

Electronic Supplementary Information

Bond Dissociation Energy Controlled σ -Bond Metathesis in Alkaline-Earth-Metal Hydride Catalyzed Dehydrocoupling of Amines and Boranes: A Theoretical Study

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1. Complete reference for Gaussian 09

Gaussian 09, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2013.

2. The value of BDE

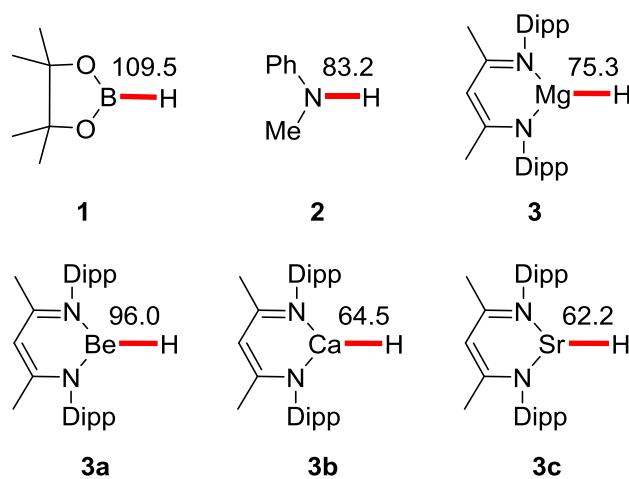


Fig. S1. The value of BDEs. The BDEs are given in kcal/mol.

3. Free energy profiles for the intermediate 3 to 7

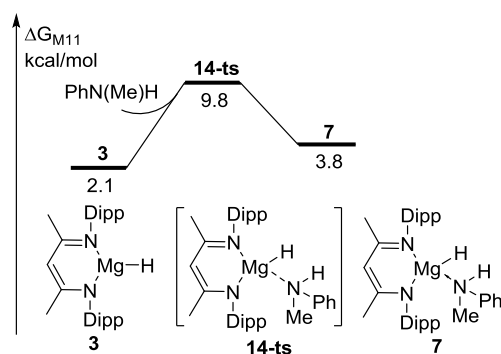


Fig. S2 Free energy profiles for the intermediate 3 to 7.

4. Free energy profiles for the intermediate 3b to 7b(b) and 3c to 7c(c)

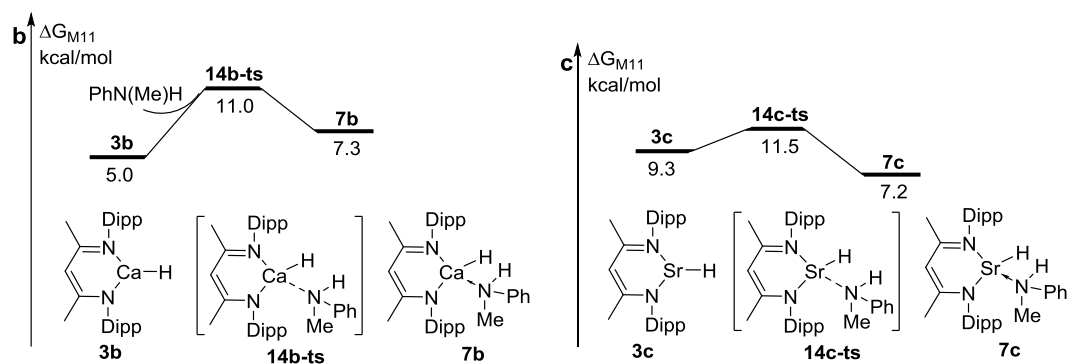


Fig. S3 Free energy profiles for the intermediate 3b to 7b(b) and 3c to 7c(c).

5. Absolute calculation energies, enthalpies, and free energies

Table S1. Absolute calculation energies, enthalpies, and free energies

Geometry	$E_{\text{(elec-B3-LYP)}}^1$	$E_{\text{(solv, M11)}}^2$	$H_{\text{(corr-B3-LYP)}}^3$	$G_{\text{(corr-B3-LYP)}}^4$	IF ⁵
1	-411.8639	-411.7595	0.202007	0.158372	
2	-326.9031	-326.7973	0.154097	0.114649	
3	-1440.027	-1439.59	0.682256	0.574688	
4	-737.6149	-737.4119	0.33736	0.275629	-1662.57
5-ts	-738.698	-738.5002	0.351344	0.288762	
6	-2880.064	-2879.224	1.369359	1.186593	
7	-1766.94	-1766.411	0.839568	0.715796	
8	-1851.897	-1851.362	0.888509	0.758353	
9-ts	-1766.917	-1766.384	0.834215	0.710537	-1245.44
10	-1765.767	-1765.229	0.819215	0.692962	
11-ts	-2177.621	-2177.008	1.023635	0.885084	-110.88

12	-2177.648	-2177.036	1.025048	0.884625	
13-ts	-2177.628	-2177.015	1.021081	0.880038	-212.17
H₂	-1.175482	-1.167608	0.01345	-0.001342	
3a	-1254.73	-1254.276	0.686521	0.583581	
6a	-2509.372	-2508.525	1.377188	1.208595	
7a	-1581.614	-1581.081	0.843507	0.725428	
9a-ts	-1581.587	-1581.045	0.837968	0.720302	-1309.32
10a	-1580.468	-1579.919	0.822889	0.703902	
11a-ts	-1992.299	-1991.667	1.026794	0.892106	-164.94
12a	-1992.303	-1991.691	1.028467	0.896268	
13a-ts	-1992.298	-1991.676	1.024581	0.888271	-118.64
3b	-1917.475	-1917.087	0.680011	0.566866	
6b	-3835.009	-3834.232	1.365364	1.174848	
7b	-2244.4	-2243.909	0.837672	0.7093	
9b-ts	-2244.386	-2243.891	0.831962	0.702302	-1143.29
10b	-2243.229	-2242.736	0.817747	0.690355	
11b-ts	-2655.098	-2654.512	1.021093	0.874835	-82.43
12b	-2655.126	-2654.543	1.022948	0.877254	
13b-ts	-2655.091	-2654.512	1.019029	0.873259	-282.63
3c	-1270.641	-1270.147	0.679564	0.56861	
6c	-2541.347	-2540.355	1.363467	1.167465	
7c	-1597.571	-1596.971	0.836667	0.706062	
9c-ts	-1597.559	-1596.956	0.831203	0.699633	-1162.9
10c	-1596.403	-1595.799	0.817163	0.686979	
11c-ts	-2008.27	-2007.575	1.021093	0.874835	-100.27
12c	-2008.298	-2007.608	1.022948	0.877254	
13c-ts	-2008.266	-2007.579	1.019029	0.873259	-379.31

¹The electronic energy was calculated by B3-LYP in gas phase. ²The electronic energy was calculated by M11 in a benzene solvent. ³The thermal correction to Gibbs free energy calculated by B3-LYP in gas phase. ⁴The thermal correction to enthalpy calculated by B3-LYP in gas phase. ⁵The B3-LYP calculated imaginary frequencies for the transition states. SDD basis set for strontium atom

6. B3-LYP geometries for all the compounds and transition state

1				O	1.08598500	1.20101000	0.36641700
B	-0.00014700	1.94531900	0.00006300	C	-0.78921900	-0.19101900	-0.04520200
H	-0.00022400	3.13519400	0.00011700	C	0.78926000	-0.19088600	0.04516100
O	-1.08617700	1.20090400	-0.36634300	C	-1.48000800	-0.48437300	1.29334800

H	-2.54923800	-0.27298100	1.19449100	C	2.80958200	2.57545300	-0.10517600
H	-1.36101600	-1.53228200	1.58820100	C	2.41140700	3.24891300	-1.43486200
H	-1.08444800	0.14891900	2.09365600	C	3.67291300	3.52460300	0.74788700
C	1.37945600	-1.07346000	1.14396900	H	1.88879200	2.38666200	0.45558000
H	1.13964800	-2.12859900	0.96880200	H	1.76182100	2.60121600	-2.03533500
H	2.46930900	-0.97061700	1.14943000	H	1.87987500	4.19030300	-1.24875600
H	1.01038900	-0.79137000	2.13268200	H	3.29609400	3.47648300	-2.04129700
C	1.48018900	-0.48411700	-1.29334000	H	3.96135000	3.06194600	1.69868000
H	2.54938900	-0.27259400	-1.19441900	H	4.59281300	3.81670000	0.22813800
H	1.36134400	-1.53203900	-1.58820300	H	3.11800700	4.44311000	0.97343600
H	1.08461200	0.14913400	-2.09367100	C	2.81053600	-2.57565600	-0.10499900
C	-1.37939800	-1.07349000	-1.14406400	C	3.67407500	-3.52419300	0.74852300
H	-1.13914400	-2.12858600	-0.96926500	C	2.41306500	-3.24959000	-1.43467100
H	-2.46928900	-0.97105400	-1.14915800	H	1.88952100	-2.38714100	0.45543900
H	-1.01073700	-0.79095600	-2.13280700	H	3.96202100	-3.06117400	1.69929000
2				H	3.11955000	-4.44291100	0.97412900
C	-0.44387600	-0.27358800	0.06097900	H	4.59427500	-3.81596800	0.22910400
C	0.52306200	-1.29858300	0.00639200	H	1.76351500	-2.60224400	-2.03555400
C	1.87904600	-0.99602700	-0.04386800	H	3.29807800	-3.47702700	-2.04071100
C	2.31529600	0.33314000	-0.04060700	H	1.88178900	-4.19110300	-1.24852300
C	1.36401100	1.35127600	0.01146700	C	-2.84949100	-0.00004400	-0.06445000
C	-0.00111100	1.06192700	0.05738900	C	-3.48801400	1.23014800	-0.35731400
H	0.19631000	-2.33694500	0.01037600	C	-3.48844100	-1.23005300	-0.35734000
H	2.60223100	-1.80682100	-0.08674600	C	-4.76624900	1.20256100	-0.92827300
H	3.37509500	0.56691000	-0.07983700	C	-4.76671400	-1.20197700	-0.92831400
H	1.68121800	2.39137400	0.01109900	C	-5.40781200	0.00043000	-1.21060800
H	-0.71811700	1.87538100	0.09229300	H	-5.26498400	2.13964300	-1.16156600
N	-1.79312100	-0.60926300	0.15133300	H	-5.26577800	-2.13889200	-1.16164800
H	-2.00221200	-1.54211200	-0.17755900	H	-6.39972600	0.00062400	-1.65468700
C	-2.83622900	0.36445700	-0.10817600	C	-2.80957300	2.57543500	-0.10508700
H	-2.74073100	0.86166400	-1.08787500	C	-3.67295800	3.52463700	0.74786600
H	-3.80470900	-0.14125800	-0.06803500	C	-2.41129700	3.24884700	-1.43477000
H	-2.83844400	1.14103400	0.66549300	H	-1.88882800	2.38667000	0.45574000
3				H	-3.96148600	3.06202700	1.69865100
C	1.28036900	-0.00003600	1.76026400	H	-3.11805400	4.44314200	0.97342300
C	-0.00000800	-0.00008500	2.35255700	H	-4.59280900	3.81673400	0.22802800
C	-1.28038600	-0.00004700	1.76023000	H	-1.76166000	2.60113700	-2.03517000
H	-0.00001500	0.00015800	3.43565500	H	-3.29593800	3.47638600	-2.04128400
Mg	0.00001800	-0.00085800	-0.95289500	H	-1.87978700	4.19025000	-1.24866200
N	1.50190500	-0.00028500	0.44064400	C	-2.81055900	-2.57564100	-0.10505800
C	2.46308200	0.00050800	2.71288900	C	-2.41304100	-3.24951700	-1.43474400
H	3.09808100	-0.87636500	2.54664000	C	-3.67416600	-3.52421400	0.74836200
H	3.09666800	0.87854200	2.54724700	H	-1.88957500	-2.38718300	0.45543600
H	2.13430400	-0.00008400	3.75402700	H	-1.76342500	-2.60217100	-2.03555300
C	-2.46307400	0.00049400	2.71288400	H	-1.88182000	-4.19106400	-1.24861600
H	-2.13427600	-0.00022500	3.75401500	H	-3.29802700	-3.47688400	-2.04085100
H	-3.09659100	0.87859300	2.54735600	H	-3.96212300	-3.06126600	1.69915600
H	-3.09814900	-0.87630300	2.54656900	H	-4.59436300	-3.81590400	0.22888600
N	-1.50193000	-0.00030900	0.44066000	H	-3.11968900	-4.44297600	0.97390300
C	2.84948000	-0.00004200	-0.06449200	H	-0.00000300	-0.00159900	-2.67317000
C	3.48801900	1.23015200	-0.35739100	4			
C	3.48844000	-1.23008200	-0.35732300	B	-0.65277700	0.46008400	-0.09766300
C	4.76626800	1.20252700	-0.92832400	C	-0.79866500	-1.05951100	0.34109800
C	4.76672200	-1.20201300	-0.92827800	H	0.16663700	-1.55116600	0.51653700
C	5.40781800	0.00038300	-1.21060200	C	-2.08173300	1.11788800	-0.32400000
H	5.26501100	2.13959800	-1.16163500	H	-2.05583000	2.17343400	-0.62785700
H	5.26578900	-2.13893500	-1.16156600	C	-1.49416600	-1.82161700	-0.82257400
H	6.39973700	0.00055500	-1.65465700	H	-0.78314000	-1.86687100	-1.66137500

H	-1.68198300	-2.86691300	-0.53358200	H	2.06522000	-1.64975900	2.29830400
C	-1.57750900	-1.09286900	1.68763300	H	0.75410300	-0.48278400	2.01222000
H	-0.92108800	-0.66566300	2.46071800	C	3.39175400	0.68087900	1.42001500
H	-1.76001100	-2.13454600	1.99259300	H	4.15726000	-0.06837000	1.65336300
C	-2.76413900	0.34143600	-1.48909200	H	3.89254200	1.64605000	1.28970200
H	-3.78654700	0.71807300	-1.64458000	H	2.71416300	0.76558100	2.27275000
H	-2.21382600	0.57943500	-2.41198400	C	3.59029100	0.40131800	-1.06599500
C	-2.85332300	1.06528100	1.02586500	H	3.94784500	1.43177500	-1.16007300
H	-2.36113500	1.76695700	1.71628900	H	4.45927200	-0.25471600	-0.94602600
H	-3.87724900	1.44601300	0.89166900	H	3.07882800	0.13537800	-1.99590200
C	-2.81169500	-1.19377000	-1.32846200	C	2.58400800	-2.26282300	-0.34222600
H	-3.07199900	-1.64307400	-2.29674300	H	3.48849300	-2.46400900	0.24405600
H	-3.63003300	-1.46581300	-0.65501800	H	1.93899900	-3.14565500	-0.28069300
C	-2.91547400	-0.32251200	1.69870400	H	2.86821100	-2.12656500	-1.38821700
H	-3.24569100	-0.19802900	2.73932300	6			
H	-3.69183200	-0.92750000	1.22076700	C	-1.19493400	4.20996600	-0.66292700
N	0.58838700	1.11244300	-0.27195300	C	0.04389600	4.80615100	-0.37315400
C	0.76228900	2.51653000	-0.65816600	C	1.25649400	4.24685100	0.07401600
H	1.34648000	3.05880700	0.09655200	H	0.05397100	5.88576800	-0.45677600
H	1.29794500	2.59651500	-1.61334100	Mg	0.01443700	1.46303800	-0.13276300
H	-0.20877000	3.00119900	-0.76015800	N	-1.45000700	2.89349900	-0.61981700
C	1.84606400	0.43228100	-0.10367000	C	-2.30709100	5.18881800	-1.01397500
C	2.40829100	-0.28161800	-1.16812000	H	-2.83013800	4.90026900	-1.92890100
C	2.53841800	0.51314500	1.11012900	H	-3.06206300	5.21559100	-0.22013700
C	3.64183800	-0.91753700	-1.01641800	H	-1.91075300	6.19830700	-1.14027700
H	1.86784600	-0.33730400	-2.10917000	C	2.32078500	5.27675700	0.43422600
C	3.77266600	-0.12148800	1.26001000	H	2.13840600	6.21524500	-0.09495600
H	2.09793400	1.06763900	1.93447900	H	2.28285600	5.49175300	1.50848600
C	4.32791400	-0.83760100	0.19712100	H	3.33260700	4.93729200	0.21075100
H	4.06593000	-1.47539400	-1.84718800	N	1.48961400	2.93842900	0.22805300
H	4.29866400	-0.05932900	2.20904100	C	-2.80015500	2.49557600	-0.92880000
H	5.28822000	-1.33221900	0.31465500	C	-3.15000200	2.15795800	-2.25981400
5-ts				C	-3.77661200	2.47505800	0.09904500
N	-0.90482800	1.25276000	-0.57550200	C	-4.48129800	1.82042100	-2.53603500
C	-2.05063200	0.45261700	-0.25953800	C	-5.08598200	2.10050200	-0.22548600
C	-3.01085500	0.88351800	0.66607000	C	-5.44545300	1.78645400	-1.53289000
C	-2.24678400	-0.77460000	-0.91777900	H	-4.76596200	1.57867400	-3.55696300
C	-4.14229100	0.10532600	0.92689600	H	-5.84099400	2.07153100	0.55494600
H	-2.88228100	1.82027900	1.19631600	H	-6.47171400	1.51699900	-1.76899600
C	-3.37539400	-1.54261700	-0.64784400	C	-2.13881400	2.18203800	-3.40578600
H	-1.50801800	-1.13139400	-1.62538400	C	-2.48308800	3.25083400	-4.46366400
C	-4.33348700	-1.10968400	0.27378000	C	-1.99887500	0.80074100	-4.07335900
H	-4.87304500	0.45915500	1.64960700	H	-1.16386300	2.44146800	-2.98305800
H	-3.50817100	-2.48781900	-1.16778000	H	-2.52671800	4.25620500	-4.03144100
H	-5.21399200	-1.71261000	0.47684700	H	-1.72443300	3.25997400	-5.25562700
C	-0.88330200	2.64286800	-0.10113000	H	-3.45241200	3.04889000	-4.93514500
H	-0.74125200	2.70145400	0.98358200	H	-1.71893700	0.03914500	-3.34029600
H	-0.04145200	3.15441900	-0.57400900	H	-2.93425900	0.48850500	-4.55317800
H	-1.81260500	3.15259800	-0.37325300	H	-1.22302300	0.83025500	-4.84836900
H	-0.37694400	1.20474300	-1.77948400	C	-3.43616700	2.86373400	1.53747800
B	0.55960700	0.61093600	-0.73482700	C	-3.24653300	1.61632400	2.41934300
H	0.56657500	0.97409300	-2.16874600	C	-4.47323100	3.81321700	2.16748000
O	0.70818000	-0.77742100	-0.66689300	H	-2.48161000	3.39776800	1.52038500
O	1.58134900	1.28245700	-0.05501600	H	-2.46003000	0.96267500	2.02840200
C	1.83855800	-1.04389300	0.20076700	H	-2.96946000	1.90267000	3.44175300
C	2.64177800	0.31418700	0.13979300	H	-4.16506200	1.02166800	2.46804700
C	1.27775200	-1.34982000	1.59788400	H	-4.64806600	4.69740200	1.54375900
H	0.55739300	-2.16979000	1.51657700	H	-5.43988300	3.32078300	2.32445100

