

Supporting Information (Computational Part) for:

Design, Scope and Mechanism of Highly Active and Selective Chiral NHC-Iridium Catalysts for the Intramolecular Hydroamination of a Variety of Unactivated Aminoalkenes

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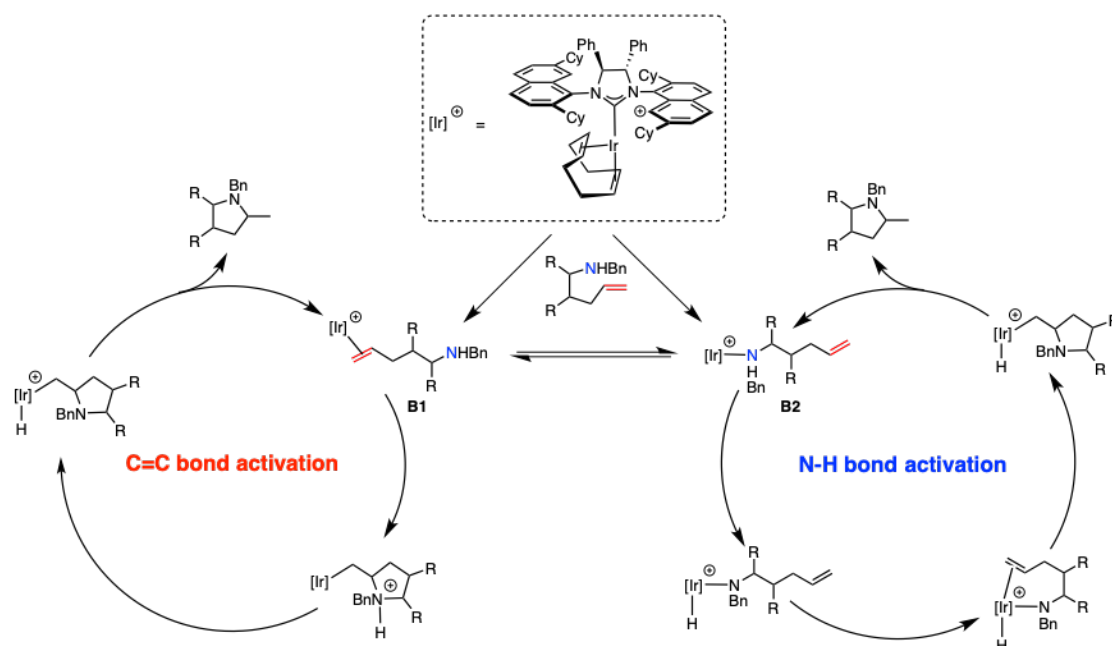
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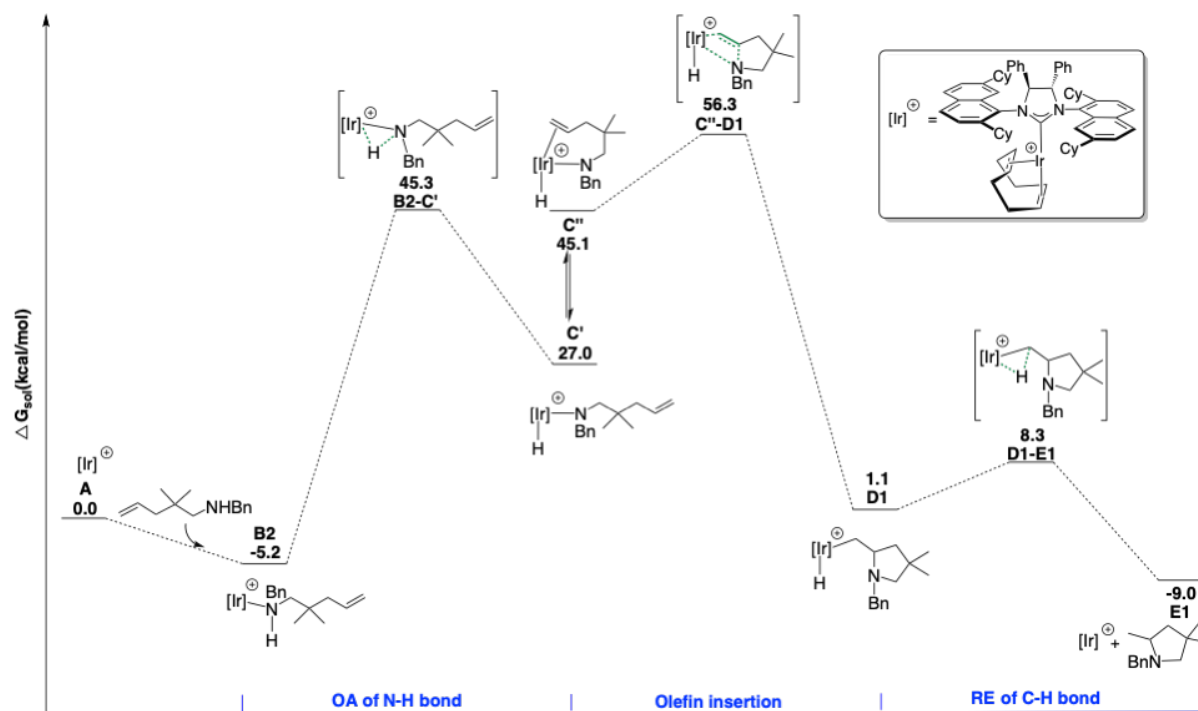
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1. Computational details.



Scheme S1 Two possible catalytic cycles for intramolecular hydroamination of aminoalkenes in the presence of cationic NHC-Iridium complex.



Scheme S2 Two possible catalytic cycles for intramolecular hydroamination of aminoalkenes in the presence of cationic NHC-Iridium complex.

Geometries were optimized with Gaussian09 package¹ using the BP86-D₃ functional of Becke and Perdew.²⁻⁴ The electronic configuration of the system was described with the split-valence SVP basis set for main group atoms (C, H and N)⁵ and the relativistic Stuttgart-Dresden effective core potential with the associated valence triple- ζ basis set for Ir.⁶ All geometries were confirmed as minimum or transition state through frequency calculations. The reported free energies were built through single point energy calculations on the BP86-D₃ geometries using the M06 functional and the triple- ζ TZVP basis set for main group atoms.^{7, 8} Solvent effects were included with the PCM model using dichloromethane as the solvent.⁸ To this M06/TZVP electronic energy in solvent, thermal corrections were added from the gas-phase frequency calculations at the BP86-D₃/SVP level.

1. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, Williams, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, *Journal*, 2016.
2. A. D. Becke, *Physical Review A*, 1988, **38**, 3098-3100.
3. J. P. Perdew, *Physical Review B*, 1986, **34**, 7406-7406.
4. J. P. Perdew, *Physical Review B*, 1986, **33**, 8822-8824.
5. A. Schäfer, H. Horn and R. Ahlrichs, *The Journal of Chemical Physics*, 1992, **97**, 2571-2577.
6. U. Häussermann, M. Dolg, H. Stoll, H. Preuss, P. Schwerdtfeger and R. M. Pitzer, *Molecular Physics*, 1993, **78**, 1211-1224.
7. V. Barone and M. Cossi, *The Journal of Physical Chemistry A*, 1998, **102**, 1995-2001.
8. J. Tomasi and M. Persico, *Chemical Reviews*, 1994, **94**, 2027-2094.

2. Cartesian coordinates of species reported in the context with energies (in a.u.).

A							
E= -2812.47100103 A.U.							
Ir	-0.560150	1.567272	1.100820	H	-4.202674	0.301446	-3.024940
C	-0.008148	-0.066618	0.043535	C	-2.218387	1.469934	-1.055476
N	0.462088	0.395652	-1.139416	H	-2.108566	0.377190	-1.082079
C	0.295588	1.817664	-1.272984	C	-1.067777	2.323857	-1.207397
C	1.400226	2.675796	-1.395552	C	0.470963	-0.626955	-2.217035
C	2.811016	2.183056	-1.168743	H	-0.401160	-0.426502	-2.877487
H	2.772398	1.078073	-1.070497	C	0.213014	-1.924940	-1.388761
C	3.313280	2.751793	0.184713	H	1.152651	-2.503404	-1.272041
H	2.617516	2.419878	0.984294	N	-0.160733	-1.401477	-0.021489
H	3.256115	3.863453	0.154995	C	-0.091252	-2.298987	1.099317
C	4.750536	2.322063	0.496322	C	-1.231632	-2.930171	1.604785
H	5.088145	2.788728	1.445955	C	-2.635445	-2.582266	1.159080
H	4.765781	1.223533	0.667844	H	-2.559469	-1.774730	0.397190
C	5.707894	2.665633	-0.653611	C	-3.464801	-2.034958	2.347022
H	5.777554	3.772340	-0.758481	H	-2.943415	-1.169241	2.800001
H	6.734882	2.311720	-0.421227	H	-3.523100	-2.812198	3.141405
C	5.216989	2.054511	-1.973611	C	-4.882750	-1.642266	1.918574
H	5.229470	0.944689	-1.888807	H	-5.459620	-1.274407	2.793598
H	5.904758	2.309448	-2.807070	H	-4.815221	-0.787319	1.209695
C	3.790084	2.509194	-2.316000	C	-5.611935	-2.810560	1.239700
H	3.793359	3.606431	-2.505886	H	-6.616645	-2.491503	0.888240
H	3.437083	2.023712	-3.248825	H	-5.788962	-3.615448	1.988566
C	1.143080	4.065818	-1.584144	C	-4.788958	-3.374359	0.071415
H	1.998519	4.746968	-1.707455	H	-4.709519	-2.602757	-0.728373
C	-0.143860	4.586422	-1.582835	H	-5.304220	-4.242924	-0.390534
H	-0.303314	5.666866	-1.724358	C	-3.373996	-3.773828	0.510808
C	-1.276693	3.751478	-1.367786	H	-2.788995	-4.158864	-0.346358
C	-2.602497	4.253002	-1.289713	H	-3.438727	-4.606796	1.246681
H	-2.761261	5.338800	-1.383981	C	-1.049881	-3.913718	2.626292
C	-3.690685	3.402472	-1.109597	H	-1.936799	-4.419539	3.036306
H	-4.703556	3.828487	-1.067907	C	0.205352	-4.258986	3.095163
C	-3.519400	1.993542	-1.019811	H	0.315392	-5.040939	3.863016
C	-4.695379	1.038305	-1.020803	C	1.374694	-3.614871	2.596307
H	-4.347554	0.091560	-0.546710	C	2.685439	-3.957477	3.041328
C	-5.924085	1.531542	-0.230258	H	2.794632	-4.743902	3.804848
H	-5.634817	1.735987	0.823408	C	3.805240	-3.328790	2.520041
H	-6.273231	2.498784	-0.655732	H	4.805315	-3.630351	2.866755
C	-7.084747	0.525453	-0.290595	C	3.678944	-2.288976	1.549018
H	-7.961180	0.928796	0.258404	C	4.907123	-1.631417	0.950345
H	-6.789074	-0.406900	0.237790	H	4.555624	-0.748565	0.367242
C	-7.464450	0.181240	-1.738488	C	5.910871	-1.121400	2.009471
H	-8.275508	-0.576707	-1.754819	H	6.228941	-1.973514	2.650429
H	-7.874133	1.087983	-2.239423	H	5.403487	-0.398855	2.684281
C	-6.245260	-0.322238	-2.526224	C	7.157892	-0.487162	1.373422
H	-6.519533	-0.536189	-3.580884	H	6.866648	0.445619	0.842217
H	-5.898733	-1.286618	-2.088039	H	7.870710	-0.180508	2.167585
C	-5.091255	0.689264	-2.480538	C	7.835283	-1.437848	0.375029
H	-5.388071	1.627485	-3.002214	H	8.708298	-0.942880	-0.100185
				H	8.235006	-2.323502	0.919510
				C	6.838288	-1.912542	-0.692954
				H	7.325973	-2.613028	-1.403637

H	6.505763	-1.033475	-1.293001
C	5.610323	-2.578031	-0.054851
H	5.922839	-3.504370	0.478289
H	4.884561	-2.902961	-0.831736
C	2.401176	-1.928722	1.120074
H	2.307890	-1.101884	0.400435
C	1.228618	-2.590056	1.594407
C	-1.700070	3.182608	2.150756
H	-2.509606	3.445576	1.445878
C	-0.402836	3.643448	1.842846
H	-0.284989	4.282549	0.949460
C	0.740199	3.719565	2.839367
H	0.576683	4.575290	3.534041
H	1.659641	3.961072	2.270802
C	0.958796	2.409619	3.639324
H	2.034720	2.312964	3.886664
H	0.427987	2.451501	4.613521
C	0.508535	1.158507	2.879613
H	1.311376	0.425213	2.682408
C	-0.834761	0.613885	2.958486
H	-0.913008	-0.481052	2.830026
C	-1.980361	1.220739	3.746673
H	-1.880771	0.969972	4.828417
H	-2.911320	0.723260	3.403499
C	-2.121768	2.748600	3.547389
H	-3.175632	3.045096	3.720379
H	-1.523060	3.296684	4.302752
C	-0.843668	-2.836577	-1.971095
C	-0.592337	-4.217919	-2.073815
C	-2.082916	-2.331585	-2.418642
C	-1.553616	-5.078667	-2.631241
H	0.369180	-4.620050	-1.716789
C	-3.042546	-3.186630	-2.979013
H	-2.308051	-1.256843	-2.333785
C	-2.777663	-4.563716	-3.090056
H	-1.342999	-6.156054	-2.710721
H	-4.001568	-2.776889	-3.330587
H	-3.528485	-5.235679	-3.533010
C	1.718344	-0.604855	-3.072755
C	1.657897	-0.018885	-4.352164
C	2.948457	-1.118467	-2.612144
C	2.804431	0.053052	-5.161538
H	0.698847	0.381320	-4.719069
C	4.092929	-1.052458	-3.420517
H	3.020055	-1.575914	-1.613668
C	4.024476	-0.464870	-4.696575
H	2.742368	0.510712	-6.160685
H	5.044057	-1.465499	-3.052657
H	4.923410	-0.415319	-5.329793

Substrate 18a

E= -600.471714138 A.U.

N	-0.302644	-0.661905	-0.031017
C	-1.561755	-1.340537	-0.289435

C	-2.808357	-0.543000	0.166727
C	-3.033742	0.730457	-0.712560
C	-1.935028	1.760529	-0.718966
C	-1.997588	2.947824	-0.085917
H	-1.605796	-2.359627	0.187084
C	-4.035759	-1.458904	-0.011639
C	-2.680797	-0.142859	1.648906
H	-3.978085	1.208197	-0.368843
H	-3.215941	0.385973	-1.756211
H	-1.635172	-1.522226	-1.386725
H	-1.021763	1.496672	-1.277312
H	-1.164716	3.668707	-0.124770
H	-2.888275	3.244537	0.495845
C	0.873669	-1.364797	-0.514358
H	-0.200254	-0.468617	0.973391
H	-2.493142	-1.030784	2.289999
H	-1.863026	0.590238	1.805592
H	-3.616106	0.337677	2.005302
H	-4.138328	-1.792064	-1.066453
H	-3.957173	-2.365615	0.624196
H	-4.970324	-0.929214	0.267026
H	0.770668	-1.478067	-1.620597
H	0.963029	-2.415075	-0.122085
C	2.158243	-0.616083	-0.210014
C	3.381952	-1.310349	-0.109710
C	4.571651	0.774884	0.298021
C	2.158111	0.784658	-0.044376
C	3.355917	1.474032	0.209520
H	3.338556	2.568030	0.338977
H	1.201207	1.324273	-0.112580
C	4.580660	-0.622055	0.136919
H	3.392545	-2.407394	-0.223222
H	5.510323	1.315528	0.497431
H	5.527216	-1.180603	0.212369

B

E= -3413.00721766 A.U.

Ir	0.574802	-0.478081	-1.891228
C	0.714107	0.170168	0.026249
N	0.583682	-0.368455	1.267940
C	-0.168749	-1.528786	1.667245
C	0.467826	-2.727832	2.008605
C	1.939514	-2.982621	1.775454
H	2.379147	-2.055900	1.342632
C	2.164333	-4.136354	0.766483
H	1.587374	-3.951485	-0.163438
H	1.749524	-5.076009	1.194000
C	3.659961	-4.330146	0.472695
H	3.803346	-5.163040	-0.248142
H	4.058014	-3.414508	-0.023553
C	4.453282	-4.587480	1.764370
H	4.145455	-5.569617	2.189534
H	5.538218	-4.671995	1.541367
C	4.201247	-3.484857	2.804320

H	4.620656	-2.524679	2.430391	H	-3.094807	3.821535	0.250619
H	4.739033	-3.708228	3.749950	H	-3.166692	5.520852	-0.256879
C	2.704552	-3.295184	3.080944	C	-1.381714	4.458364	-0.909263
H	2.291928	-4.226860	3.528812	H	-0.788511	4.731743	-0.016918
H	2.535421	-2.491404	3.821898	H	-1.142285	5.215527	-1.689229
C	-0.321800	-3.767075	2.592463	C	1.046645	3.897155	-2.727452
H	0.169184	-4.714123	2.861414	H	0.327886	4.452181	-3.348370
C	-1.674006	-3.612071	2.833062	C	2.401426	4.061324	-2.952998
H	-2.254392	-4.426400	3.294222	H	2.754188	4.727657	-3.755942
C	-2.340505	-2.401967	2.486517	C	3.361194	3.376979	-2.150283
C	-3.731078	-2.205445	2.730609	C	4.764888	3.501414	-2.356875
H	-4.310190	-3.032047	3.171913	H	5.122836	4.164440	-3.160241
C	-4.345320	-0.998387	2.441174	C	5.675223	2.795942	-1.577858
H	-5.416398	-0.870015	2.654421	H	6.750819	2.908854	-1.773258
C	-3.608103	0.080762	1.865755	C	5.227923	1.935275	-0.533180
C	-4.267583	1.432818	1.671492	C	6.168280	1.098531	0.325499
H	-3.554703	2.077015	1.107708	H	5.913104	1.321849	1.389866
C	-5.578407	1.365463	0.859457	C	5.911415	-0.417633	0.114620
H	-5.358061	0.989447	-0.158631	H	6.097210	-0.662615	-0.955931
H	-6.264262	0.617921	1.314012	H	4.842202	-0.657231	0.301303
C	-6.298316	2.718171	0.773244	C	6.803195	-1.282867	1.015615
H	-7.258787	2.589488	0.231314	H	6.514220	-1.112545	2.078354
H	-5.687177	3.420905	0.164766	H	6.615128	-2.358338	0.812774
C	-6.530099	3.335391	2.159446	C	8.290339	-0.945659	0.839012
H	-7.022630	4.326239	2.067034	H	8.910270	-1.551969	1.532464
H	-7.227275	2.690496	2.741610	H	8.608269	-1.225119	-0.191340
C	-5.203361	3.462912	2.922532	C	8.545285	0.553558	1.057913
H	-5.366304	3.900673	3.930227	H	9.615574	0.795616	0.890017
H	-4.539254	4.170187	2.373973	H	8.330625	0.813607	2.119949
C	-4.503217	2.102553	3.050232	C	7.663106	1.413852	0.139412
H	-5.130004	1.425197	3.673026	H	7.947377	1.216809	-0.919616
H	-3.534838	2.199023	3.588046	H	7.850636	2.493371	0.322511
C	-2.256224	-0.114517	1.578502	C	3.853649	1.828437	-0.315581
H	-1.697955	0.707875	1.107999	H	3.505111	1.153738	0.475921
C	-1.580486	-1.332565	1.890602	C	2.889562	2.507094	-1.105354
C	0.804869	0.645595	2.356574	C	0.788852	0.032428	-4.042235
H	-0.174536	0.803146	2.851824	H	-0.058728	0.713879	-4.244742
C	1.230727	1.912538	1.582018	C	0.497550	-1.340316	-4.034606
H	2.313112	2.096868	1.740872	H	-0.549922	-1.612351	-4.223311
N	1.048333	1.484437	0.163286	C	1.522842	-2.447371	-4.223621
C	1.470324	2.325886	-0.924020	H	2.318396	-2.099432	-4.912626
C	0.541190	3.046992	-1.692768	H	1.035034	-3.304509	-4.729827
C	-0.947606	3.061157	-1.421715	C	2.147429	-2.937403	-2.892011
H	-1.161106	2.325884	-0.615868	H	1.541979	-3.765156	-2.469701
C	-1.793385	2.677402	-2.654702	H	3.158290	-3.369102	-3.076911
H	-1.478096	1.681975	-3.021477	C	2.259338	-1.852814	-1.845545
H	-1.589995	3.396404	-3.479421	H	2.331468	-2.222790	-0.811775
C	-3.293937	2.702223	-2.333034	C	2.773128	-0.546983	-2.082926
H	-3.881639	2.418600	-3.231814	H	3.234583	-0.065536	-1.211244
H	-3.518051	1.931849	-1.559627	C	3.279052	-0.034279	-3.425541
C	-3.724747	4.083490	-1.815343	H	3.749610	-0.859202	-4.000064
H	-4.805656	4.082966	-1.561960	H	4.083529	0.704756	-3.237962
H	-3.596713	4.833772	-2.628192	C	2.159602	0.647519	-4.245430
C	-2.883159	4.504260	-0.602496	H	2.095969	1.714778	-3.956868

H	2.399522	0.641957	-5.334120
C	0.519174	3.206244	1.920377
C	1.235223	4.412184	1.769528
C	-0.815675	3.257495	2.368196
C	0.633041	5.645310	2.066448
H	2.279354	4.378486	1.418740
C	-1.415593	4.488309	2.678264
H	-1.399831	2.334101	2.492937
C	-0.693861	5.684998	2.528509
H	1.204977	6.577882	1.945086
H	-2.454184	4.511016	3.040018
H	-1.165877	6.648616	2.773853
C	1.783314	0.190263	3.417823
C	1.305152	-0.145135	4.698992
C	3.168491	0.110719	3.165300
C	2.194940	-0.529695	5.716805
H	0.222927	-0.096598	4.899985
C	4.060797	-0.261574	4.180586
H	3.563175	0.337281	2.163982
C	3.575729	-0.579613	5.461990
H	1.807644	-0.785208	6.714916
H	5.139919	-0.309001	3.969271
H	4.275217	-0.870874	6.260304
N	-4.307579	-2.572446	-2.022516
C	-3.588871	-3.390903	-1.054419
C	-2.346973	-4.086018	-1.670540
C	-1.428283	-3.030740	-2.356262
C	-1.160556	-1.819739	-1.494265
C	-1.608898	-0.510459	-1.830639
H	-3.253814	-2.727648	-0.228699
C	-2.791427	-5.097005	-2.743914
C	-1.576273	-4.817862	-0.561248
H	-0.485935	-3.549981	-2.623491
H	-1.919157	-2.710702	-3.295608
H	-4.217770	-4.180916	-0.570895
H	-1.013258	-2.054825	-0.428223
H	-2.115342	-0.379885	-2.802783
H	-1.965700	0.164999	-1.038045
H	-4.967692	-3.129401	-2.575529
C	-4.937959	-1.346391	-1.547745
H	-2.237437	-5.517489	-0.008433
H	-1.151821	-4.115341	0.180612
H	-0.738292	-5.410766	-0.983967
H	-3.377469	-4.600970	-3.545352
H	-3.419926	-5.896799	-2.298149
H	-1.916294	-5.584279	-3.223019
H	-5.048951	-0.641991	-2.402846
H	-4.217222	-0.862772	-0.850636
C	-6.287512	-1.468471	-0.855927
C	-6.473008	-2.318662	0.256511
C	-8.776587	-1.560411	0.500956
C	-7.376928	-0.683440	-1.286103
C	-8.610321	-0.721442	-0.613878
H	-9.446611	-0.096504	-0.964596

H	-7.249084	-0.020640	-2.158378
C	-7.705087	-2.365434	0.928146
H	-5.638091	-2.936988	0.614006
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H	-7.830714	-3.032618	1.795811

N-B

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N	0.619900	-0.312539	1.237299
C	0.228779	-1.605267	1.723228
C	1.185053	-2.590000	1.987690
C	2.614149	-2.446046	1.518847
H	2.776828	-1.371413	1.287544
C	2.830876	-3.214691	0.199282
H	2.095401	-2.832888	-0.541445
H	2.601766	-4.293373	0.357086
C	4.271866	-3.051981	-0.304565
H	4.425385	-3.643003	-1.232388
H	4.434544	-1.984313	-0.578058
C	5.304574	-3.447578	0.761272
H	5.217143	-4.537017	0.974857
H	6.334576	-3.289290	0.376844
C	5.081552	-2.656202	2.057375
H	5.252105	-1.572355	1.862789
H	5.818903	-2.952006	2.833060
C	3.653794	-2.852518	2.581897
H	3.520439	-3.925062	2.847065
H	3.486955	-2.270926	3.509441
C	0.771702	-3.745932	2.720340
H	1.504255	-4.545949	2.901108
C	-0.501746	-3.859150	3.253988
H	-0.774113	-4.739649	3.857110
C	-1.471948	-2.834609	3.051742
C	-2.775502	-2.871705	3.630850
H	-3.051011	-3.734416	4.256515
C	-3.692938	-1.855386	3.406420
H	-4.693720	-1.919621	3.859596
C	-3.362449	-0.741057	2.576674
C	-4.358389	0.362057	2.291868
H	-3.862343	1.076849	1.593548
C	-5.635840	-0.146505	1.584146
H	-5.360748	-0.717121	0.670402
H	-6.161396	-0.868792	2.248246
C	-6.575257	1.017660	1.237100
H	-7.491331	0.634797	0.739763
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C	-5.685246	2.321655	3.227410
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C	-4.736339	1.160671	3.561286	C	6.499450	1.855413	0.643918
H	-5.224620	0.475083	4.290066	H	7.045193	2.686325	0.142093
H	-3.814333	1.531743	4.058403	H	5.927244	2.320352	1.476025
C	-2.084796	-0.683118	2.022792	C	3.142002	2.009690	-0.572873
H	-1.828428	0.175576	1.386889	H	2.864224	1.131858	0.025635
C	-1.111265	-1.700640	2.241353	C	2.119101	2.873224	-1.055985
C	0.771417	0.685666	2.347757	C	-0.172533	-1.781456	-3.754638
H	-0.157695	0.633168	2.951321	H	-1.264210	-1.912401	-3.821815
C	0.827769	2.010461	1.591622	C	0.555063	-2.703124	-2.968814
H	1.875139	2.369551	1.532296	H	-0.004755	-3.518726	-2.480318
N	0.441173	1.613263	0.191635	C	2.023952	-3.006773	-3.194692
C	0.725942	2.652246	-0.763370	H	2.136680	-3.550203	-4.160591
C	-0.265957	3.520294	-1.227883	H	2.362775	-3.710627	-2.411199
C	-1.723820	3.397280	-0.840948	C	2.893768	-1.732428	-3.178940
H	-1.811516	2.530206	-0.148051	H	3.898309	-1.970270	-2.780890
C	-2.639121	3.128394	-2.052558	H	3.061674	-1.365139	-4.212811
H	-2.276370	2.249033	-2.614727	C	2.273282	-0.607786	-2.351150
H	-2.579683	3.989050	-2.756178	H	2.870123	-0.289802	-1.482658
C	-4.097278	2.928440	-1.619637	C	1.412327	0.371187	-2.935497
H	-4.733293	2.724560	-2.506362	H	1.418493	1.373940	-2.492530
H	-4.165602	2.017289	-0.981818	C	0.979731	0.390370	-4.388453
C	-4.619950	4.133098	-0.822590	H	1.828706	0.740204	-5.020365
H	-5.655599	3.944465	-0.466508	H	0.193955	1.167596	-4.491576
H	-4.677669	5.020050	-1.493197	C	0.443362	-0.971109	-4.885838
C	-3.693267	4.450523	0.360173	H	-0.321777	-0.806800	-5.670682
H	-3.728163	3.607638	1.087359	H	1.253262	-1.557274	-5.367223
H	-4.046878	5.347007	0.912201	C	0.015422	3.133710	2.198060
C	-2.239171	4.645750	-0.088094	C	0.589733	4.418090	2.276952
H	-1.587977	4.870001	0.775820	C	-1.273232	2.929502	2.732954
H	-2.177693	5.527493	-0.764835	C	-0.101547	5.476522	2.889452
C	0.138395	4.595891	-2.082559	H	1.595733	4.584654	1.859578
H	-0.635202	5.272336	-2.475928	C	-1.963579	3.983135	3.350996
C	1.465117	4.824728	-2.403813	H	-1.744882	1.936956	2.682415
H	1.741323	5.670641	-3.052947	C	-1.378585	5.259003	3.433882
C	2.495117	3.980673	-1.892444	H	0.361968	6.473196	2.946723
C	3.878322	4.175578	-2.185979	H	-2.966414	3.808318	3.769158
H	4.166749	5.025700	-2.824436	H	-1.919772	6.083722	3.922297
C	4.847321	3.314227	-1.690298	C	1.923842	0.393126	3.287026
H	5.906123	3.488140	-1.937396	C	1.649038	-0.248862	4.511042
C	4.486244	2.197754	-0.876236	C	3.257879	0.733053	2.980473
C	5.517288	1.214447	-0.363604	C	2.681321	-0.531279	5.420817
H	4.962162	0.416989	0.185572	H	0.609386	-0.521696	4.754028
C	6.284473	0.517360	-1.511190	C	4.291753	0.451566	3.886744
H	6.815943	1.286232	-2.115990	H	3.501849	1.230808	2.030292
H	5.559758	0.028054	-2.197366	C	4.005627	-0.177203	5.111718
C	7.298944	-0.501594	-0.972567	H	2.449540	-1.026220	6.376253
H	6.748781	-1.328134	-0.470085	H	5.327008	0.728638	3.635546
H	7.856896	-0.965044	-1.813459	H	4.816492	-0.392019	5.824450
C	8.268493	0.139021	0.032791	C	-3.406752	-0.253415	-2.472443
H	8.968329	-0.623382	0.435327	C	-2.775512	-0.496884	-1.123184
H	8.896669	0.893511	-0.493540	N	-1.797559	-1.648645	-1.091272
C	7.508443	0.827525	1.177822	C	-2.412659	-2.885931	-1.694454
H	8.216385	1.316501	1.879952	H	-1.651749	-1.848720	-0.086733
H	6.963122	0.055386	1.768411	C	-2.565155	-4.097452	-0.753479

H	-3.414009	-2.615910	-2.080984
H	-1.828819	-3.193350	-2.578734
C	-3.579589	-3.728994	0.368427
C	-3.138497	-5.246097	-1.606400
C	-1.198975	-4.515030	-0.178157
C	-3.892499	-4.831981	1.338557
H	-3.182583	-2.860095	0.935906
H	-4.522056	-3.383467	-0.110733
C	-5.115506	-5.353007	1.545913
H	-3.040332	-5.231509	1.916780
H	-5.284656	-6.160809	2.275587
H	-5.997309	-4.987032	0.992061
C	-2.641998	0.211470	-3.560519
C	-4.615105	0.225308	-4.983238
C	-4.787761	-0.466013	-2.656438
C	-5.391118	-0.227822	-3.902952
H	-6.471474	-0.396105	-4.030258
H	-5.399739	-0.815790	-1.808976
C	-3.236726	0.446141	-4.808608
H	-1.567628	0.394851	-3.400272
H	-5.085077	0.411584	-5.961233
H	-2.625707	0.816576	-5.646625
H	-0.703400	-3.696301	0.378171
H	-0.509570	-4.828954	-0.988644
H	-1.296592	-5.373708	0.513524
H	-2.448845	-5.514536	-2.433728
H	-4.117674	-4.969514	-2.050815
H	-3.299058	-6.149593	-0.985270
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H	-2.231689	0.407365	-0.784583

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C	-0.598772	-2.825147	-0.839419
C	0.333954	-3.733718	-1.367808
C	1.834174	-3.581736	-1.209456
H	2.010117	-2.639328	-0.644126
C	2.623900	-3.497379	-2.540361
H	2.188102	-2.742458	-3.219324
H	2.548327	-4.474802	-3.067142
C	4.102240	-3.183048	-2.261716
H	4.663501	-3.095389	-3.216250
H	4.167050	-2.185209	-1.766959
C	4.744914	-4.242318	-1.352477
H	4.812108	-5.204514	-1.908719
H	5.788707	-3.957053	-1.099016
C	3.920947	-4.453255	-0.074564
H	3.974192	-3.534526	0.552116
H	4.350947	-5.270684	0.542136
C	2.444893	-4.737388	-0.378843
H	2.357770	-5.683124	-0.959631

H	1.874125	-4.892467	0.552601
C	-0.169567	-4.873554	-2.067218
H	0.553249	-5.571675	-2.515418
C	-1.525654	-5.130319	-2.185200
H	-1.877071	-6.021007	-2.729519
C	-2.483516	-4.263859	-1.584208
C	-3.891096	-4.506379	-1.639874
H	-4.249607	-5.393582	-2.185529
C	-4.795551	-3.652511	-1.025571
H	-5.873974	-3.864478	-1.090583
C	-4.342099	-2.497248	-0.317398
C	-5.299267	-1.490632	0.286051
H	-4.684107	-0.763184	0.866682
C	-6.015976	-0.675696	-0.818674
H	-5.254008	-0.200932	-1.474056
H	-6.596879	-1.374000	-1.462876
C	-6.954228	0.382483	-0.220145
H	-7.482645	0.926311	-1.031716
H	-6.343071	1.142266	0.316659
C	-7.959085	-0.236951	0.763121
H	-8.598534	0.552656	1.211216
H	-8.644648	-0.916922	0.207890
C	-7.240926	-1.034560	1.863553
H	-7.976470	-1.501752	2.551741
H	-6.631765	-0.335469	2.482365
C	-6.318406	-2.108793	1.266158
H	-6.934891	-2.864467	0.729092
H	-5.779314	-2.659417	2.067230
C	-2.974706	-2.255351	-0.258029
H	-2.643590	-1.336798	0.245901
C	-2.010140	-3.100846	-0.883285
C	-0.387252	-2.062100	1.442178
H	-1.438044	-2.401230	1.529801
C	-0.224664	-0.725618	2.142527
H	0.800014	-0.633230	2.555364
N	-0.308275	0.252947	1.004818
C	0.119198	1.560049	1.443429
C	-0.801296	2.529709	1.866162
C	-2.300244	2.407744	1.705576
H	-2.514534	1.411479	1.261551
C	-2.875335	3.490693	0.764028
H	-2.360866	3.452075	-0.216852
H	-2.655385	4.494353	1.192176
C	-4.393223	3.330279	0.590690
H	-4.788975	4.130356	-0.070864
H	-4.592793	2.366212	0.069893
C	-5.138141	3.324488	1.933912
H	-6.221276	3.139598	1.770804
H	-5.060099	4.331022	2.403659
C	-4.543699	2.276700	2.885355
H	-4.723529	1.256066	2.475090
H	-5.051892	2.305449	3.872274
C	-3.035715	2.483987	3.063822
H	-2.612250	1.747021	3.767048

H	-2.859399	3.484712	3.518262	C	-1.513225	0.217261	5.607235
C	-0.300694	3.696016	2.525989	H	0.375516	0.369913	4.534386
H	-1.011245	4.489749	2.799514	C	-3.367971	-0.735931	4.356194
C	1.026548	3.824285	2.883189	H	-2.954885	-1.317928	2.316732
H	1.376626	4.712637	3.430555	C	-2.857436	-0.189240	5.546880
C	1.961035	2.803442	2.556298	H	-1.108000	0.651331	6.534015
C	3.316241	2.859055	2.990338	H	-4.421523	-1.049298	4.297180
H	3.639389	3.727591	3.584406	H	-3.508721	-0.077559	6.427217
C	4.210636	1.848134	2.681249	C	0.459506	-3.182135	2.000557
H	5.245797	1.905079	3.050411	C	-0.137010	-4.446885	2.179220
C	3.807713	0.731456	1.888318	C	1.788722	-2.987539	2.425085
C	4.779495	-0.398703	1.612298	C	0.576007	-5.496650	2.780246
H	4.296237	-1.084746	0.876789	H	-1.176800	-4.601759	1.849395
C	6.120795	0.067303	1.001867	C	2.499782	-4.031262	3.036891
H	6.637155	0.737290	1.725600	H	2.276488	-2.010838	2.289274
H	5.941069	0.672003	0.092336	C	1.895168	-5.287435	3.217866
C	7.031609	-1.128234	0.688500	H	0.097032	-6.478349	2.915613
H	6.540127	-1.767792	-0.080950	H	3.535017	-3.865809	3.370465
H	7.983903	-0.775634	0.239297	H	2.453669	-6.103875	3.700768
C	7.306665	-1.963265	1.948477	N	1.374836	2.371098	-1.473405
H	7.932660	-2.846870	1.703027	C	2.366737	2.666140	-2.544503
H	7.897729	-1.350731	2.666821	C	3.356854	1.554677	-2.927827
C	5.997249	-2.407555	2.619395	C	2.614192	0.348772	-3.536422
H	6.208595	-2.951487	3.564694	C	1.615865	-0.342512	-2.644782
H	5.474931	-3.128861	1.952351	C	0.490401	-1.009290	-3.179222
C	5.063906	-1.218934	2.897891	H	2.948877	3.567338	-2.255544
H	5.530721	-0.544623	3.650979	C	4.292987	2.145985	-4.001419
H	4.109078	-1.561255	3.349774	C	4.199354	1.117675	-1.719842
C	2.487813	0.678445	1.432185	H	3.382078	-0.403402	-3.837626
H	2.178933	-0.179763	0.814623	H	2.125911	0.665977	-4.483627
C	1.522811	1.678959	1.770898	H	1.804194	2.952294	-3.456456
C	-0.754919	1.292932	-4.270429	H	2.034214	-0.730871	-1.700194
H	0.189315	1.110322	-4.806714	H	0.088573	-1.917512	-2.721813
C	-0.795783	2.454660	-3.492722	H	0.310319	-0.948260	-4.263873
H	0.119146	3.061858	-3.513981	C	0.791308	3.632215	-0.968568
C	-2.032892	3.220744	-3.080138	H	1.850776	1.897389	-0.691172
H	-2.407009	3.801937	-3.955908	H	4.784607	1.968504	-1.314968
H	-1.732472	3.975351	-2.323500	H	3.586548	0.714288	-0.890910
C	-3.106221	2.309927	-2.483089	H	4.916532	0.324175	-2.014355
H	-3.776259	2.896685	-1.829233	H	3.721767	2.492608	-4.888091
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C	-2.269084	-0.119932	-2.377942	H	-0.033358	3.365148	-0.282713
H	-2.433174	-1.007933	-1.763728	C	1.728992	4.613014	-0.281525
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H	-3.717438	-0.461438	-3.951656	C	3.333756	6.512449	1.074601
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H	-1.711581	0.067022	-5.760931	H	1.614736	7.841071	0.908497
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C	-1.181056	-0.495797	3.292214	C	3.838737	5.236029	0.783616
C	-0.681514	0.062255	4.485861	H	3.443221	3.282494	-0.049951
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B_C_SR

