Supplementary Information for

Reduction of 1,3,5,7-Cyclooctatetraene by a Molecular Calcium Hydride: An Even Electron Polarised Insertion/deprotonation Mechanism

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Supplementary Methods

General considerations and starting materials.

All manipulations were carried out using standard Schlenk line and glovebox techniques under an inert atmosphere of argon. NMR experiments were conducted in J Young tap NMR tubes prepared in a glovebox. NMR spectra were recorded on an Agilent ProPulse spectrometer operating at 500 MHz (^{1}H) and 126 MHz (^{13}C). The spectra were referenced relative to residual protio solvent resonances. Solvents (Toluene, Hexane) were dried by passage through a commercially available (Innovative Technologies) solvent purification system, under argon and stored in ampoules over 4Å molecular sieves. C_6D_6 was purchased from Sigma-Aldrich Corp., dried over a potassium mirror then vacuum distilled and stored over 4Å molecular sieves. Cyclooctatetraene (COT)[1] and [(BDI)CaH] (BDI = HC{(Me)CN-2,6-*i*-$Pr_2C_6H_3$}$_2$) (**2**)[2] were synthesised according to literature procedures.

NMR spectra of compound 3

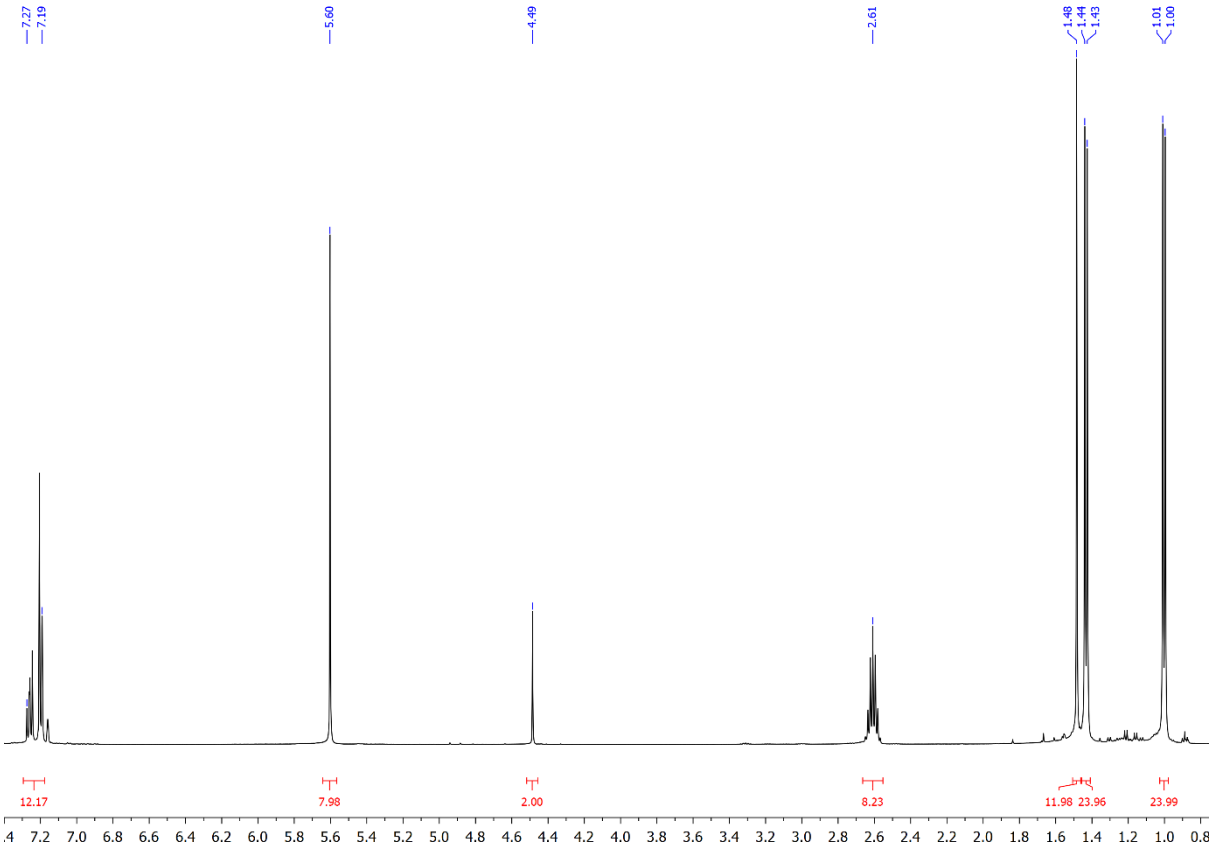

Figure S1 ^{1}H NMR spectrum (500 MHz, benzene-d_6, 298 K) of compound **3**.

