

## Supplementary Information

### **Chiral distinction of D- and L-isoleucine by permethylated $\beta$ -cyclodextrin: IRMPD spectroscopy, ion-mobility, and DFT methods**

Sung-Sik Lee<sup>1#</sup>, Jae-ung Lee<sup>2</sup>, Ju Hyeon Oh<sup>1</sup>, Soojin Park<sup>2</sup>, Yin Hong<sup>3</sup>, Byung-ki Min<sup>1</sup>, Hyun Hee Lee<sup>4</sup>, Hugh I. Kim<sup>4</sup>, Xianglei Kong<sup>3</sup>, Sungyul Lee<sup>\*1</sup> and Han Bin Oh<sup>\*2</sup>

<sup>1</sup>Department of Applied Chemistry, Kyung Hee University, Gyeonggi 17104, Republic of Korea

<sup>2</sup>Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea

<sup>3</sup>State Key Laboratory of Elemento-Organic Chemistry, Nankai University, Tianjin 300071, China

<sup>4</sup>Department of Chemistry, Korea University, Seoul 02841, Republic of Korea

**Key words:** IRMPD spectroscopy, cyclodextrin, amino acid, chirality, isoleucine, ion mobility

Corresponding authors: Prof. Han Bin Oh, [hanbinoh@sogang.ac.kr](mailto:hanbinoh@sogang.ac.kr) and Prof. Sungyul Lee, [sylee@khu.ac.kr](mailto:sylee@khu.ac.kr)

**Table S1.** Calculated cross sections of perCD/H<sup>+</sup>/*D*-Ile and *L*-Ile. The cross-sections were calculated using four different methods: projection approximation (PA), exact hard-spheres scattering (EHSS), trajectory method (TM), and modified trajectory method (MTM).

		Calculated cross section (Å <sup>2</sup> )				
		PA	EHSS	TM	MTM	
perCD/H <sup>+</sup> / <i>D</i> -Ile	292.9	D-1	293.8 (0.3 %)	353.5 (21 %)	342.6 (17 %)	323.8 (11 %)
		D-4	273.2 (-6.7 %)	325.5 (11 %)	314.0 (7.9 %)	299.4 (2.2 %)
perCD/H <sup>+</sup> / <i>L</i> -Ile	294.8	L-1	295.5 (0.2 %)	361.1 (23 %)	346.7 (18 %)	328.6 (11 %)
		L-4	272.8 (-7.5 %)	328.8 (12 %)	316.9 (8.0 %)	297.6 (0.9 %)

## XYZ Coordinates

(D-1)

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C	4.737697	-2.174785	-1.348242
C	5.912920	-1.647550	-0.536305
C	5.712799	-0.175859	-0.216630
C	4.455117	-0.090413	-2.471455
C	4.508992	0.437963	-3.906473
O	6.107167	-2.443231	0.636636
O	6.869391	0.281937	0.438803
O	4.715196	-1.499763	-2.565231
O	5.807784	0.712419	-4.378130
H	4.875861	-3.234023	-1.577332
H	6.801944	-1.754997	-1.169092
H	4.835923	-0.074012	0.437534
H	3.440308	0.060410	-2.084244
H	4.008848	-0.303961	-4.547451
H	3.957151	1.374502	-3.961276
C	0.348575	-4.618993	0.057822
C	1.158474	-4.074636	1.250740
C	1.828949	-2.781417	0.794130
C	2.787123	-3.136725	-0.338381
C	1.912881	-3.655435	-1.496357
C	2.668274	-4.068858	-2.739699
O	0.413780	-3.784901	2.409076
O	2.494497	-2.153020	1.880734
O	3.526724	-1.979386	-0.651525
O	1.189207	-4.799812	-1.046877
O	3.699174	-4.965763	-2.399597
H	-0.057875	-5.614078	0.246081
H	1.921708	-4.841607	1.485324
H	1.047676	-2.111530	0.417904
H	3.470325	-3.936225	-0.019241
H	1.219435	-2.850643	-1.767242
H	1.956416	-4.541893	-3.433092
H	3.077536	-3.170613	-3.225407
C	-3.895701	-4.847700	-1.697378
C	-2.755249	-4.803914	-0.675019
C	-1.603457	-3.927798	-1.173849
C	-2.131563	-2.558346	-1.610219
C	-1.113870	-1.630020	-2.259128
O	-4.948547	-5.560560	-1.103381
O	-2.210503	-6.076127	-0.401145
O	-0.671441	-3.687965	-0.134092
O	-3.139212	-2.748992	-2.592448
O	-0.223778	-1.127130	-1.296524
H	-3.545706	-5.365452	-2.605085
H	-3.149073	-4.356918	0.251373
H	-1.109034	-4.422032	-2.020389
H	-2.544382	-2.046017	-0.732561
H	-1.677873	-0.808424	-2.725573
H	-0.571941	-2.152840	-3.066746
C	4.452460	-5.354065	-3.524717
H	4.934908	-4.486389	-4.000196
H	5.218938	-6.049117	-3.176848
H	3.823436	-5.859690	-4.271008

C	0.506977	-0.018778	-1.776971
H	-0.150925	0.840411	-1.962956
H	1.232272	0.247978	-1.004315
H	1.052759	-0.262182	-2.699317
C	6.569937	-0.419632	-4.727991
H	7.451554	-0.055476	-5.260000
H	6.891052	-0.995799	-3.849722
H	6.001674	-1.091510	-5.387135
C	-0.472114	-4.809342	2.816376
H	-0.894855	-4.495701	3.772545
H	-1.282848	-4.941286	2.092782
H	0.051264	-5.770507	2.944278
C	2.261918	-0.746630	1.952336
H	1.191931	-0.543463	2.068253
H	2.804611	-0.376599	2.824038
H	2.637926	-0.257395	1.049881
C	7.491072	-2.714662	0.873646
H	8.058039	-1.781885	0.906355
H	7.561219	-3.220359	1.836284
H	7.883149	-3.373897	0.091086
C	6.648996	1.240741	1.465509
H	5.947993	0.851328	2.214967
H	7.618899	1.400167	1.941743
H	6.282400	2.185852	1.058104
C	-6.136629	-5.640221	-1.862065
H	-6.735957	-6.439213	-1.421731
H	-6.708052	-4.705313	-1.807983
H	-5.929217	-5.887199	-2.912826
C	-2.931602	-6.882433	0.509724
H	-2.251355	-7.679141	0.821696
H	-3.239339	-6.303244	1.393530
H	-3.824460	-7.314178	0.052559
C	4.253022	-3.609156	3.619971
H	4.283674	-3.850402	2.555722
C	5.089789	-4.588464	4.462054
H	5.012430	-4.253160	5.505091
C	6.563306	-4.515149	4.055802
H	6.967439	-3.504523	4.168386
H	7.157671	-5.179160	4.688973
H	6.704662	-4.830376	3.017080
C	4.552247	-6.033327	4.386593
H	5.242568	-6.662901	4.958000
H	3.598244	-6.115844	4.927640
C	4.392932	-6.608688	2.977619
H	5.329349	-6.567750	2.413636
H	4.087372	-7.656946	3.028974
H	3.631959	-6.080923	2.388693
C	4.649923	-2.144747	3.876731
O	5.424880	-1.527088	3.019915
H	5.534498	-1.958035	2.125808
O	4.238408	-1.618409	4.888598
H	2.764774	-3.150132	4.952332
H	2.445793	-4.588386	4.136818
H	2.254440	-3.115417	3.346776
N	2.821310	-3.643925	4.051625
C	-6.738185	0.636964	-0.039357
C	-7.454593	-0.624113	0.431514
C	-6.535487	-1.825560	0.258653
C	-5.911783	-1.888153	-1.135772

C	-5.462501	-0.518904	-1.685071
C	-5.264853	-0.526041	-3.204807
O	-7.819131	-0.446223	1.778298
O	-7.273286	-3.003993	0.509318
O	-4.818455	-2.788537	-0.985296
O	-6.430896	0.489523	-1.407231
O	-6.209060	-1.280637	-3.924468
H	-7.397120	1.504531	0.037167
H	-8.346931	-0.751689	-0.198149
H	-5.719689	-1.722175	0.983484
H	-6.651312	-2.319091	-1.821244
H	-4.511843	-0.247855	-1.205961
H	-5.264830	0.520276	-3.546776
H	-4.295786	-0.974445	-3.431061
C	-3.403999	4.157137	1.916766
C	-3.745130	3.130601	2.992513
C	-4.260342	1.816818	2.403965
C	-5.349540	2.068505	1.351089
C	-4.879652	3.140370	0.351938
C	-5.926811	3.566993	-0.674973
O	-2.611192	2.923614	3.797971
O	-4.715163	1.067982	3.503612
O	-5.567817	0.819528	0.709337
O	-4.491957	4.325067	1.044168
O	-7.220747	3.773015	-0.162827
H	-3.241399	5.131588	2.380090
H	-4.563539	3.567285	3.583910
H	-3.421056	1.302726	1.909061
H	-6.267741	2.394472	1.854498
H	-4.012036	2.731332	-0.185263
H	-5.554684	4.479599	-1.166822
H	-6.031229	2.782629	-1.428476
C	0.941170	5.806106	-0.460665
C	0.457028	6.319116	0.905357
C	-0.423136	5.284812	1.600530
C	-1.528045	4.824992	0.651777
C	-0.941197	4.362646	-0.682129
C	-1.994713	3.995667	-1.724336
O	1.506347	6.664465	1.765998
O	-1.024804	5.854308	2.739441
O	-2.252789	3.754968	1.225970
O	-0.164848	5.420543	-1.244573
O	-2.024751	2.592287	-1.872310
H	1.415371	6.614005	-1.027885
H	-0.172139	7.201392	0.703831
H	0.183775	4.411652	1.876307
H	-2.199588	5.671932	0.451412
H	-0.309564	3.480721	-0.511448
H	-1.721983	4.473436	-2.677219
H	-2.986169	4.370523	-1.428690
C	5.150302	2.961231	-1.966880
C	5.433840	4.220464	-1.134267
C	4.203626	4.627461	-0.321838
C	2.929214	4.646864	-1.166541
C	2.813385	3.375552	-2.014322
C	1.698989	3.419219	-3.034396
O	6.494758	4.073231	-0.226277
O	4.381888	5.913848	0.216785
O	1.839579	4.756795	-0.268769