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C	3.794350	-3.551138	2.073619
H	3.830831	-4.647143	1.897896
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H	6.046133	0.851475	-4.210534
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C	5.988309	0.429531	-0.070328
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C	7.200633	-2.041906	-1.164014
H	7.164846	-3.135947	-1.352348
H	8.153032	-1.678721	-1.612766
C	6.021148	-1.350192	-1.862351
H	5.057699	-1.777022	-1.498693
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C	3.627056	1.093941	-1.804054

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C	0.328446	-4.176000	-2.254628
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H	-0.234222	-5.123455	-2.133459
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C	1.654376	-2.545574	-0.818253
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C	0.933016	3.943141	0.035041
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H	-0.445187	7.554446	-0.674611
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H	-5.625433	-0.847230	-0.175489
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C	-6.091187	-4.139077	-0.788802
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C	4.601072	-4.237378	2.031812
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H	-2.134888	-4.254671	3.456265	H	2.762349	4.829331	-3.851542
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C	-1.533582	-1.175072	1.991479	C	2.937769	2.579206	-1.224076
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C	1.068355	4.000959	-2.795853	H	2.377897	4.502673	1.149510
H	0.338915	4.562165	-3.398982	C	-1.293490	4.781853	2.449567
C	2.419262	4.159173	-3.047704	H	-1.343684	2.624450	2.371917

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H	1.372567	6.753492	1.573045
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H	-0.981770	6.936494	2.432015
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C	1.034557	0.057553	4.671907
C	3.051568	0.517005	3.403106
C	1.814156	-0.307003	5.782169
H	-0.065172	0.019540	4.730595
C	3.834513	0.161997	4.511839
H	3.550130	0.829158	2.475646
C	3.216812	-0.248210	5.706550
H	1.324404	-0.632095	6.712812
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C	-1.333284	-3.175455	-0.918610
C	-1.643655	-2.051527	-1.867137
C	-1.604102	-0.648690	-1.623239
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C	-1.969857	-5.467339	-0.036999
C	-2.187843	-5.001351	-2.492872
H	-0.293752	-3.518593	-1.108760
H	-1.357189	-2.816859	0.124904
H	-3.756684	-3.479966	0.229777
H	-1.689981	-2.355714	-2.920973
H	-1.893659	-0.305093	-0.619377
H	-2.042125	-0.035985	-2.429618
H	-4.247484	-2.848443	-2.597036
C	-4.549614	-1.449965	-1.099281
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H	-2.456452	-4.286293	-3.297413
H	-1.153815	-5.351028	-2.694481
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H	-2.678460	-6.318016	-0.114282
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H	-4.067764	-1.237380	-0.124516
H	-4.328653	-0.582242	-1.756629
C	-6.047637	-1.599691	-0.927517
C	-6.932049	-1.083441	-1.896759
C	-8.843466	-1.913176	-0.639697
C	-6.582910	-2.275037	0.190519
C	-7.970557	-2.432517	0.333177
H	-8.375967	-2.957458	1.212337
H	-5.903207	-2.663840	0.964361
C	-8.321438	-1.236743	-1.755453
H	-6.525526	-0.542217	-2.767643
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C	1.929946	-2.838795	1.915388
H	2.374261	-1.947630	1.420708
C	2.128529	-4.058853	0.982081
H	1.563030	-3.907660	0.039027
H	1.687167	-4.958779	1.465943
C	3.617609	-4.317709	0.706614
H	3.734124	-5.206062	0.050148
H	4.041497	-3.455970	0.142140
C	4.406638	-4.498945	2.013243
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H	5.488000	-4.628797	1.795388
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H	4.730291	-3.468991	3.920338
C	2.698208	-3.070910	3.236654
H	2.270452	-3.957345	3.756986
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C	-0.327145	-3.564898	2.780291
H	0.162815	-4.500108	3.089670
C	-1.673560	-3.390146	3.034962
H	-2.251902	-4.175496	3.546559
C	-2.334738	-2.191073	2.640402
C	-3.723031	-1.975671	2.890656
H	-4.298753	-2.772806	3.388238
C	-4.333386	-0.776833	2.554296
H	-5.398212	-0.626432	2.785458
C	-3.597445	0.269341	1.918887
C	-4.251804	1.619038	1.688902
H	-3.541892	2.239504	1.097773
C	-5.577072	1.544798	0.898502
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H	-6.985543	4.539276	2.064705
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H	-5.297940	4.146861	3.908354
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H	-5.076978	1.668423	3.706188
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C	-2.251041	0.048971	1.617877
H	-1.694086	0.838570	1.093273
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C	0.820649	0.838419	2.300046
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C	1.453949	2.332116	-1.070522
C	0.517682	3.014900	-1.856863
C	-0.972122	2.984246	-1.592057
H	-1.150463	2.328758	-0.711155
C	-1.776928	2.408937	-2.777032
H	-1.389241	1.403734	-3.029441
H	-1.614203	3.046861	-3.674323
C	-3.277383	2.366386	-2.457568
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C	1.004201	3.822961	-2.931669
H	0.273965	4.344009	-3.569208
C	2.355955	3.977255	-3.186935
H	2.696398	4.603914	-4.026269
C	3.325953	3.334726	-2.363616
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H	5.078897	4.079388	-3.421702
C	5.648426	2.788952	-1.781591
H	6.722196	2.894943	-1.991621
C	5.212076	1.976869	-0.693352
C	6.155789	1.170982	0.191296
H	5.900421	1.425543	1.248641
C	5.901686	-0.351058	0.025137
H	6.090787	-0.626773	-1.037150
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C	6.791101	-1.188866	0.953813
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H	6.605308	-2.270514	0.782286
C	8.278350	-0.854689	0.770884
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C	8.530938	0.651224	0.943918
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H	8.312820	0.942922	1.997135
C	7.650068	1.482660	-0.002430
H	7.936860	1.254088	-1.054339
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C	3.841718	1.878829	-0.459786
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H	2.331990	-2.441566	-4.715178
H	1.163732	-3.727910	-4.390309
C	2.280845	-3.106110	-2.624621
H	1.712705	-3.900112	-2.093233
H	3.300180	-3.526279	-2.791038
C	2.363942	-1.898657	-1.711421
H	2.536268	-2.146967	-0.651621
C	2.762448	-0.592269	-2.107650
H	3.201249	0.022139	-1.314598
C	3.150214	-0.164053	-3.514279
H	3.645066	-0.998939	-4.052823
H	3.905907	0.644046	-3.443394
C	1.927502	0.357468	-4.301278
H	1.780874	1.432133	-4.071388
H	2.100311	0.295488	-5.401203
C	0.514975	3.361515	1.678337
C	1.213567	4.555791	1.402088
C	-0.806390	3.445462	2.159121
C	0.607676	5.805906	1.603899
H	2.248714	4.500329	1.028947
C	-1.411137	4.694743	2.372645
H	-1.374865	2.533565	2.392975
C	-0.707236	5.878590	2.095176
H	1.168235	6.727417	1.384302
H	-2.438627	4.741639	2.762758
H	-1.182109	6.856972	2.265207
C	1.823308	0.453446	3.367981
C	1.383645	0.230012	4.686465
C	3.197805	0.326380	3.078744
C	2.300248	-0.092453	5.702551
H	0.310136	0.318781	4.918890
C	4.117374	0.018087	4.090982
H	3.561396	0.464457	2.050081
C	3.670607	-0.190149	5.408422
H	1.942448	-0.260752	6.729876
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H	4.391301	-0.432224	6.204347
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C	-2.561200	-4.500521	-1.438383
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C	-1.602331	-0.788437	-1.757980
H	-4.587625	-4.365929	-0.545346
C	-2.726042	-5.660788	-2.431123
C	-1.987363	-5.022759	-0.109083
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H	-4.437251	-3.646676	-2.173748
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H	-2.052116	-0.682242	-2.767164

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H	-3.576378	-2.445757	0.373326
C	-4.481599	-1.351632	-1.130570
H	-2.640513	-5.808939	0.322837
H	-1.877745	-4.224635	0.649300
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H	-3.123577	-5.309718	-3.406511
H	-3.420496	-6.430931	-2.035746
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C	-5.952370	-1.434986	-0.776661
C	-6.869238	-0.683478	-1.541036
C	-8.686542	-1.334024	-0.058435
C	-6.426468	-2.151197	0.338878
C	-7.785115	-2.103132	0.695528
H	-8.140562	-2.671288	1.569232
H	-5.732664	-2.747333	0.949893
C	-8.224577	-0.626781	-1.182816
H	-6.511909	-0.124649	-2.421653
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C	0.230082	-2.569483	2.058133
C	1.692437	-2.912433	1.879849
H	2.186817	-2.039565	1.399326
C	1.896686	-4.147734	0.969936
H	1.378002	-3.997972	0.001485
H	1.411571	-5.030817	1.442120
C	3.388434	-4.447253	0.758067
H	3.508469	-5.343342	0.112872
H	3.857100	-3.600377	0.206156
C	4.119612	-4.638727	2.096372
H	3.741091	-5.562469	2.590131
H	5.205045	-4.799611	1.924092
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H	4.372679	-2.536129	2.587222
H	4.387815	-3.602281	4.008681
C	2.400137	-3.155686	3.233994
H	1.926763	-4.027051	3.739961
H	2.248656	-2.286902	3.901281
C	-0.619904	-3.539982	2.677838
H	-0.192088	-4.516653	2.949042
C	-1.938330	-3.268908	2.990660
H	-2.553076	-4.019057	3.512628
C	-2.514319	-2.006014	2.668901
C	-3.843568	-1.659283	3.053224
H	-4.443778	-2.402418	3.602019

C	-4.367750	-0.409364	2.767207
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H	-7.157194	3.074984	0.189411
H	-5.534916	3.784489	0.018347
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H	-3.399993	2.832027	3.524254
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H	-1.751269	0.935275	1.015863
C	-1.715355	-1.035162	1.964208
C	0.740325	0.822313	2.259261
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N	1.075243	1.497769	0.018717
C	1.556168	2.272532	-1.093456
C	0.675492	2.977001	-1.927219
C	-0.819011	3.042219	-1.698412
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H	-1.350002	1.607120	-3.255089
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H	-0.971546	5.180298	-2.086009
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C	5.884235	-0.546078	0.215774
H	6.116199	-0.846160	-0.831357
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H	6.373593	-1.158397	2.238423
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H	7.878692	2.330180	0.376171
C	3.904170	1.740770	-0.387898
H	3.514043	1.130261	0.435396
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C	0.562082	-1.717308	-3.903474
H	-0.473008	-2.022621	-4.114965
C	1.607495	-2.820216	-3.982695
H	2.418197	-2.521086	-4.677403
H	1.147597	-3.726008	-4.427343
C	2.194665	-3.176584	-2.595561
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H	3.208447	-3.627411	-2.703719
C	2.266863	-1.990002	-1.657675
H	2.339029	-2.257871	-0.593094
C	2.772082	-0.705662	-2.006942
H	3.202498	-0.132688	-1.177874
C	3.308906	-0.316640	-3.376892
H	3.791531	-1.190178	-3.862789
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H	2.120458	1.365543	-4.079082
H	2.459253	0.175925	-5.353171
C	0.623648	3.362419	1.650160
C	1.413712	4.505235	1.404028
C	-0.700991	3.534434	2.096713
C	0.892291	5.793758	1.598744
H	2.452409	4.377089	1.059445
C	-1.220339	4.822332	2.305524
H	-1.338849	2.662306	2.300742
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H	1.521534	6.675086	1.401526
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H	-0.837179	6.963266	2.219904

C	1.674824	0.383086	3.366766
C	1.158410	0.153611	4.656357
C	3.057131	0.212852	3.145654
C	2.008909	-0.218770	5.711642
H	0.078045	0.277471	4.834128
C	3.911259	-0.144903	4.198363
H	3.476712	0.356008	2.138891
C	3.388664	-0.359682	5.486434
H	1.592808	-0.391665	6.715955
H	4.989460	-0.262822	4.011166
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C	-3.585394	-3.671164	-0.662084
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C	-1.586722	-3.242619	-2.143282
C	-1.649938	-1.901954	-1.450961
C	-1.596469	-0.603982	-2.042879
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C	-2.975778	-5.320117	-2.505845
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H	-1.588321	-1.942742	-0.350847
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H	-1.989198	0.210128	-1.407926
H	-4.226742	-2.517773	-2.264668
C	-4.593983	-1.360058	-0.583670
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H	-3.684641	-4.807631	-3.191110
H	-3.512142	-6.173293	-2.041161
H	-2.154334	-5.735030	-3.126552
H	-4.376679	-0.395786	-1.093457
H	-4.143756	-1.300057	0.422676
C	-6.089718	-1.566274	-0.472635
C	-6.624853	-2.382292	0.546653
C	-8.876230	-2.010644	-0.302462
C	-6.968835	-0.973261	-1.401936
C	-8.353979	-1.192226	-1.319059
H	-9.030003	-0.718164	-2.047671
H	-6.561704	-0.323121	-2.194684
C	-8.008616	-2.605271	0.631043
H	-5.946747	-2.832016	1.289407
H	-9.961741	-2.181221	-0.233939
H	-8.415046	-3.240983	1.433245

C_SR

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Ir	0.337224	-0.981172	-1.614601
C	0.779209	0.230711	-0.039930
N	0.857134	-0.146222	1.275635
C	0.362334	-1.350450	1.867679

C	1.186287	-2.464504	2.057064	C	0.388889	3.088028	-1.925552
C	2.614200	-2.514643	1.561745	C	-1.090478	2.910984	-1.665394
H	2.825288	-1.551594	1.048505	H	-1.190925	2.166808	-0.845372
C	2.845283	-3.645049	0.535253	C	-1.828154	2.336858	-2.896247
H	2.148383	-3.506933	-0.315983	H	-1.348143	1.379773	-3.195477
H	2.592827	-4.624165	1.001930	H	-1.712512	3.033001	-3.756785
C	4.304817	-3.676199	0.054156	C	-3.323494	2.137622	-2.602163
H	4.453819	-4.519396	-0.653511	H	-3.846702	1.749772	-3.503404
H	4.516752	-2.744918	-0.519687	H	-3.419364	1.353383	-1.815040
C	5.298251	-3.771558	1.222893	C	-3.994821	3.422611	-2.092568
H	5.174562	-4.753762	1.733184	H	-5.063266	3.234449	-1.846315
H	6.342147	-3.747210	0.843940	H	-3.997126	4.181784	-2.906686
C	5.059798	-2.643818	2.236298	C	-3.248606	3.987346	-0.874530
H	5.272427	-1.661431	1.754579	H	-3.330342	3.268202	-0.025397
H	5.760703	-2.725266	3.093892	H	-3.719968	4.930805	-0.526748
C	3.611100	-2.648334	2.737022	C	-1.765260	4.216635	-1.190652
H	3.415412	-3.602881	3.276154	H	-1.232807	4.613867	-0.306674
H	3.442191	-1.837050	3.468730	H	-1.676174	4.990298	-1.986345
C	0.659347	-3.570124	2.797295	C	0.846818	3.999933	-2.928030
H	1.294113	-4.458351	2.937934	H	0.101881	4.562706	-3.511846
C	-0.599069	-3.540507	3.373990	C	2.196039	4.210593	-3.169111
H	-0.961841	-4.397600	3.963049	H	2.515120	4.934300	-3.935820
C	-1.445217	-2.404633	3.209447	C	3.189578	3.479323	-2.451553
C	-2.767678	-2.340419	3.743415	C	4.590799	3.590258	-2.708542
H	-3.127388	-3.177495	4.363135	H	4.933751	4.318125	-3.461083
C	-3.598677	-1.257206	3.486548	C	5.509092	2.779698	-2.054607
H	-4.614462	-1.240204	3.910943	H	6.580374	2.875092	-2.291088
C	-3.143104	-0.160195	2.691768	C	5.078624	1.796799	-1.108843
C	-4.009592	1.055646	2.424112	C	6.035014	0.804218	-0.482322
H	-3.533009	1.617970	1.586215	H	5.433317	0.169142	0.210110
C	-5.452141	0.723040	1.987906	C	6.640503	-0.149272	-1.539480
H	-5.444526	0.072086	1.084116	H	7.216378	0.449215	-2.281289
H	-5.957587	0.134255	2.785446	H	5.817892	-0.639989	-2.103383
C	-6.267680	1.994286	1.708642	C	7.560060	-1.195059	-0.892159
H	-7.304157	1.720281	1.423228	H	6.946998	-1.863746	-0.246646
H	-5.827521	2.520483	0.830291	H	8.009885	-1.843843	-1.673308
C	-6.270094	2.941997	2.917646	C	8.655146	-0.537177	-0.037872
H	-6.831350	3.869654	2.678394	H	9.280186	-1.312344	0.453895
H	-6.811091	2.457906	3.762325	H	9.339121	0.040955	-0.700531
C	-4.837921	3.277915	3.358729	C	8.052911	0.409998	1.012417
H	-4.845964	3.937348	4.252222	H	8.856141	0.904174	1.598966
H	-4.335128	3.850454	2.546122	H	7.455245	-0.186894	1.740040
C	-4.027139	2.006300	3.646607	C	7.143775	1.466170	0.364439
H	-4.466691	1.464710	4.514811	H	7.755703	2.132885	-0.284501
H	-2.984647	2.257004	3.937208	H	6.683805	2.120476	1.136400
C	-1.838554	-0.194906	2.203817	C	3.722788	1.716569	-0.815810
H	-1.486207	0.647393	1.593262	H	3.381047	0.921832	-0.136808
C	-0.962680	-1.296595	2.427125	C	2.754033	2.542270	-1.454223
C	1.140536	0.982716	2.218308	C	-0.313652	-1.670371	-3.621129
H	0.232661	1.134988	2.837765	H	-1.378744	-1.387192	-3.709933
C	1.345762	2.167844	1.263106	C	-0.014702	-2.800317	-2.821131
H	2.420132	2.443426	1.229610	H	-0.864555	-3.363757	-2.405242
N	1.002525	1.578882	-0.070500	C	1.234261	-3.652201	-2.941961
C	1.350468	2.387032	-1.198335	H	1.158706	-4.312417	-3.837862

H	1.254637	-4.335152	-2.066811
C	2.536691	-2.824337	-2.981794
H	3.368083	-3.425967	-2.564632
H	2.823813	-2.610968	-4.032736
C	2.423717	-1.509877	-2.217053
H	3.080138	-1.412854	-1.335295
C	2.017262	-0.295988	-2.828173
H	2.424957	0.619403	-2.392536
C	1.573930	-0.096402	-4.260985
H	2.458519	-0.037414	-4.937603
H	1.089677	0.902065	-4.305437
C	0.581970	-1.172549	-4.749313
H	-0.047669	-0.756960	-5.562098
H	1.126728	-2.030524	-5.195121
C	0.579510	3.443483	1.555393
C	1.153172	4.667909	1.153107
C	-0.680167	3.460956	2.186075
C	0.487717	5.883045	1.379587
H	2.137541	4.663124	0.658627
C	-1.342815	4.675774	2.426221
H	-1.151574	2.523471	2.515399
C	-0.761908	5.890359	2.022968
H	0.951199	6.828600	1.059129
H	-2.317763	4.673254	2.935992
H	-1.281852	6.841819	2.213100
C	2.279690	0.695510	3.178962
C	1.970201	0.237871	4.475472
C	3.633661	0.860450	2.821766
C	2.989632	-0.037415	5.401924
H	0.914206	0.100129	4.759029
C	4.654850	0.590729	3.745925
H	3.904976	1.212325	1.816185
C	4.335826	0.143462	5.040058
H	2.731415	-0.390978	6.411923
H	5.706144	0.730025	3.450579
H	5.136658	-0.065831	5.765691
N	-4.050956	-1.855266	-0.735478
C	-4.538449	-2.974679	0.162330
C	-3.495493	-4.108226	0.032215
C	-2.199494	-3.278351	-0.115862
C	-2.530183	-2.149811	-1.089845
C	-1.722486	-0.883320	-1.034259
H	-4.548966	-2.576374	1.196027
C	-3.756583	-4.978287	-1.215067
C	-3.497045	-4.991945	1.286953
H	-1.335953	-3.870931	-0.473198
H	-1.910250	-2.849896	0.861034
H	-5.571083	-3.255025	-0.117278
H	-2.593277	-2.540220	-2.125496
H	-1.862305	-0.433470	-0.033525
H	-2.123370	-0.160361	-1.777559
H	-4.030771	-0.979681	-0.180343
C	-4.872257	-1.591609	-1.975084
H	-4.461310	-5.529526	1.401974

H	-3.323263	-4.387546	2.198201
H	-2.693054	-5.752595	1.222689
H	-3.724796	-4.403146	-2.163153
H	-4.747404	-5.474481	-1.154768
H	-2.987825	-5.773579	-1.294078
H	-4.924306	-2.552158	-2.521744
H	-4.274729	-0.877705	-2.576709
C	-6.243737	-1.041209	-1.684614
C	-6.423929	0.347505	-1.511143
C	-8.803885	0.010390	-1.131588
C	-7.362103	-1.896332	-1.585919
C	-8.634888	-1.374374	-1.304036
H	-9.501199	-2.049772	-1.234324
H	-7.241871	-2.978762	-1.756634
C	-7.697778	0.870822	-1.242307
H	-5.562926	1.025960	-1.609218
H	-9.803817	0.421593	-0.924554
H	-7.829134	1.957506	-1.130900

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Ir	0.649619	-0.889072	-1.696039
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N	0.550562	-0.057979	1.274045
C	-0.174259	-1.185851	1.775035
C	0.486308	-2.350792	2.180782
C	1.969435	-2.560224	1.986770
H	2.388870	-1.628110	1.550080
C	2.247011	-3.711042	0.994284
H	1.740820	-3.483152	0.032221
H	1.784828	-4.647015	1.382835
C	3.753977	-3.933132	0.794494
H	3.926947	-4.792726	0.112715
H	4.187713	-3.043139	0.284615
C	4.488292	-4.145023	2.128011
H	4.152194	-5.103466	2.585235
H	5.579964	-4.248349	1.952381
C	4.203028	-2.994698	3.105016
H	4.620542	-2.046831	2.696027
H	4.714895	-3.165305	4.075657
C	2.696757	-2.817695	3.326034
H	2.288449	-3.740308	3.796556
H	2.492380	-1.989066	4.029688
C	-0.276044	-3.371568	2.829644
H	0.235686	-4.296222	3.136115
C	-1.619839	-3.212741	3.119149
H	-2.170719	-3.997698	3.661505
C	-2.303667	-2.017474	2.751800
C	-3.675264	-1.789923	3.079998
H	-4.224440	-2.577474	3.621184
C	-4.299614	-0.592681	2.763040
H	-5.347537	-0.429385	3.057724
C	-3.600327	0.433606	2.054448
C	-4.268998	1.759214	1.751270

H	-3.580505	2.332107	1.089931	H	7.282408	1.661649	0.015027
C	-5.615123	1.628150	1.003574	C	5.928457	0.562365	1.285099
H	-5.457813	1.110478	0.033945	H	4.983623	-0.020094	1.188850
H	-6.304982	0.979648	1.588809	H	5.717348	1.410961	1.970705
C	-6.281938	2.993952	0.773869	C	6.999831	-0.367629	1.872946
H	-7.260752	2.852678	0.268867	H	7.937288	0.208955	2.041790
H	-5.654131	3.593310	0.076955	H	6.678231	-0.739039	2.869596
C	-6.452986	3.772295	2.086825	C	7.284110	-1.545845	0.928468
H	-6.913504	4.763490	1.891648	H	8.076923	-2.200099	1.348453
H	-7.158082	3.224158	2.752872	H	6.367178	-2.173675	0.850692
C	-5.104792	3.936785	2.802763	C	7.674587	-1.054013	-0.473467
H	-5.229356	4.483549	3.761179	H	7.824603	-1.914226	-1.160026
H	-4.434592	4.560513	2.168206	H	8.652905	-0.524765	-0.417568
C	-4.437906	2.577620	3.056056	C	6.618784	-0.101022	-1.052439
H	-5.056977	1.989505	3.771205	H	5.660144	-0.644893	-1.218027
H	-3.446960	2.706066	3.542782	H	6.934265	0.278436	-2.047218
C	-2.270800	0.207567	1.699936	C	3.954333	1.921760	-0.503139
H	-1.743339	0.977472	1.118294	H	3.596366	1.205560	0.249044
C	-1.575061	-0.988444	2.056249	C	2.987379	2.623973	-1.285669
C	0.733859	1.068409	2.242548	C	0.326258	-0.989848	-3.840822
H	-0.267085	1.322006	2.646313	H	-0.734004	-0.733961	-4.031469
C	1.256570	2.202156	1.344976	C	0.592740	-2.326304	-3.442479
H	2.336632	2.372315	1.539256	H	-0.271434	-3.002539	-3.355499
N	1.144304	1.608487	-0.024923	C	1.916816	-3.045721	-3.675275
C	1.574044	2.411192	-1.130598	H	2.400822	-2.658049	-4.594205
C	0.644838	3.050621	-1.958763	H	1.715827	-4.118245	-3.874685
C	-0.848475	2.948521	-1.740764	C	2.866566	-2.920624	-2.465432
H	-1.012803	2.316524	-0.840741	H	2.641523	-3.729452	-1.742081
C	-1.593380	2.272485	-2.910732	H	3.926001	-3.079041	-2.775403
H	-1.137276	1.282113	-3.110239	C	2.729734	-1.585437	-1.760305
H	-1.461510	2.877811	-3.835459	H	3.135361	-1.567522	-0.731374
C	-3.091779	2.146386	-2.593719	C	2.671541	-0.336308	-2.427241
H	-3.625600	1.646513	-3.431503	H	3.015275	0.516357	-1.842730
H	-3.209971	1.488502	-1.701136	C	2.718940	-0.105766	-3.930319
C	-3.726578	3.510866	-2.281405	H	3.344391	-0.877879	-4.423943
H	-4.797490	3.386477	-2.012209	H	3.222160	0.864103	-4.120571
H	-3.706986	4.142518	-3.198157	C	1.302043	-0.067519	-4.547187
C	-2.965127	4.228161	-1.156586	H	0.901157	0.965377	-4.474937
H	-3.086272	3.659021	-0.207361	H	1.335876	-0.312111	-5.634909
H	-3.396296	5.234095	-0.967603	C	0.573105	3.551928	1.479774
C	-1.467781	4.338959	-1.464100	C	1.309861	4.705696	1.137080
H	-0.932548	4.833231	-0.631823	C	-0.755154	3.706292	1.923748
H	-1.323330	4.984988	-2.358784	C	0.734206	5.981987	1.234206
C	1.137140	3.884059	-3.008439	H	2.350883	4.597907	0.793984
H	0.413314	4.375956	-3.675988	C	-1.329314	4.983039	2.036209
C	2.491173	4.106038	-3.192231	H	-1.356896	2.829836	2.204300
H	2.843588	4.759359	-4.006027	C	-0.587998	6.124842	1.690007
C	3.450307	3.484326	-2.341920	H	1.324609	6.869918	0.960997
C	4.856832	3.638138	-2.534485	H	-2.363911	5.083452	2.397213
H	5.210253	4.314943	-3.328557	H	-1.039028	7.125128	1.777851
C	5.762823	2.923298	-1.768954	C	1.599227	0.700265	3.429294
H	6.843933	3.028843	-1.954792	C	0.981148	0.350058	4.645904
C	5.320054	2.018892	-0.753866	C	3.004481	0.684606	3.349700
C	6.330047	1.093395	-0.101598	C	1.754477	0.007980	5.767936

H	-0.118968	0.352563	4.711554
C	3.781523	0.350857	4.468977
H	3.506424	0.941066	2.406897
C	3.157667	0.014770	5.683615
H	1.259369	-0.258744	6.714275
H	4.879442	0.352159	4.390761
H	3.765596	-0.244313	6.563976
N	-3.612381	-2.554083	-1.358817
C	-3.756577	-3.762058	-0.470633
C	-2.506447	-4.620537	-0.734100
C	-1.430982	-3.512909	-0.789055
C	-2.001133	-2.375657	-1.636111
C	-1.476465	-0.994001	-1.397502
H	-4.724888	-4.262207	-0.666986
C	-2.275844	-5.618194	0.407902
C	-2.619152	-5.376021	-2.074560
H	-0.467938	-3.853563	-1.215655
H	-1.213376	-3.139135	0.230614
H	-3.750260	-3.389064	0.573386
H	-1.951799	-2.630256	-2.712277
H	-1.744234	-0.659277	-0.382601
H	-1.930356	-0.282021	-2.115091
H	-4.034046	-2.779607	-2.273741
C	-4.314424	-1.327600	-0.848781
H	-3.447257	-6.113982	-2.047084
H	-2.795662	-4.707195	-2.943609
H	-1.681403	-5.929978	-2.282409
H	-2.186875	-5.096019	1.380607
H	-3.102937	-6.355231	0.475230
H	-1.335685	-6.182351	0.241483
H	-3.931725	-1.139832	0.169866
H	-3.985450	-0.489019	-1.489930
C	-5.812320	-1.483675	-0.877021
C	-6.534207	-1.120111	-2.033910
C	-8.615818	-1.791748	-0.969058
C	-6.510393	-1.998515	0.235789
C	-7.904951	-2.151138	0.189731
H	-8.442553	-2.546866	1.065211
H	-5.954161	-2.260482	1.148774
C	-7.929160	-1.274852	-2.081471
H	-5.999640	-0.692124	-2.898774
H	-9.710089	-1.907228	-1.002373
H	-8.483939	-0.980839	-2.985666

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C	0.397046	0.387395	-0.025698
N	0.569119	-0.068442	1.256310
C	0.032793	-1.289697	1.795995
C	0.837900	-2.411061	2.037833
C	2.305273	-2.476439	1.671610
H	2.541922	-1.568684	1.072776
C	2.673619	-3.723304	0.832124
H	2.012201	-3.812005	-0.051928

H	2.492838	-4.637200	1.440611
C	4.149367	-3.682119	0.408816
H	4.398509	-4.576838	-0.200407
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C	5.078005	-3.584372	1.629836
H	5.007245	-4.528386	2.216349
H	6.137122	-3.500077	1.305790
C	4.691984	-2.402441	2.531431
H	4.885210	-1.446519	1.992101
H	5.328616	-2.374770	3.440960
C	3.210599	-2.452070	2.927122
H	3.013549	-3.369012	3.527603
H	2.944061	-1.596458	3.571062
C	0.249426	-3.531829	2.705464
H	0.872520	-4.419184	2.889516
C	-1.067774	-3.534174	3.121702
H	-1.490810	-4.416895	3.625054
C	-1.904671	-2.405423	2.883868
C	-3.284577	-2.387444	3.242136
H	-3.709663	-3.274361	3.738409
C	-4.085832	-1.284450	2.974215
H	-5.146401	-1.299724	3.267684
C	-3.544355	-0.127230	2.337442
C	-4.367898	1.125855	2.104464
H	-3.859045	1.703134	1.296314
C	-5.819293	0.877208	1.644732
H	-5.829902	0.233542	0.740318
H	-6.368603	0.316869	2.434277
C	-6.550319	2.201924	1.376093
H	-7.591676	2.003892	1.045080
H	-6.047873	2.729182	0.532803
C	-6.542831	3.105246	2.619080
H	-7.041523	4.072410	2.398182
H	-7.140598	2.621403	3.424778
C	-5.111593	3.344239	3.124430
H	-5.120748	3.954414	4.052532
H	-4.554393	3.934311	2.362284
C	-4.367668	2.022798	3.368937
H	-4.850315	1.461660	4.201070
H	-3.322868	2.212610	3.695258
C	-2.196405	-0.138688	1.977625
H	-1.794179	0.741404	1.457620
C	-1.344671	-1.254879	2.221731
C	0.780647	1.045855	2.241080
H	-0.167062	1.158808	2.807562
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C	0.937560	2.542906	-1.154465
C	0.003327	3.333785	-1.837055
C	-1.463233	3.383644	-1.468681
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H	-2.119115	2.201566	-3.202949

H	-2.284218	3.953084	-3.409147	H	2.030838	-2.133698	-0.949724
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H	-4.539904	2.902051	-3.086328	H	2.640664	0.044627	-1.653805
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C	-4.279009	4.378451	-1.490245	H	2.639364	-0.920506	-4.463985
H	-5.321835	4.301617	-1.113712	H	3.049485	0.693329	-3.854336
H	-4.272391	5.221206	-2.217934	C	0.951022	0.489852	-4.393603
C	-3.311188	4.698452	-0.340986	H	0.876756	1.563559	-4.124672
H	-3.405123	3.916334	0.446914	H	0.947213	0.449092	-5.508346
H	-3.580222	5.660064	0.144956	C	0.315499	3.543879	1.753937
C	-1.853288	4.731934	-0.816643	C	1.001923	4.761732	1.574422
H	-1.172820	4.962060	0.022143	C	-0.972480	3.566271	2.325059
H	-1.719078	5.548385	-1.561980	C	0.418398	5.978340	1.963685
C	0.477564	4.162649	-2.900409	H	2.008013	4.750005	1.125196
H	-0.249404	4.776787	-3.453063	C	-1.552980	4.778628	2.728577
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H	2.149395	4.888757	-4.062321	C	-0.859641	5.988201	2.548224
C	2.787620	3.466113	-2.533950	H	0.966804	6.921271	1.816158
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H	4.519378	4.171440	-3.656166	H	-1.316229	6.938642	2.864298
C	5.096841	2.729107	-2.152186	C	1.873272	0.798977	3.259431
H	6.163482	2.773651	-2.421999	C	1.509561	0.387753	4.557372
C	4.666653	1.854596	-1.107263	C	3.239487	0.983376	2.961930
C	5.620965	0.900347	-0.420286	C	2.488438	0.168540	5.540750
H	5.026374	0.327936	0.330528	H	0.443779	0.240500	4.795314
C	6.188188	-0.135117	-1.420398	C	4.219558	0.772337	3.943536
H	6.747049	0.402291	-2.219690	H	3.553056	1.299781	1.956515
H	5.346667	-0.658320	-1.924324	C	3.846614	0.364618	5.236379
C	7.120371	-1.140107	-0.729210	H	2.188962	-0.151883	6.550377
H	6.524569	-1.755423	-0.018378	H	5.281024	0.924480	3.694750
H	7.541017	-1.846867	-1.475593	H	4.615095	0.200607	6.007278
C	8.244836	-0.431345	0.041786	Ir	-0.050826	-0.574642	-1.756290
H	8.883013	-1.173969	0.565796	N	-2.805912	-2.529596	-1.698456
H	8.908617	0.096998	-0.680300	C	-4.006224	-3.282412	-2.180826
C	7.677609	0.588169	1.042330	C	-5.237065	-2.358823	-1.891269
H	8.499277	1.113708	1.573360	C	-4.586569	-0.971805	-1.576991
H	7.095726	0.046073	1.823960	C	-3.123460	-1.058825	-2.023863
C	6.758755	1.606736	0.349101	C	-2.110756	-0.104945	-1.433472
H	7.356949	2.220959	-0.361816	H	-3.870261	-3.441677	-3.268432
H	6.325617	2.317075	1.086124	C	-6.057828	-2.867755	-0.691078
C	3.315419	1.831446	-0.779232	C	-6.128777	-2.289955	-3.145114
H	2.992578	1.130519	0.002436	H	-5.104084	-0.137184	-2.087641
C	2.339711	2.608913	-1.468549	H	-4.620145	-0.754825	-0.489352
C	-0.289055	-0.201822	-3.858457	H	-4.045993	-4.270876	-1.685202
H	-1.211088	0.395621	-3.995362	H	-3.083639	-1.031131	-3.134250
C	-0.466414	-1.612785	-3.734286	H	-2.279680	0.869390	-1.925239
H	-1.507250	-1.960468	-3.870894	H	-2.365192	0.054380	-0.367689
C	0.587760	-2.653349	-4.103479	H	-1.934638	-2.749690	-2.227228
H	1.199123	-2.287450	-4.953450	C	-2.466688	-2.735339	-0.243397
H	0.083835	-3.568558	-4.476847	H	-6.495421	-3.296804	-3.435866
C	1.495907	-3.020795	-2.907907	H	-5.577889	-1.865183	-4.010563
H	1.030494	-3.851607	-2.338065	H	-7.015552	-1.650581	-2.959653
H	2.475141	-3.417632	-3.263267	H	-5.446205	-2.926440	0.233092
C	1.724218	-1.853805	-1.968752	H	-6.482866	-3.873708	-0.888428