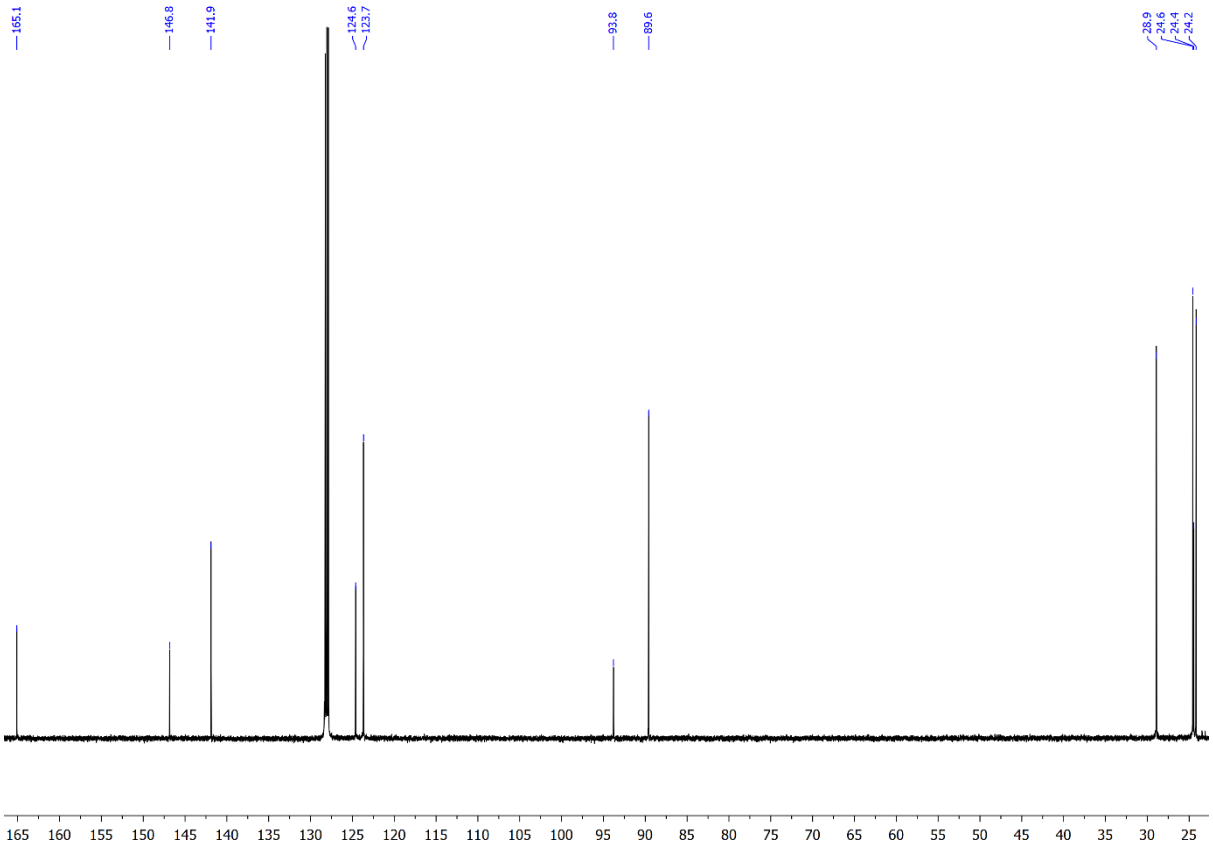

Figure S2 ^{13}C{^{1}H} NMR spectrum (126 MHz, benzene-d_6, 298 K) of compound **3**.

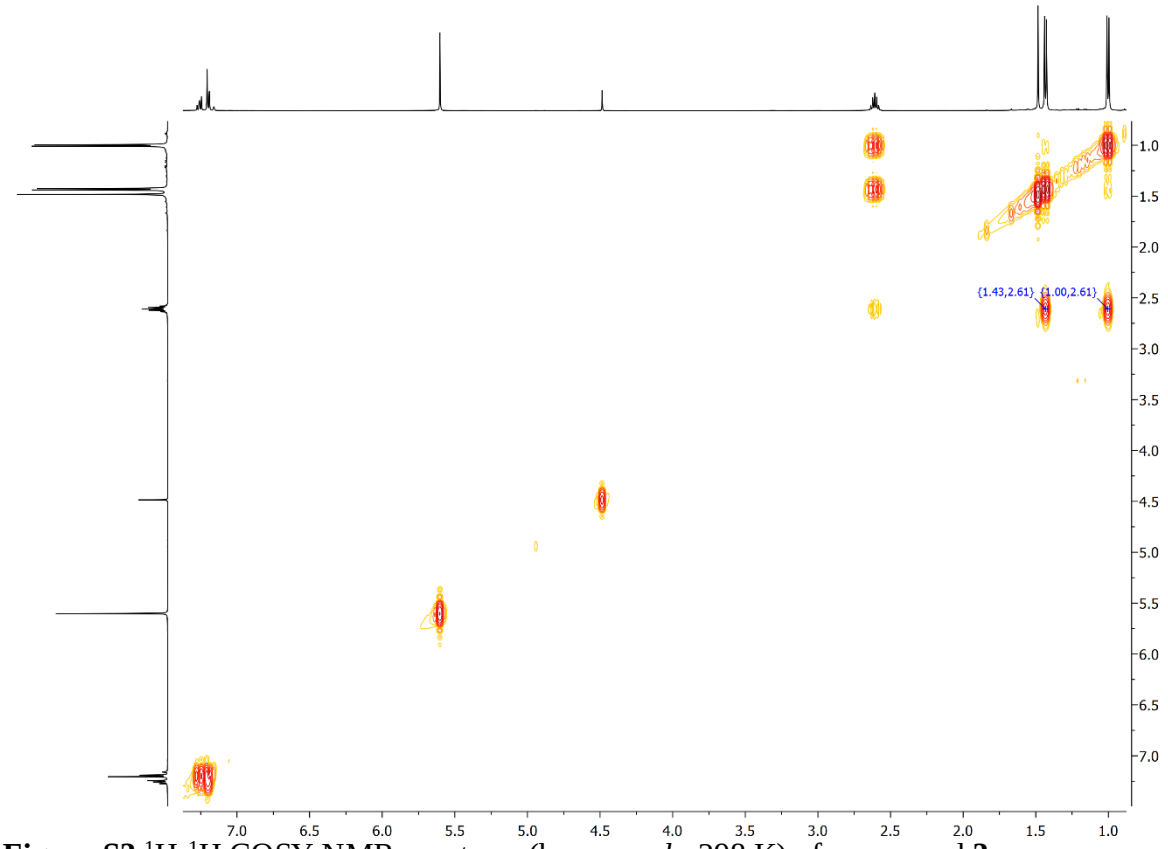

Figure S3 ^{1}H-^{1}H COSY NMR spectrum (benzene-d_6, 298 K) of compound **3**.

