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Supporting Information

Alkene Insertion Enables Ring-Opening of Vinyl Epoxides: A Theoretical Perspective

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Part 1: Complete References for Gaussian 09 and Q-Chem

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Part 2: The *s-cis* and *s-trans* conformations of vinyl epoxides and stereoselectivity of the 5,4-insertion

We studied various conformations of vinyl epoxides in terms of the orientation of the epoxide and the vinyl group across the sigma bond (*s-cis* versus *s-trans*), as well as the stereoselectivity of the 5,4-insertion. As shown in Figure S1, the calculation results indicate that *s-trans* conformation is more stable and the 5,4-insertion of *s-trans* vinyl epoxide **16** via transition state **17-ts** is more favorable.

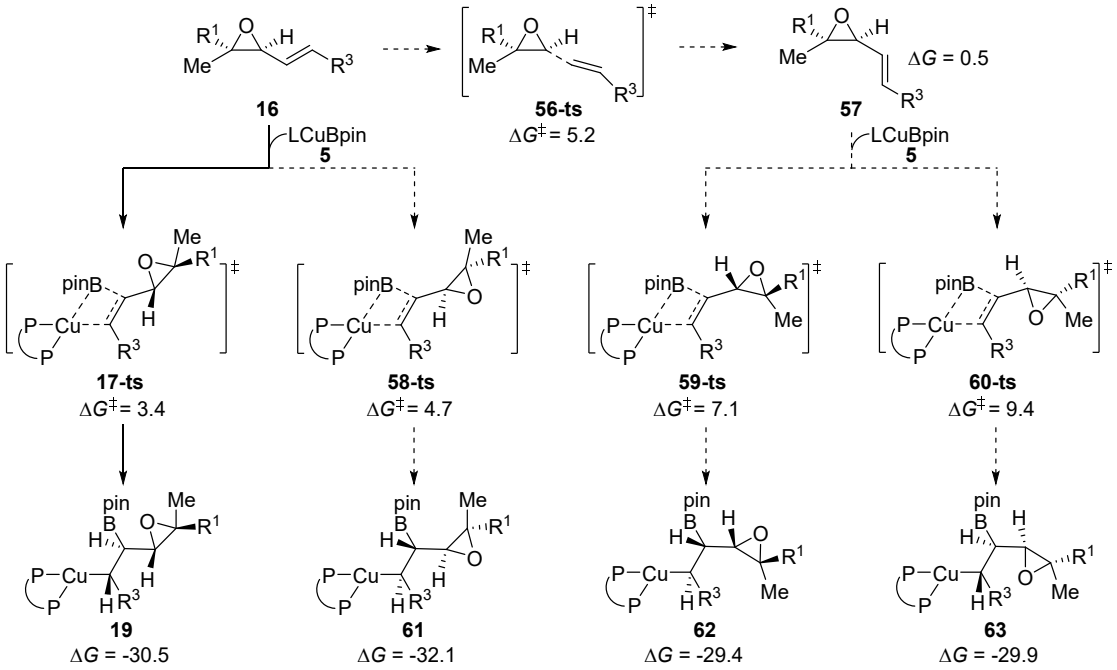

Figure S1 Gibbs free energies for the conformations of vinyl epoxides and stereoselectivity of the 5,4-insertion. Energies are in kcal/mol.

Part 3: The ring-opening pathway via 4,5-insertion followed by *β*-oxygen elimination

The ring-opening pathway involving 4,5-insertion of the olefin, followed by *β*-oxygen elimination is also considered. As shown in Figure S2, the *β*-oxygen elimination of Cu-alkyl intermediate **20** undergoes via the four-membered ring transition states **64-ts** with an activation free energy of 5.8 kcal/mol to give the copper alkoxy intermediate **44**.

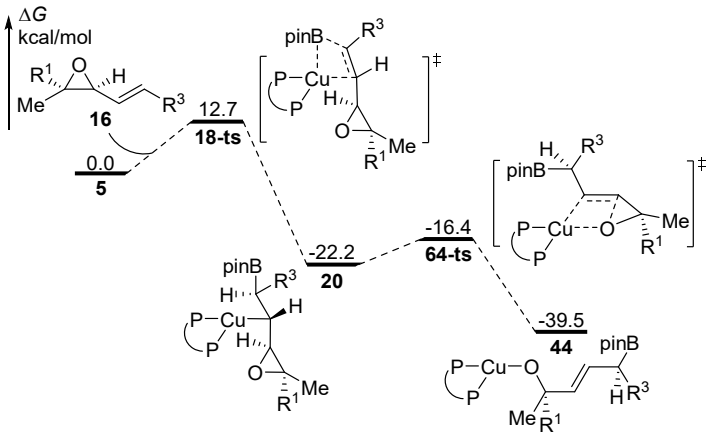

Figure S2 Free energy profile for ring-opening pathway via 4,5-insertion and *β*-oxygen elimination. Energies are in kcal/mol.

Part 4: Two different conformations that boryl and epoxide are in the *syn* and *anti* orientations in the cyclic complex.

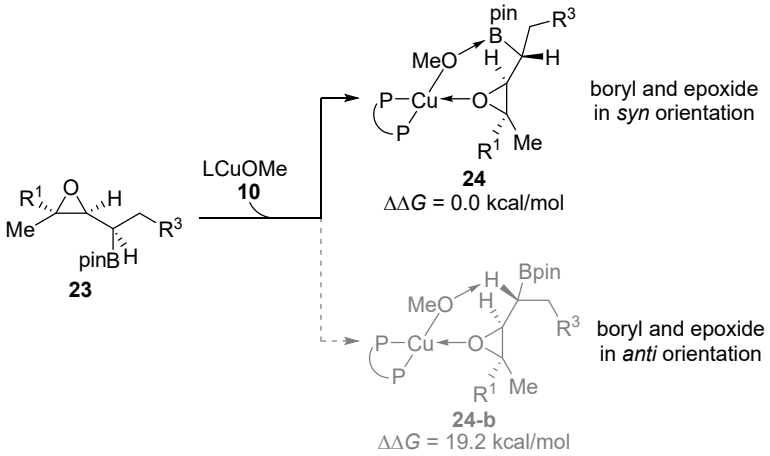

Figure S3 Gibbs free energy difference for the cyclic complex **24** and **24-b** with different conformations that boryl and epoxide are respectively in the *syn* and *anti* orientations. Energies are in kcal/mol.

Part 5: EDA study on the interaction energies.

Table S1. Energies of all components of the interaction energies in **17-ts_2.18** and **18-ts_2.17**.

ΔE	**17-ts_2.18**	**18-ts_2.17**
ΔE_{Pauli}	307.8	311.2
ΔE_{dist}	50.6	53.9
ΔE_{disp}	-46.7	-46.9
ΔE_{ct}	-108.8	-101.0
ΔE_{pol}	-39.6	-41.6
ΔE_{elstat}	-170.4	-172.4

Part 6: Cu-catalyzed reductive ring-opening of vinyl epoxides bearing the an alkyl group on the double bond

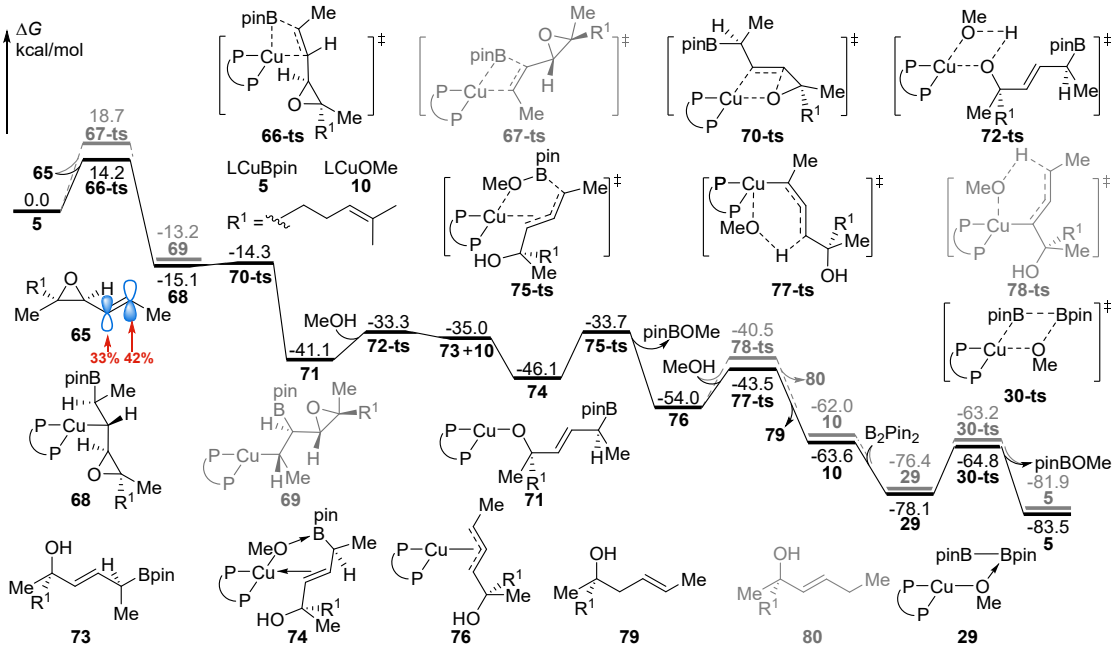

Figure S4 Free energy profiles for Cu-catalyzed reductive ring-opening of vinyl epoxides that double bond bearing a methyl group. The data in red is the p orbital of the carbon atom contributions to vacant alkenyl π* orbital. Energies are in kcal/mol.

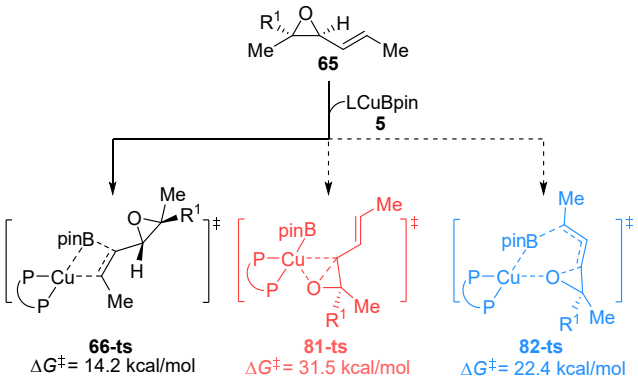

Figure S5 Gibbs free energies for the transition states in pathway determining step of the Cu-catalyzed reductive ring-opening of vinyl epoxides that double bond bearing a methyl group.. Energies are in kcal/mol.

Part 7: The copper atomic charges

Table S2. The ADCH, NPA and AIM atomic charges on the Cu center along the IRCs of **17-ts**, **31-ts** and **43-ts**. The charges are in e.

ADCH Charge			NPA Charge			AIM Charge		
17-ts	**31-ts**	**43-ts**	**17-ts**	**31-ts**	**43-ts**	**17-ts**	**31-ts**	**43-ts**
0.097	0.076	0.067	-0.089	0.125	0.123	0.426	0.334	0.324
0.096	0.075	0.068	-0.087	0.126	0.126	0.427	0.337	0.328
0.095	0.082	0.067	-0.085	0.120	0.139	0.429	0.347	0.336
0.093	0.088	0.072	-0.082	0.113	0.141	0.432	0.358	0.356
0.097	0.091	0.076	-0.074	0.111	0.130	0.436	0.379	0.383
0.104	0.130	0.117	-0.034	0.202	0.257	0.448	0.444	0.477

The ADCH, NPA and AIM atomic charges on the Cu center along the reaction coordinate were computed to account for the favor of alkene insertion. Overall, the results indicate that the oxidative addition or 1,5-vinyl epoxide insertion processes require the Cu center to donate electrons comparing with alkene insertion process, which may account for higher activation free energies.

Part 8: Energitic Information of Optimized Structures

Table S3. The single-point energies (*E*) at M06/6-311+G(d,p)/LanL08(f)/IEF-PCM$_{THF}$ level, Gibbs free energy corrections (GFEC) at M06/6-31G(d,p)/LanL08(f)/IEF-PCM$_{THF}$ level, and Gibbs free energies (*G* = *E* + GFEC), and imaginary frequencies (IF) of the stationary points (SPs) involved in the reaction. Energies are in a.u.

SP	*E*	GFEC	*G*	IF
5	-2869.897203	0.693329	-2869.203874	-
16	-828.066448	0.290311	-827.776137	-
17-ts	-3697.999390	1.024864	-3696.974526	97.7*i*
18-ts	-3697.983068	1.023355	-3696.959713	170.8*i*
19	-3698.047594	1.018927	-3697.028667	-
20	-3698.036570	1.021168	-3697.015402	-
21-ts	-2985.572748	0.739664	-2984.833084	1317.8*i*
MeOH	-115.692774	0.028660	-115.664114	-
22-ts	-3813.724988	1.063999	-3812.660989	707.83*i*
23	-1239.825768	0.476338	-1239.349430	-
10	-2573.896766	0.562036	-2573.334730	-
24	-3813.781329	1.072473	-3812.708856	-
24-b	-3813.750433	1.072128	-3812.678305	-
25-ts	-3813.755777	1.072323	-3812.683454	292.4*i*
pinBOMe	-526.268574	0.186730	-526.081844	-
26	-3287.520918	0.858327	-3286.662591	-
27-ts	-3403.225731	0.904522	-3402.321209	201.3*i*
28	-829.300121	0.313363	-828.986758	-
B_2pin_2	-822.235737	0.316525	-821.919212	-
29	-3396.184238	0.907253	-3395.276985	-
30-ts	-3396.170411	0.914528	-3395.255883	86.3*i*
31-ts	-3697.958616	1.017491	-3696.941125	263.0*i*
32	-3698.002874	1.021986	-3696.980888	-
33-ts	-3698.002268	1.020962	-3696.981306	36.5*i*
34	-3698.076625	1.019700	-3697.056925	-
35-ts	-3813.771056	1.070523	-3812.700533	200.6*i*
36	-1239.842434	0.474237	-1239.368197	-
37	-3813.810068	1.078621	-3812.731447	-
38-ts	-3813.791172	1.073352	-3812.717820	294.6*i*
39	-3287.532707	0.862331	-3286.670376	-
40-ts	-3403.215996	0.904843	-3402.311153	1431.1*i*
41-ts	-3403.208542	0.904124	-3402.304418	1604.8*i*
42	-829.307061	0.313769	-828.993292	-
43-ts	-3697.964756	1.018202	-3696.946554	92.1*i*

44	-3698.062340	1.019327	-3697.043013	-
45-ts	-3813.760633	1.067063	-3812.693570	493.8*i*
46	-1239.834890	0.469149	-1239.365741	-
47	-3813.799386	1.076481	-3812.722905	-
48-ts	-3813.784496	1.072358	-3812.712138	309.4*i*
49	-3287.515772	0.854354	-3286.661418	-
50-ts	-3403.214788	0.902568	-3402.312220	1498.5*i*
51-ts	-3403.205179	0.906129	-3402.299050	1550.8*i*
52	-3813.795909	1.074336	-3812.721573	-
53-ts	-3813.783633	1.072526	-3812.711107	299.4*i*
54	-3287.507212	0.859171	-3286.648041	-
55-ts	-3403.201855	0.900332	-3402.301523	1418.5*i*
56-ts	-828.060993	0.293195	-827.767798	96.5*i*
57	-828.066862	0.291526	-827.775336	-
58-ts	-3697.998044	1.025460	-3696.972584	115.1*i*
59-ts	-3697.992097	1.023396	-3696.968701	145.5*i*
60-ts	-3697.989691	1.024730	-3696.964961	147.5*i*
61	-3698.050640	1.019494	-3697.031146	-
62	-3698.044461	1.017574	-3697.026887	-
63	-3698.047324	1.019643	-3697.027681	-
64-ts	-3698.027668	1.021484	-3697.006184	404.2*i*
65	-544.216218	0.247373	-543.968845	-
66-ts	-3414.128279	0.978124	-3413.150155	198.9*i*
67-ts	-3414.120034	0.977117	-3413.142917	190.8*i*
68	-3414.176905	0.980192	-3413.196713	-
69	-3414.171987	0.978195	-3413.193792	-
70-ts	-3414.172628	0.977167	-3413.195461	416.8*i*
71	-3414.21248	0.974255	-3413.238225	-
72-ts	-3529.910803	1.020834	-3528.889969	85.4*i*
73	-955.987399	0.429582	-955.557817	-
74	-3529.942844	1.032615	-3528.910229	-
75-ts	-3529.919816	1.029245	-3528.890571	352.3*i*
76	-3003.646153	0.805062	-3002.841091	-
77-ts	-3119.343822	0.855335	-3118.488487	616.6*i*
78-ts	-3119.343253	0.859681	-3118.483572	1169.2*i*
79	-545.455546	0.269823	-545.185723	-
80	-545.452404	0.269303	-545.183101	-
81-ts	-3414.097936	0.975493	-3413.122443	202.7*i*
82-ts	-3414.106997	0.970018	-3413.136979	168.6*i*

Part 9: Cartesian coordinates of the stationary points

5				H	5.213079	-2.784356	-0.776127
C	-0.359045	-2.971582	3.752594	H	4.982963	-4.788956	-2.226384
C	-1.100007	-1.949939	3.159275	C	-1.003888	-2.457023	-1.595025
C	-0.839423	-1.680727	1.818246	C	-1.248952	-1.930791	-2.867792
C	0.113602	-2.360473	1.057501	C	-1.830656	-3.471093	-1.104304
C	0.822337	-3.387695	1.683167	C	-2.290157	-2.425033	-3.645045
C	0.585978	-3.687303	3.021380	H	-0.621300	-1.122817	-3.247116
H	-0.520668	-3.220040	4.798871	C	-2.883704	-3.952663	-1.876677
H	1.572630	-3.943244	1.123277	H	-1.648393	-3.888602	-0.114761
H	1.145164	-4.485889	3.502264	C	-3.110947	-3.434544	-3.148509
O	-1.541405	-0.693945	1.172446	H	-2.470894	-2.009007	-4.633769
C	-2.211353	-1.159302	3.838638	H	-3.525146	-4.739258	-1.485577
C	-2.184748	0.255266	3.273143	H	-3.933739	-3.812123	-3.751441
C	-1.875074	0.406375	1.922905	C	-1.207862	3.444497	-0.868490
C	-2.510516	1.412712	3.978452	C	-2.358721	4.201323	-1.119644
C	-1.878019	1.632837	1.255435	C	0.043411	4.067313	-0.889353
C	-2.531632	2.654012	3.346571	C	-2.257992	5.562029	-1.383393
H	-2.755105	1.353098	5.036242	H	-3.336291	3.719804	-1.107991
C	-2.218753	2.766584	1.996225	C	0.140779	5.431512	-1.152324
H	-2.791971	3.542652	3.915946	H	0.938065	3.470123	-0.702593
H	-2.221770	3.742967	1.516289	C	-1.007131	6.177445	-1.399821
P	0.400947	-1.757334	-0.652239	H	-3.155370	6.144609	-1.578518
P	-1.270794	1.657720	-0.477607	H	1.117317	5.909888	-1.170765
C	-3.560289	-1.799390	3.455465	H	-0.929386	7.241881	-1.609362
H	-3.706624	-1.808977	2.368644	C	-2.697573	1.071503	-1.472955
H	-3.602748	-2.834977	3.815833	C	-2.664701	1.293721	-2.855684
H	-4.386524	-1.236883	3.908035	C	-3.755984	0.339864	-0.929823
C	-2.073594	-1.173967	5.356055	C	-3.680528	0.814128	-3.672814
H	-2.895718	-0.624138	5.826857	H	-1.839359	1.854332	-3.295815
H	-2.129336	-2.199183	5.737404	C	-4.763273	-0.156075	-1.753530
H	-1.125453	-0.731536	5.683597	H	-3.803873	0.158123	0.142717
Cu	0.793700	0.563306	-0.439730	C	-4.731136	0.082857	-3.123217
C	1.833128	-2.767807	-1.186941	H	-3.647445	1.004027	-4.743441
C	1.710396	-3.900910	-1.994717	H	-5.579774	-0.728061	-1.318333
C	3.105245	-2.367996	-0.754313	H	-5.521953	-0.301730	-3.763339
C	2.841525	-4.622085	-2.369759	B	2.661298	1.201089	0.002605
H	0.727169	-4.223069	-2.334577	O	3.418322	2.104325	-0.747485
C	4.229797	-3.099261	-1.120960	O	3.457504	0.679585	1.026304
H	3.210583	-1.483856	-0.121032	C	4.804707	1.946647	-0.385382
C	4.101094	-4.223647	-1.933758	C	4.704379	1.400374	1.061830
H	2.735794	-5.500283	-3.002622	C	5.405725	0.943136	-1.362693

H	5.256722	1.314386	-2.382893	H	-1.438042	-1.789870	-0.281527
H	6.482104	0.806306	-1.202350	C	-3.169121	-0.517273	-0.010875
H	4.909644	-0.033132	-1.284937	C	-4.045759	-1.584097	-0.257956
C	5.514900	3.278614	-0.517626	C	-3.715440	0.755804	0.219749
H	6.548152	3.205017	-0.153622	C	-5.418049	-1.399506	-0.267108
H	5.550408	3.577333	-1.571657	H	-3.634510	-2.574800	-0.441281
H	5.004525	4.069401	0.040221	C	-5.083197	0.954005	0.215431
C	5.811584	0.446741	1.464133	H	-3.060969	1.605253	0.398325
H	6.793828	0.931773	1.390904	C	-5.945032	-0.125324	-0.027939
H	5.668496	0.130252	2.503807	H	-6.087732	-2.233655	-0.457992
H	5.817463	-0.450750	0.837262	H	-5.497973	1.942471	0.393960
C	4.561640	2.500221	2.105478	C	-7.358945	0.078123	-0.036749
H	4.281649	2.044865	3.061911	N	-8.511137	0.244863	-0.043842
H	5.499134	3.050858	2.249891	H	0.862613	-1.316542	0.127927
H	3.775061	3.209909	1.824121				
				17-ts			
16				C	2.796284	-1.377375	-0.506385
C	0.658374	-0.249152	0.269823	C	3.875676	-2.251608	-0.989108
C	1.724543	0.682452	-0.157511	C	3.593302	-3.454170	-1.844784
C	1.419058	2.094199	-0.576093	H	3.554378	-4.357151	-1.223286
H	2.184940	2.778083	-0.193062	H	2.642344	-3.365177	-2.377714
H	1.413779	2.176279	-1.669013	H	4.383656	-3.595720	-2.591694
H	0.452845	2.438772	-0.199395	C	5.165708	-2.279163	-0.207336
C	2.998966	0.087068	-0.707540	H	5.186058	-1.411639	0.467832
H	3.063065	-0.964474	-0.395293	H	5.190832	-3.175219	0.430411
H	2.958143	0.091137	-1.807093	C	6.409938	-2.232578	-1.099665
C	4.256616	0.819219	-0.230341	H	6.491144	-3.163946	-1.676416
H	4.234595	1.856923	-0.597347	H	6.272577	-1.427953	-1.836151
H	4.232879	0.877881	0.865776	C	7.662683	-2.023879	-0.302648
C	5.499538	0.151587	-0.724881	H	8.198139	-2.924349	0.008128
H	5.596860	0.123850	-1.814993	C	8.147616	-0.842356	0.100635
C	6.472114	-0.428780	-0.009896	C	9.393106	-0.747545	0.927661
C	7.644380	-1.074332	-0.686182	H	9.840171	-1.730074	1.112462
H	7.585181	-1.000073	-1.777062	H	10.146427	-0.115159	0.436753
H	8.588330	-0.613768	-0.361998	H	9.185577	-0.277001	1.899664
H	7.715966	-2.137880	-0.418027	C	7.511701	0.475893	-0.224421
C	6.514231	-0.503860	1.485757	H	6.539252	0.380926	-0.720078
H	5.655942	-0.036279	1.975142	H	7.365733	1.062777	0.694470
H	6.561037	-1.551289	1.814696	H	8.167488	1.079986	-0.867384
H	7.425061	-0.023105	1.868997	O	3.611693	-0.976342	-1.599671
O	1.507231	0.393070	1.221431	C	1.351129	-1.669090	-0.722853
C	-0.767186	0.098131	0.317117	C	0.727875	-2.294671	0.428162
H	-1.010251	1.111395	0.638285	C	-0.249609	-3.343804	0.402617
C	-1.732032	-0.774749	-0.003737	C	-0.692345	-3.920614	1.623360

C	-0.814521	-3.865234	-0.788614	C	2.108859	0.753587	2.321970
C	-1.672698	-4.886765	1.658043	C	2.506612	-0.169132	3.294519
H	-0.251294	-3.568589	2.556238	C	3.091736	1.421860	1.578225
C	-1.804766	-4.823189	-0.760720	C	3.858919	-0.420520	3.518371
H	-0.477179	-3.487353	-1.751321	H	1.756618	-0.704951	3.875973
C	-2.266032	-5.343450	0.464164	C	4.439283	1.183534	1.818459
H	-2.003955	-5.297407	2.610157	H	2.797299	2.103136	0.781893
H	-2.241867	-5.175241	-1.693904	C	4.827999	0.256098	2.783877
C	-3.304455	-6.311125	0.498192	H	4.153242	-1.146062	4.273052
N	-4.160949	-7.104020	0.529509	H	5.189246	1.713222	1.234465
H	2.993411	-0.831325	0.420334	H	5.884756	0.056346	2.955291
H	1.115747	-2.085838	-1.705481	C	-0.575013	0.409286	3.328696
H	1.238131	-2.151990	1.385249	C	-1.321474	-0.767993	3.267618
C	-0.326764	5.446088	1.247366	C	-0.537767	1.139708	4.521319
C	-1.236196	4.523233	0.733818	C	-2.021494	-1.219214	4.383478
C	-1.012444	3.178926	1.026261	H	-1.350331	-1.330810	2.333590
C	0.094039	2.721039	1.743642	C	-1.237157	0.690016	5.635000
C	0.965507	3.680594	2.265849	H	0.040607	2.061983	4.575801
C	0.752489	5.032670	2.023311	C	-1.977963	-0.490400	5.567140
H	-0.463444	6.506586	1.050280	H	-2.606621	-2.135454	4.314273
H	1.830803	3.364517	2.844479	H	-1.206828	1.260623	6.560407
H	1.438403	5.770156	2.432167	H	-2.524877	-0.836592	6.441228
O	-1.901206	2.226105	0.593566	C	-2.878514	-1.446267	-2.097661
C	-2.474226	4.887099	-0.071899	C	-4.159335	-2.002348	-2.163860
C	-2.739265	3.752072	-1.051541	C	-1.959375	-1.725009	-3.114682
C	-2.487165	2.446920	-0.628000	C	-4.507043	-2.842634	-3.217331
C	-3.276511	3.912873	-2.327756	H	-4.888393	-1.786098	-1.385078
C	-2.800590	1.316020	-1.385144	C	-2.312407	-2.559720	-4.170392
C	-3.574425	2.810096	-3.123477	H	-0.968624	-1.272141	-3.082312
H	-3.473735	4.911151	-2.710413	C	-3.583445	-3.127076	-4.219030
C	-3.354048	1.520451	-2.651571	H	-5.504025	-3.275366	-3.254658
H	-3.995693	2.957415	-4.114637	H	-1.589599	-2.770665	-4.955428
H	-3.601115	0.664188	-3.275398	H	-3.855815	-3.786264	-5.040022
P	0.349738	0.905604	1.828445	C	-3.614622	-0.685773	0.558334
P	-2.354453	-0.340116	-0.730543	C	-4.471127	0.278841	1.090534
C	-3.673406	4.975169	0.892118	C	-3.661396	-1.991055	1.066807
H	-3.827089	4.030710	1.427567	C	-5.349006	-0.052519	2.121012
H	-3.504057	5.764516	1.635326	H	-4.467559	1.293641	0.697072
H	-4.589506	5.208472	0.335077	C	-4.547360	-2.322835	2.082970
C	-2.312212	6.225456	-0.783317	H	-3.007404	-2.759481	0.656113
H	-3.218183	6.479867	-1.343652	C	-5.389597	-1.350212	2.619420
H	-2.158555	7.034038	-0.061069	H	-6.011356	0.708449	2.527294
H	-1.463631	6.214808	-1.478993	H	-4.576874	-3.345798	2.455713
Cu	-0.131274	-0.420395	-0.042056	H	-6.079322	-1.605526	3.420420

B	0.897840	0.420043	-1.596829	H	6.381678	-0.742712	-0.741256
O	1.785773	1.445797	-1.381608	H	7.034269	-0.665816	0.885648
O	0.495527	0.353411	-2.909843	O	3.122390	1.522096	1.053663
C	1.755436	2.295945	-2.552686	C	0.803757	2.238454	0.416983
C	1.262324	1.324398	-3.667113	C	-0.147036	2.294133	-0.718954
C	0.765754	3.412453	-2.244774	C	-1.187478	3.358568	-0.700892
H	1.067792	3.903489	-1.309947	C	-1.445272	4.096199	-1.862850
H	0.738522	4.168394	-3.038884	C	-1.926171	3.653390	0.453951
H	-0.249738	3.017976	-2.103638	C	-2.420664	5.082023	-1.888871
C	3.140229	2.866998	-2.768961	H	-0.874134	3.877986	-2.764710
H	3.181954	3.447666	-3.699338	C	-2.903119	4.630420	0.443378
H	3.393155	3.538026	-1.939333	H	-1.752290	3.083828	1.365034
H	3.896015	2.077388	-2.810398	C	-3.161930	5.351478	-0.732856
C	0.347378	1.953916	-4.697981	H	-2.614398	5.644876	-2.798824
H	0.860463	2.768014	-5.226207	H	-3.479772	4.838194	1.342119
H	0.058845	1.201082	-5.440277	C	-4.175850	6.356012	-0.749165
H	-0.567649	2.348496	-4.243298	N	-5.004828	7.174113	-0.762206
C	2.382765	0.560303	-4.354746	H	2.467207	1.934691	-0.922415
H	1.936844	-0.214782	-4.988708	H	0.500170	2.771854	1.320670
H	2.982382	1.216270	-4.997199	H	0.356708	2.247183	-1.692441
H	3.035654	0.068796	-3.624680	C	-4.079344	-3.899123	1.219441
				C	-2.905257	-3.794055	0.475048
18-ts				C	-2.012619	-2.785175	0.839279
C	2.245347	2.200452	0.121561	C	-2.283099	-1.841424	1.835778
C	3.337857	2.918260	0.809926	C	-3.458211	-2.004267	2.575342
C	3.074267	3.808950	1.991180	C	-4.343792	-3.032201	2.275798
H	3.045928	4.862028	1.685299	H	-4.799734	-4.678720	0.985044
H	2.122861	3.563196	2.474288	H	-3.691283	-1.303890	3.374806
H	3.869119	3.701482	2.740799	H	-5.254495	-3.150299	2.857232
C	4.633162	3.160236	0.071254	O	-0.805551	-2.674753	0.202828
H	4.634060	2.525346	-0.826237	C	-2.531283	-4.743216	-0.659141
H	4.695040	4.202433	-0.273476	C	-1.609440	-4.006808	-1.624963
C	5.857069	2.792756	0.928272	C	-0.757002	-3.027302	-1.122466
H	6.127760	3.637277	1.576927	C	-1.484491	-4.310257	-2.983006
H	5.565244	1.972412	1.598139	C	0.199255	-2.360798	-1.893498
C	7.038325	2.382176	0.102795	C	-0.537447	-3.672840	-3.779514
H	7.694190	3.182705	-0.249429	H	-2.122156	-5.069113	-3.429536
C	7.328813	1.128802	-0.272882	C	0.307922	-2.708149	-3.238379
C	8.529924	0.821831	-1.114652	H	-0.454405	-3.936545	-4.830916
H	9.107761	1.721172	-1.353111	H	1.050111	-2.216427	-3.864459
H	9.196926	0.111547	-0.605161	P	-1.166391	-0.392865	2.012101
H	8.239788	0.340056	-2.060065	P	1.200196	-1.107025	-1.008796
C	6.515162	-0.070739	0.119987	C	-1.752393	-5.931243	-0.064639
H	5.520871	0.185006	0.504103	H	-0.849512	-5.594921	0.458423

H	-2.381120	-6.475379	0.651543	H	2.392709	-3.798774	-1.505062
H	-1.449749	-6.622917	-0.861046	C	3.764680	-2.473806	1.869558
C	-3.774399	-5.268266	-1.374365	H	2.533872	-0.736330	1.500886
H	-3.500669	-5.968147	-2.170615	C	4.181868	-3.709323	1.384441
H	-4.419535	-5.826717	-0.688332	H	4.013660	-5.148682	-0.211223
H	-4.357790	-4.450085	-1.814801	H	4.144546	-2.096046	2.817042
Cu	-0.088045	0.417573	0.183567	H	4.892077	-4.306790	1.951758
C	-2.238987	0.833621	2.863832	B	-1.531020	0.872287	-1.283221
C	-1.832378	1.490507	4.028286	O	-2.844978	0.955708	-0.885274
C	-3.447485	1.209584	2.259594	O	-1.428913	0.560497	-2.618976
C	-2.616824	2.502126	4.579104	C	-3.680908	0.426914	-1.937240
H	-0.899011	1.212900	4.514671	C	-2.754581	0.494086	-3.197787
C	-4.236098	2.205269	2.822858	C	-4.053974	-0.991108	-1.529478
H	-3.755928	0.741316	1.325556	H	-4.553383	-0.956439	-0.553353
C	-3.820748	2.859045	3.981526	H	-4.742664	-1.452450	-2.247765
H	-2.285662	3.005649	5.484465	H	-3.168017	-1.632099	-1.431774
H	-5.171506	2.485307	2.342504	C	-4.930245	1.282836	-2.012198
H	-4.434550	3.645088	4.415344	H	-5.573214	0.970842	-2.844913
C	0.034208	-0.889270	3.303707	H	-5.501349	1.171383	-1.082785
C	1.146166	-0.059866	3.495362	H	-4.685328	2.343592	-2.130821
C	-0.103394	-2.041716	4.079270	C	-2.813309	-0.724922	-4.097770
C	2.092655	-0.366857	4.465920	H	-3.815596	-0.841579	-4.529446
H	1.284241	0.808116	2.846834	H	-2.101738	-0.599406	-4.923159
C	0.858858	-2.359030	5.035723	H	-2.545215	-1.642796	-3.564901
H	-0.962327	-2.695915	3.936260	C	-2.942296	1.749386	-4.035148
C	1.951220	-1.520234	5.235603	H	-2.133483	1.804066	-4.773178
H	2.953379	0.284627	4.604186	H	-3.896190	1.731031	-4.575307
H	0.750757	-3.263673	5.629673	H	-2.905938	2.656994	-3.423766
H	2.698282	-1.769567	5.985799				
C	2.292962	-0.377886	-2.288181	**19**			
C	3.679094	-0.350910	-2.106264	C	-3.984489	-0.435057	0.093513
C	1.732884	0.334269	-3.358141	C	-5.167276	0.073463	-0.615363
C	4.490122	0.384064	-2.966913	C	-5.063340	0.747193	-1.955130
H	4.130080	-0.891082	-1.274607	H	-5.067526	1.837745	-1.838416
C	2.549105	1.052118	-4.225870	H	-4.154300	0.455291	-2.490803
H	0.651984	0.335351	-3.495569	H	-5.916812	0.475660	-2.587820
C	3.927924	1.088194	-4.027276	C	-6.403417	0.400985	0.190166
H	5.565978	0.414378	-2.797141	H	-6.298933	-0.031948	1.195064
H	2.104052	1.596565	-5.055940	H	-6.474863	1.491396	0.321676
H	4.561041	1.665569	-4.696891	C	-7.691680	-0.135583	-0.438945
C	2.352254	-2.183652	-0.070816	H	-7.842681	0.335092	-1.422877
C	2.775805	-3.425432	-0.555495	H	-7.562192	-1.209409	-0.626475
C	2.852706	-1.712877	1.142773	C	-8.882426	0.141331	0.421660
C	3.687048	-4.183841	0.170467	H	-9.102400	1.204371	0.564537

C	-9.674645	-0.735508	1.052260	C	2.524746	-0.648512	-3.857957
C	-10.821262	-0.269648	1.898749	H	3.309352	-1.936943	-5.388892
H	-10.900723	0.822239	1.922810	H	1.900422	-0.079338	-4.543458
H	-11.774022	-0.674291	1.528342	P	1.794148	-0.072321	2.014897
H	-10.718931	-0.628853	2.932605	P	1.369407	0.873043	-1.735929
C	-9.527396	-2.225435	0.992002	C	6.341007	-2.124490	-0.991091
H	-8.674722	-2.559074	0.394996	H	6.196875	-1.076592	-0.701925
H	-9.413113	-2.640317	2.003180	H	6.995534	-2.597694	-0.248293
H	-10.434078	-2.685615	0.574646	H	6.845752	-2.144082	-1.965179
O	-4.850365	-1.325858	-0.617153	C	5.265016	-4.321494	-1.490184
C	-2.544107	-0.347291	-0.366778	H	5.772253	-4.363234	-2.459510
C	-1.689749	0.477456	0.587810	H	5.930375	-4.817151	-0.775792
C	-1.696064	1.918982	0.518313	H	4.333813	-4.897366	-1.557705
C	-1.292581	2.692585	1.646679	Cu	0.330002	0.300558	0.247610
C	-2.009794	2.653878	-0.660109	C	0.958489	-0.444125	3.598056
C	-1.188389	4.064334	1.599908	C	1.394897	0.039099	4.833692
H	-1.057204	2.166657	2.573884	C	-0.158632	-1.287601	3.539444
C	-1.915820	4.028623	-0.708427	C	0.722911	-0.320267	5.999420
H	-2.310856	2.118921	-1.559829	H	2.264901	0.692594	4.885624
C	-1.498183	4.766489	0.416212	C	-0.816608	-1.655106	4.708085
H	-0.872420	4.618538	2.482540	H	-0.514700	-1.655441	2.574048
H	-2.154129	4.553716	-1.632337	C	-0.378347	-1.169161	5.938112
C	-1.383404	6.178878	0.357533	H	1.065151	0.061138	6.958726
N	-1.279685	7.341439	0.308578	H	-1.679873	-2.314753	4.657492
H	-4.077990	-0.525660	1.184828	H	-0.899573	-1.449417	6.850525
H	-2.510364	0.078678	-1.379319	C	2.921504	1.315325	2.401093
H	-1.760746	0.110120	1.620907	C	2.403274	2.612700	2.337658
C	4.482004	-3.763163	1.295935	C	4.259362	1.128268	2.759992
C	4.326126	-2.807028	0.291136	C	3.209419	3.705670	2.633774
C	3.549586	-1.692427	0.599615	H	1.362814	2.768765	2.045292
C	2.923001	-1.506064	1.834244	C	5.067344	2.225219	3.043882
C	3.120080	-2.475807	2.818659	H	4.670979	0.121781	2.821893
C	3.895265	-3.598331	2.547199	C	4.544610	3.513737	2.980081
H	5.077764	-4.652788	1.106906	H	2.795667	4.710478	2.574803
H	2.645153	-2.359416	3.791334	H	6.108696	2.071509	3.317335
H	4.042060	-4.353683	3.314864	H	5.178091	4.369685	3.200774
O	3.348556	-0.707133	-0.333254	C	0.214045	1.262994	-3.098854
C	4.999528	-2.877514	-1.074206	C	0.174841	2.485145	-3.770991
C	4.111649	-2.160202	-2.084169	C	-0.730410	0.276388	-3.408764
C	3.337334	-1.085617	-1.650745	C	-0.813428	2.726488	-4.723367
C	4.075647	-2.452471	-3.447985	H	0.905902	3.258771	-3.543217
C	2.512577	-0.337726	-2.496609	C	-1.706716	0.515163	-4.368286
C	3.305919	-1.697511	-4.328794	H	-0.707060	-0.683563	-2.888489
H	4.667256	-3.276198	-3.839451	C	-1.757091	1.747594	-5.018858

H	-0.843559	3.685091	-5.236220	H	-4.708586	1.970920	-0.959293
H	-2.437199	-0.258894	-4.595513	H	-5.840814	0.770965	-0.329910
H	-2.530025	1.941538	-5.758788	C	-5.491622	2.474264	0.982182
C	2.352941	2.390331	-1.473950	H	-5.984675	1.962948	1.820172
C	3.733443	2.446984	-1.672968	H	-4.602389	2.965562	1.404253
C	1.685429	3.511960	-0.963019	C	-6.425362	3.487133	0.391549
C	4.433641	3.615359	-1.381085	H	-7.493101	3.262685	0.455113
H	4.266644	1.579273	-2.060029	C	-6.064198	4.610167	-0.243360
C	2.384352	4.681681	-0.693807	C	-7.082131	5.544365	-0.823022
H	0.609755	3.472765	-0.781218	H	-8.105858	5.193997	-0.653476
C	3.761441	4.734547	-0.900113	H	-6.987475	6.549535	-0.387769
H	5.509162	3.650993	-1.538161	H	-6.936274	5.665718	-1.905804
H	1.853425	5.549950	-0.307626	C	-4.640835	5.037086	-0.443710
H	4.311537	5.645591	-0.676196	H	-3.911532	4.326858	-0.040745
B	-1.960031	-1.793702	-0.505708	H	-4.427721	5.160614	-1.514919
O	-1.560324	-2.572725	0.554283	H	-4.458246	6.017947	0.017942
O	-1.773390	-2.414329	-1.716357	O	-2.626528	1.381716	0.524173
C	-0.825160	-3.688617	-0.002052	C	-1.764390	-0.786710	-0.435187
C	-1.416570	-3.787686	-1.439455	C	-2.074911	-1.785099	-1.591869
C	0.645371	-3.299293	0.009352	C	-3.336124	-2.534302	-1.274904
H	0.963866	-3.127682	1.044398	C	-4.565707	-2.132612	-1.814077
H	1.283720	-4.086495	-0.411172	C	-3.335042	-3.582239	-0.341416
H	0.819081	-2.370044	-0.555949	C	-5.752654	-2.743655	-1.439213
C	-1.047408	-4.904437	0.871592	H	-4.586582	-1.317461	-2.537103
H	-0.559189	-5.787142	0.440140	C	-4.509405	-4.204011	0.044413
H	-0.611140	-4.727271	1.861994	H	-2.385682	-3.907744	0.080807
H	-2.111094	-5.120997	1.003092	C	-5.731373	-3.785908	-0.503502
C	-0.445792	-4.262536	-2.499381	H	-6.700328	-2.420558	-1.863647
H	-0.082237	-5.272058	-2.270421	H	-4.494224	-5.016187	0.767758
H	-0.949576	-4.297403	-3.471588	C	-6.947433	-4.422760	-0.112481
H	0.416002	-3.592152	-2.587706	N	-7.939510	-4.943453	0.206412
C	-2.703446	-4.596329	-1.497073	H	-2.852104	0.775072	-1.488851
H	-3.160397	-4.467830	-2.484103	H	-1.894810	-1.344095	0.503658
H	-2.514429	-5.664620	-1.340697	H	-2.235773	-1.196850	-2.511274
H	-3.423190	-4.252034	-0.744811	C	5.084299	-2.078684	2.427245
				C	4.851465	-1.055319	1.509291
20				C	3.579474	-0.485320	1.508250
C	-2.725523	0.353281	-0.477988	C	2.542863	-0.903331	2.346251
C	-3.846131	0.622263	0.445096	C	2.824247	-1.918804	3.263681
C	-4.112074	-0.256398	1.635631	C	4.087189	-2.499107	3.303712
H	-4.923630	-0.962459	1.416939	H	6.060312	-2.555757	2.468320
H	-3.225500	-0.834224	1.920334	H	2.039781	-2.272357	3.930229
H	-4.413239	0.346679	2.502214	H	4.296102	-3.291275	4.018138
C	-5.014435	1.440575	-0.045420	O	3.280623	0.528982	0.632108

C	5.899575	-0.488463	0.560437	C	1.049425	3.210443	-3.577557
C	5.187523	-0.035795	-0.708019	C	0.208146	0.955508	-3.802118
C	3.903612	0.491888	-0.589728	C	0.612379	3.499503	-4.866483
C	5.753993	-0.036540	-1.983571	H	1.549193	3.978738	-2.988359
C	3.173750	1.000630	-1.667806	C	-0.217544	1.245845	-5.095163
C	5.066992	0.484200	-3.076863	H	0.054913	-0.038576	-3.379439
H	6.752799	-0.439954	-2.131320	C	-0.020192	2.517621	-5.625741
C	3.785647	1.003045	-2.922977	H	0.766634	4.493413	-5.280320
H	5.535196	0.481890	-4.057814	H	-0.711817	0.478137	-5.686292
H	3.245901	1.390412	-3.785140	H	-0.361252	2.746313	-6.632877
P	0.856291	-0.262620	2.006901	C	1.492800	3.039840	-0.465146
P	1.424009	1.454436	-1.369633	C	2.643128	3.824909	-0.360991
C	6.532682	0.749686	1.224217	C	0.301066	3.474912	0.124841
H	5.777358	1.508291	1.461595	C	2.598149	5.039381	0.318021
H	7.034296	0.462392	2.156823	H	3.573915	3.489838	-0.818232
H	7.273213	1.200999	0.551961	C	0.256378	4.697845	0.784803
C	6.996844	-1.504047	0.259676	H	-0.592816	2.848313	0.072051
H	7.749886	-1.076200	-0.410397	C	1.404406	5.479938	0.882779
H	7.526466	-1.789458	1.174761	H	3.496642	5.647218	0.397546
H	6.590860	-2.410585	-0.205807	H	-0.674581	5.033737	1.235999
Cu	0.079203	-0.026126	-0.256442	H	1.370689	6.431689	1.408432
C	-0.186723	-1.393801	3.008124	B	-0.737209	-2.569025	-1.798707
C	-0.533089	-1.143722	4.339707	O	-0.225376	-3.552438	-0.981420
C	-0.644275	-2.567531	2.395442	O	0.111730	-2.266454	-2.837159
C	-1.328348	-2.044290	5.042200	C	1.158995	-3.755717	-1.355342
H	-0.181573	-0.237481	4.830230	C	1.201521	-3.210539	-2.819712
C	-1.434022	-3.469495	3.102462	C	2.012908	-2.944393	-0.393246
H	-0.395708	-2.775645	1.353460	H	1.808810	-3.268465	0.634842
C	-1.781508	-3.206958	4.424675	H	3.084519	-3.084612	-0.585173
H	-1.592890	-1.837086	6.076638	H	1.786284	-1.869188	-0.459617
H	-1.786396	-4.376588	2.614668	C	1.489767	-5.226607	-1.214042
H	-2.406346	-3.907012	4.974350	H	2.512114	-5.425514	-1.559236
C	0.744190	1.318989	2.917097	H	1.426960	-5.517119	-0.159418
C	-0.527110	1.897878	3.024420	H	0.799880	-5.855950	-1.782973
C	1.847300	1.976539	3.463902	C	2.476503	-2.479518	-3.188323
C	-0.692333	3.098774	3.702001	H	3.342051	-3.152736	-3.139990
H	-1.382666	1.405922	2.558448	H	2.397401	-2.098217	-4.213637
C	1.679531	3.193484	4.120075	H	2.659069	-1.626442	-2.525888
H	2.840508	1.535068	3.387664	C	0.880120	-4.267735	-3.865202
C	0.411020	3.750522	4.249818	H	0.748039	-3.776748	-4.835462
H	-1.684928	3.536010	3.790734	H	1.688059	-5.002132	-3.959798
H	2.543786	3.699607	4.544766	H	-0.048186	-4.799258	-3.625633
H	0.282459	4.696227	4.771699				
C	0.848484	1.936473	-3.038167	**21-ts**			

