



Supporting Information

for

Computational studies of Brønsted acid-catalyzed transannular cycloadditions of cycloalkenone hydrazones

Manuel Pedrón, Jana Sendra, Irene Ginés, Tomás Tejero, Jose L. Vicario and Pedro Merino

Beilstein J. Org. Chem. **2023**, *19*, 477–486. doi:10.3762/bjoc.19.37

Computational methods, energies, and Cartesian coordinates

Computational methods

All of the calculations were performed using the Gaussian16 program [1]. Computations were done using the m062x functional [2] in conjunction with standard basis sets 6-31G(d) and 6-311+G(d,p)[3,4]. Geometry full optimizations were made at the m062x/6-31G(d) level. Single point calculations using the 6-311+G(d,p) basis set were carried out over optimized geometries to obtain the energy values. Solvent effects (toluene) were considered using the SMD model [5]. The nature of stationary points was defined on the basis of calculations of normal vibrational frequencies (force constant Hessian matrix). Minimum energy pathways for the reactions studied were found by gradient descent of transition states in the forward and backward direction of the transition vector (IRC analysis) [6]. Analytical second derivatives of the energy were calculated to classify the nature of every stationary point, to determine the harmonic vibrational frequencies, and to provide zero-point vibrational energy corrections. The thermal and entropic contributions to the free energies were also obtained from the vibrational frequency calculations, using the unscaled frequencies. Correction to free energy was made by subtracting S_{trans} contribution and considering a 1 M concentration [7]. The conformational searches were performed with the software Macromodel as implemented in the Schrödinger package [8]. A mixed torsional/low-mode sampling method with OPLS4 force field and chloroform as a solvent was used. The cutoff for maximum atom deviation was 0.5 and an energy window of 20 kcal/mol was selected. The resulting conformers in a range of 5.0 kcal/mol were optimized at the level m062x/6-31G(d,p) to locate the global minimum in the case of starting compounds. The conformational variability of the transition structures was carried out in a similar way by using constrained searches. Structural representations were generated using CYLView [9].

ELF analysis

The electronic structures of stationary points were analyzed by the topological analysis of the gradient field of electron localization function (ELF) [10] developed by Silvi and Savin [11,12]. The ELF study was performed with the TopMod program [13] using the corresponding wavefunctions of the all structures of the IRC. The topological analysis of the

gradient field of ELF has showed to be a powerful tool for the study of the bonding changes along an organic reaction [14-16].

NCI Calculations

NCI (non-covalent interactions) were computed using the methodology previously described [17]. Data were obtained with the NCIPLOT4 program [18]. A density cutoff of $\rho = 0.1$ a.u. was applied and the pictures were created for an isosurface value of $s = 0.35$ and colored in the $[-0.03, 0.03]$ a.u. $\text{sign}(\lambda_2)\rho$ range using VMD software[19].

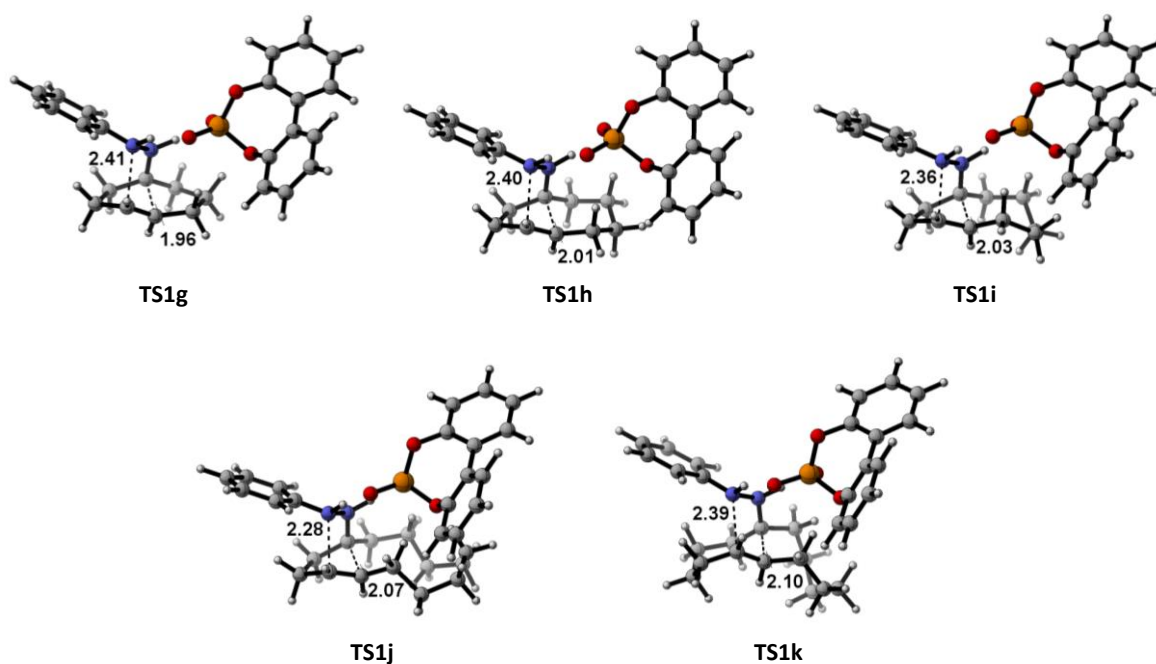


Figure S1: Optimized (m062x/6-31G(d)) geometries for transition structures of series **g–k**.

Energies

Table S1: Calculated (m062x/6-311+G(d,p)/SMD=toluene//m062x/6-31G(d)) absolute (hartree) and relative (kcal/mol) energies for transannular cycloadditions of compounds **1**.

	E_0	ΔE_0	G	ΔG	im. freq
1a	-1797.447918	0.0	-1797.529036	0.0	
TS1a	-1797.413925	21.3	-1797.492133	23.2	-380.8
2a	-1797.471650	-14.9	-1797.548721	-12.4	
1b	-1836.729861	0.0	-1836.813253	0.0	
TS1b	-1836.697226	20.5	-1836.777615	22.4	-404.0
2b	-1836.766268	-22.8	-1836.843608	-19.0	
1c	-1876.006876	0.0	-1876.090586	0.0	
TS1c	-1875.963502	27.2	-1876.044729	28.8	-385.0
2c	-1876.028483	-13.6	-1876.109301	-11.7	
1d	-1915.286933	0.0	-1915.372402	0.0	
TS1d	-1915.235568	32.2	-1915.318738	33.7	-405.4
2d	-1915.295914	-5.6	-1915.377698	-3.3	
1e	-1954.557859	0.0	-1954.646316	0.0	
TS1e	-1954.511988	28.8	-1954.595926	31.6	-433.1
2e	-1954.569735	-7.5	-1954.653154	-4.3	
1f	-1993.803082	0.0	-1993.893454	0.0	
TS1f	-1993.746446	35.5	-1993.833212	37.8	-430.6
2f	-1993.841907	-24.4	-1993.927252	-21.2	
1g	-1758.190032	0.0	-1758.268049	0.0	
TS1g	-1758.153318	23.0	-1758.229741	24.0	-416.8
2g	-1758.116045	46.4	-1758.190950	48.4	
1h	-1797.445530	0.0	-1797.526123	0.0	
TS1h	-1797.411541	21.3	-1797.488085	23.9	-420.2
2h	-1797.479896	-21.6	-1797.557943	-20.0	
1i	-1836.728570	0.0	-1836.810278	0.0	
TS1i	-1836.683966	28.0	-1836.763629	29.3	-458.8
2i	-1836.748536	-12.5	-1836.827086	-10.5	
1j	-1954.560027	0.0	-1954.646694	0.0	
TS1j	-1954.507496	33.0	-1954.590663	35.2	-486.1
2j	-1954.565691	-3.6	-1954.647864	-0.7	
1k	-1954.561858	0.0	-1954.651974	0.0	
TS1k	-1954.508163	33.7	-1954.592010	37.6	-411.9
2k	-1954.575287	-8.4	-1954.658337	-4.0	

Table S2: Calculated (m062x/6-311+G(d,p)/SMD=toluene//m062x/6-31G(d)) absolute (hartree) and relative (kcal/mol) energies for bimolecular reactions.

	E_0	ΔE_0	G	ΔG	im. freq
8a	-1564.12925672	0.0	-1564.20746098	0.0	
TS4a	-1564.09905418	19.0	-1564.17129663	22.7	-407.6
9a	-1564.17401478	-28.1	-1564.24538807	-23.8	
8b	-1721.23428241	0.0	-1721.32057330	0.0	
TS4b1	-1721.22339271	6.8	-1721.30281127	11.1	-452.5
TS4b2	-1721.21820334	10.1	-1721.29790940	14.2	-432.8
9b1	-1721.28739838	-33.3	-1721.36520349	-28.0	
9b2	-1721.26418383	-18.8	-1721.34256928	-13.8	

Cartesian coordinates

1a

0 1

C	3.5348847800	-0.1536675381	0.6585497237
N	2.6584844737	0.6691170458	0.2015516999
N	2.7165154750	1.1307998226	-1.1307712291
H	1.9433698475	0.6227578259	-1.5918012418
O	0.2560512509	-0.1702624973	-1.4360447987
C	3.1396812261	-2.7990405834	-0.2843875177
C	2.0112230676	-2.4978829648	0.3631897633
H	1.2544762282	-1.9255364987	-0.1757836170
H	3.9300841056	-3.3593150974	0.2220542606
O	0.1814037177	1.0502811849	0.8506782134
P	-0.5008880070	0.2140012353	-0.2039703665
O	-1.0336140192	-1.1204853833	0.5958784053
O	-1.9122470776	0.8788334155	-0.6652032524
C	-2.0167374755	-1.9102117750	0.0379901315
C	-2.9444751280	0.9958080569	0.2428598447
C	-3.3480120562	-1.4712242035	0.0512712335
C	-1.6726524878	-3.1680907678	-0.4429131761
C	-3.7015920737	-0.1342103567	0.5782967670
C	-3.2591452745	2.2559349201	0.7355756097
C	-4.3286149239	-2.3460548595	-0.4271736455
C	-2.6658159902	-4.0191878278	-0.9149290778
H	-0.6272882810	-3.4604946613	-0.4356230995
C	-4.8063722647	0.0471660572	1.4168382218
C	-4.3608432088	2.4101458635	1.5694555260
H	-2.6326288468	3.0930600338	0.4477683293
C	-3.9972279248	-3.6091260854	-0.9043421397
H	-2.3985884498	-5.0010567314	-1.2926236959
C	-5.1392302321	1.3046463028	1.9071348123
H	-4.6098382784	3.3932264743	1.9563350753
H	-4.7750473085	-4.2677196005	-1.2769674867
H	-5.3625050404	-2.0122856208	-0.4383169862
H	-5.3941857681	-0.8220307058	1.6987719757
H	-5.9976017379	1.4198851416	2.5610725048
C	2.4527792465	2.5333008461	-1.2002103412
C	1.4660214478	3.0011428917	-2.0675642512
C	3.2116931306	3.4280347083	-0.4470892458
C	1.2583526260	4.3708038481	-2.1927282263
H	0.8552923608	2.2877650216	-2.6147589820
C	2.9822614601	4.7943831799	-0.5650868351
H	3.9793445332	3.0504389681	0.2232243759
C	2.0115170833	5.2712469709	-1.4429666679
H	0.4890310754	4.7331885195	-2.8672730001
H	3.5710538149	5.4895011053	0.0254482362
H	1.8388998755	6.3384029648	-1.5369470893
C	3.4495911563	-2.1992973560	-1.6233719048
H	2.5488414600	-1.6867546952	-1.9812382078
H	3.7145208230	-2.9543584519	-2.3718375279

C	3.3766008952	-0.6280363473	2.0886910645
H	3.5654749420	0.2445203894	2.7276182560
H	4.1722975025	-1.3511471146	2.2922698904
C	1.8063824226	-2.6366349861	1.8363720141
H	0.7932745704	-2.9774910620	2.0744971291
H	2.5229162569	-3.3499202252	2.2627625823
C	2.0136859791	-1.2435660484	2.4681114827
H	1.9763671747	-1.3251748827	3.5591682279
H	1.1956841634	-0.5777466805	2.1723491934
C	4.7720977142	-0.4867136241	-0.1379378361
H	5.2965564456	0.4629879957	-0.3034555608
H	5.4034969926	-1.0982552953	0.5106501545
C	4.6163435979	-1.1875297979	-1.5144932069
H	4.5028435994	-0.4288395142	-2.2901092679
H	5.5672930396	-1.6995688878	-1.6959676016
H	1.7235622927	0.8971379382	0.6896523785

1b

0 1

C	3.5232971746	-0.7294440241	0.7684440795
N	2.5837704364	0.0757270555	0.4225202090
N	2.6047578734	0.7387089536	-0.8247641326
H	1.8815186824	0.2464381171	-1.3761563294
O	0.1952425418	-0.5681215139	-1.3804245199
C	2.6086983202	-2.9154829200	-0.7566722719
C	2.3752469917	-3.5298108131	0.4035038782
H	3.1511779856	-4.1807316773	0.8188314656
H	1.8346764237	-2.2675086884	-1.1784678659
O	0.0957396458	0.2733895177	1.0681056670
P	-0.6127945841	-0.0950512677	-0.2135262298
O	-1.7603316817	-1.1734116867	0.2228860583
O	-1.5406657107	1.1388303671	-0.7419927333
C	-2.8605977849	-1.3872072836	-0.5796839033
C	-2.5767941635	1.5860096269	0.0499226106
C	-3.8896271065	-0.4356647050	-0.6230610466
C	-2.9602534388	-2.5952478955	-1.2590224789
C	-3.7686756690	0.8518231467	0.0970738156
C	-2.4350321886	2.7958222935	0.7177597382
C	-5.0355080632	-0.7487804473	-1.3614316437
C	-4.1085923855	-2.8819694914	-1.9884341856
H	-2.1311962583	-3.2918334993	-1.1945080452
C	-4.8345658020	1.3871380732	0.8273494933
C	-3.5087161617	3.3055406643	1.4394199230
H	-1.4826916071	3.3124028029	0.6509258194
C	-5.1511182291	-1.9588865927	-2.0360557290
H	-4.1877893898	-3.8249344047	-2.5201312770
C	-4.7115479167	2.6029001780	1.4906096775
H	-3.4054029904	4.2501032837	1.9642557276
H	-6.0477993170	-2.1758300589	-2.6075270381
H	-5.8342273166	-0.0142918083	-1.4173678956
H	-5.7617246481	0.8237129155	0.8865669437
H	-5.5496125016	2.9960465068	2.0570929363
C	2.2070981452	2.1042281386	-0.6718475231
C	2.8445541106	2.9208689837	0.2617203176