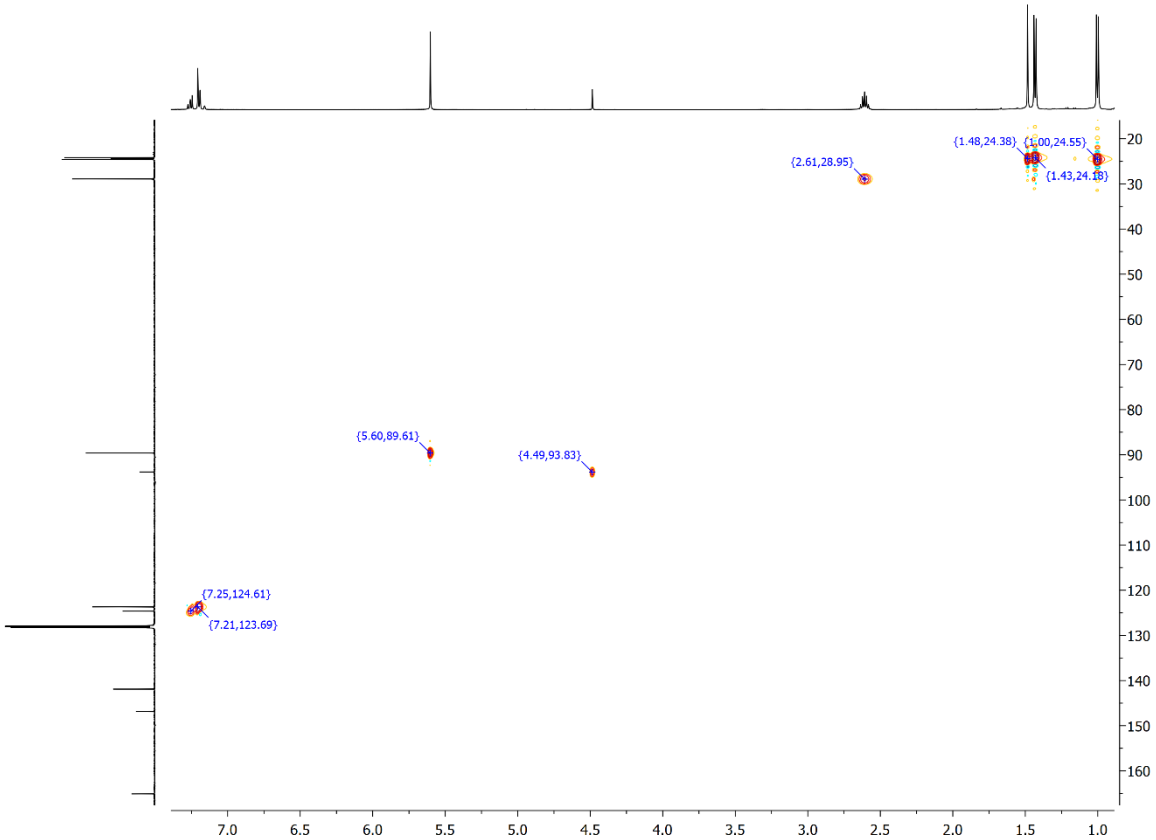

Figure S4 ^{1}H-^{13}C HSQC NMR spectrum (benzene-d_6, 298 K) of compound **3**.

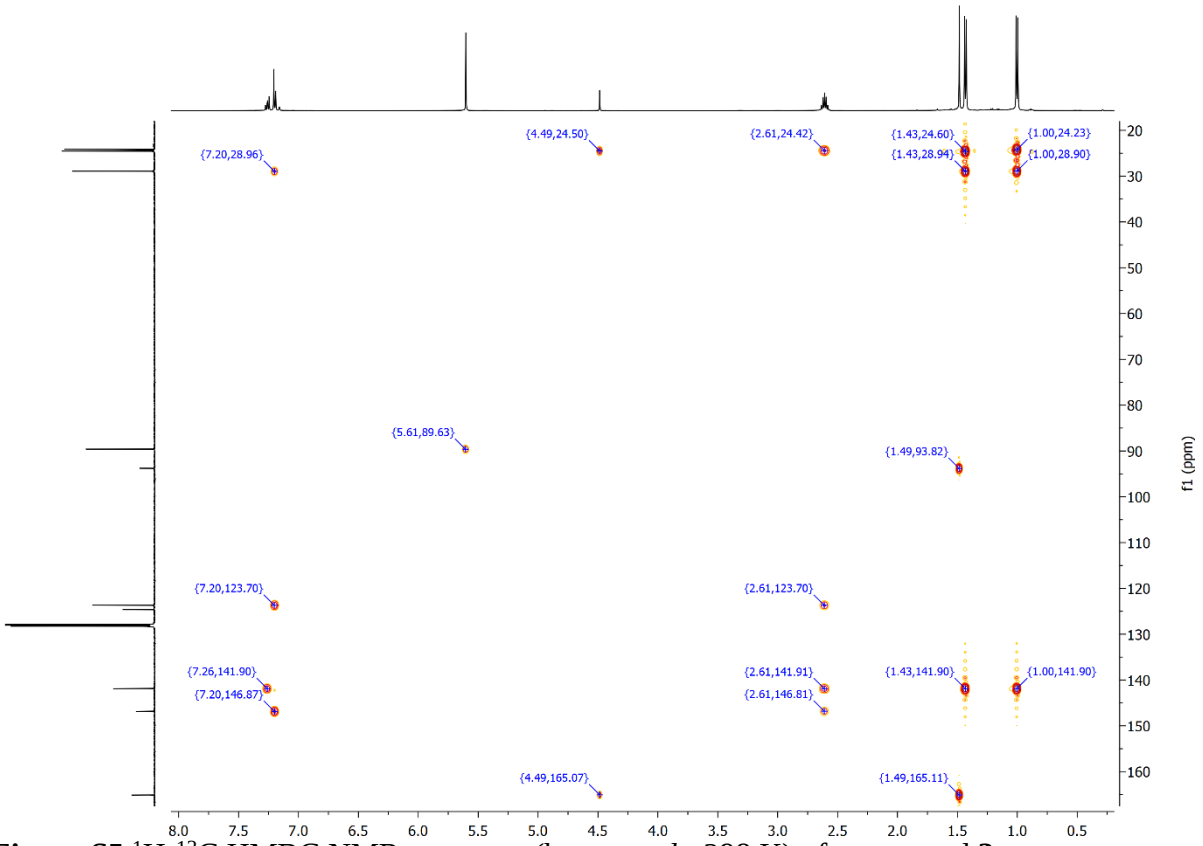

Figure S5 ^{1}H-^{13}C HMBC NMR spectrum (benzene-d_6, 298 K) of compound **3**.