C	-1.351404	-2.450377	3.597313	C	-3.998848	0.865144	0.771261
C	-0.834804	-1.195958	3.272711	C	-4.244761	2.689240	-1.321694
C	-1.105779	-0.711102	1.995923	H	-2.722104	1.532238	-2.310085
C	-1.872744	-1.398063	1.053211	C	-4.892118	1.928196	0.872179
C	-2.377674	-2.647132	1.417387	H	-3.910895	0.151418	1.589601
C	-2.112575	-3.169472	2.679487	C	-5.019264	2.837366	-0.173570
H	-1.161012	-2.877602	4.578571	H	-4.326703	3.408860	-2.133349
H	-2.967182	-3.218500	0.703175	H	-5.493837	2.042832	1.770908
H	-2.505387	-4.145376	2.952648	H	-5.716898	3.667647	-0.091186
O	-0.599295	0.507348	1.605506	C	2.435548	2.553583	-1.264199
C	-0.049430	-0.297215	4.219019	C	2.751379	3.914489	-1.188443
C	0.994873	0.437154	3.389178	C	3.301979	1.677040	-1.925393
C	0.639197	0.836372	2.101901	C	3.916728	4.393349	-1.776262
C	2.273772	0.775578	3.827610	H	2.083141	4.600287	-0.669525
C	1.487340	1.552452	1.253030	C	4.470471	2.161541	-2.506725
C	3.144847	1.493543	3.011860	H	3.068375	0.612698	-1.965783
H	2.602313	0.475475	4.819602	C	4.775519	3.517436	-2.437318
C	2.757304	1.881555	1.734163	H	4.156398	5.452458	-1.717679
H	4.136300	1.749965	3.375975	H	5.141576	1.476504	-3.019470
H	3.448090	2.429159	1.096405	H	5.685858	3.894921	-2.897396
P	-2.026255	-0.655917	-0.615030	C	-0.221836	3.248384	-0.403477
P	0.949298	1.843537	-0.475301	C	-0.600514	3.834286	-1.618238
C	-1.020698	0.745566	4.806594	C	-0.794651	3.708528	0.783053
H	-1.508103	1.332163	4.018188	C	-1.518973	4.875382	-1.641102
H	-1.802070	0.244238	5.391398	H	-0.166553	3.475685	-2.552407
H	-0.479489	1.436674	5.464753	C	-1.727565	4.742439	0.755460
C	0.581820	-1.080954	5.363222	H	-0.505764	3.270015	1.737062
H	1.108620	-0.407844	6.048379	C	-2.088238	5.328983	-0.452854
H	-0.186796	-1.587760	5.956269	H	-1.798637	5.328730	-2.589468
H	1.293351	-1.832864	4.999473	H	-2.169727	5.092462	1.685474
Cu	0.169906	-0.200221	-1.202879	H	-2.814055	6.138775	-0.470684
C	-2.949544	-1.908187	-1.569521	B	1.580201	-1.804143	-1.137719
C	-4.329766	-2.090284	-1.424849	O	2.937267	-1.539925	-1.101368
C	-2.229256	-2.717607	-2.454145	O	1.231114	-2.843032	-0.292804
C	-4.983061	-3.076854	-2.154101	C	3.552799	-2.687313	-0.476111
H	-4.892841	-1.457860	-0.738671	C	2.413872	-3.198595	0.450306
C	-2.890606	-3.706262	-3.178989	C	3.894070	-3.661690	-1.596117
H	-1.154393	-2.574495	-2.592599	H	4.584268	-3.166295	-2.289190
C	-4.262092	-3.885836	-3.030889	H	4.382094	-4.568036	-1.218758
H	-6.055774	-3.214656	-2.040185	H	2.989156	-3.928697	-2.156553
H	-2.327720	-4.333252	-3.866460	C	4.807108	-2.241105	0.244632
H	-4.774639	-4.656635	-3.602066	H	5.247537	-3.073246	0.808805
C	-3.221758	0.709361	-0.379509	H	5.550020	-1.897726	-0.484244
C	-3.344568	1.635444	-1.420003	H	4.603242	-1.416954	0.935705

C	2.411607	-4.692773	0.694770	H	-8.507756	0.154518	1.863854
H	3.342120	-5.008078	1.184385	H	-8.747826	1.204240	3.269047
H	1.575981	-4.955210	1.354066	H	-10.009875	0.072004	2.809298
H	2.298063	-5.253020	-0.237670	O	-5.949582	-0.325252	-0.155088
C	2.343467	-2.449198	1.773675	C	-3.551166	0.201662	-0.757088
H	1.389788	-2.690996	2.261368	C	-2.369838	0.403260	0.171308
H	3.158929	-2.728673	2.452433	H	-4.790747	1.176959	0.789515
H	2.374044	-1.362902	1.616317	H	-3.384884	0.762264	-1.693232
C	1.836022	-1.838934	-4.116069	H	-2.415377	-0.223135	1.069903
H	2.864693	-2.244177	-4.222280	C	3.079877	-4.726277	-0.700849
H	1.967627	-0.774915	-3.797586	C	3.560179	-3.445140	-0.970029
H	1.408743	-1.790427	-5.137044	C	3.101715	-2.409345	-0.158024
O	1.057234	-2.553861	-3.236512	C	2.198080	-2.596609	0.890269
H	0.812592	-1.623419	-2.222358	C	1.756552	-3.897667	1.139666
				C	2.191586	-4.953256	0.346192
MeOH				H	3.405365	-5.565625	-1.310538
C	0.046730	0.654434	0.000000	H	1.051454	-4.079693	1.948506
H	1.090740	0.982580	0.000000	H	1.836689	-5.961352	0.544651
H	-0.438224	1.081198	0.890505	O	3.541005	-1.124113	-0.373289
H	-0.438224	1.081198	-0.890505	C	4.599947	-3.113132	-2.030746
O	0.046730	-0.752947	0.000000	C	4.279596	-1.726847	-2.571547
H	-0.868507	-1.048005	0.000000	C	3.794876	-0.772412	-1.677232
				C	4.505880	-1.314944	-3.884044
22-ts				C	3.548561	0.557374	-2.031433
C	-4.880934	0.633621	-0.159704	C	4.272097	0.000726	-4.271889
C	-6.109935	0.870704	-0.928607	H	4.877207	-2.025372	-4.618364
C	-6.150793	0.666637	-2.418038	C	3.802189	0.932030	-3.353402
H	-7.103657	0.209220	-2.713063	H	4.459472	0.302214	-5.299147
H	-6.069312	1.629571	-2.937418	H	3.613377	1.956032	-3.668822
H	-5.345587	0.011944	-2.765231	P	1.604883	-1.112118	1.789470
C	-7.154905	1.798441	-0.356807	P	2.765474	1.671395	-0.801486
H	-6.957000	1.926993	0.716756	C	5.980563	-3.050296	-1.347968
H	-7.064192	2.793758	-0.816397	H	5.998838	-2.301688	-0.547077
C	-8.579323	1.260218	-0.534181	H	6.229630	-4.025515	-0.911257
H	-8.856096	1.289909	-1.596821	H	6.752671	-2.787187	-2.081801
H	-8.577209	0.198135	-0.249536	C	4.647099	-4.162942	-3.134730
C	-9.588735	2.025134	0.268634	H	5.423558	-3.920177	-3.867853
H	-10.096287	2.847499	-0.241679	H	4.908713	-5.143903	-2.724182
C	-9.885292	1.817451	1.558328	H	3.687326	-4.249122	-3.657736
C	-10.892911	2.662070	2.276291	Cu	1.074568	0.522631	0.212418
H	-11.334051	3.421790	1.622358	C	0.229342	-1.787152	2.787446
H	-11.706641	2.044816	2.682744	C	0.264653	-1.945355	4.173996
H	-10.438129	3.172846	3.136932	C	-0.938050	-2.118862	2.088496
C	-9.249879	0.753150	2.401409	C	-0.853839	-2.434127	4.847411

H	1.164425	-1.689651	4.731208	C	-3.829442	-3.181418	-2.418365
C	-2.049387	-2.612805	2.760204	C	-1.786070	-3.839348	-1.001577
H	-0.975219	-1.985037	1.006815	H	-1.460027	-4.000055	0.032943
C	-2.007353	-2.769797	4.144742	H	-1.537513	-4.739111	-1.576154
H	-0.820173	-2.553231	5.927954	H	-1.217714	-2.987895	-1.399488
H	-2.946007	-2.847571	2.187369	C	-4.021846	-4.705641	-0.335687
H	-2.876983	-3.147570	4.677537	H	-3.942915	-5.624163	-0.930831
C	2.937605	-0.780453	2.993262	H	-3.575652	-4.901760	0.646320
C	3.223896	0.550042	3.303289	H	-5.080422	-4.474278	-0.187250
C	3.654970	-1.803424	3.623884	C	-3.108300	-3.824682	-3.583533
C	4.210714	0.859830	4.234679	H	-3.202985	-4.916958	-3.541456
H	2.688113	1.347320	2.785976	H	-3.555065	-3.484078	-4.524282
C	4.639294	-1.493653	4.555146	H	-2.045470	-3.565887	-3.598298
H	3.437126	-2.844600	3.385613	C	-5.332247	-3.381236	-2.555264
C	4.916461	-0.162242	4.861375	H	-5.667649	-2.895902	-3.478986
H	4.435549	1.900765	4.457031	H	-5.598947	-4.442770	-2.610884
H	5.193231	-2.292009	5.043410	H	-5.871411	-2.923613	-1.717382
H	5.690282	0.076716	5.587135	C	-0.336698	-0.270918	-2.288049
C	2.406880	3.168770	-1.781296	H	0.656445	-0.204169	-2.758242
C	1.113679	3.309338	-2.287254	H	-0.844442	0.702083	-2.428889
C	3.370343	4.141673	-2.068989	H	-0.927696	-1.024074	-2.836031
C	0.784205	4.405293	-3.078423	O	-0.224894	-0.599779	-0.926254
H	0.357735	2.564327	-2.036006	H	-1.235231	-0.203612	-0.432592
C	3.037503	5.239733	-2.853540	C	-1.777375	1.681894	0.401799
H	4.381122	4.038860	-1.675968	C	-2.024243	2.837740	-0.390249
C	1.745378	5.371327	-3.358760	C	-0.757553	1.803314	1.398869
H	-0.227856	4.509950	-3.463616	C	-1.288819	3.991533	-0.236378
H	3.787259	5.996946	-3.069490	H	-2.823981	2.812593	-1.128695
H	1.487183	6.233986	-3.968453	C	-0.009457	2.959051	1.541086
C	4.133003	2.204902	0.294597	H	-0.627226	0.985578	2.110202
C	3.885244	3.274058	1.165723	C	-0.248490	4.070302	0.711772
C	5.377753	1.574346	0.325657	H	-1.500730	4.859844	-0.858057
C	4.867311	3.705070	2.048335	H	0.755800	3.019257	2.314653
H	2.924218	3.790475	1.139097	C	0.573882	5.222896	0.790197
C	6.357058	2.001987	1.219765	N	1.269127	6.160286	0.845320
H	5.589951	0.748315	-0.351419				
C	6.104796	3.063978	2.080866	**23**			
H	4.666205	4.544015	2.710457	C	0.214080	0.121685	-0.074157
H	7.323716	1.504026	1.236069	C	0.211713	1.256281	-1.005416
H	6.873018	3.398173	2.774238	C	-0.527319	1.196188	-2.313447
B	-3.577627	-1.321952	-1.153284	H	-0.962597	2.175495	-2.547231
O	-3.504075	-2.354610	-0.251018	H	0.161462	0.936679	-3.126635
O	-3.602239	-1.754539	-2.455839	H	-1.343995	0.469094	-2.291300
C	-3.284060	-3.567670	-1.009969	C	1.342053	2.254533	-0.927134

H	1.841750	2.141715	0.045355	C	1.963499	-3.187156	-0.761807
H	2.093219	2.029733	-1.698271	C	2.449784	-2.294401	1.418963
C	0.856347	3.702046	-1.064428	C	3.306689	-3.457822	-0.961784
H	0.514792	3.882674	-2.092689	H	1.244436	-3.439724	-1.539831
H	-0.028074	3.825466	-0.423038	C	3.799916	-2.557269	1.236220
C	1.916375	4.700979	-0.708813	H	2.109745	-1.842770	2.349575
H	2.535299	5.067138	-1.531590	C	4.233216	-3.140999	0.041170
C	2.192216	5.147776	0.523349	H	3.649662	-3.915336	-1.886099
C	3.288099	6.139110	0.769186	H	4.521946	-2.315775	2.011764
H	3.802063	6.422558	-0.155393	C	5.621692	-3.417270	-0.156339
H	2.893839	7.053400	1.235274	N	6.752440	-3.642209	-0.317219
H	4.035164	5.737741	1.468421	H	-0.526595	-3.220540	0.456833
C	1.455523	4.713266	1.754373				
H	0.687564	3.958129	1.559293	**24**			
H	2.157091	4.293090	2.488630	C	-2.805219	-0.047298	0.158857
H	0.976673	5.571158	2.247105	C	-2.702080	0.600598	1.479743
O	-0.615578	1.266199	0.167346	C	-2.626287	-0.224864	2.732305
C	-0.483096	-1.205630	-0.322745	H	-1.881558	0.198728	3.420616
C	0.053978	-2.300822	0.618802	H	-3.595579	-0.227886	3.246151
H	1.068490	0.069376	0.612326	H	-2.328917	-1.255733	2.507576
H	-0.306588	-1.514665	-1.365159	C	-3.163356	2.027585	1.636986
H	-0.131903	-1.999327	1.658490	H	-3.230748	2.484447	0.637881
B	-2.032694	-1.008925	-0.108920	H	-4.181021	2.038835	2.055308
O	-2.611160	-1.003499	1.129518	C	-2.233837	2.868096	2.507650
O	-2.931215	-0.853052	-1.129820	H	-2.270266	2.509666	3.548275
C	-4.044340	-1.001143	0.922111	H	-1.195534	2.698514	2.171332
C	-4.171637	-0.419816	-0.518179	C	-2.576826	4.329682	2.441404
C	-4.503800	-2.447774	1.024595	H	-3.508241	4.576652	1.922853
H	-4.199578	-2.846679	1.998240	C	-1.866258	5.342086	2.954346
H	-5.593552	-2.531370	0.944654	C	-2.304961	6.766346	2.804791
H	-4.047923	-3.069222	0.244774	H	-3.258997	6.849756	2.273963
C	-4.696203	-0.168651	2.005147	H	-2.411468	7.254337	3.783640
H	-5.773702	-0.073259	1.822226	H	-1.553199	7.348764	2.251371
H	-4.561855	-0.657315	2.976501	C	-0.583312	5.155124	3.703937
H	-4.260280	0.832303	2.066417	H	-0.245034	4.113604	3.725155
C	-5.333029	-0.960328	-1.323990	H	0.215494	5.769309	3.260230
H	-6.284916	-0.723221	-0.832792	H	-0.687082	5.495780	4.743456
H	-5.341254	-0.495172	-2.315794	O	-1.549416	0.493894	0.627746
H	-5.268560	-2.043934	-1.457083	C	-2.979860	-1.530996	-0.079804
C	-4.164150	1.101003	-0.558807	C	-3.842362	-1.737105	-1.341331
H	-4.044921	1.420950	-1.600494	C	-5.228399	-1.175274	-1.225340
H	-5.102513	1.519959	-0.178122	C	-6.160640	-1.795555	-0.381607
H	-3.326609	1.511752	0.016596	C	-5.622240	-0.024518	-1.916682
C	1.513766	-2.601652	0.427766	C	-7.440206	-1.291349	-0.229432

H	-5.867488	-2.694627	0.160195	C	4.117321	-0.548045	-3.253735
C	-6.899817	0.497992	-1.774782	C	3.178144	0.078421	-2.435269
H	-4.910515	0.465914	-2.580560	C	3.940833	-0.427842	-4.631176
C	-7.816730	-0.135110	-0.928262	C	2.064861	0.768210	-2.924052
H	-8.157591	-1.782492	0.423212	C	2.871211	0.291788	-5.156530
H	-7.195759	1.392578	-2.317098	H	4.648316	-0.898459	-5.309579
C	-9.135329	0.393261	-0.779256	C	1.935891	0.878315	-4.311923
N	-10.210450	0.823857	-0.657669	H	2.758236	0.381726	-6.233757
H	-3.204310	0.597329	-0.635358	H	1.080372	1.403036	-4.732419
H	-3.571955	-1.926297	0.763634	P	2.103213	-0.477929	1.483208
H	-3.899179	-2.818000	-1.521792	P	0.746978	1.251981	-1.739715
H	-3.334292	-1.295769	-2.211034	C	6.355375	-0.207686	-2.230746
B	-1.638053	-2.509836	-0.137523	H	5.951103	0.568310	-1.569735
O	-1.947580	-3.827754	-0.686979	H	7.200221	-0.687046	-1.720287
O	-1.121960	-2.783601	1.215675	H	6.726583	0.277653	-3.142207
C	-1.975334	-4.774987	0.359716	C	5.915162	-2.304374	-3.502310
C	-0.980855	-4.180066	1.405286	H	6.313132	-1.836553	-4.409032
C	-3.403829	-4.877441	0.900360	H	6.763045	-2.789832	-3.007284
H	-4.075920	-5.101670	0.062361	H	5.194906	-3.076937	-3.796182
H	-3.511825	-5.675048	1.646074	Cu	0.392258	-0.259371	0.016237
H	-3.731324	-3.935540	1.357462	C	1.924482	-1.124795	3.186709
C	-1.568154	-6.133864	-0.186880	C	2.963115	-1.038727	4.122991
H	-1.487405	-6.877604	0.617090	C	0.681308	-1.623755	3.578388
H	-2.323667	-6.488169	-0.898745	C	2.757273	-1.450938	5.433259
H	-0.608694	-6.081183	-0.711808	H	3.931209	-0.635462	3.826021
C	-1.320191	-4.535034	2.845849	C	0.474144	-2.018646	4.899549
H	-1.412148	-5.622011	2.974300	H	-0.111802	-1.724024	2.835765
H	-0.524847	-4.188912	3.516812	C	1.508151	-1.932823	5.825159
H	-2.258300	-4.063186	3.160607	H	3.567008	-1.383910	6.156130
C	0.470369	-4.582208	1.141004	H	-0.503473	-2.393122	5.200238
H	1.121595	-3.941814	1.751556	H	1.344418	-2.238752	6.855979
H	0.666055	-5.627609	1.413495	C	2.951956	1.115182	1.813484
H	0.750509	-4.440956	0.091995	C	2.147215	2.191626	2.197005
C	5.236126	-3.060300	-0.725853	C	4.335419	1.290120	1.736258
C	4.778626	-1.868340	-1.288805	C	2.718405	3.417937	2.516017
C	3.846077	-1.140104	-0.554959	H	1.062012	2.065986	2.237888
C	3.401275	-1.512463	0.716055	C	4.904567	2.523471	2.040550
C	3.897484	-2.700606	1.254224	H	4.974129	0.459234	1.437455
C	4.795809	-3.476237	0.527672	C	4.098248	3.586458	2.434971
H	5.954142	-3.672476	-1.266328	H	2.081561	4.251212	2.805420
H	3.571123	-3.022965	2.241525	H	5.982697	2.650822	1.973791
H	5.168192	-4.407062	0.947612	H	4.543551	4.550126	2.671638
O	3.311196	0.015317	-1.071661	C	-0.655453	1.585114	-2.870367
C	5.286573	-1.260124	-2.588283	C	-0.887512	2.829529	-3.464418

C	-1.479146	0.501947	-3.194425	H	-1.915395	8.400917	-2.825538
C	-1.928024	2.987041	-4.375215	H	-3.010798	7.750446	-1.613438
H	-0.248268	3.676883	-3.219321	C	-2.535890	5.740009	-3.481202
C	-2.507231	0.660062	-4.120156	H	-2.135261	4.830950	-3.942233
H	-1.310747	-0.459748	-2.704513	H	-3.523615	5.491511	-3.061741
C	-2.734781	1.901671	-4.708435	H	-2.712849	6.475001	-4.277213
H	-2.103169	3.958100	-4.832625	O	0.608719	1.515131	-0.648479
H	-3.135458	-0.190148	-4.382241	C	2.923213	0.506976	-0.270027
H	-3.540657	2.024032	-5.428398	C	3.207910	-0.358383	-1.501181
C	1.173894	2.915948	-1.121122	C	4.082462	-1.541663	-1.185735
C	0.217434	3.526568	-0.299049	C	5.232042	-1.795410	-1.940021
C	2.367695	3.580985	-1.397221	C	3.738272	-2.424969	-0.151310
C	0.439794	4.795888	0.216817	C	6.022334	-2.906879	-1.689607
H	-0.709784	2.995808	-0.070490	H	5.510473	-1.105796	-2.735280
C	2.599953	4.844967	-0.855813	C	4.524109	-3.537437	0.111797
H	3.115486	3.117486	-2.039609	H	2.827588	-2.229020	0.427491
C	1.637373	5.455403	-0.058104	C	5.668792	-3.785761	-0.658322
H	-0.323828	5.257428	0.842711	H	6.912815	-3.101222	-2.282203
H	3.535570	5.357549	-1.068633	H	4.255419	-4.225459	0.910316
H	1.820036	6.444994	0.356014	C	6.476119	-4.934109	-0.392179
O	-0.628361	-1.813728	-1.016627	N	7.134243	-5.870349	-0.176951
C	0.354120	-2.552194	-1.701437	H	2.160993	2.409749	0.425649
H	-0.040230	-3.518845	-2.039651	H	3.683988	0.236078	-2.292699
H	0.684966	-1.976709	-2.581042	H	2.264398	-0.749605	-1.910017
H	1.243931	-2.740453	-1.073630	C	-3.745275	-5.089147	0.496092
				C	-3.850867	-3.807839	1.037420
24-b				C	-3.206582	-2.778201	0.356198
C	2.011375	1.707361	-0.408284	C	-2.462294	-2.969348	-0.811781
C	1.362198	2.314614	-1.583138	C	-2.397257	-4.263968	-1.331455
C	1.438174	1.760980	-2.980900	C	-3.035102	-5.314705	-0.679992
H	0.571850	2.090191	-3.566690	H	-4.227562	-5.927074	0.993847
H	2.338700	2.117081	-3.495334	H	-1.823496	-4.450809	-2.237814
H	1.435534	0.669132	-2.986535	H	-2.973606	-6.320366	-1.088029
C	1.040626	3.789607	-1.492478	O	-3.270171	-1.495754	0.838563
H	1.010221	4.068985	-0.428057	C	-4.668719	-3.445139	2.270249
H	1.864296	4.363979	-1.943757	C	-3.954762	-2.305038	2.985136
C	-0.281824	4.182860	-2.140236	C	-3.310194	-1.346339	2.205791
H	-0.236307	4.023787	-3.227769	C	-3.954721	-2.105769	4.365161
H	-1.067470	3.501328	-1.765485	C	-2.679045	-0.215983	2.734126
C	-0.656942	5.604436	-1.839336	C	-3.342024	-0.989330	4.928057
H	-0.084698	6.094607	-1.045554	H	-4.441087	-2.829030	5.015303
C	-1.643279	6.302015	-2.416817	C	-2.709277	-0.050519	4.120473
C	-1.976319	7.696497	-1.984452	H	-3.355502	-0.853589	6.006488
H	-1.311894	8.050955	-1.189409	H	-2.213386	0.808281	4.569514

P	-1.494939	-1.549064	-1.451806	C	-2.923238	1.980089	0.845696
P	-1.698550	0.834053	1.589904	C	-2.527364	3.260682	0.441472
C	-6.043404	-2.928375	1.802416	C	-4.216298	1.547513	0.526151
H	-5.942984	-2.058702	1.142273	C	-3.407236	4.090735	-0.248235
H	-6.576107	-3.715551	1.254084	H	-1.520874	3.616562	0.665236
H	-6.649506	-2.632503	2.667945	C	-5.085680	2.371080	-0.179919
C	-4.882528	-4.645577	3.184867	H	-4.554921	0.557503	0.824068
H	-5.498073	-4.370422	4.048087	C	-4.686798	3.646922	-0.566891
H	-5.422567	-5.440892	2.660018	H	-3.073295	5.082869	-0.551148
H	-3.932613	-5.052894	3.550824	H	-6.082597	2.011325	-0.425619
Cu	-0.430179	-0.516822	0.247316	H	-5.368963	4.292702	-1.116110
C	-0.409349	-2.331538	-2.692415	O	1.039741	-1.495842	1.103245
C	-0.703535	-2.435007	-4.053366	C	0.556349	-2.517858	1.888505
C	0.797147	-2.847304	-2.199781	H	1.362452	-3.217122	2.202543
C	0.202600	-3.049303	-4.914377	H	0.074185	-2.169124	2.831945
H	-1.640388	-2.034361	-4.439806	H	-0.211063	-3.150721	1.379384
C	1.693787	-3.469799	-3.062199	B	4.245383	0.979528	0.431594
H	1.033392	-2.728072	-1.137007	O	4.296244	1.235848	1.778075
C	1.397203	-3.567885	-4.420076	O	5.435892	1.207639	-0.204268
H	-0.025583	-3.124536	-5.975185	C	5.549857	1.914479	2.020354
H	2.635112	-3.858099	-2.674109	C	6.423965	1.407887	0.835774
H	2.102103	-4.044097	-5.097715	C	5.250607	3.405303	1.951234
C	-2.692021	-0.532817	-2.383200	C	6.057182	1.541505	3.396005
C	-2.381127	0.824004	-2.529743	C	7.465642	2.390354	0.346397
C	-3.892872	-1.023791	-2.900290	C	7.058330	0.049793	1.097213
C	-3.247959	1.673069	-3.207408	H	4.449105	3.635606	2.663672
H	-1.459263	1.209249	-2.088606	H	6.127267	4.010210	2.209872
C	-4.768729	-0.167092	-3.562084	H	4.907190	3.697335	0.951097
H	-4.144236	-2.077600	-2.780728	H	7.053042	1.968805	3.567705
C	-4.445123	1.178164	-3.719673	H	5.381842	1.943443	4.160215
H	-2.998754	2.727981	-3.316952	H	6.112455	0.457441	3.528580
H	-5.706150	-0.551814	-3.957594	H	8.180366	2.622374	1.145771
H	-5.133064	1.845367	-4.234190	H	8.024174	1.949959	-0.486791
C	-0.656214	1.866392	2.677911	H	7.015032	3.324050	-0.002245
C	-1.108336	2.983541	3.389781	H	7.488226	-0.325029	0.161673
C	0.691857	1.496033	2.761456	H	7.860343	0.113220	1.841286
C	-0.221132	3.725611	4.162533	H	6.313751	-0.679220	1.441136
H	-2.155630	3.278901	3.332061	H	2.411143	-0.129841	0.473736
C	1.578291	2.243940	3.533458				
H	1.038909	0.611759	2.216808	**25-ts**			
C	1.122885	3.360238	4.228477	C	-2.584576	-0.383968	0.324747
H	-0.577096	4.594553	4.711458	C	-2.481694	0.088525	1.711211
H	2.628117	1.956212	3.561842	C	-2.884375	-0.915830	2.778724
H	1.815589	3.951388	4.824128	H	-2.447393	-1.896767	2.555052

H	-2.497343	-0.588898	3.751038	H	-3.341462	-6.042051	0.930922
H	-3.975809	-1.011171	2.854513	H	-3.572783	-4.283548	0.868082
C	-3.084270	1.472753	1.942527	H	-3.840533	-5.264787	-0.585804
H	-2.841794	2.102106	1.069939	C	-1.322551	-6.252323	-0.852793
H	-4.183315	1.403333	1.980116	H	-1.259162	-7.091164	-0.147339
C	-2.548771	2.139287	3.206528	H	-2.053302	-6.517115	-1.626312
H	-2.948233	1.613246	4.088780	H	-0.349336	-6.128602	-1.338325
H	-1.458634	1.996127	3.238774	C	-1.219650	-4.982109	2.384736
C	-2.905895	3.590972	3.287223	H	-1.257709	-6.078423	2.435395
H	-3.883598	3.854105	2.870156	H	-0.485349	-4.636895	3.123210
C	-2.185594	4.581018	3.832866	H	-2.199217	-4.585083	2.672433
C	-2.691014	5.992196	3.851062	C	0.651421	-4.899511	0.768838
H	-3.688231	6.079484	3.407206	H	1.272128	-4.322388	1.469063
H	-2.736136	6.383601	4.877123	H	0.828152	-5.967659	0.948322
H	-2.011227	6.659150	3.299520	H	0.982287	-4.661415	-0.247629
C	-0.843304	4.398011	4.475002	C	5.464414	-2.495690	-1.328151
H	-0.413605	3.404046	4.310280	C	4.893864	-1.262953	-1.647450
H	-0.129362	5.146761	4.098948	C	3.906267	-0.787000	-0.790318
H	-0.907854	4.557026	5.560443	C	3.524486	-1.428880	0.390263
O	-1.098539	0.127431	1.529765	C	4.123809	-2.655563	0.679468
C	-2.827367	-1.691829	-0.170333	C	5.073206	-3.191241	-0.186576
C	-3.513950	-1.668256	-1.544361	H	6.230713	-2.920707	-1.971977
C	-4.892771	-1.077367	-1.479114	H	3.839312	-3.196492	1.580430
C	-5.122843	0.271395	-1.775020	H	5.528296	-4.152231	0.039434
C	-5.971408	-1.867636	-1.066079	O	3.246240	0.383771	-1.075594
C	-6.392250	0.818698	-1.666458	C	5.336604	-0.350733	-2.782913
H	-4.292432	0.896321	-2.105858	C	4.101756	0.370036	-3.308278
C	-7.246351	-1.338010	-0.953747	C	3.097067	0.703191	-2.398400
H	-5.797372	-2.917607	-0.831268	C	3.924683	0.776514	-4.629189
C	-7.461833	0.013359	-1.255778	C	1.912867	1.350365	-2.763150
H	-6.566579	1.865304	-1.903171	C	2.790868	1.486573	-5.015626
H	-8.081283	-1.958556	-0.638304	H	4.684297	0.546735	-5.372288
C	-8.773433	0.569787	-1.149465	C	1.788192	1.761881	-4.094135
N	-9.841987	1.024259	-1.063829	H	2.682492	1.811653	-6.047100
H	-2.406981	0.410077	-0.408994	H	0.886047	2.281734	-4.412008
H	-3.401366	-2.286930	0.551120	P	2.172517	-0.637043	1.330685
H	-3.561917	-2.701228	-1.909345	P	0.548822	1.482436	-1.536871
H	-2.890995	-1.099679	-2.245221	C	6.294642	0.701346	-2.188461
B	-1.360742	-2.697984	-0.368155	H	5.814942	1.271274	-1.383519
O	-1.698866	-3.902905	-1.074358	H	7.185198	0.209832	-1.776764
O	-0.908849	-3.094709	0.939406	H	6.611986	1.406265	-2.967213
C	-1.761536	-4.978701	-0.149717	C	6.063514	-1.112801	-3.883563
C	-0.808400	-4.510349	0.999370	H	6.413064	-0.427889	-4.663376
C	-3.210131	-5.151049	0.304892	H	6.955471	-1.608420	-3.485402

H	5.420912	-1.870444	-4.347284	H	2.465006	6.048641	-0.831892
Cu	0.301404	-0.168726	0.046044	H	0.889123	6.566599	1.011948
C	2.079729	-1.553556	2.912153	O	-0.466684	-1.830907	-1.147230
C	3.191105	-1.739074	3.744490	C	0.637461	-2.438413	-1.778295
C	0.819033	-1.980647	3.335180	H	0.329489	-3.317207	-2.360149
C	3.044177	-2.363063	4.977012	H	1.101488	-1.706929	-2.456429
H	4.173369	-1.387545	3.428845	H	1.405952	-2.752527	-1.051368
C	0.674798	-2.591822	4.580030				
H	-0.035585	-1.830850	2.677322	pinBOMe			
C	1.783190	-2.787261	5.396912	B	-1.172187	-0.379594	-0.112573
H	3.910534	-2.510042	5.617819	O	-0.691437	0.824761	0.342411
H	-0.312825	-2.912673	4.908876	O	-0.188821	-1.261287	-0.487051
H	1.667946	-3.264733	6.367583	C	0.721689	0.830911	0.039221
C	2.916590	0.948020	1.892379	C	1.053140	-0.692950	-0.019902
C	2.023479	1.913139	2.367242	C	0.884315	1.528307	-1.303017
C	4.283289	1.233757	1.868587	H	0.427017	2.521729	-1.240995
C	2.490682	3.143780	2.816998	H	1.940021	1.654656	-1.568026
H	0.952082	1.696786	2.362142	H	0.387293	0.973870	-2.107491
C	4.748049	2.469024	2.311350	C	1.454282	1.599620	1.117776
H	4.990854	0.493117	1.495056	H	2.538667	1.540812	0.962442
C	3.853419	3.425036	2.785618	H	1.165416	2.655817	1.080403
H	1.782172	3.892311	3.168769	H	1.223003	1.218833	2.116476
H	5.813785	2.685653	2.284526	C	2.159931	-1.063725	-0.983919
H	4.219346	4.390555	3.127586	H	3.096398	-0.565421	-0.704213
C	-0.884384	1.743459	-2.654238	H	2.330856	-2.145385	-0.951296
C	-1.513066	2.976545	-2.839171	H	1.911598	-0.790352	-2.013454
C	-1.341817	0.628099	-3.368100	C	1.331628	-1.291092	1.351174
C	-2.578415	3.094180	-3.730758	H	1.347556	-2.382666	1.263845
H	-1.164245	3.853022	-2.295175	H	2.300542	-0.963494	1.744684
C	-2.392695	0.752333	-4.269899	H	0.552915	-1.018264	2.072908
H	-0.876140	-0.344415	-3.198198	C	-3.475423	0.240906	0.127559
C	-3.013514	1.987180	-4.452562	H	-4.290781	-0.268629	0.649817
H	-3.060445	4.059396	-3.868191	H	-3.877710	0.690300	-0.787800
H	-2.738201	-0.120496	-4.820248	H	-3.086694	1.039216	0.769127
H	-3.839875	2.083027	-5.152844	O	-2.480058	-0.710338	-0.192474
C	0.755479	3.113054	-0.744750				
C	-0.107142	3.396271	0.320747	**26**			
C	1.678695	4.073060	-1.160169	C	-3.047189	-0.489115	-2.084103
C	-0.077294	4.642360	0.933218	C	-2.092607	-1.603429	-1.714001
H	-0.790656	2.621153	0.676620	C	-2.333256	-2.866908	-2.544700
C	1.736515	5.306473	-0.513459	H	-2.191410	-2.648560	-3.610252
H	2.350803	3.859155	-1.990181	H	-1.598705	-3.629802	-2.257460
C	0.852247	5.596165	0.521315	H	-3.337831	-3.288542	-2.403695
H	-0.778382	4.853554	1.739691	C	-2.393124	-1.896290	-0.224186

H	-2.343274	-0.936737	0.317155	O	2.635727	1.729929	-0.123198
H	-3.435032	-2.246305	-0.127660	C	3.782597	4.093495	-1.091192
C	-1.461667	-2.885683	0.462712	C	2.416795	4.095454	-0.416435
H	-1.646469	-3.904994	0.085953	C	1.914187	2.883651	0.053029
H	-0.418965	-2.651166	0.174027	C	1.652285	5.235722	-0.172173
C	-1.625904	-2.830935	1.955930	C	0.686582	2.759120	0.709900
H	-2.459882	-2.217398	2.313618	C	0.446707	5.157021	0.519660
C	-0.861673	-3.424923	2.880831	H	2.002476	6.205264	-0.517958
C	-1.114602	-3.232598	4.344718	C	-0.034982	3.928589	0.958661
H	-2.005352	-2.620407	4.527727	H	-0.123952	6.061404	0.713931
H	-1.244134	-4.193954	4.861379	H	-0.986883	3.873786	1.482849
H	-0.258601	-2.732270	4.823850	P	2.588337	-1.012659	-1.011842
C	0.309199	-4.296995	2.545073	P	0.112276	1.063592	1.106560
H	0.443844	-4.434855	1.467093	C	4.863524	4.141557	0.006397
H	1.242700	-3.876221	2.951894	H	4.774248	3.296556	0.699187
H	0.199177	-5.290421	3.001798	H	5.862442	4.109544	-0.446475
O	-0.786965	-1.184293	-1.925434	H	4.771279	5.068943	0.585566
C	-4.216795	-0.555970	-2.719885	C	3.963902	5.296531	-2.009936
C	-5.123796	0.623782	-2.899227	H	3.888309	6.231426	-1.444632
C	-6.388284	0.538547	-2.076944	H	4.960732	5.290279	-2.463374
C	-6.363394	0.012097	-0.780375	H	3.216357	5.312561	-2.811665
C	-7.601514	1.010053	-2.586204	Cu	0.358741	-0.404073	-0.612884
C	-7.512703	-0.034145	-0.007359	C	2.814932	-2.453345	-2.112924
H	-5.422928	-0.365450	-0.380003	C	4.054148	-3.081057	-2.294572
C	-8.761463	0.969969	-1.827806	C	1.679191	-2.953305	-2.759134
H	-7.634284	1.413746	-3.596737	C	4.158772	-4.189843	-3.125291
C	-8.720471	0.445311	-0.530447	H	4.936344	-2.704132	-1.776860
H	-7.487399	-0.446021	0.998702	C	1.793190	-4.067576	-3.589783
H	-9.701608	1.336877	-2.231613	H	0.709899	-2.466557	-2.597323
C	-9.910998	0.395236	0.258368	C	3.026220	-4.683768	-3.772851
N	-10.880473	0.355249	0.901697	H	5.122695	-4.673859	-3.265308
H	-2.714828	0.485566	-1.707339	H	0.908393	-4.457615	-4.089534
H	-4.592537	-1.515241	-3.085482	H	3.109082	-5.555503	-4.418240
H	-5.401605	0.761022	-3.954082	C	3.626853	-1.459251	0.435821
H	-4.579336	1.536380	-2.606219	C	3.404685	-2.710473	1.024316
C	4.655854	2.610027	-3.022652	C	4.561737	-0.596579	1.011482
C	3.930593	2.777073	-1.843954	C	4.112425	-3.095467	2.156111
C	3.367840	1.632937	-1.281935	H	2.676943	-3.394108	0.584035
C	3.505740	0.352559	-1.823960	C	5.261412	-0.979136	2.153723
C	4.244519	0.228534	-3.002536	H	4.752876	0.378569	0.567014
C	4.811562	1.350942	-3.596353	C	5.040217	-2.226685	2.727304
H	5.112830	3.471326	-3.503737	H	3.938872	-4.076373	2.594935
H	4.362125	-0.749702	-3.463797	H	5.986910	-0.297418	2.591784
H	5.381342	1.245180	-4.515908	H	5.591740	-2.524075	3.616191

C	-1.617924	1.283588	1.659541	H	-0.102607	5.823069	0.869562
C	-2.073022	0.762267	2.872613	H	-1.072122	5.966585	2.345365
C	-2.548661	1.796366	0.745794	H	0.483849	6.773697	2.251044
C	-3.436281	0.742085	3.160465	O	0.642476	1.710290	-1.882276
H	-1.362167	0.357917	3.592664	C	4.044529	0.947376	-2.584657
C	-3.905199	1.791053	1.041587	C	4.928744	-0.254779	-2.708003
H	-2.206660	2.191073	-0.212005	C	6.112594	-0.256856	-1.770798
C	-4.353303	1.250147	2.246233	C	6.020840	0.302356	-0.493404
H	-3.779848	0.323762	4.104193	C	7.303865	-0.886056	-2.145080
H	-4.617532	2.192228	0.322347	C	7.087851	0.243555	0.389610
H	-5.417977	1.228487	2.468502	H	5.090483	0.781702	-0.191663
C	1.019398	0.639537	2.635399	C	8.378541	-0.962121	-1.272589
C	1.278610	-0.707686	2.900102	H	7.386352	-1.324026	-3.138528
C	1.423564	1.612963	3.554242	C	8.273831	-0.392544	0.002795
C	1.927736	-1.076373	4.075050	H	7.009305	0.680787	1.382038
H	0.964828	-1.472346	2.186738	H	9.301624	-1.452814	-1.570303
C	2.082137	1.242270	4.721482	C	9.377138	-0.460909	0.908550
H	1.220690	2.664876	3.355945	N	10.274489	-0.518351	1.648048
C	2.332793	-0.102666	4.983168	H	2.584143	0.010874	-1.413735
H	2.137139	-2.127017	4.270430	H	4.403547	1.867443	-3.050451
H	2.399331	2.004219	5.429583	H	5.292906	-0.371928	-3.737786
H	2.849545	-0.391353	5.895528	H	4.334560	-1.155071	-2.485211
				C	-5.623490	-2.459937	-1.622274
27-ts				C	-4.562307	-2.678611	-0.745667
C	2.901378	0.943740	-1.897932	C	-3.713739	-1.601081	-0.492934
C	1.970946	2.102186	-1.642613	C	-3.893633	-0.331826	-1.046514
C	2.296579	3.306371	-2.522913	C	-4.980747	-0.149580	-1.905186
H	2.270862	3.019353	-3.580794	C	-5.831521	-1.209224	-2.197164
H	1.544452	4.087645	-2.371511	H	-6.307359	-3.271669	-1.857944
H	3.284748	3.729688	-2.300600	H	-5.149051	0.825330	-2.358677
C	2.105264	2.462235	-0.152383	H	-6.668126	-1.059578	-2.874729
H	1.957181	1.532246	0.425604	O	-2.646204	-1.759788	0.357336
H	3.136440	2.793403	0.051455	C	-4.320053	-3.970246	0.023634
C	1.107913	3.504763	0.335183	C	-2.815203	-4.140522	0.178273
H	1.317346	4.476106	-0.135995	C	-2.042722	-2.992768	0.353926
H	0.113057	3.202488	-0.035662	C	-2.154026	-5.366867	0.223430
C	1.109835	3.637814	1.830610	C	-0.657064	-3.017020	0.534666
H	1.567023	2.806397	2.377779	C	-0.782405	-5.431816	0.449605
C	0.614247	4.649452	2.555957	H	-2.713361	-6.289604	0.090918
C	0.695118	4.652220	4.052695	C	-0.038465	-4.267884	0.604384
H	1.186926	3.752584	4.440059	H	-0.288772	-6.398871	0.500780
H	1.250503	5.528471	4.416495	H	1.035693	-4.330768	0.763329
H	-0.305653	4.717656	4.506443	P	-2.655641	0.969102	-0.671053
C	-0.046897	5.855668	1.961541	P	0.224512	-1.405647	0.614918

C	-4.935237	-3.806812	1.427568	C	-0.070118	-1.778918	3.408413
H	-4.504632	-2.949022	1.957718	C	-0.413265	0.943218	3.901025
H	-6.018596	-3.652502	1.347495	H	-0.249062	1.197914	1.769608
H	-4.752689	-4.707486	2.026973	C	-0.249278	-1.323930	4.709399
C	-4.963454	-5.172358	-0.657618	H	0.067902	-2.842947	3.216992
H	-4.809667	-6.081276	-0.066129	C	-0.419856	0.037755	4.956427
H	-6.047147	-5.036687	-0.738800	H	-0.552809	2.008228	4.079959
H	-4.556252	-5.337197	-1.662200	H	-0.256383	-2.032453	5.534333
Cu	-0.509974	0.121314	-0.898296	H	-0.560508	0.390544	5.975504
C	-3.122144	2.293197	-1.840728	O	-0.236536	-0.148803	-3.011639
C	-4.068838	3.280697	-1.553238	H	0.410890	0.853906	-2.631244
C	-2.525752	2.249909	-3.106444	C	0.522002	-1.233391	-3.434937
C	-4.409353	4.222801	-2.518931	H	1.578435	-1.171756	-3.105785
H	-4.543599	3.311980	-0.573537	H	0.122331	-2.189104	-3.046107
C	-2.878283	3.188825	-4.070829	H	0.542283	-1.326684	-4.535710
H	-1.789991	1.473513	-3.325623				
C	-3.814382	4.177116	-3.777361	**28**			
H	-5.144056	4.991401	-2.290062	C	0.362091	-1.838313	-0.502567
H	-2.414419	3.152498	-5.053935	C	1.662051	-1.747194	0.253679
H	-4.081398	4.914454	-4.531061	C	1.542752	-2.198392	1.701589
C	-3.182454	1.613790	0.962935	H	2.533738	-2.238022	2.163922
C	-2.541426	2.761230	1.448295	H	0.913624	-1.518899	2.288996
C	-4.142772	0.987683	1.759848	H	1.104722	-3.202714	1.758715
C	-2.870257	3.279658	2.694195	C	2.173136	-0.308146	0.138408
H	-1.778247	3.257408	0.845581	H	2.206269	-0.048230	-0.930452
C	-4.456370	1.498375	3.017658	H	1.426260	0.357347	0.598685
H	-4.658827	0.099198	1.398927	C	3.550577	-0.053511	0.749279
C	-3.826504	2.646270	3.485403	H	3.511221	-0.257425	1.830453
H	-2.371246	4.178622	3.052490	H	4.266300	-0.767338	0.324784
H	-5.204614	0.998840	3.628616	C	3.981722	1.363027	0.540270
H	-4.077906	3.047489	4.464306	H	3.311694	2.110495	0.978083
C	1.988729	-1.908137	0.601079	C	5.053626	1.819061	-0.120764
C	2.870835	-1.563406	1.628705	C	5.321019	3.290147	-0.234713
C	2.486562	-2.580260	-0.523652	H	4.557892	3.889289	0.273115
C	4.219923	-1.897710	1.540778	H	6.299630	3.546561	0.195485
H	2.504313	-1.032496	2.505522	H	5.358849	3.603858	-1.287561
C	3.830107	-2.929277	-0.599678	C	6.078875	0.958359	-0.793877
H	1.816275	-2.836659	-1.345129	H	5.863171	-0.111512	-0.731635
C	4.701968	-2.583490	0.430817	H	6.164495	1.224651	-1.856591
H	4.897119	-1.617795	2.344816	H	7.072584	1.128527	-0.356123
H	4.200382	-3.464690	-1.471926	O	2.629532	-2.553438	-0.424359
H	5.757562	-2.839880	0.361219	C	-0.855945	-2.045753	-0.003839
C	-0.060990	-0.872794	2.342014	H	-0.998300	-2.175095	1.071166
C	-0.238425	0.487268	2.597246	C	-2.101818	-2.072011	-0.835802

C	-3.031906	-0.926996	-0.517403	C	3.225469	1.908772	-0.389265
C	-2.552853	0.387508	-0.529161	H	3.004267	2.782446	0.233240
C	-4.376613	-1.152723	-0.217551	H	4.268180	1.977771	-0.719800
C	-3.394274	1.453831	-0.259678	H	2.576261	1.948186	-1.271313
H	-1.501282	0.567033	-0.749669	C	3.904338	0.624793	1.628984
C	-5.233181	-0.096841	0.058590	H	4.947083	0.500684	1.310810
H	-4.757102	-2.172325	-0.201836	H	3.827940	1.574542	2.169609
C	-4.742709	1.213135	0.036825	H	3.651129	-0.182408	2.321857
H	-3.019882	2.474109	-0.273335	C	3.904848	-0.624712	-1.628811
H	-6.278998	-0.278057	0.292557	H	4.947487	-0.500557	-1.310308
C	-5.617483	2.307315	0.321207	H	3.828660	-1.574461	-2.169462
N	-6.329912	3.198219	0.552973	H	3.651819	0.182483	-2.321759
H	0.477483	-1.697282	-1.582437	C	3.225428	-1.908731	0.389217
H	-1.825844	-2.027345	-1.899668	H	3.004434	-2.782403	-0.233366
H	2.312528	-3.464023	-0.398933	H	4.268047	-1.977706	0.720050
H	-2.640306	-3.018655	-0.690607	H	2.575970	-1.948191	1.271080

