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AH

C	2.15847	0.71298	-0.49154
H	2.59577	0.55901	-1.48900
C	2.48138	2.13330	-0.01955
H	2.02168	2.85150	-0.70607
H	2.03026	2.28186	0.96939
C	3.99325	2.41629	0.04217
H	4.12943	3.40757	0.48849
C	4.72698	1.40496	0.94558
H	5.79927	1.63270	0.95456
H	4.35792	1.46233	1.97301
C	4.59215	-0.02638	0.49446
O	2.81606	-0.19535	0.43247
H	4.77382	1.60643	-1.55671
O	4.57335	2.50680	-1.25150
O	4.90344	-0.93733	1.40688
O	4.97165	-0.25555	-0.77058
H	4.96091	-1.82174	0.94508
H	4.96309	-1.25848	-0.90856
C	3.55169	-3.25993	-0.54150
O	2.50954	-2.59439	-0.30848
O	4.75263	-2.84882	-0.47038
H	3.40763	-4.31466	-0.83639
H	2.67654	-1.20051	0.11942
C	-2.21477	4.54328	0.07685
C	-1.57397	3.82189	1.07833
C	-1.65625	2.43104	1.06121
C	-2.35856	1.75103	0.04982
C	-2.99446	2.51995	-0.94098
C	-2.92945	3.91376	-0.93397
F	-2.14237	5.89288	0.09095
H	-1.03901	4.35112	1.86062
H	-1.17745	1.85778	1.84899
C	-2.46304	0.27712	0.03818
H	-3.53847	2.01623	-1.73472
C	0.68285	0.44031	-0.56122
H	-3.41663	4.50972	-1.69903
C	-1.43518	-0.65140	0.12805
C	0.01055	-0.43391	0.19940
H	0.56246	-1.03180	0.92102
C	-3.69063	-0.47150	0.00454
C	-3.34875	-1.85013	0.07998
C	-4.34221	-2.84231	0.08147
C	-5.67054	-2.43946	0.01534
C	-6.02201	-1.07603	-0.04349
C	-5.04407	-0.09237	-0.04421
H	-4.09744	-3.89623	0.14270
H	-6.45256	-3.19399	0.01678
H	-7.07095	-0.79541	-0.08386

H	-5.31483	0.95920	-0.07832
N	-1.96716	-1.94433	0.15989
C	-1.16498	-3.18140	0.08559
H	-0.12283	-2.85705	0.05544
C	-1.41633	-3.94887	-1.22123
H	-1.23991	-3.30011	-2.08504
H	-0.72565	-4.79687	-1.28484
H	-2.43627	-4.33706	-1.29020
C	-1.34344	-4.04864	1.34041
H	-0.65899	-4.90311	1.29893
H	-1.11700	-3.47241	2.24355
H	-2.36171	-4.43726	1.43620
H	0.15702	1.03136	-1.30853

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AL1

C	2.22841	0.62168	-0.32439
H	2.70274	0.49942	-1.30642
C	2.57443	2.00561	0.22253
H	2.16847	2.75967	-0.45930
H	2.08422	2.13689	1.19547
C	4.09370	2.21440	0.34752
H	4.26273	3.20261	0.79198
C	4.70432	1.17993	1.31204
H	5.79406	1.28416	1.33675
H	4.33804	1.36061	2.33093
C	4.40741	-0.27646	1.04328
O	2.81923	-0.37191	0.57819
H	4.90156	1.30618	-1.16266
O	4.73089	2.24021	-0.91256
O	4.73807	-1.23906	1.65745
O	5.02750	-0.44008	-0.75889
H	4.57928	-1.50588	-1.27928
H	5.96612	-0.63901	-0.59796
C	3.19991	-3.06047	-1.31652
O	2.44604	-2.63163	-0.41586
O	4.24638	-2.50297	-1.79004
H	2.95235	-4.02790	-1.77669
H	2.69321	-1.35756	0.17501
C	-2.02348	4.58878	-0.13843
C	-1.46100	3.90203	0.93215
C	-1.58911	2.51541	0.98164
C	-2.25966	1.80532	-0.03042
C	-2.81613	2.53961	-1.09250
C	-2.70448	3.92916	-1.15333
F	-1.90670	5.93407	-0.18936
H	-0.95023	4.45506	1.71410
H	-1.17250	1.96993	1.82275
C	-2.41573	0.33671	0.02938