H	-4.12097700	4.15522000	3.14788900	C	-1.31516800	-1.20755300	4.08000200
C	2.78687400	2.57055000	0.73437500	H	-0.90924600	-3.00595100	2.99986500
C	3.01818300	2.57128100	2.13566200	H	-2.59089100	-4.45880900	4.22925800
C	3.83032600	2.23731000	-0.16636200	H	-1.38428500	-3.70802800	5.29179200
C	4.29969900	2.26474600	2.60825700	H	-3.02645100	-3.06248900	5.22094500
C	5.09354700	1.93857400	0.36720200	H	-0.91703900	-0.54934100	3.30270600
C	5.33931900	1.96030300	1.73581700	H	-2.14439700	-0.68787300	4.57519500
H	4.48598500	2.26955100	3.67898300	H	-0.52698600	-1.36853000	4.82614700
H	5.90189900	1.69310900	-0.31744200	C	-3.43982500	-2.67926700	-1.39370300
H	6.33114100	1.73470700	2.11949000	C	-4.34030000	-1.84101800	-2.31453200
C	1.92428500	2.90794000	3.15077900	C	-3.60559700	-4.17239200	-1.75224300
C	2.33480600	4.04368000	4.11017300	H	-2.40082000	-2.40849200	-1.61864600
C	1.50479100	1.66450700	3.96007500	H	-4.31545100	-0.78043600	-2.05498400
H	1.04451700	3.24822100	2.59707400	H	-4.00473100	-1.94691900	-3.35266400
H	2.66650700	4.93837700	3.57253500	H	-5.38417100	-2.17723200	-2.27993900
H	1.48669900	4.32541600	4.74558900	H	-2.86197400	-4.80506100	-1.26268200
H	3.15175000	3.73708700	4.77420500	H	-4.60251400	-4.53116600	-1.46698100
H	1.14088700	0.86937900	3.30361100	H	-3.49649600	-4.31196300	-2.83472500
H	2.34747600	1.26839200	4.53988000	C	2.79901900	-2.42760700	-1.01427700
H	0.70430000	1.92030400	4.66555500	C	3.04148000	-2.18328300	-2.39163800
C	3.74190800	2.25002800	-1.69970500	C	3.81693200	-2.19037500	-0.05085400
C	3.99370700	3.65302100	-2.29284200	C	4.29075900	-1.65307200	-2.75367200
C	2.49153600	1.62605800	-2.33874000	C	5.03824900	-1.65418700	-0.47295800
H	4.58087000	1.62206700	-2.02498100	C	5.27904200	-1.37800800	-1.81509500
H	4.90333400	4.10583800	-1.88236600	H	4.48820000	-1.46294300	-3.80659100
H	4.11226300	3.58457200	-3.38149300	H	5.81400300	-1.45571700	0.26085900
H	3.15513800	4.32886200	-2.09615100	H	6.23479900	-0.96665500	-2.12980400
H	2.24840700	0.65644900	-1.89390300	C	2.12011300	-2.53938600	-3.57171400
H	1.62065600	2.28461200	-2.26801000	C	0.61109700	-2.29429600	-3.42495200
H	2.67703800	1.45009800	-3.40548300	C	2.37333100	-3.98078900	-4.06696700
H	-0.24166000	-0.05447700	-1.27793100	H	2.45150700	-1.87859400	-4.38436100
H	0.20795000	0.03227000	1.15459800	H	0.39672500	-1.29046900	-3.04916900
C	-1.00898800	-4.26047700	0.60927300	H	0.13582700	-2.39111600	-4.40936800
C	0.20038800	-4.81627600	0.15258100	H	0.13820500	-3.02104800	-2.75829400
C	1.36519000	-4.20772100	-0.35152800	H	3.44152000	-4.17404800	-4.21648500
H	0.26573600	-5.89327800	0.25377000	H	1.98834400	-4.72095400	-3.35787200
Mg	0.03231800	-1.47718900	-0.04600400	H	1.86120200	-4.14530800	-5.02315600
N	-1.32162700	-2.95848200	0.57561600	C	3.62967000	-2.53241400	1.42890500
C	-1.97061200	-5.27252100	1.22084300	C	3.44384400	-1.27247100	2.29202300
H	-1.81543400	-5.32162200	2.30525600	C	4.78683500	-3.38951500	1.98075000
H	-3.01775600	-5.01547800	1.05701900	H	2.71624700	-3.12466100	1.52613200
H	-1.78464500	-6.27092400	0.81735100	H	2.58912800	-0.67741800	1.95645600
C	2.51579700	-5.17364900	-0.60395800	H	3.27231500	-1.54911300	3.34015500
H	2.13376100	-6.16958800	-0.84281100	H	4.32718000	-0.62776000	2.25217100
H	3.17558900	-4.84621000	-1.40759100	H	4.95943800	-4.28423400	1.37213900
H	3.12896200	-5.26587800	0.30082900	H	5.72755400	-2.82815800	2.01857400
N	1.51623000	-2.89570900	-0.56133300	H	4.55985900	-3.71247800	3.00381100
C	-2.62621700	-2.57345100	1.04582500	7			
C	-2.86293400	-2.36081400	2.42645200	C	0.71812800	-2.07758000	1.63937300
C	-3.66897400	-2.40785300	0.09589300	C	-0.63279500	-2.28577700	1.99636200
C	-4.14879100	-1.97803200	2.83116400	C	-1.81070100	-1.64955300	1.54953100
C	-4.93534900	-2.02875200	0.55708900	H	-0.77869700	-2.97256300	2.82176700
C	-5.17946600	-1.81519800	1.91177000	Mg	-0.26046400	-0.70460800	-0.80929400
H	-4.34568800	-1.81056100	3.88687000	N	1.12931900	-1.30504200	0.62960400
H	-5.74562700	-1.89722900	-0.15246200	C	1.73612800	-2.78183600	2.52285500
H	-6.17166500	-1.52470800	2.24790100	H	2.59230400	-3.14076800	1.94686100
C	-1.77784600	-2.55247900	3.48658000	H	2.12617900	-2.09668900	3.28421400
C	-2.22410400	-3.50234200	4.61728800	H	1.27808200	-3.62725000	3.04196000

C	-3.05825600	-1.93972700	2.36884900	H	-3.48916100	-2.85589400	-3.45526900
H	-3.95285400	-1.99407700	1.74438200	H	-4.57358400	-1.45709800	-3.45366300
H	-2.95130200	-2.87806300	2.91845400	H	-4.89720400	-3.10185900	0.00365200
H	-3.22706600	-1.14292800	3.10338900	H	-5.82752900	-2.63870700	-1.42786100
N	-1.87340200	-0.81661400	0.50686100	H	-4.64479000	-3.95378900	-1.52943200
C	2.52957800	-1.03602500	0.45727600	H	-0.28232200	-1.42815300	-2.41904700
C	3.15322900	-0.01647300	1.22390400	C	0.99304200	2.29966100	-1.87201100
C	3.26654000	-1.73620400	-0.53397700	C	2.32810100	1.89102900	-2.01562700
C	4.49474800	0.29240300	0.96844900	C	3.36489900	2.80571000	-1.85462500
C	4.60759200	-1.38764500	-0.74499900	C	3.09100100	4.14197200	-1.54850000
C	5.22293200	-0.38009100	-0.00855800	C	1.76582000	4.54867600	-1.40444800
H	4.97690300	1.07615000	1.54704300	C	0.71716700	3.63823900	-1.56756800
H	5.18187000	-1.92494400	-1.49520500	H	2.55485200	0.85255100	-2.24434000
H	6.26513000	-0.12788600	-0.18750300	H	4.39071900	2.46619500	-1.96395100
C	2.41495800	0.76373200	2.31258700	H	3.90123900	4.85465700	-1.42467700
C	2.21761600	2.24113600	1.92036700	H	1.53504000	5.58432700	-1.16941400
C	3.12743800	0.67296100	3.67781000	H	-0.30631700	3.97978200	-1.46077000
H	1.42064400	0.32345400	2.42916300	N	-0.04546600	1.31895400	-2.02859800
H	1.66026600	2.33946200	0.98467900	H	0.23811100	0.64086300	-2.74054700
H	1.66622900	2.77430200	2.70509900	C	-1.38465000	1.82160700	-2.39797300
H	3.17991100	2.74840000	1.78447500	H	-1.33951800	2.52398100	-3.24077100
H	3.30664100	-0.36487800	3.97897900	H	-2.00356600	0.96570600	-2.67563500
H	4.09849500	1.18187800	3.66064100	H	-1.85832800	2.31391000	-1.54693800
H	2.52052300	1.15201200	4.45557200	8			
C	2.66881700	-2.88923200	-1.34072500	C	-1.27962700	-2.90937900	0.09953000
C	3.27958000	-4.24201000	-0.91802400	C	0.00242100	-3.49195600	-0.00303600
C	2.81798800	-2.68793100	-2.85982800	C	1.28384000	-2.90767300	-0.10435900
H	1.59685500	-2.93119100	-1.12820700	H	0.00300200	-4.57497600	-0.00395700
H	3.13376800	-4.43727900	0.14991400	Mg	0.00052300	-0.26650200	-0.00111500
H	2.81289800	-5.06252300	-1.47628000	N	-1.52062200	-1.59248700	0.08056600
H	4.35792500	-4.27221200	-1.11667900	C	-2.44332500	-3.87625500	0.22738100
H	2.34291100	-1.75681200	-3.18366700	H	-3.08660500	-3.59999900	1.06899200
H	3.86995900	-2.66796900	-3.16980400	H	-3.07373500	-3.85548700	-0.66817700
H	2.32890800	-3.50858000	-3.39718900	H	-2.09098200	-4.89917200	0.37426800
C	-3.08949400	-0.11962700	0.20204500	C	2.44853100	-3.87316000	-0.23326000
C	-3.37462800	1.11316100	0.84593100	H	2.09726100	-4.89598400	-0.38332300
C	-3.95338500	-0.61354200	-0.81090800	H	3.09270400	-3.59420500	-1.07323100
C	-4.50017600	1.84129600	0.43944400	H	3.07773300	-3.85436200	0.66316800
C	-5.06895300	0.15336000	-1.17324400	N	1.52328000	-1.59075400	-0.08318800
C	-5.34226000	1.37503900	-0.56594700	C	-2.87343300	-1.09745300	0.10380400
H	-4.72346000	2.78916900	0.92305600	C	-3.61346400	-1.01858200	-1.10333000
H	-5.73909600	-0.21829600	-1.94417300	C	-3.41748000	-0.60815200	1.31588100
H	-6.21145100	1.95453900	-0.86614000	C	-4.90311800	-0.47626500	-1.06146500
C	-2.50193600	1.67107700	1.97084600	C	-4.71489300	-0.08053300	1.30225000
C	-3.30956100	1.89846300	3.26510700	C	-5.45871500	-0.01659000	0.12919100
C	-1.79003200	2.97396700	1.55777100	H	-5.47995000	-0.40586100	-1.97971000
H	-1.72460300	0.93418500	2.19060200	H	-5.14484100	0.29250300	2.22788900
H	-3.83702100	0.99111900	3.57859900	H	-6.46291600	0.39873000	0.13958800
H	-2.64393600	2.20405500	4.08131700	C	-3.02995500	-1.45277200	-2.44752700
H	-4.06018300	2.68776300	3.13920700	C	-2.66844000	-0.22350600	-3.30735100
H	-1.13074900	2.81631600	0.69803700	C	-3.96116200	-2.40068200	-3.22773700
H	-2.51181900	3.75640200	1.29283200	H	-2.10100300	-1.99790200	-2.25598300
H	-1.17370200	3.35397700	2.38141700	H	-1.96611600	0.43675400	-2.78614400
C	-3.73862100	-1.96955000	-1.48499700	H	-2.20856100	-0.53487800	-4.25345900
C	-3.65208700	-1.86333600	-3.01906500	H	-3.56136100	0.36690900	-3.54463100
C	-4.84120700	-2.97181800	-1.08253100	H	-4.23979600	-3.27799500	-2.63266700
H	-2.78276100	-2.37148200	-1.13682600	H	-4.88757400	-1.90141200	-3.53405500
H	-2.81230700	-1.23222900	-3.32455000	H	-3.46387000	-2.75387400	-4.13881500

C	-2.63697800	-0.62229600	2.62823100	C	1.53885700	5.21773500	-0.80967300
C	-3.29055100	-1.54510800	3.67614600	H	1.24572500	6.25527900	-0.60835200
C	-2.44916200	0.80135800	3.19272900	H	2.61499300	5.12837000	-0.62525500
H	-1.64182700	-1.03090000	2.42088900	H	1.36106700	5.00222800	-1.86609800
H	-3.38500300	-2.57260300	3.30638300	9-ts			
H	-2.68996200	-1.56978500	4.59340600	C	0.64696300	-2.39262200	1.22922000
H	-4.29425200	-1.19501300	3.94485500	C	-0.71381300	-2.66367500	1.48835200
H	-2.00047800	1.47564300	2.45540500	C	-1.87816700	-1.94596900	1.14980300
H	-3.40836000	1.23665000	3.49805300	H	-0.88681500	-3.53770200	2.10401200
H	-1.80317300	0.77540700	4.07899400	Mg	-0.20096000	-0.15515700	-0.54889700
C	2.87539700	-1.09420100	-0.10467000	N	1.09836800	-1.37910400	0.48071300
C	3.41960800	-0.60186500	-1.31533500	C	1.63586800	-3.32682200	1.90742300
C	3.61459400	-1.01692800	1.10298000	H	2.45867200	-3.59802000	1.24170100
C	4.71649800	-0.07293600	-1.29992100	H	2.08399400	-2.84035800	2.78193400
C	4.90374400	-0.47342200	1.06303900	H	1.14033800	-4.23843100	2.24835000
C	5.45967200	-0.01077000	-0.12634800	C	-3.17603200	-2.46451200	1.74366900
H	5.14652400	0.30255200	-2.22454800	H	-3.90720000	-2.68535300	0.95977000
H	5.47998800	-0.40434600	1.98175200	H	-3.00955400	-3.37072400	2.32940200
H	6.46351000	0.40551900	-0.13536900	H	-3.63394000	-1.71144600	2.39386300
C	2.64006500	-0.61423300	-2.62824500	N	-1.90126900	-0.85740500	0.37121500
C	3.29491800	-1.53522100	-3.67704600	C	2.51802400	-1.15737500	0.37739000
C	2.45197500	0.81008400	-3.19086800	C	3.17573900	-0.37002500	1.35695600
H	1.64492300	-1.02359500	-2.42237900	C	3.23111000	-1.66026000	-0.74051800
H	3.38966500	-2.56318000	-3.30874200	C	4.53929000	-0.09911100	1.19374100
H	2.69505400	-1.55886400	-4.59481400	C	4.59683300	-1.36423500	-0.84976200
H	4.29862900	-1.18411300	-3.94443200	C	5.25121600	-0.58947800	0.10282200
H	2.00200900	1.48300400	-2.45306200	H	5.05156500	0.51079900	1.93296600
H	3.41115400	1.24650200	-3.49464700	H	5.15611500	-1.74985000	-1.69804000
H	1.80690400	0.78497800	-4.07785000	H	6.31058500	-0.37073300	-0.00301200
C	3.03041100	-1.45374600	2.44596700	C	2.44364400	0.21237000	2.56585500
C	2.66664200	-0.22596800	3.30705200	C	2.30328800	1.74396700	2.45222300
C	3.96193800	-2.40151700	3.22593200	C	3.11874300	-0.16516000	3.89947000
H	2.10231200	-1.99970900	2.25301000	H	1.43392900	-0.20813400	2.58314000
H	1.96433000	0.43431400	2.78595700	H	1.79920800	2.03773900	1.52612000
H	2.20595700	-0.53908500	4.25219200	H	1.72939400	2.14018500	3.29910100
H	3.55870100	0.36497300	3.54625000	H	3.28501400	2.23228400	2.45454900
H	4.24165100	-3.27814500	2.63035900	H	3.23322200	-1.24984300	4.00580900
H	4.88777000	-1.90181400	3.53327800	H	4.11529600	0.28235500	3.99064400
H	3.46438500	-2.75589300	4.13640400	H	2.51902500	0.19619500	4.74334400
H	0.18597100	1.28577300	1.02499800	C	2.57542800	-2.52787700	-1.81512800
H	-0.18556500	1.28710600	-1.02423800	C	3.10742100	-3.97570500	-1.77800800
B	-0.00063800	2.08378400	0.00139700	C	2.74607300	-1.93500100	-3.22730400
O	1.13229000	2.90238700	-0.28762700	H	1.50207200	-2.56765900	-1.60585200
O	-1.13582100	2.89910800	0.29145200	H	2.94837800	-4.44453700	-0.80083100
C	0.77956500	4.24590800	0.09455500	H	2.59812000	-4.58856200	-2.53143800
C	-0.78718800	4.24347400	-0.09122800	H	4.18251000	-4.00938800	-1.99184200
C	1.20042900	4.45663000	1.55881400	H	2.33997400	-0.92080300	-3.28700600
H	2.26693000	4.22814400	1.65555200	H	3.80031700	-1.89930000	-3.52664500
H	1.03813000	5.48898700	1.88924500	H	2.21496200	-2.55221700	-3.96164500
H	0.64716700	3.78894900	2.22684500	C	-3.13620100	-0.14816400	0.16586100
C	-1.54934300	5.21347000	0.81258200	C	-3.48603100	0.90584200	1.04831300
H	-1.25891000	6.25173900	0.61106300	C	-3.94303100	-0.43916800	-0.96309300
H	-2.62518900	5.12119400	0.62791500	C	-4.62228100	1.67191600	0.76045000
H	-1.37121300	4.99866400	1.86907200	C	-5.07027600	0.35802100	-1.20249100
C	-1.20873100	4.45249200	-1.55560400	C	-5.40859300	1.41079000	-0.35809200
H	-2.27455800	4.22075100	-1.65218600	H	-4.89542100	2.48775900	1.42472200
H	-1.04953500	5.48521500	-1.88637300	H	-5.69407200	0.14775700	-2.06740700
H	-0.65349900	3.78625200	-2.22349300	H	-6.28474700	2.01944800	-0.56556000