EPR investigation of the reaction of Compound 2 and 1,3,5,7-C_8H_8

Samples for EPR measurements were prepared under an N_2 atmosphere in a glovebox. A solution of compound **2** was prepared by dissolving ca. 21 mg in 500 μL of dry benzene and transferred to a 4 mm medium wall low pressure/vacuum suprasil EPR tube (727-LPV-250M, Wilmad Labglass). *Ca.* 10 μL of 1,3,5,7-C_8H_8 was suspended at the top of the EPR tube, prior to dissolution with compound **2** before rapid transfer to the pre-cooled EPR cavity. The X-band CW EPR measurements were performed on a Bruker EMX spectrometer utilising an ER4119HS resonator, 20 or 100 kHz field modulation and 1 mW microwave power. Spectra were recorded at 20 K intervals between 140 and 298 K.

X-ray diffraction analysis of compound 3

Single crystals of $C_{66}H_{90}Ca_2N_4$ (**3**) were isolated from a saturated hexane solution at −30°C. A suitable crystal was selected and mounted on a SuperNova, Dual, Cu at zero, EosS2 diffractometer. The crystal was kept at 150.01(10) K during data collection. Using Olex2,[3] the structure was solved with the olex2.solve[4] structure solution program using Charge Flipping and refined with the ShelXL[5] refinement package using Least Squares minimisation. The asymmetric unit in **3** comprises half of a dimer. A crystallographic inversion centre coincident with the centroid of the C_8 ring serves to generate the remainder of the molecule.

Computational studies

Calculations were carried out using the Gaussian09 package[6] at the DFT level by means of the hybrid density functional B3PW91.[7] A triple-zeta 6-311G basis set augmented by a polarization and diffuse function was used for the Ca atom. Polarized all electron triple-zeta 6-311G(d,p) basis set were used for N, whereas a polarized all electron double-zeta 6-31G(d,p) basis set were used for the C and H atoms. The nature of the optimized stationary point, minima or transition state, has been verified by means of analytical frequency calculation at 298.15 K and 1 atm. The geometry optimisations have been achieved without any geometrical constraints. IRC calculations were carried out in order to confirm the connectivity between reactant(s), transition state and product(s). Energy data are reported in the gas phase.

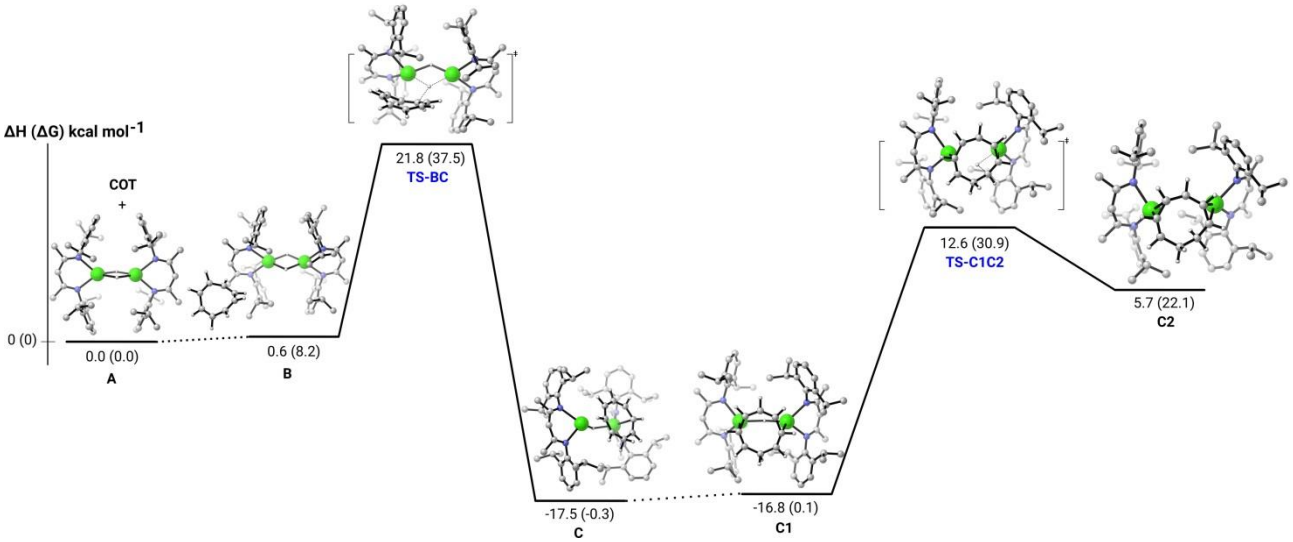

Figure S6: Computed enthalpy pathway at room temperature of the two nucleophilic attack of the COT by the hydrides.

Cartesian coordinates of all optimized structures

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C 23.366332 22.119129 2.859594
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C 26.979550 19.658640 0.912866
C 21.850637 22.266262 2.844515
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C	22.707476	21.131150	10.539486
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C	23.136553	22.512357	8.659964
C	24.441332	22.671973	8.134433
C	24.801445	23.892781	7.554477
C	23.913300	24.958360	7.495404
C	22.633507	24.799362	8.013643
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C	25.465085	21.551252	8.163810
C	26.787907	21.965009	8.823278
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C	2.657416	-0.049033	1.901935
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C	1.560022	-2.356026	2.375482
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164
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C -4.867196 -1.682507 1.828250
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C	-1.921534	2.783671	4.168787
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C	1.034875	-5.572073	-3.516080
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H	-2.219041	-0.632823	-6.320917
H	-2.221334	1.483169	-6.614606
H	-0.476638	1.756947	-6.635528
H	-1.474314	2.655922	-5.503732
H	-2.925704	-3.115882	-2.919588
H	-3.699198	-4.913358	-4.515560
H	-4.876273	-4.586076	-3.229137
H	-3.854889	-6.028524	-3.153959
H	-3.035621	-5.353473	-0.820311
H	-4.100636	-3.946262	-0.900519
H	-2.374119	-3.742659	-0.539850
H	-1.728398	-6.593373	-2.257961
H	0.540023	-7.404358	-2.797646
H	2.171901	-5.879858	-3.847585

