.39208402
C	10.46147837	3.64135928	-1.52706837
C	11.03453210	2.93071482	0.75674299
C	7.39870082	7.42587199	-2.22967488
C	9.11786189	5.29393873	4.62175873

C	8.22860877	6.40124923	-2.75674308
C	9.94776984	4.26931598	4.09469054
H	5.67489658	9.55097931	1.51285316
H	6.24795030	8.84033484	3.79666451
H	11.09852036	2.85485312	-1.93164886
H	11.67157409	2.14420866	0.35216249
H	6.86024014	8.09187249	-2.90391793
H	8.32719014	6.28074348	-3.83556667
H	9.01928052	5.41444448	5.70058232
H	10.48623053	3.60331548	4.76893358
H	5.90190504	9.27348443	-0.97140994
H	9.85857896	4.38848707	-3.48426331
H	7.48789170	7.30670089	5.34927896
H	11.44456562	2.42170353	2.83642559
C	-2.21532649	-0.61437509	-1.64532434
C	-3.59568047	-2.52447724	-0.06047981
C	-2.04421876	-2.00157988	-1.89589386
C	-3.07661121	-0.18222137	-0.60233255
C	-2.73439575	-2.95663096	-1.10347160
C	-3.76678820	-1.13727245	0.19008972
C	-1.52514951	0.34067598	-2.43774661
C	-1.18293404	-2.43373360	-2.93888565
C	-3.24771894	1.20498342	-0.35176303
C	-4.28585746	-3.47952831	0.73194246
C	-2.56328802	-4.34383575	-1.35404112
C	-4.62807292	-0.70511873	1.23308151
C	-0.49275706	-1.47868253	-3.73130792

C	-2.55754195	2.16003449	-1.14418529
C	-3.25346501	-5.29888682	-0.56161885
C	-5.31824991	-1.66016980	2.02550377
C	-0.66386476	-0.09147769	-3.48073843
C	-1.69625721	1.72788082	-2.18717712
C	-4.11474975	-4.86673315	0.48137297
C	-5.14714220	-3.04737464	1.77493428
C	-1.01182641	-3.82093822	-3.18945505
C	-4.10900356	1.63713696	0.69122864
C	-1.70200340	-4.77598929	-2.39703279
C	-4.79918055	0.68208589	1.48365090
H	-0.13408104	0.64162486	-4.08900620
H	-1.16647349	2.46098337	-2.79544488
H	-4.64453347	-5.59983570	1.08964074
H	-5.67692592	-3.78047719	2.38320205
H	-0.35069935	-4.15266189	-3.99006150
H	-1.57066012	-5.84081560	-2.58937140
H	-4.24034684	2.70196327	0.88356725
H	-5.46030761	1.01380956	2.28425735
H	0.16836993	-1.81040599	-4.53191427
H	-3.12212185	-6.36371299	-0.75395731
H	-2.68888511	3.22486066	-0.95184684
H	-5.97937689	-1.32844634	2.82611012
C	2.19834581	-0.38804545	4.51043170
C	2.13542646	-2.38088054	2.48799532
C	3.41140166	-0.87648185	3.95696493
C	0.95383029	-0.89602659	4.05268029

C	3.37994198	-1.87289940	2.94574673
C	0.92237062	-1.89244414	3.04146210
C	2.22980549	0.60837210	5.52164990
C	4.65591717	-0.36850071	4.41471634
C	-0.25922555	-0.40759019	4.60614707
C	2.10396679	-3.37729809	1.47677712
C	4.59299783	-2.36133580	2.39227996
C	-0.32214490	-2.40042528	2.58371068
C	4.68737685	0.62791684	5.42593454
C	-0.22776588	0.58882736	5.61736526
C	4.56153815	-3.35775335	1.38106176
C	-0.35360457	-3.39684283	1.57249249
C	3.47432100	1.11635329	5.97940136
C	1.01674964	1.09680855	6.07511672
C	3.31702263	-3.86573454	0.92331030
C	0.85945127	-3.88527928	1.01902567
C	5.86897278	-0.85693711	3.86124957
C	-1.50374083	-0.91557133	4.14839564
C	5.83751311	-1.85335466	2.85003138
C	-1.53520050	-1.91198888	3.13717745
H	3.49846963	1.88120898	6.75561810
H	1.04089826	1.86166424	6.85133346
H	3.29287401	-4.63059023	0.14709356
H	0.83530265	-4.65013497	0.24280892
H	6.82427000	-0.46700790	4.21262216
H	6.76866170	-2.22828122	2.42518714
H	-2.43488943	-0.54064477	4.57323988

H	-2.49049772	-2.30191809	2.78580486
H	5.64267383	1.01784610	5.77730717
H	5.49268651	-3.73267996	0.95621749
H	-1.15891423	0.96375397	6.04220954
H	-1.30890155	-3.78677209	1.22111985
C	2.46297508	2.21182571	-0.91687674
C	0.72757693	4.20249647	-1.96149279
C	2.29827605	2.34432038	-2.32105603
C	1.75997504	3.07466642	-0.03500548
C	1.43057697	3.33965575	-2.84336405
C	0.89227597	4.07000180	-0.55731350
C	3.33067416	1.21649033	-0.39456872
C	3.00127609	1.48147966	-3.20292729
C	1.92467408	2.94217176	1.36917381
C	-0.14012215	5.19783185	-2.48380081
C	1.26587793	3.47215042	-4.24754334
C	0.18927593	4.93284252	0.32455776
C	3.86897516	0.48614428	-2.68061926
C	2.79237316	1.94683638	1.89148183
C	0.39817885	4.46748580	-4.76985136
C	-0.67842315	5.92817790	-0.19775027
C	4.03367424	0.35364958	-1.27643996
C	3.49537324	1.08399562	1.00961059
C	-0.30482122	5.33032655	-3.88798012
C	-0.84312223	6.06067260	-1.60192957
C	2.83657700	1.61397440	-4.60710635
C	1.22167409	3.80501240	2.25104485

C	1.96887792	2.60930978	-5.12941438
C	0.35397502	4.80034778	1.72873682
H	4.69972491	-0.41037543	-0.87551339
H	4.16142390	0.31997062	1.41053715
H	-0.97087189	6.09435156	-4.28890668
H	-1.50917289	6.82469761	-2.00285614
H	3.37620383	0.95165295	-5.28403578
H	1.84245401	2.71101342	-6.20727041
H	1.34809800	3.70330876	3.32890088
H	-0.18565182	5.46266923	2.40566625
H	4.40860198	-0.17617713	-3.35754845
H	0.27175486	4.56918956	-5.84770719
H	2.91879716	1.84513262	2.96933766
H	-1.21804997	6.59049931	0.47917892
Cs	0.20465800	0.10074000	0.48149700

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n = 5, Energy = -510.864568502620 (26.6)