C	-2.66632400	1.22849000	2.29827800	C	-5.00369700	0.38184100	0.02360800
C	-3.52804200	1.20556100	3.57683400	C	-5.44831200	-0.63548000	-0.81388200
C	-1.93098500	2.57771700	2.17139400	H	-4.93801300	-2.47708900	-1.78712100
H	-1.90250100	0.45311300	2.40843200	H	-5.66958600	1.20829800	0.25584500
H	-4.05702200	0.25267300	3.69167300	H	-6.45204300	-0.60384600	-1.22928700
H	-2.89730800	1.35127700	4.46185500	C	-2.40107200	-2.92596900	-0.99384900
H	-4.27998700	2.00318900	3.57407500	C	-2.02510100	-2.84592200	-2.48757600
H	-1.23851800	2.57950500	1.32300200	C	-3.03235800	-4.29589000	-0.67566800
H	-2.63760800	3.40437900	2.02968800	H	-1.47460300	-2.85463700	-0.41606300
H	-1.35071200	2.78598000	3.07852500	H	-1.55068700	-1.88891300	-2.73315400
C	-3.63984800	-1.59644200	-1.91559900	H	-1.33043800	-3.65075700	-2.75704700
C	-3.32888300	-1.10881300	-3.34489400	H	-2.91236400	-2.94220300	-3.12442700
C	-4.79039800	-2.62404900	-1.94686300	H	-3.30806300	-4.37941300	0.38134900
H	-2.74865600	-2.11199700	-1.54456600	H	-3.93776000	-4.47177500	-1.26793800
H	-2.45813100	-0.44613900	-3.36267100	H	-2.32675400	-5.10311100	-0.90589000
H	-3.11162900	-1.96257600	-3.99810000	C	-3.28967700	1.52724300	1.47479200
H	-4.17940300	-0.56776000	-3.77664800	C	-4.04376100	1.51454100	2.82087600
H	-5.02981400	-3.00104300	-0.94639400	C	-3.46506900	2.89131700	0.77952400
H	-5.70640700	-2.18754700	-2.36229000	H	-2.22453400	1.40389400	1.69872000
H	-4.51800200	-3.48091600	-2.57449200	H	-3.88245500	0.58270800	3.37349000
H	-0.03501000	-0.23268500	-2.51600800	H	-3.70606000	2.34321300	3.45480700
C	1.05566700	2.67088100	-1.38481500	H	-5.12388500	1.62925600	2.66984800
C	2.35567900	2.12180700	-1.36634700	H	-2.92618600	2.93144600	-0.17121100
C	3.48262700	2.93731200	-1.37755500	H	-4.52178400	3.10891400	0.58414400
C	3.35583900	4.32975300	-1.40310800	H	-3.07574200	3.69389200	1.41605500
C	2.07784300	4.88592600	-1.41940000	C	2.87762800	-0.68792500	0.26717800
C	0.94043500	4.07467300	-1.41285700	C	3.32439600	-1.71844600	-0.59916300
H	2.48469100	1.04326500	-1.35071300	C	3.71950500	0.41212400	0.56551300
H	4.46630900	2.47534500	-1.36312400	C	4.61562000	-1.63570100	-1.13377400
H	4.23663900	4.96567100	-1.40880500	C	5.00566400	0.43987300	0.01024100
H	1.95475800	5.96646500	-1.43534000	C	5.45845300	-0.57149700	-0.82991000
H	-0.03820900	4.54167600	-1.41806600	H	4.96608300	-2.41966100	-1.79999500
N	-0.05714900	1.80069600	-1.39010700	H	5.66250100	1.27431100	0.23991800
H	0.04875400	0.74086500	-2.23562300	H	6.45967800	-0.52767300	-1.25021300
C	-1.34741600	2.41080600	-1.72324300	C	2.43905900	-2.89984400	-0.99388000
H	-1.28176400	3.03765300	-2.62425500	C	3.08930400	-4.26082200	-0.67519800
H	-2.07642900	1.61629000	-1.92028400	C	2.05582200	-2.82821200	-2.48614300
H	-1.75157200	3.02621500	-0.90987400	H	1.51420300	-2.83912800	-0.41232800
10				H	3.37033300	-4.33833100	0.38088900
C	-1.27032500	-1.45972600	1.91285300	H	2.39325300	-5.07764100	-0.90059000
C	0.01550500	-1.69281200	2.44578700	H	3.99444400	-4.42626200	-1.27082100
C	1.29749000	-1.44180200	1.91253100	H	1.56802200	-1.87799200	-2.73194400
H	0.01944900	-2.24767000	3.37600300	H	2.94149200	-2.91461100	-3.12661400
Mg	0.00224800	0.17558200	-0.19629300	H	1.37039300	-3.64252300	-2.75075200
N	-1.51884800	-0.75958600	0.79805000	C	3.28660100	1.56476200	1.46987500
C	-2.41715300	-2.11290400	2.66536300	C	3.41516100	2.92669900	0.75987800
H	-3.28555700	-1.45408800	2.73456200	C	4.07059600	1.58043800	2.79854600
H	-2.74798600	-3.01724300	2.14118700	H	2.22986400	1.41809800	1.71828600
H	-2.10854100	-2.40300100	3.67210000	H	2.85034900	2.94832800	-0.17629100
C	2.45491000	-2.07333800	2.66714600	H	3.02759000	3.72711400	1.40033100
H	2.14573000	-2.38586000	3.66688000	H	4.46172900	3.16250200	0.53343200
H	2.81782600	-2.95964800	2.13371300	H	3.95042900	0.64594100	3.35721100
H	3.30297200	-1.39016700	2.75405500	H	5.14301800	1.72797200	2.62334100
N	1.53584500	-0.74101300	0.79553900	H	3.72171700	2.40075900	3.43723300
C	-2.86193000	-0.72134300	0.27196900	C	-0.02877900	2.80734000	-1.47395500
C	-3.29958600	-1.75662200	-0.59315700	C	-0.05061900	3.79785500	-2.48964300
C	-3.71464300	0.36985800	0.57258200	C	-0.06849800	5.15740900	-2.17555800
C	-4.59407700	-1.68924800	-1.12207700	C	-0.06560800	5.60226800	-0.85332100

C	-0.04399300	4.64390900	0.16673300	C	2.87200300	-2.27740100	0.97368900
C	-0.02620800	3.28888300	-0.13690400	C	5.14051200	-0.66652700	0.65300600
H	-0.05374900	3.50173100	-3.53260900	C	3.97498700	-2.40761400	1.82543700
H	-0.08489600	5.88085200	-2.98834300	C	5.10007200	-1.60059300	1.68024100
H	-0.07932200	6.66275600	-0.61993300	H	6.02958800	-0.05472000	0.52671100
H	-0.04044200	4.95547100	1.20912200	H	3.95965400	-3.15535300	2.61144700
H	-0.00736900	2.57182900	0.69025500	H	5.94455700	-1.71147600	2.35535600
N	-0.00983600	1.44676700	-1.70984100	C	4.24552100	0.50622500	-1.38023600
C	-0.00815500	1.02884200	-3.10224500	C	5.41932400	0.09536300	-2.29874300
H	0.87083100	1.39499600	-3.65946700	C	4.47253400	1.94960400	-0.89373400
H	0.00991000	-0.06686400	-3.16257400	H	3.33159000	0.51024100	-1.98051600
H	-0.90264600	1.36548500	-3.65345100	H	5.33610000	-0.93697000	-2.65077300
11-ts				H	5.45982400	0.75310400	-3.17536200
C	-0.77235900	-0.95330800	-2.70064800	H	6.37851800	0.18797400	-1.77564300
C	0.56374800	-1.29404500	-2.97099700	H	3.61840800	2.32333100	-0.32894700
C	1.66976500	-1.48004000	-2.11059700	H	5.36752300	2.02438800	-0.26392800
H	0.73944900	-1.62385500	-3.99045800	H	4.61639500	2.61553000	-1.75281700
N	-1.23396100	-0.49153200	-1.52583600	C	1.69003300	-3.23923400	1.10446100
C	-1.71171400	-1.20568700	-3.87665600	C	1.52139700	-3.83785900	2.51147000
H	-1.78366900	-2.27816200	-4.08656900	C	1.79099000	-4.38679900	0.07617900
H	-2.71817600	-0.82386000	-3.71115700	H	0.77622900	-2.67992400	0.86591800
H	-1.29967000	-0.73384300	-4.77551200	H	1.53374300	-3.07115900	3.29278600
C	2.82861600	-2.22308600	-2.76410600	H	0.56851500	-4.37551800	2.57621000
H	3.29605400	-1.59317900	-3.52874100	H	2.31245000	-4.56144900	2.74093100
H	3.59535700	-2.51929700	-2.04869700	H	1.79540300	-4.01374100	-0.95069700
H	2.45539200	-3.11868500	-3.27112000	H	2.71199600	-4.96124400	0.23284200
N	1.72179000	-1.08003600	-0.83988700	H	0.94186400	-5.07379000	0.18079100
C	-2.65151800	-0.58131500	-1.27966600	H	-1.47784900	2.49909300	0.72240600
C	-3.22552600	-1.84750200	-0.97861800	N	1.02982100	1.90912700	0.62152200
C	-3.47059500	0.57981600	-1.30477400	C	1.10489500	3.10245000	-0.08336000
C	-4.59230600	-1.91660000	-0.67539900	C	1.64108300	4.30631900	0.43932200
C	-4.83126500	0.44960000	-0.99679900	C	0.61329000	3.16089500	-1.41288700
C	-5.39458100	-0.78174400	-0.67507100	C	1.65818200	5.47982000	-0.31515700
H	-5.03519300	-2.88161100	-0.44176000	H	2.04276400	4.32713900	1.44652600
H	-5.46483800	1.33063200	-1.01592900	C	0.63068800	4.33627300	-2.15636100
H	-6.45297600	-0.85601000	-0.43901900	H	0.23936300	2.24979500	-1.87944500
C	-2.42977400	-3.15623600	-0.99680000	C	1.15175700	5.51610000	-1.61506000
C	-2.99947100	-4.15665200	-2.02531300	H	2.07597600	6.38186400	0.12761300
C	-2.37323100	-3.82671700	0.38949400	H	0.24896500	4.32525300	-3.17521400
H	-1.40105600	-2.93133100	-1.28860600	H	1.17155300	6.43382300	-2.19582000
H	-3.08553100	-3.71277500	-3.02161700	C	1.83995200	1.83973500	1.83246200
H	-2.35122200	-5.03820000	-2.09947300	H	1.50378300	2.52970900	2.62384900
H	-3.99726300	-4.50501100	-1.73352800	H	1.79713000	0.82418000	2.24452300
H	-1.90384800	-3.17380600	1.13136300	H	2.90346200	2.05567500	1.65000900
H	-3.37483500	-4.08085200	0.75614000	B	-1.24168900	1.83638900	1.66861800
H	-1.79117000	-4.75531600	0.34271400	O	-1.46468100	2.29791400	2.93164800
C	-2.92827600	1.94767300	-1.71719400	O	-1.11731800	0.42151000	1.64728300
C	-3.62359800	3.13055400	-1.01902800	C	-1.52195100	1.19641200	3.87345000
C	-2.99523900	2.15383700	-3.24586100	C	-1.65221400	-0.07501500	2.93318700
H	-1.87235900	1.98581300	-1.44045200	C	-0.25351600	1.23030700	4.73526300
H	-3.69710900	2.98442400	0.06294900	H	-0.17633200	2.21775500	5.20064700
H	-3.04914100	4.04640000	-1.19508800	H	-0.29629300	0.48016700	5.53226500
H	-4.63479700	3.29960800	-1.40900000	H	0.65145800	1.06684000	4.14963000
H	-2.39765200	1.41567600	-3.78659900	C	-0.82850100	-1.27359600	3.38432200
H	-4.02961000	2.08197300	-3.60450200	H	-1.17769900	-1.63008000	4.35985100
H	-2.61521800	3.14864400	-3.50750200	H	-0.93812300	-2.09767400	2.67460300
C	2.90677700	-1.29234000	-0.05139800	H	0.23296200	-1.03164700	3.46895500
C	4.06799700	-0.49355000	-0.23381100	C	-3.10121700	-0.49045900	2.66037200

H	-3.12143200	-1.25513200	1.88103600	C	5.78972000	-0.15634400	0.56081100
H	-3.57228800	-0.89938000	3.56020700	H	5.92969400	1.77496600	-0.34934100
H	-3.70118600	0.35180900	2.30504500	H	5.35865300	-2.08229000	1.38771400
C	-2.73678800	1.43607400	4.77608000	H	6.79839100	-0.12407900	0.96410700
H	-2.87523300	0.60766900	5.48005200	C	3.54167000	2.12406800	-1.51160500
H	-2.57546700	2.34988500	5.35613900	C	4.11632400	2.17043300	-2.94431800
H	-3.65472600	1.56358800	4.19898200	C	3.91334200	3.44467400	-0.80187500
Mg	0.18866100	0.17866500	-0.11000700	H	2.45108300	2.07470500	-1.59497600
12				H	3.78941400	1.32718300	-3.55500900
C	-0.74876300	-1.41132900	-2.46986300	H	3.79753800	3.09130100	-3.44773800
C	0.53878900	-1.14252000	-2.98502200	H	5.21298100	2.16515900	-2.92168700
C	1.75205500	-0.82304300	-2.34021200	H	3.66969200	3.42672600	0.26397400
H	0.66277000	-1.43635000	-4.02262800	H	4.98429500	3.65957600	-0.89355100
Mg	0.08115200	0.11998800	-0.08846900	H	3.37902000	4.28345400	-1.26319300
N	-1.16053200	-1.09954600	-1.23776500	C	2.83799900	-2.58207400	0.54820100
C	-1.64464000	-2.17972700	-3.43352300	C	3.08865600	-3.18698300	1.94248200
H	-1.32348000	-3.22642900	-3.48828300	C	3.05781900	-3.66961800	-0.52443400
H	-2.69421400	-2.16627500	-3.14249000	H	1.78233100	-2.29034000	0.49993900
H	-1.54871800	-1.76287500	-4.44118800	H	3.04890700	-2.42928900	2.73066600
C	2.97520900	-1.13098100	-3.20179000	H	2.32919800	-3.94586400	2.16075600
H	2.86437100	-0.65425100	-4.18134100	H	4.06364600	-3.68466200	2.00180200
H	3.91460400	-0.80880800	-2.75725500	H	2.75861500	-3.32935400	-1.51832600
H	3.03884000	-2.20929200	-3.38375100	H	4.11440700	-3.96070800	-0.56841000
N	1.86970500	-0.35064100	-1.08927700	H	2.47126300	-4.56576700	-0.28706900
C	-2.39939600	-1.66389100	-0.75623400	H	-2.23970600	1.38788900	1.29446900
C	-2.40921200	-2.98681800	-0.24354400	N	-0.32204700	2.21412700	0.42357500
C	-3.59217600	-0.89419300	-0.77229600	C	-1.09107600	3.13130600	-0.39171000
C	-3.61169400	-3.51118100	0.24914900	C	-1.95541900	4.06492200	0.19706300
C	-4.76723300	-1.47394400	-0.27735600	C	-0.92862900	3.14066400	-1.78300800
C	-4.78575200	-2.76794500	0.23349500	C	-2.65277500	4.97800700	-0.59597900
H	-3.62633000	-4.52334000	0.64550100	H	-2.07449000	4.06752700	1.27635600
H	-5.68702600	-0.89801000	-0.28949300	C	-1.62653900	4.05490100	-2.57514600
H	-5.71028400	-3.19319500	0.61538200	H	-0.25035800	2.42642200	-2.24576100
C	-1.16765700	-3.87863200	-0.21402700	C	-2.49245700	4.97712100	-1.98375000
C	-1.35951700	-5.16325900	-1.04689600	H	-3.32256900	5.69359600	-0.12591400
C	-0.76593600	-4.24586100	1.22758100	H	-1.49236400	4.04452100	-3.65375000
H	-0.33605700	-3.32207900	-0.65505900	H	-3.03614000	5.68936500	-2.59856700
H	-1.65727500	-4.93918700	-2.07620000	C	0.93370300	2.89725300	0.83434900
H	-0.42761600	-5.74085400	-1.08063900	H	0.73165500	3.66359700	1.59120300
H	-2.13275000	-5.80894800	-0.61408900	H	1.63605600	2.17448400	1.25985600
H	-0.57215200	-3.35077400	1.82690700	H	1.39896300	3.36684700	-0.03224800
H	-1.55574800	-4.81619100	1.73027000	B	-1.09611100	1.58744700	1.65368400
H	0.14127200	-4.86251400	1.23075200	O	-0.97201400	2.25429900	2.92741100
C	-3.64232400	0.52046700	-1.34685600	O	-0.33959600	0.26237900	1.86646500
C	-4.59099000	1.45707200	-0.57720500	C	-0.44821400	1.38691700	3.93241600
C	-4.02261500	0.52609100	-2.84301600	C	-0.49397200	-0.05530600	3.26954900
H	-2.63773400	0.94429000	-1.27000100	C	0.98117900	1.84222300	4.28160300
H	-4.39436700	1.43102100	0.49831100	H	0.95273800	2.90823400	4.52955400
H	-4.44687800	2.48640700	-0.92103700	H	1.38690900	1.30176600	5.14471900
H	-5.64441400	1.20067600	-0.74472900	H	1.66817900	1.71224700	3.44147300
H	-3.30414300	-0.02603900	-3.45492400	C	0.63196500	-0.98745400	3.71038700
H	-5.01217500	0.07739900	-2.99668400	H	0.58924700	-1.15546600	4.79268700
H	-4.05606300	1.55645600	-3.21637800	H	0.53319700	-1.96165100	3.22110300
C	3.19123100	-0.25281900	-0.51350300	H	1.61553800	-0.57976300	3.46483100
C	4.00167600	0.89650000	-0.72054300	C	-1.85081400	-0.75372900	3.45396600
C	3.67609700	-1.33148700	0.27549100	H	-1.89108400	-1.64690500	2.82294800
C	5.29634100	0.90893000	-0.18194800	H	-2.00018300	-1.06184100	4.49416400
C	4.97498000	-1.25873000	0.79408200	H	-2.67776300	-0.10259600	3.16108100