H 1.568941 -2.254123 -4.406649
H 2.575417 -2.839023 -6.600749
H 0.863773 -3.297523 -6.536048
H 2.117114 -4.536517 -6.362485
H 3.322122 -3.400712 -2.950377
H 3.953592 -2.709340 -4.458337
H 3.713275 -4.448691 -4.323271
H 1.591199 0.333027 -4.977800
H 3.397885 2.466209 -6.235949
H 1.830104 1.962200 -6.880165
H 3.170038 0.804032 -6.794330
H 4.010618 -0.037925 -4.549611
H 3.182372 0.413406 -3.047693
H 4.168572 1.601997 -3.901659
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H 1.859775 5.541372 -3.186256
H -0.442017 5.175865 -2.367470
H -2.288503 1.943268 -2.680779
H -2.715796 4.942918 -3.133632
H -3.987794 3.737682 -2.881157
H -2.981378 3.672707 -4.335925
H -1.388320 2.642532 -0.421288
H -3.092426 3.089073 -0.635363
H -1.826643 4.311910 -0.776949
H 0.079947 -3.007320 2.993361
H -0.586776 -3.200035 0.883185
H 0.543620 -3.017180 -1.066002
H 1.959052 -2.183888 3.994239
H 3.468454 -0.597597 3.323352
H 3.742455 0.561786 1.428395
H 2.266866 -1.615653 -1.765541
H 3.290642 0.155140 -0.721497
164
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C -2.716699 -0.404436 2.936961
C -2.806332 -1.206083 4.103264
C -3.646386 -2.323695 4.096001
C -4.389857 -2.668803 2.974216
C -4.288696 -1.888836 1.828935
N -1.844645 0.727383 2.929938
C -2.351211 1.903544 3.318118
C -3.855321 2.046195 3.477743
C -2.028150 -0.879872 5.369296
C -1.155646 -2.059496 5.820949
C -3.353287 0.025098 0.491802
C -2.505788 -0.763706 -0.518259
C -1.610098 3.058226 3.629402
C -0.226968 3.275274 3.862454
C 0.068299 4.592100 4.562298

N	0.746503	2.442754	3.529121
C	2.097589	2.700648	3.917264
C	2.638463	1.975563	5.011033
C	3.983881	2.154257	5.342246
C	4.799846	3.018139	4.620469
C	4.263523	3.726986	3.554612
C	2.920493	3.592093	3.185201
C	1.765878	1.059920	5.856897
C	2.500672	-0.177108	6.386438
C	2.407623	4.419184	2.014600
C	3.089352	4.021417	0.697360
C	1.133203	1.838129	7.022248
C	2.579394	5.927249	2.257766
C	-2.958417	-0.437992	6.509745
C	-4.707597	0.392580	-0.127512
Ca	0.386093	0.572262	2.086403
C	1.237163	-2.917116	-0.112119
C	2.218468	-2.439098	-1.004220
C	2.771015	-1.147238	-1.138882
C	2.835196	-0.044647	-0.248969
C	2.880379	0.058337	1.167724
C	2.476962	-0.802610	2.208470
C	1.473983	-1.795903	2.227339
C	0.830137	-2.514669	1.188274
Ca	0.279467	-1.138907	-1.919165
N	-0.303645	0.567728	-3.490064
C	0.410963	1.803932	-3.543292
C	1.476919	1.952872	-4.466734
C	2.185904	3.157501	-4.497118
C	1.872568	4.209185	-3.645083
C	0.834525	4.055519	-2.734562
C	0.096010	2.870587	-2.666609
C	1.869583	0.846419	-5.434570
C	3.337109	0.432813	-5.253283
C	-0.999684	2.745763	-1.620309
C	-0.368093	2.577709	-0.229927
C	-1.373101	0.435198	-4.282933
C	-1.929491	1.661490	-4.985855
C	-2.044472	-0.767980	-4.569330
C	-1.705384	-2.128849	-4.352440
C	-2.534450	-3.100485	-5.175839
N	-0.764796	-2.561746	-3.527612
C	-0.415406	-3.946524	-3.476335
C	-1.178960	-4.875455	-2.726791
C	-0.730802	-6.197912	-2.634564
C	0.432879	-6.617521	-3.263653
C	1.171759	-5.703589	-4.006556
C	0.774173	-4.369458	-4.124910
C	-2.473376	-4.502364	-2.017758
C	-2.338046	-4.621992	-0.492784
C	1.584624	-3.412047	-4.986704

C	3.095121	-3.670453	-4.943918
C	1.086372	-3.434767	-6.441149
C	-3.660835	-5.348536	-2.504484
C	1.604304	1.243294	-6.894930
C	-1.986033	3.920507	-1.615377
H	-3.444892	8.006502	1.587206
H	-3.039078	8.623786	1.667921
H	-0.655439	4.771372	5.363092
H	1.074991	4.621931	4.982798
H	-0.026081	5.421799	3.850906
H	-2.224200	3.910865	3.901787
H	-4.129307	3.048991	3.812555
H	-4.371382	1.843936	2.532680
H	-4.243631	1.321240	4.200510
H	0.942304	0.712986	5.220021
H	0.529128	2.677558	6.664678
H	0.485036	1.184562	7.619093
H	1.910663	2.240016	7.683741
H	3.246589	0.083475	7.146724
H	1.788008	-0.861040	6.860652
H	3.012544	-0.723595	5.586970
H	4.404101	1.605374	6.180109
H	5.846328	3.137643	4.889360
H	4.901003	4.405622	2.992481
H	1.335032	4.220161	1.911141
H	2.112236	6.501103	1.447807
H	2.127989	6.242585	3.203753
H	3.639032	6.207303	2.287711
H	2.946041	2.960220	0.472743
H	2.686778	4.600562	-0.142254
H	4.169118	4.207347	0.740482
H	-2.827485	0.958672	0.717696
H	-5.259711	-0.495187	-0.456147
H	-5.341047	0.931128	0.585393
H	-4.564911	1.031729	-1.007002
H	-2.356966	-0.192907	-1.445133
H	-1.542089	-1.037554	-0.054070
H	-2.994800	-1.705970	-0.785042
H	-4.866657	-2.159847	0.948342
H	-5.040442	-3.539522	2.991413
H	-3.723090	-2.934892	4.992467
H	-1.365322	-0.039400	5.138188
H	-3.660227	-1.236365	6.780628
H	-2.376803	-0.186357	7.404976
H	-3.546548	0.443851	6.234679
H	-0.471863	-2.380104	5.027692
H	-0.556401	-1.779288	6.695375
H	-1.762382	-2.927356	6.105989
H	-2.693709	-2.711544	-6.185860
H	-3.523244	-3.227451	-4.717998
H	-2.068146	-4.085002	-5.244760