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C	-2.072724	-4.149409	0.060753
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H	-0.099587	-3.859490	-0.775858
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C	1.768084	-2.815546	2.000849
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C	1.883243	-4.075012	1.108191
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H	1.359275	-4.921375	1.606804
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H	3.386546	-5.398286	0.243821
H	3.840660	-3.679001	0.249495
C	4.122617	-4.647981	2.168222
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C	-0.480490	-3.398640	2.975036
H	-0.020024	-4.346578	3.291154
C	-1.790009	-3.133513	3.325074
H	-2.368371	-3.859232	3.918388
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C	-3.746438	-1.589914	3.308093
H	-4.316435	-2.321318	3.903433
C	-4.314798	-0.376675	2.956130
H	-5.341059	-0.142772	3.278126
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H	-3.497162	2.481719	1.225315
C	-5.535190	1.790482	1.058575
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C	0.823110	0.932130	2.249698
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H	-1.155389	2.166502	-0.846349
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C	-1.538538	4.203710	-1.471564
H	-0.965882	4.663959	-0.644636
H	-1.364385	4.841906	-2.366575
C	0.949271	3.575067	-3.164662
H	0.202255	4.029638	-3.832863
C	2.295491	3.755514	-3.433697
H	2.615769	4.334212	-4.314367
C	3.284546	3.203804	-2.569196
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H	5.012680	3.935554	-3.676785
C	5.624847	2.780217	-1.953149
H	6.695964	2.906246	-2.168384
C	5.212165	2.032765	-0.810809
C	6.170886	1.302508	0.116517
H	5.779394	1.440931	1.152627
C	6.143343	-0.222794	-0.167074
H	6.494336	-0.393189	-1.210253
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C	7.023844	-1.002827	0.819516
H	6.581966	-0.920374	1.840076
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C	8.462217	-0.462633	0.846296
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H	9.530160	1.430889	1.095552
H	8.106824	1.245480	2.147644
C	7.620125	1.819052	0.108461
H	8.053949	1.689482	-0.909089
H	7.637944	2.908835	0.323976
C	3.846863	1.902613	-0.570466
H	3.532100	1.313899	0.298920
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H	-0.306465	-0.174634	-4.175518
C	0.526942	-2.087715	-3.651732
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C	1.688105	-3.067807	-3.763122
H	2.393891	-2.733639	-4.551056
H	1.306149	-4.052448	-4.102315
C	2.429239	-3.246041	-2.417171
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H	3.474441	-3.596273	-2.585298
C	2.439917	-1.983269	-1.576830
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H	3.173557	0.000857	-1.308064
C	3.130480	-0.350071	-3.491667
H	3.649826	-1.201989	-3.977806
H	3.852716	0.490906	-3.491849
C	1.876501	0.061360	-4.295425
H	1.683816	1.141532	-4.138777
H	2.043521	-0.070147	-5.390417
C	0.545162	3.423688	1.465656
C	1.239981	4.577668	1.043723
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C	0.651443	5.847668	1.144848
H	2.256829	4.473283	0.633341
C	-1.338137	4.840550	2.108864
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H	-1.102772	6.978111	1.770871
C	1.874341	0.553757	3.273393
C	1.534082	0.484562	4.636905
C	3.205526	0.288710	2.889114
C	2.509200	0.181246	5.603678
H	0.493462	0.678647	4.943078
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H	2.229410	0.131862	6.667214
H	5.221982	-0.185788	3.534164
H	4.606736	-0.272750	5.969519
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C	-3.949939	-3.889245	-1.367823
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C	-2.029822	-2.285795	-1.056280
C	-1.564013	-1.017793	-1.733601
H	-4.780476	-4.139668	-0.680343
C	-2.593516	-5.975796	-1.893643
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H	-0.556731	-3.882623	-1.185114
H	-1.518626	-3.652474	-2.668537
H	-4.303058	-4.047218	-2.405054
H	-1.872989	-2.216983	0.037286
H	-1.939975	-1.019497	-2.788511
H	-2.029796	-0.149539	-1.220072
H	-3.799427	-1.942818	-2.112019
C	-4.345334	-1.677655	-0.148779
H	-3.291268	-5.664860	0.755163
H	-2.573414	-4.047527	1.033484
H	-1.517211	-5.421306	0.633000
H	-2.668231	-5.787019	-2.985079
H	-3.418679	-6.659471	-1.604348
H	-1.639006	-6.508894	-1.707338
H	-3.819691	-0.709338	-0.038720
H	-4.207791	-2.236188	0.794585
C	-5.797108	-1.467023	-0.476886
C	-6.806985	-2.040063	0.319571
C	-8.513764	-0.997481	-1.068103
C	-6.159244	-0.652451	-1.572201
C	-7.510469	-0.422626	-1.869936
H	-7.783648	0.218524	-2.721966
H	-5.377541	-0.166864	-2.181867
C	-8.161306	-1.803749	0.027067
H	-6.527407	-2.661258	1.185743
H	-9.574428	-0.811854	-1.296838
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C	0.812849	-2.898632	-2.175601
C	2.253829	-2.634473	-1.801136
H	2.252497	-1.998594	-0.890173
C	3.043448	-1.888542	-2.898156
H	2.521111	-0.947534	-3.161079
H	3.063335	-2.505352	-3.824333
C	4.485589	-1.606413	-2.451581
H	5.036868	-1.074373	-3.255682

H	4.465203	-0.916648	-1.576860	H	-4.416513	1.935053	-0.048908
C	5.212143	-2.902525	-2.058649	C	-5.349113	2.512848	1.821495
H	5.331647	-3.543251	-2.961467	H	-6.373603	2.362207	1.419530
H	6.238978	-2.677875	-1.699806	H	-5.399909	3.410869	2.477863
C	4.423284	-3.674690	-0.991785	C	-4.911744	1.303159	2.661203
H	4.394900	-3.079922	-0.050273	H	-4.963035	0.379324	2.038684
H	4.930878	-4.628804	-0.736405	H	-5.610031	1.140546	3.509349
C	2.983375	-3.951683	-1.441614	C	-3.479566	1.469678	3.182894
H	2.993468	-4.615518	-2.335516	H	-3.172753	0.590510	3.778184
H	2.422939	-4.491639	-0.656117	H	-3.439060	2.344952	3.869745
C	0.523263	-3.625083	-3.374405	C	-0.707131	2.879579	3.393143
H	1.357809	-3.901717	-4.036212	H	-1.489448	3.587175	3.705002
C	-0.763031	-4.017634	-3.705889	C	0.578506	3.026057	3.886386
H	-0.946377	-4.590899	-4.628491	H	0.813420	3.840551	4.589887
C	-1.868029	-3.688480	-2.865660	C	1.620569	2.138011	3.488776
C	-3.216952	-4.033591	-3.184250	C	2.968108	2.269064	3.940807
H	-3.409603	-4.619688	-4.096879	H	3.213664	3.085894	4.637920
C	-4.273912	-3.620577	-2.384558	C	3.957416	1.394472	3.514068
H	-5.305016	-3.882351	-2.667822	H	4.987862	1.521372	3.880272
C	-4.041484	-2.828871	-1.218287	C	3.660976	0.343760	2.592122
C	-5.175215	-2.215466	-0.424775	C	4.736801	-0.591968	2.080995
H	-4.720635	-1.721026	0.465377	H	4.267447	-1.225511	1.292199
C	-5.872703	-1.099318	-1.242404	C	5.914363	0.157395	1.417879
H	-5.113672	-0.358886	-1.576684	H	6.392153	0.826018	2.168946
H	-6.304028	-1.546214	-2.166924	H	5.529046	0.815849	0.612962
C	-6.982584	-0.416397	-0.430347	C	6.963535	-0.817327	0.865107
H	-7.489774	0.352249	-1.051055	H	6.507599	-1.407394	0.038772
H	-6.521003	0.127383	0.424309	H	7.807945	-0.253269	0.415616
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H	-8.766436	-0.926165	0.727282	H	8.197735	-2.500315	1.522804
H	-8.542643	-1.898639	-0.746340	H	8.026022	-1.197319	2.723351
C	-7.303883	-2.541208	0.920198	C	6.306428	-2.523641	2.621318
H	-8.044012	-3.287269	1.278317	H	6.678758	-3.187982	3.429701
H	-6.846327	-2.090955	1.831924	H	5.820663	-3.185259	1.867708
C	-6.205478	-3.237503	0.100969	C	5.256782	-1.549817	3.179742
H	-6.670103	-3.771727	-0.758571	H	5.704205	-0.949173	4.003789
H	-5.689063	-4.011405	0.708444	H	4.403176	-2.101437	3.630103
C	-2.725881	-2.526981	-0.877175	C	2.348408	0.204571	2.149454
H	-2.557435	-1.862529	-0.018242	H	2.131992	-0.562311	1.392957
C	-1.614587	-2.938546	-1.667312	C	1.302860	1.073052	2.576019
C	-0.291564	-2.638868	1.165542	C	0.417181	0.932954	-3.796317
H	-1.285013	-3.126099	1.088814	H	1.496656	0.716951	-3.881873
C	-0.331452	-1.517667	2.219046	C	0.066633	2.199986	-3.318947
H	0.616753	-1.504552	2.794163	H	0.883558	2.849853	-2.973036
N	-0.344363	-0.264827	1.383976	C	-1.274225	2.880140	-3.545697
C	-0.049049	0.938769	2.105249	H	-1.688314	2.557899	-4.520600
C	-1.059546	1.821080	2.498532	H	-1.103075	3.971502	-3.638707
C	-2.487725	1.693243	2.020139	C	-2.290992	2.630913	-2.410181
H	-2.538248	0.796415	1.362344	H	-2.111298	3.355777	-1.592837
C	-2.920144	2.923063	1.189435	H	-3.326683	2.831185	-2.768764
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H	-2.844541	3.836381	1.818553	H	-2.630576	1.130306	-0.816315
C	-4.360173	2.780990	0.674979	C	-2.067456	0.067379	-2.577461
H	-4.648269	3.692826	0.110053	H	-2.359884	-0.856489	-2.070019

C	-1.940412	-0.046459	-4.087623
H	-2.527067	0.750591	-4.585826
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C	-0.469105	-0.028037	-4.561825
H	-0.039107	-1.046625	-4.449434
H	-0.409110	0.203422	-5.650543
C	-1.461492	-1.573803	3.226304
C	-1.205496	-1.153528	4.547332
C	-2.757417	-2.018511	2.893957
C	-2.218229	-1.188976	5.519962
H	-0.196941	-0.798647	4.813512
C	-3.771894	-2.056247	3.863164
H	-2.987935	-2.355144	1.872846
C	-3.503786	-1.644745	5.180611
H	-2.001260	-0.861902	6.548270
H	-4.776774	-2.410803	3.586610
H	-4.297760	-1.677800	5.942239
C	0.721980	-3.743137	1.380727
C	0.368120	-5.055552	1.006540
C	2.002728	-3.509075	1.921164
C	1.273465	-6.116468	1.171860
H	-0.631285	-5.243523	0.581980
C	2.905523	-4.569261	2.096609
H	2.304438	-2.495110	2.221235
C	2.544326	-5.875156	1.721493
H	0.982963	-7.136293	0.876612
H	3.898287	-4.373273	2.528620
H	3.253705	-6.705341	1.859953
N	1.734108	3.419721	-0.724863
C	2.566654	4.419463	-1.431654
C	3.867639	3.713718	-1.895203
C	3.986119	2.582045	-0.842036
C	2.537170	2.178416	-0.485310
C	2.070854	0.913901	-1.238923
H	2.815887	5.256259	-0.735855
C	3.733321	3.163207	-3.329930
C	5.070521	4.671046	-1.846269
H	4.491809	2.980310	0.063084
H	4.591206	1.726972	-1.207298
H	2.025550	4.880810	-2.288281
H	2.481478	1.955753	0.595094
H	2.493415	0.045744	-0.689496
H	2.556584	0.894656	-2.235141
H	0.034445	1.991753	-0.870691
C	1.140360	3.950389	0.498338
H	4.928096	5.528327	-2.537321
H	5.223467	5.077614	-0.824861
H	6.002828	4.150579	-2.149821
H	2.841625	2.520864	-3.455590
H	3.649417	3.993600	-4.061761
H	4.622772	2.558972	-3.604617
H	1.921342	4.381584	1.179999
H	0.692832	3.101038	1.050480
C	0.042345	4.972723	0.298160

C	-0.557646	5.191614	-0.954438
C	-2.161006	6.735970	0.033872
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C	-1.548055	6.548599	1.287158
H	-1.925167	7.087881	2.170309
H	0.025790	5.539973	2.395291
C	-1.651669	6.065292	-1.089021
H	-0.153455	4.665359	-1.828400
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C	-0.298591	-2.283213	-1.685266
C	0.667417	-2.513876	-2.677498
C	2.130051	-2.165261	-2.511479
H	2.231201	-1.578406	-1.572431
C	2.703918	-1.324224	-3.674434
H	2.088511	-0.416499	-3.834722
H	2.641501	-1.913397	-4.616161
C	4.172249	-0.952726	-3.413354
H	4.571114	-0.354912	-4.260111
H	4.225316	-0.293216	-2.515939
C	5.039797	-2.199319	-3.175795
H	5.099787	-2.788246	-4.119011
H	6.082034	-1.902679	-2.930322
C	4.452861	-3.085089	-2.067248
H	4.505350	-2.545079	-1.093906
H	5.055166	-4.009203	-1.938480
C	2.988814	-3.443667	-2.346981
H	2.923246	-4.045132	-3.281769
H	2.578036	-4.076145	-1.540636
C	0.257952	-3.193303	-3.867028
H	1.004292	-3.363345	-4.657423
C	-1.032060	-3.665157	-4.042004
H	-1.309623	-4.193049	-4.967991
C	-2.016291	-3.483562	-3.027546
C	-3.360512	-3.944405	-3.168229
H	-3.640728	-4.472086	-4.093618
C	-4.306783	-3.721583	-2.177559
H	-5.340667	-4.070075	-2.323824
C	-3.953026	-3.035633	-0.975781
C	-4.977727	-2.658342	0.074629
H	-4.412404	-2.285021	0.960844
C	-5.851869	-1.476266	-0.415585
H	-5.196817	-0.634256	-0.727451
H	-6.409197	-1.795547	-1.325448
C	-6.838915	-1.021766	0.669927
H	-7.477449	-0.198449	0.285255
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C	-7.702594	-2.188715	1.174289

H	-8.375938	-1.847663	1.988877	H	8.527472	-2.232237	0.149527
H	-8.364376	-2.537727	0.348944	H	8.437787	-1.191576	1.591128
C	-6.834483	-3.362954	1.653775	C	6.807669	-2.621852	1.443952
H	-7.471377	-4.210515	1.983630	H	7.328184	-3.389375	2.054743
H	-6.250324	-3.044223	2.548530	H	6.263200	-3.172433	0.642750
C	-5.859414	-3.827035	0.559678	C	5.792636	-1.858619	2.309705
H	-6.440017	-4.234298	-0.298628	H	6.323774	-1.388507	3.167632
H	-5.217055	-4.656126	0.926296	H	5.046332	-2.552517	2.753524
C	-2.635803	-2.614421	-0.820434	C	2.720834	0.085246	1.830201
H	-2.382272	-2.065427	0.095341	H	2.456343	-0.434100	0.896218
C	-1.641314	-2.789507	-1.823600	C	1.722269	0.843793	2.511006
C	0.069859	-2.629558	0.764849	C	-0.718749	0.986721	-3.769691
H	-0.909388	-3.147465	0.795150	H	0.269207	0.721327	-4.189107
C	0.184282	-1.655581	1.941668	C	-0.908610	2.327532	-3.407729
H	1.222266	-1.655711	2.328758	H	-0.049711	2.987979	-3.595353
N	-0.033316	-0.310785	1.295413	C	-2.258156	3.005975	-3.256052
C	0.331943	0.797883	2.133352	H	-2.968516	2.580636	-3.994375
C	-0.625298	1.585794	2.782393	H	-2.152577	4.078299	-3.510919
C	-2.113507	1.432944	2.550571	C	-2.830656	2.895729	-1.824243
H	-2.245178	0.681852	1.740210	H	-2.464594	3.745209	-1.221087
C	-2.815624	2.739445	2.115248	H	-3.940873	2.991764	-1.843510
H	-2.317714	3.167575	1.222992	C	-2.465483	1.611528	-1.118158
H	-2.707103	3.498033	2.922819	H	-2.487621	1.664077	-0.022205
C	-4.309819	2.502100	1.839490	C	-2.581614	0.328461	-1.673346
H	-4.795980	3.456174	1.544591	H	-2.700402	-0.491337	-0.957761
H	-4.413430	1.818809	0.965745	C	-3.009522	0.019800	-3.096878
C	-5.026335	1.878134	3.046963	H	-3.770890	0.753432	-3.432564
H	-6.085241	1.658394	2.793792	H	-3.507385	-0.970044	-3.111659
H	-5.050443	2.615325	3.881325	C	-1.811998	-0.015665	-4.077132
C	-4.306758	0.607809	3.526473	H	-1.359160	-1.025710	-4.067286
H	-4.383737	-0.185096	2.745928	H	-2.156547	0.149686	-5.124733
H	-4.797580	0.195171	4.433226	C	-0.717820	-1.924648	3.127452
C	-2.824320	0.878555	3.808334	C	-0.220855	-1.660114	4.420501
H	-2.315468	-0.035958	4.157798	C	-2.027100	-2.429193	2.992442
H	-2.733098	1.621929	4.632213	C	-1.012107	-1.901202	5.555260
C	-0.169019	2.481297	3.802947	H	0.800146	-1.261115	4.532602
H	-0.903182	3.137486	4.294885	C	-2.819150	-2.676499	4.124435
C	1.139167	2.470836	4.258327	H	-2.442575	-2.644621	1.997336
H	1.436147	3.107328	5.106812	C	-2.312746	-2.414841	5.409625
C	2.113448	1.621315	3.655110	H	-0.609805	-1.691752	6.558173
C	3.450559	1.496640	4.140529	H	-3.837842	-3.075108	4.000413
H	3.742718	2.068808	5.035236	H	-2.932120	-2.611491	6.298095
C	4.374772	0.685587	3.498281	C	1.118007	-3.720213	0.681401
H	5.398491	0.609131	3.895759	C	0.732935	-4.968207	0.148719
C	4.031448	-0.004405	2.293565	C	2.448424	-3.543534	1.111359
C	5.067698	-0.766057	1.493676	C	1.657062	-6.020258	0.046844
H	4.527917	-1.279961	0.664185	H	-0.306340	-5.111148	-0.188574
C	6.089978	0.191030	0.834765	C	3.371717	-4.597072	1.019171
H	6.615051	0.765119	1.631806	H	2.773826	-2.581660	1.532728
H	5.548583	0.940243	0.218967	C	2.979706	-5.837103	0.486001
C	7.114017	-0.571815	-0.017794	H	1.341989	-6.988300	-0.371744
H	6.589635	-1.036849	-0.883071	H	4.405443	-4.447378	1.364896
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C	7.821778	-1.667434	0.794306	N	1.168065	3.336411	-0.420745

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C	2.180942	2.281381	-0.787178
C	1.690417	1.363480	-1.890890
H	1.689698	3.337092	1.633097
C	3.822710	5.488865	0.002465
C	4.231016	3.571954	1.545286
H	4.373338	2.396391	-0.755028
H	3.597608	3.601923	-1.815400
H	1.413528	4.975414	0.955509
H	2.218603	1.667928	0.134625
H	2.305136	0.444917	-1.854387
H	1.857888	1.811644	-2.898035
H	0.069010	2.365632	-0.653431
C	0.906833	4.352596	-1.459889
H	4.022278	4.161091	2.462411
H	4.028542	2.511584	1.771946
H	5.312842	3.670490	1.319069
H	3.246364	5.926749	-0.837389
H	3.709064	6.168597	0.872711
H	4.893111	5.498338	-0.290598
H	1.788753	5.013815	-1.584000
H	0.782662	3.830163	-2.421422
C	-0.309670	5.209444	-1.176818
C	-0.759874	6.092054	-2.181643
C	-1.008164	5.168907	0.046252
C	-1.886138	6.902650	-1.974432
H	-0.223155	6.138983	-3.143766
C	-2.129063	5.990153	0.261467
H	-0.695972	4.469717	0.833981
C	-2.575600	6.855903	-0.748649
H	-2.228150	7.577635	-2.774201
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C	0.962073	-2.466627	2.049647
C	2.398998	-2.503411	1.575424
H	2.583022	-1.569048	0.997667
C	2.702304	-3.711658	0.657440
H	1.966640	-3.773494	-0.168219
H	2.574097	-4.649122	1.242303
C	4.137744	-3.643883	0.116482
H	4.338980	-4.511147	-0.547654
H	4.243992	-2.732858	-0.517851
C	5.162287	-3.591820	1.260665
H	5.140606	-4.559151	1.811678
H	6.191724	-3.490290	0.856074
C	4.848346	-2.449202	2.238737

H	4.994219	-1.470959	1.724680
H	5.557561	-2.455022	3.093312
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H	3.259923	-3.460484	3.331887
H	3.191294	-1.691005	3.445739
C	0.443298	-3.578548	2.785907
H	1.093454	-4.450909	2.946860
C	-0.838095	-3.585332	3.305098
H	-1.202350	-4.456465	3.870274
C	-1.711279	-2.477101	3.101949
C	-3.053043	-2.448039	3.586815
H	-3.424368	-3.315337	4.155257
C	-3.885255	-1.364240	3.343309
H	-4.916898	-1.374437	3.727924
C	-3.421881	-0.240621	2.592003
C	-4.318972	0.939801	2.279985
H	-3.751003	1.603548	1.586013
C	-5.611776	0.524363	1.544766
H	-5.350102	-0.059620	0.637494
H	-6.204004	-0.156175	2.196992
C	-6.464232	1.745955	1.174465
H	-7.394661	1.422832	0.661427
H	-5.903031	2.369114	0.441691
C	-6.795531	2.593590	2.412590
H	-7.377904	3.493605	2.122863
H	-7.449770	2.003525	3.094067
C	-5.519919	3.002587	3.166750
H	-5.774326	3.577804	4.082070
H	-4.921908	3.686029	2.521461
C	-4.658857	1.782541	3.531992
H	-5.203425	1.143538	4.263571
H	-3.719846	2.096847	4.037248
C	-2.110540	-0.254266	2.127069
H	-1.771452	0.590626	1.513205
C	-1.226840	-1.349169	2.354174
C	0.822732	0.951939	2.287605
H	-0.095944	1.000303	2.906995
C	0.931215	2.216631	1.422678
H	1.993381	2.514689	1.311472
N	0.464727	1.729761	0.085571
C	0.774733	2.560508	-1.055780
C	-0.191892	3.360694	-1.688920
C	-1.648823	3.398908	-1.284996
H	-1.823790	2.556718	-0.582329
C	-2.621160	3.256105	-2.481196
H	-2.359213	2.373288	-3.101773
H	-2.508697	4.136487	-3.151856
C	-4.078017	3.186462	-1.998327
H	-4.763711	3.072798	-2.864739
H	-4.210297	2.274489	-1.371405
C	-4.449626	4.430914	-1.176784
H	-5.482926	4.338619	-0.779404
H	-4.452351	5.320756	-1.846167
C	-3.452319	4.663748	-0.032020

H	-3.545396	3.838921	0.710624	H	1.060038	0.864593	-5.450033
H	-3.692723	5.598595	0.517081	C	0.189989	3.427606	1.945363
C	-2.001804	4.704720	-0.530576	C	0.815056	4.688007	1.866103
H	-1.304131	4.858490	0.311231	C	-1.097289	3.336528	2.514393
H	-1.860920	5.569175	-1.218138	C	0.170364	5.837978	2.351273
C	0.244603	4.234597	-2.733114	H	1.819338	4.763221	1.418952
H	-0.506221	4.852377	-3.247388	C	-1.739650	4.482150	3.007238
C	1.575243	4.350365	-3.096442	H	-1.607967	2.364921	2.579560
H	1.873838	5.046677	-3.895962	C	-1.107888	5.735872	2.926550
C	2.577075	3.583184	-2.436660	H	0.669885	6.816516	2.283955
C	3.961167	3.676717	-2.775068	H	-2.742138	4.396238	3.452908
H	4.261574	4.378269	-3.569275	H	-1.612894	6.634172	3.313454
C	4.911815	2.895509	-2.135381	C	1.974728	0.697388	3.235452
H	5.970398	2.976939	-2.426425	C	1.686777	0.202907	4.523802
C	4.527029	1.973819	-1.114464	C	3.317884	0.952503	2.889596
C	5.522425	1.024096	-0.483091	C	2.716434	-0.025595	5.451196
H	4.958505	0.392042	0.242259	H	0.639636	-0.001368	4.798847
C	6.124339	0.063588	-1.537087	C	4.349024	0.728448	3.814834
H	6.657818	0.661770	-2.309851	H	3.574886	1.339400	1.893469
H	5.302349	-0.467747	-2.064453	C	4.050953	0.240750	5.099311
C	7.097640	-0.937498	-0.898950	H	2.474984	-0.410163	6.453836
H	6.528760	-1.608778	-0.218253	H	5.391468	0.936692	3.528997
H	7.540783	-1.589507	-1.681098	H	4.859444	0.068449	5.826144
C	8.198918	-0.225419	-0.098130	Ir	-0.114126	-0.409701	-1.798961
H	8.864778	-0.968827	0.388633	N	-2.507564	-2.439863	-1.655939
H	8.840854	0.359443	-0.795808	C	-3.366167	-3.353353	-2.441760
C	7.600117	0.724318	0.951755	C	-4.799772	-2.679343	-2.496451
H	8.404642	1.256423	1.501911	C	-4.536448	-1.235239	-1.941640
H	7.045124	0.124627	1.710014	C	-3.014191	-1.094060	-2.067739
C	6.637818	1.738040	0.312628	C	-2.191118	0.017191	-1.450297
H	7.205665	2.408575	-0.371475	H	-2.940900	-3.441109	-3.463649
H	6.182592	2.394933	1.085144	C	-5.816316	-3.444214	-1.630945
C	3.184312	1.905580	-0.754360	C	-5.291825	-2.624189	-3.953884
H	2.901015	1.173731	0.013804	H	-5.075724	-0.457744	-2.518231
C	2.172076	2.675652	-1.396106	H	-4.863103	-1.143003	-0.885104
C	-0.271654	0.048077	-3.965427	H	-3.373431	-4.364064	-1.991290
H	-1.189229	0.656480	-4.065957	H	-2.829596	-1.053766	-3.162277
C	-0.434633	-1.348488	-3.935725	H	-2.448402	0.965668	-1.948335
H	-1.465702	-1.723504	-3.968710	H	-2.428340	0.145327	-0.376017
C	0.620725	-2.387347	-4.275666	H	-0.961517	-1.840553	-1.703133
H	1.324694	-1.983775	-5.029007	C	-2.620846	-2.690490	-0.202505
H	0.121518	-3.251749	-4.757546	H	-5.349435	-3.641155	-4.396078
C	1.385111	-2.876409	-3.027439	H	-4.609330	-2.020138	-4.589073
H	0.788277	-3.658419	-2.514013	H	-6.302943	-2.171473	-4.016149
H	2.341147	-3.368958	-3.318688	H	-5.474207	-3.535907	-0.579819
C	1.670513	-1.761596	-2.050103	H	-5.984927	-4.470016	-2.020198
H	1.910610	-2.091221	-1.029165	H	-6.796093	-2.922485	-1.621970
C	2.085457	-0.463828	-2.391752	H	-3.666204	-2.578044	0.155309
H	2.599454	0.083402	-1.593726	H	-2.030763	-1.907468	0.301219
C	2.291845	0.120006	-3.780751	C	-2.096728	-4.048566	0.189262
H	2.680223	-0.650625	-4.476127	C	-0.807724	-4.458750	-0.201935
H	3.080795	0.896008	-3.713554	C	-2.872849	-4.914856	0.982607
C	1.004834	0.776336	-4.340113	C	-0.305676	-5.709724	0.185414
H	0.926621	1.816104	-3.960895	H	-0.195181	-3.775199	-0.807726

C	-2.369813	-6.162948	1.386151
H	-3.880140	-4.598233	1.297782
C	-1.084382	-6.564712	0.985373
H	0.702951	-6.018115	-0.130052
H	-2.987455	-6.828316	2.009329
H	-0.690562	-7.546108	1.292023

C_D_RS

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Ir	-0.060271	0.953374	-1.600471
C	-0.243309	-0.376229	-0.107575
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C	0.034362	0.843568	2.046316
C	-0.900484	1.716952	2.612859
C	-2.385929	1.615376	2.332065
H	-2.519346	0.808821	1.575968
C	-2.998210	2.913535	1.760763
H	-2.409312	3.281948	0.899161
H	-2.930294	3.712753	2.531045
C	-4.474639	2.710063	1.389022
H	-4.895962	3.649992	0.973367
H	-4.547075	1.949997	0.575515
C	-5.294066	2.236199	2.600315
H	-5.327847	3.052587	3.356786
H	-6.347883	2.042644	2.306715
C	-4.670767	0.985509	3.236159
H	-4.746780	0.132565	2.523167
H	-5.236173	0.678852	4.141448
C	-3.191999	1.200953	3.585974
H	-3.105430	2.004557	4.351870
H	-2.758131	0.292030	4.038781
C	-0.416822	2.689556	3.542851
H	-1.136423	3.387130	3.998020
C	0.915141	2.749596	3.919550
H	1.247884	3.494900	4.658998
C	1.867379	1.827293	3.392113
C	3.226479	1.779414	3.827993
H	3.567710	2.517098	4.571299
C	4.101957	0.811449	3.353885
H	5.132520	0.778681	3.739683
C	3.681293	-0.143339	2.377377
C	4.587849	-1.267284	1.906763
H	4.067725	-1.767538	1.055985
C	5.964949	-0.807821	1.382837
H	5.826973	-0.090804	0.549486
H	6.501573	-0.254602	2.186223
C	6.826603	-1.994037	0.925186
H	7.814538	-1.629591	0.572832
H	6.340399	-2.476763	0.046764
C	6.997912	-3.033693	2.041742
H	7.597444	-3.896311	1.682005
H	7.572374	-2.581200	2.881936
C	5.631679	-3.508137	2.557893
H	5.751961	-4.240933	3.383724

H	5.107470	-4.042212	1.732729
C	4.762101	-2.329403	3.021381
H	5.232235	-1.844473	3.906757
H	3.764282	-2.683132	3.360771
C	2.368639	-0.076387	1.915667
H	2.057829	-0.801778	1.151714
C	1.424462	0.869108	2.414620
C	-0.381174	-1.616800	1.914571
H	0.617886	-1.730431	2.382828
C	-0.525225	-2.589282	0.733929
H	-1.581729	-2.913036	0.642825
N	-0.237019	-1.704561	-0.436757
C	-0.557827	-2.179473	-1.756314
C	0.437454	-2.558512	-2.671892
C	1.912808	-2.517328	-2.340080
H	2.028686	-1.911748	-1.415988
C	2.794760	-1.887046	-3.441738
H	2.405698	-0.888592	-3.734236
H	2.746810	-2.514796	-4.359060
C	4.256631	-1.790999	-2.976034
H	4.882494	-1.336061	-3.772732
H	4.312196	-1.101702	-2.102645
C	4.812879	-3.167111	-2.575421
H	5.846385	-3.063718	-2.181129
H	4.889659	-3.808291	-3.482714
C	3.909213	-3.861977	-1.546111
H	3.935661	-3.296561	-0.586034
H	4.285586	-4.880327	-1.312948
C	2.454245	-3.935324	-2.026264
H	1.816651	-4.428456	-1.271346
H	2.388498	-4.556938	-2.947891
C	0.011512	-3.095050	-3.927527
H	0.777362	-3.384131	-4.662645
C	-1.326366	-3.294198	-4.229798
H	-1.615068	-3.728104	-5.200283
C	-2.347306	-2.953716	-3.294209
C	-3.739060	-3.138948	-3.557871
H	-4.038136	-3.585133	-4.519594
C	-4.704840	-2.754921	-2.637138
H	-5.769805	-2.902609	-2.873612
C	-4.332272	-2.144795	-1.400066
C	-5.351329	-1.626168	-0.407768
H	-4.783904	-1.046342	0.358445
C	-6.364971	-0.649378	-1.044325
H	-6.939583	-1.179923	-1.836563
H	-5.818032	0.175570	-1.550269
C	-7.340334	-0.093865	0.004335
H	-6.773006	0.531226	0.730066
H	-8.075868	0.582021	-0.480539
C	-8.058608	-1.221810	0.761825
H	-8.728807	-0.799970	1.540111
H	-8.713252	-1.779721	0.054083
C	-7.053114	-2.197858	1.392815
H	-7.581986	-3.026519	1.909330

H	-6.468553	-1.660497	2.175114
C	-6.080892	-2.763145	0.345677
H	-6.638547	-3.388684	-0.387857
H	-5.333744	-3.434446	0.822099
C	-2.976731	-1.988691	-1.124405
H	-2.701837	-1.470379	-0.195423
C	-1.954825	-2.383101	-2.035241
C	0.160294	1.458171	-3.783234
H	1.186875	1.133448	-4.033954
C	0.037969	2.708742	-3.169414
H	0.983524	3.216496	-2.954853
C	-1.197616	3.589549	-3.114887
H	-1.814251	3.433040	-4.020577
H	-0.871376	4.647385	-3.137600
C	-2.031265	3.367769	-1.836361
H	-1.564117	3.922786	-0.998119
H	-3.051637	3.798444	-1.957098
C	-2.142623	1.915102	-1.448916
H	-2.436729	1.733606	-0.404385
C	-2.275511	0.830922	-2.322779
H	-2.659588	-0.089932	-1.870254
C	-2.332962	0.849632	-3.842836
H	-2.821886	1.772738	-4.210417
H	-2.975107	0.008398	-4.172211
C	-0.935192	0.676614	-4.479654
H	-0.653505	-0.399039	-4.462743
H	-0.953395	0.959801	-5.557853
C	0.302913	-3.852270	0.788709
C	-0.252258	-5.032338	0.251906
C	1.593962	-3.898195	1.351129
C	0.468934	-6.236705	0.271169
H	-1.263775	-5.001176	-0.184140
C	2.309614	-5.105115	1.386685
H	2.052083	-2.991137	1.771961
C	1.751866	-6.275508	0.843726
H	0.024401	-7.149666	-0.153652
H	3.310880	-5.130897	1.841158
H	2.316514	-7.219999	0.871961
C	-1.402198	-1.780884	3.018546
C	-0.978070	-1.622750	4.353690
C	-2.748235	-2.116940	2.766837
C	-1.877665	-1.801204	5.417187
H	0.072399	-1.359162	4.556743
C	-3.647356	-2.305274	3.827652
H	-3.110097	-2.244586	1.735861
C	-3.214377	-2.148419	5.155857
H	-1.531903	-1.674898	6.454496
H	-4.692836	-2.574917	3.614122
H	-3.919421	-2.298334	5.987756
N	2.421756	3.242050	-0.543288
C	3.477752	3.357425	0.476404
C	4.819048	3.080288	-0.252949
C	4.364567	1.888600	-1.130844
C	2.868946	2.173383	-1.493599