C	1.96804095	6.19148917	2.67226431
C	3.29194643	4.66279033	4.66624366
C	1.33093659	5.94431077	3.91701367
C	3.26709805	5.67431814	2.42450463
C	1.99288933	5.17996135	4.91400334
C	3.92905079	4.90996872	3.42149431
C	1.30608821	6.95583859	1.67527464
C	0.03187949	6.46148180	4.16477335
C	3.90420241	5.92149654	1.17975528
C	3.95389917	3.89844091	5.66323334



C	1.35578497	4.93278296	6.15875269
C	5.22810789	4.39279770	3.17373463
C	-0.63007325	7.22583122	3.16778367
C	3.24224967	6.68584596	0.18276561
C	2.01773771	4.16843353	7.15574237
C	5.89006063	3.62844828	4.17072430
C	0.00703108	7.47300965	1.92303428
C	1.94319254	7.20301702	0.43052524
C	3.31679484	3.65126248	6.90798273
C	5.25295630	3.38126985	5.41547370
C	-0.60522468	6.21430338	5.40952255
C	5.20325932	5.40432554	0.93199575
C	0.05672806	5.44995395	6.40651223
C	5.86521206	4.63997612	1.92898542
H	-0.50108755	8.05972854	1.15773942
H	1.43507391	7.78973591	-0.33476961
H	3.82491347	3.06454358	7.67327758
H	5.76107493	2.79455096	6.18076855
H	-1.60238832	6.61128680	5.59970431
H	-0.43231690	5.26021842	7.36198893
H	5.69230428	5.59406108	-0.02348095
H	6.86237570	4.24299270	1.73880366
H	-1.62723673	7.62281465	3.35796524
H	1.52869297	3.97869794	8.11121896
H	3.73129441	6.87558156	-0.77271099
H	6.88722411	3.23146485	3.98054273
C	3.05850429	0.56858824	4.38045626

C	1.32630154	2.20946141	2.84012889
C	3.45504194	1.00269948	3.08789856
C	1.79586526	0.95491358	4.90285027
C	2.58894056	1.82313607	2.31773488
C	0.92976389	1.77535016	4.13268659
C	3.92460566	-0.25184834	5.15061994
C	4.71768096	0.61637414	2.56550455
C	1.39932761	0.52080234	6.19540797
C	0.46020017	3.02989799	2.06996521
C	2.98547821	2.25724731	1.02517718
C	-0.33287513	2.16167550	4.65508060
C	5.58378234	-0.20406244	3.33566823
C	2.26542899	-0.29963425	6.96557165
C	2.11937684	3.07768390	0.25501350
C	-1.19897651	2.98211209	3.88491692
C	5.18724472	-0.63817372	4.62822596
C	3.52806805	-0.68595962	6.44317767
C	0.85673778	3.46400927	0.77740748
C	-0.80243889	3.41622337	2.59235919
C	5.11421845	1.05048538	1.27294703
C	0.13668875	0.90712768	6.71780180
C	4.24811708	1.87092197	0.50278335
C	-0.72941262	1.72756426	5.94763812
H	5.85206898	-1.26794543	5.21940792
H	4.19289231	-1.31573134	7.03435962
H	0.19191352	4.09378099	0.18622553
H	-1.46726316	4.04599508	2.00117723

H	6.08342736	0.75393986	0.87195439
H	4.55250165	2.20414823	-0.48939131
H	-0.16769583	0.57390142	7.70997646
H	-1.69862154	2.02410979	6.34863076
H	6.55299112	-0.50060800	2.93467580
H	2.42376122	3.41091019	-0.73716101
H	1.96104461	-0.63286054	7.95774616
H	-2.16818530	3.27865765	4.28590935
C	-1.54753434	-4.20162005	-0.48626855
C	0.20682328	-3.11265064	1.46359670
C	-0.22069700	-3.84503901	-0.84508984
C	-1.99719287	-4.01371638	0.84748536
C	0.65648181	-3.30055430	0.12984278
C	-1.12001406	-3.46923168	1.82241798
C	-2.42471315	-4.74610475	-1.46120118
C	0.22896153	-4.03294267	-2.17884375
C	-3.32403021	-4.37029743	1.20630665
C	1.08400209	-2.56816593	2.43852932
C	1.98331914	-2.94397326	-0.22897850
C	-1.56967259	-3.28132802	3.15617190
C	-0.64821728	-4.57742738	-3.15377638
C	-4.20120902	-4.91478213	0.23137402
C	2.86049795	-2.39948856	0.74595412
C	-0.69249378	-2.73684331	4.13110452
C	-1.97505466	-4.93400844	-2.79495513
C	-3.75155052	-5.10268582	-1.10237993
C	2.41083946	-2.21158487	2.07970807

C	0.63434359	-2.38026225	3.77228327
C	1.55579869	-3.67636165	-2.53766488
C	-3.77368856	-4.18239375	2.54006039
C	2.43297750	-3.13187694	-1.56273225
C	-2.89650976	-3.63790904	3.51499302
H	-2.64838202	-5.35195795	-3.54331887
H	-4.42487789	-5.52063532	-1.85074367
H	3.08416682	-1.79363536	2.82807181
H	1.30767096	-1.96231274	4.52064701
H	1.90095916	-3.82059756	-3.56146198
H	3.45146540	-2.85816330	-1.83816554
H	-4.79217647	-4.45610738	2.81549368
H	-3.24167022	-3.49367312	4.53879012
H	-0.30305702	-4.72166333	-4.17757336
H	3.87898572	-2.12577491	0.47052104
H	-5.21969679	-5.18849577	0.50680710
H	-1.03765404	-2.59260735	5.15490150
C	3.86580816	0.84387853	-5.00849812
C	5.33144262	2.81231258	-3.57923870
C	3.62663718	2.2242071	-5.25102391
C	4.83779638	0.44955337	-4.05134262
C	4.35945441	3.20663774	-4.53639420
C	5.57061361	1.43377040	-3.33671291
C	3.13299093	-0.14033850	-5.72312784
C	2.65464896	2.61674587	-6.20817942
C	5.07696736	-0.92898882	-3.80881683
C	6.06425985	3.79652961	-2.86460898

C	4.12028342	4.58517993	-4.77891999
C	6.54260182	1.03944524	-2.37955740
C	1.92183173	1.63252884	-6.92280913
C	4.34415013	-1.91320585	-4.52344654
C	4.85310065	5.56939695	-4.06429028
C	7.27541905	2.02366227	-1.66492769
C	2.16100269	0.25398661	-6.68028337
C	3.37216189	-1.51888073	-5.48060207
C	5.82508890	5.17507184	-3.10713474
C	7.03624810	3.40220450	-1.90745345
C	2.41547809	3.99528788	-6.45070509
C	6.04895546	-1.32331380	-2.85166144
C	3.14829532	4.97950491	-5.73607538
C	6.78177269	-0.33909677	-2.13703173
H	1.59848808	-0.50150389	-7.22883713
H	2.80964728	-2.27437123	-6.02915584
H	6.38760350	5.93056234	-2.55858098
H	7.59876270	4.15769499	-1.35889968
H	1.66937440	4.29797414	-7.18542311
H	2.96470630	6.03768175	-5.92223957
H	6.23254449	-2.38149064	-2.66549725
H	7.52787638	-0.64178303	-1.40231371
H	1.17572812	1.93521488	-7.65752706
H	4.66951177	6.62757366	-4.25045432
H	4.52773901	-2.97138256	-4.33728250
H	8.02152266	1.72097622	-0.93020976
C	-1.55273692	3.30133468	-1.73846424