O	4.013543	3.194154	-2.752395
O	1.583435	2.140557	-3.614311
H	5.948693	2.754935	-2.686958
H	5.659314	5.026944	-1.850069
H	4.056560	3.887105	0.477079
H	2.967223	5.520509	-1.832509
H	2.648318	2.519428	-1.347146
H	0.761162	3.713062	-2.551501
H	1.937634	4.172511	-3.802128
O	4.987021	1.875001	-1.096940
C	-7.382726	4.936781	0.621162
H	-6.974129	5.818524	0.108447
H	-8.457206	5.068850	0.764573
H	-6.890574	4.849218	1.596229
C	-2.981740	2.174885	-2.811642
H	-2.820563	2.644489	-3.794348
H	-2.879139	1.092384	-2.915579
H	-4.004897	2.404015	-2.479868
C	0.511684	2.070151	-4.520794
H	-0.443497	2.275069	-4.015046
H	0.636741	2.783681	-5.348288
H	0.493034	1.055731	-4.926214
C	-7.481596	-0.677361	-4.038044
H	-8.061917	-1.295433	-4.726092
H	-7.999710	-0.617733	-3.073581
H	-7.398681	0.339830	-4.446162
C	-2.877693	2.871919	5.182506
H	-1.915977	2.719559	5.679069
H	-3.311077	3.817361	5.542064
H	-3.555909	2.049424	5.430568
C	-4.820505	-0.329023	3.332755
H	-4.032034	-0.709402	2.667077
H	-4.693555	-0.778626	4.322671
H	-5.798193	-0.606245	2.929069
C	-9.069205	-1.001538	2.132145
H	-9.096422	-2.080459	1.948355
H	-9.207003	-0.804722	3.197235
H	-9.886957	-0.522060	1.574744
C	-6.631562	-3.942700	1.347290
H	-6.339005	-3.481927	2.302100
H	-7.363585	-4.729016	1.548207
H	-5.754971	-4.383293	0.860850
C	7.734855	3.743766	-0.809100
H	7.774305	2.685666	-1.103951
H	7.949737	4.374276	-1.683482
H	8.498087	3.920443	-0.048683
C	4.731915	5.926770	1.586357
H	3.896570	5.567650	2.201246
H	5.629427	5.327367	1.772826
H	4.939974	6.968142	1.841836
C	2.098384	7.912221	1.479697
H	2.748942	8.152926	2.322787
H	2.707478	7.874592	0.567578
H	1.336742	8.699354	1.384091
C	-0.443167	5.459400	3.964448
H	-0.998958	5.973939	4.752061
H	-0.543514	4.376261	4.106671
H	0.611688	5.751969	4.014859
C	5.453044	0.603980	-1.515043

H	6.417005	0.713900	-2.028843
C	-4.285543	-3.414125	-2.104912
H	-4.992743	-3.400091	-2.940462

**(D-1) Truncated**

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C	2.753657	-1.188798	0.469822
C	4.048533	-0.908380	-0.280183
C	4.086622	-1.719925	-1.568360
C	3.817393	-3.200071	-1.295248
C	2.580373	-3.411137	-0.402636
C	2.441637	-4.835515	0.139462
O	4.111287	0.476915	-0.515909
O	5.360489	-1.554012	-2.148663
O	2.661795	-2.558322	0.751119
O	3.667863	-5.455643	0.450338
H	2.749968	-0.669105	1.433404
H	4.881137	-1.230311	0.365451
H	3.299565	-1.342454	-2.238189
H	4.698116	-3.615847	-0.783598
H	1.680649	-3.155830	-0.981449
H	1.805044	-4.782897	1.037218
H	1.958344	-5.462771	-0.610094
C	-2.145107	0.639554	0.458266
C	-1.255364	1.532198	-0.388886
C	-0.040400	0.757963	-0.894459
C	0.693111	0.073319	0.270145
C	-0.281926	-0.739653	1.143312
C	0.338220	-1.330698	2.400899
O	-2.059000	2.039061	-1.417130
O	0.769156	1.693496	-1.550845
O	1.661771	-0.768174	-0.321080
O	-1.370884	0.136966	1.559919
O	1.157291	-0.427035	3.120394
H	-2.952004	1.227883	0.905812
H	-0.890788	2.349922	0.259109
H	-0.390803	-0.022035	-1.588588
H	1.180979	0.845498	0.883105
H	-0.710939	-1.552752	0.541132
H	-0.457875	-1.730554	3.047677
H	0.986660	-2.156985	2.099833
C	-6.378512	-2.185813	-0.512438
C	-6.379349	-0.659035	-0.313405
C	-5.007181	-0.107114	-0.684875
C	-3.934590	-0.849631	0.103854
C	-4.050181	-2.355261	-0.116855
C	-3.059104	-3.176665	0.696441
O	-7.336724	0.005253	-1.084732
O	-4.905152	1.272648	-0.392778
O	-2.649171	-0.398669	-0.296405
O	-5.356529	-2.752088	0.286602
O	-1.917031	-3.392873	-0.091160
H	-7.308536	-2.636584	-0.147432
H	-6.554674	-0.471532	0.762084
H	-4.830731	-0.280991	-1.755839
H	-4.077203	-0.666738	1.182357

H	-3.888041	-2.590207	-1.177032
H	-3.541327	-4.131574	0.956340
H	-2.797617	-2.667780	1.643855
C	0.498449	0.370668	4.060739
H	-0.129481	-0.228002	4.735754
H	1.267395	0.877789	4.648334
H	-0.133785	1.131425	3.563816
C	-1.003878	-4.285564	0.507308
H	-1.501649	-5.219512	0.805717
H	-0.245456	-4.516718	-0.242520
H	-0.539542	-3.842194	1.402993
C	4.283462	-4.967022	1.622902
H	5.109912	-5.640835	1.854790
H	4.669638	-3.947715	1.496174
H	3.575759	-4.958646	2.463106
C	-1.726645	3.346386	-1.848933
H	-2.468136	3.621377	-2.601225
H	-1.788173	4.060178	-1.013378
H	-0.723992	3.384569	-2.278943
C	1.626339	1.188966	-2.567281
H	1.146695	0.361981	-3.105548
H	1.799874	2.011006	-3.265534
H	2.575676	0.855240	-2.143912
C	5.421427	1.018247	-0.499266
H	6.054220	0.553118	-1.258968
H	5.320251	2.086096	-0.699052
H	5.885216	0.881826	0.487226
C	5.358766	-1.402007	-3.560229
H	4.714306	-0.562832	-3.856035
H	6.387335	-1.174298	-3.847702
H	5.037701	-2.319125	-4.061033
C	-8.672131	-0.270229	-0.706010
H	-9.300984	0.472552	-1.198992
H	-8.985954	-1.263170	-1.043224
H	-8.797106	-0.177951	0.382050
C	-5.155236	2.108393	-1.515002
H	-5.012093	3.139256	-1.181224
H	-4.434805	1.892905	-2.311689
H	-6.178288	1.973441	-1.874906
C	1.559732	4.065979	0.322817
H	0.979423	3.155891	0.186929
C	2.102456	4.187206	1.762704
H	2.848250	4.990595	1.768916
C	2.795292	2.887946	2.188247
H	3.579521	2.576828	1.496274
H	3.270263	3.036752	3.159182
H	2.085897	2.063166	2.293318
C	0.988301	4.568507	2.762666
H	1.400725	4.413209	3.762008
H	0.787062	5.647957	2.724909
C	-0.320293	3.785970	2.626806
H	-0.145562	2.721592	2.463835
H	-0.920262	3.883203	3.531994
H	-0.950628	4.135082	1.800916
C	2.659020	4.144089	-0.746184
O	3.375643	3.084863	-1.000098
H	3.070743	2.243623	-0.611889
O	2.849773	5.196323	-1.306034
H	1.311365	5.864964	-0.578589



H	0.316392	5.710906	0.792686
H	-0.091523	4.945530	-0.625261
N	0.686776	5.237107	-0.030036
H	-6.229135	-2.392637	-1.551577
H	3.713596	-3.651458	-2.259806