C	1.2064198486	2.6216036857	-1.4941340994
C	2.4745182861	4.2563163820	0.3749482979
H	3.6255125607	2.5074328312	0.8942410905
C	0.8548145499	3.9630242688	-1.3832103826
H	0.6862795781	1.9645452636	-2.1856021589
C	1.4827019208	4.7841279596	-0.4491801112
H	2.9683816916	4.8885103031	1.1063738169
H	0.0690020722	4.3594689776	-2.0186414199
H	1.1987843209	5.8277650810	-0.3606664451
C	3.9356440424	-2.9486918174	-1.4550159261
H	3.8323621287	-3.2953068161	-2.4903783703
H	4.6089974390	-3.6483469878	-0.9430331627
C	3.4991786098	-1.3298112943	2.1507598235
H	4.0649331966	-2.2658699052	2.1159664993
H	4.1194031119	-0.6340671876	2.7379446067
C	1.1554517159	-3.3407683744	1.2561291064
H	0.4934570699	-2.5889994199	0.8105536264
H	0.5854297697	-4.2778896906	1.3062819157
C	1.5310477753	-2.9375826571	2.6902983645
H	0.6303790461	-2.9751959810	3.3118360213
H	2.2229020880	-3.6882476635	3.0994875337
C	2.1481739032	-1.5432574339	2.8620254362
H	2.3263126679	-1.3928476902	3.9318790251
H	1.4116040527	-0.7884114413	2.5723349856
C	4.7518705412	-0.9070596990	-0.0899553817
H	5.1714466097	0.0956037710	-0.2389381118
H	5.4756997698	-1.4937154976	0.4847524759
C	4.5550316291	-1.5440658886	-1.4827667203
H	3.9339787305	-0.8770020749	-2.0844534190
H	5.5402585900	-1.5816511901	-1.9603762095
H	1.6278832672	0.1735293396	0.9191017816

1c

0 1

C	3.6116452867	0.7777531272	1.3124553121
N	2.5066991823	1.0901669879	0.7392298292
N	2.4743634788	1.4940479923	-0.6155597817
H	1.9847145490	0.7124982721	-1.0785407145
H	1.4836900905	0.9641072742	1.1497746715
O	0.5437729714	-0.5529652154	-0.8845819457
C	3.6604984833	-1.8229729301	-0.2752786325
C	3.8456449567	-2.6661661942	0.7432656960
H	4.8497793572	-2.7897547915	1.1595051212
H	2.6554500817	-1.7024361166	-0.6850581829
O	0.0249483584	0.8221468598	1.2402266782
P	-0.4647556595	-0.0217259869	0.0831458210
O	-1.3772608712	-1.1966616045	0.7575341316
O	-1.5926890425	0.7842216588	-0.7750952437
C	-2.3541501426	-1.8407797009	0.0280584554
C	-2.7504723043	1.1807725513	-0.1383336551
C	-3.5566720738	-1.1833777189	-0.2704401897
C	-2.1538694149	-3.1733231725	-0.3115650644
C	-3.7605249166	0.2380270736	0.0880924634
C	-2.9077367198	2.5197233858	0.1960188891

C	-4.5597037033	-1.9186642985	-0.9104107459
C	-3.1655474252	-3.8820529749	-0.9496383628
H	-1.2038269636	-3.6318495270	-0.0589720934
C	-4.9614873286	0.6913070064	0.6433813758
C	-4.1103299961	2.9448425985	0.7497803042
H	-2.0804388514	3.1980847234	0.0111938131
C	-4.3737847017	-3.2548211836	-1.2458492398
H	-3.0090298363	-4.9226694296	-1.2156155461
C	-5.1402925628	2.0312057606	0.9684853645
H	-4.2422208925	3.9893454485	1.0141966361
H	-5.1654404458	-3.8017069037	-1.7476912873
H	-5.4900097315	-1.4172749260	-1.1626550030
H	-5.7511889239	-0.0288321692	0.8391292830
H	-6.0778408656	2.3602219562	1.4050459924
C	1.7014693886	2.6849571762	-0.7833683360
C	1.9640350126	3.8094589078	-0.0019694415
C	0.7166357855	2.7262994175	-1.7699000544
C	1.2356945348	4.9758382747	-0.2081173126
H	2.7332707901	3.7664912299	0.7641854182
C	0.0051814494	3.9030757062	-1.9787693392
H	0.4887770401	1.8295207003	-2.3394687951
C	0.2585557341	5.0304056719	-1.1998728389
H	1.4376425002	5.8480622893	0.4058620175
H	-0.7674513021	3.9277751939	-2.7409488261
H	-0.3050648265	5.9437164056	-1.3606934302
C	4.7822473849	-1.0235462359	-0.9095053359
H	4.3718018414	-0.3218062705	-1.6434426260
H	5.4401894801	-1.7015179657	-1.4670241668
C	3.5918140444	0.2356720178	2.7142688320
H	4.3170525276	-0.5894138228	2.7293211598
H	4.0256483972	1.0202048403	3.3504658681
C	2.2373891171	-0.2202682834	3.2668884634
H	2.3803229586	-0.4551540573	4.3282028868
H	1.5195213381	0.6057234224	3.2263610301
C	4.9361665069	1.0187743262	0.6478249621
H	4.7876632247	1.7297853281	-0.1671166894
H	5.5868008568	1.4752896762	1.4037249922
C	5.6310916561	-0.2442348578	0.1023392812
H	6.5612879228	0.0899805250	-0.3688951198
H	5.9215953760	-0.8981282229	0.9317295720
C	1.6471007653	-1.4377912611	2.5470616711
H	1.6216458802	-1.2422575838	1.4702957194
H	0.5991014581	-1.5360316152	2.8444465360
C	2.7655135851	-3.4368477608	1.4463471077
H	1.8701175295	-3.4857184592	0.8152292155
H	3.1001525011	-4.4653135664	1.6256751639
C	2.3998616688	-2.7606377756	2.7813454037
H	3.3215757704	-2.5928125772	3.3575231705
H	1.7903586799	-3.4428886264	3.3830596915

1d

0 1

C	3.5616342085	0.6053990307	-0.9734446540
N	2.6265569070	-0.2355917171	-0.7176984134

N	2.7723583272	-1.2208217305	0.2873786754
H	2.0931034882	-0.9250939760	1.0050788025
O	0.3816711362	-0.0963587602	1.2983791989
C	3.0361085696	1.8781629338	1.8770091066
C	2.5520053429	3.1183414844	1.9687031969
H	3.2393960509	3.9500543993	2.1532604570
H	2.3218625879	1.0703454616	1.7168930243
O	0.1243670067	-0.3689500412	-1.2579175983
P	-0.5100579459	-0.2819570523	0.1116689162
O	-1.6474376095	0.8853554398	-0.0040059887
O	-1.4382818422	-1.5904595724	0.4028623132
C	-2.7170561155	0.9248336243	0.8652202206
C	-2.5157080097	-1.8411613199	-0.4214798952
C	-3.7595590989	-0.0048752785	0.7397077999
C	-2.7787964435	1.9615817458	1.7889426417
C	-3.6925658565	-1.1019646649	-0.2517246516
C	-2.4248971010	-2.8724227261	-1.3476599108
C	-4.8727583278	0.1481945840	1.5727148679
C	-3.8956710827	2.0913528322	2.6065224206
H	-1.9471323796	2.6565743668	1.8420744646
C	-4.7976970680	-1.4489483139	-1.0358175771
C	-3.5368343869	-3.1966659573	-2.1167977946
H	-1.4807530159	-3.3995360618	-1.4416817829
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H	5.6352136377	0.5695728741	-1.1807122297
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H	-4.4617432346	1.8755086412	-0.7820475948
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H	1.7105139590	2.6244716333	-1.5084155243
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H	5.5144896944	2.0387072884	0.5775979820
O	0.0574937138	-0.3723453559	-1.1170869494
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C	-3.9126801282	-0.8868277650	0.3351663804
C	-3.4337817216	0.9272178841	1.8925616474
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H	4.4812296242	-1.9630436610	-2.2718090324
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H	3.6362286258	-0.1512643710	2.9202121916
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C	1.8516540586	-2.8034892413	1.4053197206
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O	2.0767853030	1.5860504700	0.1192829980
C	2.7745493655	-1.1381037510	0.7381902237
C	3.2695784213	1.5768350013	-0.5763007578
C	3.9863867989	-0.4341423167	0.7388716137
C	2.5210406487	-2.1461928876	1.6605202888
C	4.2485364008	0.6264204009	-0.2592275444
C	3.4994758864	2.5747466923	-1.5147343035
C	4.9440361012	-0.7847907071	1.6961181739
C	3.4882857321	-2.4761934451	2.6031711293
H	1.5661415352	-2.6603129513	1.6161806505
C	5.4829929522	0.7210160333	-0.9102988674
C	4.7339920865	2.6462618649	-2.1501605111
H	2.7033377977	3.2810038138	-1.7228585570
C	4.7040129832	-1.7958364240	2.6195702257
H	3.2920084685	-3.2633510947	3.3243169063
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H	4.9170282148	3.4240399231	-2.8846801900
H	5.4603441848	-2.0458488852	3.3564778190
H	5.8814671420	-0.2361027383	1.7190318018
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H	6.6929417041	1.7698052403	-2.3414009604
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C	-3.4722229387	2.3350042900	-0.3700994839
C	-2.6808871469	1.9737976563	1.8935593487
C	-3.9093599771	3.6054706983	0.0000454977
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C	-3.1254116156	3.2416938322	2.2495799770
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C	-3.7472428666	4.0570312152	1.3057975166
H	-4.3708554221	4.2460707626	-0.7445130512
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H	-4.0873212652	5.0489935762	1.5849640726
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H	-2.3311149876	-1.6666729802	-3.2829650162
C	-1.1358330692	-2.5887943884	0.3718058833
H	-0.4882144204	-1.7189528723	0.5113039016
H	-1.0729589133	-3.1635307830	1.3045163861
C	-0.6133492139	-3.4074866304	-0.8088052927
H	0.4376566720	-3.6631015471	-0.6377497974
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H	-5.0511977650	0.3465586521	-0.6509368222
H	-6.2103199948	-0.9208937160	-0.3061542684
H	-1.5082218085	-0.0182828083	-1.5079424153

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C	-2.8895621530	-0.3189577341	1.2134347050
C	-2.6368220221	-1.6585851120	0.5139482554
H	-3.3416334441	-2.3932230524	0.9214793211
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O	0.4053984256	-0.0767273450	-1.5114141764
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O	2.0306091018	-1.0114964554	0.1755669534
O	2.2063048161	1.4368497464	-0.3775148144
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C	3.3560876307	1.1960767039	-1.1016749858
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C	2.8486155375	-1.4710726268	2.3628007488
C	4.3824582384	0.4308261905	-0.5332369246
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H	6.6643384470	0.7819749885	-3.0404117597
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C	-3.5624367564	2.6240461586	-0.4988004981
C	-2.0332408816	2.7820706864	1.3821147394
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H	-0.5131188725	-3.9155269577	-1.6011119216
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C	-1.2228271775	-2.2352009162	0.6318709104
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C	-1.2090991994	-3.7545665135	0.4273164595
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H	-0.2507909539	-4.1493326844	0.7828156314

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C	2.8013410172	0.5926243810	1.2631618744
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H	2.1678403070	0.4301131689	2.1389070142
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P	-1.0115962186	-0.4927482505	-0.2082673085
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C	2.4122282267	-2.5535755967	1.4555256387
C	4.3863760998	-3.5493899797	-0.2449073871
H	4.1767249830	-1.6737897995	-1.3137927404
C	2.9430782478	-3.8219531176	1.6673265763
H	1.6098313450	-2.1674436049	2.0770505880
C	3.9339457411	-4.3188405423	0.8236778678
H	5.1442919387	-3.9413067389	-0.9155901844
H	2.5692238547	-4.4268628498	2.4868548844
H	4.3419389228	-5.3106069631	0.9900733034
C	4.2890666901	0.4784675180	1.6096030966
H	4.6012916183	-0.5691503815	1.5856862138
H	4.4176573019	0.8118790034	2.6442803568
C	4.6175421763	1.3786427936	-0.7587473840
H	4.9170493596	0.4813403817	-1.3092766925
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H	6.1862003395	0.9771765003	0.6811739433
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H	1.2330238892	2.6317697730	-3.6104238818
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H	-6.3331929655	-0.2852187242	-0.7171872085
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H	2.9681260491	2.4420224299	1.0642255014
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C	-3.5220633860	-1.9363336576	-2.5263699551
C	-5.1323595945	-0.5541085498	1.8521052858
C	-3.7457905818	0.5314128039	3.4959838689
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C	4.3834743713	-3.7513793033	-0.4221173407
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H	1.5715184790	-2.5488377201	1.9572640985
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H	2.5411207165	-4.8267140091	2.2217408298
C	4.3650819787	0.2255780376	1.4485132565
H	4.7100887545	-0.8017831651	1.3040802543
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C	4.4407448156	1.3218753752	-0.8675876081
H	4.7435436283	0.5007272080	-1.5250524746
H	4.7936060826	2.2452241515	-1.3385401528
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C	0.8845598773	1.8784612771	0.7957010287
H	0.3643162322	1.7253449039	-0.1531023897
H	0.4615794799	1.1211251036	1.4648869185
C	0.5123798650	3.2508439358	1.3686648438
H	0.9218905564	3.3431092853	2.3839388863
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H	5.1517659144	-4.0920873222	-1.1087362843
H	4.3338864555	-5.5946425293	0.6867287740
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H	2.9977758925	2.0517210895	1.4607148040
H	2.2382762174	-0.4150029291	2.2840875055
O	-0.4435133765	-0.0072329576	-1.4958225246
P	-1.1177158380	-0.6726620081	-0.3453474148
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C	-3.0246062297	0.0548966341	1.2872443811
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C	-4.2178273672	-0.5129909596	0.8213615759
C	-2.8241677156	0.3138121661	2.6377680328
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C	-3.5717731721	-1.6009967155	-2.7497952927
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H	4.7562125866	0.3878706509	-1.3298419346
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H	1.0426080313	-0.6924163813	0.4526085570

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C	2.5523352807	0.4803782662	1.2520735706
C	2.3071518636	1.7654687426	0.4397773138
H	2.9799953004	2.5408452473	0.8235313135
H	1.8072183879	0.3780879074	2.0460331043
O	-0.5294145117	-0.1083002816	-1.5604386950
P	-1.1873111091	-0.4621311247	-0.2721917378
O	-2.1909904900	0.7630312835	0.1297678995
O	-2.2378356440	-1.6994832129	-0.3835069958
C	-3.1512753104	0.5822750582	1.1023991515
C	-3.4167266508	-1.5354247863	-1.0824756992
C	-4.3052640252	-0.1582476721	0.8129182206
C	-2.9866966653	1.2199598780	2.3259972404
C	-4.4717144430	-0.8225062776	-0.4986886097
C	-3.5544011033	-2.1606353230	-2.3152354693
C	-5.2984318430	-0.2290374029	1.7952103566
C	-3.9876083842	1.1345068713	3.2870829567
H	-2.0751258777	1.7832682062	2.4960918292
C	-5.6858563064	-0.7708828871	-1.1909931461
C	-4.7705965510	-2.0928175676	-2.9855214110
H	-2.7022700813	-2.6941964378	-2.7215960694
C	-5.1476691587	0.4101941939	3.0204469454
H	-3.8610700871	1.6324980542	4.2432179295
C	-5.8400617469	-1.4006970174	-2.4206244749
H	-4.8817997036	-2.5793597772	-3.9493282520
H	-5.9296576061	0.3355250229	3.7691192988
H	-6.1910321180	-0.8137305054	1.5907982089
H	-6.5082490370	-0.2075843799	-0.7588173918
H	-6.7894707352	-1.3414175448	-2.9428471686
C	2.6634970548	-1.9491192234	0.4678106236
C	2.2357285418	-2.6014931189	1.6230039211
C	3.4875369732	-2.5788439050	-0.4545755565
C	2.6886590279	-3.8903884592	1.8788742150
H	1.5345567287	-2.1121034398	2.2928392595
C	3.9308312810	-3.8728036554	-0.1860134059
H	3.7455111230	-2.0650606538	-1.3723008773
C	3.5435169618	-4.5256849338	0.9796133084
H	2.3588911863	-4.4042140637	2.7758564197
H	4.5754238472	-4.3727930141	-0.9018021222
H	3.8905775520	-5.5342045319	1.1797346208
C	4.2648728501	1.4683218066	-1.2147598403
H	4.4573687350	1.2205337180	-2.2662917214
H	4.5411610429	2.5234459464	-1.0831910742
C	0.8522078176	2.2653191372	0.5798609469
H	0.2127397558	1.8243154020	-0.1899623210
H	0.4550440727	1.8926068261	1.5309035201
C	0.6765244438	3.7879374026	0.5806759937
H	1.3632629661	4.2245199808	1.3209543025
H	-0.3372451170	3.9964675473	0.9429531693
C	0.8581430796	4.5237000068	-0.7506281359
H	0.5734208689	5.5684538755	-0.5839099551
H	0.1395837176	4.1306337085	-1.4825018994
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H	2.5429054697	5.4660698203	-1.7367222224
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C	2.0256367412	2.0334502396	-2.1685382256