H	3.333813	2.583560	1.258769
C	5.277250	4.247027	-1.152974
C	5.935877	2.743586	0.742634
H	4.418345	0.949657	-0.540051
H	4.997573	1.748349	-2.030419
H	3.430900	4.344495	0.979606
C	2.049560	4.543675	-1.100249
H	6.227476	3.644280	1.323113
H	5.610696	1.971058	1.464841
H	6.844589	2.374284	0.223252
H	4.574743	4.444905	-1.986626
H	5.399309	5.186190	-0.573628
H	6.259971	4.005737	-1.609598
H	1.934418	4.477560	-2.201590
H	2.868767	5.287259	-0.956008
C	0.800490	5.157137	-0.496850
C	0.143227	6.208890	-1.169872
C	-1.426183	6.448977	0.674301
C	0.330363	4.758402	0.768353
C	-0.761467	5.418029	1.357423
H	-1.093057	5.119229	2.361621
H	0.828267	3.929113	1.291370
C	-0.973731	6.839171	-0.599560
H	0.514833	6.540493	-2.154331
H	-2.289084	6.954886	1.134318
H	-1.486569	7.647020	-1.144714
C	2.048091	0.876620	-1.396299
H	2.310758	0.403551	-0.432551
H	0.356340	2.119748	-0.628641
H	2.410320	0.185479	-2.184600
H	2.814198	2.579550	-2.528615

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C	-0.462377	-2.169630	-1.778245
C	0.601075	-2.436504	-2.654336
C	2.048849	-2.408281	-2.219144
H	2.083229	-1.959733	-1.203101
C	2.956404	-1.564865	-3.140823
H	2.541645	-0.543761	-3.255881
H	2.971293	-2.014668	-4.158604
C	4.392199	-1.515317	-2.598296
H	5.032640	-0.899664	-3.264690
H	4.385975	-1.002652	-1.609113
C	4.975321	-2.927809	-2.434692
H	5.090663	-3.395284	-3.438696
H	5.995501	-2.877145	-1.998063
C	4.061908	-3.806973	-1.567952
H	4.041720	-3.404053	-0.529738
H	4.463241	-4.839325	-1.489062
C	2.624847	-3.841085	-2.104605

H	2.609014	-4.318148	-3.110616	H	-3.011038	0.035609	3.995140
H	1.977239	-4.457841	-1.454235	H	-3.269907	1.748573	4.389579
C	0.274406	-2.835608	-3.989195	C	-0.532781	2.415720	3.731974
H	1.095767	-3.039026	-4.692246	H	-1.261459	3.118739	4.163434
C	-1.035379	-3.000953	-4.409700	C	0.788530	2.471000	4.142109
H	-1.248712	-3.321576	-5.441761	H	1.108214	3.220004	4.883687
C	-2.125637	-2.766251	-3.519967	C	1.755001	1.564643	3.616395
C	-3.493306	-2.896812	-3.911179	C	3.130105	1.598693	3.994773
H	-3.719094	-3.222172	-4.939138	H	3.458649	2.359026	4.720870
C	-4.525486	-2.604067	-3.029843	C	4.042932	0.694737	3.469829
H	-5.569684	-2.701026	-3.365118	H	5.094932	0.742041	3.788602
C	-4.248462	-2.154661	-1.702232	C	3.637737	-0.287608	2.516415
C	-5.346429	-1.727850	-0.752114	C	4.608755	-1.308881	1.954818
H	-4.854144	-1.446165	0.208232	H	4.150590	-1.709942	1.019793
C	-6.085061	-0.463058	-1.253160	C	5.992234	-0.737895	1.578303
H	-5.345720	0.346195	-1.440680	H	6.475526	-0.311231	2.485743
H	-6.563146	-0.683992	-2.234263	H	5.869284	0.100587	0.863776
C	-7.152188	-0.005977	-0.247247	C	6.910323	-1.820021	0.991209
H	-7.690029	0.882501	-0.640327	H	6.478609	-2.180076	0.029660
H	-6.646108	0.324858	0.687828	H	7.900488	-1.383378	0.742589
C	-8.139819	-1.135271	0.084818	C	7.068469	-3.007932	1.951920
H	-8.876303	-0.794065	0.842476	H	7.703320	-3.796422	1.495564
H	-8.725786	-1.389067	-0.827916	H	7.600953	-2.669568	2.869903
C	-7.407114	-2.393242	0.577883	C	5.699608	-3.583987	2.344620
H	-8.129011	-3.212337	0.779794	H	5.816764	-4.416813	3.070321
H	-6.909645	-2.168529	1.550200	H	5.221531	-4.019402	1.437590
C	-6.346472	-2.859899	-0.430976	C	4.774436	-2.504943	2.926727
H	-6.847776	-3.186317	-1.370337	H	5.191681	-2.126570	3.887641
H	-5.796985	-3.745593	-0.046078	H	3.777338	-2.929157	3.174219
C	-2.918327	-2.049051	-1.306026	C	2.300306	-0.316765	2.125374
H	-2.708686	-1.641446	-0.307812	H	2.008729	-1.029475	1.341567
C	-1.832437	-2.347635	-2.177479	C	1.329583	0.584495	2.652151
C	-0.548350	-2.776620	0.685253	C	0.464609	1.702520	-3.457775
H	-1.588184	-3.130970	0.528532	H	1.515029	1.390224	-3.591137
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C	-0.049015	0.567730	2.243528	H	-1.495147	3.590417	-3.759083
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H	-2.866850	3.546417	2.640441	H	-2.577337	1.527661	-0.454020
C	-4.411515	2.692640	1.383579	C	-2.120385	0.833384	-2.410893
H	-4.746278	3.677676	0.994813	H	-2.523839	-0.137967	-2.107373
H	-4.491799	1.978486	0.530895	C	-1.980580	1.029261	-3.912904
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H	-6.371774	2.113853	2.164046	H	-2.523426	0.205551	-4.417782
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C	-4.824923	0.896740	3.126016	H	-0.181988	-0.058953	-4.464813
H	-4.910456	0.087413	2.363880	H	-0.414682	1.419548	-5.412855
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H	-3.213380	-2.351131	1.501757
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H	-4.968862	-2.697780	3.217408
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C	0.332684	-4.006043	0.674636
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C	1.613331	-4.033758	1.260998
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C	1.895889	-6.356902	0.587000
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H	2.504010	-7.274015	0.560254
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C	4.342229	3.390717	-2.513802
C	6.016089	3.928346	-0.707867
H	4.822953	2.011162	0.643468
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H	3.336931	5.252579	-0.794047
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H	2.430569	-0.017975	-0.650514
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H	0.016097	1.980571	-0.241054
C	1.342910	3.817262	0.725196
H	6.177601	4.944918	-1.124184
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H	6.769811	3.256264	-1.168953
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H	4.513899	4.388412	-2.969105
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H	1.376166	5.497376	-1.501350

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C	-2.653238	3.499279	0.668619
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H	-2.438628	4.476500	1.154088
C	-4.126478	3.459695	0.240118
H	-4.345676	4.293468	-0.460430
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C	-5.061581	3.514777	1.458684
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C	-0.314709	3.516372	2.686710
H	-0.961521	4.393666	2.832823
C	0.993805	3.559950	3.129350
H	1.381856	4.465061	3.619865
C	1.865303	2.447986	2.942493
C	3.234491	2.472362	3.338123
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C	4.076334	1.394806	3.093955
H	5.131761	1.450935	3.399211
C	3.590082	0.222319	2.443487
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H	4.005020	-1.520572	1.302424
C	5.915857	-0.624205	1.731844
H	5.902092	0.102106	0.893661
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H	7.732674	-1.617212	1.037999
H	6.220146	-2.354544	0.455822
C	6.731178	-2.899192	2.502798
H	7.259454	-3.826419	2.195608
H	7.318069	-2.469916	3.346382
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C	-0.710214	-1.089597	2.303090	C	0.547818	0.540397	-3.921948
H	0.239363	-1.184619	2.868465	H	1.574653	0.133923	-3.933242
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C	-0.914934	-2.558772	-1.109106	H	-1.209546	2.437664	-4.880615
C	0.044857	-3.249467	-1.864803	H	-0.423063	3.794206	-4.058416
C	1.515847	-3.257176	-1.514361	C	-1.883925	2.771616	-2.819573
H	1.670951	-2.497054	-0.718316	H	-1.627198	3.525611	-2.049548
C	2.439919	-2.910347	-2.704710	H	-2.852361	3.110903	-3.253924
H	2.131853	-1.948874	-3.168099	C	-2.088214	1.441489	-2.132575
H	2.324507	-3.682581	-3.496974	H	-2.554040	1.492218	-1.135068
C	3.911652	-2.858393	-2.263255	C	-2.101647	0.200686	-2.772193
H	4.561647	-2.614569	-3.130158	H	-2.569243	-0.616729	-2.213225
H	4.040722	-2.027066	-1.532907	C	-1.932574	-0.051352	-4.261732
C	4.353221	-4.175795	-1.606067	H	-2.347064	0.794194	-4.845467
H	5.398051	-4.090400	-1.238618	H	-2.538721	-0.938894	-4.532682
H	4.356250	-4.984788	-2.371302	C	-0.462943	-0.322437	-4.653023
C	3.409252	-4.567606	-0.460481	H	-0.221069	-1.385532	-4.434045
H	3.493672	-3.817610	0.358794	H	-0.319976	-0.207083	-5.752478
H	3.706602	-5.541881	-0.018703	C	-0.168421	-3.578388	1.786076
C	1.947447	-4.621530	-0.921706	C	-0.811119	-4.821598	1.617432
H	1.280045	-4.900270	-0.085628	C	1.146164	-3.551568	2.292266
H	1.826437	-5.409489	-1.699082	C	-0.155707	-6.017559	1.953047
C	-0.419914	-4.050840	-2.955647	H	-1.838382	-4.846518	1.219365
H	0.320909	-4.589710	-3.565125	C	1.798105	-4.743643	2.642824
C	-1.767655	-4.200518	-3.236851	H	1.672302	-2.594368	2.420836
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C	-2.756591	-3.526513	-2.460438	H	-0.668762	-6.981665	1.815849
C	-4.155269	-3.623735	-2.731296	H	2.820612	-4.707776	3.046506
H	-4.490121	-4.284723	-3.546420	H	1.662830	-6.913755	2.747040
C	-5.080539	-2.886376	-2.006260	C	-1.805853	-0.819405	3.313630
H	-6.151177	-2.970214	-2.248624	C	-1.444573	-0.339491	4.588474
C	-4.657248	-1.989734	-0.977166	C	-3.170069	-1.034181	3.028461
C	-5.628418	-1.052765	-0.292023	C	-2.424273	-0.087870	5.563104
H	-5.046392	-0.462998	0.454572	H	-0.380818	-0.165798	4.816788
C	-6.216741	-0.038594	-1.302963	C	-4.151203	-0.788253	4.001249
H	-6.762384	-0.595686	-2.097879	H	-3.482750	-1.407673	2.042436
H	-5.385736	0.497133	-1.811787	C	-3.780395	-0.316323	5.272627
C	-7.170900	0.952186	-0.622085	H	-2.126494	0.284029	6.555323
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H	-7.603991	1.643227	-1.375837	H	-4.549050	-0.126296	6.037258
C	-8.281844	0.226035	0.151936	Ir	-0.019261	0.455433	-1.724851
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H	-8.933618	-0.321532	-0.566649	C	4.040919	3.313002	-2.152742
C	-7.694848	-0.772457	1.162153	C	5.244212	2.329292	-1.867092
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H	4.178448	4.316154	-1.702117
H	3.011052	1.137855	-3.007826
H	2.296604	-0.735371	-1.587654
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H	0.150593	1.809762	-0.985319
C	2.553934	3.017746	-0.237857
H	6.497160	3.097181	-3.502855
H	5.468516	1.705372	-3.965614
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H	5.572184	2.987180	0.210868
H	6.624969	3.802858	-0.990615
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H	3.456091	2.946612	0.415079
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C	1.915950	4.374585	-0.053460
C	0.716294	4.681787	-0.725060
C	2.449785	5.319111	0.842109
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H	0.321547	3.953223	-1.448604
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C	0.237005	-2.614255	-2.629863
C	1.673501	-2.705823	-2.164965
H	1.710236	-2.308678	-1.126498
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H	5.589567	-3.433886	-1.992657
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H	1.477852	-4.772309	-1.481576
C	-0.119173	-3.029074	-3.951856
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H	-1.674967	-3.378030	-5.409918
C	-2.497269	-2.626650	-3.530338
C	-3.866850	-2.595318	-3.934622
H	-4.125676	-2.940000	-4.948399
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H	-5.904763	-2.103280	-3.431027
C	-4.538311	-1.639833	-1.780003
C	-5.572533	-1.069860	-0.830582
H	-5.007703	-0.500584	-0.053974
C	-6.555227	-0.075040	-1.483094
H	-5.987368	0.730215	-1.996944
H	-7.145363	-0.597125	-2.269506
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H	-8.229039	1.213703	-0.930702
H	-6.935893	1.122108	0.289352
C	-8.279410	-0.589105	0.311584
H	-8.943158	-0.145718	1.083432
H	-8.944498	-1.126751	-0.401885
C	-7.310255	-1.595072	0.952024
H	-7.868163	-2.408207	1.462888
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C	-6.342316	-2.186526	-0.083752
H	-6.905331	-2.796786	-0.825902
H	-5.620347	-2.878662	0.401618
C	-3.209606	-1.695633	-1.368294
H	-2.957951	-1.276164	-0.383933
C	-2.166890	-2.186041	-2.203629
C	-0.954536	-2.681457	0.677975
H	-2.027576	-2.919155	0.525320
C	-0.787224	-1.771261	1.909884
H	0.147062	-2.029187	2.449628
N	-0.562756	-0.415762	1.296046
C	-0.048152	0.607035	2.161376
C	-0.876740	1.605973	2.684537
C	-2.333297	1.740604	2.299530
H	-2.528085	0.995908	1.495507
C	-2.683044	3.143769	1.752804
H	-1.970922	3.446733	0.960848
H	-2.559386	3.891274	2.567789
C	-4.133004	3.188068	1.248042
H	-4.370749	4.199731	0.856273
H	-4.241953	2.487128	0.387378
C	-5.123458	2.788946	2.354337
H	-6.160110	2.763726	1.955574
H	-5.114282	3.570282	3.147742
C	-4.752990	1.434584	2.978239
H	-4.890777	0.629491	2.219778
H	-5.438951	1.186951	3.815674
C	-3.296537	1.406471	3.462562
H	-3.045918	0.421908	3.896804
H	-3.156353	2.155079	4.274860
C	-0.310463	2.508083	3.638909
H	-0.951083	3.296332	4.063224

C	1.004371	2.400355	4.060115	H	-3.552824	-1.951873	1.490525
H	1.408491	3.104789	4.804144	C	-3.927960	-1.984327	4.893852
C	1.854227	1.377264	3.547024	H	-2.306979	-1.838034	6.340639
C	3.214472	1.227178	3.951248	H	-5.320003	-2.105865	3.223268
H	3.629565	1.940085	4.681163	H	-4.715252	-2.053831	5.659966
C	4.003968	0.201005	3.451791	C	-0.209434	-3.999908	0.689433
H	5.045119	0.103991	3.795323	C	-0.807330	-5.107000	0.053185
C	3.485980	-0.727748	2.497133	C	1.057307	-4.158706	1.286608
C	4.323649	-1.880592	1.978165	C	-0.156833	-6.350875	0.017263
H	3.777866	-2.321394	1.110699	H	-1.796947	-4.988096	-0.416704
C	5.717466	-1.454481	1.469203	C	1.704860	-5.403930	1.261556
H	6.273300	-0.953009	2.293152	H	1.548476	-3.312936	1.789893
H	5.603093	-0.700167	0.664644	C	1.100758	-6.502686	0.626200
C	6.536765	-2.654686	0.972543	H	-0.636870	-7.206416	-0.481929
H	6.038961	-3.087518	0.075879	H	2.687988	-5.515401	1.742873
H	7.539932	-2.315847	0.638066	H	1.609860	-7.478431	0.608302
C	6.661674	-3.740191	2.051295	N	2.857350	3.265920	-0.156713
H	7.232840	-4.609665	1.663260	C	4.118094	4.011832	-0.078193
H	7.245748	-3.339707	2.911135	C	5.123161	3.128931	-0.842654
C	5.276429	-4.184819	2.543725	C	4.713249	1.733726	-0.301210
H	5.367945	-4.950480	3.342928	C	3.195519	1.828212	0.014216
H	4.735932	-4.672295	1.699697	C	2.359115	0.872958	-0.871395
C	4.449264	-2.993160	3.049060	H	4.453330	4.132674	0.986879
H	4.930774	-2.562665	3.956387	C	4.880395	3.224058	-2.361871
H	3.435234	-3.320006	3.366550	C	6.579266	3.481312	-0.514567
C	2.166886	-0.574361	2.077149	H	5.269506	1.518591	0.633462
H	1.786950	-1.258847	1.306660	H	4.947008	0.918349	-1.016645
C	1.319027	0.456269	2.579072	H	4.018732	5.031173	-0.505150
C	0.785622	1.560360	-3.481590	H	3.040603	1.543180	1.076051
H	1.785265	1.113985	-3.631897	H	2.518146	-0.154667	-0.494606
C	0.725351	2.741830	-2.733830	H	2.763586	0.949132	-1.898167
H	1.650714	3.098963	-2.243916	H	1.054845	1.641183	-0.315681
C	-0.423095	3.728358	-2.784119	C	1.832049	3.703205	0.773484
H	-0.932472	3.675657	-3.764901	H	6.829580	4.508165	-0.854061
H	-0.016058	4.752585	-2.692213	H	6.772070	3.426372	0.577346
C	-1.415851	3.492319	-1.631423	H	7.279335	2.783624	-1.019721
H	-1.007335	3.947341	-0.705559	H	3.825239	3.001175	-2.617996
H	-2.382327	4.013059	-1.825683	H	5.110788	4.243201	-2.736869
C	-1.681763	2.028867	-1.379965	H	5.526616	2.507684	-2.910573
H	-2.162506	1.813133	-0.412133	H	2.232625	3.765832	1.820046
C	-1.815762	1.016534	-2.372418	H	1.046276	2.910805	0.825513
H	-2.424393	0.158644	-2.064101	C	1.128408	4.998315	0.431475
C	-1.725268	1.198385	-3.885342	C	1.368859	5.708226	-0.759957
H	-2.148345	2.177964	-4.186510	C	-0.328523	7.353860	-0.161573
H	-2.367611	0.431360	-4.362101	C	0.158752	5.494354	1.330988
C	-0.282550	1.025164	-4.417098	C	-0.570104	6.655360	1.036141
H	-0.082746	-0.058625	-4.559832	H	-1.328362	7.021997	1.745679
H	-0.168134	1.489610	-5.423798	H	-0.026103	4.949715	2.270532
C	-1.908277	-1.825832	2.923802	C	0.649308	6.881735	-1.051624
C	-1.578420	-1.790343	4.293569	H	2.120720	5.331214	-1.468440
C	-3.264227	-1.929337	2.551969	H	-0.894157	8.269509	-0.393206
C	-2.580423	-1.865502	5.274816	H	0.854728	7.429432	-1.984991
H	-0.520355	-1.708099	4.590117				
C	-4.267033	-2.015859	3.529821				

D_E_R

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C	-0.419027	-0.403482	-0.013412	H	-2.016538	-2.882973	0.525523
N	-0.627827	-0.351233	1.330798	N	-0.545909	-1.702952	-0.413047
C	-0.178696	0.672001	2.234983	C	-0.801019	-2.121771	-1.764084
C	-1.063272	1.612849	2.771965	C	0.228749	-2.531711	-2.619001
C	-2.515968	1.709041	2.361488	C	1.675885	-2.601385	-2.182755
H	-2.690226	0.948099	1.567974	H	1.749815	-2.119375	-1.182374
C	-2.867657	3.096391	1.779419	C	2.649271	-1.873198	-3.136400
H	-2.165104	3.353822	0.965073	H	2.337092	-0.815288	-3.274210
H	-2.718704	3.868045	2.567751	H	2.594500	-2.337065	-4.146020
C	-4.323708	3.145021	1.295592	C	4.093396	-1.958255	-2.618749
H	-4.557642	4.150817	0.886544	H	4.781533	-1.428330	-3.310712
H	-4.451977	2.428448	0.450951	H	4.157459	-1.422931	-1.645079
C	-5.300602	2.776741	2.423751	C	4.541202	-3.413069	-2.413981
H	-5.261459	3.564465	3.209809	H	5.570990	-3.443230	-1.998336
H	-6.344889	2.768294	2.045666	H	4.588346	-3.927190	-3.400488
C	-4.939941	1.421388	3.050794	C	3.564321	-4.161830	-1.497373
H	-5.091277	0.613510	2.297630	H	3.600693	-3.716981	-0.476754
H	-5.620924	1.185019	3.895519	H	3.863355	-5.224792	-1.380194
C	-3.481206	1.387782	3.525654	C	2.126048	-4.074856	-2.020017
H	-3.338679	2.141590	4.332507	H	1.429275	-4.609056	-1.348565
H	-3.231728	0.406254	3.967458	H	2.057592	-4.581319	-3.009206
C	-0.562033	2.502464	3.774495	C	-0.133470	-2.982694	-3.927159
H	-1.243288	3.255211	4.199555	H	0.664698	-3.298635	-4.615713
C	0.740130	2.430929	4.239480	C	-1.453420	-3.060084	-4.340253
H	1.088702	3.124325	5.020916	H	-1.697552	-3.424438	-5.350660
C	1.645623	1.459246	3.723206	C	-2.514557	-2.672338	-3.469947
C	2.994167	1.345078	4.172915	C	-3.888774	-2.700188	-3.859201
H	3.350399	2.039038	4.950623	H	-4.144546	-3.075412	-4.862838
C	3.849933	0.385761	3.648747	C	-4.887310	-2.245065	-3.009719
H	4.883989	0.320593	4.019507	H	-5.936029	-2.264282	-3.344472
C	3.402854	-0.516142	2.636556	C	-4.567170	-1.722467	-1.718728
C	4.303051	-1.586699	2.053295	C	-5.615701	-1.090038	-0.828185
H	3.816067	-1.937683	1.112110	H	-5.112783	-0.821734	0.130658
C	5.705476	-1.074620	1.671271	C	-6.138502	0.233076	-1.439006
H	5.605918	-0.196360	1.001500	H	-6.607377	0.014959	-2.425263
H	6.232155	-0.713478	2.582773	H	-5.279349	0.908678	-1.643544
C	6.544012	-2.176434	1.009130	C	-7.162192	0.911845	-0.517326
H	7.552093	-1.787811	0.752232	H	-6.648931	1.231195	0.417227
H	6.066451	-2.465795	0.045169	H	-7.547915	1.838557	-0.992565
C	6.655416	-3.412228	1.916039	C	-8.317291	-0.035259	-0.157376
H	7.227081	-4.217224	1.407987	H	-9.021961	0.463626	0.540888
H	7.236055	-3.144087	2.827773	H	-8.901699	-0.268300	-1.076632
C	5.267879	-3.925002	2.334137	C	-7.795149	-1.345403	0.453369
H	5.362669	-4.788866	3.025807	H	-8.635866	-2.033516	0.682404
H	4.736595	-4.300618	1.430227	H	-7.298777	-1.121721	1.426585
C	4.421087	-2.818975	2.983132	C	-6.784819	-2.035222	-0.476868
H	4.883668	-2.500101	3.944625	H	-7.300492	-2.347957	-1.412876
H	3.407923	-3.196232	3.240879	H	-6.388474	-2.963935	-0.013051
C	2.087737	-0.409641	2.188519	C	-3.234478	-1.722945	-1.319094
H	1.760354	-1.088801	1.389054	H	-2.988443	-1.264623	-0.351036
C	1.179093	0.561308	2.698626	C	-2.181327	-2.194198	-2.156487
C	-0.829348	-1.713833	1.933957	C	0.681335	1.770565	-3.388606

H	1.733455	1.450939	-3.503200
C	0.457485	2.939140	-2.646347
H	1.328955	3.411393	-2.169903
C	-0.767625	3.826786	-2.735141
H	-1.211191	3.764546	-3.747197
H	-0.443734	4.876388	-2.592181
C	-1.804277	3.479293	-1.649783
H	-1.510307	3.981886	-0.708039
H	-2.809024	3.883141	-1.915434
C	-1.916645	1.996239	-1.397881
H	-2.420451	1.726359	-0.454359
C	-1.897647	0.989406	-2.400772
H	-2.415824	0.065144	-2.126962
C	-1.758407	1.191346	-3.907093
H	-2.236203	2.140171	-4.222948
H	-2.320687	0.382534	-4.415302
C	-0.284347	1.127814	-4.365987
H	0.011373	0.061764	-4.475392
H	-0.156455	1.583693	-5.375171
C	-0.182032	-3.921281	0.731675
C	-0.767289	-5.060516	0.142707
C	1.092388	-4.035993	1.322321
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H	-1.762705	-4.974689	-0.321925
C	1.760069	-5.270376	1.339930
H	1.573224	-3.160844	1.783385
C	1.169039	-6.401669	0.750811
H	-0.564373	-7.175216	-0.316464
H	2.749113	-5.348505	1.815108
H	1.693949	-7.369084	0.765280
C	-1.968314	-1.799961	2.927530
C	-1.666655	-1.766979	4.303841
C	-3.314376	-1.932664	2.529237
C	-2.685934	-1.874580	5.264265
H	-0.617066	-1.662201	4.622584
C	-4.334951	-2.045681	3.485698
H	-3.581131	-1.959347	1.462447
C	-4.023142	-2.019272	4.856447
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H	-4.823172	-2.111401	5.606820
N	3.512493	2.916688	0.012894
C	4.911501	2.890859	0.414461
C	5.645088	2.440232	-0.868876
C	4.636288	1.378396	-1.370763
C	3.244996	1.994783	-1.097338
H	5.114607	2.166596	1.248893
C	5.749428	3.605069	-1.873273
C	7.038630	1.862735	-0.593185
H	4.751403	0.453373	-0.766227
H	4.776617	1.102960	-2.435676
H	5.246002	3.893583	0.761521
C	2.492684	3.353389	0.925333
H	7.713643	2.637922	-0.174259

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H	7.503287	1.486953	-1.528297
H	4.758037	4.052903	-2.087827
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H	1.813909	2.518748	1.234441
C	1.626473	4.506056	0.434643
C	2.049165	5.336400	-0.620322
C	0.032452	6.687700	-0.402520
C	0.396141	4.777350	1.064815
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H	-1.349929	6.068345	1.162480
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C	1.257218	6.419591	-1.039721
H	3.017031	5.121194	-1.099610
H	-0.586248	7.538972	-0.726395
H	1.601480	7.063308	-1.864610
C	2.184259	0.925445	-0.802137
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H	-2.018489	3.343076	0.955814
H	-2.528864	3.959694	2.539799
C	-4.185697	3.289215	1.302102
H	-4.364058	4.293557	0.862480
H	-4.359600	2.555047	0.481521
C	-5.175464	3.012050	2.445493
H	-5.088410	3.820822	3.205998
H	-6.220056	3.049852	2.070512
C	-4.889391	1.658760	3.114450
H	-5.088653	0.837589	2.387388
H	-5.580555	1.488674	3.966820
C	-3.433192	1.555564	3.588382
H	-3.246643	2.322711	4.373509
H	-3.238459	0.573708	4.057444
C	-0.460766	2.491418	3.810863
H	-1.107578	3.263016	4.255137
C	0.845037	2.363697	4.253920
H	1.232171	3.028679	5.041760
C	1.704065	1.364970	3.709162
C	3.046767	1.173618	4.153996

H	3.441202	1.837531	4.939418	H	-4.277122	-3.112583	-4.848800
C	3.845874	0.173664	3.618929	C	-5.027959	-2.221756	-3.027591
H	4.874682	0.045242	3.988745	H	-6.071053	-2.226061	-3.378570
C	3.350792	-0.691866	2.595533	C	-4.717320	-1.683278	-1.741124
C	4.201701	-1.799825	2.009198	C	-5.761355	-1.010634	-0.873228
H	3.646737	-2.212394	1.133546	H	-5.325923	-0.914594	0.149434
C	5.564513	-1.299945	1.486006	C	-6.037172	0.431926	-1.367111
H	5.396673	-0.494221	0.741012	H	-6.432361	0.385089	-2.407397
H	6.133291	-0.833610	2.321669	H	-5.077567	0.991171	-1.423097
C	6.396437	-2.437970	0.879530	C	-7.038599	1.155045	-0.454778
H	7.380041	-2.050713	0.538750	H	-6.575111	1.291185	0.548411
H	5.880442	-2.820230	-0.029536	H	-7.243002	2.174879	-0.844376
C	6.583389	-3.591234	1.877260	C	-8.343608	0.359145	-0.299423
H	7.155776	-4.419714	1.409631	H	-9.033889	0.881132	0.396330
H	7.193535	-3.235978	2.738702	H	-8.865598	0.314505	-1.282473
C	5.228596	-4.100037	2.394274	C	-8.068208	-1.071735	0.189779
H	5.372172	-4.913100	3.136967	H	-9.014426	-1.647673	0.265512
H	4.662655	-4.545960	1.544140	H	-7.643995	-1.032008	1.220177
C	4.395852	-2.965239	3.009141	C	-7.078980	-1.799886	-0.733878
H	4.904537	-2.577520	3.920736	H	-7.545620	-1.921582	-1.737215
H	3.403928	-3.337684	3.345306	H	-6.866927	-2.824163	-0.359559
C	2.045914	-0.505011	2.145939	C	-3.390180	-1.696424	-1.323542
H	1.679353	-1.146421	1.331929	H	-3.146655	-1.223703	-0.361071
C	1.190927	0.505045	2.674751	C	-2.335206	-2.205020	-2.135971
C	-0.927230	-1.674352	1.957053	C	0.748316	1.869474	-3.263514
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C	-1.098915	-2.581225	0.727535	C	0.422299	3.017546	-2.513830
H	-2.171203	-2.824692	0.582212	H	1.236971	3.545944	-1.992865
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C	2.471758	-1.849627	-2.971123	H	-2.951957	3.718677	-2.087368
H	2.137117	-0.789588	-2.989038	C	-1.931855	1.931625	-1.442742
H	2.415095	-2.204003	-4.024621	H	-2.514462	1.636960	-0.550659
C	3.918598	-1.969745	-2.471640	C	-1.770093	0.913692	-2.444676
H	4.598506	-1.368325	-3.110177	H	-2.268331	-0.030350	-2.213541
H	3.982513	-1.532902	-1.448608	C	-1.597897	1.142356	-3.944029
C	4.381002	-3.432448	-2.407251	H	-2.155641	2.048334	-4.257338
H	5.421704	-3.490664	-2.023497	H	-2.063374	0.292099	-4.481503
H	4.405227	-3.857793	-3.436053	C	-0.109480	1.233918	-4.340312
C	3.430040	-4.262366	-1.534868	H	0.279910	0.208570	-4.512427
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C	-0.280544	-3.090664	-3.853859	H	-1.950856	-4.910430	-0.318668
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C	-2.659411	-2.714022	-3.441116	H	-0.799240	-7.133975	-0.333949
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H	-2.916189	4.153316	1.362551
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H	4.955179	-2.433726	-2.927770	H	-1.627396	-0.702687	-2.593558
H	4.341736	-1.980401	-1.326932	C	-1.202133	0.557345	-4.316836
C	4.679934	-4.111796	-1.537986	H	-2.103252	0.381118	-4.949128
H	5.706198	-4.052781	-1.116471	H	-0.489006	-0.249554	-4.586055
H	4.719192	-4.869985	-2.353044	C	-0.567996	1.930100	-4.632277
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H	3.952476	-5.574963	-0.073197	C	-0.049366	-3.537909	1.436408
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H	0.793278	-4.637812	-3.582129	C	1.847845	-4.662610	2.483288
C	-1.308970	-4.212767	-3.466291	H	1.713592	-2.518394	2.221901
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C	-2.353646	-3.501632	-2.805477	H	-0.513659	-6.945530	1.488438
C	-3.729708	-3.643486	-3.157759	H	2.831763	-4.607374	2.972322
H	-3.995490	-4.337356	-3.970995	H	1.726350	-6.831959	2.618799
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H	-5.772008	-3.058427	-2.793799	C	-1.674664	-0.762911	4.372129
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H	-4.912593	-0.514097	-0.037855	H	-0.646008	-0.505730	4.671733
C	-6.308390	-0.344720	-1.669533	C	-4.287713	-1.427889	3.601659
H	-6.824401	-1.003736	-2.403382	H	-3.486940	-1.700093	1.612563
H	-5.649951	0.327683	-2.261400	C	-4.017130	-1.095421	4.940682
C	-7.354317	0.464593	-0.887589	H	-2.488618	-0.489174	6.368468
H	-6.829124	1.201070	-0.239335	H	-5.310600	-1.691334	3.292722
H	-7.979551	1.056917	-1.588506	H	-4.827724	-1.099986	5.685319
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C	-7.378156	-1.302549	0.931772	C	2.460531	3.110348	-1.163217
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C	-3.047040	-1.870256	-1.103650	C	1.162125	4.474440	0.577603
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C	-2.001274	-2.595282	-1.746589	C	3.477909	6.490117	0.432875
C	0.211326	2.489226	-3.451740	H	4.186753	5.090117	-1.033033
H	1.306856	2.549804	-3.573913	H	2.580637	5.786757	-1.386990
C	-0.373938	3.303833	-2.467410	C	2.841814	7.675630	0.455537
H	0.286274	3.970703	-1.898608	H	4.248934	6.287120	1.198883
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C	5.105046	0.646507	-1.704431
C	5.974429	0.542048	-2.803978
H	7.063336	0.581424	-2.646463
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H	0.545378	5.011075	-0.174013
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C	-2.660497	2.087635	1.822230
H	-2.743271	1.156612	1.216878
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H	-3.524996	1.185552	3.614085
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C	1.320776	2.234468	3.640737
C	2.592270	2.197884	4.288188
H	2.813251	2.954184	5.057914
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H	4.512528	1.236395	4.477372
C	3.276167	0.265910	2.948843

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H	5.525053	0.686692	1.428640
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H	6.196910	-1.609538	0.643252
C	6.806605	-2.365412	2.594952
H	7.455718	-3.154214	2.159806
H	7.340372	-1.983159	3.494682
C	5.457259	-2.963836	3.026305
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H	4.903937	-1.448679	4.500080
H	3.514775	-2.330505	3.827129
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H	1.839657	-0.440239	1.522776
C	1.032185	1.244545	2.637661
C	-0.746745	-1.167015	2.118984
H	0.170908	-1.246377	2.736726
C	-0.790666	-2.298044	1.096266
H	-1.837150	-2.626399	0.937980
N	-0.374047	-1.613386	-0.178256
C	-0.636769	-2.425357	-1.336351
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C	1.812963	-3.155237	-1.497076
H	1.878268	-2.492804	-0.605397
C	2.770904	-2.591853	-2.565988
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H	2.709746	-3.217728	-3.485016
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C	4.688709	-3.959894	-1.611769
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H	4.731080	-4.640766	-2.492362
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C	-4.737155	-2.936804	-2.453485
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H	-6.876920	-1.076972	-2.325945
H	-5.716721	0.267806	-2.211012
C	-7.408718	0.401779	-0.822511
H	-6.886040	1.150307	-0.186320
H	-8.045818	0.980092	-1.524477
C	-8.271987	-0.502646	0.071379
H	-8.991437	0.107368	0.657272
H	-8.884092	-1.176986	-0.569814
C	-7.401460	-1.353124	1.010402
H	-8.032937	-2.030554	1.623256
H	-6.874455	-0.680450	1.725325
C	-6.358420	-2.166055	0.229196
H	-6.871814	-2.913527	-0.417048
H	-5.710955	-2.749080	0.919643
C	-3.073950	-1.884348	-1.041509
H	-2.829572	-1.166877	-0.245636
C	-2.023528	-2.588377	-1.696774
C	0.154340	2.591236	-3.408391
H	1.237297	2.774402	-3.366222
C	-0.665965	3.279813	-2.506399
H	-0.200851	4.027089	-1.844127
C	-2.162861	3.427282	-2.699901
H	-2.341975	4.168471	-3.511931
H	-2.587265	3.881182	-1.785052
C	-2.888801	2.097110	-3.000694
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H	-3.021547	1.955782	-4.093490
C	-2.190949	0.865094	-2.423349
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C	-1.163699	0.136326	-3.093966
H	-1.083955	-0.926377	-2.836368
C	-0.599004	0.435360	-4.463886
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H	0.345997	-0.137479	-4.574183
C	-0.334762	1.934978	-4.683503
H	0.434191	2.071145	-5.470221
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C	-0.002527	-3.535806	1.459690
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C	0.067628	-5.973134	1.635828
H	-1.598372	-4.850010	0.796008
C	1.943024	-4.644248	2.431549
H	1.765773	-2.497974	2.206227
C	1.338102	-5.897819	2.231607
H	-0.410259	-6.951129	1.472614
H	2.939953	-4.580527	2.892284
H	1.859599	-6.816856	2.539745
C	-1.916843	-1.097024	3.079971
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C	-2.707787	-0.672260	5.355128
H	-0.641629	-0.441478	4.711080
C	-4.274745	-1.402135	3.645616
H	-3.462613	-1.732123	1.671083
C	-4.013767	-1.026805	4.975010
H	-2.495632	-0.372002	6.392582
H	-5.295323	-1.676035	3.338067
H	-4.829365	-1.008418	5.713955
C	3.767491	0.687988	-1.894596
C	2.749413	0.744426	-0.759433
N	1.716555	1.749636	-1.039072
C	2.299100	3.085416	-1.214979
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C	2.445231	4.017885	0.028480
H	3.309758	2.976797	-1.666455
H	1.706670	3.665776	-1.944241
C	3.036762	5.348306	-0.541196
C	1.074372	4.289043	0.659040
C	3.414245	3.419970	1.060197
C	3.247129	6.433146	0.479011
H	4.008823	5.111443	-1.032734
H	2.359569	5.725414	-1.339901
C	2.548569	7.581907	0.534678
H	4.038305	6.257931	1.231238
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H	1.755708	7.807797	-0.199604
C	3.349689	0.609147	-3.238445
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C	5.146441	0.734146	-1.618245
C	6.091856	0.676301	-2.656728
H	7.166669	0.709880	-2.420649
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C	4.287505	0.551301	-4.279969
H	2.271100	0.599919	-3.459760
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H	4.409030	3.222302	0.607092
H	3.029110	2.472890	1.474152
H	3.559730	4.106700	1.917246
H	0.565373	3.343611	0.916582
H	0.416650	4.854394	-0.035583
H	1.170658	4.898623	1.577673
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H	2.264158	-0.246510	-0.647413