**(L-1)**

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H	4.343636	-3.700682	0.484070
C	5.042190	-1.674399	-1.457135
C	6.195710	-0.684024	-1.334201
C	5.652526	0.674566	-0.909170
C	3.556168	0.039810	-2.201263
C	2.720275	0.356936	-3.424767
O	7.188224	-1.176646	-0.440906
O	6.705874	1.608282	-0.840126
O	4.175509	-1.231058	-2.448849
O	3.580652	0.631709	-4.498111
H	5.419755	-2.652710	-1.773866
H	6.637590	-0.595109	-2.333785
H	5.163206	0.581429	0.069846
H	2.894287	-0.041629	-1.328051
H	2.073859	-0.509099	-3.645119
H	2.072240	1.213946	-3.213384
C	1.204862	-4.329287	0.797090
C	1.950532	-3.576972	1.909403
C	2.756004	-2.436249	1.297124
C	3.650619	-2.914810	0.140429
C	2.704858	-3.566148	-0.898119
C	3.280115	-4.174728	-2.168279
O	1.118822	-3.018928	2.885270
O	3.560683	-1.813432	2.291582
O	4.408957	-1.762584	-0.206714
O	2.115938	-4.665352	-0.219164
O	2.189830	-4.715569	-2.869626
H	0.818446	-5.289612	1.139924
H	2.652308	-4.297035	2.367829
H	2.058777	-1.693168	0.889594
H	1.944263	-2.835386	-1.197585
H	3.765534	-3.409914	-2.782724
H	4.012093	-4.959031	-1.910791
C	-2.607215	-5.375861	-1.398928
C	-1.542053	-5.107967	-0.326950
C	-0.608720	-3.962130	-0.742010
C	-1.440908	-2.755626	-1.179650
C	-0.616081	-1.608043	-1.717906
O	-3.446960	-6.365754	-0.874134
O	-0.844116	-6.271232	0.067316
O	0.178507	-3.497642	0.356394
O	-2.328662	-3.150871	-2.210076
O	-1.453701	-0.492669	-1.833956
H	-2.132123	-5.731040	-2.329076
H	-2.069289	-4.788877	0.578643
H	0.046195	-4.271666	-1.565953
H	-2.005907	-2.387764	-0.314998
H	0.211497	-1.395719	-1.020342

H	-0.182208	-1.888696	-2.693036
C	2.898678	1.199565	-5.595962
H	2.148734	0.501914	-5.999553
H	2.397897	2.130280	-5.305496
H	3.647262	1.397559	-6.365937
C	2.557114	-5.238821	-4.123189
H	1.649906	-5.636309	-4.580921
H	2.979591	-4.461066	-4.776532
H	3.292409	-6.050511	-4.019970
C	-0.798736	0.612283	-2.403348
H	-1.503091	1.445323	-2.423683
H	0.081775	0.904762	-1.806401
H	-0.455108	0.396052	-3.424912
C	-4.580702	-6.669897	-1.655420
H	-4.318860	-6.812232	-2.714372
H	-4.987832	-7.603732	-1.262999
H	-5.349895	-5.891330	-1.569498
C	-0.233196	-7.026450	-0.960002
H	-0.981547	-7.513856	-1.596790
H	0.449974	-6.425533	-1.574437
H	0.346945	-7.801288	-0.454684
C	0.266522	-3.945796	3.525966
H	0.832053	-4.802459	3.920961
H	-0.204373	-3.415575	4.355034
H	-0.512389	-4.310323	2.845983
C	2.987640	-0.637236	2.864086
H	2.023192	-0.870063	3.317300
H	3.688540	-0.296424	3.628871
H	2.865763	0.138220	2.097064
C	8.520128	-0.909876	-0.872322
H	9.192780	-1.262350	-0.088009
H	8.736742	-1.456602	-1.797624
H	8.664806	0.160970	-1.031296
C	6.971855	2.070674	0.465532
H	7.243660	1.238510	1.135140
H	7.824863	2.747928	0.394177
H	6.114745	2.619520	0.869654
C	6.314056	-2.881573	2.927400
H	5.542267	-3.555764	2.548303
C	7.672590	-3.608193	2.875937
H	7.481282	-4.546718	3.409700
C	8.034829	-3.979941	1.434941
H	8.888579	-4.662862	1.432622
H	7.202406	-4.485489	0.932504
H	8.310399	-3.113247	0.828328
C	8.817008	-2.904239	3.629365
H	8.603479	-2.924777	4.704973
H	9.709572	-3.524827	3.494086
C	9.141351	-1.464130	3.220013
H	8.411848	-0.751886	3.621346
H	10.112447	-1.168269	3.625084
H	9.195513	-1.339148	2.132898
C	5.923864	-2.469203	4.337661
O	5.666297	-3.520546	5.104546
H	5.445225	-3.200797	5.995859
O	5.886778	-1.316650	4.703051
H	5.203477	-1.494237	1.915780
H	6.552029	-0.844477	2.661715
H	6.708341	-1.652628	1.191133

N	6.222259	-1.641136	2.110200
C	-6.721045	-0.722778	0.276400
C	-7.113849	-2.134694	0.697989
C	-5.928499	-3.077322	0.533435
C	-5.248683	-2.935420	-0.831449
C	-5.081670	-1.470222	-1.279627
C	-4.730076	-1.306111	-2.758602
O	-7.553639	-2.087448	2.033559
O	-6.381870	-4.402772	0.714406
O	-4.003078	-3.602394	-0.659330
O	-6.301412	-0.754991	-1.066696
O	-5.391236	-2.192427	-3.632306
H	-7.586498	-0.057539	0.319159
H	-7.926963	-2.459689	0.032637
H	-5.188965	-2.815596	1.300966
H	-5.851437	-3.472548	-1.574562
H	-4.280173	-1.007556	-0.690229
H	-4.945107	-0.260584	-3.030481
H	-3.664067	-1.488266	-2.889391
C	-4.334489	3.533879	2.111993
C	-4.415088	2.498740	3.232840
C	-4.639272	1.080554	2.709685
C	-5.771959	1.031201	1.673651
C	-5.581026	2.142863	0.627100
C	-6.713693	2.295739	-0.388504
O	-3.249320	2.583923	4.012963
O	-4.905307	0.295996	3.846027
O	-5.687259	-0.263554	1.101310
O	-5.451448	3.412351	1.267780
O	-8.012666	2.189167	0.139814
H	-4.394997	4.534849	2.544966
H	-5.298727	2.769732	3.830211
H	-3.715940	0.739403	2.215003
H	-6.735673	1.152892	2.183662
H	-4.658743	1.912185	0.073106
H	-6.577589	3.268719	-0.886852
H	-6.629676	1.505676	-1.137583
C	-0.322274	5.853684	-0.354192
C	-0.751350	6.246620	1.068701
C	-1.495077	5.102396	1.749340
C	-2.622918	4.596672	0.854804
C	-2.149973	4.331380	-0.578918
C	-3.324619	4.083131	-1.506416
O	0.321751	6.629233	1.884507
O	-2.083338	5.538300	2.951397
O	-3.139161	3.393269	1.396297
O	-1.450701	5.463649	-1.093508
O	-2.932859	3.236892	-2.563492
H	0.072828	6.724675	-0.888141
H	-1.460091	7.083791	0.960666
H	-0.798947	4.272581	1.932051
H	-3.407344	5.366247	0.821806
H	-1.495741	3.449850	-0.580813
H	-3.683895	5.049016	-1.892552
H	-4.139991	3.623465	-0.938655
C	4.007832	3.443916	-2.217428
C	4.214936	4.669017	-1.318499
C	3.015653	4.868715	-0.400358
C	1.722585	4.905636	-1.210393

C	1.633905	3.744963	-2.215008
C	0.537731	3.967358	-3.236188
O	5.372365	4.590497	-0.529137
O	3.134886	6.090609	0.284484
O	0.647491	4.848388	-0.292122
O	2.839425	3.610260	-2.965300
O	0.397566	2.802597	-4.011583
H	4.807673	3.363453	-2.960230
H	4.274375	5.543505	-1.985480
H	2.956438	4.028373	0.304413
H	1.701435	5.858171	-1.759967
H	1.438337	2.820569	-1.654906
H	-0.405250	4.215621	-2.735814
H	0.825360	4.821060	-3.872707
O	3.982056	2.288469	-1.417603
C	-8.436632	3.284918	0.922361
H	-8.277089	4.234716	0.392860
H	-9.505171	3.145450	1.099098
H	-7.910983	3.336432	1.882944
C	-4.029412	2.770966	-3.311296
H	-4.566513	3.596506	-3.800809
H	-3.638345	2.092921	-4.073456
H	-4.737421	2.218404	-2.675267
C	-0.570723	2.952542	-5.022763
H	-1.534628	3.257171	-4.596344
H	-0.255153	3.699047	-5.766939
H	-0.676448	1.982243	-5.513837
C	-6.759831	-1.915240	-3.831127
H	-7.093725	-2.548614	-4.656259
H	-7.362497	-2.130636	-2.940031
H	-6.915802	-0.859940	-4.097814
C	-3.468983	2.504627	5.404562
H	-2.491581	2.614808	5.881344
H	-4.121776	3.319605	5.751909
H	-3.913063	1.544981	5.686357
C	-4.716808	-1.099008	3.720164
H	-3.831916	-1.325804	3.107506
H	-4.554274	-1.482778	4.731780
H	-5.592058	-1.585028	3.280505
C	-8.631176	-2.949043	2.336229
H	-8.376806	-3.996331	2.144156
H	-8.850012	-2.809872	3.396977
H	-9.524964	-2.684746	1.752106
C	-5.560304	-5.211069	1.533110
H	-5.401191	-4.740773	2.514537
H	-6.097090	-6.151848	1.678559
H	-4.596416	-5.418999	1.058275
C	6.562944	4.894850	-1.219700
H	6.858863	4.087258	-1.902223
H	6.467023	5.833571	-1.782684
H	7.343133	5.020361	-0.465547
C	3.499399	5.957920	1.641643
H	2.697212	5.472664	2.211788
H	4.437509	5.400394	1.747079
H	3.643923	6.969724	2.026868
C	0.822820	7.919277	1.613822
H	1.482262	8.181790	2.443722
H	1.405651	7.942695	0.684464
H	0.010895	8.658752	1.561356