C	-3.47013148	1.85614971	-0.22167883
C	-1.65410759	1.89204520	-1.87998175
C	-2.41006352	3.98803168	-0.83855403
C	-2.61280487	1.16945271	-1.12158904
C	-3.36876081	3.26543920	-0.08016132
C	-0.59403964	4.02392717	-2.49685695
C	-0.79678099	1.20534820	-2.77989197
C	-2.30869285	5.39732117	-0.69703652
C	-4.42882876	1.13355722	0.53671388
C	-2.71417555	-0.23983678	-1.26310655
C	-4.22608741	3.95213620	0.81974890
C	0.16191630	1.92794068	-3.53828467
C	-1.34999557	6.11991366	-1.45542923
C	-3.67287283	-0.96242927	-0.50471384
C	-5.18478469	3.22954371	1.57814160
C	0.26328701	3.33723020	-3.39676720
C	-0.49266892	5.43321669	-2.35533947
C	-4.53019948	-0.27573230	0.39519640
C	-5.28615541	1.82025419	1.43662413
C	-0.89815173	-0.20394109	-2.92140937
C	-3.16601938	6.08401797	0.20287360
C	-1.85684901	-0.92653358	-2.16301667
C	-4.12471666	5.36142548	0.96126630
H	0.99918841	3.89189624	-3.97891368
H	0.24323248	5.98788272	-2.93748596
H	-5.26610087	-0.83039833	0.97734289
H	-6.02205681	1.26558815	2.01877061

H	-0.24006295	-0.73105364	-3.61218558
H	-1.93466171	-2.00831222	-2.27164633
H	-3.08820669	7.16579661	0.31150325
H	-4.78280545	5.88853803	1.65204251
H	0.82000505	1.40082837	-4.22906081
H	-3.75068564	-2.04420774	-0.61334337
H	-1.27218276	7.20169213	-1.34679970
H	-5.84287345	3.75665603	2.26891774
Cs	0.20465800	0.10074000	0.48149700

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n = 5, Energy = -508.185673612407 (29.2)

C	-0.84602633	-2.99569709	-0.35717635
C	-0.98256605	-2.89011179	2.47757376
C	-2.10485432	-2.87694467	0.28908215
C	0.34453179	-3.06165686	0.41394020
C	-2.17312417	-2.82415202	1.70645721
C	0.27626193	-3.00886421	1.83131526
C	-0.77775648	-3.04848975	-1.77455140
C	-3.29541244	-2.81098491	-0.48203440
C	1.60335977	-3.18040928	-0.23231830
C	-1.05083590	-2.83731913	3.89494881
C	-3.43195215	-2.70539960	2.35271571
C	1.46682006	-3.07482397	2.60243181
C	-3.22714258	-2.86377756	-1.89940945
C	1.67162963	-3.23320193	-1.64969335
C	-3.50022201	-2.65260695	3.77009076
C	1.39855020	-3.02203132	4.01980686

C	-1.96831460	-2.98252998	-2.54566801
C	0.48107151	-3.16724217	-2.42080996
C	-2.30966389	-2.71856671	4.54120737
C	0.13972222	-2.90327890	4.66606542
C	-4.55424019	-2.69223251	0.16422411
C	2.79391766	-3.24636903	0.53879824
C	-4.62251004	-2.63943985	1.58159917
C	2.72564780	-3.19357637	1.95617329
H	-1.91591028	-3.02305392	-3.63365304
H	0.53347583	-3.20776610	-3.50879499
H	-2.36206821	-2.67804277	5.62919239
H	0.08731789	-2.86275496	5.75405044
H	-5.46811940	-2.64160141	-0.42768933
H	-5.58879359	-2.54828482	2.07767086
H	3.76020121	-3.33752406	0.04272655
H	3.63952702	-3.24420747	2.54808674
H	-4.14102156	-2.81314649	-2.49132295
H	-4.46650533	-2.56145193	4.26616253
H	2.63791294	-3.32435695	-2.14576512
H	2.31242918	-3.07266239	4.61172035
C	5.11911242	3.63988482	-2.67469292
C	3.88827359	5.80044835	-1.30261402
C	5.54139671	3.98033517	-1.36237832
C	4.08140871	4.37971624	-3.30096807
C	4.92597730	5.06061693	-0.67633887
C	3.46598930	5.45999801	-2.61492862
C	5.73453183	2.55960306	-3.36073238



C	6.57910042	3.24050375	-0.73610317
C	3.65912442	4.03926590	-4.61328268
C	3.27285418	6.88073012	-0.61657456
C	5.34826159	5.40106728	0.63597573
C	2.42828559	6.19982943	-3.24120377
C	7.19451983	2.16022198	-1.42214263
C	4.27454383	2.95898413	-5.29932213
C	4.73284218	6.48134904	1.32201519
C	1.81286618	7.28011120	-2.55516432
C	6.77223556	1.81977159	-2.73445726
C	5.31224756	2.21915267	-4.67304701
C	3.69513844	7.22118051	0.69574007
C	2.23515044	7.62056159	-1.24284968
C	7.00138457	3.58095413	0.57621124
C	2.62142085	4.77909728	-5.23955764
C	6.38596516	4.66123590	1.26225069
C	2.00600144	5.85937905	-4.55351818
H	7.24463495	0.99054126	-3.26106498
H	5.78464695	1.38992234	-5.19965473
H	3.22273906	8.05041084	1.22234779
H	1.76275106	8.44979191	-0.71624196
H	7.79793185	3.01305532	1.05694363
H	6.71011300	4.92256751	2.26959087
H	2.29727301	4.51776567	-6.24689781
H	1.20945416	6.42727785	-5.03425057
H	7.99106700	1.59232317	-0.94141045
H	5.05698986	6.74268074	2.32935520