H	-2.904792	-0.643628	-5.219343
H	-2.198566	2.440545	-4.264493
H	-2.813405	1.416947	-5.578831
H	-1.179585	2.104316	-5.649856
H	-2.693416	-3.454987	-2.252950
H	-3.774036	-5.307722	-3.592536
H	-4.594217	-4.994253	-2.049616
H	-3.540111	-6.401707	-2.224372
H	-2.117237	-5.654173	-0.195923
H	-3.267724	-4.324810	0.006927
H	-1.532834	-3.988589	-0.108601
H	-1.310835	-6.913233	-2.056081
H	0.763226	-7.649588	-3.177605
H	2.079305	-6.035463	-4.502643
H	1.407549	-2.398516	-4.604925
H	1.658793	-2.731091	-7.058221
H	0.029271	-3.160214	-6.510158
H	1.203164	-4.436459	-6.873127
H	3.473439	-3.722227	-3.917276
H	3.627270	-2.863603	-5.459866
H	3.365809	-4.605150	-5.449371
H	1.244980	-0.024587	-5.210027
H	2.205973	2.112451	-7.187778
H	0.551725	1.495595	-7.061874
H	1.861466	0.417620	-7.569592
H	3.586652	-0.398291	-5.923494
H	3.539808	0.114669	-4.224995
H	4.021442	1.257708	-5.485081
H	2.999867	3.275168	-5.208943
H	2.433772	5.139150	-3.688513
H	0.588587	4.876060	-2.064296
H	-1.568422	1.837709	-1.846408
H	-1.500783	4.858503	-1.322206
H	-2.797761	3.736320	-0.901396
H	-2.431840	4.073555	-2.604012
H	0.365983	1.753837	-0.257204
H	-1.134411	2.408054	0.539071
H	0.191183	3.474536	0.055022
H	-0.008568	-3.107945	1.558425
H	0.765011	-3.847738	-0.434383
H	2.430543	-3.116356	-1.834173
H	1.166221	-2.116520	3.226647
H	2.858934	-0.518978	3.191410
H	3.436158	0.933828	1.510770
H	3.298960	-0.971120	-2.080328
H	3.210964	0.856154	-0.738418

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C	-1.562554	-2.278884	3.720795
C	-2.179609	-3.500064	3.436315
C	-3.096800	-3.632703	2.398567
C	-3.413471	-2.523709	1.625367
N	-1.249384	0.095766	3.179395
C	-1.911822	0.999048	3.906067
C	-3.349316	0.725542	4.330390
C	-0.567911	-2.172987	4.870582
C	0.121674	-3.499496	5.209287
C	-3.201074	-0.092128	0.996999
C	-2.453837	-0.182796	-0.345470
C	-1.407061	2.232408	4.348876
C	-0.111567	2.803969	4.313156
C	-0.018793	4.112528	5.086677
N	0.939363	2.298517	3.689372
C	2.203855	2.942412	3.837522
C	3.141154	2.403190	4.757431
C	4.406797	2.987077	4.850966
C	4.765759	4.073687	4.059552
C	3.839222	4.602998	3.171572
C	2.553350	4.064878	3.048932
C	2.767478	1.239584	5.666089
C	3.949374	0.336737	6.036225
C	1.577023	4.723743	2.083710
C	2.023463	4.561778	0.625343
C	2.078414	1.733906	6.948662
C	1.366473	6.211674	2.406165
C	-1.208226	-1.595634	6.143837
C	-4.708942	0.060711	0.765753
Ca	0.993172	0.329293	2.170665
C	1.196089	-2.161352	1.063347
C	0.996614	-1.376852	-0.093157
C	1.511403	-0.133672	-0.559879
C	2.465528	0.790719	-0.065542
C	3.343933	0.831397	1.035170
C	3.608499	-0.006128	2.136167
C	3.066649	-1.214919	2.618445
C	2.052112	-2.091997	2.182435
Ca	-0.543481	-0.724245	-2.395405
N	-0.260654	0.542591	-4.309255
C	0.433637	1.760039	-4.029844
C	1.835602	1.845835	-4.235844
C	2.491102	3.029824	-3.885119
C	1.801975	4.114434	-3.356006
C	0.430226	4.020676	-3.153751
C	-0.273641	2.854572	-3.469865
C	2.652575	0.702266	-4.825354
C	3.650152	0.128069	-3.806641
C	-1.780380	2.811642	-3.251360
C	-2.199760	3.367046	-1.883114
C	-0.608120	0.253438	-5.563557