C	-1.362567	5.200476	4.117039
H	-1.962573	5.545441	4.962567
H	-1.237484	4.113231	4.193138
H	-0.384877	5.694557	4.137281
C	-3.312638	-4.060393	-1.774053
H	-3.984388	-4.180239	-2.629852
C	4.608919	1.131116	-1.926232
H	5.118890	1.351183	-2.870763

**(L-1) Truncated**

114

H	-1.104019	0.696439	-0.815026
C	-2.870306	-0.472960	0.373150
C	-3.729304	-0.658133	1.623154
C	-3.853469	-2.122953	2.021244
C	-4.182629	-3.030353	0.830096
C	-3.215374	-2.721522	-0.328834
C	-3.471883	-3.474391	-1.636126
O	-3.201887	0.099137	2.678311
O	-4.843245	-2.180113	3.018743
O	-3.334580	-1.328856	-0.641852
O	-4.817122	-3.805572	-1.877515
H	-3.001358	0.542293	-0.005152
H	-4.732299	-0.300384	1.353619
H	-2.883141	-2.437906	2.433724
H	-5.205931	-2.828728	0.497291
H	-2.190421	-2.931683	-0.003080
H	-3.072697	-2.851880	-2.448981
H	-2.917357	-4.411941	-1.622108
C	2.171405	0.891822	-0.382737
C	1.209039	1.823679	0.364880
C	0.027782	1.070643	0.963471
C	-0.591065	0.108572	-0.042888
C	0.480889	-0.750919	-0.720114
C	-0.088351	-1.612123	-1.820441
O	1.829743	2.542085	1.391931
O	-0.977444	1.974985	1.342439
O	-1.519759	-0.709669	0.647157
O	1.476690	0.088642	-1.301256
O	0.898560	-2.499188	-2.305508
H	2.860094	1.481166	-0.991663
H	0.799234	2.510750	-0.391061
H	0.377316	0.488171	1.826310
H	0.931260	-1.404640	0.029267
H	-0.925250	-2.178182	-1.405809
H	-0.462330	-0.976260	-2.636139
C	6.688157	-1.530517	0.701261
C	6.639395	-0.057028	0.267433
C	5.273177	0.553236	0.585086
C	4.143529	-0.337925	0.058573
C	4.343340	-1.786179	0.498075
C	3.277620	-2.693748	-0.102174
O	7.610908	0.747995	0.856476
O	5.134145	1.879473	0.125305
O	2.895346	0.114608	0.536857
O	5.630779	-2.220993	0.056560

O	3.803818	-4.001704	-0.288861
H	7.599707	-2.017348	0.337854
H	6.782691	-0.080851	-0.829076
H	5.172367	0.620046	1.670775
H	4.142309	-0.330959	-1.040068
H	4.315449	-1.847430	1.590076
H	2.424076	-2.748724	0.575047
H	2.910477	-2.311174	-1.059255
C	-5.605645	-2.728468	-2.341231
H	-5.657679	-1.913034	-1.612331
H	-5.201919	-2.325893	-3.279438
H	-6.605681	-3.121918	-2.521160
C	0.355910	-3.456030	-3.181461
H	1.177787	-4.084217	-3.530111
H	-0.388778	-4.084217	-2.672971
H	-0.119531	-2.983534	-4.051393
C	2.784811	-4.979665	-0.474229
H	3.250199	-5.843945	-0.954250
H	2.388833	-5.281325	0.495447
H	1.987017	-4.581711	-1.107221
C	8.941828	0.383521	0.562571
H	9.070275	0.186950	-0.512883
H	9.569634	1.229831	0.837922
H	9.257254	-0.486068	1.148581
C	5.600519	2.169679	-1.171112
H	6.695019	2.175565	-1.213836
H	5.209085	1.476185	-1.929335
H	5.239571	3.170350	-1.409595
C	2.518392	3.700139	0.970066
H	1.861445	4.354035	0.381429
H	2.827038	4.228256	1.871760
H	3.413674	3.446590	0.394627
C	-1.000230	2.293792	2.720498
H	-0.076630	2.793402	3.025264
H	-1.846455	2.965208	2.868047
H	-1.159554	1.389413	3.317182
C	-4.159891	0.825766	3.420126
H	-3.614362	1.346195	4.207981
H	-4.665342	1.571165	2.791606
H	-4.904367	0.161565	3.866493
C	-4.731052	-3.223050	3.965082
H	-3.686355	-3.351610	4.279641
H	-5.325113	-2.926523	4.830733
H	-5.101823	-4.171233	3.568348
C	-3.690398	3.212589	-1.153568
H	-4.761772	3.419385	-1.109490
C	-2.974401	4.386906	-1.829025
H	-3.171138	4.228924	-2.893781
C	-3.645798	5.706204	-1.432901
H	-3.130790	6.547726	-1.899655
H	-4.688532	5.731888	-1.757334
H	-3.628307	5.889785	-0.352537
C	-1.437822	4.423169	-1.677841
H	-1.029930	3.423593	-1.851201
H	-1.073189	5.033725	-2.507837
C	-0.877164	5.014462	-0.380531
H	-0.926379	4.330627	0.471455
H	0.181088	5.237154	-0.519444
H	-1.357907	5.957378	-0.111069

C	-3.523302	1.864081	-1.866593
O	-4.556130	1.070053	-1.585782
H	-4.343577	0.153377	-1.842549
O	-2.583407	1.565570	-2.542374
H	-2.305015	2.619838	0.448866
H	-3.276712	3.939646	0.755994
H	-3.919960	2.422023	0.787752
N	-3.267272	3.031130	0.289582
H	6.626952	-1.603154	1.767036
H	-4.154916	-4.015472	1.246838

**(D-2) Truncated**

114

C	-2.820486	-0.880266	-0.280511
C	-4.061590	-0.726110	0.587672
C	-4.078123	-1.804444	1.663023
C	-3.897691	-3.194503	1.052215
C	-2.717711	-3.246846	0.064069
C	-2.677685	-4.517110	-0.788456
O	-4.042669	0.572069	1.128893
O	-5.312299	-1.724424	2.339353
O	-2.811785	-2.153963	-0.864278
O	-3.947353	-5.003855	-1.157041
H	-2.837280	-0.157753	-1.102872
H	-4.939766	-0.862378	-0.063443
H	-3.241398	-1.617790	2.352708
H	-4.822112	-3.450420	0.513440
H	-1.779195	-3.163002	0.631400
H	-2.083567	-4.288486	-1.687755
H	-2.190936	-5.314945	-0.226858
C	2.159280	0.708985	-0.149783
C	1.358010	1.421817	0.925378
C	0.131394	0.601008	1.316397
C	-0.691470	0.224474	0.073745
C	0.197664	-0.408207	-1.014006
C	-0.511890	-0.677060	-2.332978
O	2.235202	1.653217	1.991669
O	-0.596985	1.395403	2.210741
O	-1.671623	-0.690538	0.518728
O	1.308071	0.497118	-1.288295
O	-1.318150	0.396040	-2.784155
H	2.972236	1.351420	-0.501770
H	1.004233	2.377682	0.498007
H	0.475163	-0.327969	1.797874
H	-1.168821	1.132875	-0.322418
H	0.613713	-1.351760	-0.633987
H	0.230628	-0.951545	-3.098027
H	-1.185925	-1.524332	-2.185763
C	6.286448	-2.422874	-0.081763
C	6.354862	-0.891630	0.064099
C	5.032020	-0.385044	0.628821
C	3.886225	-0.889408	-0.241034
C	3.936074	-2.409412	-0.367923
C	2.866411	-2.988193	-1.284012

O	7.380921	-0.455090	0.906372
O	4.985867	1.027941	0.657445
O	2.646208	-0.490927	0.324162
O	5.199553	-2.755270	-0.925417
O	1.754434	-3.331896	-0.498667
H	7.173665	-2.815436	-0.591772
H	6.487045	-0.473983	-0.951120
H	4.899184	-0.788363	1.642734
H	3.985397	-0.474315	-1.258294
H	3.813900	-2.870315	0.621070
H	3.286525	-3.878021	-1.777617
H	2.585330	-2.269646	-2.077495
C	-0.666211	1.358825	-3.560470
H	-0.102873	0.903583	-4.387366
H	-1.436128	2.014254	-3.974428
H	0.027070	1.963491	-2.944723
C	0.769322	-4.031385	-1.226114
H	1.204137	-4.892744	-1.753446
H	0.037463	-4.395893	-0.503344
H	0.285088	-3.380460	-1.971935
C	-4.593626	-4.240800	-2.153384
H	-5.463385	-4.812941	-2.480479
H	-4.921137	-3.262020	-1.780685
H	-3.928017	-4.070926	-3.010685
C	1.990760	2.841757	2.722169
H	2.780848	2.911841	3.471982
H	2.047695	3.722241	2.064186
H	1.013374	2.820783	3.207925
C	-1.428253	0.708576	3.137950
H	-0.965503	-0.236071	3.449713
H	-1.525887	1.358609	4.010502
H	-2.412685	0.515334	2.707360
C	-5.323007	1.153229	1.309917
H	-5.940903	0.553865	1.982886
H	-5.158361	2.144113	1.735940
H	-5.840434	1.260048	0.346726
C	-5.234382	-1.893887	3.746776
H	-4.534699	-1.168122	4.183528
H	-6.234949	-1.697284	4.137493
H	-4.936198	-2.911772	4.011329
C	8.680726	-0.689482	0.398239
H	9.369534	-0.101304	1.006352
H	8.959911	-1.744128	0.487147
H	8.757256	-0.359787	-0.647445
C	5.332079	1.579703	1.920811
H	5.225240	2.663939	1.833674
H	4.641184	1.218451	2.690439
H	6.363255	1.328060	2.181066
C	-1.671081	3.514583	-0.544091
H	-0.907550	2.814141	-0.876029
C	-1.383794	4.906115	-1.140727
H	-2.035663	5.612146	-0.611338
C	-1.754990	4.956978	-2.623022
H	-2.828526	4.830763	-2.774436
H	-1.473868	5.925932	-3.039025
H	-1.236036	4.186531	-3.196512
C	0.081474	5.317540	-0.895174
H	0.170991	6.374173	-1.161529
H	0.320875	5.283797	0.177823