H	3.95039615	2.69765244	-6.30666214
H	1.01631901	7.84801001	-3.03589649
C	-5.67887819	0.51107638	2.11278812
C	-3.43209480	1.11528037	3.74143832
C	-4.53258173	1.12465003	1.54188369
C	-5.70178296	0.19960473	3.49801766
C	-3.40919003	1.42675203	2.35620879
C	-4.57839127	0.50170673	4.31234275
C	-6.80226988	0.20897439	1.29846303
C	-4.50967696	1.43612168	0.15665416
C	-6.84807942	-0.41396891	4.06892209
C	-2.30870311	1.41738237	4.55576342
C	-2.26289357	2.04032567	1.78530435
C	-4.60129603	0.19023508	5.69757229
C	-5.63306865	1.13401969	-0.65767094
C	-7.97147112	-0.71607091	3.25459699
C	-1.13950187	2.34242767	2.59962945
C	-3.47790434	0.49233707	6.51189738
C	-6.77936516	0.52044603	-0.08676654
C	-7.94856640	-0.40459927	1.86936743
C	-1.16240660	2.03095603	3.98485901
C	-2.33160783	1.10591073	5.94099298
C	-3.36338061	2.04969524	-0.41425009
C	-6.87098408	-0.72544048	5.45415143
C	-2.23998891	2.35179724	0.40007501
C	-5.74759238	-0.42333848	6.26847653
H	-7.64168691	0.28855085	-0.71184704

H	-8.81088815	-0.63649445	1.24428693
H	-0.30008485	2.26285121	4.60993952
H	-1.46928608	1.33780591	6.56607348
H	-3.34579876	2.28878266	-1.47756018
H	-1.36008522	2.82277987	-0.03815451
H	-7.75088777	-1.19642311	5.89238095
H	-5.76517423	-0.66242591	7.33178662
H	-5.61548696	1.37310701	-1.72098087
H	-0.25959825	2.81341022	2.16140015
H	-8.85137475	-1.18705346	3.69282629
H	-3.49548603	0.25324975	7.57520732
C	-3.75614442	5.39492590	1.07513932
C	-3.67411723	4.87323040	3.86560610
C	-4.88256735	4.82350604	1.72402360
C	-2.58870789	5.70549801	1.82148843
C	-4.84155376	4.56265829	3.11925699
C	-2.54769430	5.44465026	3.21672183
C	-3.79715802	5.65577365	-0.32009407
C	-6.05000388	4.51293394	0.97767449
C	-1.46228496	6.27691786	1.17260416
C	-3.63310363	4.61238265	5.26083949
C	-5.96797669	3.99123844	3.76814127
C	-1.38025777	5.75522236	3.96307094
C	-6.09101747	4.77378169	-0.41755890
C	-1.50329856	6.53776561	-0.22262923
C	-5.92696309	3.73039069	5.16337466
C	-1.33924417	5.49437461	5.35830433

C	-4.96459455	5.34520155	-1.06644324
C	-2.67073509	6.22719351	-0.96897841
C	-4.75952656	4.04096278	5.90972383
C	-2.46566710	4.92295475	6.00718867
C	-7.17642659	3.94151417	1.62655877
C	-0.29484866	6.58748988	1.91895326
C	-7.13541299	3.68066642	3.02179216
C	-0.25383506	6.32664213	3.31418665
H	-4.99607681	5.54542974	-2.13743220
H	-2.70221735	6.42742171	-2.03996737
H	-4.72804429	3.84073459	6.98071279
H	-2.43418484	4.72272655	7.07817762
H	-8.07255753	3.70311724	1.05365695
H	-8.00006167	3.24204128	3.51987942
H	0.56980002	7.02611502	1.42086600
H	0.64229588	6.56503906	3.88708847
H	-6.98714820	4.53538485	-0.99046077
H	-6.79161154	3.29176562	5.66146198
H	-0.63865011	6.97639068	-0.72071656
H	-0.44311345	5.73277144	5.93120620
C	3.16225588	0.07381831	-2.69731087
C	3.15045329	1.56364687	-0.27948724
C	4.06397891	-0.26091072	-1.65268073
C	2.25463155	1.15346163	-2.53302919
C	4.05807761	0.48400355	-0.44376892
C	2.24873025	1.89837590	-1.32411738
C	3.16815717	-0.67109596	-3.90622268

C	4.97160324	-1.34055404	-1.81696241
C	1.35290852	1.48819067	-3.57765933
C	3.14455199	2.30856114	0.92942458
C	4.95980065	0.14927451	0.60086122
C	1.34110593	2.97801922	-1.15983570
C	4.97750453	-2.08546831	-3.02587423
C	1.35880981	0.74327639	-4.78657114
C	4.95389935	0.89418879	1.80977303
C	1.33520463	3.72293349	0.04907612
C	4.07578150	-1.75073931	-4.07050441
C	2.26643414	-0.33636695	-4.95085287
C	4.04627502	1.97383213	1.97405476
C	2.23692766	3.38820449	1.09370630
C	5.87332610	-1.67528294	-0.77233236
C	0.44528437	2.56783384	-3.41337756
C	5.86742480	-0.93036867	0.43657945
C	0.43938307	3.31274812	-2.20446575
H	4.08031137	-2.32253967	-4.99847189
H	2.27096401	-0.90816732	-5.87882034
H	4.04174515	2.54563250	2.90202224
H	2.23239779	3.96000485	2.02167378
H	6.57002371	-2.50402330	-0.89843590
H	6.55959255	-1.18730860	1.23844349
H	-0.24688338	2.82477378	-4.21524160
H	-0.25731455	4.14148848	-2.07836221
H	5.67420198	-2.91420857	-3.15197790
H	5.64606692	0.63724902	2.61163704

H	0.66664224	1.00021616	-5.58843515
H	0.63850719	4.55167375	0.17517979
Cs	0.20465800	0.10074000	0.48149700

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n = 5, Energy = -476.820309156298 (60.6)

C	4.28756190	4.41991195	-3.28292108
C	2.50028323	3.26384105	-5.16301005
C	4.63381266	3.20995240	-3.94057478
C	3.04767180	5.05183604	-3.56531187
C	3.74017333	2.63191695	-4.88061926
C	2.15403246	4.47380059	-4.50535635
C	5.18120123	4.99794740	-2.34287659
C	5.87370276	2.57802831	-3.65818399
C	2.70142103	6.26179559	-2.90765817
C	1.60664389	2.68580560	-6.10305454
C	4.08642409	1.42195741	-5.53827296
C	0.91414236	5.10572469	-4.78774714
C	6.76734210	3.15606376	-2.71813950
C	3.59506037	6.83983104	-1.96761368
C	3.19278476	0.84392196	-6.47831745
C	0.02050303	4.52768924	-5.72779163
C	6.42109137	4.36602333	-2.06048576
C	4.83495050	6.20790697	-1.68522285
C	1.95289462	1.47584603	-6.76070828
C	0.36675376	3.31772967	-6.38544537
C	6.21995337	1.36806895	-4.31583765
C	1.46153109	6.89371950	-3.19004899