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H	2.2270376455	1.4199253877	-3.0568273934
C	2.4468386490	3.4692390038	-2.4828143275
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H	1.8351195057	3.8051460675	-3.3293936268
C	5.1268369030	0.9565948522	1.1446053245
H	5.1125399338	2.0480278161	1.2645375682
H	6.0399553973	0.6117494107	1.6417599946
C	3.9417424412	0.3285769385	1.8816055675
H	3.8724017800	0.7777761015	2.8790518079
H	4.1388747182	-0.7357612838	2.0484637362
C	5.1887293699	0.6177090728	-0.3437815480
H	4.9730128285	-0.4469542935	-0.4891739486
H	6.2119478166	0.7737863581	-0.7033687939
H	1.4236722275	-0.1556103794	-1.5223200579

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C	2.5646115152	-1.9719108508	-0.8342570270
C	2.2408632184	-2.5153677439	0.3947327080
H	2.9930724024	-3.1855173718	0.8123176645
H	1.7905149502	-1.6355493153	-1.5201607852
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C	-3.0782216028	-1.2560018880	-0.5509423626
C	-3.2303226082	1.6746624685	0.2774088122
C	-4.2059037596	-0.4309898324	-0.6641431807
C	-2.9556154405	-2.4199358309	-1.3006193343
C	-4.3212332765	0.8056381260	0.1400758340
C	-3.3200122416	2.8378358821	1.0322479658
C	-5.2176753732	-0.8239151180	-1.5459459479
C	-3.9735272214	-2.7890528044	-2.1726392425
H	-2.0603246555	-3.0204279522	-1.1784254505
C	-5.5180718837	1.1532815454	0.7746957421
C	-4.5197787756	3.1608416387	1.6561151010
H	-2.4429574577	3.4709769636	1.1090196491
C	-5.1097142102	-1.9916284111	-2.2928792622
H	-3.8785728729	-3.6978437516	-2.7587109322
C	-5.6228972680	2.3197594540	1.5237467443
H	-4.5922868198	4.0688838685	2.2464208622
H	-5.9050359116	-2.2724281953	-2.9757582986
H	-6.0898006280	-0.1850698569	-1.6546547500
H	-6.3671209559	0.4805918314	0.6895186431
H	-6.5599429159	2.5661025521	2.0126758988
C	3.2668432635	1.4104533416	-0.6384675849
C	3.3818106942	1.6447663221	-2.0144842042
C	4.0206131156	2.1683997419	0.2601852579

C	4.2563607971	2.6172625845	-2.4809948749
H	2.7693991819	1.0664739803	-2.7020584518
C	4.9018731257	3.1324468711	-0.2224853158
H	3.8828221469	2.0176777931	1.3260143841
C	5.0292000544	3.3603603211	-1.5893104506
H	4.3340128743	2.7956075601	-3.5489863144
H	5.4808414415	3.7209285029	0.4827699963
H	5.7134489950	4.1175103894	-1.9571789548
C	4.0115589888	-1.8901200483	-1.2115074159
H	4.1879487720	-0.9594185085	-1.7616573108
H	4.2686509621	-2.7101158794	-1.8969113901
C	2.3520143059	-1.6545027058	2.7722501427
H	2.3527280404	-0.9073730825	3.5730896015
H	3.0047035940	-2.4740549073	3.0884699571
C	0.8714563992	-2.6846125469	1.0001605142
H	0.1280818087	-2.1435833381	0.4114513432
H	0.5903132344	-3.7422563443	0.9796812421
C	0.9219895488	-2.1587242922	2.4669787964
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C	2.7204900807	-1.9361041489	-1.0950159793
C	2.2112235574	-2.5480409418	0.0401474618
H	2.8602145538	-3.3014365792	0.4957278431
H	2.0409538886	-1.5352864497	-1.8425149094
O	-0.4003937525	0.8190476253	1.2665662885
P	-1.0414034486	0.4766191448	-0.0440754651
O	-2.0393289704	-0.7971874137	0.2615623766
O	-2.1287864960	1.5976102132	-0.5137804211
C	-3.0323257117	-1.1238154196	-0.6333317610
C	-3.2740263767	1.7946857257	0.2264164085
C	-4.1956624524	-0.3437369137	-0.6975972791
C	-2.8963068612	-2.2808285700	-1.3917222509
C	-4.3316259802	0.8815297921	0.1207373800
C	-3.3843862829	2.9475311800	0.9942953334
C	-5.2248993786	-0.7724661117	-1.5417699746
C	-3.9323849081	-2.6863618172	-2.2253292522
H	-1.9744911036	-2.8471685445	-1.3079357165
C	-5.5179318903	1.1738712652	0.8015926278
C	-4.5729061136	3.2151801884	1.6640005607

H	-2.5323688830	3.6165250711	1.0444819446
C	-5.1016697938	-1.9323714943	-2.2983817847
H	-3.8257779137	-3.5893680143	-2.8183222120
C	-5.6439645746	2.3292408825	1.5643178366
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H	-6.1247588527	-0.1676901167	-1.6128059507
H	-6.3407237578	0.4667334399	0.7413567369
H	-6.5720134928	2.5322371372	2.0890081489
C	3.2656773929	1.4828495159	-0.5717774965
C	3.9628038781	2.1195181041	0.4558898981
C	3.4299732158	1.9033366303	-1.8950755302
C	4.8369289941	3.1593151497	0.1497536005
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C	4.2965333756	2.9493580136	-2.1844685438
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H	4.4142662917	3.2745552893	-3.2134838507
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C	4.1978581966	-1.9361137539	-1.3216048880
H	4.4523027386	-1.4950582181	-2.2881585229
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C	2.2407310287	-1.7305471053	2.6553550445
H	2.7778274269	-2.6559807253	2.8934588891
H	2.5018832418	-1.0046910653	3.4361600162
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H	0.1913012939	-1.8909687879	-0.1542696051
H	0.4258820318	-3.6071811263	-0.4255663005
C	0.3298665145	-3.0864026507	1.6610028181
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H	0.7918037718	-4.0392447549	1.9594273027
C	0.7292797986	-1.9973209001	2.6566594560
H	0.4477217595	-2.3090013019	3.6679216295
H	0.1649814750	-1.0817186036	2.4460748725
C	4.3063052748	-1.3258148578	1.1916642117
H	4.7422275379	-0.5711787004	1.8611280999
H	4.5771853811	-2.3023012223	1.6080429697
C	4.9365170771	-1.1673322038	-0.1960227058
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H	1.2174905413	0.1687688436	1.2643063671

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H	1.1448530613	0.0832030932	1.2592587010
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C	2.5182390757	-1.1006550626	-1.5968204592
C	2.1634887421	-2.0460674141	-0.6603191823
H	2.9317211818	-2.7873688725	-0.4447624470

H	1.7542037551	-0.5896239599	-2.1787966106
O	-0.5496416417	0.0646677327	1.4257305387
P	-1.1789172194	0.3624594043	0.0944665078
O	-2.1965776843	-0.8845693492	-0.2209499743
O	-2.2453737509	1.5950604272	0.2019791292
C	-3.2036573640	-0.7380974365	-1.1482628145
C	-3.3778426465	1.4462121069	0.9720066881
C	-4.3524950815	-0.0043938648	-0.8199122845
C	-3.0951816050	-1.4027366060	-2.3642746670
C	-4.4559779495	0.7010455188	0.4763262480
C	-3.4553509746	2.1129376788	2.1886854111
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C	-4.1466260661	-1.3568237981	-3.2727003084
H	-2.1839266466	-1.9532649273	-2.5720615257
C	-5.6288613208	0.6614789165	1.2370052204
C	-4.6309621820	2.0567537667	2.9286659037
H	-2.5880628092	2.6687673482	2.5275738400
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H	-4.0615663051	-1.8758694519	-4.2223063637
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H	-6.1249013522	-0.6009062283	-3.6704318272
H	-6.2862523314	0.6046343007	-1.5121880993
H	-6.4673143025	0.0748942650	0.8715127296
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C	3.8844221482	2.3952418253	0.8342165913
C	3.2382415681	2.6599233969	-1.4824754530
C	4.7593287761	3.4704209102	0.7006340506
H	3.7507602731	1.8979128215	1.7895551489
C	4.1054035625	3.7381942932	-1.5979229398
H	2.6283647298	2.3396471053	-2.3235854448
C	4.8788802243	4.1441199687	-0.5108016761
H	5.3385161219	3.7918987886	1.5608690544
H	4.1775138651	4.2645494542	-2.5445401933
H	5.5578487420	4.9848075317	-0.6056343380
C	3.9680846548	-0.8560435860	-1.8805774910
H	4.1366040949	0.2143353896	-2.0425031840
H	4.2546548246	-1.3572336221	-2.8158419178
C	2.4216122942	-1.8755629798	2.1722377923
H	3.0627567052	-1.5451446943	3.0000156602
H	1.3963572184	-1.5975979384	2.4460480220
C	2.5110543937	-3.4078236581	2.0426844285
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H	4.6728871210	0.0546343856	0.8678497376
H	4.8539264060	-1.6065553249	1.4003896317
C	4.8432902791	-1.3777999467	-0.7367261966
H	5.8661215399	-1.0099574223	-0.8581184502
H	4.9091116319	-2.4698642432	-0.7927623309
C	1.1977030189	-4.0851744257	1.6095957699
H	0.3974342171	-3.6818881524	2.2436170837
H	1.2709394828	-5.1520770033	1.8507337154
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H	0.2613774714	-1.8682799899	0.3527301329

H	0.1528245089	-2.4371141514	-1.2936851414
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H	1.4267519092	-4.5635015583	-0.4913279985
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C	-2.5990303381	-1.1729732969	1.5655462430
C	-2.1026333814	-1.9840534972	0.5589862867
H	-2.7640372747	-2.8018198311	0.2668833293
H	-1.9106282024	-0.6507565463	2.2247172492
O	0.5521126214	0.3657842323	-1.4365655451
P	1.1863289162	0.5824510292	-0.0929730597
O	2.1844208071	-0.7014883170	0.1467719004
O	2.2754146473	1.7990974559	-0.1262639667
C	3.1812719416	-0.6373063065	1.0929954994
C	3.4183978553	1.6762196695	-0.8841408571
C	4.3431201784	0.1031505256	0.8324102519
C	3.0513949298	-1.3914503273	2.2537747604
C	4.4774812863	0.8877474348	-0.4147615178
C	3.5275653183	2.4128035875	-2.0575389093
C	5.3750525780	0.0548416788	1.7750582927
C	4.0904884527	-1.4232444636	3.1768938549
H	2.1347746189	-1.9520844010	2.4064453470
C	5.6633382882	0.8764807685	-1.1561792683
C	4.7155925156	2.3836994600	-2.7789491514
H	2.6745476854	3.0011325429	-2.3772572478
C	5.2567456473	-0.6999316060	2.9365227045
H	3.9885287601	-2.0115273267	4.0834941895
C	5.7880513852	1.6179643262	-2.3254235264
H	4.8031359795	2.9584233254	-3.6956516663
C	-3.1520098942	2.0529435593	0.3906600444
C	-3.2900110088	2.7148099531	1.6144912904
C	-3.8722977452	2.4865644113	-0.7233860133
C	-4.1520156364	3.7985678629	1.7201401602
H	-2.7159573528	2.3714602271	2.4710968659
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O	0.6158250261	0.1828849934	-1.4409815338
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C	4.2974094989	-1.3731997526	1.1618966376
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H	-1.7872666198	-2.7645295266	-1.3623393659
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H	5.0725005275	2.6029328856	-3.3425372851
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N	2.4779894633	0.4428068926	-0.3849574683
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C	2.4031174256	-2.4010674425	-0.2280961692
H	2.8730765641	-3.1533540835	0.4091749354
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O	-0.3551196851	0.6992419991	1.3762162684

P	-0.9811420873	0.6814592151	0.0122146404
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O	-2.1173878295	1.8361569802	-0.1623702006
C	-2.8850789093	-0.8041443202	-0.9959635118
C	-3.2791715177	1.7806946753	0.5770010541
C	-4.0854002936	-0.0886529395	-0.8849456480
C	-2.6788765436	-1.7164819942	-2.0239011018
C	-4.2892555414	0.8784899549	0.2162067658
C	-3.4551141935	2.6910164551	1.6119773767
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C	3.7210065157	1.8134179153	-1.9141761033
C	5.2166347649	2.9132672111	0.1584244938
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H	5.0034848680	-0.4690760088	-0.9411140934
H	5.3151799492	-2.1884382992	-0.7382300670
C	2.3232583702	-1.6989877671	2.5839966863
C	0.9273429400	-2.5184560640	-0.4959668705
H	0.4988886694	-1.5122653211	-0.4207180103
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H	4.9008507072	-0.4052663974	1.4466763242
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H	-0.1034082807	-4.1038619508	2.4444973431
H	0.5638861080	-2.2683003243	3.6264742975
H	0.1972488900	-1.4092951130	2.1507044784
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C	-2.2707597846	-2.3918796847	-0.4593020116
H	-2.8340508224	-3.0620406529	-1.1143753533
H	-2.5487279447	-1.6197011747	1.5504543891
O	0.5522117880	0.3549797574	-1.5694220810
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C	4.2398115823	-0.4831020568	0.7470804270
C	2.8086137399	-2.1268434048	1.8332452664
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C	3.6603312341	2.3310530644	-1.7233015816
C	5.2196796402	-0.7481017855	1.7089342136
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C	5.6843538606	0.5586075895	-1.0199254420
C	4.8795379679	2.3689016299	-2.3903305677
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H	-5.5736374696	3.5432484179	-0.3251240463
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H	-4.7230498614	-0.5628004481	0.8632508660
H	-5.0741134695	-2.2379430620	0.4534215639
C	-4.3739595089	-1.0481808210	-1.2558902643
H	-4.9298329713	-0.1288899388	-1.4726950680
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C	-0.7741383163	-2.5596059967	-0.3928832630
H	-0.3344573780	-1.8785900030	-1.1288723889
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H	-0.1887832617	-4.5257406671	0.3044725436
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H	-3.0815070710	-0.3422136552	-3.7517314436
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H	-0.9312796263	-4.5443569417	-1.2709684720