H	-3.33473	2.01142	-1.88739
C	0.74979	0.38853	-0.44621
H	-3.13032	4.49873	-1.97312
C	-1.42533	-0.62156	0.19626
C	0.02360	-0.45133	0.30455
H	0.53390	-1.05384	1.05249
C	-3.66870	-0.36778	-0.00050
C	-3.38114	-1.75182	0.15629
C	-4.41151	-2.70535	0.18407
C	-5.72125	-2.25788	0.06057
C	-6.01915	-0.88762	-0.08107
C	-5.00493	0.05800	-0.10713
H	-4.20896	-3.76254	0.30932
H	-6.53131	-2.98189	0.08171
H	-7.05535	-0.57170	-0.16510
H	-5.23378	1.11550	-0.20469
N	-2.00671	-1.89165	0.27853
C	-1.25210	-3.15998	0.29335
H	-0.19852	-2.87522	0.26530
C	-1.50598	-3.99295	-0.97246
H	-1.29086	-3.40181	-1.86832
H	-0.84576	-4.86726	-0.97232
H	-2.53745	-4.34915	-1.04077
C	-1.48804	-3.94480	1.59200
H	-0.83952	-4.82754	1.61448
H	-1.25435	-3.32639	2.46481
H	-2.52353	-4.28461	1.68841
H	0.26978	0.98767	-1.21727

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AL2

C	2.18402	0.75189	-0.59515
H	2.60425	0.73529	-1.61005
C	2.43936	2.13150	0.03033
H	1.95465	2.89362	-0.58876
H	1.96804	2.15733	1.02066
C	3.93738	2.46305	0.15476
H	4.03777	3.40212	0.71147
C	4.64994	1.34274	0.94221
H	5.71679	1.57459	1.03389
H	4.21788	1.22946	1.93865
C	4.51094	0.05989	0.14798
O	2.89833	-0.25389	0.18970
H	4.83861	1.82066	-1.44857
O	4.54187	2.68666	-1.10854
O	4.86815	-1.16477	1.23643
O	5.01903	-0.11687	-0.94834
H	5.84095	-1.20093	1.17666

H	2.73437	-1.32537	-0.30078
C	3.26719	-3.39778	-0.44331
O	4.24247	-3.34303	0.35260
O	2.50451	-2.44789	-0.79085
H	3.04547	-4.37981	-0.88280
H	4.52995	-2.19263	0.80891
C	-2.13055	4.56080	0.12316
C	-1.46620	3.82306	1.09695
C	-1.55748	2.43299	1.06471
C	-2.29223	1.77008	0.06530
C	-2.95091	2.55510	-0.89755
C	-2.87705	3.94824	-0.87503
F	-2.05004	5.90947	0.15241
H	-0.90530	4.33911	1.86976
H	-1.05992	1.84720	1.83140
C	-2.40907	0.29711	0.03939
H	-3.52022	2.06480	-1.68190
C	0.71696	0.43829	-0.65575
H	-3.38150	4.55664	-1.61881
C	-1.38808	-0.64188	0.08677
C	0.06168	-0.43512	0.12092
H	0.63160	-1.02979	0.83212
C	-3.64546	-0.43842	0.03583
C	-3.31683	-1.82099	0.08618
C	-4.31992	-2.80292	0.10961
C	-5.64545	-2.38573	0.08940
C	-5.98361	-1.01827	0.05512
C	-4.99552	-0.04486	0.03351
H	-4.08482	-3.86004	0.15287
H	-6.43508	-3.13204	0.10802
H	-7.03016	-0.72615	0.05060
H	-5.25587	1.00974	0.01861
N	-1.93422	-1.92970	0.12118
C	-1.14927	-3.17178	0.00179
H	-0.10787	-2.84943	-0.06191
C	-1.45183	-3.91945	-1.30590
H	-1.29292	-3.26232	-2.16654
H	-0.77726	-4.77753	-1.40213
H	-2.47898	-4.29194	-1.34662
C	-1.28999	-4.05513	1.25054
H	-0.62118	-4.91962	1.17160
H	-1.02243	-3.49524	2.15272
H	-2.30926	-4.43101	1.37901
H	0.16924	1.02984	-1.38666