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C	-2.461810	2.378270	1.714874
H	-2.617776	1.361828	1.287273

C	-3.078476	3.402266	0.739881	C	2.722672	-3.526329	-2.469622
H	-2.545327	3.355084	-0.229348	H	2.375835	-2.740565	-3.165382
H	-2.907734	4.428742	1.134039	H	2.574767	-4.491190	-3.003604
C	-4.585331	3.170280	0.554449	C	4.215363	-3.355355	-2.151035
H	-5.009045	3.927889	-0.139475	H	4.804648	-3.314341	-3.091792
H	-4.742206	2.177613	0.071050	H	4.364066	-2.374659	-1.644723
C	-5.337647	3.185174	1.893576	C	4.728879	-4.477503	-1.237321
H	-5.289982	4.208511	2.329280	H	5.789888	-4.298880	-0.961111
H	-6.414798	2.965008	1.734329	H	4.707749	-5.441301	-1.794633
C	-4.715421	2.185120	2.877564	C	3.858906	-4.599050	0.021664
H	-4.857819	1.149490	2.492634	H	3.992106	-3.688120	0.647468
H	-5.233537	2.221734	3.859011	H	4.187651	-5.453205	0.650598
C	-3.216660	2.443248	3.062947	C	2.369003	-4.741182	-0.317597
H	-3.074417	3.453829	3.506392	H	1.763765	-4.838570	0.599462
H	-2.775604	1.727810	3.778492	H	2.207330	-5.677556	-0.897969
C	-0.517616	3.774006	2.544322	C	-0.130290	-4.673364	-2.197474
H	-1.251605	4.557869	2.784796	H	0.584711	-5.385872	-2.634734
C	0.798092	3.934363	2.938746	C	-1.484440	-4.853876	-2.419465
H	1.110076	4.838147	3.484440	H	-1.839759	-5.696844	-3.032814
C	1.765812	2.922978	2.674313	C	-2.439150	-3.976950	-1.828705
C	3.094359	2.982473	3.186531	C	-3.848168	-4.159854	-1.974726
H	3.389694	3.857642	3.784992	H	-4.208064	-4.996702	-2.593992
C	3.997977	1.960296	2.943583	C	-4.751532	-3.320079	-1.341675
H	5.010918	2.018280	3.370660	H	-5.831743	-3.495051	-1.462235
C	3.651088	0.861944	2.101521	C	-4.296144	-2.231767	-0.535060
C	4.651547	-0.234161	1.799197	C	-5.269796	-1.320055	0.183231
H	4.166540	-0.929524	1.073508	H	-4.671883	-0.515098	0.672405
C	5.949050	0.277232	1.133228	C	-6.266240	-0.629185	-0.774554
H	5.703016	0.873933	0.232400	H	-6.831074	-1.405996	-1.337313
H	6.472166	0.966489	1.833868	H	-5.702456	-0.043273	-1.533174
C	6.880565	-0.890142	0.773823	C	-7.257082	0.267752	-0.015983
H	7.807600	-0.508411	0.296237	H	-6.702747	1.117249	0.441241
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C	7.220314	-1.737894	2.009935	C	-7.992332	-0.505344	1.089665
H	7.860024	-2.600518	1.727357	H	-8.678189	0.170672	1.642238
H	7.819888	-1.122333	2.718560	H	-8.632766	-1.289297	0.624914
C	5.946931	-2.225009	2.719771	C	-7.000990	-1.171583	2.055902
H	6.204829	-2.790634	3.640524	H	-7.540910	-1.754417	2.831699
H	5.411365	-2.938036	2.051960	H	-6.430804	-0.381745	2.596424
C	5.005785	-1.059564	3.059502	C	-6.015844	-2.080120	1.306237
H	5.493982	-0.389752	3.802811	H	-6.568170	-2.936436	0.857049
H	4.077172	-1.426601	3.546413	H	-5.275117	-2.526652	2.004620
C	2.364145	0.810274	1.568252	C	-2.926084	-2.029770	-0.408813
H	2.107433	-0.009818	0.882377	H	-2.590951	-1.154643	0.164201
C	1.376729	1.786647	1.884716	C	-1.961137	-2.875525	-1.036319
C	-0.298335	-0.677597	2.160440	C	-0.618409	1.736256	-4.138092
H	0.716361	-0.567254	2.593311	H	0.396544	1.665308	-4.557845
C	-0.400894	-1.996998	1.418576	C	-0.820457	2.779022	-3.228433
H	-1.446952	-2.361332	1.443836	H	0.034638	3.446956	-3.052282
N	-0.148377	-1.595486	-0.014615	C	-2.162054	3.362277	-2.856571
C	-0.541101	-2.667684	-0.898717	H	-2.503175	4.041241	-3.671336
C	0.382426	-3.595656	-1.409424	H	-2.015504	4.009029	-1.967914
C	1.879674	-3.541332	-1.169250	C	-3.225099	2.290017	-2.559818
H	2.097261	-2.612784	-0.593741	H	-3.989010	2.699771	-1.874701

H	-3.769852	2.025974	-3.489038
C	-2.658826	1.003026	-1.960322
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C	-2.352780	-0.097054	-2.778886
H	-2.405900	-1.091296	-2.325345
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H	-3.588065	0.015674	-4.515338
H	-2.183452	-1.033142	-4.696154
C	-1.729870	1.098519	-4.968553
H	-1.288993	0.733276	-5.917613
H	-2.433694	1.905510	-5.262049
C	0.445445	-3.100375	2.004439
C	-0.157143	-4.351037	2.247539
C	1.777822	-2.889207	2.413145
C	0.554732	-5.374781	2.893667
H	-1.199736	-4.515989	1.931587
C	2.487421	-3.907363	3.067407
H	2.265133	-1.920690	2.227069
C	1.877973	-5.151118	3.310374
H	0.072444	-6.346527	3.079584
H	3.525228	-3.732110	3.387078
H	2.436633	-5.946508	3.827044
C	-1.283943	-0.501161	3.294732
C	-0.826248	0.062749	4.502380
C	-2.623322	-0.934201	3.207747
C	-1.685135	0.181658	5.607372
H	0.218050	0.406711	4.572921
C	-3.482416	-0.821053	4.311586
H	-3.007978	-1.376594	2.277096
C	-3.014319	-0.266414	5.515886
H	-1.313151	0.621744	6.545158
H	-4.523748	-1.168275	4.230179
H	-3.687117	-0.181725	6.382958
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C	2.370313	2.278717	-2.675067
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C	2.407708	0.018820	-3.780550
C	1.360700	-0.610217	-2.911165
C	0.175749	-1.059924	-3.451157
H	3.054873	3.102395	-2.377356
C	4.222338	1.662065	-4.230559
C	4.093900	0.543393	-1.985228
H	3.079041	-0.814468	-4.098354
H	1.942319	0.389898	-4.719859
H	1.842053	2.694716	-3.577498
H	1.683449	-0.977646	-1.925408
H	-0.421738	-1.846365	-2.983608
H	-0.028906	-0.839792	-4.508953
C	1.214665	3.324176	-0.903487
H	4.831759	1.288909	-1.630578
H	3.445604	0.278470	-1.126870
H	4.660288	-0.354765	-2.305188
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H	4.878018	2.457681	-3.820777

H	4.873520	0.855846	-4.628251
H	0.765539	4.078410	-1.607068
H	0.452434	3.191160	-0.116081
C	2.395106	4.048235	-0.264561
C	3.641479	3.449605	-0.018684
C	4.485702	5.505472	0.979187
C	2.207697	5.391287	0.127719
C	3.234330	6.110619	0.756064
H	3.064505	7.155599	1.060204
H	1.233819	5.875376	-0.057233
C	4.682871	4.173638	0.585196
H	3.780352	2.395506	-0.280509
H	5.299779	6.073127	1.456052
H	5.651679	3.681405	0.764872
H	-0.857130	1.996160	-0.923345

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C	-0.246218	0.894071	2.135160
C	-1.347763	1.542801	2.703050
C	-2.781827	1.272016	2.300350
H	-2.771704	0.473480	1.525444
C	-3.482139	2.508957	1.697482
H	-2.901163	2.884063	0.832386
H	-3.483234	3.329791	2.449028
C	-4.926525	2.187564	1.285467
H	-5.416801	3.092334	0.866610
H	-4.901409	1.435130	0.463735
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H	-6.767117	1.329435	2.089496
C	-5.042148	0.401652	3.067626
H	-4.997122	-0.424047	2.321501
H	-5.615741	0.004880	3.931567
C	-3.614561	0.753538	3.497698
H	-3.654093	1.543493	4.280777
H	-3.114977	-0.115234	3.960633
C	-1.103802	2.477939	3.757951
H	-1.957981	3.026698	4.180885
C	0.161018	2.692070	4.272055
H	0.313355	3.409333	5.093459
C	1.283777	1.978297	3.761572
C	2.600581	2.143941	4.285755
H	2.751476	2.853814	5.114270
C	3.671580	1.426131	3.776138
H	4.673632	1.563026	4.210674
C	3.493302	0.521368	2.684759
C	4.650105	-0.293952	2.143618
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C	5.890035	0.543888	1.763712
H	5.600902	1.348081	1.058036

H	6.284842	1.049699	2.673421	H	-5.140171	-0.318364	-2.148576
C	6.990518	-0.344073	1.162729	C	-6.947204	-0.458441	-0.913205
H	7.874878	0.271195	0.893523	H	-6.531163	0.240445	-0.153435
H	6.617797	-0.789110	0.210796	H	-7.568649	0.159041	-1.595769
C	7.391625	-1.470480	2.128890	C	-7.807447	-1.516320	-0.204778
H	8.158297	-2.126290	1.664884	H	-8.612635	-1.028401	0.383930
H	7.867847	-1.022562	3.030560	H	-8.317220	-2.146689	-0.968768
C	6.171878	-2.299133	2.561556	C	-6.951552	-2.415840	0.701006
H	6.467493	-3.069816	3.304936	H	-7.578666	-3.195481	1.182432
H	5.776229	-2.849813	1.678706	H	-6.525031	-1.802075	1.527334
C	5.056487	-1.412741	3.135875	C	-5.802575	-3.071027	-0.080807
H	5.401672	-0.940340	4.083155	H	-6.222718	-3.767726	-0.840951
H	4.166061	-2.019837	3.406561	H	-5.168174	-3.691600	0.588682
C	2.217066	0.371439	2.148463	C	-2.463605	-2.265808	-1.237931
H	2.097275	-0.263640	1.258350	H	-2.314532	-1.542006	-0.424632
C	1.083015	1.062229	2.672030	C	-1.333064	-2.740440	-1.969318
C	-0.266480	-1.503981	1.903140	C	-0.587740	2.805292	-3.270828
H	0.672566	-1.444630	2.488564	H	0.423438	2.985742	-3.659072
C	-0.099860	-2.482025	0.756428	C	-0.953472	3.516212	-2.110898
H	-1.069660	-2.970699	0.538187	H	-0.211943	4.203673	-1.673230
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C	0.018403	-2.354489	-1.642175	H	-2.796610	4.600376	-2.345227
C	1.112350	-2.940673	-2.305234	H	-2.383635	4.173866	-0.676412
C	2.563217	-2.731551	-1.917099	C	-3.274735	2.523132	-1.800319
H	2.584141	-2.004940	-1.074028	H	-4.115455	2.610518	-1.088927
C	3.447828	-2.184592	-3.065823	H	-3.744134	2.446077	-2.801985
H	2.978475	-1.311735	-3.556058	C	-2.516947	1.224493	-1.524527
H	3.530015	-2.962825	-3.857111	H	-2.804996	0.688967	-0.604567
C	4.855265	-1.847841	-2.551345	C	-1.958884	0.447790	-2.567704
H	5.475984	-1.432594	-3.374094	H	-1.894356	-0.629261	-2.402736
H	4.781176	-1.045902	-1.779459	C	-2.014309	0.823682	-4.032914
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H	6.517477	-2.802575	-1.494939	H	-1.369470	0.116796	-4.591802
H	5.753215	-3.815402	-2.743260	C	-1.570959	2.275123	-4.308368
C	4.639131	-3.740483	-0.878721	H	-1.094027	2.334964	-5.306886
H	4.542244	-3.058961	-0.003722	H	-2.447331	2.952914	-4.355022
H	5.104514	-4.671695	-0.492206	C	0.880064	-3.597413	1.034533
C	3.231988	-4.035368	-1.414588	C	0.493459	-4.919887	0.736616
H	2.612231	-4.519701	-0.642629	C	2.116186	-3.373540	1.674336
H	3.295108	-4.755563	-2.260916	C	1.320455	-6.002064	1.079579
C	0.837285	-3.811792	-3.404625	H	-0.472171	-5.096808	0.236394
H	1.688062	-4.244979	-3.951083	C	2.940494	-4.453406	2.024997
C	-0.450530	-4.142960	-3.787409	H	2.438765	-2.349737	1.913564
H	-0.621276	-4.823519	-4.636325	C	2.544000	-5.769986	1.731259
C	-1.570649	-3.634026	-3.071082	H	1.005119	-7.029936	0.843916
C	-2.916431	-3.989658	-3.393194	H	3.900469	-4.266164	2.528876
H	-3.090552	-4.667540	-4.243730	H	3.190102	-6.615987	2.011458
C	-3.985820	-3.502580	-2.657984	C	-1.363214	-1.860190	2.883534
H	-5.011681	-3.794787	-2.930526	C	-1.089494	-1.765452	4.262654
C	-3.770384	-2.616899	-1.557459	C	-2.619669	-2.348712	2.469266
C	-4.926163	-2.012523	-0.788072	C	-2.047101	-2.159722	5.211689
H	-4.490646	-1.363330	0.007819	H	-0.109642	-1.382920	4.590438
C	-5.787807	-1.097891	-1.691350	C	-3.576994	-2.746312	3.414626
H	-6.193484	-1.702066	-2.533951	H	-2.858725	-2.433953	1.399614

C	-3.292454	-2.655663	4.788611
H	-1.818032	-2.083693	6.285581
H	-4.552092	-3.128342	3.075773
H	-4.042426	-2.971583	5.529809
N	1.590509	2.473240	-1.019949
C	2.327483	3.318635	-1.952348
C	3.667145	2.680612	-2.399571
C	3.239717	1.416551	-3.176314
C	2.198663	0.591614	-2.493963
C	0.986612	0.297710	-3.113679
H	2.536967	4.311123	-1.501227
C	4.426237	3.638530	-3.329712
C	4.545235	2.288057	-1.202175
H	4.128854	0.766000	-3.335402
H	2.865625	1.710074	-4.179972
H	1.766699	3.561705	-2.878691
H	2.476207	0.058053	-1.572764
H	0.496035	-0.661853	-2.909020
H	0.826680	0.705322	-4.123392
C	1.733429	3.012365	0.342076
H	4.839271	3.177961	-0.607825
H	4.006803	1.591651	-0.529148
H	5.477160	1.791418	-1.544223
H	3.795044	3.955706	-4.187186
H	4.735822	4.553200	-2.782493
H	5.342953	3.165717	-3.739325
H	1.304601	2.292258	1.038741
H	2.812376	3.089956	0.603927
C	1.086264	4.366116	0.604773
C	1.798928	5.573630	0.428836
C	-0.165520	6.885082	1.026413
C	-0.252503	4.453406	1.042842
C	-0.877104	5.693107	1.248312
H	-1.921233	5.728101	1.598726
H	-0.804366	3.527312	1.247446
C	1.180657	6.820160	0.626800
H	2.866681	5.538860	0.156628
H	-0.649890	7.860838	1.186645
H	1.757716	7.746953	0.481916
H	-0.864787	2.144313	-0.166437

Substrate 29a

E= -674.244963528 A.U.

N	0.458326	-0.527967	1.282266
C	3.009834	-1.153561	0.104766
C	2.249294	-2.190548	-0.692371
H	2.069429	-1.930120	-1.752252
C	1.768815	-3.352819	-0.208378
C	2.394735	0.231870	0.012910
C	1.114713	0.490469	0.595526
C	0.565029	1.792623	0.487306
H	-0.430592	2.003359	0.901607
C	1.266806	2.814673	-0.167561
H	0.813657	3.816450	-0.236850

C	2.523649	2.566751	-0.742102
H	3.074295	3.366349	-1.260236
C	3.067731	1.274502	-0.646045
C	-0.905503	-0.388453	1.745257
H	-0.973885	0.471550	2.448665
C	-1.972651	-0.235843	0.661627
C	-3.225567	0.326900	0.978039
H	-3.416282	0.685408	2.003899
C	-4.228482	0.440051	0.001470
H	-5.202252	0.883357	0.263964
C	-3.986465	-0.002818	-1.310877
H	-4.769021	0.090742	-2.080167
C	-2.737097	-0.557982	-1.635891
H	-2.535977	-0.899790	-2.663622
C	-1.737451	-0.673262	-0.655739
H	-0.755705	-1.099119	-0.915300
H	0.721097	-1.473898	0.994752
H	4.055439	1.061465	-1.088660
H	3.080781	-1.482105	1.167081
H	4.050751	-1.098115	-0.282736
H	1.930682	-3.647264	0.844321
H	1.214013	-4.060251	-0.845059
H	-1.139050	-1.287568	2.357121

29-B

E= -3486.77655157 A.U.

Ir	0.516260	-0.057125	-1.940442
C	0.802518	0.262968	0.038425
N	0.752949	-0.485533	1.171858
C	-0.017609	-1.685480	1.387093
C	0.573172	-2.952226	1.458971
C	2.041658	-3.209384	1.208276
H	2.511357	-2.246597	0.903392
C	2.272784	-4.242279	0.078178
H	1.712685	-3.953544	-0.835288
H	1.848059	-5.221728	0.390604
C	3.770689	-4.411537	-0.215686
H	3.920985	-5.151842	-1.030014
H	4.178412	-3.444295	-0.592416
C	4.538795	-4.834541	1.047272
H	4.219206	-5.861076	1.337672
H	5.627557	-4.897615	0.836268
C	4.272607	-3.872561	2.214968
H	4.710290	-2.878696	1.976735
H	4.785223	-4.221762	3.136225
C	2.773605	-3.691964	2.481799
H	2.329988	-4.659654	2.807680
H	2.603944	-2.977456	3.308408
C	-0.260709	-4.061983	1.797453
H	0.192227	-5.063058	1.849009
C	-1.610969	-3.917403	2.053818
H	-2.229110	-4.793448	2.299703
C	-2.229519	-2.638307	1.978589
C	-3.624015	-2.450170	2.205445

H	-4.237692	-3.330312	2.452734	H	5.380350	4.332057	-2.700954
C	-4.200651	-1.195237	2.108857	C	5.863234	2.729919	-1.329803
H	-5.278054	-1.073875	2.286450	H	6.940806	2.797564	-1.533863
C	-3.420450	-0.054362	1.751136	C	5.374302	1.767722	-0.398810
C	-4.070124	1.307291	1.624735	C	6.280689	0.778203	0.321078
H	-3.297437	2.020523	1.253176	H	6.010596	0.826066	1.403780
C	-5.230984	1.297185	0.605790	C	6.003782	-0.675505	-0.143791
H	-4.846952	0.986169	-0.389516	H	6.202984	-0.741059	-1.237627
H	-5.963683	0.519119	0.902626	H	4.927587	-0.922563	-0.011703
C	-5.949930	2.648713	0.519911	C	6.872482	-1.691987	0.611030
H	-6.803294	2.569459	-0.185153	H	6.569268	-1.697994	1.682888
H	-5.261276	3.411177	0.096746	H	6.674377	-2.715299	0.228642
C	-6.428540	3.121148	1.899517	C	8.367267	-1.354239	0.516415
H	-6.925806	4.111078	1.821518	H	8.965368	-2.080865	1.105518
H	-7.195887	2.410747	2.283537	H	8.700326	-1.458447	-0.541400
C	-5.257429	3.183384	2.892797	C	8.636777	0.080704	0.992802
H	-5.606792	3.511987	3.894596	H	9.713019	0.332142	0.889036
H	-4.526615	3.950747	2.546868	H	8.401520	0.159786	2.079094
C	-4.551866	1.824281	3.001882	C	7.783921	1.094216	0.214757
H	-5.256314	1.079828	3.436636	H	8.087008	1.066121	-0.856587
H	-3.689447	1.875319	3.701900	H	7.981508	2.126962	0.573335
C	-2.057567	-0.223816	1.529111	C	3.998500	1.716395	-0.166068
H	-1.469715	0.649338	1.212769	H	3.617675	0.956397	0.527866
C	-1.421267	-1.495512	1.645460	C	3.071391	2.571536	-0.819513
C	1.017052	0.343589	2.400257	C	0.678209	0.693301	-4.020812
H	0.046251	0.440448	2.927575	H	-0.114092	1.461145	-4.101314
C	1.444939	1.713537	1.823947	C	0.273562	-0.645281	-4.157148
H	2.537325	1.854431	1.954998	H	-0.802277	-0.815005	-4.314902
N	1.181217	1.530593	0.364763	C	1.191451	-1.796635	-4.539732
C	1.645038	2.485449	-0.609787	H	1.981459	-1.425854	-5.223094
C	0.764303	3.377123	-1.245788	H	0.610342	-2.540200	-5.121037
C	-0.712655	3.483457	-0.932675	C	1.831956	-2.499139	-3.316034
H	-0.995029	2.629241	-0.279342	H	1.185992	-3.333750	-2.974375
C	-1.598499	3.452067	-2.198413	H	2.798928	-2.971864	-3.604934
H	-1.413956	2.516467	-2.762162	C	2.069352	-1.570730	-2.147125
H	-1.301325	4.284512	-2.873552	H	2.147924	-2.075659	-1.172410
C	-3.086429	3.610952	-1.858817	C	2.683568	-0.289064	-2.243291
H	-3.692208	3.595880	-2.789726	H	3.220357	0.039096	-1.343143
H	-3.423277	2.738397	-1.254144	C	3.175953	0.347787	-3.537621
C	-3.336924	4.904577	-1.068015	H	3.551300	-0.433767	-4.230761
H	-4.412412	5.003786	-0.811181	H	4.047043	0.991062	-3.301657
H	-3.090731	5.779818	-1.710925	C	2.088682	1.217484	-4.209911
C	-2.470110	4.945071	0.197310	H	2.124911	2.237347	-3.778542
H	-2.774312	4.120663	0.881019	H	2.290065	1.340482	-5.299321
H	-2.631534	5.887776	0.761454	C	0.768882	2.934412	2.413765
C	-0.983240	4.787785	-0.139118	C	1.523603	4.117624	2.548201
H	-0.364154	4.801683	0.776591	C	-0.582075	2.937449	2.818983
H	-0.650718	5.654414	-0.753732	C	0.943353	5.281477	3.079067
C	1.316516	4.319665	-2.170784	H	2.580164	4.121640	2.234825
H	0.634093	5.013911	-2.682184	C	-1.162564	4.097628	3.354490
C	2.673379	4.404499	-2.418889	H	-1.195371	2.028977	2.731327
H	3.063708	5.148256	-3.131331	C	-0.402110	5.272659	3.485560
C	3.588510	3.540305	-1.750862	H	1.545717	6.197183	3.179949
C	4.992040	3.592006	-1.983533	H	-2.216697	4.081772	3.670583

H	-0.858226	6.181423	3.907162
C	1.993179	-0.288374	3.367198
C	1.506956	-0.833324	4.571622
C	3.378301	-0.337414	3.108297
C	2.387806	-1.401866	5.507307
H	0.424680	-0.807663	4.776078
C	4.262098	-0.895087	4.043495
H	3.781873	0.065548	2.168048
C	3.768539	-1.427560	5.247904
H	1.993723	-1.822424	6.445013
H	5.341621	-0.917534	3.829466
H	4.461239	-1.864828	5.983067
N	-4.473834	-2.166289	-1.690591
C	-1.661924	-2.425245	-2.441648
C	-1.332668	-1.218080	-1.578656
C	-1.667647	0.135843	-1.866185
H	-0.729015	-2.890193	-2.809258
H	-2.241995	-2.117309	-3.340004
H	-1.241107	-1.496286	-0.522463
H	-2.131208	0.380069	-2.839788
H	-1.961698	0.803967	-1.040640
H	-3.900491	-1.354918	-1.920177
C	-5.883006	-2.089675	-2.049923
H	-6.232867	-3.121752	-2.269003
H	-5.978813	-1.531976	-3.007546
C	-6.813240	-1.448177	-1.028642
C	-7.604815	-0.340634	-1.391820
C	-8.619234	-0.284144	0.819930
C	-6.938238	-1.964082	0.278427
C	-7.834762	-1.390871	1.194087
H	-7.926353	-1.812397	2.207743
H	-6.315963	-2.816721	0.586519
C	-8.501944	0.239627	-0.478010
H	-7.519944	0.072642	-2.410692
H	-9.323373	0.164503	1.537468
H	-9.113892	1.102824	-0.782724
C	-2.414690	-3.485901	-1.662875
C	-1.750550	-4.662560	-1.273646
C	-3.805191	-3.336190	-1.361554
C	-2.419573	-5.721876	-0.642559
H	-0.676293	-4.757072	-1.502469
C	-4.479502	-4.424726	-0.748362
C	-3.797475	-5.597485	-0.399266
H	-1.877464	-6.637156	-0.362467
H	-5.554840	-4.346877	-0.533973
H	-4.353933	-6.420900	0.075548

29_B_C_SR

E= -3486.75770601 A.U.

Ir	0.048513	-0.798953	-1.508089
C	0.674298	0.298488	0.101595
N	0.750301	0.014436	1.439639
C	0.041068	-1.016635	2.141957
C	0.656948	-2.224242	2.492152

C	2.072165	-2.573397	2.095195
H	2.456769	-1.743861	1.461163
C	2.138121	-3.879658	1.269752
H	1.441818	-3.817033	0.408823
H	1.779820	-4.726788	1.896203
C	3.574689	-4.169522	0.810285
H	3.606387	-5.110246	0.220751
H	3.908737	-3.359296	0.122238
C	4.540053	-4.244968	2.004892
H	4.284476	-5.134595	2.624203
H	5.580597	-4.400468	1.649775
C	4.450562	-2.982634	2.875797
H	4.826893	-2.107557	2.297907
H	5.110958	-3.070534	3.764337
C	3.010083	-2.695464	3.318557
H	2.650134	-3.523788	3.970288
H	2.961542	-1.774333	3.928075
C	-0.102905	-3.175562	3.243774
H	0.373635	-4.128530	3.518308
C	-1.411846	-2.939219	3.622191
H	-1.979346	-3.702185	4.176667
C	-2.053524	-1.713250	3.284502
C	-3.419644	-1.456980	3.601472
H	-3.991741	-2.235353	4.129833
C	-4.027041	-0.259846	3.246607
H	-5.081198	-0.087781	3.512718
C	-3.295646	0.752337	2.551745
C	-3.921060	2.088471	2.203237
H	-3.250895	2.582750	1.462011
C	-5.312753	1.969458	1.546014
H	-5.229139	1.365064	0.615494
H	-5.999844	1.414879	2.223714
C	-5.920759	3.345469	1.233648
H	-6.934920	3.222146	0.798444
H	-5.304425	3.843801	0.453771
C	-5.970796	4.240393	2.481091
H	-6.382789	5.238166	2.221749
H	-6.669721	3.797508	3.226925
C	-4.578482	4.381159	3.114719
H	-4.623580	5.009876	4.028868
H	-3.906600	4.909170	2.399587
C	-3.976944	3.008498	3.448039
H	-4.588266	2.510449	4.234567
H	-2.955826	3.114320	3.873958
C	-1.963457	0.502053	2.225351
H	-1.417045	1.271287	1.663512
C	-1.307265	-0.717789	2.558214
C	1.196785	1.181516	2.267793
H	0.320483	1.514039	2.861227
C	1.556262	2.236223	1.204878
H	2.658868	2.335893	1.131250
N	1.085286	1.591048	-0.061191
C	1.430924	2.217152	-1.307770
C	0.493873	2.944226	-2.050889

C	-0.943355	3.133873	-1.614657	C	1.409263	-3.418285	-2.361632
H	-1.104693	2.517612	-0.703155	H	0.947722	-4.090614	-1.606709
C	-1.963773	2.684128	-2.684089	H	2.341013	-3.932941	-2.694362
H	-1.779367	1.625911	-2.954606	C	1.760789	-2.112520	-1.682037
H	-1.806026	3.274383	-3.613857	H	2.203582	-2.226357	-0.678889
C	-3.408976	2.892185	-2.206550	C	2.070521	-0.895037	-2.353013
H	-4.120629	2.579964	-3.001060	H	2.719917	-0.216399	-1.790584
H	-3.603261	2.232297	-1.328858	C	2.105316	-0.665718	-3.857843
C	-3.664595	4.352991	-1.804341	H	2.415431	-1.589764	-4.387251
H	-4.704451	4.478368	-1.434649	H	2.883788	0.091390	-4.080291
H	-3.577368	4.999718	-2.706406	C	0.742874	-0.157326	-4.380377
C	-2.647632	4.817369	-0.752608	H	0.691626	0.944250	-4.253092
H	-2.792723	4.235618	0.186739	H	0.636935	-0.350185	-5.473472
H	-2.812984	5.882090	-0.483771	C	1.010040	3.634212	1.420284
C	-1.209143	4.612356	-1.239970	C	1.780599	4.725204	0.967285
H	-0.483144	4.943902	-0.476273	C	-0.224687	3.891485	2.049860
H	-1.030103	5.247529	-2.136598	C	1.331378	6.043951	1.142298
C	0.941239	3.586767	-3.247114	H	2.746670	4.532891	0.473400
H	0.210630	4.152290	-3.844833	C	-0.672567	5.209239	2.234815
C	2.260244	3.533881	-3.664892	H	-0.848030	3.064518	2.419958
H	2.571686	4.043375	-4.590382	C	0.103944	6.289531	1.781790
C	3.234068	2.824180	-2.904046	H	1.945975	6.883618	0.783438
C	4.600725	2.720028	-3.301984	H	-1.633984	5.391599	2.738566
H	4.920800	3.230459	-4.224260	H	-0.246606	7.322489	1.929178
C	5.512548	1.976975	-2.564188	C	2.292018	0.844726	3.258681
H	6.555064	1.902421	-2.907467	C	1.953793	0.677293	4.616021
C	5.108623	1.298900	-1.374849	C	3.639211	0.697287	2.871320
C	6.022838	0.356106	-0.615357	C	2.941753	0.382986	5.570626
H	5.652916	0.319316	0.436665	H	0.901708	0.784905	4.925600
C	5.888502	-1.083344	-1.177021	C	4.630499	0.411273	3.821896
H	6.205839	-1.078065	-2.244591	H	3.930077	0.811933	1.816847
H	4.818657	-1.384739	-1.174679	C	4.284464	0.255249	5.175938
C	6.735705	-2.082327	-0.376429	H	2.662177	0.258497	6.627968
H	6.321693	-2.154206	0.655101	H	5.678847	0.307852	3.502393
H	6.648026	-3.097615	-0.818442	H	5.061845	0.033084	5.922870
C	8.207117	-1.646682	-0.297502	C	-2.417007	-1.712411	-0.847719
H	8.788882	-2.359533	0.324314	C	-1.997042	-0.353059	-0.891837
H	8.655268	-1.683225	-1.316714	H	-1.958181	0.179364	0.066864
C	8.336679	-0.219227	0.257632	H	-2.506542	0.228959	-1.677883
H	9.400952	0.096687	0.275634	H	-2.863434	-2.101452	-1.775041
H	7.989318	-0.203139	1.316862	C	-4.387794	-2.965289	0.696258
C	7.503026	0.779009	-0.561758	C	-5.499550	-3.609958	1.270451
H	7.913517	0.821295	-1.595775	C	-3.122392	-3.585900	0.685984
H	7.590149	1.805165	-0.144998	C	-5.344036	-4.881981	1.843315
C	3.783498	1.421953	-0.964117	H	-6.482547	-3.114389	1.281387
H	3.462449	0.860112	-0.075704	C	-2.976718	-4.858535	1.266366
C	2.814104	2.163195	-1.697250	C	-4.081697	-5.505043	1.842240
C	-0.431408	-0.762303	-3.636915	H	-6.211072	-5.389542	2.293044
H	-1.373665	-0.192688	-3.739368	H	-1.988996	-5.345801	1.261932
C	-0.578254	-2.121533	-3.273174	H	-3.962693	-6.505563	2.285751
H	-1.611685	-2.472655	-3.136597	C	-1.972698	-2.809982	0.088645
C	0.434385	-3.225272	-3.544187	H	-1.330617	-2.404599	0.887943
H	0.994760	-3.011373	-4.476390	N	-4.432180	-1.655619	0.114955
H	-0.108257	-4.174062	-3.730161	C	-5.534029	-1.302906	-0.810085

H	-6.481222	-1.795037	-0.496653
H	-5.695822	-0.209770	-0.735973
C	-5.173650	-1.674947	-2.232683
C	-4.725648	-0.685419	-3.130589
C	-5.137178	-3.028544	-2.630294
C	-4.214297	-1.039719	-4.389939
H	-4.759962	0.373361	-2.829875
C	-4.621560	-3.385249	-3.887485
H	-5.491552	-3.809816	-1.939235
C	-4.148543	-2.392748	-4.765439
H	-3.863609	-0.257019	-5.080385
H	-4.589045	-4.444776	-4.185115
H	-3.739320	-2.673799	-5.747903
H	-1.330276	-3.505999	-0.491578
H	-4.272629	-0.926829	0.828903

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Ir	0.640844	-0.562627	-1.868362
C	0.854457	0.268019	-0.014453
N	0.646223	-0.195837	1.256133
C	-0.196349	-1.283619	1.659332
C	0.327296	-2.549840	1.949056
C	1.786615	-2.903145	1.774369
H	2.291436	-2.025968	1.312123
C	1.994829	-4.126947	0.850473
H	1.474373	-3.972486	-0.117497
H	1.520246	-5.019236	1.316012
C	3.489485	-4.410764	0.636409
H	3.620390	-5.294703	-0.023110
H	3.951289	-3.550386	0.098845
C	4.218166	-4.619107	1.974183
H	3.847201	-5.556295	2.447706
H	5.305457	-4.765977	1.802435
C	3.976746	-3.442293	2.932162
H	4.452467	-2.523577	2.520357
H	4.464024	-3.628206	3.912555
C	2.480477	-3.172023	3.130720
H	2.002439	-4.054729	3.612772
H	2.320162	-2.318154	3.813227
C	-0.562580	-3.549983	2.451414
H	-0.163040	-4.553914	2.659199
C	-1.894080	-3.284405	2.713248
H	-2.550193	-4.069048	3.120810
C	-2.435244	-1.988739	2.474704
C	-3.788093	-1.661074	2.786684
H	-4.428263	-2.440162	3.230509
C	-4.289044	-0.389549	2.557620
H	-5.332064	-0.160902	2.822859
C	-3.477532	0.618181	1.953055
C	-4.030793	2.008264	1.713421
H	-3.281387	2.563258	1.104626
C	-5.358290	2.004222	0.922815
H	-5.200456	1.526917	-0.065854