C	-1.32081200	1.51623000	5.18914700	C	-3.28335500	2.81244800	-3.48034500
H	-1.00161800	0.82485600	5.97896600	C	-3.19841700	0.45757200	-2.55963600
H	-1.23732800	2.53590900	5.58025300	H	-1.56663700	1.83549300	-2.65698300
H	-2.37354100	1.33182400	4.96374300	H	-2.91196700	3.84117800	-3.40890200
13-ts				H	-3.06582300	2.44400700	-4.48973200
C	2.50757600	1.75700400	-1.65412600	H	-4.37386400	2.84736200	-3.37384100
C	1.63742900	2.85660600	-1.79509600	H	-2.68171200	-0.24027700	-1.89479600
C	0.35575700	3.10183200	-1.26801300	H	-4.26916500	0.42806700	-2.32304200
H	2.02776700	3.65611200	-2.41307700	H	-3.07531300	0.09401700	-3.58720200
N	2.27289500	0.67936000	-0.89453300	C	-0.70846300	3.42022100	2.11081900
C	3.77413100	1.85543300	-2.49648600	C	-0.80792100	2.57414500	3.39436700
H	4.05922300	2.89927600	-2.65061300	C	-0.58545400	4.91612200	2.46484800
H	4.61933100	1.31819900	-2.06593100	H	0.21187500	3.12896000	1.59558400
H	3.57941500	1.42139900	-3.48490700	H	-0.85455800	1.50730400	3.15524000
C	-0.21856000	4.47703200	-1.57218100	H	0.06389800	2.74662100	4.03799000
H	0.51891600	5.10784900	-2.07230200	H	-1.70298800	2.82687200	3.97555300
H	-1.10136900	4.40301600	-2.21513200	H	-0.47598200	5.53696800	1.56900400
H	-0.54221000	4.97998800	-0.65595400	H	-1.46658100	5.27402300	3.01048300
N	-0.36394400	2.22350500	-0.55800300	H	0.29119500	5.08706000	3.10151300
C	3.32508400	-0.29242300	-0.74800800	H	-0.50919200	-1.18772500	-0.95545700
C	4.23785100	-0.15798900	0.33691700	N	-2.68420000	-1.57593200	0.65168700
C	3.43114300	-1.38538000	-1.64506900	C	-3.49479900	-2.50064700	-0.04091300
C	5.23187700	-1.13148400	0.49744700	C	-4.89953600	-2.44894300	0.04427000
C	4.43985400	-2.33456100	-1.42677500	C	-2.92026400	-3.49122100	-0.86446400
C	5.33431600	-2.21644000	-0.37013200	C	-5.69272600	-3.36286500	-0.65226300
H	5.94005900	-1.04410700	1.31548200	H	-5.38536400	-1.70211900	0.66092000
H	4.52805000	-3.17828600	-2.10619100	C	-3.72223200	-4.39795700	-1.54986400
H	6.11203400	-2.96149100	-0.22365600	H	-1.84393300	-3.54243600	-0.96668000
C	4.17888800	1.03180000	1.30233200	C	-5.11572200	-4.34695800	-1.45193300
C	4.96454600	2.25575800	0.78180000	H	-6.77442900	-3.29775600	-0.56083800
C	4.68164900	0.70094400	2.72100200	H	-3.24849800	-5.14913300	-2.17740800
H	3.12834600	1.33615600	1.37945900	H	-5.73586300	-5.05639300	-1.99273000
H	4.53788700	2.66286700	-0.13663700	C	-3.34420800	-0.41088000	1.23599500
H	4.95569700	3.05560600	1.53247200	H	-3.99053100	-0.69709100	2.07883500
H	6.01081700	1.99042600	0.58625100	H	-2.59568800	0.28467500	1.61032300
H	4.24684400	-0.22171100	3.11647900	H	-3.95818600	0.11292000	0.49776400
H	5.77252700	0.59425400	2.74853700	B	-1.28656900	-1.80273900	0.90860400
H	4.42458000	1.51855100	3.40421400	O	-0.77136300	-3.07148700	1.10732300
C	2.52067500	-1.56028100	-2.86208300	O	-0.45360900	-0.81833300	1.56697600
C	1.67921100	-2.84931200	-2.78476800	C	0.37433400	-3.00385000	1.98200700
C	3.32779800	-1.53888500	-4.17795400	C	0.22183700	-1.57695600	2.63897800
H	1.82189300	-0.71874700	-2.88774600	C	0.26855300	-4.16461100	2.97611200
H	1.01481500	-2.83690800	-1.91710900	H	0.36381100	-5.11122500	2.43519200
H	1.05389200	-2.94327000	-3.68080300	H	1.07106200	-4.11908900	3.72183400
H	2.31634800	-3.74050800	-2.72871800	H	-0.69394500	-4.17115900	3.49210700
H	3.95055100	-0.64234800	-4.26435800	C	-0.72091500	-1.56990100	3.85037700
H	3.99136400	-2.40857500	-4.25398800	H	-0.27116400	-2.08843800	4.70303200
H	2.64876800	-1.56679900	-5.03842100	H	-0.92195800	-0.53704500	4.14924000
C	-1.68313000	2.61621000	-0.13720900	H	-1.67618400	-2.05109000	3.62016100
C	-2.78841200	2.43120800	-1.00813800	C	1.53047000	-0.88714800	2.98714200
C	-1.87534600	3.15040800	1.16179400	H	1.34056600	0.11517400	3.38490000
C	-4.06738400	2.76398800	-0.54337500	H	2.06281800	-1.45669800	3.75733700
C	-3.17631900	3.46252000	1.57721200	H	2.18615200	-0.80285800	2.11927000
C	-4.26928000	3.27014400	0.73776900	C	1.64110000	-3.17293600	1.13822900
H	-4.92189000	2.62308700	-1.19990700	H	2.54258100	-3.21875000	1.75821500
H	-3.33324600	3.87165100	2.57212900	H	1.56205400	-4.11028500	0.57930600
H	-5.27135500	3.52044200	1.07625900	H	1.76547400	-2.36944300	0.41050400
C	-2.63548400	1.88727200	-2.42977100	Mg	0.28512100	0.24697100	-0.30240800

H₂				C	2.10180800	-3.21122900	-1.46720700
H	0.00000000	0.00000000	0.37139400	H	1.70094000	-2.39025300	0.46664400
H	0.00000000	0.00000000	-0.37139400	H	3.84109800	-3.10657800	1.57349700
3a				H	2.93855700	-4.46368400	0.87461200
C	-1.24573200	-0.00010800	1.86223400	H	4.37308500	-3.84021300	0.05388900
C	0.00001400	-0.00016100	2.50843600	H	1.42177200	-2.53839500	-1.99976500
C	1.24575200	-0.00010500	1.86221800	H	2.94615700	-3.43174400	-2.13162900
H	0.00002000	-0.00026700	3.59133800	H	1.57395300	-4.15256800	-1.27006400
N	-1.33800600	0.00002300	0.52298700	C	2.58677500	2.57418200	-0.14866400
C	-2.49271500	-0.00023000	2.71742900	C	2.10211000	3.21153300	-1.46686800
H	-3.11291600	0.87756400	2.50668800	C	3.48985800	3.54685000	0.63345000
H	-3.11272700	-0.87816200	2.50669200	H	1.70105300	2.39031200	0.46684000
H	-2.23615700	-0.00020800	3.77911300	H	1.42206000	2.53883300	-1.99957300
C	2.49274300	-0.00022500	2.71739900	H	1.57431600	4.15288300	-1.26961800
H	2.23619700	-0.00018300	3.77908700	H	2.94652000	3.43208500	-2.13120200
H	3.11274200	-0.87816900	2.50667200	H	3.84119500	3.10628400	1.57393100
H	3.11295300	0.87755700	2.50663700	H	4.37336300	3.84007400	0.05445900
N	1.33801100	0.00002600	0.52297100	H	2.93884300	4.46357900	0.87517300
C	-2.64382600	0.00002300	-0.09526700	H	-0.00000700	0.00039400	-1.78101800
C	-3.25933800	-1.23029900	-0.41965400	Be	-0.00000100	0.00012400	-0.42045900
C	-3.25941700	1.23034300	-0.41951500	6a			
C	-4.50898200	-1.20256700	-1.05135900	C	-1.09461500	3.69187600	-0.18030400
C	-4.50905900	1.20259700	-1.05122300	C	0.11467500	4.27218300	0.19898600
C	-5.13634200	0.00001200	-1.36163500	C	1.26696600	3.57955600	0.57255100
H	-4.99450800	-2.13931600	-1.31124800	H	0.15603200	5.35258300	0.23212300
H	-4.99464800	2.13934400	-1.31100500	N	-1.29136300	2.35902400	-0.21811700
H	-6.10627400	0.00001000	-1.85212000	C	-2.18750500	4.68547100	-0.54655900
C	-2.58660400	-2.57411800	-0.14892500	H	-2.45173900	4.61202200	-1.60393400
C	-2.10181700	-3.21123100	-1.46720100	H	-3.10939400	4.52043800	0.01403600
C	-3.48962700	-3.54698500	0.63300800	H	-1.84128800	5.70292300	-0.35248800
H	-1.70092300	-2.39025500	0.46664500	C	2.41841400	4.46872000	1.01963300
H	-1.42179100	-2.53839500	-1.99976800	H	2.03725200	5.46170400	1.26998400
H	-1.57395800	-4.15257000	-1.27006600	H	2.95248100	4.07191600	1.88305700
H	-2.94617600	-3.43174700	-2.13161100	H	3.15350700	4.58648700	0.21954900
H	-3.84106000	-3.10658700	1.57353100	N	1.36391100	2.24117000	0.52325900
H	-4.37307200	-3.84022200	0.05393000	C	-2.65711200	2.04500400	-0.58391800
H	-2.93852900	-4.46369100	0.87463000	C	-3.03011200	2.02914000	-1.94964500
C	-2.58678700	2.57417800	-0.14862500	C	-3.63091200	1.99133200	0.44463800
C	-3.48987000	3.54684500	0.63349100	C	-4.39623300	2.05971300	-2.26064000
C	-2.10212700	3.21152900	-1.46683100	C	-4.98147000	2.02679200	0.07572400
H	-1.70106400	2.39031000	0.46687700	C	-5.36364700	2.09660500	-1.26218400
H	-3.84120600	3.10627800	1.57397200	H	-4.70528400	2.07762800	-3.30265800
H	-2.93885500	4.46357400	0.87521300	H	-5.74715700	2.01743300	0.84496900
H	-4.37337600	3.84007000	0.05450100	H	-6.41697100	2.15082900	-1.52548800
H	-1.42207600	2.53883100	-1.99953600	C	-2.00803600	2.02461300	-3.08993400
H	-2.94653900	3.43207900	-2.13116300	C	-2.17679400	3.20780500	-4.06579000
H	-1.57433500	4.15288100	-1.26958300	C	-2.06421400	0.70144400	-3.87923100
C	2.64382400	0.00002800	-0.09529500	H	-1.01171600	2.09764100	-2.64657400
C	3.25933800	-1.23029300	-0.41968100	H	-2.09031100	4.17798100	-3.56644800
C	3.25940600	1.23034700	-0.41955600	H	-1.40111000	3.16559800	-4.83953500
C	4.50897600	-1.20255900	-1.05139800	H	-3.14809600	3.17946900	-4.57370400
C	4.50904200	1.20260400	-1.05127500	H	-1.83663000	-0.15323000	-3.23699900
C	5.13632800	0.00002100	-1.36168700	H	-3.05467900	0.54363900	-4.32377400
H	4.99450400	-2.13930800	-1.31128600	H	-1.33101400	0.71331600	-4.69409100
H	4.99462500	2.13935200	-1.31106600	C	-3.23868300	1.96187700	1.92709600
H	6.10625600	0.00002000	-1.85218100	C	-4.25117800	1.18959700	2.79072400
C	2.58661200	-2.57411200	-0.14893900	C	-3.03957000	3.36384400	2.54639500
C	3.48965000	-3.54697800	0.63298000	H	-2.27827200	1.43700200	1.99108000

H	-4.50630900	0.22160200	2.35669500	H	-5.99840300	-2.07961800	0.24732000
H	-3.82875800	1.01510300	3.78695600	H	-5.89757100	-2.56693700	2.64805900
H	-5.17819600	1.75943200	2.93251400	C	-1.24277700	-2.34251300	2.80077100
H	-2.19353700	3.90318600	2.11489700	C	-0.95005900	-3.77906100	3.28093300
H	-3.94201300	3.97593100	2.42267200	C	-1.22646400	-1.37669100	3.99941300
H	-2.85140600	3.26729100	3.62275400	H	-0.43220200	-2.04188100	2.13360200
C	2.66018900	1.77467400	0.97177200	H	-0.84289400	-4.47629200	2.44422100
C	2.80722700	1.45535700	2.35161900	H	-0.01495500	-3.80538300	3.85382400
C	3.78286900	1.81909900	0.10911400	H	-1.74925600	-4.15349400	3.93231400
C	4.08922200	1.18760000	2.84208900	H	-1.38293100	-0.34247400	3.67555700
C	5.03500700	1.49090100	0.65864500	H	-2.00166600	-1.62122000	4.73478800
C	5.20026600	1.19800600	2.00286500	H	-0.26125800	-1.43179000	4.51179700
H	4.22698200	0.97040600	3.89602800	C	-4.02336000	-1.59663100	-1.53761100
H	5.90392100	1.47938800	0.00743700	C	-5.46278400	-1.19347800	-1.91393200
H	6.18789600	0.97403000	2.39795000	C	-3.60817800	-2.68576100	-2.55504900
C	1.61872000	1.47837500	3.32318600	H	-3.38152200	-0.72763700	-1.71628200
C	1.30379500	2.89045100	3.86737500	H	-5.87961200	-0.44200900	-1.24260700
C	1.80292900	0.53811100	4.52785100	H	-5.46782300	-0.77315100	-2.92504600
H	0.73997700	1.13399600	2.76749000	H	-6.12991500	-2.06527300	-1.92301200
H	0.96068300	3.57678600	3.09107200	H	-2.55237700	-2.95208700	-2.51342900
H	0.50884900	2.82789500	4.62064400	H	-4.20431400	-3.59737700	-2.42561400
H	2.18598600	3.32815300	4.35148000	H	-3.80756400	-2.31250600	-3.56658000
H	2.05667800	-0.48048800	4.22231600	C	2.71451300	-1.72410200	-0.97673300
H	2.58531700	0.89304900	5.20958900	C	3.39600100	-1.26094400	-2.13117100
H	0.87444000	0.49926300	5.10623000	C	3.44437200	-2.09622600	0.19326000
C	3.83458400	2.20429400	-1.38860800	C	4.79821600	-1.14479300	-2.05191500
C	4.78697400	3.39498800	-1.66128400	C	4.83525000	-1.98189400	0.19176400
C	2.52691200	2.44386000	-2.15973300	C	5.51655900	-1.50602300	-0.92437300
H	4.30911200	1.33529000	-1.85982400	H	5.33906500	-0.76516800	-2.91457600
H	5.75653200	3.28429500	-1.16778000	H	5.39811500	-2.26935600	1.07287900
H	4.96887600	3.47848100	-2.73968400	H	6.59994100	-1.41738700	-0.91199300
H	4.35575400	4.34773300	-1.33449500	C	2.82086900	-0.85099500	-3.51055900
H	1.81469100	1.62659800	-2.03808800	C	1.30164100	-0.84356700	-3.72672100
H	2.02758900	3.37206200	-1.86832100	C	3.47246500	-1.62984200	-4.68125200
H	2.76560000	2.52832900	-3.22761100	H	3.14557100	0.19124700	-3.63642100
H	-0.06290400	0.26003500	-1.18281200	H	0.77137100	-0.29164400	-2.95173800
H	0.01555900	-0.08977400	0.87605900	H	1.09300600	-0.36341800	-4.69101000
C	-1.26607400	-3.45123100	-0.59681300	H	0.87783700	-1.85200700	-3.77149100
C	-0.18083800	-3.89938300	-1.35413300	H	4.56500500	-1.62846500	-4.64505700
C	1.04976100	-3.25372600	-1.48126700	H	3.14521000	-2.67515100	-4.70664300
H	-0.24304400	-4.90656200	-1.74268200	H	3.17096400	-1.17422400	-5.63191500
N	-1.38911200	-2.18445700	-0.15331100	C	2.75744700	-2.70353300	1.42362200
C	-2.26590400	-4.54625700	-0.24541400	C	3.50490600	-2.42220100	2.73992300
H	-2.23296300	-4.75198600	0.82891900	C	2.57106600	-4.23417600	1.30760800
H	-3.29881000	-4.29216100	-0.47692800	H	1.76396000	-2.25052500	1.50215900
H	-2.00599200	-5.46606300	-0.77342700	H	3.77801900	-1.37013700	2.83955400
C	2.12580600	-4.07777800	-2.17273500	H	2.86862100	-2.69930700	3.58871800
H	1.74492500	-5.07744000	-2.39227500	H	4.41910100	-3.02280600	2.82327800
H	2.43081900	-3.61922700	-3.11501400	H	1.88889000	-4.52113500	0.50596700
H	3.02767400	-4.17722400	-1.56494500	H	3.53675900	-4.72592900	1.13483600
N	1.29496800	-2.03263700	-0.97866200	H	2.15994100	-4.63020900	2.24426700
C	-2.61207300	-2.03501200	0.62698700	Be	-0.04113000	-1.03816600	-0.35751500
C	-2.55569200	-2.24274100	2.02522000	Be	0.01100000	1.22849100	0.02138100
C	-3.87025300	-1.92730200	-0.03832600	7a			
C	-3.75133700	-2.42367100	2.73574200	C	-0.60792700	-1.64313600	1.97998100
C	-5.02838000	-2.12517600	0.72685900	C	0.68679200	-1.59061500	2.53028600
C	-4.97891700	-2.39806300	2.09194200	C	1.80658900	-0.98582600	1.93714600
H	-3.71166900	-2.61213700	3.80489100	H	0.86651700	-2.18844800	3.41742300

N	-0.96028700	-0.90622800	0.92438000	C	2.73312500	2.54092800	1.21635900
C	-1.59261200	-2.55957300	2.68375500	C	2.68177700	3.98967800	0.69668600
H	-1.99589000	-2.04739400	3.56610700	C	3.50745300	2.49817800	2.55101500
H	-2.43590500	-2.83973800	2.05166700	H	1.70411600	2.23064800	1.42926300
H	-1.09197900	-3.46639700	3.03539600	H	2.23002400	4.05627200	-0.30080700
C	3.14385500	-1.30205500	2.58458000	H	2.08490900	4.60620600	1.37843200
H	3.08225700	-1.07917700	3.65591200	H	3.67653200	4.44802200	0.63540900
H	3.37910000	-2.36798700	2.49494300	H	3.48892600	1.49878600	2.99545100
H	3.96788900	-0.72929600	2.15779400	H	4.55716700	2.78537500	2.40787200
N	1.70314900	-0.18510400	0.87053500	H	3.06077100	3.19279500	3.27272700
C	-2.27322400	-1.04744400	0.35699600	H	-0.22755200	1.57028300	1.38088700
C	-2.45896800	-1.91454500	-0.75281900	C	-1.07046500	2.11729500	-1.38018400
C	-3.35865900	-0.29688300	0.87276600	C	-0.97569000	3.46722000	-1.02734600
C	-3.73164300	-2.00141400	-1.33183200	C	-2.03486100	4.33659500	-1.28631000
C	-4.60890500	-0.41788000	0.25038000	C	-3.19716800	3.86816100	-1.90191300
C	-4.80147600	-1.25547000	-0.84245700	C	-3.29243600	2.51918100	-2.24430100
H	-3.89180500	-2.66589100	-2.17580000	C	-2.23702300	1.64260500	-1.98572300
H	-5.44759900	0.15592400	0.63581400	H	-0.07932100	3.83350900	-0.53605900
H	-5.78128400	-1.33580200	-1.30661900	H	-1.94677500	5.38284700	-1.00647600
C	-1.32090300	-2.78395200	-1.29047300	H	-4.02096600	4.54610400	-2.10646800
C	-1.35848500	-2.97260300	-2.81925400	H	-4.19564500	2.13507700	-2.70997600
C	-1.29463200	-4.17054300	-0.61175400	H	-2.33953600	0.59332200	-2.23796700
H	-0.38093200	-2.28323400	-1.03431700	N	0.05295900	1.22922700	-1.12708200
H	-1.46931500	-2.02297600	-3.35483300	H	0.85167700	1.82903300	-0.91391600
H	-0.43130100	-3.44776300	-3.15997300	C	0.43003100	0.42459200	-2.31787400
H	-2.18474200	-3.62241000	-3.13033200	H	0.45687500	1.04220700	-3.22339500
H	-1.14392900	-4.09301500	0.46794500	H	1.41563300	-0.00341200	-2.14159600
H	-2.23699600	-4.70514800	-0.78386700	H	-0.28629300	-0.38260600	-2.45915300
H	-0.48059300	-4.78198100	-1.02078800	Be	0.07710200	0.44339300	0.60954300
C	-3.23020900	0.61112800	2.09577200	9a-ts			
C	-4.15421800	0.14784000	3.24169800	C	0.63495700	-1.70289400	1.90549600
C	-3.51102400	2.08607300	1.75289500	C	-0.68952800	-1.88133900	2.32613300
H	-2.19630700	0.56383500	2.44519400	C	-1.81845100	-1.30259000	1.73557500
H	-3.98774900	-0.90205500	3.50568400	H	-0.84692200	-2.46524100	3.22378700
H	-3.97840400	0.75504500	4.13793100	N	0.96225500	-0.98911400	0.81680500
H	-5.21268500	0.25573900	2.97467800	C	1.70353100	-2.34677700	2.76538500
H	-2.80822500	2.45391000	1.00248900	H	2.40586000	-2.93130700	2.16650200
H	-4.53079400	2.22696300	1.37312400	H	2.29543600	-1.59125500	3.29054000
H	-3.40112500	2.70599500	2.65128100	H	1.24747100	-3.00118600	3.51143000
C	2.87560000	0.20499900	0.14119300	C	-3.13325600	-1.48249200	2.46624700
C	3.54113800	-0.72355500	-0.70824000	H	-3.95089300	-1.73853500	1.78953300
C	3.32968000	1.55124400	0.21446300	H	-3.04327000	-2.26225400	3.22603100
C	4.61119700	-0.27080000	-1.49259100	H	-3.42111700	-0.55294400	2.97093700
C	4.40307600	1.94637300	-0.59523300	N	-1.75045200	-0.59095300	0.60047400
C	5.03734600	1.05191500	-1.45209400	C	2.37736900	-0.84759300	0.54548900
H	5.12098700	-0.97275100	-2.14745400	C	3.10248300	0.21010600	1.14831100
H	4.75660400	2.97179500	-0.54530200	C	3.02435800	-1.77595400	-0.30892500
H	5.86670600	1.38069500	-2.07291200	C	4.46543700	0.33633800	0.85236400
C	3.17044100	-2.20789300	-0.78804200	C	4.39078600	-1.60187200	-0.56723700
C	4.33616100	-3.10049600	-0.30833100	C	5.10963300	-0.55397100	-0.00049500
C	2.74832000	-2.64713600	-2.20518400	H	5.03163200	1.14905500	1.29929200
H	2.31892600	-2.38476300	-0.12570900	H	4.90015100	-2.30510200	-1.22101000
H	4.69021400	-2.81195300	0.68539700	H	6.16893500	-0.43771400	-0.21490200
H	4.02127400	-4.15030500	-0.26767000	C	2.46896000	1.20787000	2.12020500
H	5.19047000	-3.03845200	-0.99302700	C	2.47816100	2.64538600	1.56480800
H	1.86759000	-2.10310500	-2.55806500	C	3.15793500	1.18507800	3.50148300
H	3.55317900	-2.48988300	-2.93289300	H	1.42371800	0.91948200	2.26629100
H	2.50385200	-3.71638800	-2.21054500	H	1.95287200	2.71403900	0.61012700