C	1.131531	4.515392	-1.663869
H	1.029089	4.656039	-2.741496
H	2.133892	4.846479	-1.387067
H	1.083321	3.440099	-1.463969
C	-3.100482	3.045233	-0.867868
O	-3.286873	2.172447	-1.833584
H	-2.500575	1.645367	-2.081972
O	-4.005277	3.544531	-0.254813
H	-2.592828	3.826446	1.244224
H	-0.995753	4.309488	1.271192
H	-1.338009	2.679268	1.417237
N	-1.636325	3.583129	0.952712
H	6.177407	-2.852156	0.892263
H	-3.770171	-3.854863	1.884420

**(L-2) Truncated**

114

H	-1.10978900	0.81437100	-0.68935100
C	-2.96121500	-0.73936600	-0.06143400
C	-4.07453200	-0.51190500	0.96590100
C	-4.18475800	-1.68515000	1.94820700
C	-4.24192500	-3.03937700	1.20958900
C	-3.18762600	-3.13891500	0.07731700
C	-3.39371800	-4.31017500	-0.89239000
O	-3.85583000	0.73405100	1.61340200
O	-5.35152800	-1.44953200	2.71661900
O	-3.20913100	-1.93983200	-0.74168400
O	-4.74797200	-4.55280700	-1.24248200
H	-2.99882300	0.05090000	-0.81963600
H	-5.00907700	-0.47140200	0.38788700
H	-3.29710700	-1.69375500	2.59814400
H	-5.24125800	-3.15172800	0.77172900
H	-2.19244300	-3.23993100	0.52658800
H	-2.78964000	-4.11246400	-1.78978800
H	-3.02058200	-5.21818900	-0.42045700
C	2.12062100	0.86179700	-0.43187300
C	1.16222900	1.71081800	0.45363800
C	0.11778800	0.78106300	1.09108900
C	-0.65515700	0.05753000	-0.03369400
C	0.37323500	-0.75951000	-0.84525600
C	-0.17809400	-1.53812900	-2.02699500
O	1.81643700	2.47350700	1.47217400
O	-0.78852300	1.50784700	1.93409900
O	-1.67716200	-0.73429700	0.56015800
O	1.35009300	0.15356100	-1.37970300
O	0.77674500	-2.53156400	-2.35637700
H	2.76003900	1.51455800	-1.02947900
H	0.65279400	2.40403600	-0.23748000
H	0.64631800	0.04371500	1.70615700
H	0.85594700	-1.47269300	-0.16673000
H	-1.14333400	-1.99089600	-1.76999700
H	-0.33596600	-0.84687600	-2.87134800
C	6.72903000	-1.27113800	1.01561200
C	6.67681500	0.09988000	0.30959200
C	5.24047700	0.63179500	0.31795800
C	4.17869700	-0.39254700	-0.12642100
C	4.45311300	-1.79594200	0.44621100

C	3.71612100	-2.91754600	-0.27179700
O	7.47080400	1.11223100	0.88780600
O	5.08018100	1.85843100	-0.41099300
O	2.89048100	0.03133800	0.39273100
O	5.84015300	-2.12729500	0.32010500
O	3.70442900	-4.04261100	0.59112900
H	7.70996100	-1.74175000	0.90390700
H	7.00753300	-0.10231800	-0.72239400
H	5.01132200	0.89655300	1.35439300
H	4.13010400	-0.44270300	-1.22166200
H	4.16205500	-1.79443400	1.50302100
H	2.69700100	-2.61962200	-0.54789700
H	4.26095000	-3.13752000	-1.20198700
C	-5.25790500	-3.74786100	-2.29489200
H	-5.33153700	-2.68948600	-2.01664900
H	-4.62869100	-3.82499700	-3.19361800
H	-6.25435200	-4.12986600	-2.52946600
C	0.40741500	-3.29501200	-3.49059500
H	1.19560800	-4.03280700	-3.65219700
H	-0.54593500	-3.82138700	-3.33448800
H	0.31620600	-2.66665900	-4.38920100
C	3.66301200	-5.28893300	-0.08451500
H	3.62645300	-6.05818800	0.68950700
H	2.77181300	-5.38403600	-0.72112000
H	4.55734400	-5.43471000	-0.70774500
C	8.86702600	0.84269400	0.91599500
H	9.22717000	0.46748000	-0.05332300
H	9.36305800	1.79172300	1.13070200
H	9.12697200	0.13023800	1.70659000
C	5.75171700	1.97615900	-1.65991600
H	6.83470400	2.05925600	-1.52211400
H	5.53327100	1.14071100	-2.33897700
H	5.38366000	2.89716700	-2.11797300
C	2.74987400	3.45100700	0.97503400
H	2.26062400	4.12586200	0.25493400
H	3.08080300	4.02666100	1.84371700
H	3.62076400	2.98970000	0.50555600
C	-1.13720900	0.81192300	3.14717100
H	-0.26367600	0.73818500	3.80752700
H	-1.92948800	1.38920700	3.62515000
H	-1.52012600	-0.17947300	2.91502000
C	-5.04769700	1.45791000	1.91344500
H	-4.73610100	2.38829100	2.39572700
H	-5.60419400	1.70518100	0.99714800
H	-5.70023400	0.89532400	2.58449700
C	-5.35359700	-1.95590600	4.05168400
H	-4.41754500	-1.70260600	4.57044600
H	-6.18145100	-1.45871000	4.56423400
H	-5.50081000	-3.03751100	4.07610500
N	-2.20354700	5.83184000	-1.43816700
H	-2.47225300	6.70873500	-0.99481300
H	-2.33758800	5.91669800	-2.44493400
H	-1.19903000	5.63427000	-1.20798600
C	-2.91843300	4.64116100	-0.85234200
H	-3.77156200	4.99524900	-0.27339000
C	-3.38480100	3.68229500	-1.97014000
C	-1.85731000	4.01242000	0.07051300
H	-3.94865500	4.30125700	-2.68356800
C	-2.20228700	3.04526200	-2.70506600

C	-4.36865200	2.65120000	-1.39589400
O	-0.70196000	4.37635000	-0.05028500
H	-1.67016700	2.33715000	-2.06461800
H	-2.55098100	2.50320000	-3.58366300
H	-1.46803700	3.77722800	-3.05675200
H	-5.20494500	3.19441200	-0.94215800
H	-3.88604000	2.10514100	-0.58225700
C	-4.91236400	1.67096100	-2.43048500
H	-4.13919500	0.99388500	-2.80192600
H	-5.69175600	1.05183900	-1.98181900
H	-5.35260800	2.18654200	-3.28892000
O	-2.34457500	3.11870400	0.84945300
H	-4.09679200	-3.77411400	1.97378700
H	6.47386100	-1.16492800	2.04929900
H	-1.66021800	2.50272900	1.33654800

**(D-3) Truncated**

114

C	3.719607	-0.618011	-0.363517
C	4.980567	-0.963057	0.416719
C	5.491324	0.271848	1.147194
C	5.638858	1.455903	0.191080
C	4.385675	1.659235	-0.680536
C	4.590610	2.629993	-1.845699
O	4.661785	-2.013787	1.295861
O	6.737077	-0.048791	1.723653
O	3.998247	0.409387	-1.274548
O	5.871133	2.566914	-2.429748
H	3.387226	-1.478854	-0.952633
H	5.742654	-1.283851	-0.311311
H	4.759370	0.542080	1.922972
H	6.498269	1.255781	-0.465951
H	3.569026	2.027958	-0.042699
H	3.818824	2.404025	-2.598870
H	4.461513	3.653126	-1.491593
C	-1.418572	-0.391007	0.579073
C	-0.705029	-1.051590	1.745525
C	0.756973	-0.614819	1.799972
C	1.443727	-0.838458	0.442979
C	0.621566	-0.224998	-0.706700
C	1.157282	-0.527633	-2.098411
O	-1.427879	-0.719342	2.897534
O	1.348488	-1.368751	2.821314
O	2.710737	-0.221294	0.541726
O	-0.737625	-0.749661	-0.634735
O	1.522407	-1.881619	-2.294789
H	-2.431885	-0.792441	0.481308
H	-0.726680	-2.143169	1.573838
H	0.788683	0.461744	2.030190
H	1.557540	-1.920143	0.278662
H	0.573331	0.864677	-0.572224
H	0.417863	-0.213123	-2.850951
H	2.068219	0.058172	-2.242957
C	-4.353766	3.850761	0.090480
C	-4.852333	2.509595	0.659136
C	-3.668617	1.743526	1.240002