C	5.32631404	0.79003350	-5.25588214
C	0.56789175	6.31568405	-4.13009348
H	7.10705392	4.80972658	-1.33890235
H	5.52091306	6.65161021	-0.96363944
H	1.26693207	1.03214278	-7.48229168
H	-0.31920880	2.87402642	-7.10702878
H	7.17170008	0.88300039	-4.09907288
H	5.59209812	-0.13873835	-5.76070086
H	1.19574701	7.82249135	-2.68523027
H	-0.38385496	6.80075260	-4.34685825
H	7.71908869	2.67099541	-2.50137466
H	3.45856865	-0.08484973	-6.98313617
H	3.32927648	7.76860273	-1.46279496
H	-0.93124356	5.01275758	-5.94455647
C	-2.43829577	-4.78363162	6.26805056
C	-3.75943534	-2.58282364	5.05288225
C	-1.78517541	-4.03593794	5.25277324
C	-3.75198591	-4.43092131	6.67574372
C	-2.44574519	-2.93553395	4.64518908
C	-4.41255570	-3.33051732	6.06815957
C	-1.77772599	-5.88403561	6.87563471
C	-0.47148526	-4.38864825	4.84508007
C	-4.40510628	-5.17861499	7.69102104
C	-4.42000512	-1.48241965	4.44529810
C	-1.79262483	-2.18784027	3.62991177
C	-5.72624584	-2.97780701	6.47585274
C	0.18908452	-5.48905224	5.45266422

C	-3.74453649	-6.27901898	8.29860519
C	-2.45319461	-1.08743629	3.02232761
C	-6.38681562	-1.87740302	5.86826859
C	-0.46403582	-6.23674596	6.46794157
C	-2.43084632	-6.63172933	7.89091205
C	-3.76688479	-0.73472593	3.43002076
C	-5.73369529	-1.12970930	4.85299124
C	0.18163491	-3.64095461	3.82980289
C	-5.71879623	-4.82590464	8.09871407
C	-0.47893488	-2.54055062	3.22221874
C	-6.37936601	-3.72550065	7.49112992
H	0.04302125	-7.08142222	6.93432656
H	-1.92378926	-7.47640559	8.35729705
H	-4.27394185	0.10995033	2.96363576
H	-6.24075235	-0.28503304	4.38660625
H	1.19003095	-3.91169704	3.51685528
H	0.02240405	-1.96661670	2.44288608
H	-6.22013516	-5.39983856	8.87804673
H	-7.38776206	-3.45475822	7.80407753
H	1.19748040	-5.75979476	5.13971677
H	-1.95185590	-0.51350236	2.24299507
H	-4.24587520	-6.85295290	9.07793774
H	-7.39521151	-1.60666050	6.18121603
C	1.09385451	0.60727359	-2.97722894
C	1.72827153	2.67389598	-1.13544001
C	2.32655205	0.57694223	-2.27300110
C	0.17836547	1.67091614	-2.76056231



C	2.64376056	1.61025343	-1.35210663
C	0.49557398	2.70422733	-1.83966784
C	0.77664600	-0.42603760	-3.89812340
C	3.24204109	-0.48670032	-2.48966773
C	-1.05433207	1.70124750	-3.46479015
C	2.04548004	3.70720717	-0.21454554
C	3.87645811	1.57992207	-0.64787880
C	-0.41991505	3.76786988	-1.62300122
C	2.92483258	-1.52001151	-3.41056219
C	-1.37154058	0.66793630	-4.38568461
C	4.19366662	2.61323326	0.27301567
C	-0.10270654	4.80118108	-0.70210675
C	1.69213502	-1.48968020	-4.11479007
C	-0.45605156	-0.39570629	-4.60235128
C	3.27817760	3.67687586	0.48968234
C	1.12999102	4.77084976	0.00212113
C	4.47473842	-0.51703157	-1.78543994
C	-1.96982090	2.76488994	-3.24812347
C	4.79194693	0.51627962	-0.86454547
C	-1.65261239	3.79820114	-2.32722901
H	1.44864399	-2.28285565	-4.82167382
H	-0.69954259	-1.18888174	-5.30923503
H	3.52166862	4.47005131	1.19656608
H	1.37348204	5.56402522	0.70900487
H	5.17747304	-1.33348965	-1.95175446
H	5.73817260	0.49299708	-0.32397617
H	-2.91604657	2.78817248	-3.78869277

H	-2.35534701	4.61465922	-2.16091448
H	3.62756697	-2.33646953	-3.57687681
H	5.13989209	2.58995087	0.81358496
H	-2.31776606	0.69121869	-4.92625390
H	-0.80544094	5.61763910	-0.53579214
C	-2.25157717	-3.40824284	0.15256537
C	-3.66701584	-4.96627185	2.05904865
C	-3.58053344	-3.05800018	0.50978434
C	-1.63034024	-4.53749999	0.74858804
C	-4.28825278	-3.83701469	1.46302598
C	-2.33805957	-5.31651450	1.70182968
C	-1.54385784	-2.62922833	-0.80067626
C	-4.20177038	-1.92874303	-0.08623832
C	-0.30138397	-4.88774265	0.39136907
C	-4.37473518	-5.74528636	3.01229028
C	-5.61720905	-3.48677204	1.82024495
C	-1.71682264	-6.44577166	2.29785234
C	-3.49405104	-1.14972852	-1.03947996
C	0.40633537	-4.10872814	-0.56187257
C	-6.32492838	-4.26578655	2.77348659
C	-2.42454197	-7.22478617	3.25109398
C	-2.16509474	-1.49997114	-1.39669897
C	-0.21490154	-2.97947095	-1.15789527
C	-5.70369148	-5.39504374	3.36950929
C	-3.75349827	-6.87454355	3.60831299
C	-5.53072646	-1.57850052	0.27098067
C	0.31985278	-6.01699966	0.98739171

C	-6.23844579	-2.35751503	1.22422231
C	-0.38786656	-6.79601417	1.94063335
H	-1.62184542	-0.90199524	-2.12841258
H	0.32834779	-2.38149505	-1.88960889
H	-6.24694080	-5.99301963	4.10122291
H	-4.29674760	-7.47251944	4.34002660
H	-6.00759149	-0.71167629	-0.18652972
H	-7.25856021	-2.08866675	1.49842562
H	1.33996719	-6.28584793	0.71318840
H	0.08899847	-7.66283840	2.39814374
H	-3.97091585	-0.28290440	-1.49699036
H	-7.34504264	-3.99693845	3.04768996
H	1.42644962	-4.37757623	-0.83607594
H	-1.94767716	-8.09161029	3.70860438
C	0.97809698	-0.30998584	5.30349139
C	-1.61432426	0.45965911	6.17101562
C	0.35364692	-1.00137479	6.37514597
C	0.30633642	0.76622558	4.66559893
C	-0.94256369	-0.61655231	6.80890808
C	-0.98987420	1.15104806	5.09936104
C	2.27430760	-0.69480832	4.86972928
C	1.02540749	-2.07758621	7.01303843
C	0.93078647	1.45761453	3.59394435
C	-2.91053487	0.84448159	6.60477773
C	-1.56701375	-1.30794126	7.88056266
C	-1.66163476	2.22725948	4.46146858
C	2.32161810	-2.46240869	6.57927632