B_2pin_2

B	-0.850110	-0.000042	-0.000311
O	-1.610527	-0.710520	0.892152
O	-1.610850	0.710441	-0.892488
C	-2.982405	-0.648756	0.428473
C	-2.982546	0.648726	-0.428265
C	-3.225554	-1.908636	-0.389690
H	-3.004317	-2.782511	0.232523
H	-4.268291	-1.977520	-0.720166
H	-2.576413	-1.947785	-1.271800
C	-3.904288	-0.625261	1.628987
H	-4.947044	-0.501040	1.310896
H	-3.827879	-1.575172	2.169324
H	-3.651035	0.181732	2.322088
C	-3.904911	0.625264	-1.628407
H	-4.947540	0.501089	-1.309879
H	-3.828687	1.575170	-2.168780
H	-3.651980	-0.181744	-2.321609
C	-3.225326	1.908629	0.389976
H	-3.004291	2.782480	-0.232341
H	-4.267932	1.977571	0.720853
H	-2.575848	1.947782	1.271837
B	0.850108	-0.000045	-0.000360
O	1.610541	0.710200	0.892279
O	1.610831	-0.710219	-0.892792
C	2.982400	0.648628	0.428517
C	2.982551	-0.648587	-0.428622

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C	3.305610	1.871296	3.667239
C	3.454474	0.923418	2.657093
C	2.654801	1.066165	1.523244
C	1.744528	2.111400	1.345747
C	1.629885	3.044336	2.380677
C	2.400014	2.920139	3.531919
H	3.896487	1.793353	4.576328
H	0.916791	3.860702	2.291826
H	2.294232	3.648661	4.331532
O	2.723374	0.117941	0.529506
C	4.427636	-0.248060	2.685330
C	3.705404	-1.434117	2.060779
C	2.897598	-1.179750	0.955765
C	3.802647	-2.757684	2.488577
C	2.211849	-2.174176	0.253545
C	3.124770	-3.774433	1.821104
H	4.411345	-3.004022	3.355177
C	2.339393	-3.488769	0.707913
H	3.212336	-4.800094	2.170095
H	1.809655	-4.289570	0.195638
P	0.653913	2.076256	-0.128832
P	1.102223	-1.627803	-1.096294
C	5.642126	0.104819	1.805037
H	5.345347	0.327508	0.772818
H	6.157181	0.984108	2.211418
H	6.347946	-0.734815	1.784300

C	4.912041	-0.555269	4.095687	H	4.039783	-2.045789	-1.597655
H	5.622052	-1.389437	4.085172	C	3.911752	-0.340713	-4.534580
H	5.443909	0.303930	4.518609	H	2.145307	0.575011	-5.363320
H	4.079502	-0.813662	4.761885	H	5.497346	-1.330346	-3.464428
Cu	-0.310314	0.042303	-0.417853	H	4.553610	-0.027797	-5.354995
C	-0.517535	3.451995	0.118127	O	-2.212028	-0.127812	-1.232557
C	-0.141279	4.801043	0.107856	C	-2.442126	0.533273	-2.446591
C	-1.860064	3.108421	0.295248	H	-2.609778	1.613756	-2.296507
C	-1.098874	5.790384	0.295134	H	-1.568231	0.405385	-3.103066
H	0.902226	5.073745	-0.051407	H	-3.318437	0.110506	-2.957819
C	-2.816709	4.103640	0.478684	B	-2.642672	-1.026038	1.116055
H	-2.178842	2.064768	0.268871	O	-3.159828	-1.744073	2.174523
C	-2.437189	5.441496	0.483098	O	-1.340996	-0.601275	1.441654
H	-0.804816	6.837415	0.290265	C	-2.115223	-1.950847	3.148284
H	-3.857650	3.814382	0.612758	C	-1.159798	-0.763587	2.868408
H	-3.183442	6.220139	0.624969	C	-2.724249	-1.958904	4.534323
C	1.716225	2.648745	-1.510008	H	-3.380543	-2.829261	4.645177
C	1.078105	3.038658	-2.693920	H	-1.940988	-2.026357	5.300145
C	3.111100	2.646279	-1.457657	H	-3.318459	-1.059336	4.720116
C	1.822233	3.428262	-3.799980	C	-1.477883	-3.300537	2.843502
H	-0.010947	3.044615	-2.747554	H	-0.728524	-3.575695	3.595240
C	3.854921	3.028162	-2.571399	H	-2.259786	-4.067622	2.841078
H	3.625488	2.352036	-0.543846	H	-0.996279	-3.300365	1.856584
C	3.214192	3.418586	-3.742342	C	-1.605291	0.545494	3.504665
H	1.314404	3.736180	-4.711325	H	-1.455578	0.542932	4.590608
H	4.941284	3.019457	-2.520119	H	-1.005167	1.359913	3.077178
H	3.798183	3.715615	-4.610505	H	-2.661301	0.752267	3.290490
C	0.339472	-3.161717	-1.728590	C	0.294272	-1.026792	3.179576
C	1.067936	-4.165659	-2.377252	H	0.883965	-0.126381	2.967706
C	-1.042140	-3.305083	-1.564585	H	0.423151	-1.268644	4.243102
C	0.424048	-5.309025	-2.834278	H	0.698370	-1.849188	2.580602
H	2.141614	-4.047341	-2.524565	B	-3.387897	-0.399938	-0.323966
C	-1.683900	-4.452516	-2.024666	O	-4.400295	-1.154844	-1.054403
H	-1.615346	-2.500001	-1.102152	O	-4.076542	0.844552	0.098375
C	-0.951717	-5.453541	-2.654296	C	-5.673403	-0.685914	-0.663201
H	0.992478	-6.088457	-3.336339	C	-5.421570	0.826192	-0.339648
H	-2.759099	-4.553996	-1.897157	C	-6.659835	-0.923893	-1.795197
H	-1.453253	-6.348177	-3.016276	H	-6.796835	-2.001999	-1.944506
C	2.264259	-1.138355	-2.425060	H	-7.642033	-0.489113	-1.565990
C	1.743281	-0.390967	-3.485784	H	-6.300372	-0.497580	-2.737924
C	3.621086	-1.470952	-2.423309	C	-6.132433	-1.475556	0.563707
C	2.560320	-0.004178	-4.541557	H	-7.151725	-1.209736	0.872051
H	0.689727	-0.105836	-3.475626	H	-6.119456	-2.542963	0.311195
C	4.441509	-1.069447	-3.473959	H	-5.454583	-1.325976	1.411341

C	-5.563434	1.734356	-1.561920	C	0.002821	-5.185873	-3.112137
H	-6.612724	1.874980	-1.853075	H	-1.780287	-4.029215	-2.777248
H	-5.144245	2.718639	-1.312367	C	2.041871	-4.280345	-2.195792
H	-5.012906	1.349845	-2.426072	H	1.853853	-2.406135	-1.142673
C	-6.309823	1.381318	0.765738	C	1.377511	-5.278248	-2.902435
H	-6.084018	2.444421	0.921298	H	-0.519072	-5.965023	-3.663281
H	-7.374116	1.300711	0.505393	H	3.115786	-4.346332	-2.033744
H	-6.141888	0.860363	1.713673	H	1.929933	-6.129678	-3.293954
				C	-2.345750	-1.436172	-2.294931
30-ts				C	-2.078865	-1.124174	-3.634681
C	-2.539582	-3.216708	2.870328	C	-3.673747	-1.508632	-1.869422
C	-2.610556	-1.857526	2.563175	C	-3.117608	-0.912759	-4.532058
C	-2.174187	-1.472716	1.296716	H	-1.044509	-1.058213	-3.977937
C	-1.650809	-2.360430	0.354959	C	-4.714455	-1.277690	-2.766242
C	-1.604564	-3.711603	0.698815	H	-3.903073	-1.753990	-0.832960
C	-2.053018	-4.135755	1.945273	C	-4.440290	-0.985161	-4.097546
H	-2.874668	-3.570897	3.842339	H	-2.895935	-0.683078	-5.572219
H	-1.192378	-4.431500	-0.005444	H	-5.744439	-1.336597	-2.421326
H	-2.012620	-5.190884	2.204265	H	-5.254076	-0.812239	-4.798129
O	-2.248466	-0.155350	0.916593	C	-0.015838	3.704428	-0.237103
C	-3.199615	-0.793025	3.481218	C	-0.657696	4.905783	-0.549382
C	-2.478032	0.519845	3.204780	C	1.336546	3.714662	0.122346
C	-2.059418	0.779666	1.902118	C	0.047175	6.105005	-0.502769
C	-2.251259	1.520009	4.151802	H	-1.710463	4.904960	-0.828706
C	-1.433077	1.964668	1.511150	C	2.034367	4.916674	0.173843
C	-1.642555	2.719839	3.796282	H	1.842853	2.772980	0.338875
H	-2.555524	1.366731	5.184447	C	1.391616	6.111786	-0.139946
C	-1.236014	2.944649	2.484042	H	-0.455802	7.037335	-0.749678
H	-1.482981	3.486691	4.550120	H	3.086329	4.919273	0.452335
H	-0.751666	3.881636	2.215295	H	1.940087	7.050520	-0.106187
P	-0.910835	-1.652950	-1.169274	C	-2.409380	2.386711	-1.152268
P	-0.857605	2.079771	-0.228068	C	-2.404177	2.133791	-2.526580
C	-4.686013	-0.613039	3.117824	C	-3.575272	2.870141	-0.550858
H	-4.808806	-0.328241	2.065869	C	-3.539129	2.377306	-3.292696
H	-5.231574	-1.550579	3.284385	H	-1.506630	1.727279	-2.994988
H	-5.136296	0.170309	3.740564	C	-4.714445	3.101500	-1.315882
C	-3.093453	-1.193553	4.948857	H	-3.590391	3.070213	0.520083
H	-3.540065	-0.429526	5.593881	C	-4.695984	2.859790	-2.687027
H	-3.643955	-2.120155	5.142601	H	-3.524447	2.171813	-4.360646
H	-2.049032	-1.339766	5.253460	H	-5.618378	3.475471	-0.840265
Cu	0.432478	0.201010	-0.590324	H	-5.586991	3.042836	-3.283222
C	-0.042688	-3.090950	-1.901529	O	1.894376	0.194822	-2.260939
C	-0.704938	-4.097014	-2.614671	C	1.753135	1.304273	-3.124793
C	1.337634	-3.187969	-1.697221	H	2.688871	1.512923	-3.664332

H	0.973025	1.063687	-3.856750				
H	1.466140	2.215660	-2.581500	**31-ts**			
B	1.681025	-0.431868	0.916611	C	0.272475	5.437640	1.303516
O	2.259157	0.216992	1.998337	C	0.074206	4.696946	0.138248
O	1.457041	-1.767192	1.234239	C	-0.518925	3.442113	0.274666
C	2.230821	-0.666510	3.137658	C	-0.921102	2.913613	1.503970
C	2.111739	-2.070801	2.477632	C	-0.729818	3.699118	2.643857
C	3.485219	-0.453653	3.961863	C	-0.130570	4.949580	2.543902
H	3.497524	0.569671	4.355130	H	0.737588	6.418900	1.246652
H	3.512177	-1.144724	4.814728	H	-1.032281	3.313654	3.615839
H	4.395843	-0.599010	3.371533	H	0.023729	5.550252	3.436662
C	1.006923	-0.284527	3.960313	O	-0.749250	2.662996	-0.829631
H	0.946562	-0.861225	4.891939	C	0.373274	5.199502	-1.266839
H	1.068310	0.779342	4.218692	C	0.764293	3.999779	-2.118404
H	0.077851	-0.436450	3.394371	C	0.152120	2.773904	-1.861168
C	3.453116	-2.696312	2.120359	C	1.668191	4.052731	-3.178405
H	4.015174	-3.006472	3.009691	C	0.417294	1.612872	-2.589213
H	3.266751	-3.583755	1.502895	C	1.933065	2.925133	-3.949231
H	4.063006	-2.005140	1.527247	H	2.172416	4.986918	-3.413548
C	1.268696	-3.068473	3.247970	C	1.311467	1.716013	-3.656501
H	1.225467	-4.014550	2.694848	H	2.629960	2.989140	-4.781278
H	1.706577	-3.270219	4.234748	H	1.543196	0.832982	-4.248639
H	0.238527	-2.719471	3.380705	P	-1.501701	1.177183	1.535371
B	2.767904	0.305622	-1.131728	P	-0.315116	0.030178	-1.993765
O	3.389792	1.553596	-0.960891	C	-0.922941	5.803209	-1.841571
O	3.691351	-0.734432	-0.861712	H	-1.736364	5.068271	-1.851419
C	4.768192	1.339743	-0.642304	H	-1.242230	6.660602	-1.235363
C	4.987802	-0.151298	-1.059603	H	-0.756404	6.144650	-2.871107
C	5.597896	2.337029	-1.433125	C	1.456487	6.273686	-1.265805
H	5.406065	3.350404	-1.060695	H	1.630489	6.652427	-2.278624
H	6.670793	2.134632	-1.318350	H	1.148840	7.135814	-0.664452
H	5.347274	2.318386	-2.498414	H	2.406246	5.892537	-0.868710
C	4.965508	1.589703	0.844576	Cu	-0.108791	-0.503373	0.415465
H	6.025167	1.553976	1.126541	C	-1.561812	0.828123	3.333449
H	4.584812	2.591964	1.078944	C	-2.724327	0.897547	4.104903
H	4.396933	0.873267	1.442669	C	-0.356570	0.460995	3.947374
C	5.333166	-0.305116	-2.538145	C	-2.688591	0.587769	5.462108
H	6.331651	0.083540	-2.771144	H	-3.666308	1.189412	3.644151
H	5.308016	-1.369820	-2.796462	C	-0.320883	0.168393	5.306542
H	4.602217	0.210083	-3.172970	H	0.553712	0.393382	3.347478
C	6.010318	-0.896173	-0.225676	C	-1.488378	0.222029	6.064622
H	6.053197	-1.944084	-0.546001	H	-3.601753	0.637612	6.051065
H	7.009002	-0.459808	-0.356934	H	0.620388	-0.114583	5.773293
H	5.764409	-0.875420	0.840609	H	-1.462311	-0.020296	7.124581

C	-3.261133	1.258453	1.045665	H	3.614945	3.271219	-1.018396
C	-3.996498	0.066134	1.126007	H	2.853031	3.713790	0.517009
C	-3.873190	2.396045	0.514689	C	4.814539	0.868141	2.477213
C	-5.320852	0.021654	0.708633	H	5.534770	1.695716	2.433322
H	-3.507198	-0.832423	1.504277	H	4.685349	0.589294	3.529577
C	-5.196472	2.344684	0.082377	H	5.238937	0.011863	1.944686
H	-3.320138	3.332080	0.443347	C	2.865836	2.386475	2.752541
C	-5.924530	1.163049	0.182970	H	2.719640	2.000211	3.768724
H	-5.880265	-0.910251	0.784640	H	3.511822	3.270587	2.814851
H	-5.662768	3.238373	-0.326623	H	1.886017	2.693875	2.364114
H	-6.959470	1.130313	-0.149723	C	-0.080818	-3.157436	0.410249
C	0.697860	-1.192853	-2.912656	C	-1.267249	-3.105860	1.281485
C	0.160885	-2.139893	-3.786248	C	-1.018902	-2.859721	2.756290
C	2.072035	-1.225856	-2.633012	H	-1.943828	-2.516060	3.236203
C	0.984252	-3.098640	-4.377123	H	-0.683317	-3.772597	3.264619
H	-0.904509	-2.128721	-4.012761	H	-0.275120	-2.068956	2.901416
C	2.895197	-2.155965	-3.253164	C	-2.267221	-4.224864	1.017315
H	2.488511	-0.510847	-1.921192	H	-2.368219	-4.330585	-0.073398
C	2.351858	-3.102358	-4.122073	H	-1.871581	-5.178745	1.398621
H	0.553953	-3.834420	-5.053078	C	-3.652732	-3.952958	1.606867
H	3.962925	-2.156549	-3.037687	H	-3.608786	-4.005303	2.703043
H	2.994345	-3.840942	-4.596744	H	-3.935641	-2.919840	1.358778
C	-1.941791	0.000723	-2.840324	C	-4.682129	-4.918845	1.102708
C	-3.008982	-0.574955	-2.144120	H	-4.800557	-5.841359	1.676765
C	-2.159976	0.538428	-4.113974	C	-5.426511	-4.776321	-0.001501
C	-4.279323	-0.609273	-2.715189	C	-6.408040	-5.826087	-0.425057
H	-2.832822	-0.991537	-1.149921	H	-6.432724	-6.671473	0.270574
C	-3.428144	0.499675	-4.681864	H	-7.423403	-5.410693	-0.495667
H	-1.332705	0.992322	-4.659404	H	-6.165823	-6.212135	-1.425303
C	-4.489082	-0.072386	-3.981193	C	-5.354202	-3.587837	-0.911779
H	-5.108449	-1.044295	-2.159616	H	-4.609016	-2.846874	-0.601690
H	-3.592200	0.920409	-5.671596	H	-5.101969	-3.899728	-1.935517
H	-5.482178	-0.094535	-4.424669	H	-6.331435	-3.085929	-0.978158
B	1.723514	0.264133	0.825953	O	-1.595672	-1.946152	0.567129
O	2.217191	1.210377	-0.061007	C	1.278745	-2.910385	0.729291
O	2.565956	0.169319	1.930966	H	1.531474	-2.589498	1.737205
C	3.516001	1.644808	0.379880	C	2.252372	-3.338785	-0.138232
C	3.482960	1.290699	1.893530	H	1.938827	-3.720480	-1.112034
C	4.543184	0.847095	-0.415460	C	3.664009	-3.328725	0.117753
H	4.364817	1.024807	-1.483929	C	4.531116	-3.984282	-0.783988
H	5.570933	1.153956	-0.186219	C	4.235137	-2.678062	1.234905
H	4.448734	-0.232289	-0.228824	C	5.895104	-4.015029	-0.578745
C	3.661126	3.122627	0.068906	H	4.103182	-4.477394	-1.655603
H	4.624376	3.507583	0.429502	C	5.600146	-2.709820	1.447787

H	3.605111	-2.110338	1.917861	H	-5.090005	0.630702	1.926378
C	6.444043	-3.380000	0.547574	C	-7.850277	0.842574	-0.034867
H	6.548962	-4.528238	-1.279127	H	-7.913985	1.713028	-2.008015
H	6.031681	-2.211254	2.313281	H	-7.476493	0.044794	1.934761
C	7.851041	-3.409003	0.772081	C	-9.228801	0.477542	-0.034036
N	9.001677	-3.432559	0.955510	N	-10.354554	0.177909	-0.032999
H	-0.286794	-3.520570	-0.598855	H	-1.133062	2.155399	-0.357490
				P	1.030367	-1.517209	1.807825
32				C	0.230569	-1.891438	3.406545
Cu	-0.009979	0.325417	0.909356	C	-1.156059	-1.730783	3.502325
C	-1.358156	1.791460	0.651093	C	0.949205	-2.363276	4.509676
C	-0.510450	2.559970	1.711457	C	-1.814072	-2.042541	4.688245
C	-1.229238	2.646835	3.053864	H	-1.720911	-1.369576	2.641801
H	-0.559476	3.097924	3.795606	C	0.287594	-2.668325	5.694487
H	-2.152525	3.241714	3.008187	H	2.028428	-2.493305	4.439727
H	-1.476181	1.638332	3.412952	C	-1.093361	-2.507749	5.784505
C	-0.246359	3.956846	1.127919	H	-2.892004	-1.916457	4.757211
H	0.236055	3.817956	0.144500	H	0.851520	-3.032092	6.550056
H	-1.212718	4.456811	0.933875	H	-1.607728	-2.744728	6.712888
C	0.649823	4.860995	1.974167	C	2.760508	-1.151821	2.249446
H	0.167811	5.066248	2.940938	C	2.987479	0.020230	2.982520
H	1.574808	4.313180	2.199610	C	3.834094	-1.970470	1.895561
C	0.927428	6.160666	1.283040	C	4.275710	0.340584	3.390924
H	0.140937	6.916388	1.373516	H	2.150514	0.688241	3.193019
C	1.991662	6.472953	0.531565	C	5.126135	-1.627933	2.286024
C	2.112531	7.812143	-0.130867	H	3.664686	-2.879066	1.317098
H	1.253664	8.457365	0.084547	C	5.345829	-0.481534	3.043723
H	3.023098	8.334374	0.195087	H	4.449675	1.248114	3.965417
H	2.196019	7.707326	-1.223284	H	5.961022	-2.265906	2.006302
C	3.140584	5.547960	0.273486	H	6.355504	-0.222759	3.355473
H	3.011842	4.560886	0.729571	C	1.066812	-3.138663	0.964547
H	3.273736	5.394343	-0.807871	C	1.462065	-3.184990	-0.376374
H	4.084626	5.975866	0.639519	C	0.635888	-4.325103	1.562810
O	0.688355	1.843712	1.873025	C	1.421552	-4.348649	-1.144810
C	-2.787496	1.612083	0.840291	C	0.580663	-5.500332	0.823108
H	-3.112582	1.206253	1.800789	H	0.320765	-4.321467	2.604898
C	-3.711597	1.869642	-0.110402	C	0.960311	-5.506609	-0.516347
H	-3.369653	2.299993	-1.056690	H	0.236641	-6.419271	1.290805
C	-5.125460	1.546881	-0.035916	H	0.909060	-6.437956	-1.074641
C	-5.952167	1.833127	-1.137721	C	1.968839	-4.302437	-2.565575
C	-5.705300	0.894143	1.069145	C	1.714607	-2.910373	-3.128312
C	-7.292085	1.488401	-1.145802	C	1.738854	-1.822708	-2.260991
H	-5.518425	2.329499	-2.005093	C	1.517811	-2.634142	-4.482461
C	-7.042901	0.551351	1.076093	C	1.573786	-0.498263	-2.669565

C	1.361829	-1.326204	-4.932304	C	-3.147141	-0.718362	-2.639300
H	1.490128	-3.449221	-5.201749	C	-1.854335	-2.836462	-2.751463
C	1.392934	-0.263824	-4.032427	H	-2.909057	-3.721825	0.975384
H	1.219565	-1.134449	-5.992416	H	-2.870357	-4.366649	-0.680452
H	1.261986	0.756351	-4.388883	H	-1.432705	-3.571071	0.007421
C	3.492691	-4.525389	-2.494962	H	-4.904525	-2.886268	-1.315264
H	3.711281	-5.516100	-2.074522	H	-4.931859	-2.484228	0.411842
H	3.929317	-4.467053	-3.500061	H	-4.933065	-1.183406	-0.790912
H	3.981994	-3.772078	-1.866486	H	-2.522817	-0.328922	-3.453199
C	1.355087	-5.387303	-3.445585	H	-4.036612	-1.181587	-3.081902
H	1.566927	-6.383834	-3.045038	H	-3.466719	0.124286	-2.011807
H	0.267916	-5.271151	-3.535370	H	-2.706495	-3.420143	-3.124400
H	1.790513	-5.361725	-4.450228	H	-1.325802	-2.404711	-3.610086
O	1.914331	-2.012627	-0.910758	H	-1.161124	-3.510829	-2.238061
P	1.494836	0.761932	-1.338098				
C	3.256343	1.134881	-1.008336	**33-ts**			
C	3.529412	1.863952	0.156890	C	1.011862	-5.536240	-0.293753
C	4.307769	0.758392	-1.848784	C	1.525801	-4.409634	-0.935623
C	4.840477	2.221967	0.460164	C	1.529579	-3.214854	-0.215472
H	2.700925	2.138974	0.818574	C	1.047688	-3.104550	1.092305
C	5.617775	1.101235	-1.527889	C	0.563433	-4.261135	1.708184
H	4.100987	0.195910	-2.758374	C	0.544876	-5.467195	1.016391
C	5.884600	1.836603	-0.376027	H	0.984401	-6.489180	-0.816571
H	5.047072	2.793930	1.363460	H	0.176143	-4.208681	2.723724
H	6.432089	0.799194	-2.183101	H	0.159006	-6.361298	1.499042
H	6.909377	2.108296	-0.129742	O	2.030303	-2.073329	-0.781049
C	0.926939	2.255421	-2.242726	C	2.162030	-4.410386	-2.319475
C	-0.397629	2.267723	-2.706402	C	1.877200	-3.058992	-2.961056
C	1.690681	3.419067	-2.358624	C	1.865079	-1.934023	-2.140323
C	-0.940751	3.416164	-3.268647	C	1.692730	-2.847321	-4.327701
H	-1.007158	1.366823	-2.609206	C	1.682291	-0.631985	-2.607696
C	1.141525	4.572940	-2.913771	C	1.522569	-1.562004	-4.834624
H	2.720726	3.429184	-2.002154	H	1.690108	-3.692810	-5.011303
C	-0.173214	4.575569	-3.367258	C	1.522929	-0.461042	-3.982975
H	-1.969838	3.409724	-3.623496	H	1.394330	-1.417808	-5.904602
H	1.749553	5.472061	-2.997033	H	1.381245	0.538989	-4.387981
H	-0.600857	5.478817	-3.795345	P	0.965208	-1.441094	1.847643
B	-1.411474	-0.672215	-0.048847	P	1.556787	0.686751	-1.339897
O	-2.559282	-1.223610	0.449723	C	3.686993	-4.545184	-2.137298
O	-1.164021	-1.011403	-1.349266	H	4.089924	-3.736997	-1.515324
C	-3.022510	-2.198356	-0.524670	H	3.926487	-5.501317	-1.654952
C	-2.329940	-1.722144	-1.843655	H	4.188283	-4.508835	-3.112599
C	-2.527034	-3.548481	-0.037783	C	1.666605	-5.567672	-3.178761
C	-4.535486	-2.177514	-0.562730	H	2.158737	-5.558486	-4.157215

H	1.914781	-6.529653	-2.717748	H	5.028501	2.857457	1.367600
H	0.581834	-5.526571	-3.336525	H	6.509066	0.716289	-2.052976
Cu	0.035401	0.371214	0.751650	H	6.930325	2.120172	-0.050244
C	0.089917	-1.723581	3.427071	B	-1.412609	-0.627526	-0.191208
C	0.751064	-2.188036	4.568983	O	-1.225926	-0.917051	-1.511806
C	-1.284328	-1.468522	3.481459	O	-2.507034	-1.237339	0.353276
C	0.045782	-2.391311	5.750285	C	-2.364891	-1.698698	-1.958905
H	1.821156	-2.388939	4.531889	C	-2.974716	-2.217175	-0.613919
C	-1.986641	-1.675849	4.665467	C	-3.271735	-0.747414	-2.721011
H	-1.805013	-1.116389	2.591273	H	-2.711501	-0.327430	-3.565127
C	-1.322205	-2.132723	5.799776	H	-4.153479	-1.261559	-3.120033
H	0.565798	-2.749837	6.635451	H	-3.605777	0.079630	-2.082804
H	-3.054512	-1.472953	4.702261	C	-1.853759	-2.781207	-2.886750
H	-1.869923	-2.286922	6.726509	H	-2.677611	-3.424147	-3.221252
C	2.672983	-1.055359	2.362200	H	-1.396819	-2.315263	-3.768268
C	2.865804	0.169020	3.014487	H	-1.090511	-3.402571	-2.406022
C	3.759517	-1.898843	2.126355	C	-4.487392	-2.260458	-0.581910
C	4.133582	0.520491	3.460843	H	-4.860272	-2.979280	-1.322890
H	2.023304	0.855544	3.116317	H	-4.824477	-2.590025	0.407721
C	5.031958	-1.525447	2.551715	H	-4.936694	-1.282990	-0.784092
H	3.615063	-2.850366	1.615824	C	-2.399631	-3.549421	-0.164376
C	5.217131	-0.324286	3.229341	H	-2.712233	-3.739020	0.869818
H	4.281864	1.470801	3.969554	H	-2.747436	-4.379670	-0.789882
H	5.877969	-2.182084	2.362383	H	-1.304529	-3.528155	-0.181602
H	6.211042	-0.039951	3.567835	C	-1.398019	1.850427	0.497173
C	0.984833	2.143211	-2.298531	C	-0.546004	2.616709	1.553673
C	1.702394	3.339741	-2.363832	C	-1.241969	2.662734	2.910989
C	-0.308457	2.098767	-2.841005	H	-0.572058	3.129414	3.642117
C	1.137225	4.470568	-2.950596	H	-2.186272	3.225728	2.893235
H	2.704621	3.397399	-1.941054	H	-1.442208	1.640508	3.262215
C	-0.865617	3.224100	-3.435537	C	-0.329808	4.028486	0.985474
H	-0.879461	1.171657	-2.775098	H	0.155574	3.909859	0.001113
C	-0.145719	4.417050	-3.484840	H	-1.308990	4.504888	0.800472
H	1.705783	5.398613	-2.986031	C	0.545702	4.942019	1.842808
H	-1.869081	3.172255	-3.853975	H	0.038157	5.160059	2.793899
H	-0.586105	5.302163	-3.937912	H	1.461585	4.393238	2.098773
C	3.304583	1.086942	-0.971093	C	0.850565	6.232275	1.145615
C	3.546175	1.867209	0.166895	H	0.075136	7.001192	1.214270
C	4.377773	0.678293	-1.768009	C	1.934343	6.519555	0.412213
C	4.847391	2.247082	0.484065	C	2.094910	7.850855	-0.257342
H	2.699011	2.167180	0.793919	H	1.247101	8.515819	-0.060654
C	5.677967	1.042780	-1.431504	H	3.011251	8.355869	0.081059
H	4.196495	0.074022	-2.656112	H	2.195113	7.737084	-1.346726
C	5.913681	1.831471	-0.308175	C	3.071491	5.569930	0.191628

H	2.889514	4.575572	0.611499	P	0.438837	-0.136153	-1.885239
H	3.263498	5.443716	-0.884628	C	5.375596	-3.159829	-1.910573
H	4.005217	5.960628	0.622116	H	5.258433	-2.088710	-2.111945
O	0.676157	1.942530	1.690238	H	6.326876	-3.309695	-1.384833
C	-2.815959	1.631221	0.707215	H	5.421439	-3.683644	-2.873613
H	-3.115739	1.239517	1.681299	C	4.419017	-5.198212	-0.838230
C	-3.762230	1.843744	-0.233333	H	4.471439	-5.735130	-1.791081
H	-3.448474	2.266597	-1.192904	H	5.370254	-5.379551	-0.326573
C	-5.164782	1.485569	-0.122369	H	3.610653	-5.632838	-0.236472
C	-6.027559	1.750518	-1.201460	Cu	0.485130	0.445050	0.325038
C	-5.699572	0.820332	0.999011	C	2.733755	1.479894	2.894174
C	-7.358614	1.374814	-1.173354	C	3.944997	1.890196	3.468110
H	-5.629084	2.254922	-2.080521	C	1.539285	1.633674	3.606484
C	-7.028321	0.447084	1.041947	C	3.963721	2.433485	4.746291
H	-5.056142	0.568929	1.839172	H	4.874658	1.785139	2.908629
C	-7.871993	0.718450	-0.046649	C	1.567667	2.183453	4.888151
H	-8.009235	1.583204	-2.018852	H	0.592209	1.335254	3.141699
H	-7.426178	-0.069180	1.912034	C	2.772542	2.579717	5.457508
C	-9.241395	0.322031	-0.006905	H	4.906258	2.748410	5.188350
N	-10.359393	-0.003698	0.027134	H	0.637414	2.306120	5.439672
H	-1.186069	2.206805	-0.517560	H	2.788733	3.009264	6.456831
				C	3.810660	1.836083	0.281554
34				C	3.592792	3.217915	0.340465
C	4.699682	-3.388213	1.452651	C	4.845447	1.348994	-0.519095
C	4.163227	-2.938642	0.247469	C	4.391738	4.093262	-0.384281
C	3.572207	-1.675836	0.245885	H	2.798783	3.613716	0.974561
C	3.538909	-0.836411	1.362135	C	5.643073	2.227274	-1.248753
C	4.092210	-1.323531	2.549279	H	5.040607	0.279371	-0.571653
C	4.657238	-2.593035	2.594690	C	5.418718	3.598526	-1.185313
H	5.156234	-4.373398	1.508094	H	4.210764	5.164764	-0.323705
H	4.065655	-0.710190	3.446997	H	6.448115	1.834527	-1.865716
H	5.075834	-2.964354	3.526593	H	6.044337	4.280993	-1.755805
O	2.959469	-1.212063	-0.894620	C	-1.180228	-0.140844	-2.752595
C	4.208546	-3.706279	-1.066686	C	-1.521422	0.866173	-3.660203
C	2.906872	-3.425895	-1.804054	C	-2.140652	-1.105702	-2.415272
C	2.340964	-2.157891	-1.677442	C	-2.792279	0.901578	-4.229304
C	2.247579	-4.341776	-2.622579	H	-0.792186	1.628696	-3.928090
C	1.142456	-1.784653	-2.291759	C	-3.400742	-1.079715	-3.002403
C	1.079536	-3.989105	-3.291319	H	-1.900799	-1.870612	-1.676222
H	2.651406	-5.343308	-2.748346	C	-3.730346	-0.074164	-3.909507
C	0.531096	-2.722068	-3.128010	H	-3.043805	1.691738	-4.932824
H	0.590283	-4.709237	-3.942004	H	-4.135303	-1.837171	-2.735398
H	-0.391544	-2.464547	-3.642905	H	-4.717718	-0.051316	-4.365318
P	2.646545	0.760703	1.213489	C	1.449413	1.001452	-2.900788

C	1.650264	2.298226	-2.424327	H	-2.900383	5.193760	0.409799
C	1.993364	0.629568	-4.133793	C	-0.922753	5.392949	-0.205495
C	2.380248	3.217183	-3.172042	C	-1.209263	6.588253	-1.062952
H	1.235794	2.585451	-1.456044	H	-2.261884	6.886686	-1.012913
C	2.733519	1.544581	-4.874532	H	-0.596302	7.448862	-0.758008
H	1.834406	-0.378414	-4.516020	H	-0.958538	6.391882	-2.115143
C	2.925861	2.838621	-4.394609	C	0.509467	4.953001	-0.205827
H	2.542724	4.222151	-2.786153	H	0.653033	3.978869	0.277613
H	3.159226	1.248668	-5.830529	H	0.886044	4.878018	-1.236678
H	3.506403	3.551826	-4.975232	H	1.153761	5.685329	0.303924
B	-1.955861	-1.389835	1.370073	O	-0.755483	0.765036	1.762786
O	-1.018307	-2.080000	0.625459	C	-4.236424	-0.265672	0.969707
O	-2.166329	-1.964103	2.601929	H	-4.619529	-0.614254	1.933925
C	-0.674197	-3.268481	1.373823	C	-5.103126	0.011858	-0.018925
C	-1.060074	-2.864715	2.825282	H	-4.694981	0.324572	-0.984805
C	-1.526332	-4.396949	0.812286	C	-6.555007	-0.105103	0.038996
H	-1.347350	-4.460946	-0.268022	C	-7.287456	-0.050425	-1.158209
H	-1.268036	-5.363517	1.260261	C	-7.264490	-0.270038	1.241605
H	-2.594592	-4.210386	0.972242	C	-8.665734	-0.172501	-1.167859
C	0.792574	-3.576492	1.173411	H	-6.750607	0.084693	-2.096179
H	1.108835	-4.413096	1.811249	C	-8.640907	-0.393281	1.246823
H	0.969729	-3.862942	0.128874	H	-6.726586	-0.288702	2.186704
H	1.424198	-2.710383	1.400767	C	-9.354236	-0.347918	0.039335
C	-1.519619	-4.009610	3.701568	H	-9.218842	-0.133826	-2.102875
H	-0.718752	-4.750748	3.817104	H	-9.178391	-0.518101	2.183533
H	-1.775006	-3.631932	4.697880	C	-10.775698	-0.474344	0.042628
H	-2.401883	-4.508962	3.290443	N	-11.935732	-0.579269	0.045542
C	0.028551	-2.060843	3.525048	H	-2.514625	-0.001682	-0.222045
H	-0.382740	-1.649851	4.455176				
H	0.894949	-2.684755	3.775786	**35-ts**			
H	0.346821	-1.214869	2.902890	C	5.028224	0.098793	-3.974895
C	-2.762576	-0.147628	0.839229	C	4.864860	0.620567	-2.692704
C	-2.099492	1.060044	1.604849	C	4.030218	-0.080871	-1.823045
C	-2.723875	1.224103	2.993074	C	3.351668	-1.248787	-2.182211
H	-2.129453	1.939001	3.575662	C	3.566249	-1.753307	-3.467286
H	-3.760253	1.588411	2.948191	C	4.397261	-1.081972	-4.356116
H	-2.712141	0.267236	3.527677	H	5.665212	0.612297	-4.690647
C	-2.304626	2.330750	0.765364	H	3.058841	-2.663002	-3.779945
H	-1.789754	2.170312	-0.200138	H	4.551530	-1.478546	-5.356261
H	-3.375817	2.463258	0.536074	O	3.836991	0.373116	-0.544134
C	-1.752962	3.604130	1.402972	C	5.588275	1.850879	-2.160697
H	-2.297614	3.810464	2.336694	C	4.669332	2.536506	-1.158429
H	-0.707571	3.421730	1.691378	C	3.860906	1.735328	-0.357309
C	-1.886306	4.792576	0.504982	C	4.637871	3.910064	-0.914369

C	3.053182	2.229634	0.668244	C	-1.046318	3.282709	3.073262
C	3.843607	4.439963	0.097870	H	-0.678061	2.063683	1.333667
H	5.247261	4.580650	-1.515183	C	-0.546024	3.751871	4.284039
C	3.059090	3.606667	0.889886	H	1.128565	3.759203	5.642046
H	3.838733	5.512816	0.272747	H	-2.044812	3.551334	2.734649
H	2.436166	4.027527	1.676700	H	-1.155929	4.397098	4.912827
P	2.091373	-1.914963	-1.027767	C	3.163797	0.176030	2.667248
P	1.987178	1.030172	1.552006	C	2.687261	-0.945056	3.352256
C	6.844246	1.376495	-1.403212	C	4.481980	0.590631	2.873441
H	6.583323	0.704012	-0.576595	C	3.505507	-1.633814	4.238803
H	7.517289	0.839448	-2.083443	H	1.664201	-1.280336	3.181800
H	7.381071	2.238278	-0.986838	C	5.305933	-0.107745	3.752777
C	6.014409	2.790293	-3.283235	H	4.867371	1.465426	2.350837
H	6.551405	3.656234	-2.882120	C	4.819482	-1.216839	4.438207
H	6.707924	2.289491	-3.967110	H	3.120052	-2.507388	4.761693
H	5.154511	3.150123	-3.860329	H	6.331308	0.221333	3.906111
Cu	0.931257	-0.169383	-0.114151	H	5.465982	-1.760411	5.123392
C	1.206846	-3.147883	-2.054307	B	-3.373830	2.154966	-0.369312
C	1.297875	-4.529275	-1.880413	O	-2.809111	3.121218	0.416434
C	0.337865	-2.639944	-3.027219	O	-3.736822	2.617352	-1.607396
C	0.517133	-5.385302	-2.654801	C	-2.936105	4.381079	-0.279305
H	1.971535	-4.942754	-1.132754	C	-3.144947	3.930848	-1.759937
C	-0.427781	-3.493865	-3.810063	C	-4.146761	5.085669	0.313698
H	0.263892	-1.560486	-3.165863	H	-4.003903	5.183944	1.395886
C	-0.346533	-4.871948	-3.616288	H	-4.275829	6.089625	-0.106647
H	0.589178	-6.460014	-2.505046	H	-5.067192	4.514738	0.143720
H	-1.100377	-3.082901	-4.559661	C	-1.681152	5.193808	-0.034247
H	-0.956166	-5.543444	-4.216117	H	-1.683374	6.106927	-0.642812
C	3.022281	-2.903219	0.198224	H	-1.630838	5.488294	1.020708
C	2.290463	-3.674859	1.110658	H	-0.781321	4.613528	-0.264722
C	4.413594	-2.857500	0.305888	C	-4.086208	4.801348	-2.565390
C	2.944517	-4.407723	2.093290	H	-3.703347	5.827966	-2.623352
H	1.201051	-3.722303	1.042842	H	-4.160390	4.412113	-3.586900
C	5.063267	-3.575627	1.306903	H	-5.092916	4.826624	-2.138440
H	4.998741	-2.264530	-0.395652	C	-1.839601	3.730973	-2.510484
C	4.332680	-4.355538	2.196791	H	-2.056918	3.216917	-3.455111
H	2.365350	-5.013100	2.788669	H	-1.359404	4.687887	-2.747050
H	6.146906	-3.527821	1.385465	H	-1.137969	3.110766	-1.936896
H	4.843358	-4.917066	2.975800	C	-3.627970	0.682479	0.129893
C	1.016099	2.087261	2.681178	C	-2.499301	-0.274878	-0.396308
C	1.517127	2.564318	3.897575	C	-2.614543	-0.489143	-1.902420
C	-0.271370	2.448401	2.271101	H	-1.755740	-1.069405	-2.261316
C	0.736192	3.392399	4.696071	H	-3.526916	-1.036719	-2.171937
H	2.521772	2.289675	4.217979	H	-2.624031	0.474637	-2.429050

C	-2.629374	-1.600278	0.365924	O	0.461857	-2.713234	-1.198256
H	-2.597547	-1.366217	1.442109	O	1.602159	-2.516586	0.772901
H	-3.625023	-2.029902	0.176919	C	0.676431	-4.063029	-0.716806
C	-1.552168	-2.638793	0.064067	C	1.837930	-3.870223	0.301197
H	-1.606711	-2.956791	-0.987221	C	-0.623947	-4.505696	-0.063789
H	-0.571178	-2.149343	0.175120	H	-1.433159	-4.418362	-0.796510
C	-1.638146	-3.844824	0.952211	H	-0.572016	-5.548603	0.268443
H	-2.123340	-4.730220	0.533396	H	-0.877771	-3.876785	0.798162
C	-1.214812	-3.917412	2.222450	C	1.003043	-4.958229	-1.892028
C	-1.376284	-5.164578	3.036411	H	1.249480	-5.970079	-1.547300
H	-1.872211	-5.962136	2.473217	H	0.131844	-5.029743	-2.551976
H	-0.401907	-5.542224	3.379037	H	1.842807	-4.573077	-2.477169
H	-1.964042	-4.969830	3.944753	C	1.815446	-4.814273	1.482943
C	-0.564766	-2.777560	2.947158	H	1.900432	-5.853794	1.143139
H	-0.379316	-1.907884	2.302968	H	2.665371	-4.603727	2.140977
H	-1.190323	-2.444513	3.787613	H	0.897116	-4.712234	2.067826
H	0.394287	-3.097789	3.384994	C	3.213475	-3.866650	-0.347982
O	-1.272960	0.327216	-0.079791	H	3.952923	-3.535030	0.389963
C	-5.012710	0.251658	-0.210740	H	3.500500	-4.867498	-0.688919
H	-5.275278	0.279574	-1.272220	H	3.254804	-3.180860	-1.202906
C	-5.933723	-0.131522	0.687116	C	0.659262	-0.312313	-0.264369
H	-5.648120	-0.140437	1.742624	C	1.707383	0.479358	0.565879
C	-7.307614	-0.538928	0.410695	C	1.421936	0.399067	2.061327
C	-8.151334	-0.850513	1.488754	H	2.275015	0.791984	2.624228
C	-7.832485	-0.638395	-0.889579	H	0.534089	0.982833	2.333971
C	-9.464478	-1.240522	1.289777	H	1.260060	-0.639643	2.374052
H	-7.758965	-0.780277	2.501553	C	1.740641	1.922094	0.069071
C	-9.141134	-1.027389	-1.103161	H	2.036996	1.896464	-0.990594
H	-7.204722	-0.408996	-1.747201	H	0.715137	2.322669	0.096462
C	-9.969762	-1.331485	-0.012700	C	2.683860	2.856988	0.823311
H	-10.105035	-1.477559	2.135199	H	2.343736	2.949177	1.866892
H	-9.535681	-1.101795	-2.113265	H	3.681902	2.403136	0.861251
C	-11.321778	-1.734609	-0.229759	C	2.714099	4.216525	0.200753
N	-12.424949	-2.063875	-0.405686	H	1.735624	4.703424	0.127907
O	0.315350	1.404704	-1.447307	C	3.765473	4.888104	-0.286403
C	0.476780	1.196001	-2.810551	C	3.598075	6.249653	-0.892224
H	-0.267769	0.489139	-3.231101	H	2.555329	6.583920	-0.875563
H	0.366433	2.131397	-3.389624	H	4.205195	6.995563	-0.359717
H	1.479181	0.793864	-3.055446	H	3.945012	6.262406	-1.935254
H	-0.713823	0.917292	-0.892923	C	5.179351	4.392281	-0.282245
H	-3.509921	0.695077	1.226327	H	5.291598	3.390737	0.141182
				H	5.584073	4.375587	-1.303830
36				H	5.824119	5.074210	0.289860
B	0.914717	-1.869062	-0.226420	O	3.000050	-0.056029	0.287021

C	-0.762695	-0.044394	0.112559	H	5.435535	-0.523941	2.264967
H	-1.059693	-0.347081	1.120742	H	4.191745	0.745147	2.261800
C	-1.672627	0.508877	-0.702357	H	3.719814	-0.968714	2.333361
H	-1.348982	0.816983	-1.699969	C	5.173890	0.839464	-0.236010
C	-3.079059	0.760483	-0.398744	H	5.165550	0.709883	-1.329421
C	-3.861982	1.437725	-1.346352	H	4.621429	1.769743	-0.023569
C	-3.691139	0.354475	0.799135	C	6.622933	0.984475	0.227327
C	-5.199355	1.710516	-1.114567	H	6.637938	1.203854	1.306687
H	-3.403040	1.754789	-2.280861	H	7.129502	0.019854	0.100399
C	-5.024825	0.621366	1.044526	C	7.326193	2.085315	-0.500025
H	-3.117042	-0.184332	1.549053	H	6.867396	3.073132	-0.381168
C	-5.790216	1.303499	0.087208	C	8.410337	2.010698	-1.283254
H	-5.793129	2.236725	-1.857245	C	8.967328	3.233104	-1.950139
H	-5.488011	0.302179	1.974517	H	8.389590	4.132735	-1.712397
C	-7.168935	1.578181	0.337711	H	10.010265	3.406969	-1.648495
N	-8.293181	1.802010	0.542141	H	8.982454	3.114514	-3.043084
H	3.034068	-0.932616	0.695706	C	9.174194	0.754974	-1.574783
H	0.792020	-0.017605	-1.319262	H	8.749069	-0.134164	-1.101934
				H	9.218134	0.574020	-2.657941
37				H	10.216713	0.850893	-1.239731
B	2.133890	-1.807780	-0.181703	O	5.115385	-1.520908	-0.029237
O	2.916914	-2.904146	-0.764576	C	2.136084	0.666694	0.483915
O	1.733469	-2.284085	1.132611	H	1.971129	0.514361	1.554400
C	2.510363	-4.105853	-0.110493	C	1.620617	1.793933	-0.083058
C	2.197131	-3.614761	1.335679	H	1.848794	1.999464	-1.132624
C	1.272083	-4.666654	-0.808497	C	0.929991	2.874938	0.628533
H	1.503915	-4.833759	-1.867475	C	0.365641	3.921119	-0.119499
H	0.966525	-5.626781	-0.374631	C	0.824037	2.929773	2.030023
H	0.434824	-3.961434	-0.740408	C	-0.316836	4.959814	0.490424
C	3.636260	-5.119368	-0.210677	H	0.466282	3.904711	-1.204775
H	3.401233	-6.025447	0.362772	C	0.147157	3.964255	2.651557
H	3.777897	-5.410032	-1.258435	H	1.272770	2.151683	2.646648
H	4.583152	-4.711449	0.158006	C	-0.437712	4.983204	1.885969
C	1.124074	-4.419574	2.047364	H	-0.761814	5.753996	-0.104595
H	1.435161	-5.465884	2.172004	H	0.061920	3.988329	3.735344
H	0.952306	-3.998536	3.047289	C	-1.162602	6.034898	2.523485
H	0.171198	-4.398016	1.510484	N	-1.762538	6.889578	3.038942
C	3.440390	-3.581856	2.221433	H	4.456834	-2.162984	-0.360231
H	3.194410	-3.049556	3.150401	H	3.046551	-0.074873	-1.260168
H	3.769824	-4.592083	2.494922	C	-3.046541	-3.336047	-3.455984
H	4.271003	-3.058279	1.736022	C	-3.018549	-3.042509	-2.091768
C	2.963917	-0.358240	-0.194046	C	-2.633560	-1.750919	-1.738947
C	4.416181	-0.348316	0.371682	C	-2.271832	-0.767993	-2.668036
C	4.435649	-0.263621	1.899438	C	-2.325716	-1.103867	-4.021206