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HL1

C	2.14467	0.87852	-0.44670
H	2.60439	0.75924	-1.43620

C	2.43903	2.28889	0.07081
H	2.04230	3.01842	-0.64215
H	1.92384	2.43855	1.02819
C	3.95526	2.50641	0.23123
H	4.12484	3.48354	0.69662
C	4.51435	1.41939	1.16779
H	5.60674	1.42852	1.18310
H	4.17202	1.59944	2.19603
C	4.02519	0.03368	0.81956
O	2.76541	-0.12367	0.41565
H	4.76644	1.62089	-1.29884
O	4.62127	2.54749	-1.01538
O	4.51072	-0.95678	1.48875
O	4.90487	-0.17782	-0.90975
H	4.11763	-1.87796	1.10547
H	5.83772	-0.31947	-0.67517
C	3.68891	-3.19295	-0.76444
O	4.07414	-2.34326	-1.63195
O	3.66180	-3.08248	0.48327
H	3.33515	-4.14679	-1.18927
H	4.49473	-1.24774	-1.25196
C	-2.34883	4.50221	-0.00107
C	-1.73329	3.81729	1.04125
C	-1.76149	2.42417	1.03766
C	-2.38470	1.70720	0.00050
C	-2.99819	2.43936	-1.03094
C	-2.98636	3.83487	-1.03880
F	-2.32833	5.85336	-0.00065
H	-1.25953	4.37555	1.84257
H	-1.30160	1.87756	1.85528
C	-2.43783	0.22947	0.00761
H	-3.48309	1.90582	-1.84335
C	0.68214	0.56163	-0.53317
H	-3.45642	4.40336	-1.83483
C	-1.37999	-0.66511	0.10564
C	0.05676	-0.40075	0.16007
H	0.65644	-1.02793	0.81467
C	-3.64185	-0.55432	-0.01038
C	-3.26065	-1.92102	0.08540
C	-4.22647	-2.94037	0.10371
C	-5.56548	-2.57530	0.03421
C	-5.95534	-1.22322	-0.04520
C	-5.00532	-0.21315	-0.06320
H	-3.95401	-3.98662	0.17831
H	-6.32602	-3.35131	0.04803
H	-7.01178	-0.97299	-0.08869
H	-5.30414	0.83008	-0.11500
N	-1.87679	-1.97355	0.16149
C	-1.04745	-3.19255	0.13734
H	-0.01406	-2.84041	0.12256

C	-1.25476	-4.00141	-1.15244
H	-1.07176	-3.37471	-2.03110
H	-0.55166	-4.84134	-1.17735
H	-2.26708	-4.40696	-1.23067
C	-1.22513	-4.02823	1.41371
H	-0.51680	-4.86390	1.41035
H	-1.03148	-3.41923	2.30261
H	-2.23400	-4.44141	1.50175
H	0.12888	1.19623	-1.22112