H	1.99288800	3.32613800	2.27553800	C	-1.27580700	1.26457200	-2.22560400
H	3.50227200	3.00468600	1.40864300	H	-1.02826000	1.64362800	-3.22537800
H	3.17718700	0.18295200	3.94297600	H	-1.91768300	0.38824800	-2.34172900
H	4.19492200	1.53496200	3.43644700	H	-1.86633700	2.02536100	-1.70491400
H	2.63036200	1.84835700	4.19732600	Be	-0.26669500	-0.43616500	-0.22582900
C	2.30617300	-2.96981100	-0.94225700	10a			
C	2.88692400	-4.31416100	-0.45580000	C	-1.19486700	-1.11837500	2.04108600
C	2.34085800	-2.91282600	-2.48244100	C	0.05467800	-1.21858100	2.67136200
H	1.25606200	-2.93103900	-0.64340500	C	1.29622000	-0.96248400	2.07241900
H	2.84227700	-4.41142600	0.63432900	H	0.06642100	-1.60757300	3.68161800
H	2.32215900	-5.14871700	-0.88847700	N	-1.32576800	-0.59420700	0.80880200
H	3.93490100	-4.43261900	-0.75584500	C	-2.39354200	-1.64910500	2.79686200
H	1.88528900	-1.99228900	-2.85912300	H	-3.15506900	-0.87672500	2.92921500
H	3.36703000	-2.96770300	-2.86541600	H	-2.87468800	-2.46557200	2.24969900
H	1.78321000	-3.75734700	-2.90464800	H	-2.09527600	-2.01825900	3.78052900
C	-2.98405000	-0.02021100	0.11101700	C	2.53500400	-1.28947700	2.87760100
C	-3.39049200	1.25582100	0.57024300	H	2.26364200	-1.64962900	3.87228200
C	-3.75829700	-0.73158600	-0.83902400	H	3.14383900	-2.05241000	2.38463100
C	-4.54415400	1.82678800	0.01727000	H	3.17345800	-0.40849700	2.98666700
C	-4.90912200	-0.11778500	-1.35052500	N	1.39157300	-0.46174000	0.82676400
C	-5.29597800	1.15507100	-0.94219000	C	-2.63381400	-0.68237100	0.18063700
H	-4.86146700	2.81252300	0.34697700	C	-2.93419700	-1.82082100	-0.61046800
H	-5.51270700	-0.64828400	-2.08214900	C	-3.60348000	0.33245100	0.37012800
H	-6.18765000	1.61591900	-1.35917000	C	-4.22274600	-1.94878200	-1.14428700
C	-2.62428900	2.02157300	1.65070500	C	-4.87626400	0.15103900	-0.18867600
C	-3.54472200	2.47753400	2.80085100	C	-5.19636700	-0.98042900	-0.92846800
C	-1.85510700	3.22528200	1.07300100	H	-4.46655600	-2.82488700	-1.73860500
H	-1.87921800	1.34439000	2.07807800	H	-5.62985600	0.91917700	-0.04037800
H	-4.12276000	1.64412400	3.21593600	H	-6.19286000	-1.10082700	-1.34524800
H	-2.94773700	2.91352200	3.61054300	C	-1.91728400	-2.92271900	-0.91012000
H	-4.25840300	3.24248200	2.47326600	C	-1.80078900	-3.19612500	-2.42329400
H	-1.10264200	2.90063700	0.34927000	C	-2.23756600	-4.23340800	-0.16228400
H	-2.53293400	3.92870500	0.57353500	H	-0.93767000	-2.58206600	-0.56191300
H	-1.33862700	3.76950800	1.87313900	H	-1.59948000	-2.27737000	-2.98289400
C	-3.40701400	-2.14871700	-1.30008600	H	-0.98633500	-3.90278200	-2.61961700
C	-3.23864200	-2.25342500	-2.82884800	H	-2.71916200	-3.63750700	-2.82675400
C	-4.45981400	-3.17186000	-0.82274400	H	-2.23319000	-4.09637400	0.92389300
H	-2.44797700	-2.41975400	-0.85142300	H	-3.22383600	-4.61848500	-0.44727500
H	-2.44539000	-1.59403000	-3.19251400	H	-1.49532200	-5.00400500	-0.40382700
H	-2.97027900	-3.27968800	-3.10656000	C	-3.33717100	1.63220700	1.12811200
H	-4.16437200	-1.99939800	-3.35886000	C	-4.19760400	1.76892000	2.40167800
H	-4.57420400	-3.16718200	0.26631100	C	-3.57183100	2.85526200	0.21730900
H	-5.44399900	-2.96523100	-1.26011300	H	-2.28662200	1.64093600	1.43028800
H	-4.16816200	-4.18528100	-1.12349100	H	-4.02772400	0.95537400	3.11474300
H	-0.22578800	-1.38568700	-1.52351400	H	-3.96613600	2.71096000	2.91292600
C	1.04105600	1.74272000	-1.77738700	H	-5.26701700	1.77863300	2.15987600
C	2.32654600	1.24196100	-2.04323700	H	-2.98374600	2.79102300	-0.70111600
C	3.38454700	2.09840200	-2.34443900	H	-4.63003200	2.94719000	-0.05595100
C	3.19040100	3.47949600	-2.40986100	H	-3.27974800	3.77509700	0.73497200
C	1.91432900	3.99043900	-2.17138200	C	2.70592800	-0.45256700	0.20618400
C	0.85397800	3.13710600	-1.86278100	C	3.14813200	-1.62373000	-0.46285200
H	2.49849900	0.17314500	-2.02353700	C	3.53977900	0.68957400	0.27451800
H	4.36559900	1.67385200	-2.54051100	C	4.43538000	-1.63865500	-1.01384900
H	4.01558100	4.14352500	-2.65223200	C	4.81887600	0.61676600	-0.29470900
H	1.73562200	5.06180100	-2.22537200	C	5.27439600	-0.53379000	-0.92635000
H	-0.12942300	3.55973000	-1.68556600	H	4.78508500	-2.53423800	-1.52012400
N	-0.05199500	0.86920300	-1.50553900	H	5.46906400	1.48514000	-0.23941600
H	0.02820300	-0.42294200	-1.78173300	H	6.27242600	-0.56659300	-1.35532200

C	2.28734700	-2.87923000	-0.61582000	H	4.19582700	0.92571700	-3.08126400
C	2.84958400	-4.07777200	0.17657200	H	4.88219800	-2.57564800	-0.73115000
C	2.11518000	-3.27016700	-2.09752500	H	5.76255000	-0.67124300	-2.03354400
H	1.29334900	-2.66128100	-0.21470000	C	1.50694600	0.95015200	-3.07536300
H	2.92027900	-3.86513400	1.24803600	C	1.41604400	0.62078400	-4.58099000
H	2.20204100	-4.95433300	0.05322700	C	1.93383800	2.41541400	-2.88133500
H	3.85122800	-4.35154500	-0.17533400	H	0.50023100	0.85244100	-2.65897300
H	1.71608200	-2.44071800	-2.68944100	H	1.01687500	-0.38215800	-4.76163400
H	3.06831700	-3.56919900	-2.54830900	H	0.75989300	1.33763300	-5.09001400
H	1.42870400	-4.12012400	-2.18988200	H	2.40425000	0.67743500	-5.05370400
C	3.12226500	2.00343600	0.93136100	H	1.98816800	2.65350900	-1.81746900
C	3.22124400	3.18103200	-0.05928700	H	2.90716600	2.62453700	-3.34058400
C	3.95041600	2.31839100	2.19492700	H	1.20534300	3.08306800	-3.35691900
H	2.07574600	1.91351400	1.23228600	C	2.37024500	-3.29148100	-0.20848400
H	2.65348200	2.98591000	-0.97235600	C	2.87614700	-3.25106700	1.24754600
H	2.81534800	4.09121500	0.39432500	C	2.84193900	-4.60646200	-0.86758100
H	4.26334400	3.38146400	-0.33627500	H	1.27755700	-3.30307800	-0.17704000
H	3.86143300	1.53855300	2.95885600	H	2.55611200	-2.34234100	1.76039700
H	5.01521600	2.42683600	1.95642500	H	2.48801300	-4.11078700	1.80492000
H	3.61257200	3.26131400	2.64095500	H	3.97155800	-3.29472200	1.28406100
C	-0.13813700	2.30658400	-1.25630000	H	2.53500600	-4.68961800	-1.91524500
C	-0.21257800	3.11229800	-2.42098900	H	3.93456700	-4.69316200	-0.84191600
C	-0.31666600	4.50210000	-2.33434700	H	2.43238700	-5.46688900	-0.32482500
C	-0.35218500	5.15481100	-1.10248600	C	-3.09939800	0.49053900	-0.36988800
C	-0.28384000	4.37680500	0.05953100	C	-4.00984400	-0.00772700	0.59866300
C	-0.18240600	2.99367900	-0.01310700	C	-3.18187000	1.83191800	-0.81232900
H	-0.18897300	2.65197800	-3.40225400	C	-4.96715600	0.87040300	1.12263700
H	-0.37026000	5.08002400	-3.25483300	C	-4.14979900	2.66908400	-0.24077600
H	-0.43104900	6.23651900	-1.04526900	C	-5.03599300	2.20066300	0.72147300
H	-0.31070800	4.85483800	1.03682300	H	-5.66960000	0.50342400	1.86579500
H	-0.13117400	2.41927400	0.91047700	H	-4.21258300	3.70435800	-0.56449100
N	-0.02107000	0.93078100	-1.28107300	H	-5.78187200	2.86444100	1.15062700
C	0.06502000	0.30302600	-2.58837300	C	-4.01110600	-1.45524700	1.09698100
H	0.92495600	0.66336500	-3.17682000	C	-5.28905300	-2.21138400	0.67328700
H	0.18701300	-0.77867100	-2.46982600	C	-3.85227200	-1.54647500	2.62848200
H	-0.83874800	0.46206000	-3.20062900	H	-3.15697000	-1.96921600	0.65007300
Be	0.01208600	0.01795100	0.03999200	H	-5.41827400	-2.23984600	-0.41328000
11a-ts				H	-5.24873300	-3.24728800	1.03052300
C	-0.12215400	-1.97214200	-2.43478000	H	-6.18506700	-1.74739300	1.10230100
C	-1.50729500	-1.94929600	-2.64518500	H	-2.94797000	-1.04111800	2.97559700
C	-2.41635200	-1.10746000	-1.99653000	H	-4.71186100	-1.10556600	3.14720800
H	-1.88924100	-2.54634200	-3.46341600	H	-3.78158600	-2.59602700	2.93494900
N	0.47493500	-1.25904500	-1.45988600	C	-2.28221000	2.40823600	-1.90542800
C	0.67745400	-2.84903300	-3.37652100	C	-1.35465000	3.51356300	-1.36401300
H	1.59432900	-2.36824400	-3.72013300	C	-3.10466000	2.93912400	-3.09826200
H	0.97202800	-3.76935300	-2.86132100	H	-1.64687000	1.60251400	-2.28453000
H	0.07523500	-3.12855800	-4.24387800	H	-0.65236900	3.12334200	-0.62157100
C	-3.79647800	-1.00436400	-2.60985900	H	-0.76542600	3.94954700	-2.17874800
H	-3.97444400	-1.84041600	-3.29022200	H	-1.93011700	4.32320600	-0.89964900
H	-4.59180400	-0.97372900	-1.86510500	H	-3.77799500	2.17479000	-3.50222200
H	-3.87347600	-0.07739300	-3.19096100	H	-3.71883900	3.80133200	-2.81380300
N	-2.06937600	-0.37563300	-0.92124600	H	-2.43662900	3.26202600	-3.90540300
C	1.92470100	-1.12294600	-1.57658300	H	2.35427700	-0.23520400	0.98309500
C	2.41961000	-0.03661800	-2.34299800	N	-0.10298900	-0.08642400	1.25004800
C	2.81336000	-2.06194300	-1.00072500	C	-0.10500600	-1.25691400	2.09310100
C	3.80478100	0.10149200	-2.49228200	C	0.33941200	-1.20709500	3.43019200
C	4.19005300	-1.86749600	-1.17768200	C	-0.56445400	-2.49852600	1.61568500
C	4.69020300	-0.79810500	-1.90930500	C	0.31299100	-2.34128200	4.24001600

H	0.74572500	-0.28141000	3.81795500	C	-1.26889100	-4.08400900	-2.44210600
C	-0.58379300	-3.63594700	2.42696600	C	-0.53083900	-4.55055300	-0.08385200
H	-0.93244800	-2.58753000	0.59642300	H	-0.20527500	-2.72949800	-1.16680900
C	-0.15063500	-3.56484600	3.74989600	H	-1.56812100	-3.33490600	-3.18025100
H	0.66975800	-2.26733000	5.26460400	H	-0.36396200	-4.58087500	-2.81311200
H	-0.95156400	-4.57489700	2.01977700	H	-2.06677300	-4.83471300	-2.38911600
H	-0.17161900	-4.44478500	4.38704400	H	-0.33824400	-4.15070900	0.91661600
C	-0.89406700	0.99888300	1.87582100	H	-1.26234100	-5.35980800	0.01745300
H	-0.49785000	1.24587500	2.86234400	H	0.39417400	-5.00354800	-0.45655800
H	-0.82625800	1.89483700	1.25523800	C	-3.96815800	0.77083000	-0.39024200
H	-1.94975200	0.74061800	1.99286100	C	-4.67644700	1.35742900	0.84829000
B	1.87040000	0.78123700	1.36304200	C	-4.85999600	1.02913700	-1.62570700
O	2.13045700	1.18509200	2.68805600	H	-3.03683000	1.31704600	-0.53182900
O	1.77815700	1.93223600	0.54056000	H	-4.13112300	1.13748400	1.76901700
C	2.37135900	2.60519900	2.74147300	H	-4.74726000	2.44534500	0.74715900
C	2.48924900	2.99716400	1.20983900	H	-5.69842600	0.97292100	0.95156000
C	1.21774200	3.30370100	3.47964800	H	-4.39735700	0.69161300	-2.55592200
H	1.07145900	2.81551600	4.44939700	H	-5.82354200	0.51345100	-1.52839000
H	1.44820600	4.35918600	3.66517300	H	-5.06128200	2.10262100	-1.72173800
H	0.27648800	3.25298700	2.93075100	C	2.93366000	-0.04876900	-0.54961500
C	1.85530400	4.34070400	0.84154700	C	3.81063100	1.07684100	-0.50162700
H	2.34928000	5.16352500	1.37189100	C	3.42669100	-1.32312000	-0.13995300
H	1.96617100	4.52206000	-0.23272700	C	5.09317300	0.91289700	0.04552100
H	0.78943400	4.36891500	1.07851000	C	4.71722900	-1.41837200	0.39682000
C	3.93970600	2.96844600	0.69253100	C	5.54615900	-0.30986600	0.51202100
H	3.93323100	3.10594100	-0.39288600	H	5.75408200	1.77308600	0.09264900
H	4.54886800	3.76415400	1.13560800	H	5.08942500	-2.38287700	0.72109000
H	4.41657600	2.00604600	0.90041200	H	6.54167500	-0.40647000	0.93698700
C	3.65421000	2.81646400	3.55787700	C	3.51772400	2.47199900	-1.06832500
H	3.94635000	3.87321600	3.58061400	C	4.38564900	2.78360200	-2.31166300
H	3.48298400	2.49201800	4.58998900	C	3.78433600	3.60019400	-0.04179000
H	4.48531800	2.23073900	3.15941900	H	2.46821100	2.51046000	-1.37177300
Be	-0.49584800	-0.47830800	-0.32651200	H	4.27216400	2.04961700	-3.11020300
12a				H	4.11786600	3.76786000	-2.71511600
C	-1.10508800	-0.36674500	-2.38650800	H	5.44781300	2.81598700	-2.04315300
C	0.10169300	0.05279900	-2.97203900	H	3.37853900	3.38260500	0.94791300
C	1.36852500	0.08742200	-2.36605500	H	4.86009600	3.77251600	0.07736000
H	0.09494400	0.14762500	-4.05275800	H	3.34635100	4.54182900	-0.39307000
N	-1.24968100	-0.51425000	-1.06473800	C	2.63793800	-2.61824300	-0.34769400
C	-2.21769600	-0.66253600	-3.37787800	C	3.10926700	-3.78417400	0.54282200
H	-1.83261700	-1.23899100	-4.22413400	C	2.70427600	-3.08154400	-1.82056000
H	-3.05377200	-1.20129600	-2.93579900	H	1.59044300	-2.41327500	-0.10977000
H	-2.59377400	0.28553600	-3.78105300	H	3.20570400	-3.49917500	1.59418900
C	2.51539300	0.11557200	-3.36465100	H	2.39240200	-4.60850200	0.48229700
H	2.52752900	1.08088800	-3.88204800	H	4.07642200	-4.17871200	0.20946400
H	3.48973500	-0.04689700	-2.90854200	H	2.22194400	-2.37665500	-2.49989000
H	2.35821700	-0.65124200	-4.12914300	H	3.74705900	-3.20461600	-2.13744500
N	1.55813900	0.05261900	-1.03589600	H	2.20320600	-4.04986900	-1.93812000
C	-2.38985900	-1.30218500	-0.59885300	H	-2.06658800	0.88916600	1.70391400
C	-2.25131100	-2.71728600	-0.55002700	N	-0.30849900	1.85049800	0.61123900
C	-3.63347600	-0.71283500	-0.24097200	C	-1.18389400	2.85309200	0.03420100
C	-3.32251100	-3.49811100	-0.09641100	C	-1.96314100	3.67395000	0.86062800
C	-4.66853900	-1.54731000	0.20718300	C	-1.17499000	3.08993900	-1.34595500
C	-4.52436900	-2.92448900	0.29526700	C	-2.73628700	4.69858400	0.31167000
H	-3.21629900	-4.57824500	-0.06565200	H	-1.95916900	3.50403200	1.93319000
H	-5.61814300	-1.09855300	0.48116400	C	-1.95127600	4.11408800	-1.89257400
H	-5.34512400	-3.54494700	0.64576400	H	-0.56658300	2.46139300	-1.99018200
C	-1.01225800	-3.45640900	-1.05449900	C	-2.73570400	4.92223400	-1.06703900