C	-0.369106	1.256953	-6.674622
C	-1.158691	-0.970672	-5.983867
C	-1.398987	-2.159304	-5.268918
C	-1.845422	-3.334750	-6.116700
N	-1.253190	-2.276382	-3.954595
C	-1.505691	-3.486357	-3.248060
C	-2.828704	-3.907872	-2.951957
C	-3.004608	-5.002836	-2.099256
C	-1.922848	-5.678497	-1.549104
C	-0.629268	-5.282747	-1.871538
C	-0.391312	-4.200029	-2.723025
C	-4.060870	-3.246017	-3.558195
C	-4.973580	-2.609927	-2.500696
C	1.034244	-3.866151	-3.153912
C	2.113136	-4.236377	-2.131541
C	1.346866	-4.525469	-4.508371
C	-4.871682	-4.242958	-4.403050
C	3.403297	1.131405	-6.096666
C	-2.533944	3.547814	-4.370829
H	-3.125543	4.163898	2.652230
H	-3.572815	4.650706	2.309917
H	-0.603359	4.056434	6.010055
H	1.009186	4.380681	5.335501
H	-0.442494	4.927175	4.486582
H	-2.120210	2.820670	4.917580
H	-3.660763	1.408231	5.124588
H	-4.039807	0.858925	3.489399
H	-3.478480	-0.301316	4.683356
H	2.039269	0.624946	5.122539
H	1.158732	2.283404	6.730894
H	1.816456	0.887374	7.595969
H	2.745394	2.397769	7.513183
H	4.643545	0.832287	6.726180
H	3.584125	-0.563989	6.543500
H	4.515456	0.022514	5.153700
H	5.131066	2.582983	5.552801
H	5.759451	4.507596	4.141747
H	4.115470	5.460328	2.561242
H	0.610693	4.218240	2.188021
H	0.584307	6.635533	1.763725
H	1.071980	6.366368	3.449145
H	2.281731	6.790617	2.233290
H	2.117662	3.505713	0.358854
H	1.297171	5.023720	-0.055033
H	2.995467	5.040384	0.452136
H	-2.841137	0.817332	1.487513
H	-5.125360	-0.769812	0.185148
H	-5.250833	0.098445	1.716242
H	-4.921804	0.986491	0.217424
H	-2.722369	0.659314	-0.999672
H	-1.374137	-0.167582	-0.125154

H	-2.716713	-1.129925	-0.842230
H	-4.130642	-2.628729	0.814381
H	-3.560020	-4.595002	2.195497
H	-1.936090	-4.372117	4.036189
H	0.213238	-1.471011	4.551800
H	-2.059450	-2.210078	6.463852
H	-0.477453	-1.583394	6.962048
H	-1.556431	-0.570182	5.998821
H	0.518612	-3.996551	4.318102
H	0.957175	-3.317059	5.894720
H	-0.558751	-4.198052	5.712488
H	-1.216470	-3.417006	-7.008921
H	-2.874993	-3.184933	-6.462644
H	-1.804509	-4.278858	-5.569666
H	-1.364505	-1.034518	-7.048284
H	-0.361743	2.286023	-6.309359
H	-1.132197	1.158046	-7.451930
H	0.602923	1.071723	-7.146486
H	-3.723711	-2.441244	-4.219745
H	-4.251789	-4.740264	-5.155254
H	-5.690486	-3.728356	-4.920325
H	-5.318151	-5.022945	-3.775238
H	-5.336275	-3.354767	-1.782469
H	-5.849609	-2.152234	-2.976117
H	-4.456475	-1.827840	-1.936713
H	-4.013585	-5.332779	-1.862160
H	-2.085094	-6.518599	-0.879008
H	0.212179	-5.827394	-1.455020
H	1.098800	-2.779709	-3.325081
H	2.364693	-4.273910	-4.829523
H	0.654877	-4.201331	-5.290729
H	1.277329	-5.616790	-4.424885
H	1.912491	-3.819279	-1.139706
H	3.080989	-3.845039	-2.463365
H	2.222986	-5.323606	-2.038975
H	1.959672	-0.099833	-5.102742
H	4.186432	1.863788	-5.867701
H	2.736685	1.584676	-6.837883
H	3.890909	0.265306	-6.559757
H	4.190088	-0.721627	-4.242154
H	3.162608	-0.211676	-2.887130
H	4.393912	0.879322	-3.516451
H	3.565595	3.103522	-4.033919
H	2.332073	5.026843	-3.096583
H	-0.104961	4.872166	-2.741845
H	-2.091945	1.758313	-3.305111
H	-2.240630	4.604101	-4.402234
H	-3.617059	3.502724	-4.203088
H	-2.326600	3.112647	-5.353176
H	-1.633088	2.912736	-1.062446
H	-3.267399	3.186356	-1.708963

H -2.046313 4.450316 -1.822217
H 1.878119 -2.908415 2.879807
H 0.507275 -3.002626 1.114278
H 0.298769 -1.922741 -0.743602
H 3.505384 -1.525927 3.565397
H 4.360169 0.415008 2.800341
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C -4.826525 -1.313191 2.495655
C -5.730238 -0.406356 1.950029
C -5.429646 0.949348 1.967064
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H	0.626831	-2.091610	-6.543409
H	-0.556074	1.212755	-6.698585
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164
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C	1.695249	-2.315531	2.386776
C	1.615792	-3.182455	1.176207
C	2.140451	-2.961957	-0.200776
C	2.913567	-2.006951	-0.806747
C	3.303511	-0.659482	-0.517969
C	3.172744	0.163687	0.605260
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N	1.372864	0.556503	-3.695891
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164
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C	-3.104061	3.475527	0.282223
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H	-1.211982	3.453518	5.850167
H	0.535388	3.272732	5.974830
H	-0.337954	1.079791	6.021291
H	-2.545162	-0.148738	6.547875
H	-2.404461	-1.739179	5.785290
H	-1.009846	-1.010205	6.615147
H	2.177068	2.924521	3.585427
H	2.021215	4.946075	5.112764
H	3.685779	4.386148	4.877455
H	3.102035	5.818611	4.021776
H	3.868015	4.797991	1.844010
H	4.430245	3.351351	2.689715
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H	2.145460	6.249463	1.950030
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H	-2.441227	2.615117	2.125081
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H	-3.167612	4.461442	3.629369
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H	-4.059889	2.940085	0.293717
H	-3.280709	4.449121	-0.190263
H	-3.544661	1.116843	3.278002
H	-6.073891	0.620710	4.938810
H	-4.447839	0.856490	5.591745
H	-5.256404	2.179301	4.731698
H	-5.568986	2.081288	2.212596
H	-4.996812	0.676292	1.290229
H	-6.412612	0.539293	2.340337
H	-6.337836	-1.327926	3.451174
H	-6.044061	-3.783896	3.452898
H	-3.766391	-4.731571	3.395359
H	-0.630185	-2.759582	3.230690
H	-1.836972	-5.045192	4.878717
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H	-1.116916	-3.572407	5.544058
H	-1.408694	-4.009825	1.229498