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H	-2.8021856962	-2.5256416616	0.6075317758
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O	0.7437706938	0.1921762525	-1.4305891646
P	1.3802506625	0.5028404790	-0.1061340316
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C	4.5336273459	0.0286055938	0.8329253685
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C	4.6701811403	0.6944437019	-0.4811354718
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H	2.2845725401	-1.7885498539	2.6256254006
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H	2.8932589674	2.6828008908	-2.5925171448
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C	-2.9559919652	2.9804178737	1.3944589466
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C	-3.7904324657	4.0895143221	1.4603757185
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H	-3.5999090226	2.0047059771	-1.7973855270
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H	-5.1109138092	3.9693714131	-1.6612086888
H	-5.2321125870	5.3114709546	0.4243094825
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H	-4.5013486383	-0.4489727403	-1.8296267052
H	-4.3820573500	-1.9844766642	-1.0026389808
C	-0.5806132100	-2.3128307491	0.4760299483
H	-0.1049517600	-1.7975438022	-0.3659321343
H	0.0331827917	-2.0410795473	1.3413449362
C	-0.4918992817	-3.8272444196	0.2589085454
H	-1.1001956493	-4.3402052520	1.0174214132
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H	-0.9648117185	-1.6508306109	-2.1304827073
H	-2.2544407612	-0.9918562099	-3.0912391064
C	-2.6080248515	-3.0174707020	-2.5417513611
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H	-5.6156012254	-0.8347868579	2.2528339281
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H	-3.4439641010	-1.0174107157	3.3598573319
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C	0	5.8617810000	-3.1044290000	0.6912140000
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H	0	2.7066960000	-4.3101740000	0.3370580000
H	0	2.5956892800	-3.1147411400	-1.0758660900
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O	-1.6060538887	-1.1222356358	1.0206194326
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C	-2.9238008110	-1.3260077906	0.6320886889
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C	-1.4221123412	2.7285196474	-0.2348454118
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H	-2.7417213091	-3.4364993942	0.8723496349
C	-3.3826290568	3.5015303426	0.9335236160
H	-1.7367878793	4.7678477753	0.3568477416
C	-5.5919763955	-1.7600311030	0.0516350876
H	-5.1534307878	-3.8503634386	0.3399864070
H	-3.9467460750	4.3034304989	1.3981303974
H	-4.8463414099	1.9970069121	1.4062331953
H	-5.7194217884	0.3731749098	-0.2017484228
H	-6.6385265953	-1.9256280218	-0.1819404336
C	3.9325466531	0.0251721859	0.1754753019
C	4.9761350610	-0.7952087194	0.6003632295

C	3.9418862891	1.3862515617	0.4943819271
C	6.0331133597	-0.2426365336	1.3190727330
H	4.9400562741	-1.8521948711	0.3683205864
C	5.0028172077	1.9253554877	1.2123983991
H	3.1074175072	2.0152840758	0.1956083299
C	6.0573072368	1.1145903487	1.6253353202
H	6.8456127679	-0.8862825148	1.6425509115
H	4.9984547336	2.9830987170	1.4567366453
H	6.8842353698	1.5358030135	2.1875937596
H	1.9716475285	-2.2542857945	-0.7582358053
H	1.3608781070	-1.1378603906	-3.0278128060
H	3.2379245655	1.0091461760	-1.9868728707
H	4.3104434171	-1.7139871290	-2.4194036540
H	3.0169429317	-2.9049953864	-2.6968407908

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C	0	-2.8060080000	1.7454320000	0.9120920000
N	0	-2.6265490000	0.5205030000	0.5588900000
N	0	-3.0201270000	0.0630520000	-0.7112840000
H	0	-2.1561270000	0.1266740000	-1.2826200000
H	0	-1.9082250000	-0.1123130000	1.0341220000
O	0	-0.3695050000	0.0328410000	-1.4813090000
C	0	-1.1959490000	3.1556550000	-0.5372300000
C	0	-0.9270260000	3.9020850000	0.5346800000
H	0	-1.6117240000	4.7173860000	0.7839010000
H	0	-0.5596360000	2.3047870000	-0.7891810000
O	0	-0.4595230000	-0.8343650000	0.9687280000
P	0	0.3359700000	-0.4462980000	-0.2505290000

O	0	1.4002430000	0.6966810000	0.2743280000
O	0	1.3596730000	-1.6313210000	-0.6912900000
C	0	2.5257020000	0.9865270000	-0.4680210000
C	0	2.3821400000	-2.0021570000	0.1573400000
C	0	3.6076550000	0.0948420000	-0.4615370000
C	0	2.5956140000	2.2064370000	-1.1311970000
C	0	3.5239160000	-1.1966020000	0.2564380000
C	0	2.2856620000	-3.2143620000	0.8290260000
C	0	4.7715270000	0.4757120000	-1.1367980000
C	0	3.7640960000	2.5616590000	-1.7966310000
H	0	1.7302050000	2.8622260000	-1.1130220000
C	0	4.5828780000	-1.6606620000	1.0439220000
C	0	3.3506400000	-3.6529740000	1.6076550000
H	0	1.3746470000	-3.7926260000	0.7210100000
C	0	4.8558500000	1.6964500000	-1.7968780000
H	0	3.8192010000	3.5129440000	-2.3163260000
C	0	4.5036170000	-2.8772010000	1.7119370000
H	0	3.2789760000	-4.5996600000	2.1337380000
H	0	5.7675750000	1.9668830000	-2.3195700000
H	0	5.6114030000	-0.2132920000	-1.1542310000
H	0	5.4691990000	-1.0400420000	1.1429050000
H	0	5.3355680000	-3.2140380000	2.3219490000
C	0	-3.4529430000	-1.2955190000	-0.6585460000
C	0	-4.4384520000	-1.6844530000	0.2477910000
C	0	-2.9154890000	-2.2165830000	-1.5578030000
C	0	-4.8854840000	-3.0015110000	0.2535110000
H	0	-4.8547400000	-0.9542490000	0.9362200000
C	0	-3.3848520000	-3.5255660000	-1.5561630000
H	0	-2.1199330000	-1.9033680000	-2.2284700000
C	0	-4.3668530000	-3.9240290000	-0.6516670000
H	0	-5.6496520000	-3.3044990000	0.9625850000

H	0	-2.9650480000	-4.2423940000	-2.2548020000
H	0	-4.7221330000	-4.9493040000	-0.6484310000
C	0	-2.5801470000	3.1679380000	-1.1483700000
H	0	-2.6390310000	2.4926230000	-2.0041980000
H	0	-2.8940620000	4.1636780000	-1.4767000000
C	0	-3.5451840000	2.6800610000	-0.0201410000
H	0	-4.4140850000	2.1613950000	-0.4344860000
H	0	-3.8783770000	3.5390030000	0.5679700000
H	0	-2.4064772800	2.0409098500	1.8597037600
H	0	-0.2754365400	3.5730299600	1.3170187800

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C	0	3.6335510000	-0.0025420000	0.5500630000
N	0	2.5363990000	0.5934110000	0.2471240000
N	0	2.3455760000	1.1835380000	-1.0221440000
H	0	1.6936150000	0.5367530000	-1.4975950000
O	0	0.1972830000	-0.5785220000	-1.3420050000
C	0	3.0508080000	-2.3967440000	-0.8172130000
C	0	3.0183570000	-2.9834430000	0.3797160000
H	0	3.9306190000	-3.4551760000	0.7585430000
H	0	2.1405370000	-1.9278760000	-1.2025190000
O	0	0.1061900000	0.3542250000	1.0735750000
P	0	-0.6047260000	-0.2058920000	-0.1352330000
O	0	-1.4931590000	-1.4563090000	0.4280650000
O	0	-1.7846400000	0.8033930000	-0.6370600000
C	0	-2.5845450000	-1.9135050000	-0.2792260000
C	0	-2.8306250000	1.0885940000	0.2145490000
C	0	-3.7766440000	-1.1751860000	-0.2793680000

C	0	-2.4980800000	-3.1521290000	-0.9030290000
C	0	-3.8546230000	0.1474590000	0.3804640000
C	0	-2.8769770000	2.3362550000	0.8235990000
C	0	-4.8893900000	-1.7350560000	-0.9154640000
C	0	-3.6176550000	-3.6861080000	-1.5310030000
H	0	-1.5489830000	-3.6767420000	-0.8760890000
C	0	-4.9507560000	0.5103670000	1.1696250000
C	0	-3.9764490000	2.6721510000	1.6057360000
H	0	-2.0474090000	3.0180280000	0.6646110000
C	0	-4.8178340000	-2.9784530000	-1.5332700000
H	0	-3.5516390000	-4.6532820000	-2.0192380000
C	0	-5.0169100000	1.7601160000	1.7753280000
H	0	-4.0196200000	3.6450590000	2.0852270000
H	0	-5.6935090000	-3.3886980000	-2.0257870000
H	0	-5.8154200000	-1.1671360000	-0.9376070000
H	0	-5.7472510000	-0.2130290000	1.3208570000
H	0	-5.8739880000	2.0178390000	2.3891820000
C	0	1.7062090000	2.4563620000	-0.8906540000
C	0	2.2383520000	3.4249120000	-0.0400440000
C	0	0.5715950000	2.7340460000	-1.6527110000
C	0	1.6290670000	4.6713730000	0.0509160000
H	0	3.1250520000	3.1982480000	0.5458690000
C	0	-0.0209370000	3.9897020000	-1.5656840000
H	0	0.1404040000	1.9564730000	-2.2770940000
C	0	0.5010160000	4.9608610000	-0.7140480000
H	0	2.0419890000	5.4216860000	0.7180590000
H	0	-0.9093490000	4.1986390000	-2.1534860000
H	0	0.0300210000	5.9359430000	-0.6433400000
C	0	4.3090300000	-2.2165520000	-1.6134410000
H	0	4.2034450000	-2.6291630000	-2.6240790000
H	0	5.1367150000	-2.7503440000	-1.1286190000

C	0	4.8120680000	0.0093290000	-0.3926690000
H	0	5.0216300000	1.0638470000	-0.6109580000
H	0	5.6719120000	-0.4009320000	0.1465320000
C	0	4.6458820000	-0.7240540000	-1.7413640000
H	0	3.8695180000	-0.2170440000	-2.3183450000
H	0	5.5853350000	-0.6008440000	-2.2913140000
H	0	1.6154900000	0.5357440000	0.8114640000
H	0	3.7648937500	-0.3733572600	1.5451233600
H	0	2.1820910000	-2.9829537200	1.0472180200

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C	0	2.3604790000	-1.9046850000	-0.5560380000
N	0	1.4512450000	-1.0062640000	-0.5573120000
N	0	1.1367810000	-0.4116240000	-1.8090320000
H	0	0.3582200000	-0.9520300000	-2.1980150000
O	0	-1.4853550000	-1.6054260000	-1.5526370000
C	0	5.3918440000	1.1497760000	-0.2891870000
C	0	6.1333700000	0.7705870000	0.7509630000
H	0	7.0212790000	0.1574890000	0.5762570000
H	0	4.5040340000	1.7594390000	-0.1001870000
O	0	-0.7933230000	-0.6416170000	0.7612140000
P	0	-1.8968550000	-0.9083200000	-0.3196500000
O	0	-3.0241020000	-1.6229220000	0.5846520000
O	0	-2.5890680000	0.5021180000	-0.6746880000
C	0	-4.3658790000	-1.5371610000	0.2439580000
C	0	-3.1359450000	1.2624340000	0.3475220000
C	0	-5.0610120000	-0.3352420000	0.4299560000
C	0	-5.0028820000	-2.6936840000	-0.1850130000

C	0	-4.3720320000	0.8925600000	0.8862590000
C	0	-2.4606270000	2.4049310000	0.7514290000
C	0	-6.4365080000	-0.3387930000	0.1744590000
C	0	-6.3706380000	-2.6692890000	-0.4333880000
H	0	-4.4126500000	-3.5950760000	-0.3079190000
C	0	-4.9336270000	1.7351510000	1.8516240000
C	0	-3.0403950000	3.2239990000	1.7139170000
H	0	-1.5005630000	2.6282260000	0.2956470000
C	0	-7.0895180000	-1.4902190000	-0.2495170000
H	0	-6.8724820000	-3.5705110000	-0.7702660000
C	0	-4.2787730000	2.8911240000	2.2609800000
H	0	-2.5232950000	4.1213510000	2.0383580000
H	0	-8.1562010000	-1.4643590000	-0.4466250000
H	0	-6.9886080000	0.5889810000	0.2946560000
H	0	-5.8856960000	1.4592040000	2.2960710000
H	0	-4.7295440000	3.5267260000	3.0162240000
C	0	0.7705310000	0.9457870000	-1.6824850000
C	0	1.3867600000	1.7744410000	-0.7394870000
C	0	-0.1769250000	1.4844370000	-2.5604090000
C	0	1.0784370000	3.1322330000	-0.7020340000
H	0	2.0975320000	1.3480980000	-0.0381050000
C	0	-0.4744490000	2.8397520000	-2.5146280000
H	0	-0.6889710000	0.8277780000	-3.2585270000
C	0	0.1569470000	3.6758420000	-1.5930880000
H	0	1.5668310000	3.7671190000	0.0316210000
H	0	-1.2158520000	3.2438340000	-3.1969130000
H	0	-0.0782980000	4.7347660000	-1.5625650000
C	0	3.2043860000	-2.3009150000	-1.7404210000
H	0	3.3803860000	-3.3804050000	-1.6799630000
H	0	2.6920820000	-2.0848560000	-2.6793330000
C	0	4.4511830000	-0.1147350000	-2.2178720000

H	0	3.5036120000	0.3393850000	-1.9044650000
H	0	4.4263190000	-0.1408980000	-3.3133810000
C	0	5.6074130000	0.7711180000	-1.7252810000
H	0	5.6553130000	1.6765000000	-2.3421260000
H	0	6.5655350000	0.2483160000	-1.8419790000
C	0	4.5478810000	-1.5445270000	-1.6817880000
H	0	4.9052890000	-1.5177190000	-0.6425840000
H	0	5.3002480000	-2.0999450000	-2.2532260000
H	0	0.1537610000	-0.7557100000	0.3867300000
H	0	5.9056276100	1.0088393800	1.7689360900
H	0	2.5463838800	-2.4292548000	0.3578361200

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C	0	-2.8060080000	1.7454320000	0.9120920000
N	0	-2.6265490000	0.5205030000	0.5588900000
N	0	-3.0201270000	0.0630520000	-0.7112840000
H	0	-2.1561270000	0.1266740000	-1.2826200000
H	0	-1.9082250000	-0.1123130000	1.0341220000
O	0	-0.3695050000	0.0328410000	-1.4813090000
C	0	-1.1959490000	3.1556550000	-0.5372300000
C	0	-0.9270260000	3.9020850000	0.5346800000
H	0	-1.6117240000	4.7173860000	0.7839010000
H	0	-0.5596360000	2.3047870000	-0.7891810000
O	0	-0.4595230000	-0.8343650000	0.9687280000
P	0	0.3359700000	-0.4462980000	-0.2505290000
O	0	1.4002430000	0.6966810000	0.2743280000
O	0	1.3596730000	-1.6313210000	-0.6912900000
C	0	2.5257020000	0.9865270000	-0.4680210000