C	2.22699709	1.07279205	3.16018224
C	-2.86322437	-0.92311878	8.31432477
C	-2.95784538	2.61208196	4.89523069
C	2.94606822	-1.77101976	5.50762172
C	2.89875771	-0.00341939	3.79807468
C	-3.53498498	0.15309266	7.67643233
C	-3.58229549	1.92069303	5.96688529
C	0.40095743	-2.76897499	8.08469284
C	0.25902592	2.53382578	2.95605206
C	-0.89525319	-2.38415251	8.51845495
C	-1.03718470	2.91864826	3.38981417
H	3.94104674	-2.06641165	5.17466350
H	3.89373623	-0.29881128	3.46511646
H	-4.52996351	0.44848455	8.00939055
H	-4.57727401	2.21608492	6.29984351
H	0.91660465	-3.59508102	8.57434274
H	-1.37458460	-2.91486662	9.34106312
H	0.73835733	3.06453989	2.13344389
H	-1.55283192	3.74475429	2.90016427
H	2.83726538	-3.28851457	7.06892604
H	-3.34255584	-1.45383270	9.13693279
H	2.70632856	1.60350597	2.33757422
H	-3.47349265	3.43818784	4.40558097
Cs	0.20465800	0.10074000	0.48149700

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n = 5, Energy = -472.350921319022 (65.1)

C	-2.32788067	-1.67154275	1.71000805
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C	-0.67154707	-0.53614237	3.71824721
C	-2.61190073	-0.37529939	2.21546411
C	-1.21569381	-2.40008592	2.20867157
C	-1.78373394	0.19240080	3.21958369
C	-0.38752701	-1.83238573	3.21279115
C	-3.15604747	-2.23924293	0.70588847
C	-3.72408760	0.35324379	1.71680059
C	-0.93167374	-3.69632928	1.70321551
C	0.15661973	0.03155782	4.72236678
C	-2.06775400	1.48864416	3.72503975
C	0.72465985	-2.56092890	3.71145466
C	-4.55225440	-0.21445640	0.71268101
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H	7.41800587	3.46077183	-7.84926377
H	-1.14058049	1.17816336	-10.61669904
H	0.01047578	7.23614859	-7.82227885
H	5.44020384	-0.40518046	-9.89489619
H	6.59126010	5.65280477	-7.10047601
C	3.02416830	-2.76418989	-1.69500508
C	3.21577978	-1.50898387	0.84533789
C	4.00047704	-1.75738671	-1.47236487
C	2.14366530	-3.14339007	-0.64747380
C	4.09628278	-1.12978369	-0.20219339
C	2.23947104	-2.51578705	0.62269768
C	2.92836256	-3.39179291	-2.96517656
C	4.88098004	-1.37818653	-2.51989615
C	1.16735656	-4.15019326	-0.87011401
C	3.31158552	-0.88138085	2.11550937
C	5.07259152	-0.12298051	0.02044682
C	1.35896804	-2.89498723	1.67022895
C	4.78517430	-2.00578955	-3.79006763
C	1.07155082	-4.77779627	-2.14028549
C	5.16839726	0.50462251	1.29061830
C	1.45477378	-2.26738421	2.94040044

C	3.80886555	-3.01259276	-4.01270789
C	1.95205381	-4.39859612	-3.18781682
C	4.28789426	0.12542236	2.33814963
C	2.43108252	-1.26058100	3.16304070
C	5.85728860	-0.37138348	-2.29725586
C	0.28685374	-4.52939330	0.17741718
C	5.95309434	0.25621953	-1.02708438
C	0.38265948	-3.90179028	1.44758867
H	3.73532453	-3.49434435	-4.98769863
H	1.87851279	-4.88034771	-4.16280756
H	4.36143529	0.60717395	3.31314037
H	2.50462355	-0.77882941	4.13803144
H	6.53316773	-0.08030725	-3.10134683
H	6.70251450	1.02904740	-0.85618450
H	-0.46256643	-5.30222116	0.00651731
H	-0.29321966	-4.19286651	2.25167964
H	5.46105324	-1.71471348	-4.59415857
H	5.91781725	1.27745027	1.46151831
H	0.32213083	-5.55062403	-2.31118550
H	0.77889483	-2.55846028	3.74449138
Cs	0.20465800	0.10074000	0.48149700

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C	2.29297219	-0.99953327	-2.97147154
C	3.78913102	-1.41159023	-0.59295996
C	2.82093990	-2.28475876	-2.67847728
C	2.51308389	0.07966373	-2.07521000

C	3.56901931	-2.49078723	-1.48922149
C	3.26116330	-0.12636475	-0.88595421
C	1.54489277	-0.79350480	-4.16072733
C	2.60082819	-3.36395576	-3.57473882
C	1.98511618	1.36488921	-2.36820426
C	4.53721043	-1.61761870	0.59629583
C	4.09698702	-3.77601271	-1.19622723
C	3.48127501	0.95283226	0.01030732
C	1.85274878	-3.15792729	-4.76399461
C	1.23703677	1.57091769	-3.55746005
C	4.84506644	-3.98204119	-0.00697144
C	4.22935442	0.74680378	1.19956311
C	1.32478104	-1.87270179	-5.05698891
C	1.01692503	0.49172069	-4.45372163
C	5.06517817	-2.90284419	0.88929014
C	4.75732217	-0.53842171	1.49255742
C	3.12879587	-4.64918101	-3.28174450
C	2.20522791	2.44408599	-1.47194278
C	3.87687529	-4.85520949	-2.09248871
C	2.95330733	2.23805751	-0.28268699
H	0.75055109	-1.71455318	-5.96986831
H	0.44269508	0.64986930	-5.36660103
H	5.63940812	-3.06099281	1.80216954
H	5.33155211	-0.69657032	2.40543682
H	2.95983689	-5.47757880	-3.96971996
H	4.28214631	-5.84175591	-1.86758467
H	1.79995689	3.43063241	-1.69684683

H	3.12226632	3.06645530	0.40528846
H	1.68378973	-3.98632484	-5.45197005
H	5.25033746	-4.96858739	0.21793271
H	0.83176574	2.55746389	-3.78236420
H	4.39831347	1.57520133	1.88753856
C	-3.07518970	4.35411105	4.52066441
C	-0.94135682	3.59177313	6.23273848
C	-1.89521679	5.14196292	4.57857326
C	-3.18824617	3.18509022	5.31879260
C	-0.82830035	4.76079396	5.43461029
C	-2.12132973	2.80392126	6.17482963
C	-4.14210614	4.73528001	3.66462737
C	-1.78216032	6.31098375	3.78044507
C	-4.36821908	2.39723834	5.26088375
C	0.12555963	3.21060417	7.08877552
C	0.35167256	5.54864583	5.49251914
C	-2.23438619	1.63490042	6.97295782
C	-2.84907676	6.69215271	2.92440803
C	-5.43513552	2.77840730	4.40484671
C	1.41858900	5.16747687	6.34855618
C	-1.16746975	1.25373146	7.82899486
C	-4.02904972	5.90430086	2.86649915
C	-5.32207910	3.94742815	3.60671849
C	1.30553258	3.99845603	7.14668440
C	0.01250320	2.04158332	7.88690374
C	-0.60218754	7.09883544	3.83835399
C	-4.48127542	1.22821770	6.05901186