C	-2.711453	-2.381534	-4.410731	C	-5.194504	3.557131	-1.177937
H	-3.348910	-4.326977	-3.786416	H	-3.776490	5.168791	-1.387548
H	-2.035716	-0.373003	-4.772819	H	-6.362469	1.754870	-1.025115
H	-2.746773	-2.637968	-5.466181	H	-6.036685	4.215301	-0.977571
O	-2.596901	-1.362202	-0.429450	C	-0.465134	0.023176	3.395885
C	-3.488849	-4.016445	-1.015720	C	-0.984203	0.846239	4.400366
C	-2.877032	-3.627736	0.325077	C	0.775370	-0.600696	3.595996
C	-2.462134	-2.318473	0.541005	C	-0.269678	1.055234	5.577863
C	-2.793805	-4.496665	1.417333	H	-1.945309	1.339626	4.265514
C	-1.915251	-1.867819	1.746778	C	1.479933	-0.391839	4.777635
C	-2.314640	-4.066801	2.650203	H	1.192854	-1.243918	2.816363
H	-3.126904	-5.526903	1.311741	C	0.964821	0.442510	5.767159
C	-1.864407	-2.759658	2.814658	H	-0.682145	1.703434	6.347830
H	-2.274326	-4.761914	3.485041	H	2.443800	-0.877555	4.920089
H	-1.454341	-2.434321	3.769144	H	1.523655	0.613811	6.684315
P	-1.565550	0.807003	-2.028252	C	-2.787348	0.852403	1.961812
P	-1.271656	-0.154127	1.752798	C	-2.738938	2.199889	1.597222
C	-5.018506	-3.884285	-0.900039	C	-3.943395	0.348862	2.564869
H	-5.303607	-2.856443	-0.642355	C	-3.811628	3.042577	1.865346
H	-5.497987	-4.145672	-1.851804	H	-1.849630	2.594517	1.106831
H	-5.402239	-4.553276	-0.119576	C	-5.026825	1.187089	2.810339
C	-3.128940	-5.457102	-1.379837	H	-3.990251	-0.699007	2.858982
H	-3.505428	-6.157472	-0.627513	C	-4.958172	2.535973	2.470943
H	-3.589246	-5.750939	-2.328717	H	-3.755596	4.092037	1.582138
H	-2.043373	-5.588054	-1.463285	H	-5.923529	0.787559	3.278689
Cu	-0.100073	0.244441	-0.277325	H	-5.801930	3.191569	2.674297
C	-0.859776	1.585548	-3.531197	O	0.883023	-1.542628	-1.003253
C	-1.655120	2.186544	-4.514917	C	1.052930	-1.692240	-2.390574
C	0.526486	1.552463	-3.704549	H	0.172662	-1.307255	-2.914674
C	-1.070147	2.737690	-5.648841	H	1.940288	-1.153562	-2.765407
H	-2.736730	2.222050	-4.390817	H	1.173340	-2.747286	-2.668839
C	1.112269	2.104430	-4.840204				
H	1.147681	1.083962	-2.941914	**38-ts**			
C	0.313330	2.697541	-5.812110	B	-2.023364	-1.588608	-0.018245
H	-1.695466	3.200290	-6.408585	O	-2.961618	-2.597727	0.299932
H	2.192102	2.073218	-4.962015	O	-1.552670	-1.741979	-1.321045
H	0.767909	3.132342	-6.699068	C	-2.634281	-3.682661	-0.594624
C	-3.032237	1.859636	-1.700679	C	-2.155119	-2.929071	-1.872747
C	-2.854722	3.247701	-1.658919	C	-1.514888	-4.477079	0.070471
C	-4.303693	1.331782	-1.467257	H	-1.860992	-4.824557	1.050806
C	-3.928612	4.091558	-1.406606	H	-1.230961	-5.352601	-0.525535
H	-1.869404	3.674341	-1.842078	H	-0.623736	-3.851719	0.224625
C	-5.376668	2.178576	-1.202812	C	-3.854659	-4.556867	-0.785066
H	-4.468018	0.256095	-1.499512	H	-3.649464	-5.348786	-1.516327

H	-4.119495	-5.034975	0.164704	H	-1.240200	2.880272	-2.219635
H	-4.717820	-3.980375	-1.131329	C	0.683584	5.376140	-0.952371
C	-1.104042	-3.667911	-2.673714	H	1.290307	5.548706	1.116006
H	-1.497360	-4.625636	-3.039103	H	-0.077310	4.903458	-2.917050
H	-0.819480	-3.064029	-3.544784	C	1.375115	6.543638	-1.375128
H	-0.198477	-3.854888	-2.087821	N	1.948073	7.499467	-1.721295
C	-3.302498	-2.532280	-2.788554	H	-4.543181	-1.742255	-0.006107
H	-2.926539	-1.826729	-3.541139	H	-3.350329	0.162371	1.234194
H	-3.699033	-3.406112	-3.319942	C	2.069161	-4.372325	2.493808
H	-4.119048	-2.057164	-2.235219	C	2.339297	-3.724230	1.286560
C	-3.333433	0.274751	0.140528	C	2.206268	-2.338155	1.281562
C	-4.731353	0.157777	-0.457625	C	1.875837	-1.582080	2.409789
C	-4.797006	0.597284	-1.917079	C	1.639773	-2.267192	3.600757
H	-5.752062	0.277869	-2.347978	C	1.719873	-3.656530	3.635128
H	-4.718912	1.686659	-2.022027	H	2.151868	-5.454777	2.556275
H	-3.997536	0.133677	-2.505227	H	1.374692	-1.713798	4.499776
C	-5.669904	1.030108	0.398106	H	1.522696	-4.186094	4.563613
H	-5.596913	0.674113	1.437487	O	2.432210	-1.617786	0.141991
H	-5.295169	2.066524	0.394013	C	2.899650	-4.420464	0.049844
C	-7.138937	1.007642	-0.023558	C	2.532380	-3.612613	-1.188373
H	-7.232361	1.444074	-1.030833	C	2.287622	-2.247901	-1.063682
H	-7.464725	-0.036164	-0.105868	C	2.506027	-4.136705	-2.482929
C	-7.994686	1.785314	0.924383	C	1.923144	-1.426108	-2.133407
H	-7.722415	2.841888	1.021245	C	2.227889	-3.331461	-3.583214
C	-9.016410	1.350403	1.673907	H	2.719271	-5.191327	-2.642313
C	-9.754075	2.280675	2.590142	C	1.916398	-1.986348	-3.409890
H	-9.355860	3.300193	2.551513	H	2.230220	-3.762884	-4.580925
H	-10.822660	2.320946	2.334518	H	1.647861	-1.370412	-4.266567
H	-9.702927	1.932002	3.631605	P	1.695072	0.228253	2.157763
C	-9.532413	-0.056422	1.688393	P	1.402542	0.289217	-1.749000
H	-8.984348	-0.729352	1.023692	C	4.434523	-4.429008	0.181339
H	-9.486204	-0.472803	2.704567	H	4.827210	-3.407958	0.270350
H	-10.592016	-0.081901	1.397175	H	4.737234	-4.992094	1.073292
O	-5.239441	-1.177666	-0.381388	H	4.890861	-4.896568	-0.700353
C	-2.434863	1.218782	-0.337094	C	2.393769	-5.856990	-0.060998
H	-2.519453	1.475516	-1.397961	H	2.831883	-6.361826	-0.928029
C	-1.414177	1.878028	0.384332	H	2.683748	-6.445054	0.815837
H	-1.508502	1.838460	1.473874	H	1.301227	-5.889775	-0.156057
C	-0.699570	3.038154	-0.114053	Cu	0.270997	0.531482	0.290912
C	0.052704	3.829256	0.792444	C	1.290096	0.853182	3.839207
C	-0.708103	3.460416	-1.467430	C	2.224995	0.830471	4.881797
C	0.727468	4.963028	0.392087	C	0.019300	1.381604	4.081898
H	0.084522	3.530216	1.840797	C	1.886967	1.314456	6.139793
C	-0.046306	4.602273	-1.871818	H	3.223606	0.431170	4.706818

C	-0.318477	1.871929	5.340778				
H	-0.713503	1.407709	3.276772	**39**			
C	0.615431	1.837055	6.370114	C	-0.259420	0.445306	-3.003571
H	2.619137	1.287897	6.943289	C	-1.209251	-0.581092	-3.571979
H	-1.309803	2.284036	5.512474	C	-0.966347	-0.832340	-5.054049
H	0.355910	2.220608	7.353922	H	-1.638883	-1.606257	-5.443121
C	3.430117	0.799989	1.992080	H	-1.127553	0.088850	-5.625842
C	3.631582	2.139738	1.647700	H	0.066415	-1.162623	-5.215178
C	4.534149	-0.017111	2.247998	C	-2.643662	-0.107059	-3.305209
C	4.919548	2.658886	1.582374	H	-2.726595	0.072569	-2.219033
H	2.773841	2.776271	1.417345	H	-2.795595	0.871845	-3.787929
C	5.822783	0.504008	2.174642	C	-3.738148	-1.087543	-3.731453
H	4.386420	-1.063721	2.513532	H	-3.884670	-1.035890	-4.818498
C	6.016066	1.843130	1.848345	H	-3.383105	-2.104603	-3.516540
H	5.067496	3.699582	1.302132	C	-5.039063	-0.828634	-3.028736
H	6.676924	-0.137975	2.377650	H	-5.790566	-0.246981	-3.567803
H	7.022948	2.250231	1.790067	C	-5.326513	-1.209633	-1.776955
C	0.601401	0.824774	-3.312825	C	-6.630504	-0.863143	-1.125634
C	1.227195	1.655188	-4.245814	H	-7.290513	-0.301342	-1.795287
C	-0.717476	0.409258	-3.541585	H	-7.162591	-1.767434	-0.796332
C	0.535685	2.091676	-5.373064	H	-6.466438	-0.257140	-0.221625
H	2.254127	1.978696	-4.086931	C	-4.385280	-1.979718	-0.901384
C	-1.399431	0.838493	-4.675248	H	-3.461828	-2.292768	-1.401326
H	-1.202677	-0.252428	-2.821834	H	-4.097963	-1.368983	-0.030342
C	-0.779331	1.691125	-5.586605	H	-4.870449	-2.879983	-0.496195
H	1.029261	2.747675	-6.086434	O	-1.012343	-1.854003	-2.936856
H	-2.424494	0.514147	-4.846351	C	1.114037	0.233877	-2.832322
H	-1.319401	2.037496	-6.464711	H	1.490463	-0.773736	-3.031193
C	2.980965	1.225405	-1.755674	C	2.003468	1.181052	-2.276085
C	2.920869	2.614687	-1.587478	H	1.646195	2.209394	-2.166037
C	4.224538	0.614569	-1.923801	C	3.348603	0.922222	-1.871420
C	4.078351	3.380716	-1.630958	C	4.095753	1.947147	-1.230402
H	1.957236	3.103439	-1.442965	C	4.001963	-0.329332	-2.038580
C	5.386632	1.382198	-1.939354	C	5.370494	1.734530	-0.755450
H	4.290896	-0.464494	-2.054730	H	3.627214	2.922905	-1.096201
C	5.315974	2.764666	-1.803683	C	5.279984	-0.544620	-1.571277
H	4.014994	4.461381	-1.515037	H	3.481517	-1.151353	-2.527379
H	6.351235	0.895373	-2.064786	C	5.988796	0.478041	-0.910894
H	6.224724	3.362094	-1.824535	H	5.908631	2.536781	-0.254235
O	-1.106456	-1.176512	0.953305	H	5.748075	-1.518122	-1.704876
C	-1.429101	-1.475133	2.296128	C	7.295258	0.248087	-0.406662
H	-0.803434	-0.865880	2.954498	N	8.368873	0.060583	0.012790
H	-2.481360	-1.257268	2.521241	H	-1.001337	-1.665407	-1.983440
H	-1.236742	-2.534609	2.514831	H	-0.616072	1.479137	-3.014783

C	-4.734342	0.775994	2.078257	C	-0.216424	3.374440	2.668369
C	-3.625594	-0.061248	2.198366	C	2.549678	3.044474	2.506960
C	-2.422822	0.394647	1.660152	H	2.154929	1.903316	0.719813
C	-2.288706	1.618428	0.998875	C	0.609971	3.928219	3.639827
C	-3.416434	2.439677	0.925154	H	-1.295650	3.513671	2.725962
C	-4.630005	2.017392	1.456363	C	1.992349	3.766571	3.557709
H	-5.695776	0.461871	2.478067	H	3.626999	2.900857	2.443419
H	-3.346492	3.407051	0.432111	H	0.175599	4.491694	4.462279
H	-5.503318	2.660603	1.387120	H	2.635078	4.203846	4.318206
O	-1.294810	-0.382061	1.760298	C	1.991386	-2.885827	-0.390458
C	-3.621491	-1.407740	2.909827	C	3.013034	-3.531739	0.312678
C	-2.650671	-2.314703	2.163769	C	1.735072	-3.254317	-1.716719
C	-1.484299	-1.740115	1.661311	C	3.784568	-4.508130	-0.309276
C	-2.801798	-3.690575	1.997601	H	3.215673	-3.263420	1.347759
C	-0.461245	-2.473160	1.054302	C	2.503779	-4.237500	-2.332168
C	-1.812395	-4.450837	1.379121	H	0.927783	-2.776752	-2.273232
H	-3.701629	-4.183936	2.356807	C	3.536247	-4.857238	-1.633787
C	-0.643057	-3.852431	0.923016	H	4.582498	-4.997906	0.243822
H	-1.950435	-5.522563	1.263133	H	2.298341	-4.513487	-3.363760
H	0.131100	-4.453617	0.450257	H	4.144294	-5.616524	-2.119786
P	-0.663553	1.987615	0.236514	C	1.973076	-1.057386	1.815712
P	0.972173	-1.562399	0.365529	C	3.239230	-0.513373	1.560270
C	-3.074915	-1.200782	4.336563	C	1.525923	-1.153801	3.133501
H	-2.069071	-0.765322	4.324027	C	4.047385	-0.092830	2.608138
H	-3.732686	-0.526009	4.898237	H	3.601031	-0.430467	0.534299
H	-3.026059	-2.161650	4.863750	C	2.331370	-0.711822	4.181209
C	-5.020002	-2.006210	3.005339	H	0.547183	-1.579270	3.350332
H	-4.994757	-2.969363	3.526078	C	3.592192	-0.185268	3.922111
H	-5.676346	-1.355871	3.593597	H	5.034177	0.315214	2.395547
H	-5.474100	-2.154729	2.017320	H	1.971749	-0.789635	5.204562
Cu	0.273973	0.239191	-0.888992	H	4.221112	0.151762	4.742742
C	-0.969373	3.462189	-0.805235				
C	-0.167748	4.602606	-0.703490	**40-ts**			
C	-1.926017	3.394241	-1.827893	C	2.353534	-2.151882	1.636457
C	-0.324897	5.655499	-1.601825	C	3.497646	-2.879888	0.936805
H	0.584802	4.673111	0.080353	C	3.488892	-4.384133	1.160269
C	-2.086929	4.450542	-2.716431	H	4.284571	-4.875961	0.587776
H	-2.554033	2.509127	-1.927503	H	3.631996	-4.612241	2.223552
C	-1.283374	5.583579	-2.606878	H	2.532530	-4.815081	0.840168
H	0.305286	6.537010	-1.511286	C	4.816358	-2.252761	1.404797
H	-2.839083	4.385241	-3.499270	H	4.751835	-1.168198	1.214418
H	-1.404368	6.407004	-3.306418	H	4.904233	-2.363433	2.496947
C	0.338949	2.645475	1.612715	C	6.064160	-2.804606	0.714329
C	1.723563	2.479237	1.540326	H	6.277454	-3.814471	1.090775

H	5.835511	-2.918431	-0.353772	C	1.331804	2.224017	-4.415288
C	7.269311	-1.934151	0.912759	C	-0.145335	0.469047	-2.808572
H	7.927059	-2.189331	1.747576	C	1.108094	0.913465	-4.827872
C	7.583052	-0.855236	0.183482	H	1.911781	2.888422	-5.051136
C	8.803204	-0.036761	0.475908	C	0.370747	0.042077	-4.033550
H	9.371390	-0.435834	1.322917	H	1.511779	0.569555	-5.776644
H	9.471216	0.001275	-0.396548	H	0.208720	-0.984879	-4.354984
H	8.537219	1.005710	0.702145	P	-0.669430	1.593634	1.563389
C	6.760200	-0.364928	-0.970063	P	-0.987806	-0.639101	-1.616920
H	5.856371	-0.959416	-1.142205	C	-0.372889	4.872151	-3.146857
H	6.449485	0.676637	-0.801475	H	-1.262815	4.384946	-2.731051
H	7.349269	-0.359240	-1.898219	H	-0.350355	5.909409	-2.789496
O	3.366952	-2.700216	-0.483262	H	-0.465206	4.880203	-4.240182
C	1.016616	-2.570386	1.360587	C	2.113365	4.859345	-3.339235
H	0.900548	-3.221547	0.487921	H	2.032724	4.893702	-4.430844
C	-0.139281	-2.118510	1.967566	H	2.151760	5.899805	-2.999354
H	-0.041548	-1.509654	2.872081	H	3.058554	4.370505	-3.074342
C	-1.470120	-2.655338	1.722362	Cu	-0.009933	-0.320894	0.464922
C	-2.543462	-2.202971	2.518083	C	-0.255449	1.701165	3.341334
C	-1.755097	-3.639385	0.749711	C	-1.019007	2.396118	4.282361
C	-3.827349	-2.688523	2.357761	C	0.913318	1.049250	3.752332
H	-2.346552	-1.446088	3.278042	C	-0.613397	2.441927	5.613498
C	-3.030936	-4.147224	0.595905	H	-1.932081	2.903768	3.974812
H	-0.964715	-4.015975	0.101990	C	1.321575	1.103492	5.080106
C	-4.086492	-3.676785	1.395286	H	1.502133	0.497198	3.017279
H	-4.637989	-2.315147	2.979678	C	0.555502	1.799569	6.012269
H	-3.226298	-4.910022	-0.154723	H	-1.212907	2.983072	6.341686
C	-5.404157	-4.190598	1.225599	H	2.232288	0.595805	5.388986
N	-6.484983	-4.603430	1.082698	H	0.867696	1.836486	7.053177
H	3.124225	-1.765450	-0.618086	C	-2.430726	2.071909	1.460076
H	2.552609	-1.862866	2.675904	C	-3.377438	1.049775	1.373214
C	1.693789	5.030043	-0.427653	C	-2.858937	3.403606	1.486062
C	0.982761	4.118779	-1.208591	C	-4.735587	1.347441	1.338979
C	0.245762	3.147006	-0.534413	H	-3.046572	0.013021	1.312309
C	0.196724	3.045709	0.857323	C	-4.217145	3.700396	1.438870
C	0.902678	3.989699	1.603971	H	-2.127362	4.209153	1.545768
C	1.648990	4.973147	0.962758	C	-5.156234	2.673035	1.369913
H	2.290728	5.802023	-0.906900	H	-5.460807	0.538941	1.265869
H	0.884774	3.939273	2.691272	H	-4.544136	4.737413	1.456503
H	2.203180	5.700716	1.550092	H	-6.217124	2.909552	1.334413
O	-0.458913	2.204370	-1.241431	C	-0.740340	-2.303923	-2.332890
C	0.916485	4.138706	-2.729478	C	-1.716794	-3.043488	-3.001899
C	0.814781	2.696386	-3.209732	C	0.514019	-2.879294	-2.101157
C	0.085569	1.795597	-2.434890	C	-1.444110	-4.348833	-3.407328

H	-2.697649	-2.610413	-3.190138	H	-7.087124	0.682354	-2.840688
C	0.787313	-4.178291	-2.509597	C	-5.330594	-1.088935	-4.061870
H	1.281000	-2.317011	-1.571543	H	-4.384554	-1.638512	-4.088598
C	-0.198905	-4.919934	-3.158120	H	-5.984452	-1.567274	-3.316561
H	-2.212836	-4.922879	-3.919725	H	-5.825278	-1.222839	-5.034166
H	1.767608	-4.602899	-2.301787	O	-0.105713	-0.769136	-2.615829
H	0.001528	-5.942648	-3.468860	C	2.080767	1.172034	-1.882374
C	-2.770254	-0.282390	-1.843440	H	2.420590	0.171450	-2.168511
C	-3.693218	-1.101337	-1.179817	C	3.056683	2.064799	-1.267328
C	-3.238534	0.804205	-2.584900	H	2.843021	3.122340	-1.473138
C	-5.056182	-0.853916	-1.279214	C	4.487229	1.746260	-1.359287
H	-3.341605	-1.944964	-0.585579	C	5.435003	2.766589	-1.557051
C	-4.604703	1.066136	-2.660987	C	4.969143	0.436969	-1.171335
H	-2.537236	1.448524	-3.113343	C	6.791398	2.499771	-1.585757
C	-5.515391	0.236482	-2.015180	H	5.085864	3.788569	-1.697001
H	-5.762274	-1.507281	-0.769659	C	6.321858	0.154947	-1.206391
H	-4.956100	1.918326	-3.238070	H	4.265277	-0.370203	-0.974212
H	-6.581663	0.439153	-2.082931	C	7.251208	1.185079	-1.417013
H	2.302902	-1.030694	0.927558	H	7.508132	3.301742	-1.746545
C	2.841479	0.979662	0.212458	H	6.668985	-0.866215	-1.060495
H	3.914020	0.776481	0.036908	C	8.646618	0.899572	-1.453312
H	2.749446	1.392447	1.235775	N	9.788219	0.665504	-1.483819
H	2.546118	1.780560	-0.483623	H	-0.355910	-0.797042	-1.679475
O	2.068147	-0.168068	0.021877	H	0.432224	2.495636	-1.950237
				C	-5.225651	-0.668866	-0.356178
41-ts				C	-4.080952	-1.386341	-0.005685
C	0.761052	1.461012	-2.104262	C	-2.974600	-0.645392	0.404712
C	-0.133888	0.608057	-2.998180	C	-2.967310	0.750287	0.479340
C	0.391112	0.631837	-4.428571	C	-4.138562	1.428195	0.140754
H	-0.223342	0.008459	-5.088014	C	-5.258677	0.719408	-0.277710
H	0.395297	1.656521	-4.817398	H	-6.119501	-1.200603	-0.676337
H	1.417682	0.249237	-4.454310	H	-4.168690	2.514436	0.196999
C	-1.570885	1.128735	-2.923735	H	-6.166947	1.254113	-0.545472
H	-1.871421	1.142005	-1.863490	O	-1.816502	-1.273346	0.795914
H	-1.576729	2.177684	-3.264485	C	-4.013503	-2.905162	0.081874
C	-2.614369	0.337555	-3.699692	C	-2.574416	-3.338381	-0.161657
H	-2.324033	0.280543	-4.761412	C	-1.537448	-2.493395	0.236238
H	-2.621175	-0.700144	-3.335060	C	-2.215699	-4.579098	-0.685966
C	-3.974155	0.961468	-3.580016	C	-0.183364	-2.818105	0.095934
H	-3.980548	2.031521	-3.342942	C	-0.881573	-4.957872	-0.793353
C	-5.160158	0.364045	-3.744919	H	-2.988778	-5.272900	-1.006667
C	-6.442671	1.126672	-3.614398	C	0.127063	-4.085178	-0.406094
H	-6.272212	2.177529	-3.355182	H	-0.627630	-5.938289	-1.187514
H	-7.021931	1.093893	-4.548199	H	1.168258	-4.381011	-0.511623

P	-1.403130	1.538496	1.019989	C	1.426831	-1.794990	2.276030
P	1.092283	-1.552030	0.495729	C	2.330695	-0.906866	2.874020
C	-4.404440	-3.313690	1.515579	C	0.871047	-2.828793	3.030252
H	-3.746846	-2.850391	2.260516	C	2.693822	-1.075409	4.205110
H	-5.434656	-3.001763	1.728550	H	2.722869	-0.069610	2.291968
H	-4.337384	-4.402937	1.629663	C	1.219079	-2.977606	4.371208
C	-4.972263	-3.572876	-0.899631	H	0.171022	-3.525735	2.571809
H	-4.958361	-4.661122	-0.780700	C	2.135560	-2.109123	4.955659
H	-6.004465	-3.259157	-0.712197	H	3.404277	-0.390025	4.662203
H	-4.716672	-3.333170	-1.938650	H	0.778416	-3.781307	4.956428
Cu	0.574863	0.747128	0.076841	H	2.413106	-2.234505	5.999769
C	-1.756248	3.335424	0.875542	O	2.042216	1.821193	1.105560
C	-1.752662	4.184161	1.985782	C	1.758194	3.149983	1.431300
C	-1.926282	3.891884	-0.399584	H	1.254398	3.232086	2.409384
C	-1.912661	5.558132	1.823711	H	2.679215	3.756602	1.495978
H	-1.614485	3.773932	2.984351	H	1.097028	3.645110	0.690945
C	-2.098658	5.261577	-0.557809	H	2.716031	1.943440	-0.030143
H	-1.933856	3.248669	-1.278655				
C	-2.086012	6.099532	0.554878	**42**			
H	-1.903091	6.205781	2.697218	C	-0.607382	-0.675579	-0.743998
H	-2.237803	5.676666	-1.553277	C	-1.617662	-0.060602	0.242957
H	-2.210937	7.172532	0.431184	C	-1.208669	-0.349663	1.675486
C	-1.447599	1.247400	2.829356	H	-1.876456	0.153903	2.381667
C	-0.240484	1.085032	3.511786	H	-1.236581	-1.428162	1.871734
C	-2.651924	1.220742	3.541642	H	-0.189723	0.007582	1.861110
C	-0.237737	0.903047	4.892542	C	-3.009485	-0.608070	-0.083280
H	0.695079	1.091021	2.949523	H	-3.230143	-0.372229	-1.138231
C	-2.645098	1.039184	4.919609	H	-2.983211	-1.707365	-0.022251
H	-3.598982	1.347909	3.017749	C	-4.143726	-0.069110	0.786629
C	-1.437003	0.881351	5.596430	H	-3.987646	-0.393600	1.827036
H	0.707603	0.768324	5.414105	H	-4.094891	1.026782	0.796218
H	-3.584430	1.020051	5.467428	C	-5.473404	-0.565145	0.314815
H	-1.433658	0.737383	6.674433	H	-5.579919	-1.654960	0.321235
C	2.579935	-2.293784	-0.299516	C	-6.517533	0.146085	-0.130088
C	3.670197	-2.772922	0.431325	C	-7.774979	-0.532637	-0.584667
C	2.617038	-2.365022	-1.700560	H	-7.710106	-1.622493	-0.499796
C	4.780384	-3.302750	-0.224202	H	-8.640310	-0.194562	0.002939
H	3.659822	-2.736059	1.518518	H	-8.001025	-0.283356	-1.631257
C	3.722442	-2.902603	-2.349070	C	-6.563712	1.640905	-0.221005
H	1.769907	-2.001261	-2.283542	H	-5.635972	2.128452	0.089989
C	4.809978	-3.369197	-1.612846	H	-6.784360	1.956528	-1.250297
H	5.622358	-3.669146	0.358641	H	-7.378237	2.038924	0.400109
H	3.735940	-2.953950	-3.435218	O	-1.603510	1.359921	0.115223
H	5.676884	-3.784609	-2.121380	C	0.780988	-0.163556	-0.580347

H	0.881623	0.923758	-0.577453	C	0.466466	-3.622970	-0.615383
C	1.857317	-0.946404	-0.433830	H	0.663473	-3.922140	0.415234
H	1.710556	-2.029675	-0.424277	C	1.505388	-3.166532	-1.403066
C	3.243922	-0.508911	-0.287269	C	2.918054	-3.387213	-1.152311
C	4.240606	-1.478811	-0.102955	C	3.403748	-3.849585	0.084770
C	3.630507	0.841104	-0.328256	C	3.835091	-3.213839	-2.204824
C	5.572393	-1.127698	0.038139	C	4.745131	-4.129589	0.263840
H	3.956019	-2.528806	-0.071648	H	2.719930	-3.977425	0.921058
C	4.956004	1.206551	-0.188201	C	5.177517	-3.502996	-2.041124
H	2.882668	1.616426	-0.475378	H	3.472313	-2.839923	-3.160367
C	5.938549	0.222563	-0.003967	C	5.643370	-3.964459	-0.801778
H	6.333997	-1.889917	0.180151	H	5.112070	-4.487751	1.222851
H	5.244659	2.253887	-0.221278	H	5.875581	-3.373219	-2.864560
C	7.308786	0.598373	0.138760	C	7.028099	-4.259066	-0.622003
N	8.425882	0.905521	0.255169	N	8.158241	-4.498940	-0.475004
H	-1.922663	1.578878	-0.769276	H	-1.039353	-3.341058	-2.104585
H	-0.623008	-1.771180	-0.649829	H	1.254829	-2.799800	-2.400010
H	-0.963476	-0.443198	-1.762739	C	2.664624	3.772309	2.893491
				C	1.664394	3.815797	1.922696
43-ts				C	0.895664	2.666538	1.748461
C	-0.846559	-3.486905	-1.040316	C	1.082892	1.494536	2.482003
C	-1.972940	-3.101217	-0.157221	C	2.081626	1.496664	3.456158
C	-1.817979	-3.439776	1.314625	C	2.867438	2.627502	3.658708
H	-2.535548	-2.861170	1.908488	H	3.291729	4.643665	3.064232
H	-2.000651	-4.506772	1.498188	H	2.256819	0.600758	4.048779
H	-0.818242	-3.183590	1.683606	H	3.644402	2.616791	4.419090
C	-3.342855	-3.494084	-0.702392	O	-0.106999	2.649890	0.807671
H	-3.369430	-3.181567	-1.758257	C	1.311847	5.042243	1.092656
H	-3.448332	-4.589678	-0.691984	C	0.854652	4.556869	-0.275984
C	-4.514877	-2.852242	0.041239	C	0.116613	3.373887	-0.335654
H	-4.665159	-3.341311	1.012735	C	1.041869	5.250587	-1.471034
H	-4.241303	-1.808308	0.263212	C	-0.438545	2.870774	-1.514731
C	-5.765936	-2.857848	-0.777176	C	0.489288	4.787940	-2.662719
H	-5.675907	-2.329504	-1.733739	H	1.616983	6.173620	-1.475242
C	-6.947198	-3.429589	-0.506728	C	-0.251029	3.611120	-2.684468
C	-8.090946	-3.330049	-1.471389	H	0.638711	5.350285	-3.580972
H	-7.829795	-2.751700	-2.363891	H	-0.666291	3.245947	-3.621970
H	-8.421760	-4.327535	-1.793939	P	0.055800	0.043041	2.024657
H	-8.963882	-2.856864	-0.999698	P	-1.259611	1.230587	-1.448387
C	-7.260425	-4.209743	0.733411	C	0.120479	5.754896	1.763757
H	-6.417957	-4.290979	1.425249	H	-0.749333	5.092566	1.847013
H	-8.099944	-3.752051	1.275066	H	0.397189	6.085261	2.772913
H	-7.584072	-5.227331	0.473685	H	-0.172829	6.633904	1.175750
O	-1.664429	-1.767618	-0.470521	C	2.473796	6.024344	0.995117

H	2.185907	6.907902	0.415155	C	-5.580139	2.075781	-0.010464
H	2.758786	6.386181	1.988881	H	-5.918149	-0.006662	-0.482795
H	3.355669	5.572468	0.524657	H	-4.942011	4.096697	0.367540
Cu	-0.078663	-0.493545	-0.287872	H	-6.596632	2.247901	0.336114
C	0.786164	-1.295390	3.043197	B	1.890794	-0.332473	-0.934216
C	0.110509	-1.900828	4.105761	O	2.493407	-0.302302	-2.183259
C	2.047001	-1.782769	2.669075	O	2.673650	0.345288	-0.011318
C	0.684071	-2.971980	4.787055	C	3.553834	0.682617	-2.150217
H	-0.874134	-1.539929	4.399215	C	3.912832	0.742418	-0.635979
C	2.626477	-2.834844	3.369643	C	4.684194	0.238768	-3.054644
H	2.572967	-1.320619	1.830042	H	4.333531	0.201366	-4.092752
C	1.943656	-3.437213	4.425332	H	5.515887	0.953521	-3.005535
H	0.145185	-3.439657	5.607981	H	5.063652	-0.751495	-2.784138
H	3.618038	-3.186763	3.089414	C	2.946768	1.976242	-2.671575
H	2.395404	-4.267226	4.963485	H	3.688017	2.780557	-2.754682
C	-1.526010	0.415411	2.876644	H	2.520882	1.793736	-3.666190
C	-2.707866	-0.017669	2.271403	H	2.132290	2.312204	-2.019864
C	-1.586683	1.087237	4.102887	C	4.961856	-0.273458	-0.211988
C	-3.935560	0.204502	2.890277	H	5.959543	-0.018157	-0.590101
H	-2.646374	-0.527134	1.307516	H	5.004451	-0.293069	0.884311
C	-2.813694	1.311173	4.717509	H	4.700796	-1.278334	-0.560756
H	-0.668019	1.429370	4.579535	C	4.290638	2.118076	-0.124494
C	-3.988576	0.867813	4.112293	H	4.495891	2.063443	0.951736
H	-4.852843	-0.129659	2.408461	H	5.193581	2.488898	-0.627172
H	-2.855013	1.833038	5.671042	H	3.480017	2.840121	-0.272151
H	-4.947502	1.045145	4.594354				
C	-1.491237	0.845821	-3.225428	**44**			
C	-2.593439	1.281668	-3.967732	C	-1.924655	2.276975	-0.193230
C	-0.482373	0.112011	-3.860581	C	-0.895372	3.084613	0.572050
C	-2.686894	0.986289	-5.324104	C	-1.128053	3.011358	2.083467
H	-3.381635	1.855380	-3.481550	H	-0.320661	3.539244	2.605676
C	-0.576657	-0.175509	-5.219550	H	-2.086741	3.462023	2.379704
H	0.384646	-0.218545	-3.285250	H	-1.109037	1.972263	2.432953
C	-1.679138	0.257625	-5.951191	C	-0.995903	4.549040	0.095954
H	-3.548557	1.327259	-5.893689	H	-0.781511	4.541810	-0.984504
H	0.212683	-0.743008	-5.707767	H	-2.023219	4.929733	0.218007
H	-1.754276	0.027213	-7.011516	C	0.006625	5.476703	0.790856
C	-2.961978	1.636745	-0.896401	H	-0.383376	5.769857	1.776385
C	-3.899614	0.595558	-0.902050	H	0.918861	4.894470	0.977755
C	-3.348586	2.896653	-0.437185	C	0.321005	6.704763	-0.004950
C	-5.201606	0.814987	-0.471554	H	-0.384098	7.536244	0.086425
H	-3.582077	-0.397119	-1.226798	C	1.349979	6.862340	-0.848708
C	-4.651934	3.111502	0.009009	C	1.545072	8.133371	-1.618618
H	-2.631750	3.717905	-0.428369	H	0.771082	8.874738	-1.392577

H	2.524180	8.583409	-1.399035	P	1.374239	-0.227577	2.082723
H	1.532336	7.945514	-2.701892	P	1.298830	-0.054495	-1.893132
C	2.383758	5.809494	-1.116646	C	4.743905	-4.347898	-0.257620
H	2.211512	4.880993	-0.560024	H	4.955765	-3.273048	-0.239184
H	2.404305	5.552599	-2.186081	H	5.269396	-4.816094	0.584020
H	3.391045	6.180186	-0.873070	H	5.143613	-4.760057	-1.192729
O	0.359389	2.599344	0.226785	C	3.014932	-6.139457	-0.188995
C	-2.745082	1.332394	0.278340	H	3.416013	-6.570826	-1.112274
H	-2.760149	1.108616	1.349414	H	3.548346	-6.625649	0.634614
C	-3.632908	0.488038	-0.584972	H	1.951125	-6.398106	-0.116755
C	-5.110106	0.554177	-0.252381	Cu	0.544914	0.648703	0.140419
C	-5.602516	1.282948	0.833879	C	0.278465	-0.025004	3.532606
C	-6.021687	-0.149162	-1.054708	C	0.656166	0.651056	4.693200
C	-6.959953	1.307931	1.120032	C	-1.033624	-0.500004	3.407576
H	-4.916687	1.852690	1.456349	C	-0.270370	0.858270	5.713367
C	-7.378510	-0.130705	-0.784318	H	1.672602	1.028224	4.798011
H	-5.649675	-0.718643	-1.905952	C	-1.950925	-0.303972	4.432555
C	-7.856056	0.599121	0.312940	H	-1.351072	-0.997113	2.488255
H	-7.333402	1.880146	1.965461	C	-1.571593	0.383170	5.584744
H	-8.076188	-0.676153	-1.414502	H	0.027439	1.394783	6.611344
C	-9.254858	0.622160	0.602386	H	-2.968479	-0.673195	4.322805
N	-10.395170	0.639101	0.836835	H	-2.293700	0.551302	6.380295
H	-1.905592	2.456782	-1.276333	C	2.857205	0.775282	2.467724
H	-3.515363	0.797358	-1.637334	C	2.841467	2.121878	2.076824
C	2.511553	-4.703486	2.316350	C	3.973211	0.257676	3.131750
C	2.703301	-4.007211	1.124020	C	3.940243	2.931598	2.347706
C	2.419766	-2.640613	1.123457	H	1.970876	2.521455	1.541845
C	1.932212	-1.965499	2.246748	C	5.067296	1.075821	3.398366
C	1.775425	-2.696983	3.428264	H	3.987740	-0.786506	3.441924
C	2.064527	-4.055063	3.463606	C	5.052484	2.411875	3.005581
H	2.716309	-5.770175	2.357738	H	3.927611	3.974385	2.033406
H	1.400900	-2.195754	4.319284	H	5.934285	0.667745	3.913044
H	1.933563	-4.614553	4.386180	H	5.911400	3.046726	3.211725
O	2.579465	-1.912609	-0.033130	C	0.304141	0.402906	-3.352760
C	3.232864	-4.631019	-0.159317	C	0.799993	1.097685	-4.456725
C	2.537294	-3.935154	-1.319912	C	-1.038074	0.008949	-3.333366
C	2.280384	-2.569169	-1.204548	C	-0.042421	1.393936	-5.526623
C	2.179596	-4.554851	-2.516975	H	1.844346	1.405439	-4.482001
C	1.699013	-1.811857	-2.225816	C	-1.872349	0.289995	-4.407069
C	1.613231	-3.828462	-3.560148	H	-1.430399	-0.539949	-2.476238
H	2.352332	-5.620155	-2.647487	C	-1.374240	0.989875	-5.505340
C	1.381611	-2.464557	-3.419678	H	0.346546	1.939471	-6.383264
H	1.353044	-4.329613	-4.488948	H	-2.910734	-0.035707	-4.380980
H	0.931445	-1.901745	-4.235372	H	-2.025150	1.221889	-6.344966

C	2.899402	0.805669	-2.106692	H	0.445715	4.684001	-2.035190
C	3.031156	2.079233	-1.537816	H	-0.625533	3.687752	-1.064730
C	3.974152	0.239693	-2.798928	C	0.043487	5.497283	-0.101060
C	4.234733	2.767977	-1.658846	H	0.456535	6.456360	-0.423530
H	2.185319	2.525805	-1.004496	C	-0.571160	5.459394	1.088608
C	5.172983	0.936068	-2.916600	C	-0.706111	6.680952	1.944967
H	3.873159	-0.747274	-3.249110	H	-0.252843	7.561430	1.477170
C	5.305346	2.197795	-2.342468	H	-1.762417	6.907285	2.149352
H	4.337762	3.751207	-1.202030	H	-0.230401	6.531515	2.924885
H	6.006372	0.490435	-3.454900	C	-1.149214	4.210029	1.682370
H	6.246386	2.736557	-2.427609	H	-1.120813	3.353366	0.995663
B	-3.213744	-1.033840	-0.519672	H	-0.599559	3.925866	2.592877
O	-3.228082	-1.838703	-1.626307	H	-2.194089	4.366124	1.992313
O	-2.842330	-1.685893	0.623165	O	0.403369	1.536386	-1.453720
C	-3.066489	-3.202243	-1.159093	C	3.886832	1.031618	-0.881905
C	-2.373989	-3.001618	0.225725	H	4.317069	1.372340	-1.827475
C	-4.464674	-3.788836	-1.048295	C	4.809989	0.234890	0.015301
H	-4.960944	-3.706968	-2.021700	C	6.176348	0.857187	0.121176
H	-4.435876	-4.846881	-0.764741	C	7.000545	0.993522	-1.003595
H	-5.070365	-3.246958	-0.311358	C	6.642813	1.325826	1.353255
C	-2.248350	-3.966765	-2.178040	C	8.249656	1.583422	-0.903695
H	-2.023432	-4.977266	-1.814152	H	6.660840	0.616625	-1.965844
H	-2.817846	-4.061877	-3.109043	C	7.891841	1.916009	1.471054
H	-1.304291	-3.459680	-2.407348	H	6.009916	1.228461	2.233708
C	-2.773017	-3.999038	1.292265	C	8.701911	2.049350	0.337653
H	-2.493151	-5.016119	0.991205	H	8.884704	1.684264	-1.779971
H	-2.245817	-3.765575	2.224996	H	8.245145	2.279425	2.432593
H	-3.847657	-3.976594	1.493360	C	9.989119	2.660068	0.445851
C	-0.860974	-2.920561	0.130454	N	11.038027	3.157707	0.532986
H	-0.450849	-2.665147	1.115622	H	2.206981	0.961278	0.374944
H	-0.420371	-3.877417	-0.178577	H	4.354075	0.204468	1.015470
H	-0.538852	-2.142098	-0.576400	C	-4.727475	-2.997340	-2.913120
				C	-4.145768	-3.000455	-1.646223
45-ts				C	-3.734562	-1.772344	-1.130562
C	2.620924	1.320209	-0.576801	C	-3.880510	-0.560491	-1.810517
C	1.657880	2.174608	-1.363469	C	-4.476337	-0.601403	-3.073109
C	2.152640	2.474385	-2.772922	C	-4.895051	-1.809826	-3.618157
H	1.389323	3.039119	-3.320139	H	-5.060324	-3.931307	-3.359170
H	3.080456	3.059517	-2.772430	H	-4.596483	0.317947	-3.641653
H	2.331978	1.537403	-3.316305	H	-5.352365	-1.827495	-4.604098
C	1.440740	3.459663	-0.548157	O	-3.157287	-1.716692	0.116015
H	1.252288	3.162990	0.496558	C	-3.997732	-4.229602	-0.761437
H	2.373880	4.043295	-0.539844	C	-2.714858	-4.068113	0.041622
C	0.268269	4.325387	-1.011313	C	-2.385204	-2.789312	0.486883

C	-1.881182	-5.114024	0.434690	H	-0.354502	-0.258741	4.582630
C	-1.291217	-2.518002	1.313123	C	2.934575	-1.366096	2.861713
C	-0.787709	-4.882969	1.264500	H	1.797595	-1.475557	1.044687
H	-2.089523	-6.127888	0.102071	C	2.925667	-1.064092	4.222055
C	-0.500779	-3.597586	1.711801	H	1.731102	-0.416611	5.892823
H	-0.157049	-5.714057	1.570408	H	3.846114	-1.698569	2.368786
H	0.358751	-3.428458	2.356606	H	3.839506	-1.148358	4.805674
P	-3.149267	0.953351	-1.068819	C	-2.230649	-0.282092	2.874296
P	-0.930223	-0.755144	1.680482	C	-2.457061	1.081491	3.076631
C	-5.179585	-4.251930	0.229104	C	-2.940770	-1.217773	3.629719
H	-5.210357	-3.342426	0.841449	C	-3.357531	1.507566	4.047014
H	-6.127572	-4.329034	-0.318027	H	-1.922194	1.808520	2.464794
H	-5.092821	-5.114094	0.902358	C	-3.860976	-0.790240	4.582355
C	-4.010905	-5.522807	-1.566913	H	-2.768958	-2.282904	3.477713
H	-3.932275	-6.391639	-0.904683	C	-4.062022	0.570797	4.798297
H	-4.957123	-5.633443	-2.107140	H	-3.520284	2.571744	4.204984
H	-3.189131	-5.560680	-2.291604	H	-4.415524	-1.522332	5.164898
Cu	-1.048096	0.323435	-0.305015	H	-4.775935	0.902565	5.548833
C	-3.315111	2.185728	-2.411698	B	4.808941	-1.247445	-0.529570
C	-4.542757	2.770617	-2.747836	O	3.903270	-2.164887	-0.072334
C	-2.169906	2.519960	-3.140671	O	5.629640	-1.735322	-1.505864
C	-4.622255	3.675463	-3.799155	C	4.270902	-3.443367	-0.642657
H	-5.438419	2.513465	-2.182816	C	5.075532	-3.016265	-1.908465
C	-2.255348	3.428202	-4.193841	C	5.117568	-4.153779	0.403040
H	-1.207505	2.090737	-2.855822	H	4.537328	-4.228201	1.330112
C	-3.477349	4.004171	-4.523880	H	5.386273	-5.167501	0.085778
H	-5.578509	4.125865	-4.055264	H	6.038734	-3.600978	0.621952
H	-1.359816	3.690513	-4.753433	C	3.009672	-4.235039	-0.912644
H	-3.541036	4.715210	-5.344494	H	3.252939	-5.211959	-1.348457
C	-4.404139	1.514406	0.145913	H	2.480756	-4.404604	0.034141
C	-4.314111	2.833099	0.608236	H	2.328187	-3.709907	-1.587574
C	-5.394464	0.679697	0.667258	C	6.210070	-3.943840	-2.285020
C	-5.203708	3.311182	1.561694	H	5.824834	-4.944040	-2.519539
H	-3.547964	3.498235	0.206383	H	6.718488	-3.561206	-3.176556
C	-6.276845	1.156481	1.633985	H	6.948323	-4.032720	-1.482962
H	-5.486980	-0.346268	0.314673	C	4.193626	-2.742497	-3.116619
C	-6.184795	2.469544	2.082362	H	4.799756	-2.267879	-3.895659
H	-5.127527	4.341853	1.902875	H	3.773537	-3.668885	-3.524913
H	-7.041099	0.494931	2.035763	H	3.366412	-2.065386	-2.867713
H	-6.878047	2.839196	2.834510	O	-0.242294	-0.688349	-1.987538
C	0.571647	-0.855907	2.724795	C	0.701490	-1.657744	-1.694799
C	0.568533	-0.561340	4.090912	H	1.042003	-2.203905	-2.599772
C	1.770040	-1.243866	2.111492	H	1.620059	-1.234633	-1.227680
C	1.744358	-0.655215	4.831852	H	0.324682	-2.435658	-0.996863