C	0	2.3821400000	-2.0021570000	0.1573400000
C	0	3.6076550000	0.0948420000	-0.4615370000
C	0	2.5956140000	2.2064370000	-1.1311970000
C	0	3.5239160000	-1.1966020000	0.2564380000
C	0	2.2856620000	-3.2143620000	0.8290260000
C	0	4.7715270000	0.4757120000	-1.1367980000
C	0	3.7640960000	2.5616590000	-1.7966310000
H	0	1.7302050000	2.8622260000	-1.1130220000
C	0	4.5828780000	-1.6606620000	1.0439220000
C	0	3.3506400000	-3.6529740000	1.6076550000
H	0	1.3746470000	-3.7926260000	0.7210100000
C	0	4.8558500000	1.6964500000	-1.7968780000
H	0	3.8192010000	3.5129440000	-2.3163260000
C	0	4.5036170000	-2.8772010000	1.7119370000
H	0	3.2789760000	-4.5996600000	2.1337380000
H	0	5.7675750000	1.9668830000	-2.3195700000
H	0	5.6114030000	-0.2132920000	-1.1542310000
H	0	5.4691990000	-1.0400420000	1.1429050000
H	0	5.3355680000	-3.2140380000	2.3219490000
C	0	-3.4529430000	-1.2955190000	-0.6585460000
C	0	-4.4384520000	-1.6844530000	0.2477910000
C	0	-2.9154890000	-2.2165830000	-1.5578030000
C	0	-4.8854840000	-3.0015110000	0.2535110000
H	0	-4.8547400000	-0.9542490000	0.9362200000
C	0	-3.3848520000	-3.5255660000	-1.5561630000
H	0	-2.1199330000	-1.9033680000	-2.2284700000
C	0	-4.3668530000	-3.9240290000	-0.6516670000
H	0	-5.6496520000	-3.3044990000	0.9625850000
H	0	-2.9650480000	-4.2423940000	-2.2548020000
H	0	-4.7221330000	-4.9493040000	-0.6484310000
C	0	-2.2395040000	2.1643970000	2.2557330000

H	0	-2.6888280000	3.1218520000	2.5345780000
H	0	-2.5764940000	1.4200160000	2.9867320000
C	0	-0.0123890000	3.4401900000	1.6328500000
H	0	0.9532200000	3.1021040000	1.2431770000
H	0	0.1784360000	4.2477310000	2.3452190000
C	0	-0.6866590000	2.2316750000	2.3474610000
H	0	-0.4317600000	2.2399600000	3.4117350000
H	0	-0.2826380000	1.3007900000	1.9405010000
H	0	-2.1747574800	3.1643406800	-0.9693856700
H	0	-3.3287790100	2.4064341800	0.2527843500

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C	0	3.6335510000	-0.0025420000	0.5500630000
N	0	2.5363990000	0.5934110000	0.2471240000
N	0	2.3455760000	1.1835380000	-1.0221440000
H	0	1.6936150000	0.5367530000	-1.4975950000
O	0	0.1972830000	-0.5785220000	-1.3420050000
C	0	3.0508080000	-2.3967440000	-0.8172130000
C	0	3.0183570000	-2.9834430000	0.3797160000
H	0	3.9306190000	-3.4551760000	0.7585430000
H	0	2.1405370000	-1.9278760000	-1.2025190000
O	0	0.1061900000	0.3542250000	1.0735750000
P	0	-0.6047260000	-0.2058920000	-0.1352330000
O	0	-1.4931590000	-1.4563090000	0.4280650000
O	0	-1.7846400000	0.8033930000	-0.6370600000
C	0	-2.5845450000	-1.9135050000	-0.2792260000
C	0	-2.8306250000	1.0885940000	0.2145490000
C	0	-3.7766440000	-1.1751860000	-0.2793680000

C	0	-2.4980800000	-3.1521290000	-0.9030290000
C	0	-3.8546230000	0.1474590000	0.3804640000
C	0	-2.8769770000	2.3362550000	0.8235990000
C	0	-4.8893900000	-1.7350560000	-0.9154640000
C	0	-3.6176550000	-3.6861080000	-1.5310030000
H	0	-1.5489830000	-3.6767420000	-0.8760890000
C	0	-4.9507560000	0.5103670000	1.1696250000
C	0	-3.9764490000	2.6721510000	1.6057360000
H	0	-2.0474090000	3.0180280000	0.6646110000
C	0	-4.8178340000	-2.9784530000	-1.5332700000
H	0	-3.5516390000	-4.6532820000	-2.0192380000
C	0	-5.0169100000	1.7601160000	1.7753280000
H	0	-4.0196200000	3.6450590000	2.0852270000
H	0	-5.6935090000	-3.3886980000	-2.0257870000
H	0	-5.8154200000	-1.1671360000	-0.9376070000
H	0	-5.7472510000	-0.2130290000	1.3208570000
H	0	-5.8739880000	2.0178390000	2.3891820000
C	0	1.7062090000	2.4563620000	-0.8906540000
C	0	2.2383520000	3.4249120000	-0.0400440000
C	0	0.5715950000	2.7340460000	-1.6527110000
C	0	1.6290670000	4.6713730000	0.0509160000
H	0	3.1250520000	3.1982480000	0.5458690000
C	0	-0.0209370000	3.9897020000	-1.5656840000
H	0	0.1404040000	1.9564730000	-2.2770940000
C	0	0.5010160000	4.9608610000	-0.7140480000
H	0	2.0419890000	5.4216860000	0.7180590000
H	0	-0.9093490000	4.1986390000	-2.1534860000
H	0	0.0300210000	5.9359430000	-0.6433400000
C	0	3.8185670000	-0.5248910000	1.9517550000
H	0	4.5487100000	-1.3388640000	1.9089290000
H	0	4.3332900000	0.3040240000	2.4631110000

C	0	1.8458630000	-2.9827570000	1.3155930000
H	0	1.0238890000	-2.3923010000	0.8941070000
H	0	1.4697420000	-4.0062600000	1.4444770000
C	0	2.2345030000	-2.4431080000	2.7005880000
H	0	1.4020010000	-2.6168340000	3.3902890000
H	0	3.0830300000	-3.0287570000	3.0834920000
C	0	2.5846940000	-0.9508790000	2.7719760000
H	0	2.8033450000	-0.7149300000	3.8186190000
H	0	1.6997210000	-0.3633640000	2.5114040000
H	0	1.6154900000	0.5357440000	0.8114640000
H	0	3.9484253100	-2.2681947800	-1.3852431600
H	0	4.4690830000	0.0058741700	-0.1183047500

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C	0	3.5123530000	0.5066710000	0.6949520000
N	0	2.3409350000	0.8752990000	0.3221410000
N	0	2.1317280000	1.4821340000	-0.9378600000
H	0	1.5907500000	0.7689810000	-1.4513610000
H	0	1.3802030000	0.6613580000	0.8342040000
O	0	0.1939500000	-0.5477030000	-1.2763720000
C	0	3.3702520000	-1.8162610000	-1.2724980000
C	0	3.6900170000	-2.8013010000	-0.4298030000
H	0	4.7401540000	-2.9618130000	-0.1685330000
H	0	2.3200590000	-1.6597820000	-1.5278000000
O	0	-0.0538450000	0.4698820000	1.0854160000
P	0	-0.6841390000	-0.1978880000	-0.1177390000
O	0	-1.4954120000	-1.4856570000	0.4750720000
O	0	-1.9178850000	0.7015430000	-0.6898020000

C	0	-2.5547120000	-2.0344720000	-0.2163190000
C	0	-2.9859570000	0.9654970000	0.1425020000
C	0	-3.7893360000	-1.3699130000	-0.2538040000
C	0	-2.3925630000	-3.2932110000	-0.7823680000
C	0	-3.9530800000	-0.0264080000	0.3450910000
C	0	-3.1061670000	2.2324770000	0.6989400000
C	0	-4.8624980000	-2.0232360000	-0.8684360000
C	0	-3.4742010000	-3.9208170000	-1.3899020000
H	0	-1.4153320000	-3.7607210000	-0.7268320000
C	0	-5.0748010000	0.3050270000	1.1119090000
C	0	-4.2295470000	2.5362910000	1.4600730000
H	0	-2.3134290000	2.9521570000	0.5189840000
C	0	-4.7140290000	-3.2865570000	-1.4291300000
H	0	-3.3475600000	-4.9036780000	-1.8326990000
C	0	-5.2175710000	1.5738180000	1.6621630000
H	0	-4.3319910000	3.5238620000	1.8988290000
H	0	-5.5608010000	-3.7696650000	-1.9058190000
H	0	-5.8203510000	-1.5129380000	-0.9194400000
H	0	-5.8286160000	-0.4566390000	1.2912820000
H	0	-6.0927250000	1.8075460000	2.2599170000
C	0	1.3370430000	2.6645090000	-0.8184660000
C	0	1.6920460000	3.6615350000	0.0892450000
C	0	0.2328770000	2.8321450000	-1.6536710000
C	0	0.9367270000	4.8267280000	0.1616110000
H	0	2.5539800000	3.5207320000	0.7356250000
C	0	-0.5061070000	4.0084590000	-1.5844870000
H	0	-0.0616270000	2.0282980000	-2.3227270000
C	0	-0.1605570000	5.0084290000	-0.6776210000
H	0	1.2114070000	5.5988170000	0.8736210000
H	0	-1.3707950000	4.1305190000	-2.2293930000
H	0	-0.7452810000	5.9208900000	-0.6212170000

C	0	3.6766680000	-0.2452480000	1.9860540000
H	0	4.4023470000	-1.0439730000	1.7801570000
H	0	4.1846450000	0.4427350000	2.6767700000
C	0	2.4074700000	-0.8153910000	2.6277790000
H	0	2.6875230000	-1.2072580000	3.6126650000
H	0	1.6858060000	-0.0116580000	2.8079290000
C	0	1.7359570000	-1.9221690000	1.8073730000
H	0	1.5706220000	-1.5637840000	0.7863290000
H	0	0.7356810000	-2.0918360000	2.2160930000
C	0	2.7139830000	-3.6984870000	0.2754450000
H	0	1.7448890000	-3.6724280000	-0.2370090000
H	0	3.0746740000	-4.7333990000	0.2481990000
C	0	2.5199920000	-3.2456190000	1.7350540000
H	0	3.5074310000	-3.1450450000	2.2089230000
H	0	1.9970640000	-4.0278000000	2.2951970000
H	0	4.0942106300	-1.1699153000	-1.7230766600
H	0	4.3862855800	0.7734616900	0.1382073800

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N	0	1.4512450000	-1.0062640000	-0.5573120000
N	0	1.1367810000	-0.4116240000	-1.8090320000
H	0	0.3582200000	-0.9520300000	-2.1980150000
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C	0	5.3918440000	1.1497760000	-0.2891870000
C	0	6.1333700000	0.7705870000	0.7509630000
H	0	7.0212790000	0.1574890000	0.5762570000
H	0	4.5040340000	1.7594390000	-0.1001870000

O	0	-0.7933230000	-0.6416170000	0.7612140000
P	0	-1.8968550000	-0.9083200000	-0.3196500000
O	0	-3.0241020000	-1.6229220000	0.5846520000
O	0	-2.5890680000	0.5021180000	-0.6746880000
C	0	-4.3658790000	-1.5371610000	0.2439580000
C	0	-3.1359450000	1.2624340000	0.3475220000
C	0	-5.0610120000	-0.3352420000	0.4299560000
C	0	-5.0028820000	-2.6936840000	-0.1850130000
C	0	-4.3720320000	0.8925600000	0.8862590000
C	0	-2.4606270000	2.4049310000	0.7514290000
C	0	-6.4365080000	-0.3387930000	0.1744590000
C	0	-6.3706380000	-2.6692890000	-0.4333880000
H	0	-4.4126500000	-3.5950760000	-0.3079190000
C	0	-4.9336270000	1.7351510000	1.8516240000
C	0	-3.0403950000	3.2239990000	1.7139170000
H	0	-1.5005630000	2.6282260000	0.2956470000
C	0	-7.0895180000	-1.4902190000	-0.2495170000
H	0	-6.8724820000	-3.5705110000	-0.7702660000
C	0	-4.2787730000	2.8911240000	2.2609800000
H	0	-2.5232950000	4.1213510000	2.0383580000
H	0	-8.1562010000	-1.4643590000	-0.4466250000
H	0	-6.9886080000	0.5889810000	0.2946560000
H	0	-5.8856960000	1.4592040000	2.2960710000
H	0	-4.7295440000	3.5267260000	3.0162240000
C	0	0.7705310000	0.9457870000	-1.6824850000
C	0	1.3867600000	1.7744410000	-0.7394870000
C	0	-0.1769250000	1.4844370000	-2.5604090000
C	0	1.0784370000	3.1322330000	-0.7020340000
H	0	2.0975320000	1.3480980000	-0.0381050000
C	0	-0.4744490000	2.8397520000	-2.5146280000
H	0	-0.6889710000	0.8277780000	-3.2585270000

C	0	0.1569470000	3.6758420000	-1.5930880000
H	0	1.5668310000	3.7671190000	0.0316210000
H	0	-1.2158520000	3.2438340000	-3.1969130000
H	0	-0.0782980000	4.7347660000	-1.5625650000
C	0	5.8135770000	1.1051380000	2.1803880000
H	0	6.5843280000	1.7686220000	2.5940350000
H	0	4.8700310000	1.6634590000	2.2127560000
C	0	5.7174910000	-0.1424420000	3.0732120000
H	0	5.3890860000	0.1659090000	4.0736940000
H	0	6.7191130000	-0.5742640000	3.1938190000
C	0	4.7751980000	-1.2236750000	2.5375130000
H	0	5.2021190000	-1.6349050000	1.6135560000
H	0	4.7426660000	-2.0528170000	3.2573180000
C	0	3.3497010000	-0.7318980000	2.2749930000
H	0	3.0075360000	-0.1459320000	3.1381830000
H	0	3.3503430000	-0.0493890000	1.4135850000
C	0	2.6232710000	-2.6462080000	0.7357990000
H	0	3.6571570000	-3.0107050000	0.7162780000
H	0	1.9940170000	-3.5469100000	0.7028250000
C	0	2.3540000000	-1.8691760000	2.0267870000
H	0	1.3316300000	-1.4802170000	2.0164300000
H	0	2.4055660000	-2.5757250000	2.8642300000
H	0	0.1537610000	-0.7557100000	0.3867300000
H	0	2.9595522200	-2.1859610000	-1.3968085300
H	0	5.5455408200	0.8797996500	-1.3130962000

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C	-3.5636741367	0.2977666210	2.2938582234
N	-2.8424768042	0.1658039461	1.2435106210
N	-3.3793879616	0.5469163183	0.0109575526

H	-2.5844933470	0.7571170714	-0.5991977792
O	-0.6595495822	0.8974223524	-0.9376155284
C	-3.3426525148	3.5952286544	2.1655968101
C	-2.1981904345	3.3291388477	2.7961397461
H	-2.1003779427	3.6125418014	3.8464287854
H	-3.4350028176	3.3091246144	1.1155861392
O	-0.3489353892	-0.5477936182	1.1823551113
P	0.2798831497	0.2131486466	-0.0265705490
O	1.3768573631	1.1595634339	0.6891091074
O	1.2080804974	-0.8346118848	-0.8235851409
C	2.4078367704	1.6836909761	-0.0767389434
C	2.3452291023	-1.3704635595	-0.2379380206
C	3.4801584130	0.8592759169	-0.4347479865
C	2.3767984731	3.0336379155	-0.3967240935
C	3.4874114233	-0.5768374095	-0.0782429237
C	2.3361188002	-2.7187706509	0.0919241041
C	4.5466375174	1.4470719764	-1.1228289793
C	3.4487570675	3.5935136481	-1.0830695562
H	1.5140551423	3.6190935673	-0.0972898298
C	4.6395739097	-1.1941775623	0.4202173006
C	3.4942246735	-3.3079203703	0.5866528163
C	4.5363471317	2.7998734119	-1.4427374143
H	3.4324919189	4.6479921145	-1.3386146701
C	4.6489441151	-2.5449659116	0.7477267155
H	5.5303627411	-0.5902513242	0.5678728050
C	-4.3155162347	-0.3116948347	-0.6147167504
C	-4.8463333028	-1.4553110321	-0.0147970367
C	-4.7295117014	0.0372520010	-1.9072685557
C	-5.7851420051	-2.2267651811	-0.6982322214
H	-4.5079640705	-1.7624488418	0.9689724561
C	-5.6578058454	-0.7429326886	-2.5797524691