H	-3.33746300	5.32548900	0.96540900	H	-0.05093800	-4.71046600	-2.63909800
H	-1.93982200	4.28096800	-2.96686900	H	-1.79866700	-4.57486700	-2.90606600
H	-3.33752000	5.72059400	-1.49302200	H	-1.23828400	-3.74453300	0.78094100
C	0.93685900	2.55972000	0.99972100	H	-2.03409700	-4.90989100	-0.29384900
H	0.77024100	3.18198700	1.88529500	H	-0.27565400	-4.90727300	-0.14649600
H	1.72327400	1.84066700	1.22601700	C	-2.92519100	1.50805900	-2.09311800
H	1.25814700	3.19335000	0.17612900	C	-3.55457000	2.39075600	-0.99785300
B	-0.87579500	1.01293000	1.82614000	C	-3.56139900	1.87482900	-3.45262100
O	-0.44478000	1.36637600	3.15591100	H	-1.85964900	1.74831700	-2.13910700
O	-0.11553100	-0.29094500	1.53069800	H	-3.13714700	2.15689800	-0.01861900
C	0.25400200	0.29499400	3.78533400	H	-3.37231100	3.44982900	-1.21412600
C	0.03848200	-0.94781300	2.81880100	H	-4.64132000	2.24276000	-0.95321000
C	1.73631400	0.68649300	3.93929700	H	-3.19442300	1.25276900	-4.27443700
H	1.78337900	1.66845900	4.42112500	H	-4.65151200	1.76143100	-3.42129500
H	2.28659500	-0.02690600	4.56363600	H	-3.34937900	2.92293400	-3.69739300
H	2.24744000	0.75943400	2.97632300	C	3.21596800	-0.40018600	0.12493100
C	1.20940100	-1.92006600	2.79121200	C	4.12669300	0.69568900	0.16411000
H	1.40364500	-2.29934300	3.80112600	C	3.38655700	-1.49648100	1.00579900
H	0.97534300	-2.77805200	2.15595300	C	5.13252800	0.69052100	1.13935900
H	2.12039100	-1.45013500	2.41625400	C	4.41414700	-1.44665500	1.95716400
C	-1.26253700	-1.71256500	3.10606900	C	5.27328500	-0.35731600	2.04295600
H	-1.44754400	-2.43118800	2.30292700	H	5.82567200	1.52629300	1.18587900
H	-1.19240900	-2.26132500	4.05103900	H	4.54723900	-2.28474700	2.63533600
H	-2.12237400	-1.04077600	3.15502800	H	6.05995300	-0.33408600	2.79255000
C	-0.33969100	0.08718600	5.18681600	C	4.11862200	1.86790500	-0.82930100
H	0.11378400	-0.77074500	5.69870800	C	5.43205800	1.91142800	-1.64479700
H	-0.14834600	0.98009200	5.79144500	C	3.91595900	3.24646300	-0.16467600
H	-1.42109500	-0.05957500	5.14295900	H	3.29327900	1.72518800	-1.53216800
Be	0.04950500	0.14403000	-0.08348900	H	5.66542800	0.95125100	-2.11168600
13a-ts				H	5.36170100	2.66780600	-2.43585000
C	-0.01719300	-0.40349300	-2.88699600	H	6.28138300	2.18207000	-1.00680000
C	1.36777500	-0.40345600	-3.08484700	H	2.93143400	3.34828000	0.29734200
C	2.34997200	-0.53112700	-2.08975800	H	4.67445900	3.43714700	0.60321300
H	1.71462500	-0.47081900	-4.10943000	H	4.00352100	4.03824700	-0.91848000
N	-0.57698500	-0.39412100	-1.66543700	C	2.54526600	-2.76594600	0.90117400
C	-0.85618500	-0.46351900	-4.15015900	C	1.96409700	-3.21039500	2.25454000
H	-1.26285300	0.52833000	-4.37343300	C	3.36233300	-3.90171700	0.25110300
H	-0.24617800	-0.77238600	-5.00228900	H	1.69593100	-2.55102100	0.25113200
H	-1.70314300	-1.14553900	-4.05733700	H	1.36161700	-2.41213200	2.69813400
C	3.71613600	-0.94542000	-2.61248700	H	1.31677400	-4.08420000	2.11492300
H	4.06998700	-0.23924300	-3.37058300	H	2.74614100	-3.49401200	2.96958300
H	4.47123600	-1.03448800	-1.83383600	H	3.73896800	-3.61026100	-0.73617200
H	3.61623800	-1.91897200	-3.10673900	H	4.22685600	-4.17703300	0.86787500
N	2.09122000	-0.38268500	-0.78603600	H	2.74181800	-4.79777500	0.12547100
C	-1.95586700	-0.85193300	-1.59709600	H	-0.03791400	-1.12360800	0.78974200
C	-2.17360800	-2.24180100	-1.39444700	N	0.15513500	1.25911400	1.02008500
C	-3.05837100	0.01815200	-1.77989900	C	-0.20629700	2.57891000	0.52149400
C	-3.48781200	-2.72142100	-1.33993400	C	-0.84784000	3.50928900	1.34950100
C	-4.35359200	-0.51682100	-1.71414100	C	0.17446400	2.96326100	-0.76802200
C	-4.57761300	-1.86940600	-1.49066400	C	-1.11904800	4.79766400	0.88959300
H	-3.65939000	-3.78497400	-1.19856600	H	-1.12594500	3.22367800	2.35956000
H	-5.20340700	0.14626500	-1.85386300	C	-0.09448100	4.25568000	-1.22601800
H	-5.59131700	-2.26029800	-1.45030400	H	0.67734400	2.24802600	-1.41087800
C	-1.02661400	-3.25245000	-1.33744500	C	-0.74287200	5.17615200	-0.40123200
C	-0.88967700	-4.00423600	-2.67884300	H	-1.62148900	5.50670700	1.54223900
C	-1.15937100	-4.25839400	-0.18093400	H	0.20581800	4.54075600	-2.23087100
H	-0.10134100	-2.69791200	-1.17280700	H	-0.95050400	6.18081900	-0.75923500
H	-0.70968900	-3.31794500	-3.51265700	C	1.34756700	1.39107700	1.91435900

H	1.09958200	1.98116400	2.80323500	H	3.17106100	4.42983600	1.07492800
H	1.67081100	0.40138100	2.23353300	C	2.84513400	-2.57388300	-0.02346600
H	2.15663100	1.87378900	1.37705400	C	3.71529800	-3.51379700	0.83272500
B	-0.89073100	0.47416400	1.75797100	C	2.44064900	-3.26714200	-1.34145700
O	-0.69358800	0.08863700	3.07112800	H	1.92842700	-2.37765000	0.54170600
O	-2.21679300	0.45550300	1.39297100	H	4.00722200	-3.03949900	1.77626500
C	-1.92078100	-0.52374400	3.54049700	H	3.16463100	-4.43156800	1.07132300
C	-3.00580400	0.08375400	2.55793500	H	4.63308900	-3.80742300	0.31004500
C	-1.75959300	-2.04353900	3.41319800	H	1.79255700	-2.63170600	-1.96046800
H	-0.89695900	-2.35965300	4.00816500	H	3.32053300	-3.50462800	-1.95054800
H	-2.64418800	-2.57468900	3.78061900	H	1.90536800	-4.20351000	-1.14228900
H	-1.57526500	-2.33227500	2.37655200	C	-2.88090500	-0.00011200	0.01455200
C	-4.09370500	-0.89479400	2.11880400	C	-3.52225800	1.22912500	-0.29194800
H	-4.67557400	-1.23943700	2.98211700	C	-3.52025000	-1.23018100	-0.29277200
H	-4.77562500	-0.39776000	1.42296300	C	-4.79061800	1.20072700	-0.88401400
H	-3.67439900	-1.76051200	1.60397000	C	-4.78864200	-1.20344300	-0.88483300
C	-3.65723100	1.37086100	3.08505200	C	-5.42698200	-0.00177400	-1.17784500
H	-4.25393900	1.82158300	2.28630900	H	-5.28736600	2.13748200	-1.12366700
H	-4.31864800	1.16635600	3.93377100	H	-5.28385600	-2.14083600	-1.12515400
H	-2.90999900	2.10438300	3.40213600	H	-6.41117200	-0.00242300	-1.63845500
C	-2.09990600	-0.14853900	5.01284900	C	-2.84931800	2.57388100	-0.02185500
H	-3.04382300	-0.54297500	5.40647000	C	-3.72043500	3.51092200	0.83650800
H	-1.28251200	-0.57986100	5.59979800	C	-2.44754900	3.26973300	-1.33933800
H	-2.08516500	0.93365600	5.16180300	H	-1.93169700	2.37864200	0.54222500
Be	0.41412000	-0.27213000	-0.24061300	H	-4.01015300	3.03488400	1.77984600
3b				H	-3.17145500	4.42960500	1.07550100
C	1.28849200	-0.00063500	1.81508300	H	-4.63949200	3.80312600	0.31525600
C	-0.00000500	-0.00078600	2.39611900	H	-1.79900700	2.63645000	-1.96009600
C	-1.28850200	-0.00072400	1.81506100	H	-3.32856500	3.50648100	-1.94707700
H	-0.00000500	-0.00193100	3.47961300	H	-1.91385100	4.20684600	-1.13939800
N	1.53486600	0.00095800	0.50341100	C	-2.84494300	-2.57396300	-0.02385300
C	2.45597000	-0.00297400	2.79106200	C	-2.44053800	-3.26708800	-1.34194000
H	3.09077400	-0.88266600	2.63666800	C	-3.71500300	-3.51399800	0.83231600
H	3.09630100	0.87229500	2.63466400	H	-1.92820300	-2.37775400	0.54126600
H	2.11349400	-0.00085900	3.82792100	H	-1.79253300	-2.63157300	-1.96095900
C	-2.45596300	-0.00313200	2.79106400	H	-1.90519400	-4.20344700	-1.14289700
H	-2.11347100	-0.00138400	3.82791700	H	-3.32046200	-3.50457300	-1.95097500
H	-3.09612000	0.87231300	2.63495100	H	-4.00683900	-3.03982400	1.77594400
H	-3.09095000	-0.88264000	2.63642500	H	-4.63284200	-3.80757200	0.30969100
N	-1.53488300	0.00088400	0.50342500	H	-3.16429800	-4.43179000	1.07074400
C	2.88090600	-0.00001400	0.01453700	H	0.00003800	0.01313600	-3.45675500
C	3.52216500	1.22923400	-0.29215600	Ca	0.00000700	0.00633900	-1.34314800
C	3.52035700	-1.23009400	-0.29257900	6b			
C	4.79053900	1.20083300	-0.88419300	C	-4.80733900	-1.63126500	-0.16069000
C	4.78875500	-1.20333700	-0.88462300	C	-5.49983500	-0.44140100	0.15657200
C	5.42699600	-0.00166300	-1.17781400	C	-5.05173700	0.87973000	0.39396100
H	5.28721600	2.13758800	-1.12398300	H	-6.57050500	-0.56876400	0.26818300
H	5.28404800	-2.14072900	-1.12478400	N	-3.48890800	-1.72898700	-0.34260800
H	6.41119300	-0.00230900	-1.63840300	C	-5.67109700	-2.88000300	-0.27457800
C	2.84911800	2.57398000	-0.02226400	H	-5.48748800	-3.40500600	-1.21718300
C	2.44744000	3.26968900	-1.33984800	H	-5.43107200	-3.58779100	0.52762600
C	3.72009500	3.51114000	0.83611200	H	-6.73448800	-2.63958000	-0.21050800
H	1.93145300	2.37872500	0.54174900	C	-6.14344500	1.85673900	0.81472600
H	1.79902000	2.63629900	-1.96062700	H	-7.12215400	1.53086900	0.45325700
H	1.91364400	4.20677500	-1.14004200	H	-6.19788100	1.91287500	1.90867600
H	3.32850300	3.50646100	-1.94750800	H	-5.95131000	2.86787500	0.44875700
H	4.00969400	3.03521200	1.77954400	N	-3.78785300	1.28918800	0.29589200
H	4.63921700	3.80330100	0.31495000	C	-2.89098300	-2.99219300	-0.65550500

C	-2.65059900	-3.34575000	-2.01057800	H	0.01148700	0.25772100	1.19954500
C	-2.42545000	-3.83495800	0.38970900	C	5.04898200	-0.72218200	0.43437800
C	-1.94694600	-4.52429200	-2.28768300	C	5.51171600	0.57004200	0.10122900
C	-1.71745900	-4.99651300	0.05788500	C	4.82346900	1.74006100	-0.30036700
C	-1.47674900	-5.34636900	-1.26779600	H	6.58362900	0.69907800	0.19976700
H	-1.76350300	-4.80195200	-3.32278000	N	3.76973700	-1.10611600	0.43549900
H	-1.34785800	-5.63937400	0.85250600	C	6.12704300	-1.72430100	0.82400700
H	-0.93003900	-6.25568900	-1.50393500	H	6.00766000	-2.04797700	1.86354200
C	-3.14624800	-2.48535600	-3.17239600	H	6.05757100	-2.62724000	0.20751900
C	-4.16750000	-3.23812100	-4.04880400	H	7.12760000	-1.30207600	0.70906000
C	-1.98306600	-1.95763300	-4.03654000	C	5.68716700	2.99007500	-0.41330900
H	-3.66149200	-1.61911300	-2.74476300	H	6.72615800	2.73411100	-0.63744000
H	-5.02094400	-3.59347400	-3.46097200	H	5.31949900	3.67724600	-1.17849600
H	-4.55197600	-2.58144600	-4.83881300	H	5.68059900	3.53131000	0.54142600
H	-3.71314000	-4.11022800	-4.53410900	N	3.51801300	1.80131600	-0.54580900
H	-1.26086900	-1.38994600	-3.43898500	C	3.40825800	-2.42317900	0.86389200
H	-1.44103900	-2.78003100	-4.51899100	C	3.15876200	-2.68228000	2.23976100
H	-2.36390800	-1.30282100	-4.83047000	C	3.17823800	-3.44076500	-0.10078200
C	-2.67136200	-3.50554000	1.86182400	C	2.67926600	-3.94354600	2.61281800
C	-1.37106400	-3.08277900	2.57534500	C	2.69323400	-4.68349100	0.32589100
C	-3.34113400	-4.66988500	2.61813800	C	2.44258000	-4.94101100	1.67021100
H	-3.35974900	-2.65588600	1.90264900	H	2.48704300	-4.14823000	3.66312600
H	-0.91993200	-2.19215900	2.12020600	H	2.51368800	-5.46441400	-0.40869300
H	-1.56696000	-2.84927000	3.62942700	H	2.07138000	-5.91371000	1.98260900
H	-0.61837000	-3.87862600	2.53846400	C	3.39230300	-1.62615100	3.31991600
H	-4.26483500	-4.99193900	2.12440400	C	4.35602800	-2.11972700	4.41787600
H	-2.68132600	-5.54247100	2.68919300	C	2.06604100	-1.15209900	3.94930900
H	-3.59181600	-4.36388200	3.64090500	H	3.85644600	-0.75788100	2.84281800
C	-3.42841400	2.64222400	0.58385300	H	5.30910200	-2.46152100	3.99900700
C	-3.19117800	3.05040800	1.92536000	H	4.56915500	-1.31188100	5.12827300
C	-3.18407400	3.54966900	-0.48570300	H	3.92719600	-2.95304500	4.98670900
C	-2.72986700	4.35000000	2.16975800	H	1.38218800	-0.74007200	3.19850500
C	-2.72413900	4.83798000	-0.17959600	H	1.54819400	-1.97895700	4.45060500
C	-2.49727600	5.24562600	1.13182800	H	2.25466000	-0.37358800	4.69918400
H	-2.54831100	4.66339500	3.19463400	C	3.46396100	-3.22229400	-1.58613700
H	-2.54195400	5.53487900	-0.99459900	C	2.17703600	-3.26426400	-2.43525000
H	-2.14227300	6.25134700	1.34091500	C	4.49617900	-4.23189100	-2.12728100
C	-3.40583200	2.11219500	3.11340700	H	3.90305800	-2.22517100	-1.69429100
C	-4.38045600	2.70090700	4.15335900	H	1.45347700	-2.49663600	-2.13367900
C	-2.07018800	1.73942100	3.78967200	H	2.40980600	-3.10115500	-3.49485700
H	-3.84910000	1.18629400	2.73478200	H	1.67044100	-4.23218000	-2.34671800
H	-5.33344700	2.99271600	3.69910500	H	5.42446500	-4.20739300	-1.54574100
H	-4.58859800	1.96399800	4.93832800	H	4.11183000	-5.25824300	-2.09596400
H	-3.96147000	3.58912100	4.64091500	H	4.74354100	-4.00275600	-3.17083900
H	-1.37294200	1.27015100	3.08645100	C	2.88493000	3.00003500	-0.99460200
H	-1.57534400	2.62695800	4.20255300	C	2.60675900	3.17193100	-2.38123300
H	-2.24330200	1.03972100	4.61704700	C	2.39739300	3.94531900	-0.05098700
C	-3.42636800	3.24463500	-1.96961100	C	1.84457400	4.28072700	-2.77465900
C	-4.91943800	3.15256200	-2.34241300	C	1.63313400	5.02847100	-0.50358000
C	-2.66270900	2.03209800	-2.53564300	C	1.35268100	5.20234300	-1.85397300
H	-3.02905000	4.11812800	-2.50263700	H	1.63340900	4.41983400	-3.83278000
H	-5.47206400	4.02683200	-1.98131200	H	1.24912900	5.74432300	0.21829800
H	-5.03317400	3.10882700	-3.43287800	H	0.75756500	6.04788000	-2.18856800
H	-5.38302700	2.25417500	-1.92441000	C	3.11777600	2.25961500	-3.50541200
H	-1.60823200	2.02779700	-2.22891700	C	2.76678900	0.76440900	-3.38049600
H	-3.14478800	1.08991600	-2.25007200	C	4.62429900	2.43133400	-3.78673700
H	-2.66613800	2.06025300	-3.63178700	H	2.59696600	2.61154100	-4.40565600
H	-0.00463600	-0.18620400	-1.53950500	H	1.70821400	0.61195600	-3.13329800