H	0.344207	0.544010	-1.886108	B	-2.269785	-0.905643	-0.409023
				O	-3.293735	-1.013194	-1.308300
46				O	-2.520878	-1.517562	0.784806
C	1.386673	-0.938693	-0.488707	C	-4.436342	-1.514009	-0.566265
C	2.617671	-1.448310	0.215092	C	-3.754861	-2.262595	0.618629
C	2.367011	-1.814048	1.670296	C	-5.234166	-0.296171	-0.126027
H	3.255771	-2.293869	2.091563	H	-5.492858	0.295902	-1.011073
H	2.130980	-0.930550	2.276360	H	-6.164004	-0.584803	0.376608
H	1.531495	-2.519937	1.755968	H	-4.655460	0.342082	0.552846
C	3.707607	-0.382134	0.071141	C	-5.269856	-2.387564	-1.477650
H	3.831117	-0.174480	-1.002360	H	-6.094080	-2.848434	-0.919578
H	3.335672	0.548192	0.528277	H	-5.703583	-1.777606	-2.277391
C	5.067964	-0.746319	0.664151	H	-4.672740	-3.179922	-1.937411
H	4.963465	-0.882261	1.752026	C	-4.526487	-2.228506	1.919865
H	5.389282	-1.713581	0.259846	H	-5.503082	-2.713703	1.800035
C	6.075200	0.328035	0.403663	H	-3.972391	-2.773642	2.691674
H	5.797324	1.314244	0.790615	H	-4.685057	-1.205850	2.273353
C	7.241595	0.236152	-0.248551	C	-3.362439	-3.691476	0.276923
C	8.124036	1.435654	-0.423585	H	-2.710591	-4.078576	1.067279
H	7.692458	2.335509	0.027368	H	-4.241775	-4.341579	0.207998
H	9.112322	1.267217	0.027557	H	-2.815781	-3.743931	-0.671766
H	8.305607	1.639418	-1.488459	H	2.414710	-3.266770	-0.452718
C	7.791257	-1.020275	-0.852202				
H	7.133830	-1.885914	-0.735799	**47**			
H	7.979645	-0.879741	-1.925681	C	-0.978154	2.224881	-0.099672
H	8.762395	-1.270129	-0.402401	C	-0.367025	3.109919	0.963742
O	3.103118	-2.592505	-0.493431	C	-0.820491	2.773378	2.378444
C	0.217231	-0.613541	0.060306	H	-0.245960	3.370438	3.093957
H	0.067891	-0.734095	1.136234	H	-1.885587	2.992934	2.523185
C	-0.954039	-0.078722	-0.703548	H	-0.656587	1.716663	2.623547
C	-1.273228	1.376004	-0.399025	C	-0.718131	4.557867	0.601570
C	-0.554284	2.115470	0.544599	H	-0.316790	4.742969	-0.406020
C	-2.323354	2.004988	-1.084038	H	-1.811311	4.654798	0.531525
C	-0.871327	3.440883	0.805427	C	-0.151053	5.610622	1.559063
H	0.277179	1.653289	1.072698	H	-0.714269	5.594655	2.501801
C	-2.646892	3.327954	-0.838894	H	0.880178	5.332602	1.811664
H	-2.894322	1.434679	-1.815091	C	-0.196408	6.990069	0.971656
C	-1.920889	4.054756	0.114382	H	-1.087938	7.584277	1.186689
H	-0.305360	4.007870	1.540122	C	0.734830	7.531299	0.175133
H	-3.459616	3.807936	-1.377945	C	0.579829	8.910882	-0.387662
C	-2.250371	5.420042	0.376627	H	-0.351405	9.385812	-0.061178
N	-2.520524	6.532230	0.589602	H	1.417616	9.556117	-0.087136
H	1.522715	-0.815020	-1.568191	H	0.587990	8.891565	-1.486667
H	-0.754856	-0.148691	-1.784910	C	1.991117	6.824708	-0.237784

H	2.087315	5.824335	0.196655	C	1.612485	-3.107263	0.519427
H	2.027274	6.718397	-1.331510	C	0.728909	-2.757363	1.542482
H	2.878711	7.409876	0.041660	C	0.065930	-3.784835	2.210898
O	1.063738	3.047393	0.888221	C	0.274640	-5.108152	1.831347
C	-1.965257	1.314845	0.099467	H	1.295950	-6.459334	0.519499
H	-2.228718	1.072404	1.133163	H	-0.625529	-3.547719	3.017721
C	-2.817572	0.709695	-0.959581	H	-0.248688	-5.907277	2.350089
C	-4.265958	0.906631	-0.653761	O	2.284848	-2.062323	-0.060570
C	-4.812732	0.579878	0.597926	C	2.923045	-4.670062	-0.933787
C	-5.133875	1.392314	-1.641302	C	2.974750	-3.470144	-1.873032
C	-6.164198	0.736560	0.856261	C	2.686462	-2.205647	-1.361754
H	-4.167800	0.173169	1.374533	C	3.359201	-3.533644	-3.211991
C	-6.488423	1.551834	-1.401492	C	2.759279	-1.031016	-2.113446
H	-4.729163	1.644371	-2.620189	C	3.464859	-2.381954	-3.987544
C	-7.014960	1.225940	-0.144655	H	3.587944	-4.495896	-3.663543
H	-6.572873	0.476656	1.830260	C	3.169610	-1.137112	-3.443760
H	-7.147347	1.931321	-2.178596	H	3.775107	-2.458074	-5.026309
C	-8.408229	1.392760	0.115867	H	3.225943	-0.244764	-4.064075
N	-9.545412	1.529043	0.328707	P	0.551623	-0.967685	1.881397
H	-2.590059	1.200336	-1.918835	P	2.156400	0.537232	-1.363012
B	-2.480633	-0.914444	-1.231595	C	4.279597	-4.767530	-0.208341
O	-3.273432	-1.488503	-2.292727	H	4.497287	-3.857214	0.365165
O	-2.727665	-1.732083	-0.056708	H	4.275373	-5.615449	0.488108
C	-4.069019	-2.561488	-1.817632	H	5.087601	-4.915226	-0.935951
C	-3.471747	-2.891595	-0.394256	C	2.671410	-5.969385	-1.692279
C	-5.527237	-2.107964	-1.778297	H	3.475585	-6.166750	-2.408668
H	-5.790207	-1.715283	-2.768118	H	2.655801	-6.822758	-1.006618
H	-6.207011	-2.937868	-1.547130	H	1.718920	-5.940941	-2.234623
H	-5.690606	-1.308886	-1.050806	Cu	0.146143	0.168864	-0.152106
C	-3.977594	-3.713769	-2.810893	C	-0.652529	-0.911585	3.263649
H	-4.544290	-4.586668	-2.460532	C	-0.280233	-0.604591	4.575044
H	-4.406347	-3.397725	-3.769567	C	-2.004613	-1.134559	2.964520
H	-2.943068	-4.022655	-2.991808	C	-1.246163	-0.517256	5.574651
C	-4.519139	-3.120567	0.688744	H	0.764974	-0.425177	4.820230
H	-5.148027	-3.991444	0.461520	C	-2.960617	-1.062098	3.972798
H	-4.010272	-3.314274	1.642957	H	-2.303979	-1.374983	1.939528
H	-5.164454	-2.245026	0.820317	C	-2.585492	-0.746809	5.277275
C	-2.530298	-4.094376	-0.387453	H	-0.947278	-0.271727	6.591093
H	-2.074968	-4.175738	0.607408	H	-4.006780	-1.249582	3.733995
H	-3.057914	-5.033344	-0.597538	H	-3.337039	-0.678441	6.060329
H	-1.716825	-3.984187	-1.112141	C	2.148139	-0.576673	2.709457
H	1.299250	2.119331	0.741392	C	2.490060	0.764717	2.914967
C	1.147183	-5.417360	0.792330	C	3.014007	-1.572699	3.171412
C	1.848523	-4.417278	0.115455	C	3.667466	1.101284	3.574078

H	1.832649	1.565095	2.576888	H	-0.229361	4.689058	-0.283053
C	4.199313	-1.233540	3.817178	H	-1.698928	4.592350	0.688946
H	2.762708	-2.622834	3.028331	C	-0.032911	5.560357	1.678289
C	4.527239	0.103105	4.021674	H	-0.476971	5.430920	2.678060
H	3.915259	2.148661	3.729505	H	1.045024	5.395224	1.794319
H	4.864126	-2.019356	4.168591	C	-0.333622	6.940072	1.186315
H	5.451952	0.366603	4.530106	H	-1.400341	7.155636	1.062775
C	1.889084	1.589102	-2.833456	C	0.525679	7.913656	0.858088
C	0.606126	1.550628	-3.394635	C	0.036400	9.238762	0.354565
C	2.885278	2.355360	-3.445568	H	-1.056449	9.282885	0.300458
C	0.325510	2.276182	-4.548108	H	0.380738	10.058800	1.000846
H	-0.167273	0.937223	-2.925865	H	0.437732	9.450815	-0.646728
C	2.596957	3.086467	-4.594066	C	2.017820	7.810588	0.951092
H	3.890057	2.380400	-3.027265	H	2.368797	6.836019	1.300828
C	1.318276	3.048836	-5.144335	H	2.478354	8.004901	-0.027664
H	-0.672299	2.240331	-4.978986	H	2.415087	8.576514	1.632100
H	3.375507	3.683446	-5.063050	O	1.175164	2.985571	1.056795
H	1.095785	3.622550	-6.040948	C	-2.115163	1.609055	0.081379
C	3.650200	1.206126	-0.531372	H	-2.575820	1.577825	1.076556
C	3.772615	2.583862	-0.311825	C	-2.899402	1.067250	-0.964690
C	4.626067	0.347633	-0.014184	C	-4.342691	1.193363	-0.961969
C	4.853388	3.089706	0.402570	C	-5.077365	1.804421	0.081121
H	3.014145	3.266046	-0.690614	C	-5.087047	0.704697	-2.061305
C	5.704175	0.857648	0.700899	C	-6.456310	1.878101	0.053556
H	4.548079	-0.727459	-0.167991	H	-4.552006	2.244465	0.926073
C	5.820976	2.228272	0.911232	C	-6.462967	0.780841	-2.103557
H	4.936823	4.162865	0.559791	H	-4.548637	0.229902	-2.879079
H	6.453766	0.176988	1.098342	C	-7.173638	1.361075	-1.036992
H	6.664625	2.624338	1.471717	H	-6.994325	2.354076	0.870570
C	-0.482111	-1.953970	-2.298340	H	-7.008519	0.388888	-2.959369
H	-0.111219	-2.728002	-1.605779	C	-8.592931	1.441555	-1.071952
H	0.359741	-1.625074	-2.923280	N	-9.757615	1.505332	-1.099733
H	-1.240467	-2.408230	-2.948130	H	-2.459885	1.112093	-1.967408
O	-1.022958	-0.853210	-1.612286	B	-2.416774	-1.133423	-0.775634
H	-0.759225	2.543435	-1.125523	O	-3.388096	-1.751196	-1.565036
				O	-2.553208	-1.484393	0.569025
48-ts				C	-3.902263	-2.835191	-0.775299
C	-0.833908	2.141563	0.007781	C	-3.726020	-2.310046	0.683885
C	-0.263076	3.046538	1.086315	C	-5.334127	-3.113915	-1.182544
C	-0.734884	2.692155	2.491104	H	-5.358623	-3.483717	-2.214144
H	-0.153143	3.255412	3.228494	H	-5.777588	-3.883048	-0.537540
H	-1.795952	2.927291	2.644606	H	-5.950389	-2.210742	-1.129290
H	-0.591151	1.623192	2.692296	C	-3.026214	-4.050296	-1.069440
C	-0.602475	4.499878	0.735296	H	-3.392021	-4.954781	-0.568229

H	-3.032122	-4.230288	-2.151075	C	-1.568098	-0.810822	3.431670
H	-1.986311	-3.880471	-0.755705	C	-0.394117	-1.812749	5.749707
C	-4.886737	-1.448239	1.155428	H	1.374659	-2.091193	4.562315
H	-5.750449	-2.061465	1.439426	C	-2.301004	-0.874689	4.614282
H	-4.565064	-0.878711	2.037771	H	-2.030733	-0.446234	2.516304
H	-5.201930	-0.731619	0.394105	C	-1.716218	-1.374552	5.773330
C	-3.470338	-3.398060	1.709512	H	0.067491	-2.203706	6.653514
H	-3.328070	-2.945447	2.699561	H	-3.333589	-0.531775	4.627375
H	-4.331592	-4.076243	1.766768	H	-2.288611	-1.420817	6.696875
H	-2.578064	-3.984235	1.473013	C	2.417375	-0.961281	2.448711
H	1.404890	2.046477	0.991115	C	2.807151	0.320793	2.849043
C	0.630525	-5.457875	0.080485	C	3.326454	-2.015189	2.571358
C	1.379351	-4.456877	-0.541052	C	4.078989	0.543898	3.364487
C	1.385127	-3.204640	0.067087	H	2.108834	1.156181	2.770192
C	0.690794	-2.910507	1.243356	C	4.602256	-1.789618	3.080121
C	-0.020378	-3.944877	1.848583	H	3.036124	-3.021673	2.270994
C	-0.055410	-5.208760	1.265025	C	4.981183	-0.510338	3.474328
H	0.591820	-6.453557	-0.355299	H	4.370205	1.547900	3.664880
H	-0.564955	-3.755265	2.771704	H	5.301488	-2.618105	3.168705
H	-0.622533	-6.006340	1.739255	H	5.980447	-0.333601	3.866186
O	2.120780	-2.176778	-0.463782	C	2.030344	1.872051	-2.657029
C	2.267180	-4.678404	-1.758497	C	0.777303	2.050149	-3.254210
C	2.363396	-3.368895	-2.529377	C	3.113488	2.626841	-3.116349
C	2.325504	-2.171939	-1.816722	C	0.607545	2.964811	-4.287616
C	2.575945	-3.277213	-3.904675	H	-0.071457	1.458826	-2.910648
C	2.483884	-0.915910	-2.407138	C	2.941096	3.548145	-4.145248
C	2.763806	-2.045008	-4.524986	H	4.097670	2.493471	-2.670968
H	2.609016	-4.181316	-4.507271	C	1.690327	3.718633	-4.731546
C	2.723473	-0.870405	-3.782709	H	-0.372128	3.092422	-4.741716
H	2.940999	-2.002127	-5.596395	H	3.790553	4.131623	-4.492394
H	2.847479	0.091275	-4.276793	H	1.559092	4.440124	-5.534335
P	0.701659	-1.172262	1.822929	C	3.793096	0.906522	-0.586856
P	2.169049	0.570026	-1.373974	C	4.026755	2.164888	-0.015789
C	3.679224	-5.036557	-1.254044	C	4.792459	-0.067249	-0.517833
H	4.090736	-4.243025	-0.616821	C	5.245465	2.444161	0.591763
H	3.646834	-5.963059	-0.666962	H	3.256326	2.933818	-0.057270
H	4.360387	-5.182240	-2.101918	C	6.002953	0.210734	0.110122
C	1.748991	-5.814103	-2.634898	H	4.628808	-1.052087	-0.952677
H	2.409990	-5.977213	-3.492288	C	6.235214	1.467366	0.658730
H	1.729499	-6.757065	-2.079051	H	5.418359	3.429111	1.019702
H	0.738381	-5.607319	-3.007313	H	6.768091	-0.560290	0.166202
Cu	0.220670	0.254835	0.020678	H	7.185428	1.684673	1.141454
C	-0.240987	-1.249793	3.399637	C	-0.956052	-1.212357	-2.667839
C	0.340482	-1.749388	4.571161	H	-1.188098	-2.257320	-2.913119

H	0.079659	-1.005780	-2.952499	N	-5.216844	5.957858	-3.374506
H	-1.624395	-0.568225	-3.259266	H	0.374673	1.159267	-2.795437
O	-1.105218	-0.980916	-1.279623	H	2.674962	-0.121436	0.977510
H	-0.501114	2.439695	-0.994106	C	-5.416659	-0.110485	1.128902
				C	-4.481050	-1.030109	0.656330
49				C	-3.138641	-0.724627	0.863792
C	2.235975	1.296443	-0.769994	C	-2.698339	0.420745	1.527107
C	3.281099	1.574930	0.282453	C	-3.665220	1.304614	2.008713
C	2.891159	2.681459	1.255053	C	-5.015188	1.043060	1.797900
H	3.618330	2.721658	2.072563	H	-6.478254	-0.297215	0.986454
H	2.870447	3.665416	0.768418	H	-3.358664	2.203569	2.539471
H	1.904424	2.493732	1.698229	H	-5.763343	1.739970	2.166350
C	4.617532	1.883843	-0.401375	O	-2.161033	-1.586006	0.432895
H	4.845100	1.035807	-1.064831	C	-4.815120	-2.378641	0.033193
H	4.491555	2.764692	-1.048734	C	-3.732081	-2.703178	-0.986942
C	5.797192	2.091403	0.553512	C	-2.429200	-2.292177	-0.710336
H	5.689575	3.056441	1.067514	C	-3.925898	-3.451990	-2.146451
H	5.747754	1.321050	1.334049	C	-1.338407	-2.568329	-1.536191
C	7.118919	2.046368	-0.153389	C	-2.855827	-3.781195	-2.974684
H	7.518385	3.000772	-0.506092	H	-4.923634	-3.796492	-2.407332
C	7.825132	0.941115	-0.425963	C	-1.570647	-3.344934	-2.674717
C	9.130316	1.006298	-1.158855	H	-3.028567	-4.379370	-3.865479
H	9.408700	2.034693	-1.412946	H	-0.744250	-3.590183	-3.338603
H	9.941803	0.570758	-0.558292	P	-0.889366	0.646386	1.686811
H	9.092359	0.421978	-2.089325	P	0.273617	-1.793185	-1.129288
C	7.393154	-0.442593	-0.042416	C	-4.750959	-3.441242	1.148784
H	6.415157	-0.473155	0.448434	H	-3.765431	-3.456481	1.631254
H	7.339684	-1.084647	-0.933152	H	-5.505091	-3.229365	1.917126
H	8.129730	-0.910768	0.626093	H	-4.944960	-4.437895	0.732786
O	3.508003	0.366124	1.041088	C	-6.207612	-2.393520	-0.585811
C	1.167524	2.155230	-1.067917	H	-6.441186	-3.382468	-0.994054
H	0.997371	2.987531	-0.379756	H	-6.969595	-2.185399	0.172877
C	0.209386	1.965701	-2.079740	H	-6.304283	-1.652801	-1.388188
C	-0.902570	2.832879	-2.339295	Cu	0.323561	0.354734	-0.251955
C	-1.041624	4.122394	-1.765621	C	-0.744966	2.309741	2.429569
C	-1.922890	2.421386	-3.233615	C	-0.312167	2.543018	3.735683
C	-2.140998	4.914740	-2.022937	C	-1.007507	3.397220	1.588039
H	-0.252828	4.512436	-1.124370	C	-0.129403	3.849255	4.185423
C	-3.019391	3.210004	-3.501503	H	-0.106428	1.705938	4.400306
H	-1.836436	1.440474	-3.701581	C	-0.835508	4.697991	2.041702
C	-3.154702	4.471659	-2.890466	H	-1.349486	3.221922	0.566427
H	-2.221311	5.899872	-1.567270	C	-0.385638	4.925175	3.341746
H	-3.791342	2.861697	-4.184255	H	0.214828	4.024501	5.201965
C	-4.286266	5.287724	-3.156837	H	-1.048750	5.534226	1.378204

H	-0.238161	5.942015	3.697515	H	-6.019059	0.195544	-0.995252
C	-0.438513	-0.503437	3.040925	H	-5.420790	-1.452339	-1.174704
C	0.919736	-0.689070	3.323392	C	-7.230650	-1.275130	0.015835
C	-1.392341	-1.201075	3.785812	H	-7.122370	-2.307488	0.376930
C	1.315429	-1.554186	4.336607	H	-7.545433	-0.680097	0.882919
H	1.675998	-0.142920	2.757702	C	-8.268670	-1.227927	-1.065606
C	-0.992750	-2.075758	4.792467	H	-8.390430	-2.131017	-1.669216
H	-2.452908	-1.064328	3.578791	C	-9.022207	-0.165615	-1.379196
C	0.359296	-2.253459	5.068902	C	-10.019493	-0.212837	-2.496140
H	2.374281	-1.691422	4.544148	H	-10.044214	-1.192934	-2.984428
H	-1.742993	-2.617430	5.363776	H	-11.031840	0.012744	-2.131130
H	0.669417	-2.938711	5.854382	H	-9.795314	0.545182	-3.260190
C	1.243577	-2.138673	-2.645607	C	-8.942012	1.151113	-0.666355
C	0.940820	-1.386437	-3.787984	H	-8.171405	1.177611	0.110727
C	2.239666	-3.114558	-2.722759	H	-8.723366	1.957587	-1.380627
C	1.622502	-1.601187	-4.979367	H	-9.907016	1.406303	-0.205703
H	0.141516	-0.645699	-3.751066	O	-5.468599	0.526745	1.476316
C	2.927708	-3.323506	-3.915623	C	-2.619857	-0.767987	-0.551384
H	2.482707	-3.718198	-1.850789	H	-2.642899	-1.823964	-0.262032
C	2.623558	-2.567982	-5.042817	C	-1.602854	-0.392610	-1.403420
H	1.371890	-1.012890	-5.858655	C	-0.675362	-1.319605	-2.040645
H	3.701706	-4.085811	-3.962807	C	-0.433486	-2.626604	-1.568243
H	3.162100	-2.733882	-5.972653	C	0.008531	-0.912208	-3.201805
C	1.009224	-2.871305	0.155173	C	0.443085	-3.473857	-2.215826
C	2.337481	-2.623233	0.526929	H	-0.924075	-2.979885	-0.662108
C	0.281562	-3.841064	0.846175	C	0.887366	-1.751938	-3.859692
C	2.925760	-3.330342	1.567380	H	-0.161771	0.092072	-3.588003
H	2.922506	-1.874399	-0.008199	C	1.117724	-3.045740	-3.369717
C	0.872705	-4.547498	1.891573	H	0.631583	-4.470565	-1.823184
H	-0.750189	-4.053756	0.569564	H	1.405021	-1.413586	-4.755098
C	2.190671	-4.293454	2.255398	C	2.041466	-3.909038	-4.025195
H	3.957885	-3.122816	1.841955	N	2.809401	-4.606144	-4.558639
H	0.296163	-5.301074	2.423101	H	-1.648470	0.603159	-1.854548
H	2.645265	-4.842639	3.076633	H	-4.845831	0.718960	2.188310
H	2.562925	0.601092	-1.552739	C	4.030467	-3.263142	-1.231310
				C	3.822208	-1.887066	-1.305453
50-ts				C	2.942213	-1.328088	-0.380906
C	-3.566043	0.087697	0.096906	C	2.261844	-2.066644	0.590015
C	-4.859858	-0.481894	0.658673	C	2.506591	-3.441249	0.637071
C	-4.611279	-1.722063	1.513043	C	3.384817	-4.031165	-0.265992
H	-5.521563	-1.993103	2.058503	H	4.705692	-3.748083	-1.932019
H	-4.309787	-2.590724	0.912021	H	1.990238	-4.057531	1.369650
H	-3.819539	-1.524072	2.249938	H	3.563987	-5.102512	-0.222300
C	-5.870855	-0.751810	-0.454562	O	2.698988	0.023324	-0.401474

C	4.530375	-0.943911	-2.269111	C	-1.545050	3.488426	-1.005630
C	3.545479	0.158311	-2.636164	C	0.447446	4.826208	-1.254860
C	2.700958	0.626764	-1.633498	C	-2.322846	4.564221	-1.425043
C	3.467870	0.792184	-3.875930	H	-2.018269	2.550251	-0.715279
C	1.834204	1.709285	-1.792344	C	-0.328840	5.899907	-1.674360
C	2.595227	1.857722	-4.081505	H	1.528973	4.936092	-1.175706
H	4.097805	0.456720	-4.696419	C	-1.714147	5.768340	-1.762101
C	1.792454	2.325078	-3.044456	H	-3.403948	4.461901	-1.479770
H	2.550630	2.337501	-5.055889	H	0.146156	6.844535	-1.928553
H	1.124238	3.167468	-3.210331	H	-2.319172	6.612069	-2.085444
P	0.985715	-1.192950	1.578198	C	2.029738	2.927631	0.788054
P	0.806095	2.158677	-0.344870	C	1.629308	3.170829	2.105483
C	5.710483	-0.292344	-1.520645	C	3.323612	3.279885	0.394197
H	5.372515	0.246799	-0.626794	C	2.497291	3.780372	3.004134
H	6.427553	-1.061235	-1.206641	H	0.637737	2.862439	2.437884
H	6.225863	0.420131	-2.176980	C	4.198033	3.870498	1.301975
C	5.067024	-1.671119	-3.495407	H	3.654001	3.089881	-0.626638
H	5.581949	-0.973279	-4.164644	C	3.784518	4.128769	2.605209
H	5.807826	-2.423677	-3.204194	H	2.174451	3.960139	4.027165
H	4.270026	-2.173730	-4.057130	H	5.204837	4.134397	0.986000
Cu	-0.370983	0.357877	0.499354	H	4.468566	4.591230	3.313046
C	0.197813	-2.526660	2.556144	H	-3.751081	1.031954	-0.438821
C	0.877613	-3.229003	3.558441	O	-1.833774	0.833990	1.872393
C	-1.144406	-2.820042	2.310603	C	-2.074027	2.142827	2.289432
C	0.227074	-4.223290	4.279483	H	-1.467866	2.893661	1.749580
H	1.918984	-2.990929	3.775327	H	-3.131373	2.428954	2.122630
C	-1.798804	-3.812695	3.035281	H	-1.868748	2.273201	3.365503
H	-1.682624	-2.243670	1.559026	H	-2.780295	0.470257	1.094136
C	-1.110452	-4.517374	4.016861				
H	0.761429	-4.767237	5.054825	**51-ts**			
H	-2.847468	-4.024723	2.836452	C	-0.344318	2.563172	0.004542
H	-1.617062	-5.292535	4.586907	C	0.469503	2.960858	1.213890
C	1.923707	-0.307544	2.882807	C	-0.321960	2.957553	2.513847
C	1.164253	0.311040	3.883990	H	0.354046	3.162180	3.351110
C	3.315299	-0.223092	2.925580	H	-1.108443	3.722032	2.512966
C	1.792172	0.976312	4.929001	H	-0.790683	1.979003	2.692546
H	0.074550	0.268152	3.833331	C	1.083450	4.333675	0.917518
C	3.941056	0.466611	3.962281	H	1.553414	4.263651	-0.074954
H	3.916371	-0.706426	2.156104	H	0.274883	5.073424	0.826928
C	3.183220	1.057657	4.967511	C	2.142528	4.805181	1.920235
H	1.195641	1.445329	5.708626	H	1.659693	5.185206	2.830059
H	5.026337	0.534100	3.986035	H	2.734087	3.932234	2.227855
H	3.675697	1.588152	5.779511	C	3.038405	5.862302	1.338067
C	-0.155162	3.606447	-0.925485	H	2.861826	6.893822	1.651223

C	4.002614	5.641938	0.433706	C	2.174579	-1.764485	-3.489652
C	4.822497	6.762251	-0.128986	H	2.164511	-2.811739	-5.365989
H	4.528180	7.733945	0.281884	H	2.796631	-0.950687	-3.857455
H	5.891940	6.612239	0.076769	P	-0.805813	-1.159217	1.585965
H	4.726074	6.810258	-1.223107	P	1.922157	-0.316081	-1.040847
C	4.332385	4.283729	-0.111701	C	0.733107	-5.943773	-1.230042
H	3.801967	3.475960	0.404337	H	1.310340	-5.411493	-0.464189
H	4.070660	4.217941	-1.180120	H	0.193017	-6.764619	-0.741500
H	5.412016	4.086486	-0.049915	H	1.437817	-6.370206	-1.955147
O	1.594098	2.075474	1.355527	C	-1.026495	-5.800261	-2.991826
C	-1.695520	2.423811	-0.046964	H	-0.340360	-6.245363	-3.720233
H	-2.233788	2.395826	0.904901	H	-1.565517	-6.633896	-2.529391
C	-2.466322	2.207865	-1.266412	H	-1.748238	-5.173390	-3.528894
C	-3.912775	2.462033	-1.292923	Cu	-0.212270	0.164243	-0.241097
C	-4.709872	2.572197	-0.138252	C	-2.176169	-0.582164	2.653866
C	-4.569638	2.548955	-2.537132	C	-2.143600	-0.643112	4.048392
C	-6.080179	2.748371	-0.216263	C	-3.286755	-0.010553	2.018500
H	-4.252487	2.523061	0.847715	C	-3.206113	-0.139865	4.796357
C	-5.935391	2.727973	-2.630081	H	-1.286489	-1.083235	4.555213
H	-3.975667	2.469274	-3.447145	C	-4.353760	0.470959	2.767393
C	-6.712385	2.827918	-1.464409	H	-3.318855	0.042318	0.928351
H	-6.672877	2.833200	0.692397	C	-4.311551	0.413130	4.159317
H	-6.416523	2.794874	-3.603093	H	-3.169493	-0.187687	5.882075
C	-8.121941	3.015013	-1.548546	H	-5.220001	0.894521	2.262194
N	-9.275402	3.169224	-1.616694	H	-5.141981	0.799173	4.745429
H	-1.962233	2.609846	-2.157520	C	0.450373	-1.759935	2.776510
H	1.270697	1.184798	1.142845	C	1.372415	-0.846538	3.299512
C	-2.434100	-4.930041	-0.542451	C	0.492041	-3.091355	3.201139
C	-1.187354	-4.409025	-0.890088	C	2.313515	-1.259427	4.236454
C	-0.738885	-3.308952	-0.164141	H	1.364043	0.196555	2.979797
C	-1.474777	-2.703077	0.857050	C	1.443929	-3.504258	4.128415
C	-2.707151	-3.266982	1.188506	H	-0.225654	-3.808535	2.805151
C	-3.181183	-4.373663	0.491209	C	2.354608	-2.588808	4.647347
H	-2.830525	-5.788545	-1.078217	H	3.025298	-0.541121	4.636998
H	-3.305943	-2.827287	1.983473	H	1.470460	-4.543385	4.448107
H	-4.144207	-4.804630	0.752466	H	3.098636	-2.911945	5.371813
O	0.488466	-2.757534	-0.440166	C	2.762263	0.927496	-2.085327
C	-0.259970	-5.003917	-1.942341	C	1.952482	1.815450	-2.801617
C	0.539380	-3.865703	-2.564352	C	4.151159	1.002985	-2.227701
C	0.911062	-2.802170	-1.745265	C	2.519267	2.771958	-3.637683
C	0.998267	-3.838518	-3.881005	H	0.867680	1.744731	-2.706122
C	1.713725	-1.741729	-2.172128	C	4.717413	1.962089	-3.061250
C	1.811717	-2.804600	-4.337981	H	4.791323	0.311919	-1.682148
H	0.727872	-4.639626	-4.564480	C	3.904033	2.848268	-3.763697

H	1.880347	3.457236	-4.189141	C	-0.674623	1.497655	-3.124094
H	5.798562	2.016627	-3.164242	C	0.370730	-1.069755	-3.345956
H	4.350266	3.597689	-4.413001	H	-1.148549	-1.667016	-1.966170
C	3.218157	-0.858585	0.144390	C	0.390532	1.268469	-3.973652
C	3.882337	0.103386	0.917264	H	-1.088875	2.501542	-3.032362
C	3.516631	-2.209809	0.343868	C	0.923831	-0.026911	-4.097184
C	4.830517	-0.281514	1.857909	H	0.760475	-2.081502	-3.448985
H	3.654220	1.159934	0.787479	H	0.824703	2.085694	-4.545915
C	4.457001	-2.591197	1.296590	C	2.035618	-0.285940	-4.952026
H	3.015101	-2.975513	-0.244319	N	2.960153	-0.506532	-5.626873
C	5.117652	-1.629725	2.053443	H	-5.078838	0.836879	-1.509140
H	5.343262	0.477943	2.443975	H	-2.949263	1.621849	-1.892719
H	4.674709	-3.646784	1.442605	B	-1.922828	1.281989	0.052568
H	5.854379	-1.930127	2.795032	O	-1.266598	2.572578	-0.053640
H	0.195054	2.682924	-0.940721	O	-3.045141	1.492170	0.958272
O	-1.696079	-0.244540	-1.563042	C	-1.875446	3.519494	0.809554
H	-2.249091	0.954483	-1.448303	C	-3.275243	2.884188	1.116559
C	-1.481930	-0.472462	-2.921027	C	-0.994173	3.686799	2.044741
H	-1.852812	-1.464463	-3.233722	H	0.022373	3.926279	1.704216
H	-2.012098	0.278743	-3.540105	H	-1.337984	4.502164	2.694086
H	-0.415949	-0.431017	-3.211149	H	-0.935778	2.769064	2.639382
				C	-1.947396	4.862284	0.095357
52				H	-2.539995	5.589272	0.666161
C	-4.695633	-0.112063	-1.117596	H	-0.936412	5.274129	-0.018154
C	-5.667957	-0.807772	-0.204713	H	-2.382830	4.760318	-0.905668
C	-5.204020	-2.187393	0.238369	C	-3.781646	3.135866	2.527697
H	-5.898994	-2.605479	0.973800	H	-3.898652	4.210272	2.721196
H	-5.134055	-2.878321	-0.612727	H	-4.764263	2.663871	2.655708
H	-4.221505	-2.120930	0.722886	H	-3.105496	2.717392	3.280352
C	-7.057272	-0.847810	-0.838410	C	-4.361965	3.313120	0.131426
H	-7.304476	0.177815	-1.152883	H	-5.237507	2.670760	0.286924
H	-7.004570	-1.453058	-1.757347	H	-4.665281	4.356533	0.280754
C	-8.176133	-1.368148	0.061864	H	-4.038740	3.193188	-0.908872
H	-7.977271	-2.421604	0.316176	H	-4.878767	0.431702	1.075744
H	-8.156946	-0.813301	1.007537	C	2.872545	2.428156	4.047968
C	-9.507891	-1.273845	-0.612175	C	2.901302	1.102379	3.616547
H	-9.553724	-1.754502	-1.595537	C	2.810334	0.880491	2.243136
C	-10.623682	-0.674061	-0.177368	C	2.716689	1.905754	1.297356
O	-5.765594	0.044659	0.951411	C	2.716519	3.219516	1.771907
C	-3.380288	-0.333122	-1.181313	C	2.784866	3.475957	3.137049
H	-2.972154	-1.250697	-0.750202	H	2.929642	2.652495	5.110020
C	-2.415230	0.749828	-1.489127	H	2.639233	4.046854	1.068938
C	-1.260471	0.460842	-2.367483	H	2.770924	4.502474	3.493892
C	-0.695083	-0.825124	-2.485886	O	2.810161	-0.403318	1.752878

C	3.110953	-0.098896	4.530487	C	-1.072382	-3.385698	-0.046015
C	2.347058	-1.275171	3.939080	C	0.662113	-4.854936	-0.868165
C	2.272254	-1.379179	2.552718	C	-2.027064	-4.358090	-0.319281
C	1.761893	-2.301396	4.680849	H	-1.371592	-2.419610	0.370659
C	1.634879	-2.430229	1.891023	C	-0.299957	-5.823104	-1.149103
C	1.145100	-3.381558	4.055047	H	1.711316	-5.055156	-1.079787
H	1.790048	-2.266277	5.766989	C	-1.640926	-5.577406	-0.873928
C	1.081620	-3.450048	2.667378	H	-3.075851	-4.161026	-0.106448
H	0.707054	-4.174050	4.656015	H	0.003026	-6.773588	-1.581838
H	0.580043	-4.286170	2.183368	H	-2.389285	-6.335072	-1.093126
P	2.445304	1.477869	-0.470383	C	3.062674	-2.892554	-0.566981
P	1.461774	-2.291676	0.074214	C	3.413877	-2.558272	-1.877299
C	4.612391	-0.446578	4.519693	C	3.923772	-3.690167	0.191639
H	4.965726	-0.667792	3.505418	C	4.598576	-3.029525	-2.431072
H	5.197359	0.395348	4.910622	H	2.765934	-1.904688	-2.460615
H	4.802021	-1.326404	5.147280	C	5.117516	-4.147499	-0.358565
C	2.683596	0.193062	5.964418	H	3.658265	-3.957026	1.213780
H	2.874753	-0.671634	6.608518	C	5.452782	-3.822174	-1.670138
H	3.265349	1.021308	6.382027	H	4.864398	-2.751195	-3.448684
H	1.619077	0.447255	6.027856	H	5.785436	-4.763633	0.238878
Cu	0.766322	-0.146900	-0.531186	H	6.386446	-4.181130	-2.097071
C	2.445028	3.134511	-1.259890	C	-0.751844	0.185025	1.947128
C	1.224933	3.780136	-1.474896	H	-0.464914	-0.830046	2.254598
C	3.638355	3.790152	-1.586004	H	-1.635274	0.487051	2.522168
C	1.200429	5.058288	-2.028882	H	0.081208	0.866437	2.199553
H	0.295544	3.289862	-1.181806	O	-1.036088	0.189931	0.563577
C	3.607531	5.067210	-2.135049	C	-10.763118	0.033885	1.135847
H	4.595834	3.301568	-1.411048	H	-9.846788	0.035554	1.731982
C	2.387957	5.701189	-2.363042	H	-11.068515	1.078083	0.979902
H	0.243787	5.549888	-2.199673	H	-11.556980	-0.428882	1.739013
H	4.539233	5.568923	-2.385952	C	-11.872787	-0.672584	-1.007235
H	2.366350	6.697764	-2.798135	H	-12.703345	-1.154919	-0.472089
C	4.056581	0.811976	-1.051955	H	-12.202894	0.354106	-1.220785
C	4.222642	0.678792	-2.435472	H	-11.735278	-1.191598	-1.961787
C	5.104865	0.446705	-0.206623				
C	5.413719	0.202346	-2.965806	**53-ts**			
H	3.417689	0.972302	-3.109498	C	-4.437699	-0.357691	-1.650234
C	6.294225	-0.047800	-0.738332	C	-5.222941	-1.249855	-0.733927
H	5.003091	0.550565	0.871874	C	-4.710694	-2.681146	-0.683423
C	6.453526	-0.165824	-2.115045	H	-5.255216	-3.253792	0.075388
H	5.518243	0.107576	-4.044733	H	-4.834163	-3.178477	-1.654105
H	7.102510	-0.334090	-0.069261	H	-3.649483	-2.706810	-0.405922
H	7.385112	-0.549393	-2.525055	C	-6.703427	-1.201787	-1.121858
C	0.281595	-3.631697	-0.314413	H	-6.994904	-0.139672	-1.143861

H	-6.821798	-1.577250	-2.150206	H	-1.089053	5.309688	-0.585456
C	-7.639164	-1.946902	-0.167634	H	-2.446925	4.718201	-1.560573
H	-7.527904	-3.031039	-0.307641	C	-4.135058	3.217038	1.769187
H	-7.313069	-1.734018	0.859232	H	-4.345804	4.290021	1.860083
C	-9.077938	-1.565716	-0.354531	H	-5.090368	2.680047	1.820369
H	-9.672724	-2.198695	-1.018181	H	-3.526076	2.904309	2.622237
C	-9.680815	-0.498734	0.186455	C	-4.438319	3.171167	-0.685183
C	-11.122617	-0.192253	-0.082810	H	-5.292610	2.491526	-0.569836
H	-11.581740	-0.929088	-0.750600	H	-4.813187	4.200775	-0.657318
H	-11.702753	-0.168917	0.850937	H	-3.992192	2.988329	-1.667727
H	-11.238443	0.801467	-0.538787	H	-4.554740	0.081478	0.544378
C	-8.991275	0.480925	1.088473	C	1.423419	2.113342	4.463231
H	-7.934001	0.250661	1.253703	C	1.532162	0.823829	3.938831
H	-9.050055	1.493978	0.664809	C	1.869303	0.721879	2.590680
H	-9.490930	0.531205	2.066462	C	2.075960	1.827221	1.756392
O	-5.115859	-0.709615	0.606824	C	1.981370	3.094422	2.331620
C	-3.110528	-0.422847	-1.879210	C	1.656563	3.235403	3.676490
H	-2.574765	-1.329011	-1.578353	H	1.173738	2.248675	5.512724
C	-2.315192	0.683603	-2.341339	H	2.147604	3.977433	1.717896
C	-1.006371	0.594349	-2.859242	H	1.578715	4.227588	4.113508
C	-0.197315	-0.585228	-2.760625	O	2.056068	-0.502910	2.005756
C	-0.383752	1.717473	-3.490894	C	1.431172	-0.440254	4.785254
C	1.075890	-0.644345	-3.318345	C	1.056789	-1.612893	3.888232
H	-0.644893	-1.511324	-2.403687	C	1.430777	-1.592148	2.547834
C	0.881120	1.661510	-4.019110	C	0.419137	-2.769323	4.341945
H	-0.953535	2.645166	-3.559069	C	1.179396	-2.642220	1.659316
C	1.648266	0.471632	-3.952464	C	0.180503	-3.847213	3.494917
H	1.620810	-1.588710	-3.295253	H	0.108015	-2.839501	5.381364
H	1.311208	2.543895	-4.490075	C	0.559267	-3.788312	2.157783
C	2.966400	0.389506	-4.462732	H	-0.306724	-4.738560	3.881088
N	4.066037	0.298725	-4.850728	H	0.350310	-4.623734	1.492460
H	-4.951996	0.569088	-1.927024	P	2.355483	1.549092	-0.040568
H	-2.869804	1.579127	-2.632976	P	1.526133	-2.318803	-0.107742
B	-1.878138	1.367005	-0.191112	C	2.824838	-0.722257	5.377255
O	-1.325591	2.608305	-0.497428	H	3.570993	-0.848671	4.582744
O	-3.115531	1.511869	0.442324	H	3.142303	0.110624	6.017153
C	-2.063084	3.588216	0.251094	H	2.805706	-1.639611	5.979120
C	-3.456733	2.907665	0.447587	C	0.423480	-0.270368	5.920088
C	-1.312447	3.795305	1.559648	H	0.390512	-1.163529	6.552190
H	-0.285297	4.097022	1.321467	H	0.706136	0.557090	6.578382
H	-1.767888	4.574229	2.182671	H	-0.584584	-0.079497	5.532954
H	-1.253874	2.865280	2.143208	Cu	0.904823	-0.146533	-0.776772
C	-2.097709	4.882650	-0.535395	C	2.471106	3.261788	-0.691547
H	-2.752873	5.618753	-0.052584	C	1.385286	3.807674	-1.376995

C	3.619889	4.040657	-0.495657	H	-2.627889	-0.789840	1.089724
C	1.450390	5.109263	-1.871654	H	-1.457245	-0.042511	2.211321
H	0.484924	3.214431	-1.515040	O	-1.069558	0.281747	0.192111
C	3.677821	5.340850	-0.982379				
H	4.473600	3.626345	0.039659	**54**			
C	2.593537	5.876156	-1.676417	C	-2.692994	1.546326	-1.914042
H	0.600917	5.517413	-2.417574	C	-3.532470	0.602641	-1.095545
H	4.573313	5.937066	-0.823843	C	-2.870402	-0.751455	-0.874904
H	2.644783	6.890558	-2.065309	H	-3.446940	-1.345173	-0.156105
C	4.115461	1.034464	-0.153452	H	-2.775744	-1.325616	-1.806494
C	4.690371	1.033682	-1.429328	H	-1.863485	-0.623588	-0.453598
C	4.896272	0.674074	0.944945	C	-4.915882	0.455527	-1.734891
C	6.024953	0.692546	-1.601887	H	-5.323894	1.466655	-1.883747
H	4.093816	1.314094	-2.297947	H	-4.784345	0.022505	-2.738408
C	6.231144	0.313914	0.767782	C	-5.928684	-0.370939	-0.941317
H	4.474649	0.689873	1.948292	H	-5.545801	-1.397136	-0.823495
C	6.797947	0.326778	-0.502188	H	-6.013295	0.044848	0.069822
H	6.456134	0.702902	-2.600697	C	-7.251875	-0.422051	-1.635949
H	6.831270	0.036369	1.631424	H	-7.220368	-0.853234	-2.642336
H	7.842245	0.053580	-0.635845	C	-8.441032	0.010895	-1.196680
C	0.687848	-3.706626	-0.963329	C	-9.669725	-0.105371	-2.048127
C	-0.713679	-3.703127	-1.013382	H	-9.458810	-0.567695	-3.018301
C	1.385482	-4.721655	-1.621713	H	-10.443525	-0.702983	-1.545272
C	-1.400732	-4.696972	-1.698012	H	-10.117688	0.882158	-2.229357
H	-1.274832	-2.917533	-0.502707	C	-8.684459	0.636676	0.142998
C	0.694730	-5.713660	-2.314532	H	-7.781189	0.734257	0.751012
H	2.473691	-4.740612	-1.595427	H	-9.122621	1.637741	0.025474
C	-0.695143	-5.703807	-2.354382	H	-9.416115	0.049438	0.715702
H	-2.488224	-4.681570	-1.725217	O	-3.775626	1.210736	0.187432
H	1.248997	-6.498338	-2.823857	C	-1.448942	1.311721	-2.394755
H	-1.230685	-6.478703	-2.897195	H	-1.050119	0.300785	-2.252958
C	3.297144	-2.715148	-0.307844	C	-0.530167	2.267796	-2.928583
C	3.966131	-2.204724	-1.423181	C	0.830956	2.019507	-3.010936
C	3.970730	-3.573512	0.565770	C	1.404140	0.680578	-3.003470
C	5.281489	-2.572443	-1.682120	C	1.795567	3.093167	-3.002259
H	3.460066	-1.505435	-2.088973	C	2.777758	0.476064	-2.860941
C	5.293707	-3.924228	0.315624	H	0.799070	-0.165248	-3.333751
H	3.454690	-3.977055	1.436083	C	3.128318	2.875312	-2.816994
C	5.945421	-3.433597	-0.813076	H	1.420287	4.114652	-3.069014
H	5.788684	-2.167896	-2.555496	C	3.662572	1.551797	-2.693962
H	5.814332	-4.590663	0.999258	H	3.165743	-0.544013	-2.895936
H	6.976954	-3.715666	-1.010838	H	3.810390	3.721011	-2.742742
C	-1.569794	-0.542864	1.237148	C	5.013598	1.327794	-2.350878
H	-0.989249	-1.469442	1.258603	N	6.120730	1.134773	-2.020621