H	-4.3144153371	0.9283024190	-2.3697880449
C	-6.1996495801	-1.8792255452	-1.9778938065
H	-5.9646137622	-0.4584081595	-3.5816743850
H	-1.3682231586	-0.3123151751	1.2520378742
H	-6.1853451196	-3.1157078279	-0.2196392522
H	-6.9310797697	-2.4840956674	-2.5031864561
H	1.4213813202	-3.2822434583	-0.0554207104
H	5.3808253622	0.8203402951	-1.4250476130
H	3.4933412615	-4.3616607839	0.8458907027
H	5.3717472576	3.2325059850	-1.9833202291
H	5.5536096986	-2.9994534579	1.1380152599
C	-1.0043040709	2.6890415819	2.1539822993
H	-0.1191811517	3.3302206672	2.2401718796
H	-0.7402355218	1.7358367968	2.6294964900
H	-1.1846021546	2.4983242127	1.0908902004
C	-4.5205242907	4.2886322230	2.7850871677
H	-4.3546527291	4.4746628022	3.8505636879
H	-4.7071071186	5.2529284572	2.2985662679
H	-5.4391875804	3.7004146411	2.6773099217
C	-4.9772523063	0.7904456016	2.2902521783
H	-5.1532643414	1.4350132104	1.4257527897
H	-5.6719990691	-0.0556622105	2.2273516814
H	-5.1816227454	1.3342390756	3.2161136295
C	-2.9401201295	-0.0607542599	3.6093527930
H	-1.9341447697	-0.4647073790	3.4782915773
H	-2.8886107323	0.8417531945	4.2296675208
H	-3.5571388603	-0.7921895546	4.1419799200

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C	-2.7100209275	0.6311687305	2.7846143850
N	-3.0295889956	-0.3397026290	1.6943655897
N	-3.0679972167	0.3985258285	0.4360841532
H	-2.0991603531	0.3012520702	-0.0705369518
O	-0.7376016952	0.3285719887	-0.6812356888
C	-3.1638797390	1.8633517564	0.7882420546
C	-2.2827343168	1.9089321134	2.0304146499
O	-0.4586370881	-1.5510457597	1.0688504182
P	0.1662377998	-0.5523612942	0.1607903479
O	1.1308453442	0.4072043977	1.0821726716
O	1.2540842028	-1.1806724593	-0.8718790558
C	2.0512520727	1.2320283048	0.4731484903
C	2.4532038954	-1.6687954763	-0.3940778551
C	3.2329783238	0.6874283076	-0.0480846151
C	1.8213595696	2.6027711336	0.4651043436
C	3.4665629497	-0.7737136022	-0.0272519663
C	2.6538851590	-3.0431670113	-0.3747122040
C	4.1856531720	1.5698247421	-0.5672170175
C	2.7825821087	3.4605545254	-0.0579311734
H	0.8912585183	2.9752617600	0.8830692381
C	4.7044027535	-1.3068738390	0.3462369033
C	3.8924187221	-3.5492723585	0.0033917474
C	3.9693684617	2.9432392932	-0.5726652811
H	2.6044092153	4.5312903850	-0.0640479720
C	4.9214317605	-2.6799253565	0.3600082491
H	5.4950443386	-0.6257745184	0.6487186698
C	-4.1111421140	-0.0739522758	-0.4670256381
C	-5.3796473825	-0.3640537380	0.0200778419
C	-3.7922427897	-0.1870912896	-1.8143972070
C	-6.3617712556	-0.7625959623	-0.8794864069

H	-5.5689575378	-0.3080222030	1.0871314451
C	-4.7875131966	-0.5879046570	-2.7037844641
H	-2.7773164760	0.0194325023	-2.1451295785
C	-6.0683201630	-0.8707338116	-2.2390603040
H	-4.5543788600	-0.6867830910	-3.7587733633
H	-2.2427851426	-0.9951404255	1.5755392827
H	-7.3570948986	-0.9990642556	-0.5175550239
H	-6.8391123835	-1.1872928256	-2.9344018170
H	1.8320364509	-3.6890478231	-0.6634272633
H	5.0990710877	1.1595016173	-0.9887566151
H	4.0526780430	-4.6226009314	0.0206289753
H	4.7208932650	3.6075812842	-0.9866800844
H	5.8881121395	-3.0712792283	0.6599531421
C	-1.5875659127	0.0736337954	3.6563619632
H	-1.3650314461	0.7743399852	4.4675232904
H	-1.8919026244	-0.8764260876	4.1076236283
H	-0.6809827000	-0.1014220726	3.0712299694
C	-3.9729625557	0.8340372157	3.6266055513
H	-4.7922192716	1.2707869622	3.0444196074
H	-4.3110950239	-0.1366661496	3.9992239866
H	-3.7767717557	1.4853644494	4.4841401435
C	-2.3863041056	3.2124964860	2.8089047385
H	-1.9655635090	4.0432472113	2.2344771369
H	-3.4268983959	3.4568708980	3.0461674809
H	-1.8296732090	3.1464991751	3.7487193581
C	-2.7393080715	2.7392519348	-0.3755400682
H	-3.3987911224	2.5991301636	-1.2368783877
H	-2.8047228382	3.7878515761	-0.0717785874
H	-1.7118425150	2.5101020846	-0.6725142074
H	-1.2439553337	1.7611623971	1.6971766377
H	-4.2118926515	2.0501105966	1.0534165562

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C	0	2.9462517535	2.0889082247	-1.4569611792
N	0	2.7971122281	0.6073778709	-1.3419806916
N	0	2.5652121466	0.3527104706	0.0630545650
H	0	1.5757554232	0.7211151648	0.3505459216
O	0	0.1401341423	1.0860278749	0.6786753407
C	0	3.5823464918	1.2194551090	0.7570415746
C	0	3.4315718571	2.5355832398	-0.0306449159
H	0	4.4218640105	2.9937932798	-0.1293732471
H	0	3.2354146896	1.3217439386	1.7904380607
O	0	0.0597310200	-0.2003200550	-1.5518176048
P	0	-0.6532122016	0.2823585597	-0.3376704934
O	0	-1.9795767782	1.1087396979	-0.8011032104
O	0	-1.3320680404	-0.9269259013	0.5293741050
C	0	-3.0057125164	1.3456345394	0.0884723182
C	0	-2.3770136985	-1.6402894518	-0.0187270691
C	0	-3.8796879592	0.3079829151	0.4417353224
C	0	-3.2010320234	2.6443216609	0.5424490936
C	0	-3.6580014735	-1.0736420311	-0.0400096142
C	0	-2.1446419907	-2.9359539307	-0.4626673759
C	0	-4.9715985590	0.6245488350	1.2565983191
C	0	-4.2926140054	2.9335493170	1.3532979786
H	0	-2.4915342961	3.4069214637	0.2401988507
C	0	-4.7125179838	-1.8636058573	-0.5090353612
C	0	-3.2090564205	-3.7007986386	-0.9266773330
C	0	-5.1832603970	1.9223155770	1.7077145925
H	0	-4.4468400672	3.9478104382	1.7077971205

C	0	-4.4958181441	-3.1654915927	-0.9460741052
H	0	-5.7095523044	-1.4334836557	-0.5469609692
C	0	2.5866598646	-1.0725703255	0.3914064906
C	0	3.3715039761	-1.9583904997	-0.3370377109
C	0	1.7953310893	-1.4908366465	1.4553124614
C	0	3.3720954007	-3.3006478959	0.0282813581
H	0	3.9456270599	-1.5950310837	-1.1812356749
C	0	1.8065701794	-2.8381455319	1.8065030361
H	0	1.1532325446	-0.7807872229	1.9688282073
C	0	2.5954459605	-3.7408090219	1.0986944987
H	0	1.1834278490	-3.1797512176	2.6262426643
H	0	1.9210360129	0.2922326071	-1.7864448528
H	0	3.9763064641	-4.0063568704	-0.5325578201
H	0	2.5965978442	-4.7910172019	1.3725628600
H	0	-1.1294170298	-3.3172479804	-0.4299171972
H	0	-5.6483115362	-0.1727725407	1.5513046209
H	0	-3.0331482126	-4.7132391405	-1.2762967955
H	0	-6.0349767502	2.1417245627	2.3434063374
H	0	-5.3279138736	-3.7576271490	-1.3131271565
C	0	4.9774146515	0.6202216661	0.7123151986
H	0	5.6744187321	1.3305688807	1.1652696801
H	0	5.0346164788	-0.3187134015	1.2678160603
H	0	5.2897448280	0.4388982931	-0.3199516295
C	0	2.5118044745	3.5123461407	0.7052625795
H	0	2.9714982244	3.8013576520	1.6558115215
H	0	2.3509910834	4.4239428149	0.1239685291
H	0	1.5370742053	3.0612487587	0.9188640430
C	0	1.6287989735	2.7391005909	-1.8944372824
H	0	1.7673539079	3.8109053712	-2.0669968455
H	0	1.2925670545	2.2860210965	-2.8322649826
H	0	0.8386937151	2.6018278743	-1.1532058641

C	0	4.0223940674	2.3520471833	-2.5099060692
H	0	4.1888429488	3.4282065201	-2.6241439451
H	0	4.9665106477	1.8780331467	-2.2258177636
H	0	3.7144672611	1.9481525082	-3.4793585502

TS2

0 1

C	2.7688086752	-1.5444013951	-1.9162760440
N	2.4426530862	-1.4998849826	-0.6363539531
N	2.8248371740	-0.4201190821	0.0799806686
H	2.1022946605	-0.1844955418	0.7944238110
O	0.4594458493	0.2140629094	1.2017326459
C	2.0956028516	1.1151544891	-1.5933547059
C	1.8020829675	0.2463401942	-2.6098190261
H	2.3947829392	0.2522584624	-3.5212276801
H	1.3596422369	1.3561664659	-0.8318337675
O	-0.0901709860	-1.8149419020	-0.3012389641
P	-0.5454759313	-0.5660363601	0.4125536061
O	-1.2342515932	0.3615871441	-0.7530009913
O	-1.8204490839	-0.8584728797	1.3753843795
C	-2.0919779864	1.3852862739	-0.4114548736
C	-3.0205677464	-1.2566690796	0.8224929513
C	-3.3916913765	1.0901407046	0.0229724865
C	-1.6720485201	2.6968461963	-0.5982685927
C	-3.8385649754	-0.3103306401	0.1928473965
C	-3.4240387887	-2.5759884282	0.9844475118
C	-4.2586191944	2.1610315963	0.2635489176
C	-2.5519802270	3.7447214417	-0.3522372168
H	-0.6606481700	2.8714781900	-0.9496985069
C	-5.0938259065	-0.7313411949	-0.2586571713

C	-4.6754111427	-2.9709033555	0.5252550709
H	-2.7471453053	-3.2658859592	1.4761798455
C	-3.8492190159	3.4766120590	0.0791113312
H	-2.2237949385	4.7691687848	-0.4969138223
C	-5.5141391328	-2.0460240466	-0.0937390019
H	-4.9944075985	-4.0007933240	0.6502938110
H	-4.5383029415	4.2906855358	0.2790305888
H	-5.2628493685	1.9467334029	0.6184395457
H	-5.7334005880	-0.0128132153	-0.7637356296
H	-6.4899886748	-2.3510962296	-0.4574677987
C	4.1837727082	-0.1461531283	0.3652536345
C	5.2140835829	-1.0402902689	0.0773612649
C	4.4639556899	1.0799190274	0.9747475806
C	6.5263397041	-0.6927856481	0.3879791614
H	4.9909587547	-2.0092676516	-0.3568090630
C	5.7759655326	1.4077935246	1.2885655465
H	3.6458567153	1.7587036068	1.2005134413
C	6.8153671405	0.5278643883	0.9893534057
H	7.3253944988	-1.3931825650	0.1661369208
H	5.9871145990	2.3587008287	1.7671502936
H	7.8401597236	0.7900494051	1.2294910436
H	1.4273720455	-1.7991513055	-0.4075411381
H	0.7968928035	-0.1621805756	-2.6797410065
H	3.0118003457	1.7005117423	-1.5971600228
H	3.7489607697	-1.1967877969	-2.2224176931
H	2.2929731379	-2.3291588171	-2.4946541917

TS3a

0 1

C	0	-2.8815100000	-1.0579200000	-1.6020120000
N	0	-2.2888340000	0.0066540000	-1.0169160000
N	0	-2.5449590000	0.1937760000	0.3241830000
H	0	-1.6268670000	0.2893460000	0.8196780000
H	0	-1.2969340000	0.2380450000	-1.2724240000
O	0	0.0359810000	0.0520360000	1.1329050000
C	0	-3.1010800000	-2.1396110000	0.5370460000
C	0	-2.3821090000	-2.6277470000	-0.5331740000
H	0	-2.9911210000	-3.2041110000	-1.2339280000
H	0	-2.7182160000	-1.9853760000	1.5401850000
O	0	0.3149370000	0.6950360000	-1.3566480000
P	0	0.9323520000	0.3646000000	-0.0286410000
O	0	1.9593470000	-0.8867650000	-0.3111150000
O	0	1.9857130000	1.5101140000	0.4585250000
C	0	2.9291950000	-1.1961690000	0.6158530000
C	0	3.1491220000	1.7211960000	-0.2492460000
C	0	4.0777510000	-0.3982160000	0.7110890000
C	0	2.7840150000	-2.3488980000	1.3785770000
C	0	4.2178550000	0.8256120000	-0.1086760000
C	0	3.2634860000	2.8723950000	-1.0189440000
C	0	5.0866140000	-0.8064560000	1.5893000000
C	0	3.7995870000	-2.7336980000	2.2465560000
H	0	1.8732000000	-2.9282650000	1.2700010000
C	0	5.4185610000	1.1343280000	-0.7561200000
C	0	4.4665880000	3.1564490000	-1.6551660000
H	0	2.4029000000	3.5276610000	-1.0966350000
C	0	4.9558320000	-1.9630870000	2.3496300000
H	0	3.6870010000	-3.6334940000	2.8432460000
C	0	5.5483040000	2.2883930000	-1.5202470000
H	0	4.5584080000	4.0552710000	-2.2567760000
H	0	5.7492760000	-2.2560250000	3.0295850000

H	0	5.9750240000	-0.1882130000	1.6843850000
H	0	6.2504280000	0.4408060000	-0.6685070000
H	0	6.4879510000	2.5042300000	-2.0185010000
C	0	-3.5551930000	1.0949610000	0.7292500000
C	0	-4.3181460000	1.8356820000	-0.1741870000
C	0	-3.7974060000	1.2031130000	2.1035670000
C	0	-5.3322170000	2.6641530000	0.3008020000
H	0	-4.0862800000	1.7856230000	-1.2328660000
C	0	-4.8047660000	2.0406410000	2.5634200000
H	0	-3.1850850000	0.6322270000	2.7966340000
C	0	-5.5840620000	2.7692580000	1.6649150000
H	0	-5.9180030000	3.2432580000	-0.4064470000
H	0	-4.9825830000	2.1239350000	3.6309960000
H	0	-6.3721000000	3.4205730000	2.0276930000
C	0	-4.5180600000	-1.7819510000	0.1376420000
H	0	-4.9204950000	-1.0070700000	0.7933210000
H	0	-5.1936910000	-2.6431290000	0.2010480000
C	0	-4.3797540000	-1.2754830000	-1.3336210000
H	0	-4.9481150000	-0.3566480000	-1.5057830000
H	0	-4.7444290000	-2.0238440000	-2.0429300000
H	0	-1.3352162200	-2.6688334000	-0.7504927000
H	0	-2.3377819500	-1.3967160700	-2.4590283500