H	-6.103687	1.368907	1.450371
C	-5.936650	3.415089	0.744688
H	-6.910261	3.356077	0.213904
H	-5.259475	4.006859	0.090023
C	-6.092319	4.141599	2.088156
H	-6.481356	5.169470	1.930238
H	-6.849705	3.611539	2.709734
C	-4.756659	4.183172	2.845954
H	-4.875073	4.691230	3.826344
H	-4.027848	4.790501	2.261639
C	-4.187721	2.771511	3.052472
H	-4.866739	2.192010	3.718435
H	-3.206601	2.809331	3.573813
C	-2.157613	0.304608	1.627752
H	-1.546492	1.070891	1.129808
C	-1.583733	-0.972300	1.909296
C	0.901337	0.841393	2.309219
H	-0.087212	1.139024	2.712909
C	1.517805	1.999623	1.507710
H	2.612620	2.047483	1.685226
N	1.317395	1.550418	0.094686
C	1.832187	2.365377	-0.972027
C	0.977270	3.183123	-1.726133
C	-0.511453	3.290216	-1.477267
H	-0.778727	2.567231	-0.675661
C	-1.360731	2.953003	-2.721167
H	-1.083439	1.950953	-3.099384
H	-1.120453	3.670462	-3.537079
C	-2.860927	3.041301	-2.406558
H	-3.459404	2.780869	-3.306059
H	-3.115713	2.285304	-1.627079
C	-3.233557	4.441909	-1.894540
H	-4.314535	4.490486	-1.644905
H	-3.070482	5.181144	-2.711083
C	-2.376252	4.832538	-0.682110
H	-2.621340	4.165599	0.174854
H	-2.616007	5.863102	-0.344702
C	-0.878415	4.711718	-0.984010
H	-0.273929	4.971927	-0.096212
H	-0.603720	5.445519	-1.774649
C	1.550522	4.010197	-2.738767
H	0.883337	4.641963	-3.343714
C	2.913913	4.049281	-2.969286
H	3.328792	4.694680	-3.759385
C	3.802144	3.256340	-2.189109
C	5.210277	3.250855	-2.420956
H	5.618293	3.908838	-3.204363
C	6.046917	2.417151	-1.698760
H	7.128219	2.404452	-1.910709
C	5.530480	1.559797	-0.678777
C	6.460038	0.547862	-0.033652
H	7.446190	1.046776	0.115656
C	5.994203	0.014456	1.331097
H	5.012958	-0.497640	1.203090

H	5.828996	0.860137	2.032837
C	6.985625	-0.999956	1.919404
H	7.953542	-0.491203	2.128690
H	6.612369	-1.374969	2.896288
C	7.218854	-2.170392	0.951602
H	7.959165	-2.882576	1.373110
H	6.267510	-2.738649	0.836935
C	7.673628	-1.671037	-0.427851
H	7.787692	-2.522270	-1.132187
H	8.680658	-1.204379	-0.336405
C	6.692220	-0.641223	-1.006277
H	5.706711	-1.123425	-1.202181
H	7.052723	-0.262146	-1.985715
C	4.166153	1.606577	-0.399993
H	3.760876	0.953033	0.382730
C	3.260307	2.410668	-1.156130
C	0.852384	-0.063707	-3.973910
H	0.020848	0.626105	-4.214797
C	0.536797	-1.444669	-3.969314
H	-0.503353	-1.698125	-4.225387
C	1.545062	-2.568637	-4.163749
H	2.365506	-2.235456	-4.830876
H	1.055538	-3.413898	-4.688208
C	2.115512	-3.064416	-2.815870
H	1.433262	-3.827067	-2.382130
H	3.092334	-3.582198	-2.961494
C	2.275805	-1.946528	-1.806499
H	2.374386	-2.292656	-0.766224
C	2.835458	-0.662738	-2.075477
H	3.309912	-0.182442	-1.212293
C	3.344384	-0.167076	-3.420662
H	3.788651	-1.001661	-4.001856
H	4.168398	0.552924	-3.243977
C	2.224107	0.534641	-4.220181
H	2.182321	1.602579	-3.926587
H	2.441034	0.522286	-5.313861
C	0.971668	3.385010	1.800645
C	1.824981	4.490763	1.603250
C	-0.339304	3.614502	2.264588
C	1.380977	5.796228	1.866731
H	2.851567	4.319578	1.241805
C	-0.782245	4.917848	2.541616
H	-1.030195	2.774945	2.428578
C	0.075894	6.012584	2.342942
H	2.059830	6.647889	1.707326
H	-1.805627	5.076673	2.913854
H	-0.271552	7.034114	2.560640
C	1.712692	0.334884	3.481585
C	1.043570	-0.055847	4.658595
C	3.115752	0.237171	3.430255
C	1.766306	-0.524510	5.768384
H	-0.055346	0.012647	4.702750
C	3.842850	-0.221282	4.539033
H	3.655419	0.524586	2.518007

C	3.168963	-0.602132	5.712929
H	1.232349	-0.824880	6.682913
H	4.940442	-0.283346	4.484481
H	3.737304	-0.960863	6.584699
N	-3.909819	-2.075502	-1.886216
C	-1.578275	-2.856635	-0.933310
C	-1.827080	-1.782857	-1.970585
C	-1.548070	-0.384152	-1.791900
H	-0.605799	-3.343963	-1.154025
H	-1.465069	-2.391894	0.060126
H	-1.806194	-2.159937	-3.005180
H	-1.842788	0.037653	-0.817270
H	-1.890847	0.240241	-2.636820
H	-4.342560	-1.960049	-2.813626
C	-4.432601	-1.065856	-0.934538
H	-3.923184	-1.239955	0.031145
H	-4.101315	-0.075625	-1.309760
C	-5.931110	-1.102581	-0.761247
C	-6.767417	-0.368875	-1.628432
C	-8.738208	-1.211497	-0.476852
C	-6.516422	-1.892899	0.249375
C	-7.912421	-1.946566	0.391726
H	-8.359593	-2.563763	1.186473
H	-5.866016	-2.463410	0.929324
C	-8.163555	-0.422138	-1.489093
H	-6.317992	0.264436	-2.411902
H	-9.832541	-1.249999	-0.362587
H	-8.806650	0.160534	-2.166712
C	-2.688041	-3.876843	-0.909289
C	-3.919765	-3.442233	-1.436270
C	-2.586346	-5.180225	-0.395331
C	-5.041142	-4.287535	-1.481281
C	-3.703833	-6.032190	-0.425201
H	-1.627830	-5.529891	0.018824
C	-4.923836	-5.592107	-0.972169
H	-5.992092	-3.927589	-1.901056
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H	-5.790530	-6.269752	-1.003599

29_B_C_RR

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C	-0.046157	-2.559184	1.809437
C	1.333348	-3.108936	1.534861
H	1.965128	-2.275086	1.157992
C	1.298069	-4.217878	0.456539
H	0.808359	-3.832660	-0.461382
H	0.658212	-5.054064	0.816959
C	2.705684	-4.753121	0.154881
H	2.651792	-5.558726	-0.607998
H	3.318094	-3.939400	-0.296499

C	3.402768	-5.257018	1.429060	C	-2.744361	4.980868	-1.846775
H	2.866379	-6.156609	1.808428	H	-3.818109	5.188194	-1.653692
H	4.437791	-5.586344	1.197017	H	-2.440520	5.671346	-2.665807
C	3.413494	-4.175989	2.520678	C	-1.897153	5.272397	-0.599899
H	4.044877	-3.323463	2.185333	H	-2.257824	4.646037	0.247237
H	3.881766	-4.560931	3.451147	H	-2.019480	6.327333	-0.274711
C	2.001265	-3.657536	2.817547	C	-0.415689	4.966252	-0.844454
H	1.380020	-4.487238	3.223887	H	0.181206	5.149447	0.068674
H	2.022740	-2.872362	3.596895	H	-0.024292	5.663122	-1.618719
C	-1.047465	-3.460527	2.293925	C	1.948291	4.024830	-2.560174
H	-0.782593	-4.520080	2.423337	H	1.363398	4.738128	-3.160280
C	-2.318453	-3.038075	2.627145	C	3.310649	3.918246	-2.778417
H	-3.058879	-3.751663	3.018340	H	3.800277	4.530947	-3.551727
C	-2.694617	-1.675197	2.450934	C	4.099676	3.019865	-2.002601
C	-4.010466	-1.208413	2.741525	C	5.503087	2.858213	-2.196357
H	-4.740390	-1.917649	3.162032	H	6.002949	3.473148	-2.961535
C	-4.374672	0.107633	2.493498	C	6.234364	1.934963	-1.458348
H	-5.394921	0.441657	2.735272	H	7.312010	1.827187	-1.646759
C	-3.445675	1.030144	1.919272	C	5.599814	1.127323	-0.469168
C	-3.848707	2.469376	1.669839	C	6.315162	0.032704	0.310862
H	-3.021593	2.955627	1.104801	H	6.043726	0.170648	1.385312
C	-5.129071	2.590270	0.814093	C	5.788105	-1.366316	-0.106123
H	-4.966408	2.088071	-0.164258	H	5.993728	-1.511132	-1.190955
H	-5.955419	2.042074	1.320389	H	4.682526	-1.406047	0.000490
C	-5.561482	4.048028	0.605034	C	6.440314	-2.490562	0.710359
H	-6.505896	4.081516	0.022054	H	6.122366	-2.393873	1.774263
H	-4.796200	4.567941	-0.010333	H	6.065288	-3.477617	0.365013
C	-5.719477	4.786881	1.941705	C	7.973492	-2.432244	0.637714
H	-5.997315	5.847257	1.766310	H	8.422430	-3.226694	1.270559
H	-6.558659	4.334170	2.518008	H	8.297459	-2.643084	-0.406952
C	-4.430443	4.699670	2.773390	C	8.493789	-1.048740	1.057840
H	-4.555872	5.215972	3.748492	H	9.599345	-1.004192	0.966502
H	-3.615579	5.235432	2.235230	H	8.263134	-0.879616	2.134880
C	-4.010469	3.240220	3.003863	C	7.850997	0.069165	0.221546
H	-4.779829	2.727927	3.625314	H	8.157776	-0.058495	-0.841495
H	-3.063060	3.182695	3.581842	H	8.228217	1.063515	0.542936
C	-2.154798	0.583611	1.633582	C	4.234755	1.306651	-0.254538
H	-1.452197	1.279110	1.152982	H	3.736818	0.663514	0.481605
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C	1.007263	0.674071	2.364643	C	0.512553	0.090702	-4.010412
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C	1.671606	1.853161	1.622307	C	0.137269	-1.270986	-3.941348
H	2.768685	1.824281	1.784651	H	-0.937748	-1.480902	-4.056656
N	1.416924	1.512569	0.189152	C	1.071827	-2.438987	-4.228113
C	2.018669	2.321764	-0.834240	H	1.820468	-2.143176	-4.990535
C	1.269782	3.248013	-1.568904	H	0.491798	-3.268153	-4.682079
C	-0.200714	3.510676	-1.326032	C	1.778129	-2.948996	-2.950123
H	-0.540880	2.830759	-0.514390	H	1.142366	-3.713903	-2.456361
C	-1.067605	3.225612	-2.571227	H	2.728686	-3.472069	-3.206073
H	-0.922280	2.171486	-2.875509	C	2.058255	-1.843859	-1.951306
H	-0.711827	3.852185	-3.419330	H	2.237981	-2.199855	-0.923033
C	-2.549143	3.529667	-2.312434	C	2.635069	-0.585305	-2.275369
H	-3.147772	3.324139	-3.225478	H	3.196832	-0.109342	-1.465642
H	-2.931819	2.838780	-1.524647	C	3.035315	-0.127605	-3.670002

H	3.372911	-0.992767	-4.278149
H	3.909319	0.548537	-3.585480
C	1.883706	0.626237	-4.371886
H	1.914187	1.692631	-4.069713
H	2.010660	0.612453	-5.479596
C	1.216436	3.252799	1.991575
C	2.148051	4.304830	1.869352
C	-0.089251	3.550445	2.430346
C	1.786771	5.624466	2.184263
H	3.170602	4.080251	1.526203
C	-0.451679	4.868220	2.752635
H	-0.835539	2.750745	2.541685
C	0.484817	5.908953	2.631010
H	2.527099	6.433014	2.085629
H	-1.472404	5.082357	3.103333
H	0.200162	6.941197	2.886110
C	1.883818	-0.036278	3.375596
C	1.371894	-0.324408	4.655098
C	3.206205	-0.419614	3.070329
C	2.171117	-0.962611	5.619545
H	0.335741	-0.038692	4.897938
C	4.011798	-1.043722	4.033107
H	3.618594	-0.232639	2.068532
C	3.496257	-1.315140	5.313251
H	1.758445	-1.178958	6.616833
H	5.045597	-1.325423	3.780943
H	4.127210	-1.805701	6.070091
N	-3.837383	-1.576585	-0.638096
C	-1.944116	-2.722560	-1.937223
C	-1.942676	-1.376803	-1.226455
C	-1.692635	-0.084575	-1.822929
H	-0.904358	-3.097150	-1.999761
H	-2.310604	-2.629945	-2.983726
H	-1.604356	-1.483876	-0.189660
H	-2.120951	0.064747	-2.834715
H	-1.939231	0.760033	-1.152426
H	-3.949646	-1.066210	0.253676
C	-4.782120	-1.042363	-1.655868
H	-4.504776	-1.484714	-2.633926
H	-4.599317	0.050448	-1.712050
C	-6.217345	-1.362336	-1.308049
C	-6.853602	-2.486892	-1.870865
C	-8.812016	-2.103199	-0.477361
C	-6.895882	-0.609798	-0.326758
C	-8.185241	-0.977686	0.087948
H	-8.708744	-0.379391	0.849950
H	-6.408112	0.273353	0.112494
C	-8.145969	-2.853825	-1.461080
H	-6.326855	-3.085541	-2.631097
H	-9.824796	-2.390586	-0.155166
H	-8.634477	-3.732117	-1.910429
C	-2.811112	-3.658308	-1.132714
C	-3.844212	-3.003130	-0.436781
C	-2.663963	-5.046846	-0.989995

C	-4.745923	-3.697480	0.381637
C	-3.553997	-5.756176	-0.163080
H	-1.849412	-5.572760	-1.512091
C	-4.590159	-5.087946	0.515870
H	-5.551401	-3.159478	0.901601
H	-3.437593	-6.844441	-0.044499
H	-5.283937	-5.655102	1.155019

29_B_C_RS

E= -3486.75838119 A.U.

Ir	0.612106	-0.466545	-1.934816
C	0.740880	0.251183	-0.037162
N	0.508628	-0.296748	1.196870
C	-0.344702	-1.404411	1.529417
C	0.146159	-2.707326	1.675928
C	1.592936	-3.084838	1.454133
H	2.123552	-2.181951	1.080374
C	1.758892	-4.215259	0.412919
H	1.269690	-3.923333	-0.539050
H	1.219957	-5.120861	0.769860
C	3.237696	-4.568055	0.188699
H	3.324512	-5.393908	-0.548999
H	3.759174	-3.692825	-0.261359
C	3.935770	-4.938950	1.506234
H	3.504635	-5.888793	1.896968
H	5.014226	-5.135663	1.328097
C	3.754684	-3.832516	2.555710
H	4.279363	-2.912405	2.213138
H	4.229970	-4.118982	3.517590
C	2.273190	-3.504652	2.779602
H	1.752071	-4.400928	3.186047
H	2.153313	-2.705031	3.534547
C	-0.754771	-3.724737	2.124916
H	-0.386533	-4.758432	2.199153
C	-2.046340	-3.439354	2.521196
H	-2.700265	-4.235226	2.908738
C	-2.546339	-2.107800	2.445104
C	-3.846765	-1.756864	2.914369
H	-4.468086	-2.541429	3.374872
C	-4.322403	-0.459416	2.800350
H	-5.322883	-0.210726	3.186246
C	-3.552673	0.547123	2.140157
C	-4.132497	1.932004	1.935803
H	-3.392472	2.518521	1.346619
C	-5.449652	1.904316	1.123473
H	-5.266925	1.447387	0.128261
H	-6.182284	1.240151	1.634161
C	-6.064570	3.301723	0.959212
H	-7.027796	3.224746	0.412139
H	-5.394131	3.922425	0.324557
C	-6.259735	4.000365	2.312544
H	-6.674439	5.019796	2.165924
H	-7.011391	3.439538	2.913868
C	-4.936764	4.065495	3.090090

H	-5.082196	4.555622	4.075905	H	9.650022	0.345851	1.144220
H	-4.217838	4.701311	2.524196	H	8.300078	0.339424	2.302936
C	-4.332523	2.666457	3.283646	C	7.772065	1.116203	0.341500
H	-5.008274	2.061803	3.930025	H	8.101297	0.978688	-0.713683
H	-3.362790	2.721943	3.824114	H	8.000294	2.169498	0.611015
C	-2.274872	0.217313	1.685819	C	4.017212	1.772147	-0.215419
H	-1.693215	0.976942	1.142603	H	3.614092	1.082951	0.536062
C	-1.710476	-1.081217	1.876641	C	3.108372	2.531790	-0.998702
C	0.813820	0.642727	2.324062	C	0.782371	0.055494	-4.041099
H	-0.141083	0.873165	2.837643	H	-0.090339	0.698795	-4.262875
C	1.359962	1.892799	1.601970	C	0.548547	-1.340262	-4.021082
H	2.448247	1.981325	1.797437	H	-0.487096	-1.661129	-4.219484
N	1.186822	1.528737	0.161995	C	1.619995	-2.394897	-4.255902
C	1.681423	2.410386	-0.859592	H	2.381328	-2.007503	-4.962738
C	0.812161	3.202541	-1.621140	H	1.165283	-3.273746	-4.756279
C	-0.682008	3.253412	-1.387998	C	2.290805	-2.847901	-2.937795
H	-0.931209	2.494309	-0.614075	H	1.731030	-3.706201	-2.511929
C	-1.517021	2.936732	-2.647129	H	3.319148	-3.232174	-3.131083
H	-1.224244	1.947614	-3.048805	C	2.351761	-1.748280	-1.895292
H	-1.283349	3.679954	-3.441676	H	2.472837	-2.107935	-0.861017
C	-3.021597	2.991882	-2.343123	C	2.815654	-0.427433	-2.145035
H	-3.607665	2.756305	-3.257191	H	3.265436	0.078018	-1.284498
H	-3.273912	2.200835	-1.597438	C	3.280536	0.097727	-3.494749
C	-3.427424	4.361447	-1.775809	H	3.762584	-0.713559	-4.079388
H	-4.511159	4.374880	-1.533042	H	4.064917	0.862504	-3.327103
H	-3.275020	5.138714	-2.558471	C	2.116048	0.734471	-4.286695
C	-2.588308	4.717572	-0.540793	H	2.010534	1.794864	-3.980592
H	-2.824197	4.008601	0.284145	H	2.332861	0.746221	-5.380365
H	-2.853198	5.726715	-0.160109	C	0.754215	3.235327	1.964536
C	-1.086122	4.642556	-0.833547	C	1.557831	4.384009	1.801913
H	-0.496548	4.871125	0.073653	C	-0.560524	3.390339	2.445781
H	-0.817851	5.418903	-1.584896	C	1.059297	5.659193	2.111130
C	1.380575	4.067347	-2.607952	H	2.589270	4.271859	1.431218
H	0.703495	4.678456	-3.223404	C	-1.057871	4.663949	2.766702
C	2.747308	4.168001	-2.803249	H	-1.208482	2.514491	2.593331
H	3.152016	4.839851	-3.576456	C	-0.251653	5.802037	2.598288
C	3.650422	3.410193	-2.002340	H	1.699865	6.544343	1.977822
C	5.065522	3.465140	-2.169733	H	-2.082970	4.765876	3.152602
H	5.478631	4.137124	-2.938655	H	-0.643361	6.799296	2.850553
C	5.917230	2.680499	-1.400700	C	1.748261	0.043244	3.353494
H	7.002031	2.738941	-1.568961	C	1.255245	-0.283030	4.631061
C	5.397557	1.805684	-0.401261	C	3.109175	-0.191290	3.068014
C	6.257081	0.862937	0.431158	C	2.108278	-0.816405	5.612819
H	5.958233	1.012472	1.496737	H	0.190466	-0.111559	4.856969
C	5.943130	-0.617470	0.085182	C	3.967376	-0.707364	4.049300
H	6.181656	-0.786630	-0.989294	H	3.508405	0.020723	2.065120
H	4.853989	-0.813205	0.187601	C	3.468532	-1.021088	5.326419
C	6.740178	-1.593080	0.962639	H	1.709707	-1.065538	6.608220
H	6.400142	-1.488886	2.018916	H	5.029407	-0.874337	3.813196
H	6.515285	-2.640241	0.667523	H	4.140831	-1.428398	6.096903
C	8.249873	-1.316920	0.891838	N	-3.643507	-2.175648	-1.355032
H	8.802097	-2.002971	1.568290	C	-1.385317	-3.086168	-2.004560
H	8.611730	-1.534495	-0.138879	C	-1.724380	-1.705871	-1.447024
C	8.561539	0.147809	1.236948	C	-1.548500	-0.418388	-2.076468

H	-0.309592	-3.295375	-1.849830
H	-1.563985	-3.129153	-3.102303
H	-1.621918	-1.691627	-0.351369
H	-1.873596	-0.346258	-3.134982
H	-1.954657	0.411690	-1.467952
H	-3.893011	-2.148450	-2.356782
C	-4.418267	-1.183757	-0.594543
H	-3.957517	-0.198313	-0.823457
H	-4.248415	-1.385139	0.475826
C	-5.896606	-1.149061	-0.909194
C	-6.848998	-1.489316	0.072047
C	-8.657006	-1.057567	-1.499685
C	-6.342788	-0.747770	-2.185832
C	-7.714096	-0.708126	-2.483035
H	-8.050567	-0.392621	-3.482737
H	-5.610679	-0.445706	-2.954844
C	-8.222354	-1.442795	-0.220026
H	-6.506170	-1.777344	1.078781
H	-9.732814	-1.022510	-1.730313
H	-8.957510	-1.707762	0.555614
C	-2.249120	-4.070498	-1.253651
C	-1.916115	-5.368088	-0.841927
C	-3.497761	-3.528498	-0.882450
C	-2.826330	-6.099507	-0.055789
H	-0.938931	-5.798308	-1.110611
C	-4.410082	-4.237349	-0.092142
C	-4.058689	-5.536285	0.321610
H	-2.566561	-7.116269	0.276462
H	-5.377020	-3.795503	0.185266
H	-4.760644	-6.115929	0.940395

29_C_SR

E= -3486.78228202 A.U.

Ir	0.402961	0.793897	-1.414794
C	-0.326549	-0.474451	-0.019436
N	-0.529255	-1.779328	-0.403016
C	-0.750638	-2.182307	-1.770690
C	0.224793	-2.858141	-2.515582
C	1.604686	-3.175595	-1.982733
H	1.703216	-2.666957	-0.999011
C	2.737158	-2.671831	-2.906726
H	2.592336	-1.599898	-3.143124
H	2.685283	-3.215150	-3.876260
C	4.115016	-2.915370	-2.274463
H	4.918157	-2.545779	-2.947496
H	4.192390	-2.317090	-1.336863
C	4.325587	-4.402210	-1.946629
H	4.383289	-4.979192	-2.897139
H	5.299358	-4.553703	-1.432819
C	3.174867	-4.951623	-1.090416
H	3.194729	-4.461135	-0.090724
H	3.307518	-6.037926	-0.901295
C	1.804421	-4.688834	-1.729966
H	1.730972	-5.232436	-2.698938

H	0.992386	-5.079058	-1.089607
C	-0.123396	-3.300454	-3.830022
H	0.641351	-3.815918	-4.430296
C	-1.391381	-3.124904	-4.357155
H	-1.629182	-3.491150	-5.368360
C	-2.410778	-2.481653	-3.597009
C	-3.736297	-2.295142	-4.092038
H	-3.978086	-2.665606	-5.100813
C	-4.705399	-1.659735	-3.329577
H	-5.719181	-1.528536	-3.737564
C	-4.398954	-1.166637	-2.024554
C	-5.433583	-0.447672	-1.182182
H	-4.899543	-0.020408	-0.300733
C	-6.094048	0.734876	-1.925022
H	-5.307570	1.440315	-2.270351
H	-6.600142	0.356261	-2.841246
C	-7.125522	1.454061	-1.042257
H	-7.607573	2.276236	-1.612284
H	-6.599776	1.934587	-0.187045
C	-8.182591	0.479191	-0.499936
H	-8.897759	1.012202	0.161626
H	-8.781181	0.077738	-1.349252
C	-7.528069	-0.690975	0.250751
H	-8.298289	-1.404531	0.612881
H	-7.012435	-0.297118	1.156731
C	-6.503402	-1.420522	-0.631296
H	-7.024090	-1.908128	-1.486475
H	-6.005906	-2.239780	-0.067916
C	-3.111944	-1.356475	-1.530540
H	-2.877502	-0.950304	-0.538121
C	-2.085686	-1.998124	-2.280907
C	-1.183932	-2.606471	0.652484
H	-2.239748	-2.762428	0.349587
C	-1.118677	-1.683270	1.879551
H	-0.260627	-1.974978	2.520897
N	-0.763126	-0.352275	1.273771
C	-0.304722	0.636151	2.208554
C	-1.137898	1.657543	2.683068
C	-2.545712	1.888970	2.169945
H	-2.702089	1.203377	1.307268
C	-2.806821	3.336833	1.687160
H	-2.052646	3.650432	0.939016
H	-2.697370	4.033004	2.548683
C	-4.217905	3.474073	1.096234
H	-4.384792	4.514365	0.744765
H	-4.291751	2.824291	0.193556
C	-5.294846	3.067559	2.113846
H	-6.303760	3.116470	1.651592
H	-5.301635	3.802122	2.950879
C	-5.024703	1.664373	2.674646
H	-5.144587	0.913410	1.860907
H	-5.771636	1.397241	3.451661
C	-3.606175	1.543416	3.244325
H	-3.428156	0.530766	3.644307

H	-3.486751	2.243523	4.102236	C	-3.292074	-1.744501	5.014995
C	-0.640166	2.483478	3.741521	H	-1.160506	-1.669169	4.576930
H	-1.275727	3.301617	4.112222	C	-4.768615	-1.787091	3.083290
C	0.597732	2.274675	4.324442	H	-3.816466	-1.728186	1.143224
H	0.937391	2.918043	5.151056	C	-4.590056	-1.793093	4.477853
C	1.449850	1.226360	3.867168	H	-3.144708	-1.748116	6.105834
C	2.736212	0.966387	4.429273	H	-5.781721	-1.822585	2.654897
H	3.083286	1.594696	5.264963	H	-5.463620	-1.837090	5.146188
C	3.540202	-0.056639	3.944511	C	-0.573857	-3.977835	0.844374
H	4.522663	-0.239061	4.406883	C	-1.261069	-5.102137	0.345760
C	3.113201	-0.868860	2.848700	C	0.650048	-4.169258	1.517721
C	3.972499	-1.990448	2.299869	C	-0.741322	-6.395449	0.521027
H	3.473840	-2.356217	1.371246	H	-2.215817	-4.957038	-0.184833
C	5.394686	-1.539201	1.900810	C	1.165568	-5.460521	1.705024
H	5.921883	-1.142132	2.797474	H	1.207997	-3.306199	1.910175
H	5.330659	-0.699392	1.177671	C	0.471973	-6.577275	1.206088
C	6.205455	-2.700928	1.307247	H	-1.288859	-7.264592	0.125521
H	5.730592	-3.022364	0.352765	H	2.116581	-5.596751	2.241550
H	7.229056	-2.358182	1.046386	H	0.877880	-7.589845	1.353143
C	6.265303	-3.895644	2.271586	N	2.711972	2.454841	-0.186328
H	6.821287	-4.738208	1.809170	C	4.748792	1.240285	-0.739285
H	6.839310	-3.603823	3.180510	C	3.293513	1.018160	-0.261876
C	4.856968	-4.348565	2.687523	C	2.435131	0.161588	-1.195344
H	4.914196	-5.184388	3.416526	H	5.463452	1.316045	0.110327
H	4.325778	-4.746142	1.793024	H	5.086105	0.396245	-1.372852
C	4.040817	-3.188613	3.277766	H	3.241402	0.631520	0.770505
H	4.503568	-2.850263	4.232622	H	2.519666	-0.879939	-0.826162
H	3.011589	-3.518757	3.535826	H	2.907965	0.169835	-2.201907
C	1.863593	-0.617122	2.286331	H	1.683874	2.271407	-0.545647
H	1.558452	-1.204368	1.409065	C	2.719078	2.997551	1.226580
C	0.999040	0.405836	2.772985	H	3.774972	2.997096	1.560150
C	0.676295	0.891869	-3.564668	H	2.159424	2.258645	1.825128
H	1.443141	0.130747	-3.802841	C	2.099229	4.360468	1.336694
C	1.140364	2.144462	-3.096888	C	0.695959	4.482396	1.303710
H	2.233247	2.258373	-3.009097	C	0.886819	6.902689	1.440787
C	0.339785	3.433413	-3.206908	C	2.891343	5.521497	1.436195
H	-0.307121	3.402836	-4.106673	C	2.287159	6.788577	1.490779
H	1.033254	4.283250	-3.366650	H	2.912292	7.691129	1.570196
C	-0.508881	3.691207	-1.942026	H	3.988979	5.432181	1.462314
H	0.109864	4.203894	-1.176185	C	0.090629	5.746518	1.350399
H	-1.348173	4.391652	-2.162624	H	0.082002	3.571051	1.248402
C	-1.053804	2.416082	-1.327992	H	0.413620	7.895957	1.480966
H	-1.334475	2.504275	-0.266253	H	-1.006553	5.829613	1.323048
C	-1.691594	1.374547	-2.040274	C	4.675876	2.553786	-1.480338
H	-2.398361	0.765151	-1.463862	C	3.505084	3.244872	-1.128200
C	-1.865604	1.297301	-3.548745	C	5.562920	3.141175	-2.394363
H	-2.062402	2.307427	-3.965298	C	3.183130	4.511563	-1.626789
H	-2.768874	0.692518	-3.767182	C	5.255873	4.409402	-2.923303
C	-0.651291	0.639320	-4.252059	H	6.483073	2.617728	-2.695901
H	-0.801808	-0.457190	-4.290130	C	4.082857	5.088914	-2.541303
H	-0.581657	0.974193	-5.313571	H	2.262530	5.028283	-1.327079
C	-2.348476	-1.694404	2.759305	H	5.941581	4.876480	-3.646577
C	-2.179494	-1.699007	4.158678	H	3.860702	6.079804	-2.965045
C	-3.655694	-1.733029	2.230903				

29_C_SS
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Ir	-0.183151	0.454599	-1.909902
C	-0.402396	-0.417517	-0.100913
N	-0.626872	-1.775103	-0.042333
C	-1.126297	-2.563075	-1.143680
C	-0.297250	-3.407626	-1.894567
C	1.191355	-3.533207	-1.652710
H	1.476583	-2.730845	-0.935631
C	2.038789	-3.365155	-2.936514
H	1.755140	-2.439747	-3.477321
H	1.818866	-4.206071	-3.630424
C	3.538816	-3.375553	-2.603836
H	4.140619	-3.240149	-3.527594
H	3.767839	-2.501573	-1.949009
C	3.943634	-4.667748	-1.876763
H	3.840609	-5.526555	-2.577890
H	5.016478	-4.631832	-1.588623
C	3.061647	-4.913190	-0.643464
H	3.262299	-4.121405	0.114740
H	3.322548	-5.876659	-0.156670
C	1.567468	-4.880559	-0.990515
H	1.325120	-5.709046	-1.693900
H	0.952987	-5.048088	-0.088305
C	-0.901282	-4.214849	-2.907934
H	-0.254520	-4.867503	-3.513102
C	-2.267137	-4.217018	-3.135377
H	-2.700124	-4.857815	-3.919573
C	-3.133236	-3.402152	-2.350757
C	-4.548359	-3.376691	-2.540690
H	-4.985451	-4.019017	-3.321621
C	-5.363104	-2.555754	-1.774488
H	-6.449303	-2.545290	-1.954880
C	-4.805075	-1.713195	-0.765077
C	-5.651639	-0.720167	0.005101
H	-4.968358	-0.180107	0.702739
C	-6.254193	0.346334	-0.941260
H	-5.436745	0.833721	-1.514584
H	-6.904099	-0.159651	-1.690248
C	-7.072867	1.391534	-0.171278
H	-7.522727	2.120630	-0.878119
H	-6.387799	1.974319	0.483328
C	-8.158102	0.735582	0.695922
H	-8.710469	1.505921	1.274643
H	-8.908079	0.243696	0.035258
C	-7.555953	-0.316240	1.641796
H	-8.353090	-0.804428	2.241440
H	-6.881977	0.191403	2.370389
C	-6.752047	-1.374423	0.868858
H	-7.439154	-1.953701	0.211494
H	-6.292422	-2.110321	1.563573
C	-3.430648	-1.756171	-0.555786
H	-3.004620	-1.085789	0.200553
C	-2.554109	-2.564834	-1.333425

C	-0.966896	-2.259683	1.328859
H	-2.056381	-2.463967	1.346102
C	-0.653614	-1.036872	2.202105
H	0.334044	-1.165989	2.691340
N	-0.492731	0.063896	1.186936
C	0.134169	1.255413	1.691539
C	-0.604940	2.392817	2.054257
C	-2.092411	2.538874	1.807942
H	-2.411830	1.676296	1.182004
C	-2.479117	3.845167	1.069952
H	-1.890739	3.975516	0.140103
H	-2.228710	4.714612	1.718261
C	-3.983594	3.868920	0.760119
H	-4.246049	4.803459	0.220710
H	-4.218319	3.030231	0.064774
C	-4.822137	3.730409	2.041431
H	-5.904203	3.690826	1.794289
H	-4.680542	4.640312	2.667595
C	-4.405417	2.494193	2.850354
H	-4.670203	1.572189	2.283682
H	-4.968544	2.438628	3.805804
C	-2.897885	2.481792	3.129568
H	-2.612664	1.591321	3.713986
H	-2.625600	3.364359	3.751885
C	0.077421	3.443632	2.746128
H	-0.494253	4.340519	3.027452
C	1.410644	3.354864	3.104444
H	1.891314	4.171684	3.665548
C	2.172262	2.194527	2.782398
C	3.527935	2.022560	3.194192
H	4.013137	2.834868	3.757735
C	4.227614	0.861520	2.903191
H	5.270465	0.757191	3.238482
C	3.617621	-0.190844	2.156433
C	4.377785	-1.450760	1.796285
H	3.728955	-2.037284	1.103719
C	5.695159	-1.156202	1.045970
H	6.370423	-0.567275	1.706548
H	5.490730	-0.509224	0.170885
C	6.398798	-2.450719	0.617946
H	5.756931	-2.986862	-0.118093
H	7.347410	-2.214197	0.090831
C	6.664803	-3.365537	1.823289
H	7.132257	-4.317070	1.493520
H	7.400776	-2.872848	2.498757
C	5.371540	-3.649406	2.604299
H	5.584454	-4.271104	3.499540
H	4.686013	-4.247254	1.961787
C	4.657205	-2.353479	3.021943
H	5.287685	-1.792442	3.748541
H	3.705127	-2.577979	3.549006
C	2.296240	-0.031271	1.740012
H	1.836160	-0.830513	1.141563
C	1.531348	1.136050	2.042523

C	-0.493243	0.040195	-4.016288
H	0.278316	-0.700586	-4.299238
C	-0.088293	1.398680	-3.978576
H	0.971379	1.591031	-4.218421
C	-1.025197	2.589533	-4.130082
H	-1.874377	2.325468	-4.792442
H	-0.489388	3.414339	-4.642571
C	-1.545042	3.089540	-2.761449
H	-0.826474	3.818305	-2.331047
H	-2.501590	3.649241	-2.883224
C	-1.738931	1.961845	-1.767161
H	-1.757101	2.287127	-0.716728
C	-2.409224	0.742409	-2.037352
H	-2.875167	0.259133	-1.171124
C	-2.964265	0.301822	-3.383236
H	-3.367889	1.174410	-3.938287
H	-3.826728	-0.373023	-3.208418
C	-1.911526	-0.450562	-4.233453
H	-1.937273	-1.528701	-3.977413
H	-2.161383	-0.386238	-5.318468
C	-1.650569	-0.767181	3.307581
C	-1.167915	-0.375217	4.572644
C	-3.040853	-0.927680	3.130909
C	-2.052453	-0.147791	5.639898
H	-0.082713	-0.252006	4.719497
C	-3.926988	-0.708048	4.196218
H	-3.447663	-1.231931	2.155866
C	-3.435396	-0.317435	5.454404
H	-1.659860	0.157172	6.622017
H	-5.008591	-0.840918	4.040655
H	-4.130477	-0.147162	6.290811
C	-0.285370	-3.550017	1.731620
C	-1.016403	-4.751063	1.633105
C	1.041450	-3.596674	2.204480
C	-0.437747	-5.975576	2.004680
H	-2.051995	-4.719105	1.258349
C	1.619131	-4.817148	2.586730
H	1.634371	-2.673999	2.284941
C	0.881618	-6.010010	2.487620
H	-1.020773	-6.905461	1.921103
H	2.653184	-4.838374	2.962233
H	1.336085	-6.966494	2.788078
N	2.702076	2.041862	-0.845958
C	4.380109	0.700992	-1.940719
C	2.959412	0.578207	-1.348031
C	1.872703	-0.038835	-2.193057
H	4.898652	-0.277866	-1.917546
H	4.341774	1.016246	-3.007799
H	3.044490	0.046194	-0.383548
H	1.960474	-1.124596	-2.012384
H	2.128654	0.114608	-3.266101
H	2.046740	1.975918	-0.038074
C	2.061801	2.939136	-1.888889
H	2.720288	2.917888	-2.777115