H	-3.135046	2.541447	-2.039178	H	0.359962	7.266043	-0.644575
H	-0.853911	3.310036	-2.970425	C	2.501722	1.598449	1.692517
H	-2.910023	1.424633	0.562849	C	3.690252	1.773317	0.971000
C	-2.671212	0.966615	3.545097	C	2.563398	1.238270	3.039080
C	-1.959456	-0.114372	3.025539	C	4.921330	1.621340	1.595368
C	-0.827753	0.177080	2.263891	H	3.652649	2.030110	-0.090080
C	-0.420685	1.485095	1.965431	C	3.800132	1.061965	3.656202
C	-1.148974	2.535879	2.532323	H	1.646694	1.093255	3.609028
C	-2.264550	2.276911	3.319081	C	4.976897	1.260167	2.940205
H	-3.558348	0.786491	4.146858	H	5.832552	1.757094	1.015940
H	-0.853990	3.563188	2.333554	H	3.841326	0.775262	4.704301
H	-2.827171	3.100875	3.749056	H	5.939533	1.122954	3.427358
O	-0.047064	-0.832222	1.764972	C	1.522499	-3.142644	-1.886728
C	-2.316165	-1.566227	3.318702	C	0.605328	-3.020268	-2.938296
C	-1.786066	-2.439160	2.189271	C	2.553280	-4.080120	-1.980045
C	-0.654209	-2.032065	1.489531	C	0.709863	-3.832561	-4.060438
C	-2.328884	-3.677598	1.841927	H	-0.207007	-2.294695	-2.866387
C	-0.072986	-2.784901	0.464761	C	2.662005	-4.885199	-3.111358
C	-1.763214	-4.463500	0.843007	H	3.272472	-4.183483	-1.168869
H	-3.208420	-4.045175	2.363990	C	1.742735	-4.763928	-4.148487
C	-0.639180	-4.021555	0.153991	H	-0.010714	-3.735351	-4.868600
H	-2.203564	-5.427027	0.600899	H	3.467672	-5.612134	-3.179692
H	-0.206303	-4.630070	-0.637754	H	1.830415	-5.395041	-5.029391
P	0.938082	1.763018	0.763099	C	2.786870	-2.325999	0.576403
P	1.311891	-2.031372	-0.453731	C	3.938656	-1.591642	0.276188
C	-1.606871	-1.983333	4.620085	C	2.818087	-3.266371	1.609311
H	-0.519275	-1.875835	4.528672	C	5.111421	-1.801090	0.991842
H	-1.944690	-1.357584	5.455672	H	3.916493	-0.848521	-0.522627
H	-1.829851	-3.031754	4.854898	C	3.990032	-3.463794	2.333625
C	-3.825781	-1.733220	3.486060	H	1.928232	-3.848178	1.846308
H	-4.085117	-2.772980	3.708910	C	5.135323	-2.734314	2.024987
H	-4.193850	-1.141296	4.330024	H	5.998946	-1.220420	0.749235
H	-4.363772	-1.421216	2.581419	H	4.009468	-4.192958	3.140081
Cu	1.131605	0.218368	-0.921247	H	6.049345	-2.893547	2.592133
C	0.785659	3.546767	0.384330				
C	-0.375958	3.970844	-0.272730	**55-ts**			
C	1.786650	4.476775	0.673020	C	-4.974784	0.614036	0.652408
C	-0.531196	5.304619	-0.630484	C	-6.049768	-0.431237	0.778963
H	-1.168515	3.255217	-0.494873	C	-5.649646	-1.772154	0.178345
C	1.633702	5.809302	0.298885	H	-6.411659	-2.526193	0.399301
H	2.692319	4.165165	1.189343	H	-5.524127	-1.713563	-0.910473
C	0.477534	6.224666	-0.354139	H	-4.701263	-2.112945	0.615701
H	-1.439597	5.621355	-1.139019	C	-7.344336	0.107022	0.163914
H	2.420744	6.524784	0.524886	H	-7.550875	1.083305	0.628171

H	-7.159376	0.303205	-0.903104	C	3.959639	-2.053074	3.578255
C	-8.577722	-0.782536	0.326752	C	3.061148	-2.842454	2.636120
H	-8.407239	-1.740455	-0.188653	C	2.618654	-2.215234	1.473687
H	-8.707354	-1.021272	1.388858	C	2.692149	-4.175307	2.816915
C	-9.794359	-0.130655	-0.249044	C	1.812948	-2.842235	0.519491
H	-9.758124	0.028251	-1.331899	C	1.918297	-4.842229	1.871169
C	-10.884065	0.308428	0.394418	H	3.014418	-4.709246	3.707170
C	-12.005219	0.972814	-0.347304	C	1.476120	-4.181034	0.730761
H	-11.810988	1.032534	-1.423432	H	1.652259	-5.883944	2.030424
H	-12.951495	0.433038	-0.199369	H	0.851647	-4.698605	0.004170
H	-12.174382	1.992574	0.027123	P	2.048837	1.778468	0.504124
C	-11.109851	0.199865	1.871845	P	1.181958	-1.822652	-0.866570
H	-10.285739	-0.280005	2.406233	C	5.402799	-2.120798	3.041624
H	-11.261331	1.196108	2.310605	H	5.471603	-1.724307	2.021543
H	-12.027029	-0.368160	2.082260	H	6.070709	-1.532936	3.683642
O	-6.341924	-0.614620	2.172982	H	5.752787	-3.160617	3.029643
C	-3.838233	0.534372	-0.053668	C	3.934623	-2.617958	4.994176
H	-3.645175	-0.378582	-0.626903	H	4.288744	-3.654151	5.004355
C	-2.766481	1.539475	-0.057905	H	4.609934	-2.055858	5.647800
C	-1.919493	1.702586	-1.232185	H	2.927348	-2.590062	5.426262
C	-1.448022	0.587855	-1.967149	Cu	0.488780	0.182665	-0.044614
C	-1.420696	2.970601	-1.610857	C	1.520166	3.499255	0.812986
C	-0.543807	0.730180	-3.006622	C	0.178467	3.712325	1.140611
H	-1.817872	-0.409023	-1.731872	C	2.400309	4.585221	0.773979
C	-0.505906	3.120793	-2.633225	C	-0.279253	4.993955	1.429026
H	-1.769994	3.850954	-1.073364	H	-0.509125	2.865820	1.155922
C	-0.049365	1.997967	-3.348785	C	1.940100	5.866620	1.057720
H	-0.208569	-0.145587	-3.561637	H	3.448014	4.425178	0.522405
H	-0.134632	4.109760	-2.895877	C	0.601082	6.071368	1.384504
C	0.937585	2.129872	-4.364724	H	-1.327365	5.150604	1.675980
N	1.767968	2.227556	-5.179062	H	2.627839	6.708175	1.024666
H	-5.185004	1.525290	1.222814	H	0.243264	7.074894	1.602243
H	-3.069583	2.496177	0.386513	C	3.521487	1.954907	-0.569878
H	-5.502235	-0.811710	2.604943	C	3.339673	2.539204	-1.828790
C	3.587511	0.287215	4.611833	C	4.784368	1.475121	-0.217913
C	3.512398	-0.597379	3.536677	C	4.401183	2.647668	-2.717675
C	3.070949	-0.081415	2.318528	H	2.355148	2.913580	-2.112726
C	2.729236	1.260474	2.128888	C	5.845868	1.575855	-1.114235
C	2.834709	2.116344	3.227680	H	4.946819	1.025023	0.760466
C	3.254532	1.630205	4.460156	C	5.657667	2.160613	-2.362099
H	3.919657	-0.069692	5.583528	H	4.240650	3.098587	-3.694602
H	2.568059	3.165634	3.118933	H	6.825409	1.197878	-0.830757
H	3.325457	2.303074	5.310703	H	6.488440	2.236617	-3.059577
O	2.963326	-0.907847	1.225767	C	-0.145733	-2.868299	-1.562292

C	-1.379126	-2.824614	-0.896015	C	7.533756	-0.892997	-0.605772
C	-0.007937	-3.654916	-2.706906	H	8.028496	0.033601	-0.915623
C	-2.451674	-3.574299	-1.364345	H	8.173535	-1.390830	0.136616
H	-1.491146	-2.182119	-0.018337	H	7.491684	-1.566568	-1.473326
C	-1.089496	-4.397122	-3.177310	C	5.436057	-1.873809	0.394518
H	0.944120	-3.688125	-3.234405	H	4.426657	-1.673528	0.767860
C	-2.307610	-4.360007	-2.506870	H	5.349102	-2.586483	-0.437563
H	-3.406302	-3.539330	-0.843485	H	5.995820	-2.394429	1.184131
H	-0.977695	-5.005450	-4.071656	O	1.433397	-0.211955	0.786196
H	-3.149961	-4.939433	-2.877076	C	-0.668113	0.344331	-0.429957
C	2.536168	-1.851399	-2.091124	H	-0.967067	1.376625	-0.619525
C	2.748542	-0.710305	-2.869747	C	-1.583323	-0.602210	-0.191457
C	3.349539	-2.974247	-2.282145	H	-1.231345	-1.619524	-0.002205
C	3.744504	-0.695409	-3.841776	C	-3.033612	-0.426738	-0.140169
H	2.136390	0.177788	-2.706530	C	-3.833365	-1.529087	0.192396
C	4.347894	-2.956424	-3.249636	C	-3.663021	0.798328	-0.412409
H	3.198140	-3.864167	-1.671213	C	-5.212707	-1.422791	0.259061
C	4.542606	-1.819227	-4.031979	H	-3.356750	-2.484524	0.402639
H	3.892560	0.198617	-4.444626	C	-5.038669	0.918883	-0.350514
H	4.976747	-3.831651	-3.394382	H	-3.068999	1.668865	-0.679781
H	5.323600	-1.809554	-4.788648	C	-5.823050	-0.193440	-0.012554
O	-1.049864	0.072376	1.236025	H	-5.822550	-2.283583	0.519701
H	-1.892035	0.893263	0.728582	H	-5.518794	1.870488	-0.562566
C	-0.820652	0.333719	2.588548	C	-7.244880	-0.069754	0.052285
H	-0.291888	1.290336	2.764563	N	-8.403263	0.032616	0.104866
H	-1.769836	0.375949	3.149613	H	1.081330	-0.675838	-1.246015
H	-0.203131	-0.455965	3.048534				

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C	0.784219	0.032518	-0.464295
C	1.818909	0.943843	0.034608
C	1.442096	2.253477	0.669270
H	2.128029	2.492747	1.489917
H	1.495375	3.069208	-0.061567
H	0.430652	2.216472	1.085005
C	3.210764	0.844406	-0.538720
H	3.312359	-0.128081	-1.040893
H	3.354811	1.616080	-1.308881
C	4.296309	0.958101	0.537070
H	4.317444	1.981831	0.934203
H	4.010328	0.310653	1.378523
C	5.656711	0.595085	0.021682
H	6.268658	1.417724	-0.356065
C	6.164737	-0.642079	-0.051411

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C	-0.697539	-0.465906	-0.909439
C	-1.620499	-0.484613	0.250671
C	-1.109534	-0.629868	1.655032
H	-1.590726	0.104237	2.311444
H	-1.339490	-1.628611	2.043860
H	-0.028552	-0.473292	1.707552
C	-3.051631	-0.896055	0.008382
H	-3.276469	-0.791734	-1.062134
H	-3.168284	-1.961671	0.256829
C	-4.058385	-0.064993	0.808608
H	-3.866638	-0.202056	1.884094
H	-3.885692	0.998548	0.597161
C	-5.464869	-0.471667	0.505845
H	-5.704524	-1.505776	0.774145
C	-6.435639	0.250550	-0.068482
C	-7.792136	-0.340767	-0.311157

H	-7.858379	-1.378345	0.032633	H	-10.242810	-1.115612	0.850019
H	-8.572419	0.240031	0.200778	H	-9.470215	0.456664	0.711713
H	-8.046195	-0.317157	-1.380312	C	-7.556210	-1.402572	1.537061
C	-6.301327	1.674073	-0.515265	H	-6.559540	-1.853680	1.482759
H	-5.301083	2.089453	-0.367351	H	-7.461262	-0.438060	2.058366
H	-6.550456	1.765258	-1.581532	H	-8.184826	-2.034410	2.180224
H	-7.016152	2.314291	0.020271	O	-3.504666	-2.742516	-0.265531
O	-1.256414	0.734701	-0.402280	C	-1.275903	-1.740633	-0.610589
C	0.762155	-0.636944	-0.818485	C	-0.563342	-2.350454	0.501094
H	1.145920	-1.570909	-1.231546	C	0.458882	-3.349269	0.404889
C	1.587077	0.286879	-0.307893	C	0.994265	-3.915736	1.595024
H	1.142307	1.216785	0.051106	C	0.984722	-3.838259	-0.820868
C	3.039982	0.190118	-0.201506	C	2.004511	-4.849494	1.568417
C	3.759905	1.318095	0.219392	H	0.594580	-3.581260	2.552983
C	3.752622	-0.982996	-0.499177	C	1.996427	-4.772541	-0.852912
C	5.139517	1.290373	0.332309	H	0.593007	-3.462137	-1.763722
H	3.218106	2.231297	0.457719	C	2.539775	-5.289100	0.340218
C	5.129961	-1.024915	-0.391731	H	2.401773	-5.252278	2.498512
H	3.219412	-1.878295	-0.809927	H	2.389542	-5.110324	-1.810467
C	5.833840	0.114709	0.024403	C	3.603669	-6.227241	0.310057
H	5.686720	2.171519	0.656628	N	4.483363	-6.995403	0.289247
H	5.673719	-1.936884	-0.623802	H	-2.986188	-0.808505	0.408033
C	7.256891	0.071675	0.138618	H	-1.038794	-2.144411	-1.598219
N	8.416855	0.035277	0.231468	H	-1.026077	-2.243503	1.485950
H	-1.130154	-0.797727	-1.860409	C	2.994276	4.072125	-2.461015
				C	2.473657	3.866871	-1.183401
58-ts				C	2.325470	2.544364	-0.763927
C	-2.742186	-1.537830	-0.372014	C	2.692106	1.444043	-1.543433
C	-3.799203	-1.855571	-1.347410	C	3.237680	1.695377	-2.804699
C	-3.469153	-2.371024	-2.722547	C	3.376564	3.000597	-3.262966
H	-3.259789	-1.535326	-3.401899	H	3.123030	5.084749	-2.835542
H	-2.594160	-3.026819	-2.703764	H	3.533616	0.861670	-3.437962
H	-4.307429	-2.945936	-3.133887	H	3.791890	3.185711	-4.250171
C	-5.156215	-1.199493	-1.208934	O	1.818646	2.267567	0.477696
H	-5.175031	-0.579060	-0.299120	C	2.174999	4.979209	-0.187094
H	-5.331326	-0.522608	-2.059782	C	1.031345	4.521083	0.705896
C	-6.294194	-2.222136	-1.127332	C	0.924271	3.164261	1.005319
H	-6.299560	-2.842571	-2.034374	C	0.115928	5.379177	1.315105
H	-6.078686	-2.904033	-0.294628	C	-0.065244	2.631384	1.834151
C	-7.633416	-1.569354	-0.962065	C	-0.848401	4.892415	2.192243
H	-8.180190	-1.346492	-1.881897	H	0.160747	6.447153	1.115809
C	-8.194798	-1.200235	0.196396	C	-0.940599	3.528543	2.449217
C	-9.536054	-0.534457	0.240791	H	-1.537589	5.581462	2.673705
H	-9.968075	-0.410875	-0.757914	H	-1.714930	3.156952	3.117012

P	2.336113	-0.242061	-0.911449	C	0.917963	0.357804	3.319071
P	-0.173366	0.801901	1.916179	C	0.929998	1.069957	4.523170
C	3.427016	5.170881	0.691746	C	1.729515	-0.769578	3.180333
H	3.698991	4.243930	1.211021	C	1.741374	0.652784	5.571496
H	4.279364	5.479617	0.073400	H	0.299604	1.951415	4.638471
H	3.244002	5.944666	1.447956	C	2.535971	-1.192459	4.233598
C	1.858174	6.299242	-0.882109	H	1.725357	-1.319900	2.238609
H	1.687144	7.092459	-0.146983	C	2.541849	-0.480831	5.428638
H	2.703249	6.627761	-1.495973	H	1.749108	1.210164	6.505407
H	0.970973	6.222082	-1.522171	H	3.159933	-2.076027	4.108340
Cu	0.227604	-0.468189	-0.020092	H	3.171803	-0.805420	6.253731
C	2.667189	-1.276023	-2.384267	B	-1.080453	0.365565	-1.373059
C	3.889192	-1.906062	-2.628216	O	-1.326622	0.226097	-2.718656
C	1.623098	-1.421559	-3.305464	O	-1.512329	1.583156	-0.899350
C	4.054259	-2.696676	-3.762646	C	-1.625405	1.549691	-3.237565
H	4.711409	-1.793157	-1.924320	C	-2.169180	2.291208	-1.976842
C	1.795870	-2.200861	-4.444220	C	-0.308223	2.119435	-3.739561
H	0.667681	-0.925921	-3.124084	H	0.115305	1.437910	-4.487302
C	3.008557	-2.849018	-4.668280	H	-0.440416	3.102678	-4.206029
H	5.005612	-3.193417	-3.938397	H	0.417187	2.211990	-2.921869
H	0.978313	-2.311524	-5.152926	C	-2.610753	1.418739	-4.378446
H	3.139552	-3.470627	-5.550843	H	-2.892215	2.409541	-4.757069
C	3.719783	-0.610685	0.230728	H	-2.148737	0.862041	-5.201579
C	3.881717	-1.936800	0.654516	H	-3.521763	0.890814	-4.078754
C	4.535898	0.382285	0.776696	C	-1.788326	3.753453	-1.869740
C	4.850989	-2.261226	1.595365	H	-2.203613	4.331242	-2.705345
H	3.251350	-2.724221	0.241848	H	-2.195712	4.161925	-0.935908
C	5.494524	0.055653	1.732793	H	-0.700473	3.887308	-1.847010
H	4.426878	1.417213	0.455866	C	-3.663183	2.116607	-1.768342
C	5.655566	-1.263637	2.143041	H	-3.935046	2.498756	-0.776699
H	4.972440	-3.298277	1.904537	H	-4.248757	2.664088	-2.515963
H	6.123390	0.837774	2.151827	H	-3.939770	1.057640	-1.808486
H	6.408240	-1.515344	2.886439				
C	-1.857473	0.481215	2.563431	**59-ts**			
C	-2.068234	-0.562917	3.470266	C	-2.674892	-3.969960	-2.926101
C	-2.969519	1.122022	1.999811	C	-2.304315	-3.799647	-1.591558
C	-3.360380	-0.958742	3.804997	C	-2.228882	-2.488961	-1.122751
H	-1.215667	-1.078377	3.912695	C	-2.456398	-1.366451	-1.924220
C	-4.259012	0.735969	2.349002	C	-2.841810	-1.584448	-3.248433
H	-2.820497	1.906449	1.259744	C	-2.954360	-2.879079	-3.742866
C	-4.457829	-0.310805	3.247256	H	-2.759746	-4.972230	-3.338974
H	-3.507823	-1.774738	4.508379	H	-3.036645	-0.733931	-3.898038
H	-5.112247	1.246089	1.903788	H	-3.254913	-3.040478	-4.774851
H	-5.466811	-0.618322	3.513361	O	-1.920013	-2.236750	0.185996

C	-2.052069	-4.953874	-0.628384	C	0.812107	-0.342992	4.599672
C	-1.102769	-4.478446	0.465116	C	2.360860	-0.464199	2.747985
C	-1.106413	-3.134599	0.827298	C	1.878354	-0.142765	5.472103
C	-0.266593	-5.323205	1.199937	H	-0.206523	-0.373159	4.983901
C	-0.301724	-2.602901	1.836907	C	3.422769	-0.266735	3.623233
C	0.520019	-4.836163	2.238941	H	2.541272	-0.585609	1.681329
H	-0.233205	-6.384896	0.967208	C	3.182704	-0.105442	4.985727
C	0.508026	-3.480649	2.555712	H	1.689206	-0.014671	6.535551
H	1.151528	-5.518307	2.802413	H	4.438046	-0.224954	3.232923
H	1.144391	-3.096741	3.351018	H	4.012297	0.055450	5.670573
P	-2.104831	0.297119	-1.228780	C	-1.806604	-0.394101	2.940322
P	-0.282660	-0.780289	2.008055	C	-2.526816	-1.331552	3.684552
C	-3.391069	-5.337984	0.027066	C	-2.228232	0.937482	2.918110
H	-3.831332	-4.483091	0.554888	C	-3.654283	-0.934812	4.398639
H	-4.105637	-5.675197	-0.734503	H	-2.203865	-2.371914	3.710238
H	-3.242452	-6.148745	0.751485	C	-3.342275	1.335565	3.647161
C	-1.479723	-6.164341	-1.363601	H	-1.679550	1.661433	2.313670
H	-1.313935	-6.999946	-0.676154	C	-4.059076	0.397769	4.385488
H	-2.176186	-6.529902	-2.125019	H	-4.215667	-1.668702	4.972533
H	-0.527792	-5.916904	-1.851033	H	-3.661338	2.375790	3.615867
Cu	-0.136276	0.397126	0.029923	H	-4.939411	0.703073	4.946819
C	-2.106908	1.335047	-2.742043	B	1.315565	-0.547001	-1.089977
C	-3.131958	2.217361	-3.085697	O	1.520797	-0.663059	-2.445017
C	-0.980241	1.239456	-3.571098	O	1.954396	-1.542136	-0.389922
C	-3.023531	3.010326	-4.226130	C	2.103981	-1.966495	-2.697707
H	-4.016422	2.299855	-2.457899	C	2.726310	-2.347504	-1.313033
C	-0.879778	2.026344	-4.712518	C	0.953965	-2.868810	-3.116249
H	-0.179755	0.539923	-3.324399	H	0.447202	-2.415649	-3.976539
C	-1.896512	2.922934	-5.036256	H	1.299261	-3.868861	-3.404316
H	-3.825991	3.699652	-4.478710	H	0.213989	-2.969732	-2.312374
H	-0.001240	1.944574	-5.348542	C	3.103564	-1.839458	-3.827736
H	-1.812886	3.547032	-5.922831	H	3.607232	-2.798260	-4.004749
C	-3.627703	0.764539	-0.326029	H	2.583084	-1.557180	-4.749712
C	-3.747054	2.090119	0.112551	H	3.863481	-1.079650	-3.619292
C	-4.624508	-0.153706	0.008650	C	2.556994	-3.804653	-0.928825
C	-4.860532	2.495787	0.836283	H	3.053689	-4.458681	-1.657101
H	-2.966174	2.812372	-0.122377	H	3.013742	-3.977851	0.052400
C	-5.726235	0.249838	0.759711	H	1.500415	-4.087123	-0.857688
H	-4.551589	-1.188585	-0.322254	C	4.182933	-1.946190	-1.137711
C	-5.852123	1.574433	1.166029	H	4.456781	-2.089564	-0.085233
H	-4.943027	3.534608	1.152861	H	4.849408	-2.562524	-1.752450
H	-6.495666	-0.475048	1.015726	H	4.358439	-0.892650	-1.380569
H	-6.718996	1.887003	1.743857	C	2.898977	1.488932	-0.684217
C	1.049019	-0.506081	3.231771	C	3.879224	2.512151	-0.260008

C	3.509655	3.849162	0.316689	C	0.404506	2.467961	1.824087
H	2.468109	3.889549	0.640222	C	1.407089	3.270121	2.373832
H	4.148382	4.075309	1.179476	C	1.359146	4.652438	2.227022
H	3.674402	4.633725	-0.431456	H	0.312427	6.332019	1.403954
C	5.264222	2.431091	-0.860825	H	2.238523	2.807128	2.901827
H	5.390113	1.444699	-1.330798	H	2.143716	5.269290	2.657644
H	5.377442	3.178559	-1.659040	O	-1.648227	2.297592	0.691438
C	6.357744	2.612866	0.200048	C	-1.920956	5.050870	0.242912
H	6.400064	3.665502	0.509708	C	-2.338322	4.032053	-0.809918
H	6.061042	2.044048	1.093329	C	-2.228528	2.677798	-0.493921
C	7.708346	2.171198	-0.278035	C	-2.894458	4.351464	-2.048090
H	8.356418	2.941643	-0.702330	C	-2.680531	1.651042	-1.325386
C	8.165485	0.912204	-0.260220	C	-3.346930	3.354697	-2.908237
C	9.527199	0.565215	-0.779048	H	-2.988523	5.392548	-2.346507
H	10.065544	1.446748	-1.142869	C	-3.253750	2.015392	-2.545995
H	10.137028	0.089962	0.002429	H	-3.784648	3.625910	-3.865455
H	9.463221	-0.161867	-1.600996	H	-3.612886	1.243725	-3.223569
C	7.379536	-0.253742	0.261181	P	0.404468	0.632468	1.811365
H	6.364963	0.008341	0.581804	P	-2.381505	-0.090017	-0.825649
H	7.294805	-1.029745	-0.513451	C	-3.078488	5.198418	1.249321
H	7.896692	-0.726890	1.108000	H	-3.323398	4.239956	1.722056
O	3.584790	1.361872	0.548659	H	-2.802487	5.907738	2.039574
C	1.402971	1.606430	-0.684225	H	-3.976593	5.571249	0.741236
H	1.063784	1.894279	-1.686184	C	-1.625438	6.413826	-0.371858
C	0.718346	2.279484	0.409981	H	-2.513133	6.813986	-0.873171
H	1.173145	2.172101	1.397649	H	-1.356800	7.139829	0.402496
C	-0.241821	3.334351	0.278750	H	-0.807029	6.362668	-1.100761
C	-0.763376	3.943036	1.455750	Cu	-0.179849	-0.465891	-0.139586
C	-0.701806	3.863702	-0.958289	C	2.074946	0.242939	2.463139
C	-1.714868	4.935449	1.409574	C	2.272091	-0.429651	3.672191
H	-0.398646	3.592590	2.421886	C	3.189912	0.613600	1.697322
C	-1.645055	4.867688	-1.009169	C	3.561773	-0.711570	4.119343
H	-0.314623	3.468434	-1.896418	H	1.416985	-0.728438	4.275939
C	-2.188187	5.413158	0.170298	C	4.474352	0.360192	2.165975
H	-2.105067	5.362361	2.331691	H	3.044982	1.097497	0.729710
H	-1.982265	5.244830	-1.972970	C	4.664462	-0.305965	3.375255
C	-3.184156	6.421567	0.114533	H	3.701170	-1.237919	5.060697
N	-4.008481	7.248104	0.071672	H	5.334571	0.675036	1.576766
H	3.276154	0.827103	-1.472513	H	5.671426	-0.511757	3.731628
				C	-0.709250	0.204641	3.198179
60-ts				C	-1.447381	-0.975502	3.093840
C	0.318027	5.251301	1.522549	C	-0.798442	0.974528	4.362616
C	-0.714485	4.486932	0.980368	C	-2.247618	-1.399111	4.150682
C	-0.649174	3.108153	1.171266	H	-1.400845	-1.556492	2.171785

C	-1.611814	0.558990	5.410691	H	-0.309792	2.941761	-3.742384
H	-0.223089	1.895928	4.450526	C	2.287550	0.803174	-4.483814
C	-2.331162	-0.630942	5.307493	H	1.681202	0.206797	-5.174024
H	-2.813407	-2.324760	4.060772	H	2.905487	1.488175	-5.075888
H	-1.681115	1.161009	6.313754	H	2.954816	0.120705	-3.944995
H	-2.960986	-0.955717	6.132611	C	2.522565	-1.777017	-1.473903
C	-3.007779	-1.020573	-2.278402	C	3.668557	-2.204353	-0.655755
C	-4.319912	-1.494455	-2.364817	C	3.570346	-2.810128	0.722342
C	-2.126786	-1.257098	-3.340214	H	2.808405	-3.591589	0.749052
C	-4.733052	-2.222032	-3.477289	H	4.528302	-3.262896	1.006823
H	-5.021777	-1.308818	-1.554300	H	3.333363	-2.050598	1.475632
C	-2.545640	-1.976124	-4.454848	C	4.991441	-1.533440	-0.961019
H	-1.110808	-0.865210	-3.297155	H	4.911418	-0.967940	-1.901402
C	-3.845922	-2.470489	-4.520360	H	5.189122	-0.792254	-0.171188
H	-5.753392	-2.594852	-3.527538	C	6.175279	-2.498477	-1.061082
H	-1.850237	-2.157824	-5.271174	H	6.234030	-3.114929	-0.153962
H	-4.168703	-3.044453	-5.385844	H	5.985967	-3.196740	-1.887135
C	-3.642565	-0.432007	0.462616	C	7.470683	-1.775035	-1.280325
C	-4.339787	0.566191	1.145300	H	7.785530	-1.642473	-2.318261
C	-3.853778	-1.771496	0.815653	C	8.242125	-1.240968	-0.324437
C	-5.235677	0.230689	2.158192	C	9.507972	-0.511116	-0.655184
H	-4.197306	1.613308	0.884205	H	9.700675	-0.489365	-1.732948
C	-4.762769	-2.104321	1.811296	H	9.473312	0.525765	-0.291878
H	-3.318579	-2.564119	0.293302	H	10.372233	-0.978899	-0.162550
C	-5.453790	-1.102128	2.489767	C	7.929263	-1.310697	1.140458
H	-5.773114	1.018663	2.680865	H	8.728188	-1.831282	1.686960
H	-4.927100	-3.152098	2.058513	H	7.878899	-0.298474	1.568439
H	-6.161103	-1.360591	3.274352	H	6.981633	-1.814502	1.361766
B	0.972597	0.349046	-1.641804	O	3.169198	-3.027536	-1.718749
O	2.043866	1.156985	-1.335983	C	1.046507	-1.781923	-1.179528
O	0.497472	0.588689	-2.907548	H	0.509892	-2.032125	-2.103522
C	2.093585	2.210522	-2.330588	C	0.502711	-2.448606	-0.000376
C	1.362078	1.564602	-3.547282	H	1.095181	-2.418121	0.912330
C	1.348404	3.396477	-1.738084	C	-0.578027	-3.388318	0.011821
H	1.797393	3.645586	-0.768798	C	-0.965479	-3.984304	1.245644
H	1.405456	4.279655	-2.385365	C	-1.305099	-3.798437	-1.137773
H	0.291376	3.155397	-1.565909	C	-2.034230	-4.845085	1.339910
C	3.543223	2.572278	-2.571812	H	-0.402572	-3.727905	2.143866
H	3.629375	3.315590	-3.374323	C	-2.377908	-4.658785	-1.049244
H	3.966896	3.008083	-1.659507	H	-1.021135	-3.426476	-2.119288
H	4.140482	1.694915	-2.838799	C	-2.780176	-5.187079	0.193293
C	0.494926	2.513697	-4.348790	H	-2.314786	-5.264755	2.304413
H	1.098321	3.329586	-4.766245	H	-2.925893	-4.931882	-1.949509
H	0.034681	1.972772	-5.183252	H	2.792468	-1.050619	-2.246238

C	-3.904491	-6.046442	0.291431	H	1.842179	-0.006064	1.665729
N	-4.832928	-6.750035	0.377503	C	-4.019149	-1.898459	-3.812744
				C	-4.082230	-1.781696	-2.425266
61				C	-3.297728	-0.793047	-1.834355
C	4.098511	-0.357291	0.049590	C	-2.446983	0.048613	-2.553451
C	5.209825	-0.632592	-0.867746	C	-2.429149	-0.085161	-3.944378
C	4.976315	-0.808946	-2.344655	C	-3.211881	-1.050926	-4.567116
H	4.875025	-1.874132	-2.589734	H	-4.609007	-2.659048	-4.318518
H	4.070564	-0.292276	-2.676194	H	-1.779482	0.554377	-4.538297
H	5.818232	-0.411495	-2.924158	H	-3.187164	-1.150833	-5.649053
C	6.467240	-1.262353	-0.318587	O	-3.318307	-0.628109	-0.471281
H	6.461843	-1.154372	0.775413	C	-4.970263	-2.624456	-1.520170
H	6.469863	-2.342341	-0.529755	C	-4.218349	-2.832635	-0.211989
C	7.741715	-0.611339	-0.867656	C	-3.452710	-1.774734	0.273403
H	7.853572	-0.854028	-1.933064	C	-4.274756	-3.985737	0.570310
H	7.613799	0.479204	-0.814212	C	-2.772875	-1.809019	1.492504
C	8.972150	-1.040790	-0.126368	C	-3.610187	-4.057210	1.791781
H	9.507729	-1.903884	-0.529753	H	-4.849858	-4.843167	0.229792
C	9.441087	-0.489100	1.000617	C	-2.872434	-2.973505	2.258045
C	10.670738	-1.014036	1.676296	H	-3.673277	-4.963757	2.388044
H	11.110737	-1.856992	1.132981	H	-2.351614	-3.037808	3.211980
H	11.435553	-0.229742	1.768654	P	-1.293028	1.122095	-1.618673
H	10.447717	-1.344613	2.700684	P	-1.723970	-0.368117	1.925328
C	8.797512	0.676852	1.688810	C	-6.253735	-1.826911	-1.217626
H	7.877282	1.015501	1.202043	H	-6.028006	-0.866602	-0.739148
H	8.549135	0.417704	2.727626	H	-6.800223	-1.626857	-2.147799
H	9.490094	1.528424	1.744777	H	-6.904477	-2.400596	-0.545932
O	4.979823	0.689168	-0.358252	C	-5.351843	-3.946442	-2.174499
C	2.647515	-0.271855	-0.354154	H	-6.005039	-4.531876	-1.518525
C	1.777799	0.453403	0.669838	H	-5.915064	-3.771980	-3.097462
C	1.765962	1.897861	0.735438	H	-4.466955	-4.549059	-2.414237
C	1.261975	2.550523	1.898145	Cu	-0.228044	0.283475	0.266482
C	2.157513	2.744065	-0.338349	C	-0.148126	1.712139	-2.918086
C	1.110393	3.917423	1.965765	C	-0.174749	3.000049	-3.454229
H	0.979326	1.933174	2.753253	C	0.834571	0.808486	-3.343559
C	2.016277	4.113845	-0.271443	C	0.782450	3.387846	-4.389416
H	2.599662	2.300769	-1.229236	H	-0.933562	3.710405	-3.130843
C	1.476028	4.731069	0.874020	C	1.775199	1.193172	-4.292111
H	0.703458	4.378815	2.864646	H	0.866827	-0.200659	-2.925185
H	2.318720	4.730522	-1.116172	C	1.757235	2.488004	-4.808171
C	1.279263	6.135062	0.922502	H	0.761750	4.397188	-4.793773
N	1.101470	7.288979	0.963430	H	2.529012	0.482581	-4.624918
H	4.241916	-0.668740	1.093781	H	2.502978	2.794230	-5.537910
H	2.578625	0.241060	-1.322784	C	-2.272424	2.584985	-1.131135

C	-1.591059	3.604276	-0.454854	H	1.993090	-4.523747	-2.850674
C	-3.649518	2.695823	-1.329893	C	0.413793	-4.503057	0.809464
C	-2.269877	4.730444	-0.009185	H	0.000924	-5.413141	0.355792
H	-0.518113	3.516754	-0.282480	H	0.928899	-4.790466	1.733896
C	-4.332732	3.814851	-0.858191	H	-0.416949	-3.840021	1.075092
H	-4.192561	1.912214	-1.856193	C	2.626196	-4.709902	-0.316358
C	-3.646047	4.833876	-0.205281	H	3.108918	-4.849670	0.656924
H	-1.723389	5.520216	0.504913	H	2.366044	-5.696276	-0.716795
H	-5.406679	3.892933	-1.010923	H	3.352614	-4.239608	-0.990789
H	-4.184053	5.707815	0.154922				
C	-0.951549	-0.921214	3.486545	**62**			
C	-1.509577	-0.683324	4.745036	C	-4.030598	-2.351707	-3.572682
C	0.224881	-1.673203	3.382517	C	-3.973898	-2.228855	-2.184726
C	-0.898251	-1.193988	5.886616	C	-3.264032	-1.143449	-1.675038
H	-2.427874	-0.104407	4.832625	C	-2.598473	-0.211773	-2.474285
C	0.824483	-2.192932	4.525115	C	-2.695222	-0.359566	-3.859916
H	0.667564	-1.857694	2.401275	C	-3.409900	-1.421591	-4.402893
C	0.265196	-1.951051	5.777578	H	-4.572047	-3.181842	-4.020098
H	-1.335921	-1.004954	6.864118	H	-2.189000	0.348895	-4.512388
H	1.734166	-2.782780	4.436536	H	-3.479350	-1.531182	-5.481937
H	0.737885	-2.351365	6.671490	O	-3.178333	-0.952101	-0.318744
C	-2.926169	0.908272	2.448850	C	-4.679274	-3.153213	-1.201236
C	-4.261922	0.621020	2.743671	C	-3.833620	-3.226191	0.063663
C	-2.459488	2.219957	2.579693	C	-3.148605	-2.080477	0.462541
C	-5.116933	1.635021	3.165275	C	-3.754561	-4.334763	0.907302
H	-4.635010	-0.397813	2.645413	C	-2.411115	-1.992282	1.645652
C	-3.312138	3.227208	3.017031	C	-3.044614	-4.278501	2.103926
H	-1.424880	2.457442	2.323644	H	-4.267536	-5.255432	0.639682
C	-4.642493	2.936211	3.306613	C	-2.382233	-3.113690	2.477330
H	-6.156301	1.406033	3.389420	H	-3.010662	-5.150969	2.751202
H	-2.937986	4.244027	3.117196	H	-1.819500	-3.078909	3.408695
H	-5.312417	3.725710	3.639199	P	-1.514435	1.015504	-1.653314
B	2.019847	-1.692353	-0.553243	P	-1.485304	-0.441476	1.956392
O	1.548329	-2.157558	-1.758120	C	-6.034473	-2.517346	-0.834703
O	1.851662	-2.600243	0.465622	H	-5.904173	-1.515873	-0.406786
C	0.780392	-3.351388	-1.481221	H	-6.662911	-2.429399	-1.729854
C	1.394866	-3.835490	-0.131504	H	-6.558396	-3.140041	-0.098755
C	-0.672650	-2.915343	-1.368655	C	-4.925422	-4.533903	-1.798846
H	-0.968000	-2.423136	-2.305097	H	-5.455359	-5.175167	-1.086876
H	-1.349857	-3.762594	-1.197527	H	-5.563540	-4.465666	-2.686055
H	-0.815316	-2.188869	-0.553992	H	-3.987129	-5.026961	-2.081314
C	0.940716	-4.319503	-2.634013	Cu	-0.233804	0.348188	0.159303
H	0.437190	-5.268507	-2.411403	C	-0.565415	1.719545	-3.048682
H	0.482897	-3.897618	-3.535582	C	-0.816051	2.974920	-3.604703

C	0.504963	0.955098	-3.530409	O	1.834950	-2.286680	0.207890
C	0.011732	3.473310	-4.607906	C	1.046408	-3.226958	-1.783958
H	-1.649195	3.575378	-3.244003	C	1.569183	-3.587216	-0.359814
C	1.321217	1.450071	-4.540744	C	-0.445789	-2.934913	-1.821457
H	0.706612	-0.030833	-3.105058	H	-0.693087	-2.484323	-2.791038
C	1.082724	2.716356	-5.072290	H	-1.044770	-3.847043	-1.703427
H	-0.182986	4.457469	-5.027733	H	-0.742485	-2.226949	-1.033573
H	2.153151	0.851134	-4.904423	C	1.406119	-4.221545	-2.866987
H	1.731233	3.110858	-5.850958	H	0.973047	-5.204820	-2.644930
C	-2.628255	2.355734	-1.101585	H	1.000228	-3.883361	-3.826872
C	-2.027426	3.510752	-0.586439	H	2.488715	-4.332470	-2.975367
C	-4.019286	2.241873	-1.086168	C	0.570212	-4.310612	0.518128
C	-2.805584	4.549364	-0.092246	H	0.301692	-5.281029	0.081536
H	-0.940705	3.598840	-0.582805	H	1.011818	-4.493972	1.505331
C	-4.796869	3.276541	-0.570822	H	-0.344704	-3.725805	0.661212
H	-4.499256	1.345446	-1.477399	C	2.897600	-4.329398	-0.374369
C	-4.194142	4.430617	-0.079583	H	3.288871	-4.367673	0.647988
H	-2.323917	5.446924	0.293285	H	2.787348	-5.357223	-0.737986
H	-5.880235	3.181118	-0.561481	H	3.638255	-3.812843	-0.997489
H	-4.806571	5.236917	0.317636	C	4.127114	-0.056719	-0.539267
C	-0.533208	-0.852377	3.461153	C	5.091963	0.698122	0.275402
C	-0.951202	-0.521735	4.752326	C	4.709806	1.784219	1.243220
C	0.666982	-1.550923	3.278358	H	3.773885	1.552423	1.753277
C	-0.177012	-0.889071	5.850038	H	5.490359	1.911620	2.002962
H	-1.884242	0.019859	4.901726	H	4.589991	2.743071	0.723333
C	1.427330	-1.929590	4.379402	C	6.520666	0.755561	-0.219711
H	1.001899	-1.799681	2.269291	H	6.653005	-0.004408	-1.002566
C	1.008409	-1.594811	5.665317	H	6.714348	1.730688	-0.690665
H	-0.504045	-0.625666	6.853295	C	7.541727	0.489711	0.894368
H	2.355578	-2.476826	4.231565	H	7.602392	1.359055	1.562134
H	1.609104	-1.881510	6.525438	H	7.164310	-0.340625	1.508146
C	-2.771251	0.719482	2.545645	C	8.907859	0.173072	0.362349
C	-4.027712	0.303293	2.993784	H	9.606248	1.008810	0.274013
C	-2.449700	2.079757	2.567637	C	9.325306	-1.032332	-0.046705
C	-4.946287	1.238115	3.462707	C	10.706974	-1.241906	-0.586560
H	-4.286239	-0.755016	2.983422	H	11.295398	-0.318254	-0.581817
C	-3.364310	3.009752	3.048532	H	11.249406	-1.996715	0.000467
H	-1.478267	2.414273	2.199595	H	10.674885	-1.622775	-1.617325
C	-4.614488	2.590069	3.494657	C	8.471060	-2.264066	-0.017025
H	-5.922841	0.907694	3.809295	H	7.456037	-2.080823	0.349815
H	-3.102363	4.066081	3.056568	H	8.388781	-2.695119	-1.024948
H	-5.333765	3.317536	3.863876	H	8.928741	-3.042115	0.610126
B	2.047881	-1.419610	-0.836690	O	4.693981	-0.634436	0.636275
O	1.722205	-1.974992	-2.051358	C	2.612944	0.036350	-0.664060

H	2.429719	0.538085	-1.627824	C	5.198581	-4.526692	-0.454835
C	1.788740	0.698832	0.425799	H	6.241092	-4.323696	-0.720878
H	1.930625	0.243764	1.413761	H	5.207881	-5.450458	0.132822
C	1.591825	2.122819	0.475786	H	4.630959	-4.705503	-1.376332
C	1.108360	2.733212	1.672746	Cu	0.178667	0.326896	-0.148082
C	1.808955	3.000154	-0.625703	C	-1.698501	-1.813080	1.813158
C	0.804928	4.073279	1.745229	C	-2.462307	-1.659118	2.971829
H	0.974454	2.101831	2.553334	C	-2.303898	-2.328322	0.657991
C	1.520763	4.346040	-0.551577	C	-3.812613	-2.007380	2.975028
H	2.213537	2.602337	-1.555526	H	-2.006415	-1.255721	3.874970
C	0.995100	4.912417	0.627434	C	-3.644048	-2.693129	0.670972
H	0.416875	4.495737	2.671367	H	-1.727332	-2.413723	-0.266073
H	1.694107	4.984567	-1.416175	C	-4.404939	-2.522533	1.827222
C	0.643349	6.284379	0.684640	H	-4.400537	-1.873425	3.880203
N	0.338210	7.411354	0.733406	H	-4.105057	-3.089938	-0.231853
H	4.559971	-0.482731	-1.458609	H	-5.462447	-2.781038	1.823727
				C	0.447775	-0.620232	3.335472
63				C	0.280534	0.736790	3.624341
C	2.633255	-4.940598	0.928447	C	0.895249	-1.486045	4.338472
C	3.169680	-3.663081	0.765970	C	0.546567	1.221371	4.901118
C	2.333000	-2.586726	1.052416	H	-0.051853	1.420778	2.841870
C	1.007283	-2.730400	1.469723	C	1.172031	-0.996965	5.610872
C	0.514583	-4.025176	1.639352	H	1.025051	-2.546366	4.124527
C	1.324716	-5.122576	1.367627	C	0.996062	0.355745	5.893561
H	3.243997	-5.814400	0.715849	H	0.417777	2.281147	5.111601
H	-0.512739	-4.170726	1.968187	H	1.524101	-1.674773	6.385084
H	0.934138	-6.128581	1.497213	H	1.212697	0.735193	6.889462
O	2.790426	-1.299133	0.912414	C	2.507786	2.662742	-1.511386
C	4.608626	-3.376721	0.355543	C	3.330060	3.762035	-1.248888
C	4.623455	-2.070365	-0.428820	C	1.850025	2.570399	-2.741517
C	3.711662	-1.075102	-0.080055	C	3.481959	4.763891	-2.202645
C	5.535561	-1.768019	-1.440024	H	3.849183	3.837588	-0.294433
C	3.664382	0.177368	-0.700233	C	2.011855	3.570004	-3.696283
C	5.540988	-0.519751	-2.056231	H	1.206325	1.714512	-2.951164
H	6.264595	-2.513128	-1.748391	C	2.822040	4.669503	-3.425319
C	4.612860	0.448081	-1.689970	H	4.117480	5.620165	-1.989509
H	6.270197	-0.304461	-2.832755	H	1.495592	3.493018	-4.650714
H	4.601826	1.410866	-2.197221	H	2.940588	5.454926	-4.168276
P	0.018158	-1.200540	1.654965	C	2.705088	2.083947	1.285324
P	2.268448	1.301474	-0.311165	C	3.787933	1.704077	2.077991
C	5.450976	-3.184513	1.631142	C	1.863511	3.113085	1.723122
H	5.069379	-2.362844	2.248415	C	4.017394	2.341648	3.296143
H	5.436688	-4.100361	2.235339	H	4.464145	0.916918	1.747229
H	6.490945	-2.957325	1.364894	C	2.101226	3.756699	2.929580