TS3b

0 1

C	0	2.7958850000	-1.1892180000	1.3361120000
N	0	2.1941510000	-0.0322940000	0.9499450000
N	0	2.4080560000	0.3778600000	-0.3524900000
H	0	1.4747700000	0.4752230000	-0.8149890000

O	0	-0.1697600000	0.1760930000	-1.2257470000
C	0	2.7178420000	-1.9374940000	-1.0981590000
C	0	2.2119910000	-2.5471320000	0.0397650000
H	0	2.8621690000	-3.2999120000	0.4946710000
H	0	2.0360610000	-1.5378240000	-1.8442270000
O	0	-0.3944980000	0.8231750000	1.2682510000
P	0	-1.0398170000	0.4785370000	-0.0396940000
O	0	-2.0372110000	-0.7943380000	0.2715050000
O	0	-2.1282990000	1.5990430000	-0.5080080000
C	0	-3.0331800000	-1.1222750000	-0.6196000000
C	0	-3.2710960000	1.7979090000	0.2354780000
C	0	-4.1964400000	-0.3418980000	-0.6815990000
C	0	-2.8999970000	-2.2807470000	-1.3762640000
C	0	-4.3293520000	0.8849390000	0.1348820000
C	0	-3.3785920000	2.9522220000	1.0015560000
C	0	-5.2285230000	-0.7718280000	-1.5216770000
C	0	-3.9388790000	-2.6874580000	-2.2057980000
H	0	-1.9781180000	-2.8472620000	-1.2943700000
C	0	-5.5133710000	1.1789750000	0.8189800000
C	0	-4.5648690000	3.2215460000	1.6745580000
H	0	-2.5261820000	3.6210010000	1.0477720000
C	0	-5.1081240000	-1.9331840000	-2.2765160000
H	0	-3.8344880000	-3.5916050000	-2.7974450000
C	0	-5.6365550000	2.3358080000	1.5799510000
H	0	-4.6514140000	4.1225940000	2.2736130000
H	0	-5.9202210000	-2.2428170000	-2.9263620000
H	0	-6.1283900000	-0.1668610000	-1.5909620000
H	0	-6.3366020000	0.4720230000	0.7626930000
H	0	-6.5628490000	2.5401150000	2.1072260000
C	0	3.2659110000	1.4822320000	-0.5830370000
C	0	3.9665450000	2.1205620000	0.4412090000

C	0	3.4261230000	1.9001950000	-1.9076350000
C	0	4.8400550000	3.1594720000	0.1303430000
H	0	3.8037630000	1.8129260000	1.4686500000
C	0	4.2921240000	2.9453640000	-2.2017450000
H	0	2.8637780000	1.4016790000	-2.6928430000
C	0	5.0107110000	3.5757940000	-1.1865570000
H	0	5.3803570000	3.6552420000	0.9311030000
H	0	4.4066810000	3.2686020000	-3.2317350000
H	0	5.6884450000	4.3900270000	-1.4201910000
C	0	4.1944780000	-1.9384570000	-1.3294690000
H	0	4.4459870000	-1.4992940000	-2.2976520000
H	0	4.5402840000	-2.9799390000	-1.3398250000
C	0	4.3111770000	-1.3235190000	1.1822990000
H	0	4.7495050000	-0.5677940000	1.8489580000
H	0	4.5830410000	-2.2993260000	1.5996280000
C	0	4.9370050000	-1.1678470000	-0.2076890000
H	0	4.9895420000	-0.1150100000	-0.4805600000
H	0	5.9698050000	-1.5259620000	-0.1552060000
H	0	1.2231400000	0.1723100000	1.2620310000
H	0	1.1614211800	-2.7034170600	0.1692950300
H	0	2.4124907500	-1.5654668300	2.2615014700

TS3c

0 1

C	0	2.6170270000	0.8378210000	-1.0355050000
N	0	1.9388710000	-0.3281510000	-0.9132720000
N	0	2.0707840000	-1.0746000000	0.2329520000
H	0	1.1117100000	-1.2454350000	0.6110070000
O	0	-0.5006960000	-0.8549700000	1.0601850000

C	0	2.2007790000	0.8260580000	1.6717960000
C	0	1.9923970000	1.8102020000	0.7235760000
H	0	2.7996450000	2.5295430000	0.6049000000
H	0	1.3184570000	0.3487340000	2.0976060000
O	0	-0.7427530000	-0.1952810000	-1.4300520000
P	0	-1.3793770000	-0.5044580000	-0.1053180000
O	0	-2.3438360000	0.7739040000	0.2495940000
O	0	-2.4953840000	-1.6894210000	-0.2389350000
C	0	-3.3553230000	0.6464450000	1.1747690000
C	0	-3.6236210000	-1.4755420000	-0.9999000000
C	0	-4.5335780000	-0.0319900000	0.8318600000
C	0	-3.2191280000	1.2796430000	2.4047160000
C	0	-4.6689730000	-0.7001040000	-0.4811650000
C	0	-3.7318660000	-2.1077280000	-2.2325210000
C	0	-5.5776900000	-0.0411850000	1.7621720000
C	0	-4.2703170000	1.2555580000	3.3142570000
H	0	-2.2870550000	1.7904210000	2.6223980000
C	0	-5.8415410000	-0.5935030000	-1.2360310000
C	0	-4.9064400000	-1.9850880000	-2.9661820000
H	0	-2.8892310000	-2.6900320000	-2.5886890000
C	0	-5.4546800000	0.5966210000	2.9912940000
H	0	-4.1636040000	1.7501400000	4.2746540000
C	0	-5.9656560000	-1.2303280000	-2.4654890000
H	0	-4.9937160000	-2.4780800000	-3.9293150000
H	0	-6.2766160000	0.5702380000	3.6993940000
H	0	-6.4895040000	-0.5776230000	1.5144390000
H	0	-6.6542340000	0.0174500000	-0.8527170000
H	0	-6.8825450000	-1.1285810000	-3.0371220000
C	0	2.9069860000	-2.2145860000	0.2283550000
C	0	2.9589170000	-2.9750670000	1.4008240000
C	0	3.6796290000	-2.5794590000	-0.8756510000

C	0	3.7944910000	-4.0831840000	1.4688360000
H	0	2.3322820000	-2.6945370000	2.2436660000
C	0	4.5189040000	-3.6862990000	-0.7901020000
H	0	3.6029450000	-2.0038690000	-1.7923740000
C	0	4.5853460000	-4.4405510000	0.3782670000
H	0	3.8254360000	-4.6713940000	2.3805940000
H	0	5.1159500000	-3.9667320000	-1.6524740000
H	0	5.2378110000	-5.3053160000	0.4352640000
C	0	4.1297690000	0.9253580000	-0.9059020000
H	0	4.5018360000	0.4506940000	-1.8282840000
H	0	4.3806500000	1.9874140000	-1.0038340000
C	0	4.7418600000	1.0564220000	1.6268150000
H	0	4.7162000000	2.1476820000	1.5050880000
H	0	5.6142410000	0.8443010000	2.2539360000
C	0	3.5017780000	0.5624900000	2.3640900000
H	0	3.4420230000	1.0264550000	3.3598970000
H	0	3.6002470000	-0.5157260000	2.5452830000
C	0	4.9457730000	0.3738970000	0.2724490000
H	0	4.8111070000	-0.7039110000	0.3860180000
H	0	5.9913510000	0.5135950000	-0.0260650000
H	0	0.9433910000	-0.2912910000	-1.2362350000
H	0	2.2239699600	1.3893829000	-1.8638682300
H	0	0.9982610000	2.1645325700	0.5473844300

TS4a

0 1

C	0	-2.8815100000	-1.0579200000	-1.6020120000
N	0	-2.2888340000	0.0066540000	-1.0169160000
N	0	-2.5449590000	0.1937760000	0.3241830000

H	0	-1.6268670000	0.2893460000	0.8196780000
H	0	-1.2969340000	0.2380450000	-1.2724240000
O	0	0.0359810000	0.0520360000	1.1329050000
C	0	-3.1010800000	-2.1396110000	0.5370460000
C	0	-2.3821090000	-2.6277470000	-0.5331740000
H	0	-2.9911210000	-3.2041110000	-1.2339280000
H	0	-2.7182160000	-1.9853760000	1.5401850000
O	0	0.3149370000	0.6950360000	-1.3566480000
P	0	0.9323520000	0.3646000000	-0.0286410000
O	0	1.9593470000	-0.8867650000	-0.3111150000
O	0	1.9857130000	1.5101140000	0.4585250000
C	0	2.9291950000	-1.1961690000	0.6158530000
C	0	3.1491220000	1.7211960000	-0.2492460000
C	0	4.0777510000	-0.3982160000	0.7110890000
C	0	2.7840150000	-2.3488980000	1.3785770000
C	0	4.2178550000	0.8256120000	-0.1086760000
C	0	3.2634860000	2.8723950000	-1.0189440000
C	0	5.0866140000	-0.8064560000	1.5893000000
C	0	3.7995870000	-2.7336980000	2.2465560000
H	0	1.8732000000	-2.9282650000	1.2700010000
C	0	5.4185610000	1.1343280000	-0.7561200000
C	0	4.4665880000	3.1564490000	-1.6551660000
H	0	2.4029000000	3.5276610000	-1.0966350000
C	0	4.9558320000	-1.9630870000	2.3496300000
H	0	3.6870010000	-3.6334940000	2.8432460000
C	0	5.5483040000	2.2883930000	-1.5202470000
H	0	4.5584080000	4.0552710000	-2.2567760000
H	0	5.7492760000	-2.2560250000	3.0295850000
H	0	5.9750240000	-0.1882130000	1.6843850000
H	0	6.2504280000	0.4408060000	-0.6685070000
H	0	6.4879510000	2.5042300000	-2.0185010000

C	0	-3.5551930000	1.0949610000	0.7292500000
C	0	-4.3181460000	1.8356820000	-0.1741870000
C	0	-3.7974060000	1.2031130000	2.1035670000
C	0	-5.3322170000	2.6641530000	0.3008020000
H	0	-4.0862800000	1.7856230000	-1.2328660000
C	0	-4.8047660000	2.0406410000	2.5634200000
H	0	-3.1850850000	0.6322270000	2.7966340000
C	0	-5.5840620000	2.7692580000	1.6649150000
H	0	-5.9180030000	3.2432580000	-0.4064470000
H	0	-4.9825830000	2.1239350000	3.6309960000
H	0	-6.3721000000	3.4205730000	2.0276930000
C	0	-2.1107810000	-1.5381600000	-2.8168240000
H	0	-2.7190250000	-2.2658410000	-3.3610900000
H	0	-1.9024470000	-0.7062300000	-3.4966380000
C	0	-0.9164070000	-2.6852700000	-0.8374310000
H	0	-0.3654370000	-2.0478990000	-0.1406620000
H	0	-0.5155780000	-3.6991890000	-0.7457390000
C	0	-0.7723760000	-2.1740030000	-2.3107040000
H	0	-0.5021260000	-2.9940410000	-2.9810030000
H	0	0.0295310000	-1.4340350000	-2.3551970000
H	0	-4.1018401100	-1.8870090800	0.2549618500
H	0	-3.9241471000	-1.2093234100	-1.4152370700

TS4b

0 1

C	0	2.7958850000	-1.1892180000	1.3361120000
N	0	2.1941510000	-0.0322940000	0.9499450000
N	0	2.4080560000	0.3778600000	-0.3524900000
H	0	1.4747700000	0.4752230000	-0.8149890000

O	0	-0.1697600000	0.1760930000	-1.2257470000
C	0	2.7178420000	-1.9374940000	-1.0981590000
C	0	2.2119910000	-2.5471320000	0.0397650000
H	0	2.8621690000	-3.2999120000	0.4946710000
H	0	2.0360610000	-1.5378240000	-1.8442270000
O	0	-0.3944980000	0.8231750000	1.2682510000
P	0	-1.0398170000	0.4785370000	-0.0396940000
O	0	-2.0372110000	-0.7943380000	0.2715050000
O	0	-2.1282990000	1.5990430000	-0.5080080000
C	0	-3.0331800000	-1.1222750000	-0.6196000000
C	0	-3.2710960000	1.7979090000	0.2354780000
C	0	-4.1964400000	-0.3418980000	-0.6815990000
C	0	-2.8999970000	-2.2807470000	-1.3762640000
C	0	-4.3293520000	0.8849390000	0.1348820000
C	0	-3.3785920000	2.9522220000	1.0015560000
C	0	-5.2285230000	-0.7718280000	-1.5216770000
C	0	-3.9388790000	-2.6874580000	-2.2057980000
H	0	-1.9781180000	-2.8472620000	-1.2943700000
C	0	-5.5133710000	1.1789750000	0.8189800000
C	0	-4.5648690000	3.2215460000	1.6745580000
H	0	-2.5261820000	3.6210010000	1.0477720000
C	0	-5.1081240000	-1.9331840000	-2.2765160000
H	0	-3.8344880000	-3.5916050000	-2.7974450000
C	0	-5.6365550000	2.3358080000	1.5799510000
H	0	-4.6514140000	4.1225940000	2.2736130000
H	0	-5.9202210000	-2.2428170000	-2.9263620000
H	0	-6.1283900000	-0.1668610000	-1.5909620000
H	0	-6.3366020000	0.4720230000	0.7626930000
H	0	-6.5628490000	2.5401150000	2.1072260000
C	0	3.2659110000	1.4822320000	-0.5830370000
C	0	3.9665450000	2.1205620000	0.4412090000

C	0	3.4261230000	1.9001950000	-1.9076350000
C	0	4.8400550000	3.1594720000	0.1303430000
H	0	3.8037630000	1.8129260000	1.4686500000
C	0	4.2921240000	2.9453640000	-2.2017450000
H	0	2.8637780000	1.4016790000	-2.6928430000
C	0	5.0107110000	3.5757940000	-1.1865570000
H	0	5.3803570000	3.6552420000	0.9311030000
H	0	4.4066810000	3.2686020000	-3.2317350000
H	0	5.6884450000	4.3900270000	-1.4201910000
C	0	2.2501510000	-1.7247810000	2.6533370000
H	0	2.7876780000	-2.6499630000	2.8914470000
H	0	2.5140550000	-0.9975660000	3.4319500000
C	0	0.7278840000	-2.7679110000	0.2227480000
H	0	0.1916900000	-1.8896960000	-0.1494170000
H	0	0.4247950000	-3.6064950000	-0.4182650000
C	0	0.3356360000	-3.0817970000	1.6676270000
H	0	-0.7486110000	-3.2234770000	1.7125550000
H	0	0.7981880000	-4.0342480000	1.9663480000
C	0	0.7386170000	-1.9910070000	2.6599710000
H	0	0.4601830000	-2.3007030000	3.6727070000
H	0	0.1739720000	-1.0755960000	2.4494860000
H	0	1.2231400000	0.1723100000	1.2620310000
H	0	3.8563002400	-1.2832030700	1.2284722500
H	0	3.7749506300	-1.9381834000	-1.2637514700