H	1.098890	2.407863	-2.117253
C	1.854450	4.326194	-1.366502
C	2.633792	5.408376	-1.821592
C	0.892887	4.543334	-0.358727
C	2.450371	6.690655	-1.278599
H	3.394763	5.241130	-2.600395
C	0.715363	5.820677	0.191209
H	0.285393	3.698377	-0.000496
C	1.494383	6.897857	-0.268613
H	3.060750	7.531727	-1.641620
H	-0.039550	5.977209	0.976131
H	1.352612	7.902802	0.158019
C	5.024525	1.754138	-1.071232
C	4.031275	2.507658	-0.425894
C	6.369991	2.057898	-0.817125
C	4.299314	3.561792	0.448372
C	6.673972	3.107924	0.071078
H	7.174953	1.480268	-1.296450
C	5.654077	3.851583	0.695271
H	3.489784	4.130435	0.925136
H	7.726742	3.351254	0.281397
H	5.915520	4.668537	1.384447

29_C_RS

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Ir	0.037096	-0.442783	-1.939360
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N	0.467445	-0.086209	1.133091
C	-0.218220	-1.255008	1.607708
C	0.487401	-2.405219	1.992228
C	1.980655	-2.565490	1.788177
H	2.336700	-1.664009	1.241814
C	2.367398	-3.812309	0.955918
H	1.812159	-3.846146	-0.001861
H	2.072620	-4.728001	1.516589
C	3.880956	-3.849636	0.696114
H	4.140621	-4.739700	0.084826
H	4.162289	-2.959308	0.087130
C	4.674986	-3.844325	2.011589
H	4.486943	-4.798347	2.554568
H	5.766236	-3.815252	1.806580
C	4.260150	-2.665505	2.902932
H	4.566967	-1.711084	2.417612
H	4.791985	-2.698390	3.877214
C	2.743977	-2.632808	3.133254
H	2.431737	-3.553056	3.677844
H	2.460765	-1.782192	3.776611
C	-0.238296	-3.447343	2.649859
H	0.306943	-4.353059	2.954804
C	-1.586812	-3.338911	2.940772
H	-2.108278	-4.151887	3.470110
C	-2.314948	-2.164770	2.591520
C	-3.684719	-1.976113	2.943881
H	-4.208338	-2.788704	3.470475

C	-4.349868	-0.795597	2.650979	C	5.519662	2.202823	-1.834709
H	-5.401654	-0.678374	2.949758	H	6.605512	2.137607	-2.004468
C	-3.684043	0.268921	1.972790	C	4.909590	1.391345	-0.829949
C	-4.347408	1.617199	1.756118	C	5.707253	0.426917	0.024106
H	-3.783234	2.133590	0.942720	H	4.969237	-0.193580	0.586127
C	-5.829325	1.562454	1.331861	C	6.575221	-0.547344	-0.801186
H	-5.950661	0.926472	0.433096	H	7.305383	0.032815	-1.409030
H	-6.424907	1.075460	2.136291	H	5.932401	-1.096266	-1.522741
C	-6.389547	2.969960	1.075678	C	7.338432	-1.524777	0.106002
H	-7.453198	2.906260	0.763005	H	6.606341	-2.182942	0.625858
H	-5.839127	3.429985	0.222642	H	7.977616	-2.194775	-0.506994
C	-6.244590	3.862716	2.317129	C	8.182157	-0.784342	1.155885
H	-6.613142	4.888247	2.104653	H	8.694107	-1.510301	1.822429
H	-6.888059	3.460623	3.132432	H	8.987142	-0.211087	0.641934
C	-4.786122	3.906544	2.797087	C	7.322729	0.186515	1.980549
H	-4.697577	4.507913	3.726769	H	7.949756	0.742097	2.709761
H	-4.168980	4.421063	2.026482	H	6.586493	-0.398175	2.579663
C	-4.216480	2.498167	3.026721	C	6.562692	1.169716	1.077719
H	-4.760754	1.997411	3.859410	H	7.284889	1.834037	0.551012
H	-3.153941	2.548952	3.345128	H	5.911045	1.839329	1.680270
C	-2.352479	0.086375	1.596987	C	3.536615	1.501476	-0.635381
H	-1.841411	0.902765	1.069179	H	3.073542	0.844004	0.113104
C	-1.626602	-1.106328	1.895568	C	2.716045	2.378423	-1.402670
C	0.674659	1.005458	2.145209	C	0.064375	0.033144	-4.052682
H	-0.319391	1.217836	2.592916	H	-0.724259	0.788383	-4.227867
C	1.123329	2.185264	1.271326	C	-0.366349	-1.319039	-3.999169
H	2.228590	2.273062	1.297727	H	-1.446607	-1.472752	-4.161165
N	0.751639	1.727737	-0.099535	C	0.514648	-2.527860	-4.305238
C	1.295231	2.478314	-1.202932	H	1.238892	-2.270935	-5.105302
C	0.518731	3.383190	-1.938790	H	-0.113489	-3.339548	-4.726708
C	-0.957022	3.595075	-1.681159	C	1.261321	-3.060454	-3.055899
H	-1.278721	2.817298	-0.955679	H	0.638836	-3.821709	-2.540185
C	-1.827138	3.454058	-2.950469	H	2.190230	-3.597207	-3.358851
H	-1.594777	2.504063	-3.474029	C	1.605764	-1.969699	-2.060185
H	-1.569757	4.266601	-3.665920	H	1.765350	-2.324510	-1.029844
C	-3.320514	3.547927	-2.601744	C	2.226757	-0.745825	-2.393295
H	-3.939083	3.438615	-3.518190	H	2.791520	-0.257966	-1.591560
H	-3.587099	2.693995	-1.937090	C	2.590832	-0.287941	-3.795285
C	-3.648654	4.866720	-1.883913	H	2.861667	-1.158328	-4.428466
H	-4.716899	4.885054	-1.577279	H	3.497151	0.348401	-3.738571
H	-3.516043	5.712141	-2.596405	C	1.445643	0.525672	-4.437599
C	-2.735524	5.084902	-0.667349	H	1.524164	1.583666	-4.114680
H	-2.963827	4.314938	0.105568	H	1.537349	0.534112	-5.549244
H	-2.940229	6.067539	-0.191937	C	0.579865	3.541938	1.658313
C	-1.250610	4.971428	-1.038176	C	1.429638	4.661247	1.550844
H	-0.611877	5.123790	-0.149904	C	-0.734225	3.725929	2.129790
H	-0.980080	5.774814	-1.760258	C	0.978854	5.940121	1.915798
C	1.170192	4.156673	-2.948382	H	2.456849	4.521676	1.177213
H	0.566855	4.858287	-3.544028	C	-1.182329	4.999443	2.513099
C	2.532200	4.064014	-3.185825	H	-1.418808	2.868479	2.207987
H	3.003672	4.682023	-3.966175	C	-0.327538	6.110087	2.405666
C	3.345551	3.182733	-2.415842	H	1.652646	6.805781	1.824822
C	4.756517	3.068090	-2.605904	H	-2.206831	5.126754	2.892191
H	5.234130	3.683950	-3.384468	H	-0.680422	7.108997	2.704620

C	1.604922	0.670931	3.290484
C	1.044544	0.302531	4.530314
C	3.008361	0.754890	3.176973
C	1.865361	0.029593	5.636899
H	-0.051341	0.235907	4.625048
C	3.831049	0.494155	4.283374
H	3.475912	1.030804	2.220402
C	3.262172	0.131565	5.516863
H	1.412389	-0.255742	6.598717
H	4.924029	0.572006	4.179295
H	3.908159	-0.070777	6.384881
N	-2.828370	-2.113833	-1.082047
C	-4.512344	-0.367058	-1.518187
C	-3.090021	-0.815013	-1.929382
H	-4.447513	0.544396	-0.886974
H	-5.124708	-0.103493	-2.403918
C	-2.234928	-3.177488	-1.990835
H	-1.305605	-2.681589	-2.348690
H	-2.951251	-3.289632	-2.825964
C	-1.949746	-4.494914	-1.341441
C	-2.707044	-5.636412	-1.676170
C	-1.408281	-6.970951	-0.111588
C	-0.914481	-4.604017	-0.393077
C	-0.647983	-5.836162	0.222022
H	0.164744	-5.913445	0.958365
H	-0.322318	-3.712719	-0.134336
C	-2.436417	-6.871054	-1.065601
H	-3.520350	-5.551989	-2.414434
H	-1.193534	-7.938310	0.368074
H	-3.030669	-7.758048	-1.333499
C	-1.988048	0.218054	-1.779816
H	-2.196725	0.796065	-0.857289
H	-2.097616	-1.865893	-0.375522
H	-2.164433	0.931954	-2.610490
H	-3.117330	-1.197173	-2.967910
C	-5.084323	-1.509849	-0.723622
C	-4.101473	-2.465624	-0.434654
C	-6.380748	-1.693527	-0.216580
C	-4.337709	-3.585815	0.369350
C	-6.654125	-2.827187	0.569444
H	-7.174191	-0.964002	-0.438074
C	-5.642076	-3.758722	0.864910
H	-3.540157	-4.295089	0.619374
H	-7.670588	-2.984953	0.961210
H	-5.866825	-4.633485	1.493467

29_C_RR

E= -3486.77001846 A.U.

Ir	0.464456	-0.556482	-1.814640
C	0.831891	0.289245	-0.004463
N	0.586893	-0.161745	1.271403
C	-0.379926	-1.140561	1.661719
C	-0.029834	-2.476180	1.888883
C	1.359959	-3.019105	1.656477

H	1.989362	-2.188005	1.271013
C	1.356403	-4.148570	0.600647
H	0.900177	-3.769601	-0.337101
H	0.703859	-4.978210	0.954066
C	2.770487	-4.694220	0.352057
H	2.735287	-5.516856	-0.393454
H	3.397729	-3.893047	-0.100725
C	3.429421	-5.169243	1.656631
H	2.876933	-6.054618	2.046524
H	4.467864	-5.511149	1.460986
C	3.419820	-4.057349	2.716438
H	4.060459	-3.217045	2.368534
H	3.866950	-4.414821	3.668032
C	2.002621	-3.527568	2.968167
H	1.372900	-4.343515	3.389755
H	2.010590	-2.716884	3.722048
C	-1.040576	-3.372769	2.361730
H	-0.774437	-4.428384	2.519870
C	-2.323739	-2.950006	2.648579
H	-3.074242	-3.660010	3.028158
C	-2.694899	-1.588283	2.451711
C	-4.015247	-1.115693	2.714707
H	-4.753726	-1.819850	3.128846
C	-4.367567	0.203274	2.463218
H	-5.387199	0.544667	2.697369
C	-3.425018	1.122548	1.905909
C	-3.810089	2.571236	1.678158
H	-2.975815	3.055197	1.122987
C	-5.087851	2.731094	0.824176
H	-4.929088	2.259685	-0.170203
H	-5.922963	2.178217	1.311114
C	-5.507079	4.198650	0.656807
H	-6.448680	4.256349	0.071130
H	-4.735206	4.730793	0.060734
C	-5.662764	4.899560	2.013341
H	-5.937073	5.965390	1.868408
H	-6.501993	4.433514	2.579014
C	-4.370476	4.783644	2.835701
H	-4.485336	5.276951	3.823852
H	-3.555720	5.326474	2.304618
C	-3.959329	3.316538	3.029142
H	-4.728498	2.796421	3.644510
H	-3.008507	3.240021	3.599287
C	-2.133533	0.666954	1.633362
H	-1.418566	1.358054	1.165272
C	-1.718838	-0.668062	1.923719
C	1.035518	0.778962	2.342524
H	0.132579	1.145945	2.873073
C	1.696751	1.919888	1.539726
H	2.793859	1.898523	1.704991
N	1.441956	1.508716	0.124636
C	2.021479	2.287071	-0.932538
C	1.249349	3.169442	-1.694506
C	-0.224147	3.404490	-1.442768

H	-0.521362	2.786517	-0.567608	H	1.341595	-3.844884	-2.285009
C	-1.105721	2.967268	-2.630892	H	2.867788	-3.546104	-3.132726
H	-0.925445	1.893356	-2.826368	C	2.164326	-1.903618	-1.909906
H	-0.794460	3.518352	-3.546713	H	2.411428	-2.199677	-0.875552
C	-2.591411	3.236183	-2.358061	C	2.656101	-0.639149	-2.316239
H	-3.204723	2.922840	-3.230290	H	3.214325	-0.086599	-1.555614
H	-2.920836	2.604810	-1.499183	C	2.944533	-0.217670	-3.747424
C	-2.840558	4.713867	-2.020070	H	3.280310	-1.088323	-4.348403
H	-3.917227	4.891461	-1.813622	H	3.789283	0.500122	-3.745839
H	-2.590190	5.338119	-2.907547	C	1.713884	0.454663	-4.394871
C	-1.974078	5.157885	-0.832301	H	1.697005	1.525999	-4.107933
H	-2.285730	4.605021	0.082790	H	1.782215	0.428965	-5.507905
H	-2.132925	6.233982	-0.607434	C	1.244801	3.338866	1.834581
C	-0.487041	4.887063	-1.087591	C	2.162715	4.384235	1.599691
H	0.121837	5.173384	-0.208479	C	-0.043016	3.661988	2.305616
H	-0.142511	5.527788	-1.929529	C	1.804452	5.721384	1.832706
C	1.903690	3.914474	-2.725316	H	3.171563	4.140288	1.230597
H	1.300718	4.591380	-3.349459	C	-0.402377	4.998044	2.546801
C	3.265635	3.818658	-2.955681	H	-0.777184	2.868726	2.507398
H	3.736415	4.403903	-3.761314	C	0.519560	6.031935	2.310708
C	4.077728	2.966254	-2.152029	H	2.534114	6.523885	1.645135
C	5.481196	2.811876	-2.354295	H	-1.408491	5.231612	2.926359
H	5.966026	3.399076	-3.150398	H	0.237104	7.078614	2.501271
C	6.231150	1.927810	-1.587017	C	1.925555	0.116161	3.374464
H	7.307653	1.823105	-1.784119	C	1.441312	-0.092130	4.679801
C	5.617255	1.155005	-0.557417	C	3.236407	-0.299384	3.061048
C	6.349045	0.100099	0.261413	C	2.255442	-0.685580	5.660355
H	6.102774	0.296273	1.333030	H	0.415135	0.221796	4.930501
C	5.808719	-1.317432	-0.067090	C	4.057254	-0.877757	4.039305
H	5.994425	-1.525098	-1.145264	H	3.626206	-0.175203	2.040248
H	4.704951	-1.345496	0.058693	C	3.568655	-1.071655	5.343978
C	6.469897	-2.396859	0.800803	H	1.864245	-0.839869	6.677690
H	6.171204	-2.238173	1.862992	H	5.082158	-1.184825	3.780672
H	6.085014	-3.400250	0.519066	H	4.211904	-1.526626	6.112638
C	8.001711	-2.350934	0.696494	N	-3.693784	-1.637991	-0.619714
H	8.459690	-3.107935	1.367737	C	-2.025131	-2.970764	-1.781359
H	8.303938	-2.627285	-0.339472	C	-2.136573	-1.618020	-1.057493
C	8.537863	-0.947735	1.021263	C	-1.665858	-0.340134	-1.683011
H	9.641391	-0.916158	0.903276	H	-0.976168	-3.320455	-1.745184
H	8.332382	-0.713626	2.091304	H	-2.303991	-2.898939	-2.855995
C	7.882190	0.124523	0.136200	H	-1.663140	-1.754585	-0.072757
H	8.165091	-0.062467	-0.924763	H	-2.109531	-0.190526	-2.692361
H	8.270016	1.133145	0.394277	H	-1.966923	0.518979	-1.047759
C	4.253554	1.328811	-0.334538	H	-3.792719	-1.087515	0.256676
H	3.768692	0.709581	0.430246	C	-4.616933	-1.036278	-1.664691
C	3.445420	2.201910	-1.110086	H	-4.355348	-1.518679	-2.625547
C	0.400678	-0.154614	-3.948372	H	-4.342562	0.034663	-1.724671
H	-0.468327	0.507565	-4.123064	C	-6.062184	-1.252043	-1.308057
C	0.110283	-1.535903	-3.812171	C	-6.791785	-2.306533	-1.893081
H	-0.954929	-1.806954	-3.889762	C	-8.704283	-1.787084	-0.480964
C	1.095207	-2.662170	-4.101235	C	-6.671051	-0.460832	-0.312259
H	1.779789	-2.365972	-4.921869	C	-7.984408	-0.728893	0.103207
H	0.540677	-3.544723	-4.481134	H	-8.452970	-0.104324	0.879543
C	1.902060	-3.068313	-2.845972	H	-6.110517	0.371297	0.137795

C	-8.109014	-2.570126	-1.484961
H	-6.319393	-2.932306	-2.666878
H	-9.736136	-1.995634	-0.158742
H	-8.672196	-3.393708	-1.949799
C	-2.987760	-3.847274	-1.023113
C	-3.043739	-5.241580	-0.878840
C	-3.937014	-3.061524	-0.351794
C	-4.049590	-5.803870	-0.070140
H	-2.305497	-5.884303	-1.382301
C	-4.951945	-3.590654	0.448399
C	-4.994434	-4.990189	0.585220
H	-4.098166	-6.896584	0.054011
H	-5.684997	-2.942338	0.947627
H	-5.775507	-5.449871	1.209269

29_C_D_SR

E= -3486.76364731 A.U.

Ir	0.247668	0.910527	-1.273248
C	-0.417543	-0.512615	-0.024000
N	-0.623803	-1.770165	-0.514677
C	-0.849464	-2.038116	-1.906938
C	0.171458	-2.509873	-2.743677
C	1.573662	-2.771489	-2.244687
H	1.628357	-2.388912	-1.202576
C	2.660923	-2.052008	-3.072194
H	2.434509	-0.967923	-3.133715
H	2.644861	-2.434765	-4.117241
C	4.054388	-2.288099	-2.470580
H	4.826200	-1.765464	-3.074157
H	4.087100	-1.830061	-1.455677
C	4.372193	-3.787241	-2.355832
H	4.458636	-4.223716	-3.376709
H	5.360345	-3.936276	-1.870401
C	3.273628	-4.528696	-1.579733
H	3.266753	-4.173386	-0.523891
H	3.485968	-5.617804	-1.536375
C	1.884698	-4.286586	-2.185728
H	1.846358	-4.707329	-3.216089
H	1.104897	-4.810776	-1.601526
C	-0.171868	-2.817062	-4.098753
H	0.620034	-3.175387	-4.773632
C	-1.470457	-2.711919	-4.570295
H	-1.703211	-2.976908	-5.613910
C	-2.525668	-2.264213	-3.719933
C	-3.875071	-2.113102	-4.162918
H	-4.123966	-2.389846	-5.199713
C	-4.857507	-1.611203	-3.320040
H	-5.886418	-1.497125	-3.694494
C	-4.542799	-1.210488	-1.984788
C	-5.566326	-0.556598	-1.081111
H	-5.041993	-0.292895	-0.132324
C	-6.102204	0.766294	-1.676880
H	-5.248580	1.443172	-1.899216
H	-6.596731	0.554355	-2.651664

C	-7.105829	1.441542	-0.730471
H	-7.501387	2.369924	-1.193995
H	-6.573650	1.757425	0.194569
C	-8.253699	0.493468	-0.350784
H	-8.944207	0.990370	0.362801
H	-8.856621	0.263212	-1.258725
C	-7.720062	-0.818340	0.246009
H	-8.555835	-1.507783	0.488875
H	-7.204911	-0.596588	1.209788
C	-6.727195	-1.504981	-0.704771
H	-7.257378	-1.821424	-1.631592
H	-6.317067	-2.431971	-0.248835
C	-3.237353	-1.384651	-1.535277
H	-2.984832	-1.016327	-0.531247
C	-2.207139	-1.917525	-2.362847
C	-1.200423	-2.706499	0.495456
H	-2.274435	-2.834372	0.248407
C	-1.058621	-1.900946	1.800561
H	-0.183252	-2.262224	2.378839
N	-0.709676	-0.524557	1.304854
C	-0.209108	0.409911	2.272005
C	-1.010956	1.438190	2.778313
C	-2.443954	1.653117	2.336782
H	-2.644389	0.942707	1.503618
C	-2.709825	3.083844	1.821409
H	-1.990919	3.336058	1.019947
H	-2.520769	3.809861	2.643051
C	-4.153741	3.245252	1.325356
H	-4.320311	4.281550	0.961828
H	-4.313926	2.577831	0.446379
C	-5.165311	2.884800	2.424175
H	-6.203608	2.960497	2.036837
H	-5.086790	3.628127	3.249321
C	-4.895301	1.479254	2.980254
H	-5.083384	0.725543	2.181405
H	-5.600782	1.236535	3.802668
C	-3.448246	1.329856	3.468773
H	-3.267167	0.311660	3.857775
H	-3.268754	2.027660	4.317643
C	-0.452494	2.278383	3.792733
H	-1.059705	3.107743	4.185461
C	0.818486	2.070087	4.300910
H	1.216697	2.731852	5.085915
C	1.628860	0.996310	3.826258
C	2.941827	0.737831	4.321885
H	3.346442	1.393274	5.109255
C	3.703097	-0.314265	3.830758
H	4.710177	-0.488883	4.238271
C	3.203273	-1.161653	2.795530
C	4.009841	-2.318184	2.236612
H	3.565206	-2.568462	1.243891
C	5.500104	-1.997884	1.999133
H	5.984885	-1.753426	2.970753
H	5.595200	-1.094531	1.364326

H	4.599322	-3.494783	-4.081919	H	-5.571085	3.015034	2.866215
H	5.732836	-2.673504	-2.985428	H	-4.247733	3.850129	3.715864
C	4.059612	-3.673162	-1.985437	C	-4.042117	1.686302	3.700745
H	4.215967	-3.109513	-1.037808	H	-4.354539	0.828320	3.064056
H	4.586147	-4.642429	-1.856251	H	-4.558330	1.553449	4.674939
C	2.556483	-3.910053	-2.167422	C	-2.523007	1.634994	3.898484
H	2.384388	-4.544010	-3.066209	H	-2.214370	0.692665	4.388591
H	2.138959	-4.466649	-1.309780	H	-2.219181	2.458044	4.582859
C	-0.151459	-3.514174	-3.632584	C	0.336563	2.640454	3.631136
H	0.578799	-3.758868	-4.418063	H	-0.298197	3.380986	4.140180
C	-1.468527	-3.902201	-3.792306	C	1.687863	2.600237	3.915275
H	-1.786895	-4.435993	-4.701542	H	2.127202	3.299362	4.642781
C	-2.427848	-3.630523	-2.775557	C	2.535051	1.660169	3.265741
C	-3.795599	-4.015586	-2.892650	C	3.934959	1.589976	3.529419
H	-4.115004	-4.547640	-3.802701	H	4.365860	2.288690	4.263331
C	-4.717598	-3.726515	-1.894340	C	4.741812	0.675010	2.874668
H	-5.765999	-4.032230	-2.020250	H	5.818832	0.638806	3.099869
C	-4.312720	-3.042108	-0.711467	C	4.195923	-0.216654	1.899489
C	-5.273833	-2.637742	0.396816	C	5.084496	-1.215587	1.185572
H	-4.770829	-2.888484	1.361399	H	4.451987	-1.749286	0.439284
C	-5.496059	-1.101950	0.397043	C	6.242017	-0.545898	0.408590
H	-4.518577	-0.575488	0.447344	H	6.855001	0.058844	1.114727
H	-5.948853	-0.810999	-0.578109	H	5.828286	0.167768	-0.336173
C	-6.399920	-0.654000	1.554242	C	7.140567	-1.579386	-0.287310
H	-6.568950	0.442687	1.502034	H	6.554055	-2.093385	-1.081221
H	-5.869290	-0.838844	2.516629	H	7.978697	-1.065338	-0.803569
C	-7.734998	-1.413836	1.562669	C	7.674238	-2.625894	0.701923
H	-8.349476	-1.108307	2.435709	H	8.293033	-3.379452	0.170910
H	-8.318964	-1.135309	0.655918	H	8.348041	-2.128330	1.436416
C	-7.507994	-2.933508	1.568149	C	6.523193	-3.309825	1.455468
H	-8.478711	-3.471402	1.538245	H	6.915498	-4.044830	2.189834
H	-7.017333	-3.230685	2.523633	H	5.907703	-3.887574	0.728250
C	-6.625740	-3.372826	0.388939	C	5.632676	-2.280008	2.166553
H	-7.162281	-3.147840	-0.560813	H	6.222216	-1.769919	2.961685
H	-6.462223	-4.471500	0.408473	H	4.785242	-2.776131	2.687444
C	-2.972726	-2.677537	-0.589443	C	2.828314	-0.162528	1.639963
H	-2.669926	-2.130487	0.310469	H	2.414684	-0.819172	0.859920
C	-1.999090	-2.929915	-1.592414	C	1.960059	0.751756	2.311449
C	-0.226664	-2.663709	1.002925	C	-0.707281	0.859038	-3.779256
H	-1.239455	-3.094816	1.132975	H	0.269849	0.600871	-4.228871
C	0.021532	-1.603380	2.091753	C	-0.875250	2.193372	-3.362722
H	1.041246	-1.712241	2.512237	H	-0.016223	2.853784	-3.530560
N	-0.006935	-0.312972	1.327963	C	-2.209085	2.909551	-3.206807
C	0.539311	0.798131	2.063247	H	-2.916595	2.541746	-3.978002
C	-0.277506	1.725999	2.720891	H	-2.057124	3.986541	-3.418045
C	-1.779447	1.793195	2.552786	C	-2.826202	2.764684	-1.796603
H	-2.088344	0.949625	1.896488	H	-2.482783	3.602369	-1.164804
C	-2.209237	3.115458	1.872309	H	-3.935334	2.861478	-1.848025
H	-1.694822	3.205830	0.892825	C	-2.471863	1.468454	-1.111784
H	-1.855731	3.969890	2.491959	H	-2.517912	1.482948	-0.013159
C	-3.733639	3.208360	1.700852	C	-2.583060	0.207359	-1.712692
H	-4.005228	4.185208	1.246743	H	-2.698998	-0.638819	-1.029471
H	-4.070260	2.428689	0.981167	C	-3.018333	-0.056756	-3.142356
C	-4.472956	3.000785	3.031345	H	-3.745080	0.714213	-3.469308

H	-3.555388	-1.025680	-3.174977
C	-1.813525	-0.121497	-4.110267
H	-1.380413	-1.141274	-4.087093
H	-2.143591	0.045945	-5.161923
C	-0.947229	-1.627169	3.255738
C	-0.445358	-1.596396	4.570971
C	-2.342458	-1.692245	3.062606
C	-1.317014	-1.656778	5.672071
H	0.642909	-1.530990	4.730200
C	-3.215479	-1.767081	4.157135
H	-2.760759	-1.675486	2.046298
C	-2.703585	-1.754180	5.467227
H	-0.909891	-1.635342	6.694534
H	-4.301424	-1.826411	3.986833
H	-3.387266	-1.812985	6.327851
C	0.729360	-3.839211	0.949829
C	0.229509	-5.076175	0.490864
C	2.083362	-3.751556	1.330342
C	1.063035	-6.203333	0.414911
H	-0.828918	-5.151912	0.193792
C	2.916603	-4.879908	1.264052
H	2.499993	-2.801745	1.695182
C	2.409865	-6.108065	0.805864
H	0.657607	-7.161254	0.054875
H	3.969409	-4.798042	1.572529
H	3.064647	-6.991447	0.755257
N	1.346306	3.126534	-0.690908
C	3.646801	2.409474	-0.613818
C	2.218817	1.878672	-0.813334
C	1.722797	0.973278	-1.909633
H	4.328583	1.612929	-0.260171
H	4.087192	2.847890	-1.537069
H	1.987431	1.366529	0.133101
H	2.238703	0.002865	-1.789386
H	1.980707	1.344660	-2.928649
H	0.200497	2.343383	-0.850252
C	1.460980	4.011618	-1.890503
H	2.433491	4.546688	-1.834038
H	1.519764	3.355817	-2.779246
C	0.355700	5.026722	-2.062392
C	0.373029	5.833173	-3.222004
C	-0.682091	5.206891	-1.133581
C	-0.624258	6.793678	-3.442635
H	1.178457	5.703801	-3.963845
C	-1.677943	6.177019	-1.345151
H	-0.734054	4.567945	-0.243074
C	-1.655236	6.971488	-2.500628
H	-0.597628	7.409108	-4.355015
H	-2.482105	6.301068	-0.603143
H	-2.435938	7.728653	-2.670162
C	3.374298	3.458231	0.448731
C	1.999662	3.809813	0.441356
C	4.236974	4.061601	1.368761
C	1.473636	4.747306	1.330263

C	3.720149	5.013748	2.269693
H	5.303025	3.789342	1.391138
C	2.355520	5.346326	2.252419
H	0.410305	5.013592	1.329481
H	4.389867	5.496917	2.997618
H	1.961644	6.082656	2.969356

29_C_D_RS

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Ir	0.131593	-0.962422	-1.427089
C	0.611424	0.357855	-0.002494
N	0.477068	0.351021	1.346073
C	-0.403994	-0.423530	2.180567
C	0.055984	-1.541580	2.880675
C	1.409138	-2.172074	2.639246
H	1.956582	-1.538308	1.906037
C	1.268349	-3.587177	2.032480
H	0.664847	-3.529144	1.101967
H	0.684416	-4.223842	2.734434
C	2.638484	-4.236225	1.779406
H	2.507545	-5.263366	1.376805
H	3.179962	-3.660949	0.994292
C	3.503286	-4.257361	3.049705
H	3.036745	-4.934896	3.800450
H	4.504073	-4.683645	2.824831
C	3.635312	-2.850890	3.653499
H	4.190118	-2.195228	2.945469
H	4.236635	-2.878675	4.586704
C	2.259376	-2.234005	3.927400
H	1.729739	-2.851925	4.685943
H	2.354585	-1.221351	4.362214
C	-0.778470	-2.085105	3.907122
H	-0.430157	-2.973488	4.454817
C	-1.974503	-1.493033	4.263491
H	-2.575429	-1.901995	5.089826
C	-2.460152	-0.353719	3.561711
C	-3.689342	0.279422	3.903276
H	-4.277219	-0.131569	4.737668
C	-4.148672	1.377660	3.195482
H	-5.106134	1.842852	3.475441
C	-3.409445	1.896046	2.092315
C	-3.935600	3.071694	1.295599
H	-3.214423	3.260020	0.466869
C	-5.307320	2.771938	0.647293
H	-5.221541	1.869709	0.004632
H	-6.038738	2.514773	1.446192
C	-5.833303	3.967218	-0.160627
H	-6.834123	3.732044	-0.580698
H	-5.162223	4.137793	-1.031506
C	-5.889302	5.246556	0.688282
H	-6.234202	6.104360	0.073202
H	-6.644453	5.118147	1.497006
C	-4.522596	5.554035	1.320353
H	-4.581736	6.461688	1.957811

H	-3.791366	5.784162	0.511735
C	-4.006489	4.363674	2.142989
H	-4.683927	4.191889	3.009531
H	-3.006097	4.580751	2.576650
C	-2.193171	1.299386	1.763245
H	-1.626017	1.703078	0.912811
C	-1.682422	0.174052	2.473047
C	0.989859	1.610331	1.981303
H	0.114506	2.129544	2.420135
C	1.548808	2.413136	0.787024
H	2.656516	2.436779	0.838882
N	1.171094	1.548442	-0.375814
C	1.644143	1.856230	-1.697428
C	0.794581	2.377585	-2.687607
C	-0.655507	2.740151	-2.450320
H	-0.965191	2.317172	-1.470329
C	-1.619047	2.200345	-3.530301
H	-1.514452	1.099598	-3.619842
H	-1.336830	2.616088	-4.522494
C	-3.071668	2.598659	-3.226334
H	-3.750078	2.191952	-4.005869
H	-3.384774	2.133998	-2.262910
C	-3.214982	4.125164	-3.123731
H	-4.261877	4.400540	-2.876294
H	-3.001923	4.579654	-4.117760
C	-2.241816	4.700707	-2.085761
H	-2.522228	4.336632	-1.071871
H	-2.313718	5.808104	-2.044452
C	-0.796552	4.282450	-2.373769
H	-0.109140	4.684911	-1.608926
H	-0.470070	4.716367	-3.345766
C	1.367023	2.696565	-3.961436
H	0.707704	3.096616	-4.745460
C	2.715709	2.546998	-4.226115
H	3.121242	2.811145	-5.215563
C	3.601317	2.054328	-3.223280
C	4.993241	1.857327	-3.455266
H	5.406396	2.123996	-4.440957
C	5.821250	1.324828	-2.473914
H	6.888660	1.178304	-2.690776
C	5.298609	0.959472	-1.199341
C	6.130500	0.292691	-0.113748
H	5.919331	0.840009	0.836248
C	5.669133	-1.173367	0.104147
H	5.807958	-1.731586	-0.849593
H	4.578787	-1.199916	0.320457
C	6.449444	-1.857796	1.235106
H	6.196663	-1.360069	2.199315
H	6.119171	-2.913265	1.337524
C	7.966819	-1.778817	1.012319
H	8.507212	-2.240862	1.865104
H	8.236451	-2.374727	0.110641
C	8.419136	-0.324516	0.810589
H	9.511001	-0.278891	0.615626

H	8.246397	0.249845	1.749697
C	7.651970	0.344997	-0.340350
H	7.899274	-0.183172	-1.289347
H	7.981947	1.398083	-0.468639
C	3.940481	1.173505	-0.961047
H	3.524494	0.854181	0.002682
C	3.059410	1.713889	-1.934928
C	-0.209690	-1.512320	-3.601879
H	-1.131971	-0.962761	-3.863079
C	-0.383169	-2.739258	-2.961266
H	-1.420206	-3.032133	-2.745025
C	0.652272	-3.845775	-2.881217
H	1.289175	-3.829256	-3.786001
H	0.129211	-4.822541	-2.903947
C	1.518960	-3.776199	-1.606977
H	0.958845	-4.211819	-0.754545
H	2.427586	-4.410443	-1.723471
C	1.937032	-2.373471	-1.236120
H	2.271222	-2.248418	-0.192808
C	2.320091	-1.369956	-2.131666
H	2.915581	-0.559336	-1.697948
C	2.371287	-1.448547	-3.649779
H	2.680918	-2.460272	-3.978447
H	3.163006	-0.757816	-4.001493
C	1.038142	-1.031089	-4.316142
H	0.994558	0.077069	-4.371109
H	1.002535	-1.381082	-5.374119
C	1.092048	3.850927	0.647886
C	1.978027	4.770356	0.048323
C	-0.173978	4.301072	1.074140
C	1.608947	6.114246	-0.122239
H	2.969868	4.423920	-0.284233
C	-0.541056	5.646625	0.912834
H	-0.884596	3.605651	1.543965
C	0.347551	6.555964	0.313576
H	2.311114	6.820448	-0.591092
H	-1.529824	5.985518	1.256348
H	0.057594	7.610499	0.188931
C	1.968060	1.342928	3.106893
C	1.544510	1.514649	4.438962
C	3.291085	0.921244	2.863558
C	2.432363	1.295842	5.506169
H	0.506850	1.826722	4.637775
C	4.183865	0.711506	3.924454
H	3.637787	0.749443	1.834611
C	3.757264	0.903650	5.250843
H	2.088220	1.437927	6.541987
H	5.216030	0.391212	3.715053
H	4.456544	0.740554	6.085050
N	-2.591428	-2.548906	0.015098
C	-4.323317	-0.980971	-0.705571
C	-2.927618	-1.573018	-1.082102
H	-4.304506	0.128059	-0.766985
H	-5.124905	-1.329638	-1.391818

C	-2.253126	-3.931007	-0.358672
H	-2.152941	-4.504727	0.585314
H	-1.246229	-3.955362	-0.817829
C	-3.248937	-4.618890	-1.285077
C	-2.783244	-5.396670	-2.364688
C	-5.060791	-5.914890	-3.040036
C	-4.644502	-4.511581	-1.088370
C	-5.539348	-5.150349	-1.961121
H	-6.623310	-5.055406	-1.791511
H	-5.036736	-3.930904	-0.241147
C	-3.676493	-6.042423	-3.236387
H	-1.698383	-5.510191	-2.519959
H	-5.766153	-6.414546	-3.721871
H	-3.288232	-6.645113	-4.072259
C	-1.905076	-0.436687	-1.214906
H	-2.041512	0.223608	-0.340029
H	-0.494330	-1.909247	-0.340129
H	-2.196747	0.161731	-2.103440
H	-3.008331	-2.145301	-2.030432
C	-4.565120	-1.481642	0.696093
C	-5.641388	-1.259002	1.560456
C	-3.558077	-2.414858	1.036832
C	-5.730034	-1.995897	2.759077
H	-6.428938	-0.538007	1.290988
C	-3.640621	-3.156573	2.227441
C	-4.739771	-2.943395	3.077148
H	-6.581725	-1.840387	3.438415
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29_C_D_RR