C	-2.579948	1.618394	0.180275
C	-2.192934	2.992926	-0.358128
C	-1.161070	2.949957	-1.476966
O	-5.812536	2.650505	1.664593
O	-4.042923	0.444603	1.654936
O	-1.441754	0.978567	0.737959
O	-3.367687	3.594286	-0.892093
O	0.113910	3.082629	-0.904066
H	-5.152996	4.381586	-0.439449
H	-5.264739	1.930634	-0.187798
H	-3.260091	2.308875	2.089600
H	-2.960867	1.030359	-0.671824
H	-1.781233	3.608471	0.452471
H	-1.369659	3.784301	-2.164203
H	-1.239022	2.012168	-2.059553
C	0.496576	-2.729730	-2.722601
H	-0.030218	-2.324110	-3.597994
H	0.958335	-3.681397	-2.996152
H	-0.237275	-2.906287	-1.912853
C	1.132651	3.222700	-1.869186
H	0.896302	4.027892	-2.579740
H	2.046233	3.485251	-1.333167
H	1.273669	2.290791	-2.440232
C	6.090777	1.419458	-3.222038
H	7.027322	1.576526	-3.759653
H	6.166231	0.505777	-2.618986
H	5.276055	1.280777	-3.945815
C	-1.435724	-1.712084	3.907689
H	-2.079299	-1.336531	4.705274
H	-1.858242	-2.653746	3.525345
H	-0.431976	-1.900826	4.293111
C	2.484787	-0.796133	3.456443
H	2.381973	0.293770	3.528771
H	2.522638	-1.214742	4.464787
H	3.399309	-1.047639	2.915843
C	5.721535	-2.925086	1.533022
H	6.590105	-2.422179	1.964983
H	5.339002	-3.674336	2.227821
H	6.021451	-3.422709	0.600659
C	6.940737	0.466216	3.030910
H	6.135888	0.138642	3.703187
H	7.885977	0.048512	3.383740
H	7.007021	1.557348	3.025268
C	-7.046839	3.173811	1.211514
H	-7.772781	3.009019	2.009049
H	-6.979938	4.250490	1.026000
H	-7.385504	2.649525	0.306838
C	-4.330361	0.355449	3.044119
H	-4.567936	-0.690819	3.252586
H	-3.448751	0.639713	3.629033
H	-5.183272	0.988245	3.301979
C	-3.018762	-2.773789	-1.726110
H	-2.306802	-2.581945	-0.924138
C	-4.486036	-2.665390	-1.260592
H	-5.085442	-3.097508	-2.073545
C	-4.947799	-1.216128	-1.094144
H	-4.795732	-0.630014	-2.002689
H	-6.018733	-1.215326	-0.882429
H	-4.463040	-0.711215	-0.257805

C	-4.737312	-3.496040	0.014080
H	-5.798273	-3.388644	0.253602
H	-4.610520	-4.570962	-0.183776
C	-3.899067	-3.104835	1.230769
H	-4.004947	-2.045206	1.470802
H	-4.214915	-3.677428	2.104333
H	-2.832472	-3.309944	1.088612
C	-2.742125	-1.902072	-2.963486
O	-2.222479	-0.721735	-2.773527
H	-1.717476	-0.658753	-1.911822
O	-3.048947	-2.347964	-4.041848
H	-3.100829	-4.139451	-3.223758
H	-3.335002	-4.861705	-1.709221
H	-1.807534	-4.437022	-2.213654
N	-2.793876	-4.173776	-2.233987
H	5.850091	2.298952	0.815219
H	-3.966276	4.438216	0.896488

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114

H	-0.975363	1.098131	0.132967
C	-2.653963	-0.468772	0.924247
C	-3.363062	-1.182887	2.073988
C	-3.531485	-2.672704	1.806272
C	-4.062212	-2.960795	0.397056
C	-3.226755	-2.176241	-0.632785
C	-3.689846	-2.274698	-2.087938
O	-2.662366	-0.970326	3.269326
O	-4.392860	-3.160111	2.805468
O	-3.293554	-0.787795	-0.287153
O	-5.073067	-2.460554	-2.260505
H	-2.764828	0.609746	1.048867
H	-4.366425	-0.739243	2.129426
H	-2.540158	-3.140833	1.901125
H	-5.103515	-2.629313	0.330959
H	-2.185235	-2.512283	-0.576907
H	-3.354259	-1.359071	-2.594503
H	-3.199347	-3.124442	-2.561269
C	2.334085	1.070796	0.148446
C	1.532868	1.581155	1.353018
C	0.388046	0.645731	1.720580
C	-0.410396	0.228172	0.491981
C	0.512653	-0.248675	-0.633640
C	-0.241681	-0.534445	-1.908665
O	2.319995	1.770880	2.493484
O	-0.502669	1.294083	2.591323
O	-1.298066	-0.807035	0.877395
O	1.481541	0.757406	-0.922239
O	-0.941806	0.618154	-2.329981
H	2.979293	1.865675	-0.231407
H	1.078431	2.532634	1.037382
H	0.802662	-0.258767	2.185247
H	1.008611	-1.167477	-0.314909
H	0.483932	-0.827579	-2.670437
H	-0.941662	-1.367629	-1.749218
C	6.784301	-1.598026	-0.570456
C	6.777638	-0.084033	-0.306757

C	5.502947	0.328729	0.431259
C	4.262145	-0.234839	-0.268949
C	4.420722	-1.729245	-0.537538
C	3.233117	-2.275271	-1.319323
O	7.863964	0.375242	0.433402
O	5.394213	1.722332	0.620173
O	3.113917	-0.034903	0.526729
O	5.613483	-1.929632	-1.298235
O	3.647053	-3.368888	-2.128734
H	7.611050	-1.878146	-1.232280
H	6.783337	0.377469	-1.311951
H	5.540763	-0.089575	1.439693
H	4.126447	0.255772	-1.242575
H	4.523280	-2.265545	0.410544
H	2.467461	-2.620021	-0.622831
H	2.776614	-1.508580	-1.952531
C	-5.411580	-3.499253	-3.156867
H	-5.039337	-3.307200	-4.168542
H	-5.000080	-4.458022	-2.815218
H	-6.499263	-3.561818	-3.173624
C	-1.008968	0.705357	-3.731828
H	-1.581568	1.601814	-3.977101
H	-0.006087	0.784641	-4.174237
H	-1.515992	-0.166241	-4.166875
C	3.813657	-4.570012	-1.381276
H	3.772459	-5.400123	-2.090647
H	4.789621	-4.564528	-0.895960
H	3.016904	-4.669154	-0.639065
C	9.122447	0.172750	-0.171402
H	9.104900	0.469973	-1.231161
H	9.832518	0.808651	0.355502
H	9.450788	-0.867282	-0.073368
C	5.715541	2.552632	-0.470593
H	6.794596	2.572702	-0.657753
H	5.190092	2.265903	-1.392952
H	5.393245	3.557274	-0.196148
C	3.024766	2.993748	2.528012
H	2.343989	3.842603	2.380908
H	3.475197	3.069095	3.517280
H	3.824390	3.016550	1.781662
C	-0.335443	0.972769	3.958804
H	0.648846	1.283425	4.319639
H	-1.112118	1.513492	4.500155
H	-0.478194	-0.101435	4.116976
C	-3.473198	-0.641628	4.378633
H	-2.802648	-0.523868	5.230492
H	-4.002946	0.306381	4.214981
H	-4.198436	-1.431824	4.589031
C	-4.232695	-4.513841	3.176450
H	-3.167741	-4.771775	3.255226
H	-4.695594	-4.627126	4.157816
H	-4.709687	-5.188614	2.461553
C	-3.024191	2.314081	-1.039378
H	-2.613188	1.388109	-0.659847
C	-3.787473	3.049566	0.078760
H	-4.439600	2.273623	0.496909
C	-2.836960	3.492567	1.197828
H	-3.421306	3.825159	2.057404
H	-2.169324	2.697372	1.544019

H	-2.219101	4.351877	0.911478
C	-4.709714	4.181912	-0.405386
H	-5.489750	3.763747	-1.048945
H	-5.225025	4.566419	0.479222
C	-4.034301	5.343731	-1.135940
H	-3.705105	5.057040	-2.138474
H	-4.745083	6.159629	-1.273052
H	-3.187432	5.755846	-0.578799
C	-3.888710	1.959398	-2.244336
O	-4.685030	0.926008	-2.094986
H	-4.410126	0.356829	-1.348439
O	-3.834995	2.622771	-3.248189
H	-2.168641	3.528069	-2.450306
H	-1.499901	3.763232	-0.925887
H	-1.120685	2.369183	-1.806857
N	-1.854197	3.070530	-1.583188
H	6.849913	-2.132861	0.353962
H	-4.047036	-4.028833	0.334090

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H	3.209815	-4.702917	1.876361
C	-5.970591	1.338713	-0.560703
C	-6.684764	0.076524	-0.050658
C	-5.741386	-1.121987	-0.013591
C	-4.970636	-1.250979	-1.320025
C	-4.360657	0.071876	-1.778919
C	-3.727548	-0.019368	-3.163957
O	-7.232622	0.231603	1.231720
O	-6.492732	-2.297807	0.165384
O	-3.965829	-2.242349	-1.128944
O	-5.397169	1.055621	-1.815665
O	-4.501100	-0.724942	-4.103872
H	-6.678833	2.154018	-0.744534
H	-7.474475	-0.157032	-0.780770
H	-5.030442	-0.980728	0.815271
H	-5.676632	-1.590079	-2.085759
H	-3.586226	0.385628	-1.070907
H	-3.514795	1.003031	-3.513571
H	-2.776971	-0.553577	-3.092172
C	-2.332708	4.771786	0.616896
C	-2.972693	4.385159	1.943393
C	-3.924172	3.193137	1.836811
C	-4.733549	3.119003	0.530888
C	-3.994833	3.689983	-0.697025
C	-4.920765	4.052166	-1.865487
O	-1.938467	4.149255	2.868341
O	-4.734200	3.283413	2.988550
O	-5.011639	1.725895	0.378717
O	-3.296497	4.893221	-0.374897
O	-6.156457	4.606129	-1.485512
H	-1.860687	5.747826	0.716145
H	-3.575259	5.252584	2.247955
H	-3.321553	2.276141	1.871363
H	-5.673910	3.667825	0.665250
H	-3.275692	2.935791	-1.038713