H	1.017419	3.420341	1.108462	H	-10.291474	-1.373141	1.770507
C	3.179183	3.366635	3.723050	C	-7.996657	0.213193	1.654475
H	4.864098	2.039777	3.908382	H	-8.825599	0.695601	2.190637
H	1.438577	4.560311	3.247606	H	-7.367184	-0.257299	2.424215
H	3.365872	3.862520	4.672893	H	-7.401593	0.996744	1.174359
B	-1.087346	-0.498879	-2.925616	O	-4.527831	0.109673	-3.199490
O	-1.141196	-1.872192	-2.858598	C	-2.166392	0.439519	-2.291067
O	0.042310	-0.050601	-3.568291	H	-2.237397	1.375360	-2.865485
C	0.142864	-2.378980	-3.284930	C	-1.727101	0.732378	-0.838809
C	0.710447	-1.199026	-4.137399	H	-2.318634	0.130882	-0.135063
C	0.952250	-2.647095	-2.027081	C	-1.577380	2.088219	-0.372164
H	0.416838	-3.367947	-1.396601	C	-1.827270	2.406308	0.996380
H	1.940412	-3.063635	-2.259270	C	-1.122502	3.160952	-1.190752
H	1.089319	-1.723059	-1.445332	C	-1.612906	3.667208	1.507110
C	-0.068350	-3.670843	-4.046563	H	-2.215298	1.620450	1.647126
H	0.883129	-4.044387	-4.445298	C	-0.904283	4.422149	-0.683581
H	-0.473263	-4.431980	-3.370501	H	-0.901023	2.966561	-2.239597
H	-0.770156	-3.544392	-4.875632	C	-1.140681	4.705275	0.678272
C	2.207794	-1.000578	-4.022353	H	-1.806907	3.870440	2.559691
H	2.746544	-1.888420	-4.378101	H	-0.529609	5.209694	-1.336076
H	2.517509	-0.147419	-4.638278	H	-3.485540	-1.286789	-2.002558
H	2.513822	-0.799666	-2.990072	C	-0.880406	5.991889	1.215042
C	0.299523	-1.259199	-5.600443	N	-0.660907	7.046466	1.667379
H	0.563348	-0.309623	-6.078760				
H	0.816362	-2.065582	-6.132864	**64-ts**			
H	-0.781576	-1.403658	-5.709067	C	-2.666811	0.461278	0.425045
C	-3.528330	-0.213858	-2.234067	C	-2.837825	1.558918	1.377119
C	-4.757411	0.461782	-1.824469	C	-2.610630	1.294794	2.848339
C	-4.794851	1.938183	-1.542668	H	-3.508274	0.860777	3.307258
H	-3.900331	2.448496	-1.911453	H	-1.771839	0.608564	3.006982
H	-5.671004	2.397877	-2.016299	H	-2.385677	2.231054	3.375171
H	-4.866601	2.117198	-0.461141	C	-3.942422	2.568818	1.105518
C	-5.795995	-0.372597	-1.116068	H	-4.147088	2.566942	0.024941
H	-5.695325	-1.415307	-1.452169	H	-4.875143	2.278805	1.610966
H	-5.557152	-0.374510	-0.039263	C	-3.512714	3.983597	1.518739
C	-7.244246	0.079219	-1.304974	H	-3.618179	4.104737	2.605396
H	-7.363394	1.105952	-0.931106	H	-2.437318	4.076079	1.299140
H	-7.468073	0.116764	-2.380598	C	-4.276948	5.064402	0.813903
C	-8.191894	-0.850734	-0.606736	H	-5.138248	5.484873	1.339012
H	-8.604300	-1.664747	-1.207983	C	-4.010967	5.528306	-0.414681
C	-8.510513	-0.816559	0.693939	C	-4.846108	6.600961	-1.044765
C	-9.412823	-1.843629	1.306848	H	-5.651740	6.937733	-0.383430
H	-9.764269	-2.574976	0.571412	H	-4.233441	7.474828	-1.309392
H	-8.897661	-2.387959	2.111808	H	-5.298118	6.250185	-1.983571

C	-2.882884	5.028772	-1.268124	C	6.233517	-0.106332	-1.461628
H	-2.329621	4.196130	-0.818354	H	5.732300	0.844387	-1.244566
H	-3.268689	4.688138	-2.240366	H	7.090753	-0.205069	-0.783761
H	-2.170052	5.836130	-1.491286	H	6.605132	-0.069895	-2.493469
O	-1.681476	1.874310	0.629244	C	6.016967	-2.594337	-1.594727
C	-2.014204	-0.802174	0.626240	H	6.406648	-2.587237	-2.617652
C	-2.354145	-1.889990	-0.410367	H	6.883976	-2.718786	-0.938139
C	-3.707300	-2.506253	-0.161953	H	5.359809	-3.465564	-1.477016
C	-4.794465	-2.197463	-0.989047	Cu	-0.145805	0.071413	0.350624
C	-3.925248	-3.359755	0.929850	C	0.972217	-0.136061	3.637330
C	-6.057865	-2.712493	-0.742698	C	1.359665	0.535448	4.800169
H	-4.640418	-1.536266	-1.841862	C	0.163878	-1.273708	3.737957
C	-5.179402	-3.885035	1.189257	C	0.943869	0.073895	6.045709
H	-3.087184	-3.614524	1.576030	H	1.988909	1.422255	4.729701
C	-6.257115	-3.562376	0.352153	C	-0.243532	-1.738342	4.984130
H	-6.894860	-2.463797	-1.390569	H	-0.156949	-1.780063	2.825963
H	-5.337741	-4.549364	2.035353	C	0.143878	-1.062156	6.138451
C	-7.553204	-4.101280	0.613307	H	1.245323	0.603385	6.946599
N	-8.610364	-4.541364	0.826063	H	-0.873685	-2.621935	5.053525
H	-3.139949	0.629873	-0.548365	H	-0.183067	-1.418550	7.112549
H	-2.049497	-1.179607	1.655806	C	1.906717	2.155476	2.188103
H	-2.385755	-1.402359	-1.395495	C	0.844825	3.053720	2.361267
C	5.395600	-1.942124	1.212160	C	3.218130	2.633365	2.198440
C	4.762306	-1.290101	0.153078	C	1.098474	4.403937	2.567212
C	3.630113	-0.538871	0.462987	H	-0.182099	2.690890	2.295830
C	3.089430	-0.451029	1.749471	C	3.466319	3.991968	2.384489
C	3.760590	-1.109970	2.780445	H	4.050383	1.942573	2.069628
C	4.910015	-1.845644	2.512416	C	2.409924	4.876093	2.578195
H	6.289058	-2.532935	1.025553	H	0.268305	5.094354	2.704640
H	3.368360	-1.062968	3.794421	H	4.491064	4.356460	2.388725
H	5.427562	-2.355479	3.320989	H	2.607106	5.934542	2.732587
O	2.970863	0.157779	-0.515431	C	-0.858098	0.790876	-3.013795
C	5.274586	-1.297240	-1.282167	C	-1.534254	1.961634	-3.370456
C	4.088366	-1.106295	-2.220436	C	-1.344436	-0.440873	-3.472302
C	2.989540	-0.370240	-1.782025	C	-2.671325	1.900378	-4.172642
C	4.051999	-1.573519	-3.535185	H	-1.180009	2.928255	-3.012675
C	1.865598	-0.111418	-2.573323	C	-2.472961	-0.496172	-4.282605
C	2.966495	-1.307374	-4.363250	H	-0.849696	-1.365424	-3.172959
H	4.887817	-2.147661	-3.927579	C	-3.142832	0.674472	-4.631476
C	1.879341	-0.580811	-3.887195	H	-3.188357	2.818036	-4.444501
H	2.968514	-1.667904	-5.388735	H	-2.837175	-1.459649	-4.633336
H	1.030670	-0.381233	-4.537906	H	-4.030111	0.630931	-5.258714
P	1.472200	0.393223	1.954745	C	1.100884	2.540110	-1.848734
P	0.492918	0.809589	-1.775439	C	2.032178	2.967268	-2.801171

C	0.586215	3.460619	-0.930547	C	2.956725	0.513797	-0.518590
C	2.446275	4.294722	-2.830398	H	3.103795	0.993938	-1.491481
H	2.437814	2.258715	-3.522660	C	3.910507	-0.330290	-0.104121
C	0.999354	4.790013	-0.968116	C	5.131010	-0.584148	-0.937436
H	-0.148694	3.133013	-0.193488	H	5.122342	-0.010629	-1.870308
C	1.930828	5.208096	-1.913348	H	6.045324	-0.324975	-0.384916
H	3.173731	4.617878	-3.571778	H	5.219179	-1.650123	-1.190756
H	0.596414	5.494467	-0.241763	C	3.883043	-1.093090	1.184980
H	2.257314	6.245406	-1.936737	H	2.985881	-0.913983	1.782864
B	-1.156932	-2.903115	-0.449027	H	3.949043	-2.172795	0.991836
O	-0.793344	-3.718308	0.596583	H	4.757087	-0.839923	1.801151
O	-0.343139	-3.061637	-1.546678	O	-1.091092	-0.166378	1.212489
C	0.490988	-4.294076	0.259345	C	-3.333562	-0.180933	0.158875
C	0.495313	-4.213926	-1.296846	H	-3.660880	0.660815	0.772389
C	1.553164	-3.414025	0.896220	C	-4.238318	-0.950219	-0.450093
H	1.382093	-3.368618	1.978725	H	-3.883725	-1.799120	-1.041185
H	2.561817	-3.809749	0.724889	H	-1.622664	-1.341959	-0.479049
H	1.506794	-2.387311	0.506716	C	-5.712070	-0.744694	-0.390137
C	0.566361	-5.695677	0.826898	H	-6.219508	-1.622609	0.029599
H	1.493638	-6.189242	0.510636	H	-5.970605	0.124926	0.223858
H	0.566162	-5.649212	1.921540	H	-6.135531	-0.592834	-1.391217
H	-0.281954	-6.310601	0.513027				
C	1.855625	-3.980181	-1.918752	**66-ts**			
H	2.531014	-4.817820	-1.700868	C	2.589063	0.768193	-1.906169
H	1.756965	-3.896900	-3.007589	C	3.863459	1.502436	-2.058318
H	2.317563	-3.055026	-1.557294	C	3.904448	2.901608	-2.602499
C	-0.189248	-5.400207	-1.959694	H	4.185062	2.897042	-3.663067
H	-0.335722	-5.175156	-3.021646	H	2.931455	3.393890	-2.503888
H	0.415473	-6.310956	-1.883388	H	4.646190	3.506085	-2.064519
H	-1.172191	-5.595183	-1.515040	C	5.157608	0.723145	-2.120189
				H	4.948285	-0.305071	-1.789262
65				H	5.529930	0.661067	-3.152927
C	-1.885355	-0.417332	0.049303	C	6.217688	1.338363	-1.189700
C	-0.854592	0.637834	0.057155	H	6.737601	2.157459	-1.706865
C	-1.213061	2.091055	0.205071	H	5.691033	1.796427	-0.341701
H	-0.500823	2.594862	0.868850	C	7.218832	0.345831	-0.683984
H	-1.177819	2.595759	-0.767463	H	8.063154	0.120753	-1.341291
H	-2.211161	2.226491	0.629344	C	7.154840	-0.298440	0.489724
C	0.463050	0.346735	-0.622061	C	8.222405	-1.261899	0.912488
H	0.566854	-0.740426	-0.746397	H	9.023111	-1.343328	0.169569
H	0.456459	0.783058	-1.632512	H	8.672024	-0.953793	1.867489
C	1.672179	0.866783	0.160410	H	7.809226	-2.266956	1.083274
H	1.603017	1.961606	0.253571	C	6.048063	-0.106236	1.487594
H	1.625126	0.465962	1.181775	H	5.139264	0.326953	1.052398

H	5.771860	-1.066700	1.948023	C	-3.142521	3.988292	-2.879394
H	6.367612	0.541070	2.317825	H	-2.637439	1.954071	-2.364984
O	3.248300	1.375849	-0.769728	C	-3.127455	5.320121	-2.470164
C	1.226776	1.210905	-2.238366	H	-2.588102	6.695557	-0.903458
C	0.304548	0.293683	-2.932230	H	-3.561526	3.718446	-3.846502
H	2.699730	-0.324912	-1.914596	H	-3.531796	6.094093	-3.118517
H	1.083828	2.274153	-2.455104	C	-0.553834	2.843674	1.564679
H	0.766573	-0.674603	-3.168245	C	0.674490	3.436211	1.245986
C	-5.282316	0.052771	1.921175	C	-1.050968	2.955673	2.863233
C	-4.057331	-0.592620	2.086577	C	1.381743	4.146329	2.207400
C	-2.919914	0.075236	1.634616	H	1.079241	3.322743	0.238298
C	-2.959299	1.318076	0.997441	C	-0.328820	3.649894	3.832243
C	-4.204690	1.939563	0.870459	H	-2.007309	2.503810	3.123292
C	-5.356087	1.311941	1.332411	C	0.882248	4.250637	3.504958
H	-6.197196	-0.428778	2.257834	H	2.332277	4.607870	1.948706
H	-4.273359	2.911456	0.385482	H	-0.720954	3.727464	4.843795
H	-6.320577	1.801836	1.224624	H	1.440598	4.797303	4.261493
O	-1.684445	-0.506098	1.780666	C	2.080222	-2.234288	-0.276708
C	-3.879795	-1.950966	2.752347	C	3.399537	-2.175306	0.180268
C	-2.710667	-2.651450	2.072608	C	1.798168	-2.966330	-1.440028
C	-1.637783	-1.873235	1.643125	C	4.419530	-2.823242	-0.511932
C	-2.599855	-4.032577	1.903904	H	3.642688	-1.600102	1.071744
C	-0.482810	-2.400084	1.061997	C	2.817213	-3.627423	-2.117260
C	-1.454479	-4.595174	1.347460	H	0.777463	-2.997093	-1.822200
H	-3.410689	-4.683844	2.221364	C	4.131984	-3.551493	-1.661749
C	-0.399795	-3.786569	0.934090	H	5.444838	-2.746311	-0.152300
H	-1.383526	-5.674414	1.236545	H	2.583903	-4.196432	-3.014907
H	0.489182	-4.232941	0.492660	H	4.928657	-4.056459	-2.203200
P	-1.424274	1.959166	0.217486	C	1.551318	-0.680874	2.061369
P	0.768501	-1.190556	0.480078	C	1.582194	-1.523862	3.177508
C	-3.515397	-1.726429	4.232161	C	2.205284	0.552223	2.116324
H	-2.600845	-1.130915	4.333065	C	2.257331	-1.139158	4.330413
H	-4.328778	-1.197745	4.745197	H	1.083489	-2.491949	3.141192
H	-3.354047	-2.690159	4.731469	C	2.884456	0.932921	3.271413
C	-5.154403	-2.784107	2.676341	H	2.211210	1.198798	1.239027
H	-5.020041	-3.748111	3.178290	C	2.911739	0.090124	4.378238
H	-5.980448	-2.281405	3.190402	H	2.276185	-1.801690	5.192982
H	-5.450305	-2.969923	1.636078	H	3.398792	1.891581	3.301775
Cu	-0.131543	0.476454	-0.897175	H	3.442928	0.389163	5.279227
C	-2.074129	3.333984	-0.808736	B	-1.314091	-0.689948	-2.170702
C	-2.074705	4.669307	-0.398119	O	-2.582056	-0.314710	-2.581255
C	-2.617007	2.999642	-2.054999	O	-1.181437	-2.065694	-2.200533
C	-2.595706	5.657965	-1.229512	C	-3.403560	-1.503068	-2.636683
H	-1.669123	4.940432	0.575045	C	-2.347262	-2.627868	-2.838422

C	-4.131460	-1.604082	-1.304067	H	7.961073	-0.276552	2.181235
H	-4.681786	-0.672789	-1.121788	O	3.618645	1.711949	0.278674
H	-4.845927	-2.436824	-1.294809	C	1.445440	1.668199	-1.055493
H	-3.422818	-1.743016	-0.478153	C	0.960850	1.205528	-2.372618
C	-4.401979	-1.352908	-3.765561	H	2.894944	0.071317	-0.841161
H	-4.979517	-2.276787	-3.897675	H	1.317415	2.744005	-0.878852
H	-5.105882	-0.546971	-3.529272	H	1.628956	0.473109	-2.841294
H	-3.911439	-1.107576	-4.712625	C	-1.388757	-3.308659	3.632183
C	-2.676722	-3.946939	-2.169584	C	-2.120817	-2.363455	2.915950
H	-3.594148	-4.378548	-2.590490	C	-1.667661	-2.042945	1.635176
H	-1.858354	-4.657075	-2.343221	C	-0.491728	-2.560718	1.084715
H	-2.798992	-3.839587	-1.086678	C	0.191484	-3.530274	1.824612
C	-1.982087	-2.866044	-4.296778	C	-0.257103	-3.906530	3.084523
H	-1.106242	-3.524073	-4.337497	H	-1.707248	-3.597457	4.630871
H	-2.798740	-3.348104	-4.847197	H	1.099353	-3.971550	1.418643
H	-1.723171	-1.930764	-4.807731	H	0.284518	-4.660143	3.650496
C	-0.398742	0.910626	-4.133073	O	-2.388378	-1.174969	0.856491
H	-1.165018	0.270031	-4.583967	C	-3.401389	-1.712288	3.424777
H	-0.883739	1.853379	-3.851508	C	-3.508488	-0.327473	2.800813
H	0.351687	1.141251	-4.901065	C	-3.022152	-0.145304	1.509294
				C	-4.120883	0.771165	3.406866
67-ts				C	-3.131842	1.055849	0.804291
C	2.822557	1.160678	-0.768214	C	-4.253315	1.981891	2.732697
C	4.052052	1.900449	-1.078500	H	-4.513327	0.681859	4.416946
C	4.016000	3.318069	-1.574845	C	-3.769484	2.123204	1.434922
H	4.057881	3.338522	-2.671110	H	-4.743575	2.819873	3.222026
H	3.105937	3.834659	-1.254462	H	-3.874054	3.072700	0.913055
H	4.875479	3.885005	-1.196440	P	0.146486	-1.838018	-0.483345
C	5.288963	1.104316	-1.415518	P	-2.350476	1.096119	-0.853959
H	5.123155	0.059955	-1.111629	C	-4.601906	-2.551872	2.948572
H	5.441210	1.096360	-2.505401	H	-4.630565	-2.629499	1.855569
C	6.546271	1.624414	-0.710894	H	-4.540418	-3.566280	3.362843
H	6.829902	2.601408	-1.127468	H	-5.540833	-2.093336	3.284236
H	6.298454	1.800286	0.345027	C	-3.422513	-1.639828	4.948860
C	7.690864	0.668211	-0.842676	H	-4.358320	-1.196050	5.304550
H	8.271700	0.738327	-1.766442	H	-3.369968	-2.640522	5.389815
C	8.027834	-0.291596	0.028667	H	-2.585065	-1.044602	5.334033
C	9.176772	-1.217003	-0.234850	Cu	-0.187829	0.409420	-0.903238
H	9.683520	-0.986906	-1.178035	C	1.927178	-2.314842	-0.435745
H	9.919314	-1.166024	0.574249	C	2.567850	-2.914967	-1.522864
H	8.839263	-2.263142	-0.273738	C	2.700805	-1.910657	0.663473
C	7.318653	-0.535602	1.327651	C	3.949974	-3.095831	-1.520857
H	6.380604	0.022160	1.423618	H	1.990887	-3.241950	-2.385672
H	7.086956	-1.605279	1.437835	C	4.075824	-2.107256	0.668526

H	2.230777	-1.389441	1.496580	H	0.302819	-0.554165	3.772909
C	4.708489	-2.691972	-0.427206	H	-0.167979	0.856749	4.748118
H	4.431358	-3.558967	-2.379309	H	-0.956183	0.547326	3.179872
H	4.660737	-1.783041	1.527575	C	2.379040	1.221585	3.795181
H	5.789856	-2.823852	-0.431568	H	2.304610	1.776011	4.739720
C	-0.564444	-2.922892	-1.783355	H	2.598106	0.174001	4.036204
C	-0.352071	-2.556127	-3.118903	H	3.217134	1.615335	3.212369
C	-1.332828	-4.054110	-1.504419	C	-0.408972	3.351638	3.536452
C	-0.868450	-3.325948	-4.154088	H	-0.024492	3.439475	4.560834
H	0.211404	-1.646145	-3.336751	H	-0.657132	4.359343	3.182645
C	-1.875298	-4.808793	-2.542816	H	-1.333729	2.764456	3.555002
H	-1.510317	-4.348198	-0.471108	C	1.793507	3.697301	2.420263
C	-1.637014	-4.452912	-3.866183	H	1.410038	4.620193	1.968879
H	-0.686042	-3.037673	-5.187154	H	2.271162	3.957797	3.372592
H	-2.480835	-5.682702	-2.313443	H	2.547045	3.269782	1.747063
H	-2.056022	-5.047849	-4.674489	C	0.377351	2.220656	-3.324386
C	-2.653428	2.807730	-1.440725	H	1.143563	2.805281	-3.866292
C	-3.461780	3.077843	-2.548096	H	-0.262311	1.752969	-4.088063
C	-1.949424	3.859759	-0.836628	H	-0.253507	2.946767	-2.792055
C	-3.567676	4.375339	-3.043595				
H	-4.007819	2.272249	-3.035683	**68**			
C	-2.073408	5.155740	-1.324842	C	2.541654	1.903793	-0.054336
H	-1.291661	3.653928	0.008812	C	3.779945	2.258714	0.677864
C	-2.877830	5.416465	-2.432400	C	3.797060	3.313460	1.745699
H	-4.195876	4.570996	-3.909724	H	4.274962	4.228621	1.372553
H	-1.529006	5.965922	-0.844269	H	2.780988	3.562705	2.069617
H	-2.963239	6.429293	-2.819460	H	4.362657	2.976531	2.624376
C	-3.540705	0.105825	-1.838738	C	5.106794	1.921027	0.041273
C	-4.902770	0.039849	-1.527545	H	4.919515	1.197399	-0.766402
C	-3.061271	-0.580205	-2.955317	H	5.546433	2.814512	-0.426247
C	-5.767000	-0.706874	-2.320976	C	6.095569	1.292756	1.035244
H	-5.288725	0.577858	-0.661950	H	6.559095	2.077114	1.649337
C	-3.925596	-1.329885	-3.748216	H	5.523390	0.659679	1.727843
H	-1.997584	-0.534243	-3.189697	C	7.155504	0.478988	0.355806
C	-5.278767	-1.394220	-3.430662	H	8.079745	0.994978	0.083766
H	-6.824831	-0.753816	-2.072216	C	7.037462	-0.812560	0.019322
H	-3.535695	-1.871960	-4.607654	C	8.140677	-1.549124	-0.676622
H	-5.955171	-1.983412	-4.045754	H	9.018300	-0.915507	-0.843623
B	0.573639	1.370919	0.783652	H	8.457359	-2.426676	-0.094624
O	1.292197	0.675565	1.730721	H	7.805685	-1.935143	-1.650502
O	0.033452	2.525287	1.323339	C	5.817882	-1.635202	0.315515
C	1.082235	1.297253	3.015010	H	4.950211	-1.032637	0.609729
C	0.630696	2.735689	2.622462	H	5.528312	-2.227896	-0.565169
C	-0.003292	0.499316	3.723820	H	6.017232	-2.363594	1.115500

O	3.038734	1.073160	1.012189	C	-2.338812	3.871093	4.595064
C	1.159543	2.449706	0.082159	H	-2.682074	2.461302	6.189034
C	0.849445	3.482997	-1.037287	H	-1.926071	5.035866	2.829289
H	2.733252	1.463983	-1.045892	H	-2.546818	4.739708	5.215669
H	1.044707	2.946410	1.060809	C	-0.560906	-0.934903	3.026853
H	1.549820	3.293521	-1.870842	C	0.691698	-0.526041	3.503107
C	-5.536064	-1.428202	0.612216	C	-1.055286	-2.189519	3.386129
C	-4.369514	-1.904801	0.014511	C	1.426851	-1.352990	4.342116
C	-3.159120	-1.444432	0.529729	H	1.092923	0.444654	3.204684
C	-3.063271	-0.515901	1.570906	C	-0.306897	-3.023408	4.214619
C	-4.256231	-0.072105	2.146850	H	-2.030876	-2.515820	3.027184
C	-5.481019	-0.530945	1.674866	C	0.929375	-2.605622	4.696811
H	-6.505055	-1.760360	0.247594	H	2.396455	-1.024585	4.710251
H	-4.226246	0.658729	2.952057	H	-0.697981	-4.000298	4.490157
H	-6.402605	-0.176721	2.129729	H	1.508879	-3.257203	5.346971
O	-1.976011	-1.882102	-0.012239	C	1.897538	-0.762379	-2.291170
C	-4.327470	-2.923265	-1.117325	C	3.175190	-1.319256	-2.203286
C	-3.120795	-2.600554	-1.989415	C	1.653935	0.238748	-3.241540
C	-1.972107	-2.119184	-1.365300	C	4.195760	-0.877086	-3.042782
C	-3.046647	-2.828118	-3.363848	H	3.383952	-2.092590	-1.465983
C	-0.773293	-1.864122	-2.038871	C	2.668822	0.661139	-4.092176
C	-1.864741	-2.603789	-4.065013	H	0.673466	0.714995	-3.290026
H	-3.917656	-3.199428	-3.898361	C	3.945741	0.111262	-3.988861
C	-0.732514	-2.132399	-3.408129	H	5.191740	-1.308681	-2.951742
H	-1.826258	-2.802477	-5.133054	H	2.467628	1.438536	-4.826159
H	0.185652	-1.951761	-3.963361	H	4.743826	0.456505	-4.641997
P	-1.417975	0.226149	1.905611	C	1.252727	-2.518907	-0.104180
P	0.581841	-1.111382	-1.062320	C	0.917925	-3.849894	-0.365957
C	-4.113063	-4.320461	-0.503558	C	2.165009	-2.226538	0.916444
H	-3.187358	-4.362422	0.082944	C	1.492000	-4.875477	0.379836
H	-4.950580	-4.575169	0.158056	H	0.206687	-4.087214	-1.156237
H	-4.051107	-5.076054	-1.296820	C	2.750953	-3.256342	1.645591
C	-5.621269	-2.927765	-1.923390	H	2.427504	-1.188056	1.131188
H	-5.585808	-3.689478	-2.709358	C	2.412817	-4.580976	1.381407
H	-6.476398	-3.180685	-1.287811	H	1.223900	-5.909009	0.171769
H	-5.809537	-1.952994	-2.390000	H	3.463316	-3.018092	2.433536
Cu	0.028847	0.788886	0.188147	H	2.865335	-5.384660	1.957968
C	-1.799213	1.639598	3.006200	B	-0.575502	3.167584	-1.588980
C	-2.144458	1.479939	4.352827	O	-1.760785	3.675378	-1.097665
C	-1.719019	2.926440	2.464311	O	-0.791645	2.326864	-2.665232
C	-2.414675	2.591587	5.142906	C	-2.842246	2.967127	-1.744627
H	-2.200582	0.479189	4.781678	C	-2.172175	2.449218	-3.053928
C	-1.993115	4.037960	3.257335	C	-3.265779	1.838879	-0.819793
H	-1.430498	3.050961	1.418632	H	-3.535250	2.254826	0.159040

H	-4.134927	1.294554	-1.210143	C	-2.081708	2.772889	0.339398
H	-2.447519	1.121151	-0.667263	C	-1.080102	2.162940	1.365897
C	-3.998891	3.922767	-1.952165	H	-3.051748	0.914190	-0.266615
H	-4.804332	3.436775	-2.517246	H	-2.423858	3.769955	0.675697
H	-4.404953	4.225077	-0.980269	H	-1.688298	1.615093	2.111762
H	-3.693081	4.826676	-2.486873	C	1.600026	-3.974070	-3.274084
C	-2.665225	1.101314	-3.541193	C	2.344817	-3.139063	-2.444016
H	-3.736972	1.137531	-3.776124	C	1.658127	-2.478376	-1.426422
H	-2.128018	0.824589	-4.456709	C	0.280736	-2.577075	-1.224763
H	-2.493306	0.307286	-2.805220	C	-0.425446	-3.441328	-2.068371
C	-2.221560	3.461408	-4.190274	C	0.231135	-4.135303	-3.078477
H	-1.563761	3.118674	-4.996540	H	2.090996	-4.511196	-4.082225
H	-3.234250	3.567337	-4.596137	H	-1.500238	-3.557793	-1.947750
H	-1.871255	4.447148	-3.862420	H	-0.331952	-4.801371	-3.727285
C	1.036530	4.920219	-0.554971	O	2.342599	-1.667285	-0.557427
H	0.877895	5.663890	-1.348442	C	3.851275	-2.941804	-2.527722
H	0.321572	5.144919	0.250362	C	4.143220	-1.502914	-2.127456
H	2.045467	5.070695	-0.145267	C	3.390419	-0.958121	-1.089595
				C	5.160000	-0.709469	-2.656875
69				C	3.632701	0.295800	-0.528566
C	-3.269219	1.865101	0.227849	C	5.414833	0.559674	-2.143670
C	-4.383983	1.827168	1.174486	H	5.768565	-1.084125	-3.475853
C	-4.490385	2.793558	2.321851	C	4.668833	1.055423	-1.078758
H	-4.218144	2.297057	3.262156	H	6.212569	1.162856	-2.569652
H	-3.833740	3.658042	2.186361	H	4.886117	2.043999	-0.678278
H	-5.518423	3.162758	2.425044	P	-0.510289	-1.442650	-0.001806
C	-5.129314	0.523872	1.334325	P	2.493214	0.863127	0.795094
H	-4.966650	-0.078253	0.428373	C	4.520250	-3.868540	-1.492789
H	-4.704061	-0.049941	2.173894	H	4.162148	-3.663895	-0.476088
C	-6.634771	0.725276	1.532037	H	4.300624	-4.917484	-1.728625
H	-6.824744	1.151676	2.527202	H	5.608141	-3.726521	-1.507449
H	-6.971987	1.481517	0.808251	C	4.395128	-3.276709	-3.911392
C	-7.409908	-0.545941	1.367206	H	5.482517	-3.148099	-3.941967
H	-7.542897	-1.157448	2.263480	H	4.198796	-4.325115	-4.160900
C	-7.906353	-1.013507	0.214376	H	3.947774	-2.645298	-4.688292
C	-8.647644	-2.313863	0.151805	Cu	0.142101	0.785020	0.567365
H	-8.758203	-2.772287	1.140447	C	-2.271628	-1.779236	-0.397441
H	-9.650987	-2.178503	-0.277008	C	-3.051238	-2.724470	0.273290
H	-8.132588	-3.033540	-0.502063	C	-2.806507	-1.114804	-1.508515
C	-7.780492	-0.294262	-1.096418	C	-4.343273	-3.006929	-0.164073
H	-7.047269	0.519247	-1.075623	H	-2.645255	-3.252790	1.133864
H	-7.478899	-0.991641	-1.890659	C	-4.091751	-1.407144	-1.951761
H	-8.747901	0.122975	-1.410965	H	-2.216093	-0.350195	-2.017410
O	-4.546091	2.406169	-0.131531	C	-4.857565	-2.359649	-1.282874

H	-4.946284	-3.742212	0.364855	H	1.025406	1.178792	-1.715108
H	-4.500781	-0.885557	-2.814459	C	-0.972839	2.005256	-4.410062
H	-5.859963	-2.595973	-1.634136	H	-0.202698	2.221251	-5.161293
C	-0.271333	-2.261887	1.618948	H	-1.294571	0.966027	-4.546728
C	-0.952933	-1.716935	2.715900	H	-1.834814	2.652036	-4.595151
C	0.585776	-3.345461	1.818122	C	1.552370	3.855410	-2.856194
C	-0.799080	-2.266624	3.982561	H	1.827259	3.754614	-3.913766
H	-1.619456	-0.864795	2.567676	H	1.808670	4.872199	-2.535009
C	0.751018	-3.883437	3.091890	H	2.160428	3.155480	-2.273550
H	1.122658	-3.778541	0.975058	C	-0.714104	4.707152	-3.409268
C	0.056813	-3.349442	4.172902	H	-0.456185	5.681130	-2.979432
H	-1.341528	-1.843564	4.825226	H	-0.470427	4.727265	-4.477526
H	1.423944	-4.725482	3.237595	H	-1.795460	4.564916	-3.300226
H	0.184818	-3.774813	5.165859	C	-0.361127	3.285695	2.101515
C	3.222807	2.497859	1.178927	H	-1.067043	3.948997	2.639359
C	4.357564	2.657211	1.979917	H	0.362999	2.913293	2.841495
C	2.661360	3.613697	0.553464	H	0.199726	3.929517	1.409990
C	4.924139	3.917152	2.145555				
H	4.806546	1.791708	2.466793	**70-ts**			
C	3.235466	4.871482	0.711216	C	5.080834	1.556323	-1.449981
H	1.758747	3.496797	-0.047142	C	4.076213	0.681978	-1.869153
C	4.366904	5.023676	1.507711	C	2.785078	0.946298	-1.417882
H	5.806084	4.035386	2.770858	C	2.467295	1.994609	-0.549531
H	2.789987	5.733577	0.218702	C	3.499672	2.848466	-0.159596
H	4.814186	6.006721	1.636788	C	4.796855	2.632685	-0.614807
C	2.960190	-0.151156	2.248415	H	6.104358	1.405407	-1.784482
C	4.085126	-0.978059	2.293320	H	3.288245	3.675041	0.516785
C	2.128938	-0.063321	3.370666	H	5.595979	3.303722	-0.310197
C	4.377667	-1.700202	3.447264	O	1.737911	0.154493	-1.810062
H	4.738942	-1.053981	1.424777	C	4.294921	-0.476584	-2.835696
C	2.431562	-0.773853	4.526434	C	3.256216	-1.551856	-2.541080
H	1.236505	0.564008	3.333616	C	2.010786	-1.168740	-2.047201
C	3.555128	-1.595487	4.565110	C	3.447714	-2.911811	-2.786287
H	5.255385	-2.342128	3.473474	C	0.976610	-2.067931	-1.772538
H	1.781906	-0.694596	5.395090	C	2.432311	-3.834240	-2.552663
H	3.787716	-2.158158	5.466403	H	4.400985	-3.261630	-3.175285
B	-1.285954	2.857619	-1.005770	C	1.204469	-3.416748	-2.050690
O	-1.491665	1.992168	-2.063380	H	2.600684	-4.887115	-2.764557
O	-0.273025	3.756634	-1.274359	H	0.419409	-4.144826	-1.858105
C	-0.420890	2.182120	-3.009579	P	0.746058	2.072754	0.086118
C	0.065382	3.626481	-2.672907	P	-0.548593	-1.406047	-0.992034
C	0.630312	1.112782	-2.739803	C	4.068582	0.036921	-4.269597
H	0.175708	0.120036	-2.855958	H	3.056066	0.439641	-4.394714
H	1.473548	1.185294	-3.438439	H	4.785731	0.833523	-4.504828

H	4.203086	-0.779311	-4.990562	C	-3.528130	0.316089	-3.207291
C	5.711048	-1.034062	-2.717983	H	-3.161378	-0.225979	-1.153850
H	5.876819	-1.838929	-3.441487	C	-2.995883	0.406878	-4.490929
H	6.456597	-0.263647	-2.939469	H	-1.273347	0.033447	-5.728739
H	5.900911	-1.425955	-1.710528	H	-4.533246	0.682772	-3.001700
Cu	-0.262606	0.103176	0.789809	H	-3.583859	0.834928	-5.299794
C	0.881702	3.366166	1.378197	B	1.152509	-1.671320	3.054629
C	0.688616	4.728325	1.137060	O	2.123476	-0.973681	3.738181
C	1.192581	2.936743	2.674007	O	1.688569	-2.464655	2.060076
C	0.812335	5.647356	2.176004	C	3.364145	-1.147199	3.017910
H	0.440761	5.072041	0.133530	C	3.119882	-2.477850	2.245080
C	1.326389	3.856798	3.707634	C	3.511431	0.042824	2.086948
H	1.310616	1.869541	2.866714	H	3.491959	0.969780	2.672804
C	1.133541	5.213757	3.459306	H	4.454951	0.006329	1.529095
H	0.657261	6.706203	1.981516	H	2.681884	0.077088	1.367337
H	1.569878	3.513739	4.710510	C	4.509246	-1.184115	4.008201
H	1.229091	5.934465	4.268118	H	5.453780	-1.410173	3.497537
C	-0.169250	2.890376	-1.270228	H	4.612814	-0.204416	4.488169
C	-1.557382	2.716051	-1.295649	H	4.348960	-1.929552	4.792482
C	0.447743	3.673787	-2.251213	C	3.790310	-2.565898	0.889908
C	-2.316672	3.335259	-2.283227	H	4.882972	-2.528829	0.991268
H	-2.035805	2.070280	-0.554645	H	3.523978	-3.513629	0.406240
C	-0.316443	4.280403	-3.243041	H	3.472895	-1.755885	0.224763
H	1.528673	3.811323	-2.236843	C	3.446436	-3.714665	3.070029
C	-1.699556	4.115034	-3.257113	H	3.068570	-4.600220	2.547443
H	-3.394759	3.185530	-2.302773	H	4.527196	-3.833386	3.208427
H	0.168886	4.885139	-4.005895	H	2.970819	-3.673628	4.057092
H	-2.294891	4.590722	-4.033354	C	-2.275560	-0.262599	2.377315
C	-1.469422	-2.941028	-0.572806	C	-3.125908	0.883724	2.046724
C	-2.683076	-3.310904	-1.156115	C	-2.645202	2.276454	2.383323
C	-0.934825	-3.741339	0.447485	H	-2.875456	2.530941	3.426023
C	-3.350899	-4.457149	-0.729005	H	-1.564665	2.367515	2.231949
H	-3.118580	-2.704045	-1.947644	H	-3.140328	3.014557	1.738707
C	-1.597595	-4.890870	0.861151	C	-4.633770	0.718959	2.175625
H	0.010514	-3.461210	0.916445	H	-4.870875	-0.352881	2.122611
C	-2.811185	-5.249928	0.277574	H	-4.987539	1.075463	3.154142
H	-4.297137	-4.729438	-1.191829	C	-5.368628	1.439403	1.036221
H	-1.167896	-5.504916	1.649834	H	-5.417216	2.516294	1.245530
H	-3.334038	-6.144356	0.608492	H	-4.751748	1.331652	0.129188
C	-1.480282	-0.709191	-2.414178	C	-6.752031	0.911842	0.787302
C	-0.951625	-0.610657	-3.703860	H	-7.586265	1.506864	1.166699
C	-2.769321	-0.214571	-2.170753	C	-7.045073	-0.235039	0.159165
C	-1.700925	-0.041825	-4.731297	C	-8.461681	-0.681119	-0.038731
H	0.049436	-0.984075	-3.915282	H	-9.180748	0.037632	0.368928

H	-8.685380	-0.820644	-1.106248	C	5.655001	0.097061	-3.123527
H	-8.641501	-1.654648	0.439483	H	5.798090	-0.457522	-4.056703
C	-6.010888	-1.170367	-0.395191	H	6.338894	0.951003	-3.167117
H	-4.982395	-0.878454	-0.155312	H	5.951882	-0.546130	-2.285452
H	-6.167393	-2.185598	-0.002404	Cu	-0.622960	0.250189	0.411555
H	-6.098643	-1.251496	-1.489169	C	0.961035	2.573558	2.422782
O	-2.669140	0.376187	0.811905	C	0.746034	3.872121	2.889153
C	-0.888572	-0.273634	2.741278	C	1.310754	1.566291	3.330802
C	-0.373570	-1.574215	3.372223	C	0.878594	4.157338	4.246418
H	-2.802237	-1.222330	2.375016	H	0.467006	4.660966	2.191405
H	-0.570954	0.613927	3.308731	C	1.451122	1.855484	4.682536
H	-0.871415	-2.413480	2.857622	H	1.451168	0.541847	2.982346
C	-0.686698	-1.653775	4.868364	C	1.229938	3.152106	5.142873
H	-0.339166	-2.590494	5.326700	H	0.703958	5.169326	4.604483
H	-0.200794	-0.826688	5.404199	H	1.717626	1.060954	5.376988
H	-1.768024	-1.570080	5.047564	H	1.324946	3.378048	6.202391
				C	-0.196101	3.458186	-0.081043
71				C	-1.595347	3.426199	-0.005415
C	5.004615	2.064698	-1.043627	C	0.441960	4.536572	-0.700873
C	3.996897	1.369796	-1.710982	C	-2.338859	4.472071	-0.544141
C	2.704592	1.458948	-1.190736	H	-2.093041	2.560920	0.449086
C	2.397734	2.179668	-0.032390	C	-0.310408	5.575374	-1.241481
C	3.433457	2.879132	0.592829	H	1.529274	4.566607	-0.759780
C	4.727109	2.823995	0.089469	C	-1.700156	5.544378	-1.162009
H	6.026370	2.023107	-1.412221	H	-3.425492	4.441753	-0.490230
H	3.221387	3.449888	1.495748	H	0.190572	6.410368	-1.726116
H	5.527308	3.366594	0.586191	H	-2.285973	6.356029	-1.587763
O	1.673446	0.796148	-1.812815	C	-1.469501	-2.588046	-1.400346
C	4.210122	0.564771	-2.986747	C	-2.731331	-2.767900	-1.968508
C	3.239191	-0.608363	-2.964700	C	-0.935565	-3.589403	-0.578469
C	1.984073	-0.413549	-2.389685	C	-3.446306	-3.939075	-1.725456
C	3.487859	-1.852087	-3.546615	H	-3.162242	-1.987716	-2.595080
C	0.991177	-1.399121	-2.365110	C	-1.646388	-4.760920	-0.349086
C	2.514548	-2.846977	-3.561477	H	0.038553	-3.447261	-0.106257
H	4.452005	-2.049725	-4.008420	C	-2.906570	-4.935760	-0.919549
C	1.272388	-2.622111	-2.978211	H	-4.430413	-4.071046	-2.170273
H	2.727030	-3.803744	-4.031744	H	-1.220201	-5.532348	0.289049
H	0.516459	-3.405334	-2.980808	H	-3.468979	-5.847085	-0.729809
P	0.712319	2.064784	0.682386	C	-1.493265	-0.031039	-2.751731
P	-0.571153	-1.001846	-1.498624	C	-1.228595	-0.145915	-4.120126
C	3.859052	1.460599	-4.190038	C	-2.516319	0.819646	-2.313198
H	2.825002	1.819259	-4.134763	C	-1.971796	0.584218	-5.041671
H	4.523803	2.333221	-4.217699	H	-0.439827	-0.812077	-4.467674
H	3.978280	0.900076	-5.125754	C	-3.258783	1.543653	-3.242720

H	-2.738875	0.892336	-1.245187	H	-8.220224	-1.833180	-0.661089
C	-2.987026	1.431149	-4.603268	C	-5.821820	-0.438196	-1.093403
H	-1.758793	0.490752	-6.104215	H	-4.808832	-0.192681	-0.752513
H	-4.053509	2.202471	-2.897005	H	-5.810876	-1.474698	-1.461444
H	-3.567304	2.002558	-5.324346	H	-6.055784	0.188917	-1.966892
B	1.208389	-2.635964	2.639571	O	-2.546791	0.472390	0.796181
O	2.227521	-1.816885	3.056814	C	-0.971134	-1.385870	3.129304
O	1.583013	-3.474741	1.622084	C	-0.217019	-2.676429	3.296853
C	3.316709	-1.974960	2.113451	H	-2.350952	-2.084282	1.720479
C	3.017372	-3.368149	1.476849	H	-0.621604	-0.549591	3.745756
C	3.209165	-0.836477	1.115406	H	-0.782534	-3.476421	2.792998
H	3.308130	0.120661	1.641289	C	-0.068830	-3.014793	4.787907
H	4.000748	-0.884238	0.357097	H	0.472701	-3.956718	4.941601
H	2.232403	-0.846033	0.608511	H	0.492049	-2.223784	5.303719
C	4.628185	-1.884378	2.864135	H	-1.047593	-3.102232	5.275039
H	5.471999	-2.055456	2.184044				
H	4.735895	-0.880822	3.290766	**72-ts**			
H	4.684798	-2.609260	3.681181	C	4.125083	-3.475150	3.001176
C	3.359318	-3.482999	0.006579	C	3.513945	-3.473078	1.748198
H	4.429322	-3.306499	-0.163622	C	3.036941	-2.250703	1.277700
H	3.120148	-4.491725	-0.350290	C	3.147035	-1.051977	1.984225
H	2.786132	-2.769737	-0.594541	C	3.777909	-1.095073	3.229927
C	3.619552	-4.526882	2.256205	C	4.258755	-2.298502	3.733273
H	3.204024	-5.464997	1.872783	H	4.509272	-4.404268	3.415208
H	4.709270	-4.563626	2.145937	H	3.874757	-0.182566	3.814716
H	3.378793	-4.460269	3.324297	H	4.741835	-2.321925	4.706771
C	-2.035020	-1.227468	2.331854	O	2.423701	-2.183481	0.050552
C	-2.852539	0.024567	2.075211	C	3.401213	-4.681608	0.829319
C	-2.580567	1.114942	3.115775	C	2.094316	-4.554379	0.058085
H	-2.841640	0.799840	4.135969	C	1.684338	-3.277714	-0.320814
H	-1.522911	1.411286	3.104205	C	1.305641	-5.624940	-0.361577
H	-3.170621	2.006091	2.866773	C	0.540245	-3.025790	-1.080976
C	-4.341627	-0.380479	2.118547	C	0.169855	-5.414709	-1.138073
H	-4.460519	-1.238880	1.439084	H	1.580702	-6.640989	-0.089349
H	-4.618566	-0.735117	3.124687	C	-0.210546	-4.126630	-1.500042
C	-5.279915	0.736951	1.654505	H	-0.425388	-6.264021	-1.463445
H	-5.425970	1.465000	2.464578	H	-1.104882	-3.974730	-2.100904
H	-4.757368	1.269392	0.846503	P	2.360956	0.446935	1.271706
C	-6.614277	0.240640	1.181710	P	0.074928	-1.275476	-1.388328
H	-7.444230	0.290296	1.891837	C	4.563674	-4.622963	-0.181685
C	-6.864838	-0.282333	-0.026090	H	4.549431	-3.690005	-0.758081
C	-8.231567	-0.762995	-0.408328	H	5.524325	-4.685679	0.344885
H	-8.961888	-0.610376	0.393881	H	4.495080	-5.461553	-0.886062
H	-8.596872	-0.242605	-1.305759	C	3.486127	-5.995004	1.597594