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C	0.865428	-2.125198	2.413472
C	2.271434	-2.383985	1.913098
H	2.522000	-1.576360	1.187603
C	2.424680	-3.746282	1.194675
H	1.662620	-3.861860	0.399304
H	2.224144	-4.562319	1.923588
C	3.839477	-3.910878	0.621173
H	3.930726	-4.888764	0.102391
H	4.007307	-3.128556	-0.155798
C	4.906530	-3.780671	1.718903
H	4.813030	-4.640410	2.420405
H	5.925294	-3.848629	1.281560
C	4.739007	-2.471136	2.503821
H	4.954824	-1.607632	1.833121
H	5.476794	-2.408891	3.331505
C	3.315260	-2.318252	3.053580
H	3.105250	-3.136170	3.779346
H	3.209009	-1.373343	3.613810
C	0.269788	-3.051623	3.327046

H	0.833971	-3.954675	3.602387
C	-0.982809	-2.845495	3.875446
H	-1.410061	-3.580583	4.574276
C	-1.745749	-1.691303	3.532150
C	-3.054846	-1.444699	4.044529
H	-3.490638	-2.174867	4.744608
C	-3.777971	-0.320904	3.668251
H	-4.787017	-0.161779	4.079363
C	-3.231280	0.625817	2.747952
C	-4.003667	1.848607	2.296948
H	-3.390412	2.344568	1.507910
C	-5.360048	1.492289	1.651164
H	-5.193851	0.775338	0.819179
H	-5.997144	0.965900	2.397227
C	-6.089826	2.746137	1.148135
H	-7.070201	2.467729	0.706857
H	-5.495343	3.204120	0.325469
C	-6.276206	3.776614	2.272595
H	-6.769761	4.691259	1.881505
H	-6.962321	3.356641	3.043000
C	-4.934396	4.133413	2.932125
H	-5.087978	4.845890	3.770032
H	-4.292802	4.657757	2.187121
C	-4.198354	2.880071	3.432670
H	-4.780692	2.407928	4.256114
H	-3.210964	3.146762	3.867945
C	-1.952271	0.397893	2.250598
H	-1.555880	1.104961	1.509824
C	-1.180125	-0.744033	2.610866
C	1.093526	1.280105	2.105232
H	0.220325	1.527470	2.742346
C	1.285764	2.374705	1.045929
H	2.364938	2.523556	0.840564
N	0.685117	1.747819	-0.174922
C	1.022259	2.352281	-1.444058
C	0.122173	3.163114	-2.155946
C	-1.292898	3.448177	-1.703028
H	-1.527715	2.745613	-0.875495
C	-2.347648	3.265458	-2.821020
H	-2.237122	2.276253	-3.313503
H	-2.167771	4.018158	-3.619934
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H	-4.514884	3.321409	-3.085278
H	-3.980118	2.667173	-1.517182
C	-3.933250	4.842577	-1.622124
H	-4.943258	4.940211	-1.169702
H	-3.869245	5.625898	-2.410790
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H	-2.988879	4.400660	0.287001
H	-2.934861	6.121925	-0.149271
C	-1.436013	4.883140	-1.137729
H	-0.669033	5.067173	-0.365367
H	-1.241233	5.614406	-1.954475
C	0.597223	3.806397	-3.341257

H	-0.103509	4.431368	-3.914113	C	-1.012123	5.150806	2.383053
C	1.907609	3.694107	-3.773104	H	-1.154260	2.996049	2.257604
H	2.239212	4.216717	-4.684186	C	-0.242288	6.293478	2.102312
C	2.848106	2.915276	-3.040762	H	1.615100	7.046481	1.251386
C	4.211823	2.781697	-3.442716	H	-1.992506	5.251473	2.872749
H	4.546412	3.309321	-4.349859	H	-0.616588	7.291927	2.375636
C	5.100077	1.997119	-2.722402	C	2.263149	1.055523	3.037647
H	6.142680	1.901575	-3.062513	C	1.999746	0.823534	4.403073
C	4.670208	1.298155	-1.553059	C	3.603606	1.101490	2.601646
C	5.589517	0.354613	-0.805663	C	3.051766	0.644771	5.316244
H	4.984817	-0.119254	0.003041	H	0.954974	0.789070	4.751474
C	6.090387	-0.788838	-1.719104	C	4.657069	0.926781	3.511981
H	6.656662	-0.351628	-2.572032	H	3.841086	1.286746	1.544333
H	5.217540	-1.316952	-2.160857	C	4.384253	0.699122	4.872270
C	6.993331	-1.769519	-0.957594	H	2.829939	0.467047	6.379591
H	6.387656	-2.295808	-0.186927	H	5.697499	0.969064	3.155216
H	7.368503	-2.555019	-1.647263	H	5.211049	0.565830	5.586617
C	8.163573	-1.046102	-0.273027	Ir	-0.243406	-0.592949	-1.667284
H	8.780578	-1.767719	0.302822	N	-2.796515	-2.224796	-1.152552
H	8.833276	-0.613616	-1.051072	C	-4.736991	-0.884905	-1.618445
C	7.663308	0.081363	0.643454	C	-3.197052	-0.889695	-1.747554
H	8.517952	0.615302	1.109956	C	-2.226393	0.181211	-1.314133
H	7.076296	-0.363837	1.479973	H	-5.214353	-0.193727	-2.340460
C	6.772951	1.074777	-0.119786	H	-5.081271	-0.592327	-0.601616
H	7.378350	1.602842	-0.891079	H	-3.042300	-1.038906	-2.835564
H	6.384519	1.863311	0.560813	H	-2.373098	1.073301	-1.944647
C	3.350776	1.451850	-1.137840	H	-2.390931	0.495076	-0.264347
H	3.027119	0.890829	-0.251551	H	-1.314557	-1.902890	-1.392974
C	2.400325	2.234994	-1.854641	C	-2.806778	-2.233732	0.339265
C	-0.461959	-0.442821	-3.857351	H	-3.805087	-1.939755	0.726334
H	-1.307962	0.247675	-4.030992	H	-2.081978	-1.465132	0.650969
C	-0.785260	-1.790889	-3.601648	C	-2.412576	-3.576946	0.892771
H	-1.853414	-2.044370	-3.561623	C	-1.165375	-4.137879	0.560700
C	0.123166	-2.989689	-3.825366	C	-3.274967	-4.289049	1.745962
H	0.819302	-2.790595	-4.663257	C	-0.789839	-5.394197	1.057869
H	-0.501396	-3.847146	-4.146236	H	-0.484707	-3.567797	-0.087772
C	0.902324	-3.378726	-2.551913	C	-2.895856	-5.538788	2.263808
H	0.258047	-4.008901	-1.904793	H	-4.253115	-3.854728	2.007111
H	1.784957	-4.009768	-2.805687	C	-1.654521	-6.097833	1.915005
C	1.353523	-2.171970	-1.763349	H	0.185894	-5.824454	0.785155
H	1.607238	-2.367670	-0.710973	H	-3.578821	-6.085064	2.932806
C	1.893518	-0.996528	-2.314639	H	-1.360982	-7.082715	2.310092
H	2.503888	-0.400621	-1.627407	C	-5.011305	-2.354980	-1.904749
C	2.098539	-0.657247	-3.782285	C	-3.834010	-3.105779	-1.659701
H	2.367021	-1.564166	-4.360074	C	-6.162267	-3.014827	-2.353109
H	2.970675	0.022863	-3.859257	C	-3.773555	-4.490293	-1.835260
C	0.866062	0.051797	-4.397228	C	-6.116570	-4.411677	-2.544233
H	0.929985	1.141114	-4.197985	H	-7.088475	-2.454770	-2.556453
H	0.867325	-0.052192	-5.507195	C	-4.939154	-5.139147	-2.289966
C	0.719998	3.729372	1.411238	H	-2.850415	-5.046893	-1.621344
C	1.485075	4.879663	1.133804	H	-7.013813	-4.939782	-2.901984
C	-0.536373	3.877971	2.034873	H	-4.925518	-6.228266	-2.448875
C	1.007100	6.156215	1.473577				
H	2.467635	4.768459	0.647758				

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Ir	-0.197763	-0.730665	-1.451161
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C	0.047106	-0.780696	2.109265
C	0.750115	-1.943122	2.441717
C	2.141431	-2.236374	1.923842
H	2.439166	-1.396217	1.256906
C	2.202936	-3.543612	1.103131
H	1.465603	-3.499803	0.275176
H	1.885778	-4.390984	1.750035
C	3.621335	-3.815115	0.578579
H	3.644734	-4.771484	0.013589
H	3.907251	-3.016864	-0.145575
C	4.651344	-3.839140	1.719847
H	4.441632	-4.708740	2.382668
H	5.672612	-3.998243	1.313707
C	4.586544	-2.547866	2.547906
H	4.893475	-1.683262	1.914488
H	5.308720	-2.583058	3.390657
C	3.169951	-2.298339	3.077346
H	2.886216	-3.122753	3.769080
H	3.125423	-1.366085	3.668737
C	0.133658	-2.859563	3.349303
H	0.665243	-3.788015	3.604151
C	-1.099177	-2.611292	3.924820
H	-1.541270	-3.339413	4.620860
C	-1.822879	-1.425837	3.607804
C	-3.111722	-1.135608	4.149589
H	-3.557231	-1.854512	4.854792
C	-3.807845	0.009261	3.784630
H	-4.807594	0.195586	4.206659
C	-3.248294	0.937762	2.853110
C	-4.001520	2.159986	2.369470
H	-3.376508	2.623946	1.569987
C	-5.357104	1.802923	1.719240
H	-5.197461	1.049088	0.917479
H	-6.013661	1.318175	2.476361
C	-6.053103	3.052339	1.159759
H	-7.032992	2.778149	0.715065
H	-5.437123	3.466559	0.328791
C	-6.232348	4.127079	2.243433
H	-6.702372	5.036669	1.813585
H	-6.936349	3.748805	3.019154
C	-4.892242	4.480144	2.908269
H	-5.039817	5.229768	3.714153
H	-4.228856	4.958747	2.150557
C	-4.190155	3.231640	3.467034
H	-4.794436	2.801380	4.297521
H	-3.203238	3.495280	3.905250
C	-1.979018	0.677014	2.346581
H	-1.566012	1.379058	1.611534
C	-1.240087	-0.493610	2.682332
C	1.100898	1.480530	2.086426

H	0.236744	1.817875	2.694264
C	1.388532	2.497338	0.966115
H	2.483061	2.626543	0.840426
N	0.889077	1.783672	-0.250980
C	1.259295	2.320377	-1.528412
C	0.351692	3.032131	-2.321093
C	-1.088500	3.245544	-1.915266
H	-1.236353	2.734418	-0.938736
C	-2.086441	2.635362	-2.925647
H	-1.863981	1.553506	-3.062712
H	-1.937746	3.108260	-3.921980
C	-3.540107	2.838918	-2.471317
H	-4.237219	2.423757	-3.228795
H	-3.712328	2.257419	-1.536578
C	-3.853896	4.318756	-2.199361
H	-4.893803	4.426162	-1.824170
H	-3.807184	4.886500	-3.156145
C	-2.852907	4.923328	-1.204644
H	-2.968470	4.426929	-0.213466
H	-3.065347	6.000135	-1.036383
C	-1.407689	4.741001	-1.685123
H	-0.692244	5.165902	-0.955595
H	-1.261409	5.300360	-2.636504
C	0.841755	3.611808	-3.534547
H	0.138720	4.164953	-4.175698
C	2.173980	3.525205	-3.904626
H	2.522318	4.000018	-4.835490
C	3.114028	2.818806	-3.095784
C	4.487509	2.659016	-3.453489
H	4.852579	3.141517	-4.374030
C	5.348172	1.893048	-2.679255
H	6.397639	1.774601	-2.990067
C	4.881493	1.228716	-1.502911
C	5.763046	0.285363	-0.712736
H	5.146408	-0.109408	0.128525
C	6.190586	-0.935553	-1.562523
H	6.770625	-0.580770	-2.444161
H	5.284138	-1.437415	-1.966396
C	7.042569	-1.918340	-0.746412
H	6.412533	-2.358223	0.058130
H	7.366481	-2.765559	-1.387213
C	8.257053	-1.223705	-0.110738
H	8.833740	-1.944049	0.506900
H	8.946941	-0.880331	-0.915053
C	7.829838	-0.014199	0.736170
H	8.717866	0.496934	1.164035
H	7.225132	-0.370596	1.602256
C	6.992325	0.979252	-0.084475
H	7.621669	1.415297	-0.892951
H	6.658065	1.832039	0.545073
C	3.555493	1.413321	-1.124158
H	3.183882	0.857415	-0.251632
C	2.645976	2.203140	-1.885606
C	-0.903231	-1.585526	-3.473026

H	-1.822743	-1.006037	-3.641071
C	-0.992439	-2.618268	-2.537141
H	-1.968550	-2.790002	-2.063076
C	-0.000068	-3.744553	-2.375605
H	-0.244000	-4.544354	-3.111774
H	-0.170175	-4.205983	-1.382259
C	1.482815	-3.326183	-2.506047
H	2.110391	-4.062509	-1.965607
H	1.806158	-3.376670	-3.565078
C	1.786418	-1.939526	-1.964930
H	2.356855	-1.895312	-1.024143
C	1.750805	-0.757372	-2.704897
H	2.361019	0.061182	-2.310168
C	1.336876	-0.576529	-4.146075
H	2.214004	-0.750340	-4.811504
H	1.074441	0.495640	-4.283869
C	0.150491	-1.468774	-4.563668
H	-0.326366	-1.043054	-5.469272
H	0.503100	-2.478716	-4.851129
C	0.795510	3.881640	1.126666
C	1.539016	4.985991	0.662944
C	-0.471645	4.106179	1.702361
C	1.032466	6.290772	0.779333
H	2.528563	4.816038	0.208730
C	-0.977431	5.409499	1.826503
H	-1.073410	3.263967	2.073273
C	-0.226564	6.505415	1.366150
H	1.625884	7.143506	0.415706
H	-1.964004	5.568657	2.287711
H	-0.623028	7.527352	1.466283
C	2.237346	1.204018	3.050623
C	1.924261	0.964430	4.404058
C	3.588684	1.172206	2.649033
C	2.939325	0.709150	5.340561
H	0.870416	0.985151	4.725196
C	4.605852	0.920254	3.582948
H	3.865806	1.357320	1.601008
C	4.284114	0.690481	4.932128
H	2.678925	0.528365	6.394594
H	5.655955	0.904810	3.253087
H	5.082108	0.496879	5.665152
N	-3.685959	-2.057105	-0.590960
C	-4.030124	-0.650799	-2.513896
C	-3.497513	-0.663155	-1.050205
C	-2.092925	-0.126958	-0.726581
H	-4.959470	-0.046209	-2.582348
H	-3.319228	-0.174128	-3.217725
H	-4.174571	-0.014116	-0.440570
H	-2.034527	-0.221125	0.370147
H	-2.105501	0.974509	-0.891867
H	-0.225264	-1.794404	-0.321842
C	-3.905157	-2.340167	0.812586
H	-4.993023	-2.476352	1.031006
H	-3.587992	-1.443447	1.385678

C	-3.143725	-3.544261	1.339115
C	-3.674719	-4.321455	2.387182
C	-1.736828	-5.796207	2.319157
C	-1.896430	-3.902321	0.798980
C	-1.201113	-5.023467	1.274958
H	-0.233723	-5.299383	0.827593
H	-1.490813	-3.287538	-0.016435
C	-2.973905	-5.434702	2.881055
H	-4.657224	-4.057410	2.811977
H	-1.197223	-6.681551	2.689566
H	-3.405984	-6.035676	3.696570
C	-4.324931	-2.105001	-2.815432
C	-4.715114	-2.732219	-3.999361
C	-4.192646	-2.853104	-1.616105
C	-4.996435	-4.117157	-3.988705
H	-4.819198	-2.150898	-4.929871
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C	-4.895644	-4.843889	-2.789488
H	-5.308528	-4.622338	-4.915018
H	-4.402607	-4.811005	-0.658938
H	-5.132126	-5.919580	-2.784493

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C	0.027123	-0.767133	2.106454
C	0.794603	-1.834713	2.583966
C	2.263112	-2.003217	2.260363
H	2.550402	-1.185919	1.561455
C	2.561860	-3.350996	1.570456
H	1.923526	-3.457135	0.671686
H	2.273197	-4.182074	2.252029
C	4.049707	-3.487779	1.215745
H	4.240309	-4.467851	0.728943
H	4.320451	-2.709098	0.464559
C	4.936179	-3.315218	2.460111
H	4.749100	-4.159721	3.161157
H	6.009888	-3.376210	2.182766
C	4.633472	-1.989408	3.172113
H	4.917238	-1.141579	2.507121
H	5.252103	-1.881774	4.087890
C	3.145734	-1.865352	3.522915
H	2.868798	-2.665789	4.245441
H	2.937718	-0.904694	4.027588
C	0.159067	-2.780506	3.448682
H	0.747031	-3.632338	3.822698
C	-1.158802	-2.639545	3.847874
H	-1.615549	-3.380022	4.523602
C	-1.948312	-1.544076	3.390841
C	-3.321617	-1.389027	3.738480
H	-3.784891	-2.135788	4.402295
C	-4.080109	-0.342437	3.233809

H	-5.145762	-0.271290	3.494366	H	6.513491	1.807126	-2.643970
C	-3.496826	0.626248	2.366333	C	4.909244	1.279957	-1.245216
C	-4.282755	1.790539	1.795259	C	5.786506	0.491374	-0.296433
H	-3.776919	2.073641	0.839993	H	5.113936	0.039238	0.469820
C	-5.748753	1.463443	1.453696	C	6.509881	-0.676458	-1.006311
H	-5.807983	0.549549	0.830437	H	7.160957	-0.269012	-1.812350
H	-6.302024	1.229600	2.390786	H	5.759029	-1.324365	-1.508699
C	-6.429259	2.654279	0.763627	C	7.364243	-1.491004	-0.024761
H	-7.481428	2.401724	0.514508	H	6.692540	-1.992618	0.706633
H	-5.917459	2.854875	-0.206809	H	7.897581	-2.301346	-0.565091
C	-6.369574	3.914456	1.641485	C	8.358625	-0.600354	0.736251
H	-6.824600	4.780586	1.115949	H	8.934450	-1.203572	1.469393
H	-6.980828	3.747445	2.557265	H	9.104329	-0.185455	0.020136
C	-4.924315	4.239790	2.052091	C	7.640675	0.559193	1.444673
H	-4.899149	5.117774	2.732481	H	8.372505	1.214792	1.962050
H	-4.349576	4.527962	1.141994	H	6.974140	0.145790	2.236774
C	-4.229014	3.038069	2.712398	C	6.796530	1.384722	0.461672
H	-4.726273	2.790379	3.677260	H	7.464924	1.885444	-0.275115
H	-3.175139	3.283354	2.965619	H	6.252933	2.197688	0.990263
C	-2.149286	0.492097	2.035654	C	3.546112	1.404989	-0.991207
H	-1.711839	1.231390	1.351669	H	3.137670	0.896571	-0.106191
C	-1.345342	-0.583442	2.502647	C	2.661403	2.078341	-1.883900
C	0.890539	1.576352	2.010745	C	-0.621369	-1.501583	-3.591016
H	-0.055829	1.876425	2.505658	H	-1.643392	-1.092313	-3.675545
C	1.203309	2.532769	0.844974	C	-0.487929	-2.706910	-2.898324
H	2.298034	2.696728	0.771803	H	-1.394043	-3.117868	-2.429702
N	0.803634	1.722281	-0.346440	C	0.659063	-3.691589	-3.039718
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C	0.373419	2.753995	-2.564153	H	0.246405	-4.710128	-2.902313
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H	-1.343556	2.418921	-1.349043	H	1.480192	-3.974372	-1.060523
C	-2.022593	2.438656	-3.405691	H	2.713967	-3.990097	-2.330972
H	-1.800540	1.370889	-3.619840	C	2.081754	-2.026689	-1.707941
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C	-3.502035	2.626177	-3.034494	C	2.095633	-0.993971	-2.647917
H	-4.152533	2.246364	-3.850717	H	2.607412	-0.076096	-2.339260
H	-3.728505	2.004167	-2.139318	C	1.858316	-1.118202	-4.146497
C	-3.829399	4.093503	-2.717234	H	2.207955	-2.103218	-4.512196
H	-4.886988	4.188343	-2.391161	H	2.485587	-0.360106	-4.656783
H	-3.732177	4.701216	-3.645396	C	0.383988	-0.878492	-4.538702
C	-2.882299	4.651702	-1.645527	H	0.188490	0.216172	-4.570223
H	-3.065970	4.124316	-0.681526	H	0.188539	-1.241068	-5.574611
H	-3.089877	5.725364	-1.452946	C	0.559694	3.898784	0.908634
C	-1.411492	4.462357	-2.036304	C	1.316949	5.019166	0.511833
H	-0.740872	4.865547	-1.255656	C	-0.767324	4.088613	1.343226
H	-1.193376	5.035803	-2.965574	C	0.762196	6.308828	0.554338
C	0.933416	3.243167	-3.787265	H	2.353687	4.873289	0.168021
H	0.260930	3.701618	-4.527690	C	-1.319290	5.377139	1.401110
C	2.292869	3.193123	-4.046157	H	-1.382288	3.227932	1.644672
H	2.693205	3.603275	-4.986832	C	-0.556485	6.489961	1.005345
C	3.195894	2.613932	-3.105826	H	1.364078	7.175670	0.241484
C	4.600550	2.512408	-3.339779	H	-2.353593	5.512208	1.749993
H	5.013133	2.937582	-4.268475	H	-0.991522	7.500114	1.049609
C	5.435520	1.876367	-2.432262	C	1.947531	1.487051	3.091297

C	1.530523	1.355951	4.431198
C	3.328110	1.538861	2.808634
C	2.472602	1.289722	5.470937
H	0.453154	1.309053	4.656833
C	4.271568	1.478552	3.845720
H	3.682451	1.637132	1.772157
C	3.846254	1.356461	5.180171
H	2.132192	1.191281	6.513010
H	5.345367	1.527957	3.609043
H	4.586259	1.312806	5.993851
N	-3.285232	-2.168090	0.025714
C	-4.483845	-0.689210	-1.399838
C	-3.100859	-1.383710	-1.215195
H	-4.432089	0.352853	-1.006749
H	-4.772033	-0.616627	-2.467581
C	-2.288561	-3.061057	0.547984
H	-2.589731	-3.340282	1.577874
H	-1.334021	-2.501437	0.679060
C	-2.004296	-4.323068	-0.247983
C	-2.910607	-4.828960	-1.199789
C	-1.408555	-6.692311	-1.671212
C	-0.802695	-5.020948	-0.008262
C	-0.507000	-6.201180	-0.708604
H	0.432134	-6.740299	-0.506462
H	-0.100030	-4.633541	0.748145
C	-2.610025	-6.003447	-1.912985
H	-3.862490	-4.304469	-1.376413
H	-1.177879	-7.614871	-2.225926
H	-3.325331	-6.388396	-2.656428
C	-1.954854	-0.365010	-1.152771
H	-2.100736	0.210292	-0.222987
H	-0.103168	-1.971458	-0.426333
H	-2.123880	0.350543	-1.988509
H	-2.954066	-2.086433	-2.071304
C	-5.423945	-1.508421	-0.549064
C	-6.815825	-1.495328	-0.439527
C	-4.641992	-2.325014	0.305165
C	-7.440287	-2.306268	0.533685
H	-7.419861	-0.856287	-1.103417
C	-5.253315	-3.144984	1.271758
C	-6.657548	-3.116295	1.376162
H	-8.536525	-2.311680	0.626244
H	-4.659096	-3.802624	1.922701
H	-7.149689	-3.756252	2.125352

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E= -3486.75741735 A.U.

Ir	0.036344	-1.421656	-0.985805
C	0.767370	0.264557	-0.075704
N	0.886177	0.543769	1.253140
C	0.261727	-0.121399	2.362997
C	0.952650	-1.069007	3.125146
C	2.350848	-1.524821	2.776250
H	2.646556	-1.004054	1.838686

C	2.418007	-3.042275	2.510528
H	1.649865	-3.313863	1.758525
H	2.147793	-3.591380	3.440045
C	3.826231	-3.464211	2.065287
H	3.863423	-4.559087	1.881076
H	4.064283	-2.975395	1.091773
C	4.884598	-3.053635	3.102231
H	4.723730	-3.636925	4.036957
H	5.901233	-3.319824	2.742311
C	4.799634	-1.553547	3.422241
H	5.076459	-0.966465	2.516136
H	5.537330	-1.275886	4.204430
C	3.386286	-1.146017	3.858967
H	3.126965	-1.665604	4.808948
H	3.335908	-0.062560	4.070660
C	0.306236	-1.589776	4.288891
H	0.830848	-2.349569	4.887800
C	-0.941391	-1.144631	4.695770
H	-1.407541	-1.553478	5.605803
C	-1.643156	-0.153946	3.949703
C	-2.940320	0.315589	4.316655
H	-3.413622	-0.092515	5.221613
C	-3.619140	1.236709	3.534371
H	-4.630330	1.553838	3.829208
C	-3.033568	1.750779	2.337746
C	-3.775467	2.706603	1.427406
H	-3.160003	2.816771	0.503005
C	-5.146084	2.148114	0.989172
H	-4.995457	1.150028	0.530312
H	-5.778524	1.984347	1.889550
C	-5.865608	3.102920	0.026722
H	-6.861609	2.692605	-0.244645
H	-5.286799	3.166560	-0.922521
C	-6.006725	4.509928	0.628306
H	-6.493455	5.195915	-0.096696
H	-6.679751	4.462451	1.514552
C	-4.642574	5.069374	1.062680
H	-4.759474	6.073188	1.523135
H	-4.005716	5.209586	0.158357
C	-3.925879	4.119678	2.035655
H	-4.503258	4.048385	2.985194
H	-2.924924	4.516620	2.312305
C	-1.754770	1.326356	1.991254
H	-1.324150	1.698907	1.051351
C	-1.030843	0.369140	2.758975
C	1.338613	1.953029	1.517722
H	0.472877	2.484666	1.961214
C	1.627556	2.490345	0.106395
H	2.722232	2.567005	-0.057254
N	1.140453	1.375760	-0.765768
C	1.497375	1.434628	-2.148694
C	0.572620	1.811822	-3.122867
C	-0.864378	2.130786	-2.775015
H	-0.970067	2.025320	-1.673113

C	-1.864741	1.148326	-3.422095	H	2.742498	-4.479163	-1.295670
H	-1.597857	0.108369	-3.130480	C	1.987774	-2.478634	-1.097457
H	-1.768835	1.193310	-4.530245	H	2.666571	-1.975962	-0.385355
C	-3.307219	1.483951	-3.015329	C	1.761648	-1.828358	-2.337716
H	-4.018768	0.790283	-3.511059	H	2.293869	-0.882937	-2.477921
H	-3.420145	1.322015	-1.917599	C	1.344196	-2.509330	-3.637737
C	-3.669122	2.940224	-3.345459	H	1.765587	-3.533429	-3.689861
H	-4.704036	3.162736	-3.010020	H	1.799612	-1.951642	-4.480172
H	-3.663709	3.076029	-4.450622	C	-0.190305	-2.532850	-3.830896
C	-2.669123	3.914863	-2.709042	H	-0.515598	-1.575916	-4.290375
H	-2.744452	3.848371	-1.599609	H	-0.488807	-3.328789	-4.551822
H	-2.917493	4.964359	-2.972795	C	1.034280	3.837850	-0.253159
C	-1.230420	3.589732	-3.128951	C	1.764300	4.677246	-1.119699
H	-0.512905	4.278913	-2.644340	C	-0.214466	4.279363	0.229802
H	-1.123831	3.740991	-4.226871	C	1.262980	5.935223	-1.490982
C	1.040154	1.923238	-4.470714	H	2.740677	4.338461	-1.501947
H	0.325425	2.213031	-5.256180	C	-0.715377	5.539046	-0.134735
C	2.367459	1.703275	-4.806124	H	-0.805820	3.649459	0.909799
H	2.699336	1.814719	-5.850538	C	0.021955	6.370936	-0.995117
C	3.322304	1.320127	-3.815649	H	1.846725	6.580469	-2.165104
C	4.688106	1.023484	-4.109740	H	-1.687690	5.871998	0.258985
H	5.044835	1.145267	-5.144867	H	-0.370387	7.359835	-1.277500
C	5.553259	0.565265	-3.124282	C	2.476509	2.055893	2.512897
H	6.597127	0.332674	-3.385625	C	2.171479	2.365707	3.853645
C	5.099851	0.359394	-1.783958	C	3.824993	1.865216	2.147256
C	5.996133	-0.208660	-0.704123	C	3.192938	2.495775	4.808915
H	5.350995	-0.390120	0.187916	H	1.119468	2.511843	4.146888
C	6.618311	-1.569932	-1.087336	C	4.848358	1.999955	3.098200
H	7.256609	-1.441689	-1.990562	H	4.093316	1.621017	1.108990
H	5.812018	-2.280387	-1.371682	C	4.535193	2.318217	4.431302
C	7.465974	-2.137724	0.061666	H	2.939657	2.742037	5.851362
H	6.797043	-2.368470	0.921946	H	5.896388	1.855408	2.794640
H	7.925218	-3.101719	-0.243049	H	5.338223	2.427491	5.176169
C	8.546226	-1.142988	0.514229	C	-2.972191	-2.051170	0.228526
H	9.118701	-1.557275	1.370684	C	-1.953402	-0.990480	-0.194091
H	9.280051	-0.998565	-0.311275	H	-1.994704	-0.169950	0.535272
C	7.933792	0.216598	0.886955	H	-0.697354	-1.730540	0.418293
H	8.727093	0.937599	1.176786	H	-2.218668	-0.557686	-1.189133
H	7.282137	0.087898	1.782345	H	-3.044225	-2.844170	-0.544404
C	7.091455	0.790038	-0.263133	C	-4.804558	-1.607468	1.654701
H	7.748978	1.018715	-1.132541	C	-6.020804	-1.151629	2.198511
H	6.621169	1.753139	0.031735	C	-3.892146	-2.342631	2.451877
C	3.782213	0.682634	-1.479298	C	-6.305650	-1.449884	3.545612
H	3.416370	0.477754	-0.463047	H	-6.736414	-0.573644	1.595337
C	2.873430	1.175222	-2.458313	C	-4.188962	-2.634278	3.783505
C	-0.960882	-2.709125	-2.538226	C	-5.406062	-2.182928	4.339328
H	-2.015768	-2.381281	-2.577097	H	-7.256505	-1.102122	3.979106
C	-0.613415	-3.581393	-1.495559	H	-3.478383	-3.214669	4.393489
H	-1.402390	-3.827948	-0.769659	H	-5.654042	-2.411850	5.386651
C	0.557119	-4.550081	-1.528932	C	-2.675375	-2.684541	1.625075
H	0.744540	-4.864412	-2.574318	H	-1.749248	-2.259001	2.071460
H	0.268627	-5.469595	-0.981836	N	-4.302162	-1.420366	0.367162
C	1.837578	-3.968602	-0.891698	C	-5.133709	-1.219406	-0.814450
H	1.833442	-4.179116	0.192765	H	-6.171322	-1.041721	-0.466093

H	-4.827349	-0.304680	-1.367909
C	-5.093948	-2.412192	-1.755833
C	-4.575271	-2.289312	-3.059142
C	-5.498101	-3.685790	-1.299873
C	-4.458891	-3.413760	-3.896706
H	-4.260194	-1.297363	-3.421174
C	-5.379066	-4.809960	-2.130529
H	-5.896786	-3.792691	-0.277745
C	-4.854874	-4.677606	-3.431021
H	-4.055365	-3.300723	-4.915224
H	-5.700369	-5.797883	-1.765181
H	-4.763491	-5.560953	-4.081826
H	-2.514382	-3.781381	1.554103

29_D_E_R

E= -3486.76374093 A.U.

Ir	0.026932	-0.849433	-1.544918
C	0.605288	0.402168	-0.059057
N	0.651881	0.253531	1.293292
C	0.013471	-0.770703	2.077349
C	0.728480	-1.876577	2.553729
C	2.196018	-2.105938	2.261873
H	2.521409	-1.324953	1.538062
C	2.478051	-3.491298	1.640291
H	1.840447	-3.646761	0.749628
H	2.187223	-4.282298	2.366898
C	3.965526	-3.655156	1.293992
H	4.147714	-4.654991	0.845935
H	4.243520	-2.908264	0.513609
C	4.851170	-3.445122	2.533089
H	4.659384	-4.265681	3.260835
H	5.925192	-3.518900	2.259791
C	4.553851	-2.095873	3.202100
H	4.852957	-1.271225	2.515070
H	5.163708	-1.966213	4.120917
C	3.063757	-1.943932	3.533013
H	2.766147	-2.721257	4.272605
H	2.863023	-0.968549	4.009841
C	0.042916	-2.802074	3.402339
H	0.592398	-3.679553	3.775168
C	-1.273419	-2.613330	3.785377
H	-1.769580	-3.342137	4.445771
C	-2.010231	-1.482051	3.329932
C	-3.382829	-1.280550	3.655737
H	-3.886448	-2.021066	4.296768
C	-4.091549	-0.196296	3.158751
H	-5.158367	-0.089457	3.401009
C	-3.453514	0.767567	2.325798
C	-4.179633	1.979596	1.774326
H	-3.668924	2.246195	0.816719
C	-5.666379	1.742139	1.448825
H	-5.787838	0.840065	0.817005
H	-6.219699	1.529388	2.390805
C	-6.285809	2.979148	0.782985

H	-7.354127	2.791284	0.545986
H	-5.776528	3.162787	-0.192144
C	-6.141437	4.221950	1.676063
H	-6.552708	5.119550	1.167689
H	-6.749465	4.078004	2.597910
C	-4.674785	4.458518	2.071181
H	-4.590850	5.323712	2.763044
H	-4.096105	4.726730	1.157476
C	-4.041974	3.210047	2.705910
H	-4.539432	2.977542	3.674450
H	-2.972325	3.390009	2.947394
C	-2.106850	0.585203	2.012155
H	-1.628343	1.321205	1.351165
C	-1.354526	-0.533729	2.465463
C	0.979483	1.543037	1.997327
H	0.042711	1.886843	2.481443
C	1.352560	2.482499	0.834763
H	2.454313	2.599702	0.780007
N	0.939789	1.687856	-0.360427
C	1.388674	2.121603	-1.653400
C	0.523868	2.731923	-2.569092
C	-0.936985	2.981527	-2.265118
H	-1.168061	2.473942	-1.302380
C	-1.897426	2.427037	-3.340725
H	-1.695299	1.349137	-3.519365
H	-1.698803	2.934401	-4.310937
C	-3.363022	2.655090	-2.940037
H	-4.042632	2.249351	-3.719291
H	-3.574151	2.079864	-2.009957
C	-3.658020	4.140387	-2.679808
H	-4.706550	4.268810	-2.336168
H	-3.570367	4.705420	-3.635396
C	-2.678193	4.724718	-1.652341
H	-2.853033	4.242440	-0.663374
H	-2.862417	5.809281	-1.501659
C	-1.219159	4.490312	-2.062944
H	-0.525229	4.906416	-1.309239
H	-1.007621	5.026915	-3.015335
C	1.083066	3.192821	-3.802734
H	0.417097	3.667875	-4.538929
C	2.436557	3.088139	-4.080815
H	2.837507	3.471529	-5.032428
C	3.331486	2.486429	-3.146670
C	4.728925	2.327735	-3.395305
H	5.145992	2.723282	-4.335067
C	5.551753	1.673523	-2.488731
H	6.623465	1.560571	-2.713702
C	5.019399	1.116984	-1.284856
C	5.870996	0.314561	-0.324029
H	5.179207	-0.112090	0.440355
C	6.571802	-0.880196	-1.009693
H	7.250839	-0.500743	-1.806320
H	5.812254	-1.511288	-1.520100
C	7.383064	-1.708771	-0.003075

H	6.683450	-2.182664	0.721527
H	7.901883	-2.540825	-0.524243
C	8.390326	-0.838910	0.765205
H	8.934840	-1.449792	1.515752
H	9.160447	-0.456029	0.057091
C	7.696355	0.351209	1.446136
H	8.438895	0.990632	1.968513
H	7.003673	-0.032095	2.231225
C	6.893865	1.188877	0.438700
H	7.587696	1.661753	-0.293154
H	6.364892	2.023013	0.948816
C	3.665482	1.297181	-1.018159
H	3.251410	0.821082	-0.117960
C	2.794371	1.986722	-1.911089
C	-0.591144	-1.420602	-3.635568
H	-1.565023	-0.923228	-3.798765
C	-0.613376	-2.622913	-2.915287
H	-1.582295	-2.954190	-2.512583
C	0.451960	-3.702194	-2.962758
H	0.957332	-3.697656	-3.947584
H	-0.049296	-4.685093	-2.866378
C	1.467606	-3.550606	-1.815950
H	1.025008	-3.992098	-0.901427
H	2.395670	-4.132543	-2.023406
C	1.828172	-2.115510	-1.519799
H	2.325838	-1.958908	-0.547556
C	2.022321	-1.094393	-2.490004
H	2.661939	-0.268450	-2.158568
C	1.937267	-1.246401	-4.006061
H	2.275296	-2.255503	-4.315854
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29_E

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