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HL2

C	2.14674	0.90028	-0.49129
H	2.58470	0.81764	-1.49762
C	2.42904	2.31312	0.04983
H	2.03962	3.05934	-0.65053
H	1.90252	2.43754	1.00436
C	3.94021	2.54838	0.25155
H	4.08440	3.50672	0.76301
C	4.52182	1.41632	1.13326
H	5.60763	1.52593	1.21245
H	4.07414	1.44001	2.13050
C	4.16796	0.11182	0.44387
O	2.78707	-0.08043	0.35857
H	4.87960	1.75026	-1.25804
O	4.63196	2.65323	-0.98357
O	4.44224	-1.10036	1.55804
O	4.86687	-0.17076	-0.61572
H	5.41330	-1.19501	1.56122
H	4.42230	-1.22558	-1.19728
C	3.65828	-3.11412	-0.91504
O	3.63785	-3.10383	0.33720
O	4.05329	-2.19333	-1.70650
H	3.29935	-4.02205	-1.41991
H	4.06421	-1.99151	1.03753
C	-2.40727	4.49069	0.00176
C	-1.75078	3.81556	1.02524
C	-1.75748	2.42226	1.02236
C	-2.39982	1.69526	0.00398
C	-3.05377	2.41784	-1.00930
C	-3.06411	3.81335	-1.01716
F	-2.40828	5.84235	0.00214
H	-1.26110	4.38111	1.81171
H	-1.26411	1.88325	1.82520
C	-2.43198	0.21716	0.01278
H	-3.55304	1.87687	-1.80799
C	0.68427	0.58135	-0.56881
H	-3.56543	4.37427	-1.79939
C	-1.36102	-0.66260	0.09918

C	0.07381	-0.38196	0.13634
H	0.68943	-0.99457	0.79012
C	-3.62624	-0.58269	0.00754
C	-3.22650	-1.94427	0.09944
C	-4.17828	-2.97621	0.12840
C	-5.52316	-2.62936	0.07325
C	-5.93133	-1.28283	-0.00168
C	-4.99456	-0.26023	-0.03002
H	-3.89139	-4.01893	0.20009
H	-6.27300	-3.41558	0.09501
H	-6.99136	-1.04618	-0.03345
H	-5.30790	0.77890	-0.07788
N	-1.84103	-1.97775	0.16035
C	-0.99632	-3.18444	0.12865
H	0.03173	-2.81745	0.10419
C	-1.20519	-3.99708	-1.15875
H	-1.03669	-3.36887	-2.03929
H	-0.49399	-4.83030	-1.18908
H	-2.21381	-4.41317	-1.22853
C	-1.14982	-4.02243	1.40686
H	-0.43116	-4.84938	1.39659
H	-0.95503	-3.41020	2.29329
H	-2.15239	-4.44824	1.50555
H	0.11806	1.21101	-1.25114

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LO

C	-1.18311	-0.01097	0.58611
C	-0.33463	-0.76092	-0.13512
C	1.12509	-0.68934	-0.07072
C	1.97691	0.40864	-0.01574
C	1.61852	1.83993	-0.06800
C	0.71404	2.34333	-1.02200
C	0.40745	3.70039	-1.08771
C	1.02254	4.57191	-0.19614
C	2.20989	2.75725	0.81935
C	1.92260	4.12189	0.75949
F	0.73725	5.89599	-0.26282
H	-0.29403	4.08739	-1.81998
H	0.24191	1.65671	-1.71639
H	2.89505	2.39234	1.57892
H	2.37624	4.82921	1.44692
H	-0.78058	-1.48706	-0.81075
C	3.32077	-0.10670	0.02957
C	3.23172	-1.52753	-0.00607
C	4.38366	-2.32732	0.00525
C	5.62449	-1.69769	0.04441
C	5.72762	-0.29434	0.06069
C	4.58843	0.50108	0.04859