C	0.46472890	6.71766648	4.69439103
C	-3.41435898	0.84704874	6.91504890
H	-4.84802075	6.19688828	2.20940033
H	-6.14105013	4.24001558	2.94961967
H	2.12450361	3.70586860	7.80378322
H	0.83147424	1.74899589	8.54400256
H	-0.51540473	7.99618250	3.22570625
H	1.37048283	7.32242608	4.73884218
H	-5.38702935	0.62345810	6.01456072
H	-3.50114179	-0.05029832	7.52769664
H	-2.76229413	7.58949960	2.31176033
H	2.32434285	5.77223627	6.39300744
H	-6.34088937	2.17364790	4.36039545
H	-1.25425239	0.35638458	8.44164256
C	0.15765985	1.77716657	3.38171666
C	2.38698382	3.52072923	3.14570094
C	1.33609725	1.52873119	4.13402328
C	0.09388444	2.89738329	2.51140219
C	2.45075923	2.40051252	4.01601541
C	1.20854642	3.76916462	2.39339432
C	-0.95700213	0.90538524	3.49972453
C	1.39987266	0.40851447	5.00433775
C	-1.08455296	3.14581867	1.75909557
C	3.50164580	4.39251056	3.02769308
C	3.62919663	2.15207713	4.76832203
C	1.14477101	4.88938133	1.52307985
C	0.28521068	-0.46326685	5.12234562

C	-2.19921494	2.27403734	1.87710344
C	4.74385861	3.02385846	4.65031417
C	2.25943299	5.76116266	1.40507199
C	-0.89322677	-0.21483151	4.37003901
C	-2.13543957	1.15382059	2.74741792
C	4.68008324	4.14407521	3.77999968
C	3.43787043	5.51272731	2.15737859
C	2.57830993	0.16007922	5.75664421
C	-1.14832825	4.26603525	0.88878126
C	3.69297192	1.03186055	5.63863635
C	-0.03366627	5.13781658	0.77077339
H	-1.74884754	-0.88401573	4.46062250
H	-2.99106035	0.48463636	2.83800141
H	5.53570402	4.81325944	3.68941619
H	4.29349121	6.18191154	2.06679510
H	2.62726432	-0.69980551	6.42470257
H	4.59754718	0.84116012	6.21611120
H	-2.05290351	4.45673569	0.31130640
H	-0.08262065	5.99770132	0.10271503
H	0.33416490	-1.32315149	5.79040383
H	5.64843379	2.83315820	5.22778886
H	-3.10379012	2.46473761	1.29962874
H	2.21047877	6.62104730	0.73701378
C	-2.35572908	-5.40839128	-2.35681195
C	-4.04726052	-5.36268131	-0.07597187
C	-3.52357724	-4.60059945	-2.35504775
C	-2.03364664	-6.19332812	-1.21815610

C	-4.36934296	-4.57774447	-1.21462771
C	-2.87941236	-6.17047313	-0.07773606
C	-1.50996335	-5.43124626	-3.49723199
C	-3.84565968	-3.81566262	-3.49370360
C	-0.86579847	-7.00111994	-1.21992029
C	-4.89302625	-5.33982632	1.06444817
C	-5.53719113	-3.76995265	-1.21286352
C	-2.55732992	-6.95540997	1.06091979
C	-2.99989396	-3.83851760	-4.63412364
C	-0.02003275	-7.02397493	-2.36034033
C	-6.38295685	-3.74709766	-0.07244348
C	-3.40309564	-6.93255499	2.20133983
C	-1.83204576	-4.64630943	-4.63588788
C	-0.34211515	-6.23903809	-3.49899623
C	-6.06087445	-4.53203450	1.06621241
C	-4.57094384	-6.12476316	2.20310407
C	-5.01350770	-3.00787095	-3.49193930
C	-0.54371618	-7.78605662	-0.08126456
C	-5.85927342	-2.98501596	-2.35151926
C	-1.38948190	-7.76320164	1.05915548
H	-1.18283125	-4.66385304	-5.51128069
H	0.30709935	-6.25658170	-4.37438903
H	-6.71008895	-4.51449088	1.94160522
H	-5.22015835	-6.10721955	3.07849687
H	-5.26074003	-2.40534895	-4.36597801
H	-6.75572033	-2.36495034	-2.35016507
H	0.35273073	-8.40612224	-0.08261874



H	-1.14224957	-8.36572364	1.93319420
H	-3.24712611	-3.23599576	-5.50816229
H	-7.27940365	-3.12703220	-0.07108914
H	0.87641405	-7.64404039	-2.36169468
H	-3.15586349	-7.53507683	3.07537848
C	-3.71077777	-1.54902875	1.22251817
C	-1.58236029	-3.33151105	1.82101242
C	-3.64328072	-2.17177349	2.49689378
C	-2.71406608	-1.81752515	0.24738968
C	-2.57907198	-3.06301464	2.79614091
C	-1.64985734	-2.70876630	0.54663681
C	-4.77498652	-0.65778760	0.92327104
C	-4.63999241	-1.90327709	3.47202227
C	-2.78156314	-1.19478041	-1.02698593
C	-0.51815154	-4.22275219	2.12025955
C	-2.51157492	-3.68575939	4.07051653
C	-0.65314565	-2.97726270	-0.42849168
C	-5.70420115	-1.01203594	3.17277514
C	-3.84577188	-0.30353926	-1.32623306
C	-1.44736618	-4.57700054	4.36976365
C	0.41106309	-3.86850385	-0.12924455
C	-5.77169825	-0.38929116	1.89839952
C	-4.84248362	-0.03504281	-0.35110458
C	-0.45065445	-4.84549698	3.39463518
C	0.47856019	-4.49124864	1.14513108
C	-4.57249526	-2.52602180	4.74639767
C	-1.78485154	-1.46327684	-2.00211420

C	-3.50828652	-3.41726295	5.04564479
C	-0.72064280	-2.35451799	-1.70286707
H	-6.58859084	0.29483054	1.66869575
H	-5.65937620	0.64907888	-0.58080835
H	0.36623814	-5.52961867	3.62433895
H	1.29545278	-5.17537033	1.37483485
H	-5.33757683	-2.31992244	5.49491187
H	-3.45647541	-3.89528536	6.02386279
H	-1.83666265	-0.98525443	-2.98033220
H	0.04443877	-2.56061735	-2.45138127
H	-6.46928268	-0.80593651	3.92128912
H	-1.39555494	-5.05502295	5.34798144
H	-3.89758312	0.17448316	-2.30445085
H	1.17614461	-4.07460328	-0.87775852
C	-5.45526251	1.37317154	-4.41416002
C	-4.32825524	3.52094447	-2.93682269
C	-6.15086123	1.90956700	-3.29844392
C	-4.19616016	1.91066255	-4.79120745
C	-5.58735759	2.98345347	-2.55977525
C	-3.63265653	2.98454901	-4.05253879
C	-6.01876615	0.29928508	-5.15282868
C	-7.40996358	1.37207599	-2.92139648
C	-3.50056145	1.37426709	-5.90692355
C	-3.76475161	4.59483094	-2.19815403
C	-6.28295631	3.51984892	-1.44405915
C	-2.37355418	3.52204002	-4.42958623
C	-7.97346721	0.29818953	-3.66006514