H	2.94719900	0.25974700	-4.33770500	H	2.20805800	-1.64235000	-3.24150800
H	3.39723300	0.26617900	-2.63547200	H	3.82328200	-2.35474100	-3.44792700
H	4.88996700	3.48792600	-3.90344800	H	2.37902000	-3.36137300	-3.62439900
H	5.23384800	2.00924400	-2.98238700	C	-3.01422300	-0.48932500	0.27785300
H	4.89421200	1.91080700	-4.71413600	C	-3.42026200	0.58430100	1.11859100
C	2.68159200	3.81823700	1.44547700	C	-3.80655300	-0.84412200	-0.84777300
C	1.39799200	3.54686000	2.25554500	C	-4.58438100	1.29295600	0.79869000
C	3.40992300	5.06111200	1.99690100	C	-4.96268100	-0.10054600	-1.12247500
H	3.34635000	2.96081400	1.58868200	C	-5.35201800	0.96475800	-0.31631100
H	0.90469500	2.61891200	1.94387200	H	-4.89820300	2.11672300	1.43546400
H	1.63248600	3.45689600	3.32359800	H	-5.57412600	-0.36887000	-1.98045900
H	0.66991600	4.35805700	2.13860600	H	-6.25248700	1.52771700	-0.54762300
H	4.32696400	5.27370600	1.43664400	C	-2.61773100	0.98936100	2.35558500
H	2.77695500	5.95496400	1.94601200	C	-3.48005900	0.99963000	3.63343100
H	3.68029000	4.90863100	3.04874200	C	-1.93009800	2.35629900	2.16849500
Ca	-1.78812200	-0.01955200	-0.15863500	H	-1.82656500	0.24851000	2.49967300
Ca	1.79319100	0.13264200	-0.20385300	H	-3.98408300	0.03917700	3.78677000
7b				H	-2.85578400	1.19931200	4.51256800
C	0.95688100	-2.37385000	1.42464400	H	-4.25325500	1.77600800	3.59581300
C	-0.38347000	-2.70230600	1.74046100	H	-1.25031300	2.35324400	1.30837700
C	-1.61004600	-2.11181300	1.36517100	H	-2.66640800	3.15365500	2.00785700
H	-0.48264600	-3.50998200	2.45606300	H	-1.34095800	2.61984200	3.05532300
N	1.33191800	-1.45027700	0.54050300	C	-3.46327600	-2.03768800	-1.74002200
C	2.01516600	-3.13963600	2.20684300	C	-3.24162600	-1.63662200	-3.21221900
H	2.80740200	-3.51253900	1.55158800	C	-4.54301200	-3.13621400	-1.64398300
H	2.49815100	-2.48161700	2.93923000	H	-2.52818000	-2.47112700	-1.36895500
H	1.58019400	-3.98315400	2.74741000	H	-2.40263100	-0.94059000	-3.32704600
C	-2.84387300	-2.66892000	2.06209600	H	-3.01188400	-2.52346000	-3.81505300
H	-3.64804100	-2.86563900	1.34655900	H	-4.13714700	-1.16936800	-3.63966900
H	-2.61629300	-3.59423100	2.59589300	H	-4.70124100	-3.46032200	-0.60953700
H	-3.23858400	-1.94874000	2.78849400	H	-5.50625600	-2.78401100	-2.03209400
N	-1.74665300	-1.11509000	0.48722400	H	-4.24771000	-4.01327400	-2.23209700
C	2.71800500	-1.14342900	0.34819600	C	0.41564000	3.22861300	-1.55089800
C	3.32827000	-0.12511100	1.12958500	C	1.70169700	3.02266500	-2.08223800
C	3.44605500	-1.76496100	-0.70237000	C	2.73787500	3.90254600	-1.77580800
C	4.64282200	0.25687600	0.83710700	C	2.51319900	5.00361900	-0.94526100
C	4.75983600	-1.34623000	-0.94960200	C	1.23538500	5.21459800	-0.42740200
C	5.35965700	-0.34307400	-0.19456100	C	0.18886300	4.33817900	-0.72406900
H	5.11345500	1.03773600	1.42947500	H	1.87643500	2.18066000	-2.74838200
H	5.32348300	-1.81880200	-1.74995000	H	3.72361800	3.72818600	-2.19834700
H	6.37992700	-0.03356400	-0.40581800	H	3.32123500	5.69079200	-0.71212800
C	2.58736700	0.56646900	2.27343300	H	1.04219200	6.07130300	0.21296900
C	2.30187700	2.04738700	1.95470700	H	-0.79728700	4.52258900	-0.31149700
C	3.34067800	0.44607200	3.61299800	N	-0.60576500	2.27040100	-1.82939500
H	1.62229200	0.06537000	2.39505700	H	-0.37891300	1.75768900	-2.69393400
H	1.71907300	2.16576800	1.03372600	C	-1.99985000	2.74336100	-1.87882200
H	1.73839900	2.51718200	2.77029500	H	-2.11168300	3.63467900	-2.51112700
H	3.23035300	2.61381600	1.81875000	H	-2.62131800	1.93869100	-2.28023700
H	3.55385300	-0.59912800	3.86261300	H	-2.36845300	2.97195900	-0.87675800
H	4.29710100	0.98172900	3.58937600	Ca	-0.06080800	-0.17569100	-0.97356100
H	2.74344500	0.87435600	4.42710000	H	0.13532700	-0.15420400	-3.12639100
C	2.85597300	-2.89057000	-1.55242900	9b-ts			
C	3.61459600	-4.21745500	-1.34019600	C	0.43076800	-2.67756500	1.14136100
C	2.81603000	-2.53372600	-3.05215600	C	-0.95009400	-2.85260700	1.38867700
H	1.82375300	-3.05051800	-1.22264100	C	-2.06623800	-2.04051200	1.08575800
H	3.62981600	-4.51544800	-0.28607500	H	-1.19145400	-3.75041000	1.94505100
H	3.13890700	-5.02340500	-1.91185400	N	0.96378200	-1.65380000	0.47178200
H	4.65505700	-4.14019200	-1.67779200	C	1.34456200	-3.74984700	1.71601200

H	2.00100900	-4.16295800	0.94331600	C	-4.85241600	-2.32860800	-2.19506100
H	1.99842600	-3.32874600	2.48818400	H	-2.82040900	-1.97779300	-1.62174200
H	0.77320000	-4.56726900	2.16080800	H	-2.31185600	-0.19557800	-3.31167700
C	-3.40459200	-2.52823300	1.61998100	H	-2.96996100	-1.64941900	-4.07937500
H	-4.14221000	-2.61270100	0.81525600	H	-3.99539500	-0.22446600	-3.85256500
H	-3.31149100	-3.49945400	2.11038400	H	-5.17357200	-2.75420800	-1.23800400
H	-3.81451600	-1.81504900	2.34444800	H	-5.71270600	-1.80700800	-2.63065300
N	-2.01488500	-0.90104700	0.39367800	H	-4.59368300	-3.15793100	-2.86418200
C	2.38352600	-1.52352900	0.33126200	C	1.37711200	3.21965800	-1.13378900
C	3.12275500	-0.79177500	1.30034100	C	2.58002700	2.47574700	-1.12126900
C	3.02823100	-2.00252000	-0.84125100	C	3.81780800	3.09885800	-1.00368500
C	4.48173000	-0.54756800	1.07040600	C	3.90506000	4.48966900	-0.88574000
C	4.39007100	-1.72814400	-1.02212400	C	2.72825600	5.23803800	-0.89412400
C	5.11726900	-1.00570100	-0.08071200	C	1.48168900	4.62118600	-1.01948000
H	5.05194400	0.01480200	1.80533600	H	2.54949700	1.39058700	-1.21783800
H	4.88962500	-2.09054500	-1.91702000	H	4.71770300	2.48905300	-0.99911800
H	6.17321600	-0.80456000	-0.24067600	H	4.87091500	4.97694500	-0.78765400
C	2.47190900	-0.25397400	2.57449300	H	2.77353400	6.32090500	-0.80184200
C	2.41002000	1.28721300	2.57588800	H	0.58662600	5.23385500	-1.01936200
C	3.17748100	-0.76027200	3.84816600	N	0.16132300	2.52697600	-1.25550100
H	1.44278800	-0.62471100	2.60444200	H	0.18320900	1.65621300	-2.27850600
H	1.89301200	1.68261900	1.69340600	C	-1.03790200	3.33448500	-1.46675300
H	1.88607800	1.65103600	3.46821600	H	-0.92268400	4.05930100	-2.28728600
H	3.41372700	1.72773800	2.57295400	H	-1.87084600	2.66867300	-1.73139300
H	3.22188000	-1.85465900	3.87641200	H	-1.33636800	3.88928400	-0.56683600
H	4.20519100	-0.38499100	3.91787300	Ca	-0.13522000	0.16875300	-0.63358200
H	2.64099700	-0.41980500	4.74191600	H	0.07418100	0.79817700	-2.83179600
C	2.28672500	-2.81797200	-1.90026600	10b			
C	2.88507900	-4.23083800	-2.05634800	C	1.44690800	-2.32095300	1.08133600
C	2.25067200	-2.10071800	-3.26540000	C	0.18969200	-2.83485200	1.47567700
H	1.25248800	-2.93908000	-1.56106000	C	-1.12039700	-2.32859800	1.32275200
H	2.90398500	-4.76991500	-1.10280300	H	0.24479400	-3.76930800	2.02189000
H	2.29260700	-4.81984700	-2.76657500	N	1.63225000	-1.17485900	0.42466500
H	3.91323300	-4.19080200	-2.43513100	C	2.65182100	-3.16164900	1.47978300
H	1.76900700	-1.11746700	-3.20295200	H	3.36591600	-3.24191100	0.65455600
H	3.26083200	-1.94771400	-3.66315200	H	3.18862400	-2.70211600	2.31793000
H	1.69288500	-2.69856200	-3.99653500	H	2.35108500	-4.16664900	1.78420800
C	-3.18967600	-0.11186000	0.17745900	C	-2.22368800	-3.13233600	1.99474200
C	-3.51737600	0.92449700	1.09324200	H	-1.82072400	-3.98188300	2.55002100
C	-3.94107600	-0.26674900	-1.01869700	H	-2.79171600	-2.50195300	2.68803200
C	-4.57490200	1.78895500	0.78638500	H	-2.94152900	-3.50996600	1.25886400
C	-4.98954100	0.62573400	-1.27655900	N	-1.43760400	-1.22290100	0.64532100
C	-5.30777100	1.64988700	-0.38922000	C	2.95062800	-0.67891100	0.16651200
H	-4.82784900	2.58635800	1.48064500	C	3.62813700	0.08703700	1.15482200
H	-5.56834000	0.51363900	-2.18989700	C	3.52134600	-0.83334400	-1.12510200
H	-6.12398400	2.33246200	-0.61030700	C	4.84921400	0.68622500	0.82461200
C	-2.74113500	1.12204400	2.39519000	C	4.74784700	-0.21507000	-1.40097600
C	-3.66045200	1.08855200	3.63197400	C	5.41101900	0.54292100	-0.44148200
C	-1.91670600	2.42558600	2.37575800	H	5.36982800	1.27870700	1.57265700
H	-2.03583400	0.29088900	2.49119900	H	5.19026000	-0.33149300	-2.38703800
H	-4.24698700	0.16393000	3.67117300	H	6.35962100	1.01771800	-0.67720500
H	-3.06585800	1.15225500	4.55107600	C	3.05296700	0.29132700	2.55660000
H	-4.36517400	1.92824100	3.63621800	C	2.57814300	1.74324800	2.76829900
H	-1.20863900	2.45070900	1.53770000	C	4.04819100	-0.10933300	3.66348300
H	-2.56434600	3.30505000	2.27910400	H	2.17519700	-0.35331200	2.65746800
H	-1.34074900	2.53391800	3.30279400	H	1.81148100	2.03061400	2.03915900
C	-3.64725900	-1.38180700	-2.02194100	H	2.15087300	1.86869600	3.77078100
C	-3.20428300	-0.82780300	-3.39160900	H	3.40887900	2.45180700	2.66651200

H	4.41025200	-1.13453500	3.52876500	Ca	-0.00499300	0.31302100	-0.51389300
H	4.92398600	0.54985200	3.68139300	11b-ts			
H	3.56879800	-0.04497300	4.64757200	C	-0.83410900	-2.35502500	-2.20096300
C	2.85036100	-1.66952200	-2.21434200	C	0.48573500	-2.85320300	-2.24216800
C	3.69713700	-2.90488700	-2.58178200	C	1.61456500	-2.65197300	-1.41126700
C	2.53130900	-0.83840900	-3.47445600	H	0.62804400	-3.64073200	-2.97542200
H	1.90292800	-2.04253800	-1.80819900	N	-1.27180500	-1.35641600	-1.42475700
H	3.90098900	-3.52874900	-1.70447300	C	-1.80226100	-3.10984100	-3.10949700
H	3.17405600	-3.52179400	-3.32236400	H	-2.14454900	-4.03082800	-2.62247500
H	4.66151200	-2.61178200	-3.01350100	H	-2.68758200	-2.52289300	-3.35887500
H	1.90080400	0.03027800	-3.24776700	H	-1.30037900	-3.40421000	-4.03599000
H	3.44757800	-0.46645800	-3.94810200	C	2.75926100	-3.62441400	-1.68164400
H	2.00755000	-1.45693700	-4.21410800	H	3.33331300	-3.29563200	-2.55634700
C	-2.80017400	-0.79985800	0.52317900	H	3.45070100	-3.69405200	-0.84033600
C	-3.29676700	0.21950200	1.37848500	H	2.37191100	-4.62254800	-1.90547700
C	-3.60930300	-1.29368400	-0.53608200	N	1.72151500	-1.71621000	-0.46952000
C	-4.58156900	0.72903000	1.15028500	C	-2.67935800	-1.14287600	-1.28533100
C	-4.88524000	-0.74894700	-0.72104000	C	-3.45511900	-2.00790500	-0.46513400
C	-5.37442500	0.25623600	0.10939000	C	-3.28923200	-0.01112800	-1.89394600
H	-4.96668400	1.51058000	1.80046600	C	-4.81054800	-1.71664400	-0.26529000
H	-5.50765200	-1.11713500	-1.53268800	C	-4.64974800	0.22990100	-1.66478200
H	-6.36733400	0.66664300	-0.05359000	C	-5.41095900	-0.60913500	-0.85576200
C	-2.47261200	0.76775500	2.54266200	H	-5.40812700	-2.37227000	0.36321900
C	-3.16673900	0.52896500	3.89863200	H	-5.12447100	1.08811900	-2.12992900
C	-2.14513700	2.26434200	2.36433800	H	-6.46531300	-0.40294700	-0.69135700
H	-1.52520200	0.21854000	2.56511100	C	-2.85749100	-3.23782400	0.22164000
H	-3.37929900	-0.53397500	4.05820500	C	-3.66592200	-4.52100800	-0.05523500
H	-2.52951900	0.87462000	4.72149100	C	-2.71323200	-3.02170700	1.74071200
H	-4.11708600	1.07146500	3.96383400	H	-1.85107400	-3.39521600	-0.17351000
H	-1.60216000	2.46916800	1.43298600	H	-3.80963200	-4.68290400	-1.12872000
H	-3.05674000	2.87234700	2.34051900	H	-3.14394900	-5.39431000	0.35381800
H	-1.52547900	2.62479200	3.19432300	H	-4.65832800	-4.48662600	0.40912100
C	-3.11431800	-2.38162000	-1.48852400	H	-2.07299700	-2.15884400	1.95660000
C	-2.84233800	-1.81381900	-2.89592900	H	-3.68656700	-2.84176300	2.21306800
C	-4.08186200	-3.57824500	-1.57292300	H	-2.26456600	-3.90119000	2.21911800
H	-2.16329200	-2.75818500	-1.10009900	C	-2.50432400	0.91151000	-2.82690100
H	-2.11957100	-0.98998500	-2.86925700	C	-2.98529600	2.37335500	-2.80917600
H	-2.44333400	-2.59176300	-3.55849200	C	-2.49627700	0.38691200	-4.27840000
H	-3.76000600	-1.42273200	-3.35108200	H	-1.45733500	0.90445300	-2.49383800
H	-4.29121800	-3.99924100	-0.58330200	H	-3.09656800	2.75749800	-1.79066900
H	-5.04126000	-3.29494200	-2.02111600	H	-2.26156000	3.01096500	-3.32807900
H	-3.65085400	-4.37228700	-2.19419100	H	-3.94689700	2.48815400	-3.32323500
C	-0.21483300	2.79506900	-1.80156600	H	-2.03463800	-0.60102800	-4.35243700
C	-1.13188700	3.87445800	-2.01102100	H	-3.51976300	0.31482700	-4.66609400
C	-1.14659100	4.98262500	-1.17575300	H	-1.93597200	1.07004700	-4.92818400
C	-0.25768400	5.11419400	-0.09633300	C	2.88073700	-1.63765100	0.36772300
C	0.68993700	4.11321300	0.09968800	C	4.07137400	-1.00372400	-0.07605700
C	0.72290700	2.98213700	-0.72472100	C	2.78523100	-2.11453200	1.70479300
H	-1.83815000	3.81976700	-2.83254800	C	5.13093000	-0.85654400	0.82904100
H	-1.87102200	5.77196400	-1.36857600	C	3.87624300	-1.94578600	2.56542500
H	-0.28404900	5.99189400	0.54199000	C	5.04340300	-1.31798600	2.13803000
H	1.44328600	4.22035200	0.87717800	H	6.04441400	-0.36987900	0.49716100
H	1.60903500	2.34007200	-0.68614000	H	3.81633100	-2.31473000	3.58516200
N	-0.19929600	1.61399900	-2.48539300	H	5.87980600	-1.19346700	2.82075300
C	-0.97993100	1.56261700	-3.70850500	C	4.24561700	-0.47708700	-1.50009800
H	-0.71585800	2.37047300	-4.41156600	C	5.44656700	-1.13242000	-2.21314900
H	-0.78424000	0.61398000	-4.22155300	C	4.38405800	1.05729200	-1.52912600
H	-2.07338500	1.62698700	-3.55167100	H	3.34506100	-0.73333000	-2.06691300