H	3.432650	-6.848589	0.913477	C	3.108752	0.320795	-4.486619
H	4.446707	-6.077693	2.117227	H	2.501477	2.266807	-3.781936
H	2.681078	-6.089005	2.335875	H	3.536965	-1.735988	-4.961975
Cu	0.214822	0.067789	0.423040	H	3.813474	0.716850	-5.214329
C	2.483837	1.636380	2.655661	O	-1.062047	0.045493	2.182358
C	3.633461	2.385563	2.926896	C	-2.282098	-0.609612	2.048433
C	1.375592	1.737017	3.503674	H	-2.864750	-0.597190	2.990300
C	3.673214	3.228025	4.032824	H	-2.922131	-0.149824	1.269693
H	4.500953	2.308326	2.272449	H	-2.154416	-1.674039	1.774061
C	1.424666	2.575606	4.613750	H	-1.106091	1.129519	1.634180
H	0.477970	1.154950	3.285170	B	-5.738109	0.358897	-0.111010
C	2.569196	3.322721	4.877125	O	-6.760612	0.818514	0.680261
H	4.569085	3.809425	4.238802	O	-5.318669	-0.900743	0.239403
H	0.561619	2.650529	5.271485	C	-6.836035	-0.079640	1.812276
H	2.602019	3.981784	5.741833	C	-6.256011	-1.397567	1.222595
C	3.599656	1.060381	0.065895	C	-5.959079	0.528660	2.897753
C	3.436271	2.365829	-0.411451	H	-6.323824	1.537851	3.118438
C	4.647718	0.283799	-0.432431	H	-5.988972	-0.057576	3.823355
C	4.316875	2.894870	-1.345791	H	-4.915720	0.610402	2.565921
H	2.612834	2.978334	-0.042761	C	-8.270896	-0.170546	2.283971
C	5.520728	0.809972	-1.382199	H	-8.364988	-0.916608	3.083019
H	4.794962	-0.733872	-0.072868	H	-8.589943	0.796724	2.687419
C	5.362999	2.115727	-1.835275	H	-8.951827	-0.439710	1.471516
H	4.176206	3.916562	-1.696028	C	-5.518406	-2.277391	2.209362
H	6.335350	0.196189	-1.760248	H	-6.201484	-2.637199	2.989187
H	6.052239	2.524717	-2.570572	H	-5.113570	-3.151903	1.686653
C	-1.452150	-1.498564	-2.375077	H	-4.685583	-1.755588	2.690108
C	-1.429355	-1.649416	-3.765222	C	-7.288724	-2.219826	0.464587
C	-2.665078	-1.632327	-1.691115	H	-6.771193	-3.009289	-0.092511
C	-2.598949	-1.944049	-4.458285	H	-8.005968	-2.695490	1.143106
H	-0.490794	-1.546799	-4.307668	H	-7.844100	-1.603990	-0.252500
C	-3.830562	-1.944971	-2.385527	C	-2.734069	1.945040	-0.491705
H	-2.709512	-1.498045	-0.608556	C	-1.700108	2.778151	0.228434
C	-3.798463	-2.100509	-3.768328	C	-2.326865	3.690469	1.279034
H	-2.571249	-2.057688	-5.539504	H	-3.000980	4.435770	0.837525
H	-4.762396	-2.041487	-1.832315	H	-2.897936	3.089833	2.000218
H	-4.710311	-2.338965	-4.311127	H	-1.538602	4.217022	1.827707
C	1.306178	-0.698268	-2.613302	C	-0.962610	3.593260	-0.847386
C	1.481940	0.682051	-2.747195	H	-0.594465	2.870194	-1.595912
C	2.054087	-1.565124	-3.413911	H	-1.675942	4.245483	-1.373750
C	2.370764	1.189920	-3.687969	C	0.219420	4.403200	-0.320534
H	0.929056	1.361508	-2.093586	H	-0.136056	5.289075	0.222208
C	2.954918	-1.055919	-4.344238	H	0.729985	3.770259	0.425932
H	1.928008	-2.642686	-3.310117	C	1.168197	4.772390	-1.414911

H	1.477297	3.923670	-2.038546	C	0.619429	0.234074	-0.603369
C	1.680161	5.970267	-1.727375	C	1.644126	-0.736579	-0.076529
C	2.630977	6.127797	-2.876801	C	1.534257	-0.968323	1.423414
H	2.815108	5.178403	-3.393602	H	1.797529	-0.068377	1.993242
H	2.246171	6.847208	-3.613610	H	0.512628	-1.260516	1.699495
H	3.598173	6.526801	-2.537039	H	2.207124	-1.777013	1.725082
C	1.385560	7.245006	-0.997360	C	3.035227	-0.235134	-0.472784
H	0.667586	7.124580	-0.181773	H	3.041989	-0.097452	-1.564843
H	2.307283	7.668303	-0.573846	H	3.181691	0.763109	-0.032638
H	0.991289	8.002671	-1.688958	C	4.198380	-1.144775	-0.074503
O	-0.751828	1.956514	0.858391	H	4.262406	-1.209238	1.019939
C	-4.060980	2.086058	-0.455080	H	3.986541	-2.161289	-0.431244
C	-5.054985	1.246116	-1.212368	C	5.494020	-0.659516	-0.649444
H	-2.299497	1.166750	-1.133233	H	5.703139	-0.971700	-1.676474
H	-4.507569	2.855717	0.184109	C	6.382247	0.151009	-0.059332
H	-4.505095	0.603619	-1.915603	C	7.631525	0.583369	-0.765444
C	-6.056576	2.128047	-1.960494	H	7.707340	0.152974	-1.769604
H	-6.783717	1.530292	-2.522375	H	7.675378	1.677921	-0.857330
H	-6.620787	2.752859	-1.256386	H	8.526267	0.288713	-0.198568
H	-5.549315	2.796346	-2.666864	C	6.229873	0.706591	1.324190
				H	5.303067	0.398345	1.817801
73				H	7.073271	0.406404	1.961822
H	0.574425	-2.280252	-0.591211	H	6.244468	1.805106	1.296638
B	-2.565021	1.013173	-0.288760	O	1.474035	-1.979389	-0.767446
O	-3.164670	0.841586	0.933668	C	-0.210882	1.000605	0.106177
O	-3.107399	0.230744	-1.271907	C	-1.276037	1.893156	-0.469942
C	-3.956349	-0.364110	0.824051	H	0.587672	0.283838	-1.696779
C	-4.274151	-0.409131	-0.699725	H	-0.195566	0.953368	1.200023
C	-3.058202	-1.506226	1.278547	H	-1.079769	2.039305	-1.541581
H	-2.705348	-1.293118	2.293864	C	-1.345662	3.233258	0.260776
H	-3.589606	-2.464374	1.291907	H	-2.134116	3.875684	-0.146659
H	-2.178329	-1.599395	0.628349	H	-1.563643	3.079662	1.325429
C	-5.165474	-0.251931	1.726381	H	-0.396704	3.778413	0.191340
H	-5.827545	-1.116093	1.591618				
H	-4.845346	-0.232784	2.773955	**74**			
H	-5.735883	0.660007	1.528805	C	-1.767424	-2.037473	-0.736654
C	-4.407957	-1.799802	-1.282123	C	-2.713002	-2.110026	0.441373
H	-5.224989	-2.344998	-0.793112	C	-2.163822	-2.902653	1.618982
H	-4.640762	-1.732157	-2.350465	H	-2.840254	-2.803630	2.474344
H	-3.485964	-2.377446	-1.172203	H	-2.065696	-3.968524	1.378364
C	-5.477418	0.438312	-1.083481	H	-1.177521	-2.533817	1.929000
H	-5.509258	0.533677	-2.174133	C	-4.028642	-2.702469	-0.073844
H	-6.415428	-0.021699	-0.752459	H	-4.358395	-2.077581	-0.918608
H	-5.412101	1.445044	-0.655064	H	-3.824977	-3.702525	-0.484293

C	-5.161181	-2.774917	0.952077	C	2.619889	0.448873	1.465928
H	-4.905315	-3.498148	1.738277	C	3.829428	-0.030772	1.959332
H	-5.247449	-1.798931	1.446672	C	5.029708	0.535414	1.534228
C	-6.461011	-3.171610	0.316346	H	5.978860	1.984340	0.278442
H	-6.692402	-4.239786	0.310572	H	3.834913	-0.865308	2.658347
C	-7.329392	-2.346948	-0.283802	H	5.972885	0.157607	1.921026
C	-8.586743	-2.860184	-0.916493	O	1.434167	2.018985	0.214751
H	-8.681963	-3.946929	-0.820084	C	3.790338	3.286758	-0.847961
H	-9.474167	-2.396823	-0.462085	C	2.421687	3.362957	-1.515132
H	-8.622996	-2.606478	-1.985435	C	1.320040	2.735618	-0.940497
C	-7.135294	-0.864663	-0.393701	C	2.182748	4.107190	-2.672203
H	-6.226309	-0.509723	0.101944	C	0.033107	2.781503	-1.487925
H	-7.077582	-0.562743	-1.449405	C	0.909173	4.213267	-3.220989
H	-7.992849	-0.325373	0.032416	H	3.006917	4.628281	-3.154257
O	-3.045785	-0.781347	0.876370	C	-0.163306	3.548430	-2.635855
C	-0.629164	-2.754510	-0.913027	H	0.754703	4.809432	-4.116381
H	-0.248692	-3.349202	-0.074189	H	-1.151319	3.601238	-3.089152
C	0.159820	-2.884950	-2.164156	P	0.978126	-0.291661	1.813503
H	-0.367599	-2.342951	-2.969513	P	-1.242374	1.665966	-0.775215
B	1.636349	-2.180142	-1.944740	C	3.992681	4.566531	-0.017326
O	2.571409	-2.436381	-3.025954	H	3.212138	4.663101	0.747942
O	2.309185	-2.633199	-0.726984	H	4.966840	4.547690	0.487422
C	3.863955	-2.532923	-2.451691	H	3.952618	5.453967	-0.661588
C	3.571614	-3.185670	-1.068303	C	4.894231	3.178109	-1.902429
C	4.748026	-3.361924	-3.367258	H	4.907890	4.057451	-2.554525
H	4.918205	-2.821647	-4.306766	H	5.882842	3.123977	-1.435619
H	5.726853	-3.554674	-2.908031	H	4.756000	2.285777	-2.525256
H	4.280200	-4.320827	-3.612456	Cu	-0.149904	-0.414329	-0.294524
C	4.471087	-1.134311	-2.306724	C	1.389481	-1.717892	2.898937
H	5.509934	-1.169860	-1.953054	C	1.431705	-1.603870	4.292907
H	4.467982	-0.650165	-3.291841	C	1.690746	-2.948746	2.302462
H	3.885526	-0.515230	-1.613836	C	1.769389	-2.702310	5.077686
C	3.439999	-4.706243	-1.150565	H	1.203000	-0.653106	4.771295
H	4.415005	-5.200324	-1.251072	C	2.035126	-4.041131	3.093453
H	2.972983	-5.062278	-0.221458	H	1.693044	-3.035831	1.213802
H	2.805332	-5.012519	-1.987493	C	2.071396	-3.922591	4.480213
C	4.594284	-2.860289	0.008411	H	1.798021	-2.601950	6.160279
H	4.314340	-3.353898	0.949400	H	2.276097	-4.990960	2.618868
H	5.589274	-3.227839	-0.278433	H	2.335674	-4.779770	5.095412
H	4.662398	-1.786040	0.201945	C	0.250974	0.887732	3.021040
H	-2.211009	-0.290989	0.931771	C	-1.083770	0.705777	3.399966
C	5.028292	1.566324	0.602927	C	0.984509	1.924469	3.603309
C	3.835223	2.091370	0.096640	C	-1.671245	1.544908	4.339483
C	2.658351	1.525872	0.572704	H	-1.676807	-0.100661	2.965058

C	0.391784	2.770708	4.536188	H	-1.816320	-4.262752	1.820331
H	2.029604	2.069920	3.334251	H	-0.965092	-2.826852	2.442522
C	-0.936683	2.583829	4.903975	C	-3.799342	-2.922499	0.424745
H	-2.712038	1.396096	4.618352	H	-4.094933	-2.286788	-0.424470
H	0.973196	3.576274	4.979073	H	-3.609587	-3.924051	0.008239
H	-1.401398	3.248352	5.629005	C	-4.963670	-2.971360	1.418148
C	-2.506497	1.636682	-2.102156	H	-4.792064	-3.759587	2.163830
C	-2.366255	0.672919	-3.106991	H	-4.977949	-2.022695	1.971867
C	-3.562104	2.550037	-2.178713	C	-6.279674	-3.199339	0.732122
C	-3.268634	0.616307	-4.163861	H	-6.685973	-4.213502	0.758068
H	-1.535669	-0.032196	-3.062453	C	-6.964291	-2.273639	0.046702
C	-4.468485	2.487954	-3.232738	C	-8.246732	-2.602291	-0.654567
H	-3.677987	3.312927	-1.411061	H	-8.523043	-3.655466	-0.534740
C	-4.324931	1.521115	-4.223870	H	-9.075033	-1.985519	-0.277272
H	-3.148498	-0.138297	-4.937367	H	-8.173584	-2.388901	-1.730766
H	-5.287987	3.201101	-3.281186	C	-6.508104	-0.853674	-0.110323
H	-5.036310	1.473408	-5.044862	H	-5.648509	-0.604075	0.521350
C	-2.018612	2.690017	0.538391	H	-6.214068	-0.654692	-1.152874
C	-3.268611	2.323491	1.055846	H	-7.321794	-0.150874	0.117940
C	-1.375884	3.818910	1.053383	O	-2.821687	-1.064706	1.504052
C	-3.867116	3.086980	2.051120	C	-0.689896	-3.264510	-0.629606
H	-3.778234	1.439490	0.675850	H	-0.403301	-4.007524	0.129220
C	-1.970013	4.567927	2.064560	C	-0.154011	-3.474599	-1.886506
H	-0.405725	4.120494	0.662341	H	-0.543892	-2.836137	-2.688923
C	-3.218185	4.208273	2.560785	B	1.705911	-2.179251	-1.679834
H	-4.842918	2.797932	2.435063	O	2.449865	-2.681263	-2.753777
H	-1.453997	5.439479	2.461024	O	2.342235	-2.426417	-0.461457
H	-3.684791	4.799115	3.345794	C	3.769644	-2.922313	-2.240763
C	1.297592	0.010570	-3.017025	C	3.509940	-3.214022	-0.726805
H	2.306325	0.305541	-3.347198	C	4.403694	-4.063606	-3.008144
H	0.703204	0.925528	-2.916077	H	4.548006	-3.771264	-4.054659
H	0.856759	-0.596797	-3.824228	H	5.386845	-4.313019	-2.589224
O	1.339184	-0.683325	-1.796471	H	3.778139	-4.961343	-2.990097
H	-2.200400	-1.534933	-1.607825	C	4.568722	-1.640844	-2.460483
C	0.250686	-4.363108	-2.541209	H	5.614799	-1.745630	-2.148036
H	0.904696	-4.497764	-3.411077	H	4.551293	-1.396276	-3.528968
H	0.682133	-4.942681	-1.713284	H	4.126173	-0.799051	-1.910909
H	-0.729608	-4.802822	-2.772345	C	3.189053	-4.672925	-0.434568
				H	4.081694	-5.305690	-0.509525
75-ts				H	2.804950	-4.746138	0.590173
C	-1.504560	-2.178892	-0.195204	H	2.426202	-5.063471	-1.111497
C	-2.479074	-2.360062	0.961888	C	4.632319	-2.766177	0.192110
C	-1.937257	-3.209765	2.104530	H	4.343555	-2.940380	1.237763
H	-2.628179	-3.167478	2.954002	H	5.546510	-3.339205	-0.011075

H	4.853378	-1.701458	0.075025	C	0.844865	1.357630	2.834235
H	-2.000916	-0.551160	1.441514	C	-0.341285	1.114719	3.534230
C	4.865899	2.080867	-0.685614	C	1.556908	2.531822	3.090233
C	3.545984	2.474815	-0.915439	C	-0.802064	2.024451	4.478297
C	2.564275	1.867404	-0.136804	H	-0.911295	0.203726	3.338533
C	2.831796	0.888899	0.825811	C	1.090744	3.445776	4.031185
C	4.165076	0.549276	1.045480	H	2.481734	2.734041	2.549774
C	5.175243	1.139456	0.290056	C	-0.088496	3.194563	4.725053
H	5.672043	2.529720	-1.260793	H	-1.729193	1.826240	5.011557
H	4.412538	-0.194096	1.800886	H	1.652048	4.358086	4.221221
H	6.212063	0.860592	0.463079	H	-0.457018	3.912693	5.454295
O	1.249991	2.235159	-0.257486	C	-3.007681	1.167202	-1.641119
C	3.145051	3.596265	-1.865112	C	-2.974404	0.153974	-2.606902
C	1.713176	3.358339	-2.326532	C	-4.139692	1.983636	-1.557419
C	0.824190	2.719191	-1.464158	C	-4.050711	-0.043206	-3.466174
C	1.194590	3.818160	-3.537719	H	-2.087916	-0.473930	-2.699220
C	-0.528614	2.519191	-1.754382	C	-5.215610	1.787692	-2.418272
C	-0.151457	3.658753	-3.852702	H	-4.177789	2.784543	-0.821398
H	1.846841	4.320634	-4.247897	C	-5.173728	0.774849	-3.372859
C	-1.010409	3.017908	-2.966847	H	-4.009067	-0.833811	-4.211483
H	-0.532398	4.036592	-4.798094	H	-6.088316	2.432747	-2.345919
H	-2.056750	2.876571	-3.230320	H	-6.014925	0.623877	-4.045330
P	1.385130	0.088722	1.619617	C	-2.085142	2.562636	0.689006
P	-1.495766	1.429642	-0.630118	C	-3.098010	2.115084	1.549273
C	3.177113	4.919220	-1.075905	C	-1.544437	3.836005	0.881620
H	2.503240	4.883638	-0.210324	C	-3.572510	2.939499	2.562197
H	4.192391	5.117283	-0.709514	H	-3.523226	1.119518	1.419588
H	2.867039	5.753440	-1.717984	C	-2.007111	4.648820	1.913129
C	4.104113	3.697643	-3.048387	H	-0.763447	4.202630	0.216461
H	3.830043	4.531761	-3.702440	C	-3.025966	4.206362	2.749964
H	5.125521	3.899063	-2.709823	H	-4.367589	2.585324	3.214817
H	4.109460	2.775090	-3.641271	H	-1.575375	5.637616	2.052748
Cu	-0.211279	-0.546155	0.066911	H	-3.393120	4.847139	3.548657
C	2.116376	-1.167388	2.740077	C	0.813998	-0.446881	-3.083766
C	2.911166	-0.810851	3.835635	H	1.772506	-0.218282	-3.570481
C	1.827107	-2.515427	2.516704	H	0.227316	0.474659	-3.012285
C	3.426989	-1.788513	4.678897	H	0.273247	-1.163797	-3.719563
H	3.122587	0.240344	4.032983	O	1.019850	-0.954420	-1.783876
C	2.327847	-3.492792	3.373728	H	-2.040853	-1.726386	-1.040736
H	1.226148	-2.789259	1.651252	C	0.273433	-4.845704	-2.333695
C	3.133052	-3.131478	4.449364	H	1.187831	-4.824555	-2.942265
H	4.049060	-1.502287	5.523801	H	0.450041	-5.504934	-1.473318
H	2.088816	-4.539926	3.197995	H	-0.503826	-5.332153	-2.941880
H	3.526802	-3.894787	5.116660				

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C	2.359261	0.090251	-1.259603
C	3.414524	0.792452	-0.431105
C	3.270289	2.311277	-0.422662
H	3.905674	2.739019	0.360462
H	3.559391	2.763228	-1.381503
H	2.234510	2.601642	-0.206441
C	4.816317	0.380459	-0.896155
H	4.866349	-0.718648	-0.862705
H	4.923352	0.665743	-1.955642
C	5.985332	0.951473	-0.092648
H	5.985240	2.049055	-0.187298
H	5.827037	0.733912	0.970980
C	7.296616	0.424112	-0.580426
H	7.496458	0.619199	-1.639839
C	8.227862	-0.261847	0.095320
C	9.486863	-0.723000	-0.577008
H	9.520823	-0.434347	-1.632954
H	10.374854	-0.306476	-0.079980
H	9.589171	-1.816053	-0.517372
C	8.140876	-0.632201	1.544828
H	7.207453	-0.320370	2.020756
H	8.238077	-1.719701	1.670356
H	8.972769	-0.185223	2.107561
O	3.295286	0.328565	0.932949
C	1.744241	0.736444	-2.401135
H	1.811533	1.830001	-2.427675
C	0.962426	0.177476	-3.376581
H	0.866294	-0.909806	-3.430726
H	2.365570	0.058674	0.986134
C	-5.375905	1.896069	-1.217579
C	-4.789494	0.731299	-0.724602
C	-3.446325	0.805344	-0.363142
C	-2.679313	1.966296	-0.459224
C	-3.309539	3.118897	-0.932555
C	-4.645896	3.077922	-1.317482
H	-6.420825	1.890426	-1.518178
H	-2.746982	4.047149	-1.009220
H	-5.126636	3.977660	-1.693000
O	-2.811463	-0.298657	0.145132
C	-5.520820	-0.577925	-0.460930
C	-4.538749	-1.714281	-0.713094
C	-3.206208	-1.513138	-0.358407
C	-4.879032	-2.970548	-1.211930
C	-2.211752	-2.485858	-0.483242
C	-3.919929	-3.971846	-1.337393
H	-5.905765	-3.178003	-1.503511
C	-2.597506	-3.734745	-0.977812
H	-4.206617	-4.946616	-1.723774
H	-1.854773	-4.520387	-1.097730
P	-0.914957	1.849743	0.026031
P	-0.473591	-1.986340	-0.148576
C	-5.915277	-0.609334	1.029258
H	-5.037111	-0.510579	1.679378
H	-6.603206	0.215144	1.255284
H	-6.414277	-1.557111	1.267468
C	-6.780639	-0.709834	-1.307607
H	-7.306516	-1.643130	-1.078918
H	-7.481316	0.102446	-1.086254
H	-6.553796	-0.692072	-2.380117
Cu	0.375545	0.098103	-0.729595
C	-0.277298	3.502327	-0.439040
C	0.110670	4.464939	0.494373
C	-0.082746	3.755298	-1.802898
C	0.704345	5.652065	0.070336
H	-0.037696	4.283253	1.557527
C	0.502174	4.942102	-2.224514
H	-0.390217	3.009302	-2.536881
C	0.906929	5.889590	-1.285056
H	1.011106	6.392689	0.805225
H	0.650939	5.124124	-3.286785
H	1.376880	6.814061	-1.612120
C	-0.980411	1.901532	1.857305
C	0.204304	1.653367	2.560065
C	-2.151081	2.180197	2.566537
C	0.217684	1.696087	3.948969
H	1.124500	1.433836	2.015200
C	-2.136596	2.211671	3.958375
H	-3.079421	2.374266	2.030351
C	-0.953540	1.972162	4.650376
H	1.143588	1.498168	4.484556
H	-3.053712	2.426454	4.502259
H	-0.943978	1.995817	5.737625
C	0.459314	-3.501050	-0.589265
C	1.172796	-3.525674	-1.789289
C	0.458047	-4.639553	0.225618
C	1.870590	-4.667050	-2.175044
H	1.187303	-2.639264	-2.421041

C	1.153199	-5.779677	-0.159771	H	9.095375	0.765067	-1.015205
H	-0.094102	-4.632067	1.165119	H	9.889100	2.134118	-0.217029
C	1.860931	-5.794179	-1.360443	H	10.744115	0.608684	-0.382830
H	2.426315	-4.671669	-3.109589	O	5.081312	0.196260	-1.627976
H	1.144983	-6.659895	0.478799	C	2.441936	-0.021357	0.989959
H	2.409016	-6.685288	-1.657259	H	2.522719	-1.092409	1.213397
C	-0.335526	-1.983099	1.683017	C	1.400903	0.623004	1.638157
C	0.956491	-1.874922	2.214484	H	1.381484	1.718337	1.609062
C	-1.427820	-2.000786	2.550116	H	4.358481	0.030949	-2.246082
C	1.150573	-1.776763	3.585842	C	-3.435091	-2.938499	3.246464
H	1.818993	-1.876429	1.545591	C	-3.457173	-1.652218	2.708934
C	-1.231430	-1.896791	3.926121	C	-2.738483	-1.443015	1.533548
H	-2.438713	-2.093082	2.154812	C	-1.965444	-2.427241	0.913839
C	0.053324	-1.780678	4.444856	C	-1.987329	-3.708219	1.472402
H	2.159198	-1.690580	3.984039	C	-2.724359	-3.961105	2.624447
H	-2.090623	-1.906755	4.593165	H	-3.982413	-3.152622	4.161409
H	0.201043	-1.691089	5.518763	H	-1.403911	-4.505126	1.015486
H	2.612589	-0.967962	-1.417593	H	-2.732757	-4.960646	3.051550
C	0.311581	0.965826	-4.469831	O	-2.748254	-0.206058	0.937653
H	0.654434	0.658290	-5.468658	C	-4.237930	-0.478260	3.283966
H	-0.783718	0.865612	-4.477634	C	-3.427006	0.781775	3.012285
H	0.543036	2.035191	-4.369167	C	-2.766752	0.873864	1.789171
				C	-3.347267	1.887669	3.859114
77-ts				C	-2.096736	2.020236	1.355911
C	3.323663	0.473784	-0.022143	C	-2.656910	3.034201	3.476360
C	4.613009	-0.259267	-0.347123	H	-3.832009	1.860810	4.832059
C	4.405296	-1.770749	-0.419783	C	-2.047657	3.109161	2.227053
H	5.268743	-2.245197	-0.898793	H	-2.605616	3.882993	4.153436
H	4.275270	-2.225936	0.571281	H	-1.522044	4.013820	1.927793
H	3.511669	-2.003472	-1.016507	P	-0.826715	-1.905343	-0.428261
C	5.726625	0.108326	0.635680	P	-1.258750	1.923476	-0.269534
H	5.829706	1.204243	0.625538	C	-5.573828	-0.358504	2.524505
H	5.385182	-0.160840	1.648155	H	-5.416357	-0.214488	1.449050
C	7.094789	-0.520900	0.369004	H	-6.168674	-1.269648	2.665163
H	7.004733	-1.617302	0.427858	H	-6.147791	0.496191	2.904018
H	7.398522	-0.291689	-0.659511	C	-4.533842	-0.661223	4.767317
C	8.110685	-0.064403	1.366493	H	-5.109405	0.187498	5.152434
H	7.864682	-0.305608	2.406492	H	-5.147612	-1.553350	4.931958
C	9.246301	0.613851	1.154707	H	-3.615401	-0.756375	5.358558
C	10.135533	1.006691	2.296738	Cu	0.220816	0.153855	-0.163295
H	9.740424	0.672093	3.261900	C	0.168408	-3.425548	-0.672238
H	11.143691	0.584934	2.175294	C	-0.152748	-4.408564	-1.612875
H	10.264603	2.097677	2.339467	C	1.269753	-3.621926	0.166765
C	9.753560	1.043832	-0.188177	C	0.619435	-5.562329	-1.712423

H	-1.010945	-4.272328	-2.269154	H	0.817432	1.866536	-2.703585
C	2.037034	-4.777561	0.072092	H	2.556735	1.578620	-2.871645
H	1.520306	-2.861352	0.906760	H	2.436696	0.261089	-1.109327
C	1.713286	-5.748806	-0.871726	C	0.673372	-0.016455	2.793303
H	0.362980	-6.320808	-2.448434	H	-0.370786	0.318352	2.868893
H	2.892184	-4.914949	0.730238	H	0.657291	-1.111046	2.688752
H	2.314717	-6.651117	-0.952641	H	1.145263	0.211739	3.761192
C	-1.844623	-1.857668	-1.946291				
C	-1.182607	-1.492841	-3.126130	**78-ts**			
C	-3.202722	-2.171873	-1.987342	C	2.190607	0.929889	-1.600256
C	-1.868874	-1.474205	-4.333720	C	3.010121	1.497896	-0.459002
H	-0.125432	-1.221437	-3.078832	C	2.747328	2.973840	-0.185563
C	-3.893765	-2.124745	-3.196846	H	3.263146	3.269905	0.734415
H	-3.723154	-2.463673	-1.075760	H	3.109184	3.612671	-1.001387
C	-3.227026	-1.786680	-4.369856	H	1.675991	3.167064	-0.047755
H	-1.346764	-1.199827	-5.248271	C	4.494421	1.244724	-0.748607
H	-4.953954	-2.366333	-3.221773	H	4.608270	0.166495	-0.938670
H	-3.766908	-1.760070	-5.313868	H	4.764479	1.757511	-1.683996
C	-0.541144	3.596129	-0.489377	C	5.454866	1.646460	0.374814
C	0.850377	3.720861	-0.518017	H	5.520292	2.741323	0.434701
C	-1.333515	4.737668	-0.659224	H	5.027108	1.311512	1.328855
C	1.443594	4.966904	-0.701400	C	6.827817	1.074264	0.178349
H	1.467782	2.829335	-0.409252	H	7.554062	1.708817	-0.336111
C	-0.740976	5.981786	-0.839909	C	7.221566	-0.156243	0.532918
H	-2.419793	4.649655	-0.654207	C	8.611395	-0.644257	0.259573
C	0.648167	6.096813	-0.860344	H	9.222391	0.115147	-0.240024
H	2.527337	5.051883	-0.726055	H	9.119305	-0.934458	1.190554
H	-1.363008	6.864127	-0.970372	H	8.597936	-1.543077	-0.373415
H	1.109638	7.070637	-1.007045	C	6.329286	-1.152262	1.211310
C	-2.669059	1.951346	-1.446733	H	5.321138	-0.769424	1.401262
C	-2.397501	1.644345	-2.783045	H	6.231144	-2.058134	0.595817
C	-3.977147	2.274142	-1.074536	H	6.762211	-1.478489	2.167690
C	-3.411220	1.674924	-3.734175	O	2.736392	0.753601	0.745068
H	-1.386217	1.360519	-3.077201	C	1.654439	1.700984	-2.618542
C	-4.993186	2.293156	-2.025601	H	1.529890	2.771765	-2.407841
H	-4.206793	2.511121	-0.035982	C	1.085448	1.254552	-3.849964
C	-4.711585	1.997713	-3.356336	H	1.491009	0.294082	-4.201211
H	-3.186055	1.430728	-4.770165	H	1.792464	0.534696	0.695615
H	-6.008258	2.543295	-1.725241	C	-5.561334	0.800510	-0.789329
H	-5.506795	2.013867	-4.098027	C	-4.696548	-0.215482	-0.382112
H	3.474384	1.564077	0.001611	C	-3.409179	0.163909	-0.012171
O	1.535140	0.088678	-1.857485	C	-2.954161	1.482820	-0.026929
C	1.572454	1.073066	-2.849604	C	-3.855106	2.473255	-0.418401
H	1.402292	0.643303	-3.850504	C	-5.147948	2.130135	-0.802106

H	-6.577180	0.559125	-1.092232	H	1.102441	1.366772	4.730331
H	-3.537442	3.514042	-0.438043	H	-3.188638	1.499326	4.947147
H	-5.842856	2.906402	-1.112311	H	-0.984648	1.325492	6.078487
O	-2.507897	-0.784029	0.405752	C	1.421225	-2.932579	-0.750150
C	-5.072352	-1.683454	-0.231803	C	1.749652	-2.723764	-2.094195
C	-3.841456	-2.513127	-0.572012	C	2.005773	-3.997668	-0.060074
C	-2.596157	-2.016313	-0.189943	C	2.647324	-3.566960	-2.740433
C	-3.861954	-3.762947	-1.189085	H	1.289577	-1.890571	-2.628647
C	-1.395179	-2.699168	-0.388504	C	2.912998	-4.833430	-0.704418
C	-2.685635	-4.480794	-1.390852	H	1.752147	-4.175456	0.983849
H	-4.806532	-4.190981	-1.515761	C	3.233757	-4.619367	-2.042713
C	-1.461055	-3.958196	-0.990626	H	2.895086	-3.396798	-3.785428
H	-2.726237	-5.457332	-1.866647	H	3.368447	-5.657740	-0.160619
H	-0.545509	-4.518270	-1.171645	H	3.943284	-5.274480	-2.542552
P	-1.191064	1.762057	0.382956	C	0.387980	-1.973748	1.782950
P	0.170838	-1.809554	-0.032593	C	1.641417	-1.678711	2.336526
C	-5.423613	-1.935416	1.248134	C	-0.670448	-2.297520	2.635913
H	-4.589577	-1.668915	1.909241	C	1.828692	-1.715837	3.713223
H	-6.294671	-1.333808	1.537058	H	2.473949	-1.404044	1.689539
H	-5.661949	-2.994836	1.405887	C	-0.481053	-2.323294	4.014709
C	-6.269891	-2.058933	-1.095573	H	-1.649449	-2.539835	2.225992
H	-6.539353	-3.110522	-0.949574	C	0.767021	-2.033957	4.556113
H	-7.151141	-1.472739	-0.813498	H	2.808458	-1.489485	4.128357
H	-6.068735	-1.895096	-2.161186	H	-1.314647	-2.575811	4.666163
Cu	0.120688	0.342685	-0.920633	H	0.912681	-2.055802	5.633807
C	-0.957146	3.532137	-0.006965	H	2.488899	-0.094201	-1.862161
C	-0.763320	4.528418	0.950180	O	-1.032126	0.424399	-2.626439
C	-0.856774	3.852794	-1.367945	H	-0.098351	0.853728	-3.334506
C	-0.456425	5.827962	0.550544	C	-1.618745	-0.689594	-3.224034
H	-0.836621	4.288129	2.009715	H	-1.697996	-0.560667	-4.318639
C	-0.564126	5.151552	-1.762663	H	-1.060632	-1.630251	-3.044925
H	-0.999962	3.066112	-2.111816	H	-2.642266	-0.855201	-2.842393
C	-0.353549	6.139657	-0.801260	C	0.875714	2.276042	-4.947753
H	-0.297460	6.598810	1.301211	H	0.159331	1.920487	-5.699092
H	-0.488786	5.392609	-2.820942	H	0.464635	3.208898	-4.535208
H	-0.108902	7.153989	-1.107735	H	1.797235	2.545558	-5.486048
C	-1.168394	1.661044	2.212860				
C	0.070115	1.564910	2.858383	**79**			
C	-2.338197	1.640946	2.977712	C	-2.315669	-0.828386	-0.779151
C	0.133711	1.453540	4.242991	C	-1.049179	-1.284994	-0.029803
H	0.995152	1.574934	2.279918	C	-1.395794	-1.794834	1.362601
C	-2.271643	1.519047	4.362546	H	-0.528169	-2.279276	1.822843
H	-3.308623	1.716859	2.488992	H	-1.727837	-0.982373	2.020137
C	-1.036400	1.426231	4.996777	H	-2.206320	-2.535038	1.308034

C	-0.027359	-0.152996	0.000083	H	2.412178	1.428344	1.282376
H	0.184042	0.127675	-1.043676	C	3.791796	0.591777	-0.029676
H	-0.492382	0.726512	0.469420	C	4.727978	1.757306	0.088519
C	1.289865	-0.481815	0.700764	H	4.349153	2.524417	0.772186
H	1.093016	-0.682481	1.765808	H	5.715225	1.434873	0.448970
H	1.696070	-1.410247	0.281459	H	4.898833	2.225590	-0.891323
C	2.259945	0.651202	0.593202	C	4.275162	-0.485671	-0.951727
H	1.906787	1.593537	1.025556	H	3.579824	-1.322840	-1.051569
C	3.470691	0.661590	0.020735	H	4.457678	-0.077140	-1.955498
C	4.299785	1.910960	-0.008513	H	5.238639	-0.885358	-0.605411
H	3.798152	2.752128	0.481641	O	-0.448802	-1.947700	-0.875405
H	5.268256	1.753756	0.487499	C	-3.271244	-0.016165	0.007100
H	4.531406	2.205484	-1.042082	H	-3.451826	-0.337083	1.037215
C	4.125088	-0.518310	-0.630919	C	-4.402012	0.706952	-0.652195
H	3.510803	-1.422276	-0.620706	H	-4.131327	0.945277	-1.690078
H	4.373295	-0.290356	-1.677017	H	-1.179225	-2.565059	-1.000520
H	5.078284	-0.751730	-0.135953	H	-1.918351	0.086539	-1.589282
O	-0.440903	-2.330169	-0.787091	C	-4.779370	1.978950	0.100978
C	-3.116204	0.237250	-0.103497	H	-5.627123	2.488457	-0.369375
H	-3.657213	-0.046171	0.804865	H	-5.057650	1.753168	1.137827
C	-3.208844	1.497321	-0.532091	H	-3.935868	2.678272	0.131239
H	-2.668473	1.774627	-1.442495	H	-5.281266	0.047131	-0.702447
H	-1.042305	-3.084149	-0.780668				
H	-2.003390	-0.490646	-1.778098	**81-ts**			
C	-4.000620	2.571679	0.132816	C	-3.976600	-3.703107	0.140407
H	-3.366153	3.419795	0.420791	C	-3.430493	-2.818845	-0.790465
H	-4.770870	2.976013	-0.536691	C	-2.137937	-2.359349	-0.549352
H	-4.498045	2.199013	1.035380	C	-1.373395	-2.744111	0.552651
H	-2.941968	-1.724433	-0.926676	C	-1.943457	-3.652722	1.444623
				C	-3.238726	-4.120688	1.244699
80				H	-4.985164	-4.084805	0.000049
C	-2.089100	-0.251295	-0.561545	H	-1.376892	-3.976402	2.315688
C	-0.897190	-0.946040	0.044620	H	-3.675660	-4.822049	1.951627
C	-1.202061	-1.588926	1.389272	O	-1.554421	-1.467958	-1.421872
H	-0.347059	-2.186073	1.721038	C	-4.111092	-2.383048	-2.080488
H	-1.419880	-0.837826	2.158391	C	-3.691748	-0.945756	-2.359537
H	-2.068410	-2.257687	1.311878	C	-2.394120	-0.559817	-2.013825
C	0.248927	0.064075	0.140258	C	-4.496554	0.001296	-2.988401
H	0.402063	0.492420	-0.861714	C	-1.889118	0.725215	-2.236510
H	-0.079991	0.892550	0.785893	C	-4.011916	1.274646	-3.273205
C	1.579546	-0.493480	0.645694	H	-5.514727	-0.255089	-3.271064
H	1.447406	-0.871889	1.671305	C	-2.721135	1.631739	-2.902703
H	1.863172	-1.356662	0.031913	H	-4.647788	1.994316	-3.782853
C	2.638272	0.562880	0.650407	H	-2.361781	2.637418	-3.110787

P	0.234763	-1.885503	0.744626	C	0.921609	0.697352	-2.898169
P	-0.232935	1.173082	-1.557386	C	2.291119	0.870825	-2.646899
C	-3.585575	-3.271087	-3.225572	C	0.518916	0.120819	-4.104669
H	-2.496593	-3.197712	-3.322152	C	3.229248	0.512640	-3.608355
H	-3.843503	-4.321088	-3.037447	H	2.612049	1.254261	-1.673507
H	-4.036408	-2.964643	-4.178100	C	1.464452	-0.265959	-5.051742
C	-5.626311	-2.535166	-2.004960	H	-0.541137	-0.025716	-4.307836
H	-6.094791	-2.255804	-2.954785	C	2.818642	-0.060681	-4.810802
H	-5.897968	-3.580450	-1.822241	H	4.289141	0.663500	-3.413459
H	-6.061901	-1.919934	-1.207913	H	1.138162	-0.719454	-5.985183
Cu	0.248150	0.588638	0.761086	H	3.556179	-0.353361	-5.554662
C	0.822367	-2.407430	2.398237	B	-1.465086	1.002593	1.747283
C	2.079090	-2.988754	2.588299	O	-2.001740	2.236341	2.128580
C	0.070382	-2.032225	3.522645	O	-2.432185	0.012169	1.940172
C	2.568509	-3.210265	3.874207	C	-3.276497	2.010962	2.760575
H	2.681143	-3.269517	1.724867	C	-3.703054	0.649597	2.150758
C	0.554365	-2.271055	4.803503	C	-3.023814	1.934834	4.260615
H	-0.893687	-1.538760	3.383149	H	-2.512489	2.851565	4.578065
C	1.806061	-2.858380	4.983376	H	-3.956377	1.846135	4.831619
H	3.548266	-3.664741	4.006937	H	-2.376541	1.083536	4.506175
H	-0.043320	-1.988234	5.667819	C	-4.190521	3.177696	2.444006
H	2.186825	-3.036211	5.986700	H	-5.208132	2.995495	2.814293
C	1.314267	-2.830688	-0.405215	H	-3.814571	4.085446	2.932035
C	2.348269	-2.131335	-1.036577	H	-4.239763	3.368631	1.366404
C	1.135135	-4.188715	-0.688354	C	-4.549806	-0.233013	3.044108
C	3.181419	-2.778537	-1.945452	H	-5.508635	0.246110	3.282068
H	2.495502	-1.075541	-0.802670	H	-4.759681	-1.176673	2.524016
C	1.970592	-4.833968	-1.594664	H	-4.035318	-0.472388	3.980332
H	0.334109	-4.742366	-0.198470	C	-4.365727	0.792717	0.784547
C	2.992365	-4.128373	-2.226955	H	-4.416811	-0.196478	0.310057
H	3.974119	-2.219704	-2.441989	H	-5.384504	1.193505	0.858429
H	1.822196	-5.889872	-1.811279	H	-3.776644	1.440621	0.120881
H	3.639809	-4.632977	-2.940869	C	2.099785	2.468544	1.437778
C	-0.313209	3.006984	-1.700343	C	2.896222	1.267694	1.785085
C	0.431965	3.754452	-2.614197	C	2.617109	0.701663	3.169801
C	-1.187542	3.674538	-0.829187	H	3.004101	-0.321653	3.240669
C	0.303176	5.142244	-2.663225	H	3.086010	1.312117	3.953448
H	1.113830	3.252678	-3.299068	H	1.538482	0.642536	3.352483
C	-1.343574	5.053162	-0.909481	C	4.392174	1.425431	1.520777
H	-1.732501	3.109158	-0.069522	H	4.510848	1.893009	0.530077
C	-0.593492	5.793316	-1.822629	H	4.848922	2.104456	2.257186
H	0.894690	5.712373	-3.376345	C	5.116194	0.075472	1.514345
H	-2.042340	5.556106	-0.242501	H	5.117861	-0.345860	2.528811
H	-0.706589	6.873674	-1.875994	H	4.524900	-0.618885	0.897690

C	6.527906	0.182996	1.022648	H	8.640984	1.052471	1.052700
H	7.296920	0.325624	1.786398	H	8.957254	1.066233	-0.674925
C	6.924690	0.168857	-0.256122	O	2.102393	0.368214	-1.121658
C	8.365885	0.322918	-0.634666	C	1.134205	1.605406	-3.451976
H	9.011097	0.443305	0.242022	H	1.058435	2.654889	-3.156627
H	8.719811	-0.548948	-1.203065	C	-0.007285	1.018329	-3.966472
H	8.511861	1.194021	-1.289375	H	2.363293	-0.146632	-3.437622
C	5.986309	0.030118	-1.415505	H	0.029736	-0.038104	-4.241049
H	4.950891	-0.176541	-1.119939	C	-4.692920	1.452757	2.457807
H	5.985457	0.956924	-2.010110	C	-3.780227	0.398347	2.459268
H	6.313745	-0.769330	-2.096164	C	-2.514353	0.647621	1.931487
O	2.294923	0.548275	0.755176	C	-2.138732	1.876118	1.380809
C	1.098936	3.121722	2.187801	C	-3.077711	2.909568	1.410660
H	0.793665	2.706795	3.147106	C	-4.342876	2.700163	1.949224
C	0.578252	4.307138	1.775124	H	-5.692304	1.304670	2.859613
H	0.869150	4.690233	0.793550	H	-2.817554	3.881458	0.995130
H	2.376126	2.918562	0.479972	H	-5.064850	3.512773	1.967308
C	-0.422167	5.076995	2.545578	O	-1.573252	-0.355870	1.921193
H	-1.414709	4.931257	2.089774	C	-4.060907	-0.989152	3.021178
H	-0.490835	4.727426	3.581311	C	-3.305683	-1.992294	2.159288
H	-0.216018	6.153549	2.536896	C	-2.049609	-1.623954	1.677923
				C	-3.762133	-3.270269	1.838635
82-ts				C	-1.233061	-2.471445	0.923529
C	2.238842	0.869101	-3.056178	C	-2.980882	-4.138746	1.081266
C	3.016620	1.159363	-1.825132	H	-4.739668	-3.599556	2.181871
C	3.049856	2.611544	-1.378475	C	-1.724393	-3.745602	0.632457
H	3.438752	2.681330	-0.355553	H	-3.355403	-5.130586	0.840189
H	3.693727	3.215974	-2.031477	H	-1.126155	-4.424592	0.028473
H	2.045226	3.049045	-1.367023	P	-0.488881	1.986308	0.581017
C	4.403606	0.518368	-1.809204	P	0.336287	-1.782328	0.272139
H	4.265745	-0.534994	-2.104055	C	-3.499396	-1.063775	4.453632
H	5.050227	0.983194	-2.569318	H	-2.423510	-0.854155	4.474287
C	5.086790	0.573158	-0.440645	H	-4.003460	-0.330806	5.096048
H	5.500081	1.574168	-0.262081	H	-3.661733	-2.065472	4.871391
H	4.310939	0.419452	0.327882	C	-5.554747	-1.289237	3.057655
C	6.134996	-0.481913	-0.289972	H	-5.741326	-2.283671	3.477352
H	5.757589	-1.506539	-0.388937	H	-6.079366	-0.577431	3.703859
C	7.449244	-0.335494	-0.073001	H	-5.997605	-1.243652	2.054385
C	8.352179	-1.527403	0.038068	Cu	0.041426	0.259719	-0.906769
H	7.805065	-2.471056	-0.059215	C	-0.542637	3.623040	-0.239849
H	9.132651	-1.502252	-0.735734	C	0.236686	4.711509	0.158031
H	8.879425	-1.534781	1.002683	C	-1.324048	3.727522	-1.399957
C	8.154021	0.979096	0.070106	C	0.239100	5.886115	-0.592079
H	7.495931	1.844483	-0.043743	H	0.855502	4.638147	1.051409

C	-1.331095	4.906784	-2.135452	H	3.134905	-1.367447	0.446023
H	-1.921245	2.871453	-1.722425	C	2.005789	-2.199870	4.052036
C	-0.543326	5.986427	-1.737462	H	0.031737	-2.424779	3.228141
H	0.854795	6.725680	-0.277097	C	3.345581	-1.929852	3.796090
H	-1.948186	4.981465	-3.029177	H	4.803020	-1.429676	2.279713
H	-0.540428	6.903621	-2.321929	H	1.679455	-2.426560	5.064816
C	0.621483	2.243453	2.017594	H	4.069290	-1.939041	4.607977
C	1.888997	1.657649	1.973441	B	-1.599141	-0.143190	-2.114846
C	0.250621	3.004339	3.131618	O	-1.887997	-1.440728	-2.520078
C	2.781297	1.843949	3.026766	O	-2.757919	0.627675	-2.152232
H	2.158387	1.051470	1.104450	C	-3.250842	-1.502951	-2.990789
C	1.143334	3.188979	4.181395	C	-3.892868	-0.247940	-2.330661
H	-0.739620	3.458744	3.172319	C	-3.202882	-1.439016	-4.511419
C	2.410625	2.609960	4.127486	H	-2.578487	-2.261955	-4.877345
H	3.764465	1.377506	2.989231	H	-4.200380	-1.543260	-4.955338
H	0.851529	3.783734	5.044217	H	-2.762941	-0.500251	-4.867090
H	3.107559	2.753550	4.950287	C	-3.860254	-2.825615	-2.566377
C	0.997590	-3.107719	-0.807566	H	-4.919382	-2.873657	-2.852170
C	1.488014	-4.320939	-0.311342	H	-3.338863	-3.647621	-3.070771
C	1.054546	-2.857446	-2.180627	H	-3.780705	-2.988566	-1.486677
C	2.013640	-5.272837	-1.177966	C	-4.934945	0.458515	-3.174352
H	1.462639	-4.515213	0.761125	H	-5.783341	-0.206667	-3.381407
C	1.586411	-3.808162	-3.047385	H	-5.316485	1.330110	-2.630451
H	0.671520	-1.906364	-2.551339	H	-4.528428	0.807775	-4.128622
C	2.064207	-5.015866	-2.546848	C	-4.457686	-0.522767	-0.944074
H	2.390739	-6.214605	-0.785316	H	-4.707806	0.432930	-0.465406
H	1.630522	-3.604074	-4.115141	H	-5.365043	-1.139095	-0.982005
H	2.482023	-5.758090	-3.223507	H	-3.718178	-1.029557	-0.312474
C	1.476442	-1.902835	1.709728	C	-1.107808	1.845427	-4.536450
C	2.827662	-1.626422	1.461166	H	-2.100647	1.430971	-4.344740
C	1.074418	-2.192766	3.014002	H	-1.080224	2.861746	-4.126237
C	3.756325	-1.646524	2.493268	H	-0.981296	1.918994	-5.626905