H	-4.363574	4.741446	-2.517170
H	-5.155455	3.148565	-2.426967
C	2.501874	4.245460	-1.400238
C	2.159845	5.160722	-0.204089
C	0.854189	4.793507	0.517624
C	-0.231837	4.369886	-0.471392
C	0.313395	3.358250	-1.475817
C	-0.727557	2.869974	-2.475123
O	3.259220	5.356642	0.657401
O	0.338296	5.901646	1.219836
O	-1.337256	3.821816	0.252571
O	1.353229	4.017102	-2.183590
O	-0.173436	2.015427	-3.445675
H	3.208905	4.764529	-2.048564
H	1.979195	6.147603	-0.643088
H	1.019425	3.950320	1.206448
H	-0.577782	5.246276	-1.031868
H	0.722862	2.482770	-0.953681
H	-1.467641	2.285030	-1.923726
H	-1.230867	3.729041	-2.945518
C	6.331477	0.714533	-1.389493
C	6.634707	2.196171	-1.644444
C	5.438567	3.067659	-1.263712
C	4.104747	2.498219	-1.757385
C	3.995620	0.979771	-1.623802
C	2.827490	0.397835	-2.409939
O	7.736117	2.652960	-0.901188
O	5.544865	4.361409	-1.817090
O	3.048996	3.034783	-0.966985
O	5.172757	0.347246	-2.106606
O	2.305320	-0.763534	-1.788885
H	7.133465	0.079758	-1.771533
H	6.822327	2.309823	-2.723929
H	5.396863	3.115297	-0.167735
H	3.973723	2.783261	-2.810351
H	3.860169	0.749056	-0.559593
H	2.032841	1.141520	-2.551891
H	3.194400	0.095803	-3.395465
C	4.966227	-2.960326	1.825155
C	5.472863	-1.837319	2.727772
C	5.601092	-0.525789	1.958544
C	6.322175	-0.705423	0.613385
C	5.780151	-1.926403	-0.159967
C	6.599555	-2.325482	-1.394974
O	4.607456	-1.718435	3.826006
O	6.286828	0.363758	2.806359
O	6.151812	0.554017	-0.021731
O	5.808387	-3.065230	0.709444
O	7.975136	-2.042733	-1.312958
H	5.045146	-3.917664	2.349687
H	6.478679	-2.136936	3.057190
H	4.586024	-0.149963	1.750742
H	7.389514	-0.862432	0.808732
H	4.745221	-1.738365	-0.475273
H	6.439704	-3.400140	-1.565040
H	6.219316	-1.786622	-2.264099
C	0.201656	-4.912008	0.572655
C	0.403781	-4.475505	2.029636
C	1.506280	-3.434710	2.183888



C	2.758365	-3.826787	1.389722
C	2.388594	-4.192558	-0.055186
C	3.521923	-4.756652	-0.899803
O	-0.793625	-3.961897	2.603471
O	1.835396	-3.326653	3.541876
O	3.635100	-2.720516	1.456025
O	1.407552	-5.230717	-0.028493
O	3.145331	-4.825053	-2.253970
H	-0.399821	-5.819437	0.528449
H	0.719178	-5.359517	2.598160
H	1.162342	-2.466231	1.784244
H	1.987839	-3.301230	-0.555050
H	4.432810	-4.168544	-0.756560
H	3.721892	-5.779713	-0.563019
C	-3.831402	-3.216706	-2.140966
C	-3.856295	-4.615130	-1.510604
C	-2.693287	-4.725590	-0.533417
C	-1.355509	-4.270344	-1.147581
C	-1.480888	-3.040120	-2.058826
C	-0.296192	-2.880650	-2.989469
O	-5.014502	-4.915822	-0.789995
O	-2.580829	-5.990277	0.087985
O	-0.470751	-3.868637	-0.102250
O	-2.641966	-3.080028	-2.860651
O	-0.290205	-1.544871	-3.407283
H	-4.622644	-3.092461	-2.881904
H	-3.727183	-5.318628	-2.349356
H	-2.925338	-4.046927	0.294462
H	-0.901888	-5.095209	-1.712604
H	-1.517702	-2.135266	-1.439462
H	0.638826	-3.141167	-2.468717
H	-0.415673	-3.571384	-3.839135
C	-6.094735	5.943862	-1.035827
H	-5.552769	6.576490	-1.751906
H	-7.125019	6.295329	-0.951614
H	-5.600780	6.031867	-0.059634
C	0.237594	2.671299	-4.630074
H	0.604054	1.898420	-5.309474
H	-0.611362	3.180650	-5.108426
H	1.032713	3.397388	-4.438096
C	1.261933	-0.468730	-0.897304
H	0.414115	-0.012302	-1.421135
H	0.944304	-1.427277	-0.469250
H	1.593130	0.190270	-0.077769
C	8.710449	-2.959710	-0.529318
H	8.419357	-2.928604	0.528211
H	8.571358	-3.986514	-0.895424
H	9.762236	-2.683919	-0.625512
C	3.538431	-3.696484	-3.003205
H	3.086229	-3.803131	-3.992606
H	3.195406	-2.754285	-2.552940
H	4.631189	-3.657376	-3.121105
C	0.621602	-1.295128	-4.447399
H	0.618602	-0.216275	-4.603309
H	1.634288	-1.618737	-4.172949
H	0.317750	-1.804272	-5.373747
C	-5.577834	0.002318	-4.656357
H	-5.969051	-0.595035	-5.482706
H	-6.374595	0.184537	-3.925500

H	-5.238741	0.972932	-5.046416
C	-2.215574	4.540465	4.200154
H	-1.305161	4.347497	4.771617
H	-2.449626	5.612801	4.253345
H	-3.048909	3.971078	4.621702
C	-5.683854	2.258379	3.183694
H	-5.238746	1.261833	3.086810
H	-6.073072	2.392778	4.195292
H	-6.507782	2.317196	2.466847
C	-8.523127	0.803514	1.239984
H	-9.232959	0.184883	0.674474
H	-8.841253	0.851500	2.283062
H	-8.527807	1.820304	0.822588
C	-6.299534	-2.956852	1.392048
H	-6.555505	-2.306865	2.237619
H	-6.962631	-3.824135	1.391564
H	-5.266649	-3.320055	1.491081
C	-6.193534	-4.977956	-1.565568
H	-6.036297	-5.561053	-2.484433
H	-6.944782	-5.477897	-0.951689
H	-6.563610	-3.977887	-1.818297
C	-2.696825	-7.126032	-0.747165
H	-3.728439	-7.258407	-1.091230
H	-2.023458	-7.078808	-1.613907
H	-2.413947	-7.983347	-0.134428
C	-1.678534	-4.970638	3.088707
H	-1.167797	-5.583650	3.839544
H	-2.515200	-4.455068	3.563026
H	-2.053658	-5.599269	2.274318
C	1.575664	-2.075449	4.127671
H	0.492020	-1.884492	4.188590
H	1.978620	-2.114163	5.141077
H	2.081128	-1.266905	3.587003
C	5.243213	-1.442928	5.057405
H	4.455877	-1.416709	5.814476
H	5.957782	-2.235848	5.321564
H	5.766306	-0.482609	5.033754
C	6.099278	1.743758	2.567456
H	5.040004	1.962967	2.367929
H	6.403141	2.259999	3.481685
H	6.697179	2.100058	1.723051
C	8.971482	2.081772	-1.273837
H	9.037435	1.021152	-0.996708
H	9.144694	2.178504	-2.355218
H	9.746260	2.633400	-0.738587
C	6.192744	5.321632	-1.000913
H	5.609142	5.512335	-0.092066
H	7.206548	5.005265	-0.740862
H	6.235721	6.241307	-1.588414
C	3.553849	4.352128	1.611741
H	2.962657	4.479599	2.527506
H	3.402091	3.346006	1.214781
H	4.609732	4.476631	1.865968
C	0.770671	6.060563	2.552277
H	0.123515	6.817800	2.999771
H	0.657346	5.123965	3.115099
H	1.810702	6.402672	2.600661
C	-1.513410	-0.541766	2.031218
H	-0.631720	-0.707878	2.657042

C	-2.771862	-0.355569	2.915047
H	-3.559918	0.051479	2.263542
C	-2.487410	0.647368	4.038149
H	-2.079789	1.587303	3.662528
H	-3.408782	0.879306	4.576498
H	-1.773107	0.222884	4.754280
C	-3.263612	-1.701905	3.472167
H	-3.513759	-2.379546	2.645367
H	-2.447147	-2.174848	4.035857
C	-4.508205	-1.581821	4.349940
H	-5.297501	-1.023422	3.833935
H	-4.903303	-2.574501	4.585137
H	-4.295831	-1.077741	5.296178
C	-1.296417	0.652979	1.112873
O	-0.770329	1.679809	1.735736
H	-0.912002	2.515046	1.203399
O	-1.627127	0.612711	-0.055243
H	-1.525631	-2.626989	1.685368
H	-2.518783	-1.742626	0.606245
H	-0.895358	-1.773616	0.452103
N	-1.642684	-1.735317	1.151080