H	-0.339217	-5.035196	2.205931
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H	-1.703880	-3.221227	-5.098635
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H	-2.740603	-1.810003	-4.928285
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H	0.804385	1.390397	-6.837815
H	2.357144	1.704566	-6.030516
H	0.925726	2.602159	-5.553108
H	-2.483055	-1.025801	-2.616545
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H	3.265104	-1.128420	-4.375414
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H	3.738149	-0.028586	-6.547171
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H	5.293648	-2.487411	-4.188443
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C	-3.774225	-3.831469	3.060927
C	-5.072870	-3.375403	2.887104
C	-5.306117	-2.006509	2.871226
N	-1.893726	-0.599462	3.399800
C	-1.604226	-0.167329	4.621978
C	-2.113060	-0.886779	5.864894
C	-1.317808	-3.569387	3.436918
C	-0.961588	-4.546930	2.308992
C	-4.601138	0.396424	3.041895
C	-5.545132	0.789153	1.897768
C	-0.804219	0.966024	4.937001
C	-0.550452	2.214951	4.277792
C	-0.554139	3.388025	5.244975
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C	-0.196833	3.677745	2.427042
C	1.024658	4.397365	2.519162
C	1.101437	5.671855	1.945171
C	0.027827	6.245480	1.278595
C	-1.156798	5.529247	1.175792
C	-1.290175	4.255275	1.735637
C	2.274462	3.866756	3.210201
C	3.470603	3.841657	2.244564
C	-2.637004	3.560474	1.641001
C	-3.157529	3.485852	0.199348
C	2.656269	4.685492	4.454489
C	-3.657669	4.254275	2.556360
C	-1.212355	-4.286175	4.792871
C	-5.198144	0.824347	4.391657
Ca	0.214091	0.061161	2.411194
C	2.596549	-0.640027	2.892933
C	1.984111	-1.919818	2.800089
C	2.299636	-2.975181	1.751529
C	2.005824	-2.686745	0.271517
C	3.036911	-1.972608	-0.536563
C	3.327164	-0.624483	-0.413011
C	2.828427	0.364533	0.486662
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Ca	1.213722	-0.704455	-1.905751
N	1.656485	0.498707	-3.887990
C	2.823944	1.307096	-3.746793
C	4.095863	0.737049	-4.013364
C	5.239057	1.504823	-3.771786
C	5.149809	2.798976	-3.270829
C	3.899374	3.351844	-3.020886
C	2.723612	2.633195	-3.259106

C	4.237854	-0.664021	-4.594461
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C	1.378364	3.290422	-2.983291
C	1.128176	3.448990	-1.478044
C	0.942433	0.557088	-5.007512
C	1.295202	1.565111	-6.084535
C	-0.177805	-0.251592	-5.288844
C	-0.740335	-1.319276	-4.567085
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C	-0.933700	-2.875436	-2.776617
C	-2.054052	-2.711215	-1.923251
C	-2.559230	-3.825729	-1.248043
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C	-0.913389	-5.244355	-2.276290
C	-0.366541	-4.159480	-2.968968
C	-2.706537	-1.347483	-1.742989
C	-2.266669	-0.678685	-0.433169
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H	2.074093	2.837899	3.528024
H	1.852418	4.721162	5.194251
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H	4.331153	3.345026	2.708357
H	3.231570	3.314975	1.316211
H	2.031290	6.229280	2.029372
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H	-2.503231	2.535716	2.002485
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H	-3.317797	4.257668	3.597644
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H	-2.425114	3.011306	-0.463886
H	-4.085396	2.904191	0.156025
H	-3.377699	4.479158	-0.209488
H	-3.660932	0.940583	2.906900

H	-6.139256	0.295349	4.588131
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H	-5.152656	0.470243	0.926245
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H	-6.322263	-1.642551	2.742281
H	-5.894599	-4.077967	2.770596
H	-3.588547	-4.902459	3.083826
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H	-1.441326	-3.620283	5.629978
H	-0.943553	-4.049858	1.334124
H	0.025386	-4.987220	2.486248
H	-1.676830	-5.375831	2.246847
H	-1.660095	-3.092939	-5.396412
H	-2.134158	-1.586805	-6.206516
H	-2.792544	-2.007154	-4.612019
H	-0.652060	-0.048179	-6.242698
H	0.906766	1.255276	-7.057951
H	2.374192	1.718116	-6.163756
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H	-2.367929	-0.708644	-2.565789
H	-4.579994	-1.915483	-2.717320
H	-4.654648	-0.389573	-1.816958
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H	-2.575761	-1.265100	0.438948
H	-2.691210	0.327679	-0.339190
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H	-2.398216	-5.941051	-0.881779
H	-0.484672	-6.234417	-2.416017
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H	1.242183	-5.443155	-5.777519
H	-0.465460	-4.997896	-5.613980
H	0.187945	-6.352969	-4.685013
H	2.376213	-4.227113	-2.415154
H	2.873545	-5.046005	-3.905943
H	1.856303	-5.887272	-2.726708
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H	5.465005	-0.087448	-6.305042
H	3.728149	-0.095414	-6.650855
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H	5.285832	-2.535988	-4.261837
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2
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16
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C 5.957351 4.002026 9.113958
C 5.393483 5.349669 8.949699
C 6.034358 6.520995 9.081992
C 7.449433 6.729110 9.421657
C 8.109311 6.248472 10.486500
C 7.570435 5.401402 11.560402
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H 9.143010 6.570944 10.626267
H 7.987704 7.412627 8.762003
H 5.741810 3.307924 8.299212
H 6.897601 2.466103 10.163172
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H 7.789629 5.743833 12.573696
H 5.477721 7.429437 8.843267
H 4.355729 5.378780 8.611631

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