C	-4.06406508	0.30038063	-6.64559222
C	-5.71945268	4.59373539	-0.70539049
C	-1.81005055	4.59592648	-3.69091756
C	-7.27786852	-0.23820597	-4.77578127
C	-5.32316745	-0.23711043	-6.26854481
C	-4.46035030	5.13122644	-1.08243790
C	-2.50564924	5.13232199	-2.57520143
C	-8.10556210	1.90847145	-1.80568053
C	-2.24145929	1.91175810	-6.28397084
C	-7.54205847	2.98235792	-1.06701186
C	-1.67795565	2.98564456	-5.54530218
H	-7.71041706	-1.06252723	-5.34278748
H	-5.75571600	-1.06143169	-6.83555101
H	-4.02780176	5.95554770	-0.51543169
H	-2.07310070	5.95664325	-2.00819523
H	-9.07205625	1.49589030	-1.51625675
H	-8.07600403	3.39409812	-0.21058182
H	-1.70751373	1.50001789	-7.14040088
H	-0.71146151	3.39822571	-5.83472596
H	-8.93996119	-0.11439166	-3.37064154
H	-6.25339802	5.00547563	0.15103944
H	-3.53011974	-0.11135962	-7.50202214
H	-0.84355657	5.00850768	-3.98034116
Cs	0.20465800	0.10074000	0.48149700

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n = 6, Energy = -598.663356527008 (35.5)

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C	-4.29907731	-3.22237640	-3.70953548
C	-2.55328904	-1.43491105	-5.05964333
C	-4.73432510	-1.90832517	-4.02612450
C	-2.55568760	-4.95674618	-3.75141136
C	-0.80989932	-3.16928084	-5.10151921
C	-5.17197145	-4.11610908	-3.03448155
C	-4.29667875	0.29945873	-5.01776746
C	-1.68039490	-0.54117838	-5.73469726
C	-6.04246703	-1.48800662	-3.66765960
C	-0.37465153	-4.48333207	-4.78493019
C	-4.73672367	-5.43016030	-2.71789253
C	-2.11564268	0.77287285	-6.05128629
C	-6.47771482	-0.17395539	-3.98424862
C	-1.24754565	-5.37706479	-4.10987625
C	-3.42858172	-5.85047891	-3.07635742
C	-3.42378463	1.19319146	-5.69282140
C	-5.60482070	0.71977734	-4.65930256
C	0.06299461	-2.27554821	-5.77657304
C	-6.48011317	-3.69579048	-2.67601675
C	-0.37225318	-0.96149698	-6.09316207
C	-6.91536096	-2.38173925	-2.99260577
H	-0.91344702	-6.38573787	-3.86686074
H	-3.09448308	-6.85915199	-2.83334191
H	-3.75788327	2.20186453	-5.93583690
H	-5.93891933	1.72845042	-4.90231807

H	1.06713182	-2.59818711	-6.05173275
H	0.29778535	-0.27546270	-6.61133731
H	-7.15015170	-4.38182476	-2.15784150
H	-7.91949817	-2.05910034	-2.71744606
H	0.62948548	-4.80597107	-5.06008979
H	-1.44560438	1.45890714	-6.56946145
H	-5.40676197	-6.11619460	-2.19971737
H	-7.48185183	0.14868361	-3.70908902
C	-5.11581679	-2.53666562	0.48831266
C	-4.49822549	-0.05083728	-0.73840570
C	-3.86487283	-2.35564434	-0.15881220
C	-6.05796510	-1.47477273	0.52207833
C	-3.55607718	-1.11273017	-0.77217138
C	-5.74916945	-0.23185855	-0.09128085
C	-5.42461244	-3.77957979	1.10167184
C	-2.92272452	-3.41753724	-0.19257788
C	-7.30890906	-1.65579401	1.16920319
C	-4.18942983	1.19207690	-1.35176488
C	-2.30513322	-0.93170889	-1.41929624
C	-6.69131775	0.83003434	-0.05751517
C	-3.23152017	-4.66045141	0.42078130
C	-7.61770471	-2.89870818	1.78256237
C	-1.99633756	0.31120528	-2.03265542
C	-6.38252210	2.07294851	-0.67087435
C	-4.48246414	-4.84147274	1.06790618
C	-6.67555641	-3.96060112	1.74879672
C	-2.93848586	1.37309823	-1.99888977

C	-5.13157813	2.25396984	-1.31799923
C	-1.67178077	-3.23651588	-0.83970267
C	-8.25105715	-0.59390120	1.20296880
C	-1.36298512	-1.99360170	-1.45306185
C	-7.94226150	0.64901298	0.58960962
H	-4.71949741	-5.79554062	1.53872412
H	-6.91258968	-4.91466900	2.21961466
H	-2.70145259	2.32716610	-2.46970770
H	-4.89454486	3.20803772	-1.78881717
H	-0.94858234	-4.05163091	-0.86562141
H	-0.40275340	-1.85464875	-1.94979858
H	-9.21128888	-0.73285414	1.69970553
H	-8.66545993	1.46412801	0.61552836
H	-2.50832197	-5.47556641	0.39486266
H	-1.03610604	0.45015836	-2.52939210
H	-8.57793623	-3.03766126	2.27929906
H	-7.10572031	2.88806351	-0.64495570
C	6.29596276	-1.33717395	-2.55887062
C	4.99635975	0.35262027	-4.43536389
C	6.36389238	0.07339244	-2.41025002
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H	0.96796239	1.75543713	-5.22492686
H	0.24017434	-0.45248965	-6.02778694
H	-1.71408054	4.36282959	0.46215047
H	-0.14329397	4.55355669	-1.48627265
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H	-2.88531224	-3.76504043	-4.51113274
H	-3.41095282	3.09701413	1.71416316
H	0.82579026	3.61144537	-3.54114543

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217

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C	1.48998226	-4.41802513	-5.99823247
C	2.17326764	-4.95053762	-3.29357873
C	2.15778241	-5.62439001	-5.65892935
C	0.49602465	-2.27155160	-5.32451182
C	1.17931003	-2.80406409	-2.61985808
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C	2.51491033	-5.21679386	-1.94125186
C	2.48393988	-6.56449865	-6.67195311
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