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H	-2.226567	5.408674	0.261432
C	5.889304	-2.478444	0.003105
C	6.838984	-1.587838	0.814483
C	6.485071	-0.113582	0.654344
C	6.203237	0.288748	-0.799611
C	5.403531	-0.766539	-1.586502
C	5.468870	-0.590642	-3.109394
O	6.813180	-1.856617	2.188519
O	7.560056	0.623920	1.172920
O	5.520410	1.534951	-0.676953
O	5.922481	-2.071238	-1.336440
O	6.709066	-0.158746	-3.607112
H	6.221930	-3.519759	-0.013741
H	7.850528	-1.751319	0.408643
H	5.566458	0.068623	1.233027
H	7.165921	0.451564	-1.298023
H	4.352517	-0.721379	-1.269273
H	5.178042	-1.549676	-3.566205
H	4.747346	0.166369	-3.415058
C	1.155412	-4.743238	0.738519
C	1.744225	-4.245093	2.067290
C	2.951243	-3.306607	1.939808
C	3.847044	-3.580929	0.731793
C	3.014456	-3.940654	-0.502873
C	3.844620	-4.352392	-1.715982
O	0.710188	-3.631341	2.806697
O	3.695886	-3.434920	3.133023
O	4.595625	-2.391330	0.547009
O	2.152120	-5.033068	-0.186701
O	4.917500	-5.206916	-1.420642
H	0.621805	-5.675284	0.918336
H	2.105415	-5.144005	2.584862

H	2.576425	-2.280382	1.823762
H	4.510394	-4.421261	0.967694
H	2.409800	-3.064042	-0.786556
H	3.163554	-4.806859	-2.452457
H	4.295541	-3.458208	-2.149312
C	-3.690664	-3.955243	-1.215901
C	-3.430543	-4.668889	0.127168
C	-2.042900	-4.382657	0.725988
C	-0.960195	-4.358198	-0.351566
C	-1.391612	-3.541354	-1.566838
C	-0.348563	-3.528341	-2.673045
O	-4.500890	-4.505546	1.032160
O	-1.650008	-5.389332	1.628601
O	0.237149	-3.803955	0.199986
O	-2.582146	-4.115446	-2.077756
O	-0.605867	-2.536947	-3.637436
H	-4.532910	-4.434636	-1.718163
H	-3.433726	-5.738975	-0.106327
H	-2.034667	-3.398557	1.220308
H	-0.760799	-5.384097	-0.683608
H	-1.590338	-2.501005	-1.269238
H	0.624551	-3.297394	-2.228933
H	-0.285196	-4.526363	-3.129893
C	-6.616452	0.293487	-1.486807
C	-7.311190	-1.072135	-1.551811
C	-6.323917	-2.172696	-1.168635
C	-4.953294	-2.002274	-1.832115
C	-4.488701	-0.555887	-2.015999
C	-3.424558	-0.456430	-3.093445
O	-8.398242	-1.163838	-0.666776
O	-6.787352	-3.452277	-1.541075
O	-3.953998	-2.601826	-1.010044
O	-5.542121	0.314603	-2.392815
O	-2.678762	0.735310	-3.013074
H	-7.290975	1.093869	-1.793175
H	-7.640604	-1.223950	-2.591530
H	-6.181308	-2.110284	-0.084076
H	-4.990448	-2.505027	-2.808606
H	-4.067653	-0.238641	-1.055254
H	-2.756402	-1.325664	-3.032649
H	-3.915513	-0.457292	-4.071315
C	-3.831411	3.680023	1.204353
C	-4.156863	2.504422	2.137621
C	-4.545979	1.310438	1.269473
C	-5.743663	1.668756	0.378726
C	-5.246831	2.809416	-0.541744
C	-6.262367	3.352230	-1.547140
O	-3.044201	2.214849	2.948637
O	-4.689276	0.111346	2.014414
O	-6.182648	0.445297	-0.172498
O	-4.896432	3.901422	0.314542
O	-7.601508	3.288440	-1.119558
H	-3.726335	4.600229	1.778120
H	-5.009556	2.814656	2.759533
H	-3.694543	1.102661	0.614736
H	-6.565451	2.079121	0.979753
H	-4.362165	2.475372	-1.101485
H	-5.971225	4.386096	-1.781684
H	-6.196610	2.766562	-2.466265

C	1.136286	5.043785	0.096829
C	0.483038	5.254774	1.478747
C	-0.847381	4.513301	1.663666
C	-1.708309	4.450527	0.398812
C	-0.846460	4.156092	-0.822698
C	-1.596828	4.159423	-2.135557
O	1.315225	4.858537	2.539427
O	-1.646458	5.136429	2.644975
O	-2.644840	3.388418	0.519503
O	0.179063	5.128477	-0.921080
O	-0.727879	3.645840	-3.116800
H	1.842238	5.847671	-0.113774
H	0.259603	6.331537	1.548060
H	-0.630324	3.475917	1.954213
H	-0.406349	3.162234	-0.687905
H	-2.498842	3.536713	-2.046066
H	-1.905103	5.186622	-2.385656
C	5.154805	2.230858	-1.820886
C	5.220332	3.741757	-1.531948
C	4.128234	4.166473	-0.542530
C	2.746264	3.628798	-0.959356
C	2.893808	2.122810	-1.192581
C	1.604805	1.420815	-1.549541
O	6.439524	4.156654	-0.986131
O	4.118218	5.553165	-0.281490
O	1.804729	3.808866	0.091564
O	3.838208	1.903620	-2.229142
O	1.753843	0.005414	-1.463472
H	5.797110	1.969094	-2.666672
H	5.049468	4.229868	-2.506690
H	4.366014	3.712895	0.424942
H	2.375096	4.104217	-1.876855
H	3.269799	1.668640	-0.271105
H	0.852509	1.705707	-0.811659
H	1.242470	1.720483	-2.538802
C	4.569810	-6.555825	-1.180577
H	3.912145	-6.940822	-1.972094
H	5.503174	-7.122068	-1.182656
H	4.064634	-6.687958	-0.216585
C	-1.378248	-2.969491	-4.744008
H	-1.476702	-2.108683	-5.407958
H	-0.867901	-3.780932	-5.280544
H	-2.370699	-3.313523	-4.434817
C	-1.644819	0.686673	-2.065910
H	-1.030584	-0.218630	-2.200140
H	-1.030197	1.568261	-2.243923
H	-2.023063	0.723005	-1.028962
C	-7.985830	4.325482	-0.239953
H	-7.435704	4.289426	0.708283
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H	-9.052375	4.193912	-0.048271
C	-1.355627	3.518234	-4.375162
H	-0.599801	3.152395	-5.073072
H	-2.185204	2.800437	-4.329275
H	-1.729300	4.488701	-4.732174
C	1.934888	-0.652990	-2.713853
H	2.427352	-1.607096	-2.507727
H	0.974239	-0.842529	-3.205140
H	2.580284	-0.059256	-3.364260

C	7.725937	-1.141294	-3.608564
H	8.558321	-0.728147	-4.181314
H	8.066599	-1.385770	-2.595332
H	7.377515	-2.066576	-4.087188
C	0.764209	-3.835376	4.210214
H	-0.030752	-3.220625	4.637023
H	0.583848	-4.890420	4.453913
H	1.729927	-3.535147	4.626081
C	4.078231	-2.230621	3.767522
H	3.203296	-1.715414	4.192741
H	4.743339	-2.513978	4.585749
H	4.622923	-1.569852	3.088835
C	7.252396	-3.144152	2.552158
H	8.184718	-3.412301	2.035264
H	7.439654	-3.120936	3.627586
H	6.490378	-3.909725	2.349244
C	7.232308	1.854115	1.785390
H	6.456537	1.715070	2.553058
H	8.144406	2.205552	2.272549
H	6.894321	2.601388	1.059454
C	7.563230	3.922529	-1.806507
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H	7.808801	2.854257	-1.872068
C	4.191974	6.418688	-1.394676
H	5.187476	6.395302	-1.852828
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H	2.958473	5.297579	3.622384
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C	-1.306497	4.872039	3.989967
H	-0.397465	5.400995	4.292457
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H	-3.926342	0.934368	4.338723
C	-5.909413	-0.095012	2.711746
H	-6.715190	-0.321573	2.007477
H	-5.741595	-0.943689	3.376859
H	-6.175060	0.777939	3.320498
C	-9.503608	-0.355193	-1.010046
H	-9.298753	0.712178	-0.852261
H	-9.801458	-0.510402	-2.056725
H	-10.325860	-0.656400	-0.358526
C	-7.515295	-4.143530	-0.539685
H	-6.857108	-4.411223	0.296586
H	-8.361757	-3.550180	-0.182354
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C	-4.587589	-3.303185	1.778010
H	-3.925134	-3.317214	2.653077
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H	-5.620383	-3.248002	2.131211
C	-2.130276	-5.267658	2.949621
H	-1.587143	-6.004406	3.544965
H	-1.924290	-4.266240	3.351220

H	-3.203799	-5.476950	3.010387
C	0.111563	-0.635717	2.010323
H	0.667443	-1.392006	2.566781
C	0.777096	0.749280	2.190006
H	0.429216	1.404170	1.376524
C	0.378669	1.409748	3.507976
H	0.872514	2.380925	3.590851
H	-0.698058	1.584420	3.540644
H	0.658022	0.791301	4.368021
C	2.303770	0.573832	2.078893
H	2.608722	-0.195585	2.795169
H	2.568087	0.177991	1.088258
C	3.108631	1.845302	2.352933
H	3.182453	2.041335	3.426680
H	4.126809	1.737399	1.965303
H	2.650345	2.719763	1.883846
C	-1.325851	-0.744080	2.512330
O	-2.214872	-0.653808	1.522990
H	-3.138058	-0.574814	1.889754
O	-1.600279	-0.908233	3.674142
H	-0.724040	-0.748598	0.118278
H	0.924802	-0.668063	0.001599
H	0.179804	-2.098417	0.492792
N	0.143435	-1.057742	0.570139