H	4.32606	-3.40962	-0.02493
H	6.52690	-2.30409	0.05497
H	6.71017	0.17113	0.07822
H	4.67272	1.58421	0.04664
N	1.88863	-1.86464	-0.06743
C	1.32004	-3.21990	0.02373
H	0.23918	-3.07282	0.04963
C	1.70019	-3.91716	1.33918
H	1.41303	-3.29699	2.19419
H	1.16686	-4.87147	1.41481
H	2.77256	-4.12119	1.41109
C	1.64215	-4.05840	-1.22198
H	1.12200	-5.02133	-1.16576
H	1.30670	-3.54231	-2.12720
H	2.71395	-4.25700	-1.32234
H	-0.80258	0.72391	1.29448
H	-5.06953	0.24762	-1.90935
C	-5.20484	-0.12508	-0.88050
C	-4.87228	1.00524	0.12174
H	-6.24674	-0.43450	-0.77229
C	-4.34867	-1.38228	-0.77551
C	-3.33710	1.21446	0.09316
H	-5.34678	1.93398	-0.24929
O	-5.31085	0.74748	1.41466
O	-3.00665	-1.16857	-0.39181
O	-4.55918	-2.39279	-1.41428
C	-2.67577	-0.10873	0.50121
H	-3.06535	1.99885	0.81020
H	-2.97972	1.51507	-0.90343
H	-3.07492	-0.34934	1.49869
H	-5.27925	-0.35563	1.49613
O	-5.17902	-1.68344	1.24662
H	-4.43212	-2.07637	1.72478

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OS

C	-1.00201	0.42935	0.58057
C	-0.27849	-0.41252	-0.17298
C	1.16513	-0.62916	-0.10256
C	2.22464	0.26938	-0.03685
C	2.16195	1.74245	-0.07688
C	1.34465	2.42691	-0.99684
C	1.31466	3.81854	-1.04845
C	2.12230	4.54135	-0.17794
C	2.95523	2.51600	0.79065
C	2.94600	3.91099	0.74381
F	2.10567	5.89749	-0.23138
H	0.68152	4.34468	-1.75605
H	0.72085	1.85587	-1.67596

H	3.57762	2.01491	1.52598
H	3.55612	4.50644	1.41616
H	-0.84892	-1.02440	-0.86902
C	3.43242	-0.51377	0.01438
C	3.04857	-1.88547	-0.02425
C	4.00795	-2.90796	-0.00358
C	5.35297	-2.55237	0.04376
C	5.74717	-1.20170	0.05935
C	4.79936	-0.18551	0.04061
H	3.72375	-3.95373	-0.03270
H	6.10835	-3.33433	0.06099
H	6.80528	-0.95156	0.08219
H	5.10998	0.85566	0.03831
N	1.66563	-1.93697	-0.09801
C	0.82466	-3.14701	-0.00665
H	-0.20657	-2.79125	-0.00273
C	1.03187	-3.88984	1.32140
H	0.87125	-3.21022	2.16433
H	0.30239	-4.70333	1.39810
H	2.03542	-4.31703	1.41282
C	0.98446	-4.05041	-1.23778
H	0.25378	-4.86491	-1.18754
H	0.79768	-3.48300	-2.15522
H	1.98424	-4.49150	-1.30835
H	-0.52562	1.07719	1.31715
O	-5.12153	1.71456	1.42859
C	-4.59524	1.84501	0.10781
H	-5.13528	0.74895	1.59692
C	-3.05396	1.86208	0.12492
H	-4.94446	2.82470	-0.25093
C	-5.14279	0.75623	-0.83377
C	-2.50922	0.46749	0.49727
H	-2.71538	2.62450	0.83969
H	-2.67393	2.13148	-0.87067
H	-6.24068	0.78464	-0.80874
H	-4.82666	0.95125	-1.86354
C	-4.70547	-0.68056	-0.51299
H	-2.87102	0.26034	1.52713
O	-2.97128	-0.48704	-0.40434
O	-4.90007	-1.60207	-1.33291
O	-5.02718	-0.94349	0.86994
H	-4.62820	-1.82656	1.03040
H	-2.81601	-2.22057	0.17901
O	-3.21737	-3.11596	0.29422
H	-3.86755	-3.03194	-0.44140