TS4c

0 1

C	0	2.8330400000	1.0032550000	-1.0347430000
N	0	2.1363310000	-0.1537190000	-0.9159440000

N	0	2.2604730000	-0.8411170000	0.2700320000
H	0	1.3069360000	-0.9912570000	0.6715870000
H	0	1.1468560000	-0.1433340000	-1.2542660000
O	0	-0.2883770000	-0.5888790000	1.1157710000
C	0	2.5025390000	1.2103250000	1.5340360000
C	0	2.1383940000	2.0990790000	0.5470190000
H	0	2.8984420000	2.8362580000	0.2919370000
H	0	1.7435350000	0.7231080000	2.1424210000
O	0	-0.5474980000	-0.1533250000	-1.4228910000
P	0	-1.1752620000	-0.3851870000	-0.0778700000
O	0	-2.2075180000	0.8654620000	0.1681500000
O	0	-2.2274510000	-1.6339540000	-0.1187940000
C	0	-3.2142020000	0.7583040000	1.1012510000
C	0	-3.3604280000	-1.5403450000	-0.8967290000
C	0	-4.3541310000	-0.0053410000	0.8125100000
C	0	-3.1150620000	1.4895330000	2.2792460000
C	0	-4.4476980000	-0.7816290000	-0.4433600000
C	0	-3.4285780000	-2.2733390000	-2.0752500000
C	0	-5.4001990000	0.0032310000	1.7405660000
C	0	-4.1672260000	1.4812390000	3.1879600000
H	0	-2.2104390000	2.0609850000	2.4574100000
C	0	-5.6198560000	-0.7970840000	-1.2060270000
C	0	-4.6036830000	-2.2711040000	-2.8181590000
H	0	-2.5545260000	-2.8368690000	-2.3825720000
C	0	-5.3150850000	0.7396490000	2.9166410000
H	0	-4.0894570000	2.0522900000	4.1078780000
C	0	-5.7036470000	-1.5355310000	-2.3808680000
H	0	-4.6596890000	-2.8429720000	-3.7391020000
H	0	-6.1373340000	0.7255500000	3.6247510000
H	0	-6.2818220000	-0.5977800000	1.5354210000
H	0	-6.4654640000	-0.2010640000	-0.8737970000

H	0	-6.6212640000	-1.5277900000	-2.9602750000
C	0	3.1518700000	-1.9282510000	0.3723500000
C	0	3.9119700000	-2.3971900000	-0.7013670000
C	0	3.2655010000	-2.5423940000	1.6257910000
C	0	4.7988750000	-3.4533820000	-0.5085580000
H	0	3.7740310000	-1.9543190000	-1.6825450000
C	0	4.1447240000	-3.6027510000	1.8006540000
H	0	2.6508010000	-2.1836860000	2.4476570000
C	0	4.9243440000	-4.0585310000	0.7379540000
H	0	5.3829300000	-3.8146850000	-1.3494810000
H	0	4.2214580000	-4.0757850000	2.7746580000
H	0	5.6127080000	-4.8849550000	0.8791060000
C	0	2.4025340000	1.7771670000	-2.2717890000
H	0	3.0485970000	1.4094190000	-3.0797640000
H	0	1.3809090000	1.4729440000	-2.5308540000
C	0	2.4743270000	3.3151390000	-2.2260220000
H	0	3.3053130000	3.6548190000	-1.5925800000
H	0	2.7211020000	3.6554320000	-3.2368990000
C	0	1.1527200000	4.0000340000	-1.8316420000
H	0	0.3580140000	3.5535980000	-2.4433530000
H	0	1.2141450000	5.0529510000	-2.1306160000
C	0	0.7247080000	2.5363350000	0.2424080000
H	0	0.2398970000	1.8444780000	-0.4563710000
H	0	0.1224920000	2.5010610000	1.1564380000
C	0	0.7223250000	3.9447120000	-0.3608700000
H	0	1.3732700000	4.5949290000	0.2402170000
H	0	-0.2853180000	4.3672470000	-0.2920440000
H	0	3.5401421100	1.0587473400	1.7468833800
H	0	3.8797720700	0.9850951800	-0.8135594000

TS4d

0 1

C	0	2.6170270000	0.8378210000	-1.0355050000
N	0	1.9388710000	-0.3281510000	-0.9132720000
N	0	2.0707840000	-1.0746000000	0.2329520000
H	0	1.1117100000	-1.2454350000	0.6110070000
O	0	-0.5006960000	-0.8549700000	1.0601850000
C	0	2.2007790000	0.8260580000	1.6717960000
C	0	1.9923970000	1.8102020000	0.7235760000
H	0	2.7996450000	2.5295430000	0.6049000000
H	0	1.3184570000	0.3487340000	2.0976060000
O	0	-0.7427530000	-0.1952810000	-1.4300520000
P	0	-1.3793770000	-0.5044580000	-0.1053180000
O	0	-2.3438360000	0.7739040000	0.2495940000
O	0	-2.4953840000	-1.6894210000	-0.2389350000
C	0	-3.3553230000	0.6464450000	1.1747690000
C	0	-3.6236210000	-1.4755420000	-0.9999000000
C	0	-4.5335780000	-0.0319900000	0.8318600000
C	0	-3.2191280000	1.2796430000	2.4047160000
C	0	-4.6689730000	-0.7001040000	-0.4811650000
C	0	-3.7318660000	-2.1077280000	-2.2325210000
C	0	-5.5776900000	-0.0411850000	1.7621720000
C	0	-4.2703170000	1.2555580000	3.3142570000
H	0	-2.2870550000	1.7904210000	2.6223980000
C	0	-5.8415410000	-0.5935030000	-1.2360310000
C	0	-4.9064400000	-1.9850880000	-2.9661820000
H	0	-2.8892310000	-2.6900320000	-2.5886890000
C	0	-5.4546800000	0.5966210000	2.9912940000
H	0	-4.1636040000	1.7501400000	4.2746540000
C	0	-5.9656560000	-1.2303280000	-2.4654890000

H	0	-4.9937160000	-2.4780800000	-3.9293150000
H	0	-6.2766160000	0.5702380000	3.6993940000
H	0	-6.4895040000	-0.5776230000	1.5144390000
H	0	-6.6542340000	0.0174500000	-0.8527170000
H	0	-6.8825450000	-1.1285810000	-3.0371220000
C	0	2.9069860000	-2.2145860000	0.2283550000
C	0	2.9589170000	-2.9750670000	1.4008240000
C	0	3.6796290000	-2.5794590000	-0.8756510000
C	0	3.7944910000	-4.0831840000	1.4688360000
H	0	2.3322820000	-2.6945370000	2.2436660000
C	0	4.5189040000	-3.6862990000	-0.7901020000
H	0	3.6029450000	-2.0038690000	-1.7923740000
C	0	4.5853460000	-4.4405510000	0.3782670000
H	0	3.8254360000	-4.6713940000	2.3805940000
H	0	5.1159500000	-3.9667320000	-1.6524740000
H	0	5.2378110000	-5.3053160000	0.4352640000
C	0	0.5783430000	2.3142000000	0.4729620000
H	0	0.1035170000	1.7970510000	-0.3683290000
H	0	-0.0354760000	2.0432140000	1.3385010000
C	0	0.4881260000	3.8281660000	0.2533490000
H	0	1.0956180000	4.3429930000	1.0112420000
H	0	-0.5498950000	4.1287990000	0.4342950000
C	0	0.8823370000	4.3407220000	-1.1374970000
H	0	0.6442170000	5.4095080000	-1.1692510000
H	0	0.2323120000	3.8697840000	-1.8876080000
C	0	2.3579930000	4.1524200000	-1.5452330000
H	0	2.7163750000	5.0687550000	-2.0274820000
H	0	2.9866820000	4.0386080000	-0.6540590000
C	0	2.0559720000	1.6251280000	-2.2179220000
H	0	0.9641530000	1.6483690000	-2.1323370000
H	0	2.2548090000	0.9891820000	-3.0915670000

C	0	2.6060850000	3.0160540000	-2.5452460000
H	0	3.6767240000	2.9544050000	-2.7726070000
H	0	2.1244100000	3.3019110000	-3.4884180000
H	0	0.9433910000	-0.2912910000	-1.2362350000
H	0	3.6813540400	0.8994098200	-0.9443196000
H	0	3.1306166200	0.6376831900	2.1665857800

TS5-cis

0 1

C	-3.0193301988	-1.9304154134	0.4894059582
N	-2.2546907440	-1.1063736626	-0.2470492904
N	-2.4654108864	0.2421008055	-0.1608106702
H	-1.5448986753	0.7023702887	-0.3876127031
O	0.0814948295	0.9472340728	-0.7265016598
C	-2.5374562908	0.2593530616	2.1656307916
C	-2.6561848084	-1.0953793375	2.4340332336
O	0.3725794447	-1.4572712865	0.1639639952
P	0.9892304313	-0.1564973110	-0.2744896123
O	1.9436991931	0.3221972458	0.9680141927
O	2.1056041082	-0.3731991455	-1.4443974834
C	2.8983890076	1.2928878205	0.7579878035
C	3.2770998523	-1.0434100715	-1.1660495852
C	4.0898841779	0.9607123966	0.0994635641
C	2.6888457417	2.5631917179	1.2808074508
C	4.2946873509	-0.3972427765	-0.4508360233
C	3.4544516260	-2.3205227927	-1.6843892724
C	5.0773452305	1.9458551444	-0.0017844165
C	3.6842250382	3.5269889830	1.1659940328
H	1.7458417415	2.7678760903	1.7765353524

C	5.5083451327	-1.0725227762	-0.2866046336
C	4.6690972061	-2.9729010045	-1.5057287708
C	4.8830721911	3.2168994260	0.5268774650
H	3.5225870681	4.5201225307	1.5732310656
C	5.7004958956	-2.3463201271	-0.8091414318
H	6.2999462995	-0.5892985405	0.2794626171
C	-3.5501523457	0.8227437991	-0.8927923142
C	-4.1225411516	0.1959914387	-1.9992854731
C	-3.9961146891	2.0799623331	-0.4867762912
C	-5.1652768562	0.8207501426	-2.6766967308
H	-3.7336438952	-0.7629053115	-2.3267808603
C	-5.0268726461	2.7031253090	-1.1814268342
H	-3.5278453875	2.5600176127	0.3676931012
C	-5.6220231511	2.0722889115	-2.2717785314
H	-5.3693453496	3.6831384356	-0.8647771799
H	-1.2241621565	-1.3225696928	-0.2110423422
H	-5.6114678733	0.3305824080	-3.5363715908
H	-6.4311787824	2.5572292088	-2.8077105810
H	2.6327368735	-2.7744910212	-2.2273074798
H	5.9997719640	1.7065324042	-0.5236985641
H	4.8093891880	-3.9704118208	-1.9101677277
H	5.6607802833	3.9675574511	0.4300016403
H	6.6489591328	-2.8532449099	-0.6636338278
C	-4.5199238891	-1.7982846358	0.4283937249
H	-4.8630213198	-0.7842447154	0.6390137391
H	-4.8487917952	-2.0618280182	-0.5840175328
H	-4.9909260101	-2.4928251563	1.1242200787
C	-2.4672959254	-3.3278304679	0.5969673827
H	-1.3738050293	-3.3120531887	0.5953163092
H	-2.8228337180	-3.7984732709	1.5173430130
H	-2.8203386058	-3.9361028016	-0.2435919877

C	-1.2129698856	0.9608146695	2.2543342938
H	-1.0810134831	1.3140220891	3.2860998215
H	-0.3959460257	0.2650394467	2.0456709599
H	-1.1204426990	1.8203025417	1.5867837742
C	-3.8111446223	-1.6231445735	3.2589895599
H	-3.5795167977	-1.5123193500	4.3236203147
H	-4.7334858691	-1.0675527004	3.0646059520
H	-4.0064140316	-2.6870626374	3.0876939338
H	-3.4356297739	0.8763698954	2.2340506330
H	-1.7090366394	-1.6202571625	2.5748206478

TS5-trans

0 1

C	-2.8819524611	0.0896331628	2.0552972140
N	-2.2846761851	-0.5619522809	1.0276038327
N	-2.5503088831	-0.1238588179	-0.2424062131
H	-1.6359761682	-0.0212420508	-0.7403190610
O	0.0088690190	0.4212697083	-0.8471419349
C	-2.6505131738	2.1615079815	0.3139305617
C	-2.3067628828	2.0342616607	1.6553186497
H	-3.0318099769	2.4277713915	2.3697486656
O	0.3847969295	-0.9029220231	1.3406733980
P	0.9524862002	-0.2226951683	0.1281582083
O	2.0496831417	0.8638348967	0.6733935945
O	1.9191217222	-1.2202664077	-0.7303023468
C	2.9833794187	1.3876712579	-0.1933403770
C	3.1064525488	-1.6600118861	-0.1865544362
C	4.0847317547	0.6118097816	-0.5798965475
C	2.8538117286	2.7117469932	-0.5951990989

C	4.2090372748	-0.7960356196	-0.1424919196
C	3.2056469854	-2.9836926349	0.2243296000
C	5.0640784195	1.2168053238	-1.3740069699
C	3.8393849214	3.2910220338	-1.3863465408
H	1.9805474778	3.2670434479	-0.2696788587
C	5.4262041904	-1.3116235936	0.3141957864
C	4.4258297148	-3.4728377467	0.6771120369
C	4.9494416304	2.5433298847	-1.7739086046
H	3.7395685685	4.3251579705	-1.7008689078
C	5.5400622619	-2.6369135262	0.7180962644
H	6.2850863491	-0.6483135884	0.3683543861
C	-3.5989017094	-0.6982141590	-0.9984847840
C	-4.4085586780	-1.7260684912	-0.5131418236
C	-3.8074973526	-0.1910303804	-2.2854733522
C	-5.4394405562	-2.2199393394	-1.3068915869
H	-4.2020053016	-2.1503882657	0.4633807219
C	-4.8348464110	-0.6997045373	-3.0705950161
H	-3.1530116103	0.5921868521	-2.6598889874
C	-5.6622167841	-1.7095944857	-2.5827881067
H	-4.9872971553	-0.3044635827	-4.0698929487
H	-1.2659506294	-0.7755285769	1.1713578088
H	-6.0624921528	-3.0235829198	-0.9266977364
H	-6.4645176211	-2.1038538860	-3.1973144115
H	2.3196461136	-3.6069432418	0.1735074208
H	5.9149375957	0.6216980657	-1.6939868899
H	4.5056252486	-4.5064929946	0.9987552492
H	5.7190078187	2.9892461772	-2.3956929013
H	6.4932220268	-3.0135296210	1.0750498774
C	-3.9924182293	2.6127108659	-0.1709566732
H	-3.8820650864	3.5652408977	-0.7025176856
H	-4.4336025064	1.9039890967	-0.8831683549

H	-4.6939289684	2.7662574843	0.6529120669
H	-1.8374377471	2.1811001625	-0.4097149034
C	-0.8459949066	2.1618624456	2.0386018631
H	-0.6566956026	3.1685990537	2.4270324926
H	-0.5169592889	1.4505111470	2.7991600753
H	-0.2116575245	2.0189707736	1.1615789469
C	-4.3848593464	0.2336727600	2.0387751294
H	-4.7685900156	0.5355919041	1.0647776640
H	-4.8262074456	-0.7394721241	2.2861089339
H	-4.7069464459	0.9501288804	2.7980800007
C	-2.2912039512	-0.2564851022	3.3998748792
H	-1.2273754528	-0.4923388931	3.3151354934
H	-2.4312155326	0.5726496946	4.0983305674
H	-2.8125003177	-1.1296168109	3.8074135894

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