H	5.38259400	-2.22552000	-2.20437500	C	2.05942600	-2.49482400	-1.20235800
H	5.49367800	-0.80105300	-3.25738900	H	1.22974700	-3.97610000	-2.43454400
H	6.39416700	-0.85285700	-1.73774300	N	-1.02258000	-1.86994700	-1.13787000
H	3.51869500	1.54599900	-1.07484700	C	-1.26641500	-3.89011100	-2.56108300
H	5.28129700	1.38536200	-0.99024300	H	-1.47258600	-4.75703200	-1.92145100
H	4.46841000	1.41489300	-2.56228000	H	-2.22920500	-3.48697100	-2.88102000
C	1.54000800	-2.85860100	2.18675300	H	-0.72528500	-4.25542600	-3.43835200
C	1.19016500	-2.59279400	3.66133700	C	3.34204700	-3.31834500	-1.26682000
C	1.67088100	-4.37648400	1.94089300	H	3.40484100	-3.87206200	-2.20771900
H	0.69448800	-2.51783800	1.57514300	H	4.24256300	-2.71479300	-1.14893500
H	1.15772000	-1.52084500	3.88625700	H	3.33816000	-4.05781200	-0.45527400
H	0.20956700	-3.02240400	3.89795400	N	2.02683600	-1.34645000	-0.51983700
H	1.91403700	-3.05247100	4.34392800	C	-2.44680800	-1.84567000	-0.99887600
H	1.81850400	-4.59880300	0.88010700	C	-3.08571400	-2.68675500	-0.04759000
H	2.52587800	-4.78441000	2.49363900	C	-3.20652000	-0.89625200	-1.73524100
H	0.76820500	-4.90307800	2.27522600	C	-4.46671800	-2.55840400	0.14490700
H	-1.27490100	2.75228100	-0.28770800	C	-4.58640700	-0.81813600	-1.50996400
N	1.24955400	2.26481500	0.20731900	C	-5.21786000	-1.63670000	-0.57814800
C	1.48420100	3.25545900	-0.73055000	H	-4.96380900	-3.19245500	0.87464100
C	2.31555800	4.38881600	-0.52780400	H	-5.17770900	-0.10080300	-2.07050700
C	0.86804300	3.16211200	-2.00877900	H	-6.28931900	-1.55514900	-0.41558400
C	2.49296300	5.34915800	-1.52409700	C	-2.31055500	-3.70956000	0.78541000
H	2.83069400	4.51930400	0.41760200	C	-2.94429700	-5.11388900	0.73695900
C	1.04924300	4.12386800	-2.99506000	C	-2.15392400	-3.24804500	2.24819600
H	0.23831900	2.29903800	-2.22919700	H	-1.30345500	-3.79397600	0.36912800
C	1.86516900	5.23715600	-2.76527900	H	-3.08476700	-5.45693300	-0.29381100
H	3.14076300	6.20021400	-1.32192900	H	-2.30213800	-5.83802400	1.25256300
H	0.55499300	3.99934600	-3.95672500	H	-3.92314900	-5.13714200	1.22962500
H	2.01213700	5.98853000	-3.53579300	H	-1.61820800	-2.29353700	2.31234800
C	2.04763600	2.36367700	1.42033700	H	-3.12947400	-3.11045600	2.72929400
H	1.88922200	3.30197600	1.97943600	H	-1.59125500	-3.98783500	2.83119900
H	1.78733000	1.54078500	2.10419300	C	-2.55777400	0.00106700	-2.79005000
H	3.13303100	2.28498300	1.23661100	C	-3.17202300	1.40923800	-2.86985200
B	-1.23208700	2.57131500	0.88281000	C	-2.57408700	-0.66501100	-4.18216700
O	-1.55826600	3.53846100	1.78266600	H	-1.49978300	0.12206500	-2.51983400
O	-1.27578100	1.27810100	1.46052900	H	-3.21588700	1.88612700	-1.88593200
C	-1.76394300	2.94509500	3.09180300	H	-2.56227400	2.04305600	-3.52266700
C	-1.96141700	1.40898400	2.75882300	H	-4.18487200	1.38775100	-3.28958400
C	-0.52876600	3.25133200	3.94704500	H	-2.03716400	-1.61819600	-4.18340300
H	-0.37540600	4.33465600	3.96115200	H	-3.60437600	-0.85663000	-4.50612600
H	-0.66359500	2.91111700	4.97952200	H	-2.10261200	-0.01049400	-4.92543200
H	0.37475500	2.79334200	3.54124500	C	3.22138700	-0.86255400	0.11097200
C	-1.31454600	0.45618900	3.75892400	C	4.06949700	0.05314300	-0.57283900
H	-1.76233200	0.58313200	4.75079800	C	3.51447700	-1.23231700	1.44989900
H	-1.47907500	-0.58259900	3.45616100	C	5.18057900	0.57355600	0.10258600
H	-0.23870400	0.62563800	3.84681100	C	4.63019200	-0.66997100	2.08303900
C	-3.42198500	1.01610900	2.51055500	C	5.46229600	0.22629700	1.42112300
H	-3.46469300	-0.00181200	2.11408300	H	5.83993700	1.26546800	-0.41337200
H	-4.00551100	1.05082200	3.43632600	H	4.85464700	-0.94694100	3.11014800
H	-3.89337700	1.67590200	1.77656400	H	6.32743900	0.64805400	1.92577900
C	-2.98994100	3.61765200	3.71452600	C	3.82692400	0.44755900	-2.03083000
H	-3.23581100	3.16676400	4.68269000	C	4.70404600	-0.37295900	-3.00158100
H	-2.77268300	4.67730800	3.87996300	C	4.04791000	1.94810800	-2.29991200
H	-3.86454400	3.55202700	3.06408100	H	2.78160000	0.21086200	-2.26255300
Ca	0.18510600	0.14007400	-0.14397500	H	4.50891400	-1.44572500	-2.92753900
12b				H	4.51324800	-0.06839800	-4.03795000
C	-0.43015900	-2.85786800	-1.81033600	H	5.76854800	-0.20863000	-2.79371600
C	0.96207300	-3.09505800	-1.86072400	H	3.48187100	2.57958100	-1.60912400

H	5.10559200	2.22410000	-2.21799100	H	-5.05526900	2.18074600	1.09238700
H	3.72937500	2.19783300	-3.31860300	H	-4.67055500	1.21447700	2.50971900
C	2.65126600	-2.22937900	2.22057600	H	-4.41575600	2.97277300	2.53729900
C	1.91122500	-1.54870900	3.38820600	C	-0.42737500	4.79252000	0.96198200
C	3.46525600	-3.43562200	2.72844100	H	-1.18869600	5.40335700	1.45117400
H	1.89499900	-2.61832200	1.53126400	H	0.51701400	4.91740700	1.50074800
H	1.30120000	-0.70445800	3.04691400	H	-0.26405600	5.18911500	-0.04667400
H	1.24928000	-2.25954800	3.89806500	N	-0.01172300	2.43360500	0.35719000
H	2.61574300	-1.15642800	4.13138100	C	-3.52568100	-0.34600800	0.76897400
H	3.99345800	-3.93548100	1.90936000	C	-4.33346700	-0.40666000	-0.40025300
H	4.21348300	-3.13420500	3.47093500	C	-3.60331700	-1.38180100	1.73830000
H	2.80429900	-4.16931000	3.20547500	C	-5.15537700	-1.52243100	-0.59860900
H	-1.86102600	1.84749000	0.12574800	C	-4.44591700	-2.47395300	1.49087600
N	0.26595100	2.48988000	0.09268700	C	-5.20920000	-2.55842700	0.33033400
C	0.02394500	3.24838600	-1.11514400	H	-5.76840000	-1.57959700	-1.49473600
C	-0.72525500	4.43600600	-1.09252800	H	-4.50957100	-3.26991100	2.22844800
C	0.53951200	2.80491700	-2.33991800	H	-5.85370700	-3.41660500	0.15860200
C	-0.95378900	5.14993600	-2.26934900	C	-4.33350100	0.71164600	-1.44471100
H	-1.13666000	4.77780300	-0.14793900	C	-5.75379300	1.23882100	-1.73169000
C	0.31473800	3.52245000	-3.51783900	C	-3.65555400	0.27729000	-2.75871200
H	1.13481200	1.89472000	-2.36950700	H	-3.75053200	1.54558200	-1.04489900
C	-0.43426700	4.69952600	-3.48579500	H	-6.26058600	1.54881900	-0.81145800
H	-1.54375000	6.06248200	-2.23584200	H	-5.70983700	2.10427600	-2.40369300
H	0.72539400	3.15975400	-4.45686100	H	-6.38113300	0.47988200	-2.21365400
H	-0.61284500	5.25987600	-4.39964900	H	-2.60724800	0.00056100	-2.59587900
C	1.41492700	3.04680700	0.84093000	H	-4.16115800	-0.58707700	-3.20577300
H	1.22614700	4.07491000	1.17864100	H	-3.67205300	1.09289400	-3.49200200
H	1.60115000	2.42653900	1.72244500	C	-2.84663400	-1.31759600	3.06637200
H	2.31881400	3.04485000	0.22278500	C	-1.90832700	-2.52092100	3.28527700
B	-1.02838000	2.26737400	0.95032600	C	-3.82436500	-1.18657100	4.25412900
O	-1.49853000	3.34466700	1.78222900	H	-2.22833800	-0.41332100	3.05428400
O	-0.71042900	1.13488700	1.93249200	H	-1.11356800	-2.56005700	2.53252600
C	-1.61769200	2.93733700	3.14598200	H	-1.42093100	-2.44271400	4.26459100
C	-1.57974400	1.35941800	3.06754400	H	-2.45843800	-3.46959700	3.26508100
C	-0.43841600	3.52550300	3.94300900	H	-4.49022600	-0.32390500	4.14242500
H	-0.40614900	4.60589900	3.76789200	H	-4.45263300	-2.08014500	4.35167200
H	-0.54481800	3.35729000	5.02112800	H	-3.26913600	-1.06597200	5.19195700
H	0.51764300	3.10508800	3.62059100	C	1.23252100	2.88467900	-0.19201900
C	-0.98935100	0.67780700	4.30174700	C	2.38915700	2.97665900	0.62806300
H	-1.57425800	0.92663200	5.19495000	C	1.32390300	3.15298100	-1.58344800
H	-1.01346900	-0.41126800	4.18346300	C	3.60712800	3.33300200	0.03469800
H	0.04678200	0.97907600	4.47356600	C	2.56668400	3.50147100	-2.12691400
C	-2.96034400	0.75618800	2.75712500	C	3.70430300	3.59443600	-1.33001400
H	-2.85124300	-0.30888300	2.52834400	H	4.49734700	3.40510900	0.65396600
H	-3.63748100	0.84626500	3.61309100	H	2.64262700	3.71032300	-3.19127400
H	-3.42626500	1.24024900	1.89514700	H	4.65989300	3.87042600	-1.76817700
C	-2.92579300	3.50598500	3.71156300	C	2.34398200	2.69063800	2.12953400
H	-3.10410700	3.16488300	4.73889800	C	2.93939000	3.84090400	2.96592600
H	-2.86688600	4.59963700	3.72592900	C	3.04458600	1.36063200	2.47574300
H	-3.78274900	3.22745900	3.09402200	H	1.29282500	2.59207300	2.41789300
Ca	0.03723100	-0.03363200	0.02730800	H	2.46471400	4.80167300	2.73617400
13b-ts				H	2.79784300	3.64043600	4.03437600
C	-2.92721900	1.88520300	1.39002700	H	4.01633500	3.95350600	2.79516200
C	-2.12239300	3.04551500	1.42710400	H	2.58110100	0.50337000	1.97459800
C	-0.84203700	3.32795100	0.90072600	H	4.10169400	1.37843600	2.18553000
H	-2.61370500	3.90406700	1.86913500	H	2.99686000	1.17409400	3.55554900
N	-2.55559800	0.69841800	0.90412300	C	0.10112400	3.07848800	-2.49720200
C	-4.34341100	2.07447900	1.91992900	C	0.22038700	1.93187500	-3.52177500

C	-0.16879100	4.41393800	-3.21794800	H	2.13809800	-0.23667700	3.95295100
H	-0.76807500	2.86718800	-1.86698900	H	3.03157700	-1.17789900	2.74523600
H	0.34684300	0.95790100	-3.03231900	H	3.15948600	0.57376200	2.74609400
H	-0.67821600	1.87789100	-4.14861100	N	1.50586200	-0.06377100	0.64547400
H	1.08184900	2.07572900	-4.18490500	C	-2.82626600	-0.02103000	0.10700500
H	-0.27844400	5.23805100	-2.50457800	C	-3.49266600	-1.22070600	-0.26640200
H	0.64501300	4.67532600	-3.90456900	C	-3.41109700	1.23882500	-0.20350800
H	-1.09170200	4.35139000	-3.80718300	C	-4.72363900	-1.12898900	-0.92689500
H	0.82061300	-1.52930900	1.31103100	C	-4.64329500	1.27263000	-0.86889700
N	2.98683900	-1.34241600	-0.51476000	C	-5.30153400	0.10100000	-1.22957100
C	4.04537500	-1.73615400	0.33366700	H	-5.23699200	-2.04205000	-1.21653100
C	5.34101300	-1.20619800	0.18315200	H	-5.09632200	2.23263100	-1.10494500
C	3.82287700	-2.66071600	1.37496100	H	-6.25659200	0.14555500	-1.74597600
C	6.37771300	-1.60513100	1.02981200	C	-2.89883200	-2.59967300	0.01617700
H	5.55486200	-0.48474000	-0.59661400	C	-2.52014900	-3.32994600	-1.28920400
C	4.86668200	-3.05218400	2.20742800	C	-3.84229100	-3.47320700	0.86740900
H	2.82676600	-3.05248900	1.53521800	H	-1.97869800	-2.45465500	0.59071400
C	6.15442800	-2.53316600	2.04454400	H	-1.80922500	-2.75267800	-1.89245600
H	7.36866900	-1.18131700	0.88465000	H	-2.06274900	-4.30098400	-1.06264600
H	4.66485700	-3.76597000	3.00251300	H	-3.40589100	-3.51556300	-1.90895000
H	6.96330700	-2.84161200	2.70106200	H	-4.12704300	-2.97510100	1.80118400
C	3.22163200	-0.20002900	-1.39559400	H	-4.76519600	-3.71586100	0.32731700
H	3.98903800	-0.42587800	-2.15026800	H	-3.35308400	-4.42020700	1.12435300
H	2.30513900	0.04410800	-1.93174700	C	-2.73139100	2.55381700	0.17758500
H	3.54678500	0.68237800	-0.83587400	C	-3.61549500	3.42614000	1.09022500
B	1.78082800	-2.11553500	-0.65795100	C	-2.30001500	3.35704600	-1.06727700
O	1.70864300	-3.49311400	-0.54937500	H	-1.82767000	2.30808700	0.74476300
O	0.69501300	-1.60414700	-1.44098300	H	-3.91206500	2.87908600	1.99139800
C	0.85247200	-3.97682100	-1.60115500	H	-3.07482500	4.32750800	1.40318000
C	-0.11781800	-2.75859500	-1.86452000	H	-4.53071700	3.74760300	0.57978400
C	1.75310000	-4.30428500	-2.80451100	H	-1.63939800	2.77595000	-1.73001200
H	2.51361200	-5.02211500	-2.48362900	H	-3.16288900	3.65008800	-1.67605900
H	1.18704400	-4.74574700	-3.63191800	H	-1.76256700	4.26916900	-0.78145000
H	2.27154900	-3.41325100	-3.17300400	C	2.82622100	-0.02104600	0.10702900
C	-0.50752400	-2.55084300	-3.32701300	C	3.49259200	-1.22072500	-0.26645600
H	-1.05549700	-3.42164200	-3.70499800	C	3.41104200	1.23882000	-0.20349000
H	-1.16332100	-1.67943000	-3.42373600	C	4.72351100	-1.12898800	-0.92704900
H	0.36690300	-2.38848900	-3.96079000	C	4.64318500	1.27262800	-0.86898000
C	-1.36748800	-2.80096900	-0.98278900	C	5.30138000	0.10100500	-1.22974100
H	-1.96271100	-1.88858200	-1.11471900	H	5.23683100	-2.04204600	-1.21675000
H	-2.02711800	-3.62839300	-1.25978800	H	5.09620000	2.23263500	-1.10503200
H	-1.10509100	-2.91243100	0.07302700	H	6.25639200	0.14556800	-1.74622800
C	0.16229700	-5.25256500	-1.11555800	C	2.89879500	-2.59969500	0.01618400
H	-0.54205800	-5.63262600	-1.86484500	C	3.84228700	-3.47311800	0.86749400
H	0.91879000	-6.02390300	-0.94056000	C	2.52016800	-3.33007000	-1.28915200
H	-0.37230700	-5.09020400	-0.17724400	H	1.97864400	-2.45466200	0.59069600
Ca	-0.27796100	0.01227800	0.31301600	H	4.12698600	-2.97493400	1.80124400
3c				H	3.35313600	-4.42013400	1.12448800
C	-1.28243800	-0.17296900	1.95428500	H	4.76522100	-3.71573900	0.32743500
C	-0.00002700	-0.21644900	2.54447700	H	1.80924400	-2.75285700	-1.89245700
C	1.28238700	-0.17297700	1.95435400	H	3.40592500	-3.51571600	-1.90886400
H	-0.00004600	-0.30215300	3.62482200	H	2.06278600	-4.30110100	-1.06252800
N	-1.50590700	-0.06375200	0.64543500	C	2.73138800	2.55380200	0.17773400
C	-2.46300400	-0.25576100	2.91033200	C	2.29998500	3.35715500	-1.06703600
H	-3.15964500	0.57362900	2.74596800	C	3.61557000	3.42600800	1.09041000
H	-3.03150000	-1.17801000	2.74532200	H	1.82768400	2.30803800	0.74493200
H	-2.13813700	-0.23652700	3.95290500	H	1.63929800	2.77615300	-1.72978200
C	2.46296000	-0.25574600	2.91037400	H	1.76259800	4.26927800	-0.78109600

H	3.16284000	3.65020900	-1.67584000	H	-2.09803100	6.23852500	1.09242800
H	3.91214600	2.87886500	1.99152800	C	-3.45344800	2.22105600	3.06480200
H	4.53079000	3.74746000	0.57995700	C	-4.38127200	2.87257900	4.11070100
H	3.07495700	4.32737800	1.40345600	C	-2.10516700	1.84339800	3.71254300
H	0.00010000	-1.13923800	-3.07769100	H	-3.92986800	1.29206300	2.73721400
Sr	0.00012200	0.21137100	-1.31277100	H	-5.34463600	3.15905600	3.67568600
6c				H	-4.57288400	2.17639400	4.93606300
C	-5.05241100	-1.57758200	0.00100700	H	-3.93104700	3.77557200	4.54008100
C	-5.74291500	-0.38826700	0.31847400	H	-1.43623600	1.33291700	3.00942900
C	-5.28533300	0.93981200	0.49115600	H	-1.57804200	2.73287700	4.07840300
H	-6.80646700	-0.51707100	0.48630500	H	-2.26795200	1.17794200	4.56961100
N	-3.74039000	-1.66287300	-0.22069900	C	-3.77193700	3.22762700	-2.03621400
C	-5.90331900	-2.83834000	-0.06631700	C	-5.29151600	3.15436100	-2.28570000
H	-5.76364100	-3.35714400	-1.02025100	C	-3.07387200	1.99144000	-2.63609300
H	-5.60930500	-3.54489400	0.71865100	H	-3.40586000	4.08467000	-2.61651800
H	-6.96536100	-2.61422100	0.05512700	H	-5.79928400	4.04507900	-1.89954400
C	-6.35101100	1.92748600	0.95328300	H	-5.49295700	3.09227500	-3.36242800
H	-7.33522200	1.64920700	0.56599200	H	-5.73445900	2.27284200	-1.81358000
H	-6.41859700	1.92266400	2.04821000	H	-1.99259300	1.99347400	-2.44011100
H	-6.12602200	2.95021900	0.64306100	H	-3.52486600	1.06341100	-2.26653700
N	-4.03275600	1.33997000	0.29786400	H	-3.19155300	1.98294400	-3.72632800
C	-3.11950400	-2.90704800	-0.54472700	H	-0.03365300	-0.06420000	-1.66918300
C	-2.91064900	-3.26112100	-1.90702700	H	0.02780700	0.21228600	1.19834000
C	-2.58105800	-3.72481500	0.48763200	C	5.26313700	-0.85937200	0.41981100
C	-2.17136100	-4.41321000	-2.20231200	C	5.77553200	0.42335400	0.12674700
C	-1.84193200	-4.86099400	0.13600000	C	5.11924900	1.62058900	-0.24412100
C	-1.63398200	-5.20979200	-1.19559800	H	6.85010000	0.51651200	0.23771100
H	-2.01334500	-4.68985700	-3.24186600	N	3.97130100	-1.18838400	0.39314900
H	-1.42066400	-5.48423100	0.92050700	C	6.29482800	-1.91227000	0.80151400
H	-1.06027700	-6.09825800	-1.44638100	H	6.17014500	-2.22416300	1.84442100
C	-3.48132600	-2.43083000	-3.05616700	H	6.17534200	-2.81327800	0.19007700
C	-4.51119500	-3.22737100	-3.88301500	H	7.31391400	-1.53973800	0.67625000
C	-2.37380300	-1.87593800	-3.97533300	C	6.00788100	2.85630300	-0.31302800
H	-4.00880000	-1.57756200	-2.61741100	H	7.04440400	2.58677000	-0.53323300
H	-5.32697600	-3.60613200	-3.25761000	H	5.66095000	3.56954200	-1.06430000
H	-4.94997400	-2.59184000	-4.66183200	H	6.00153100	3.37263000	0.65537400
H	-4.04664200	-4.08788900	-4.37923100	N	3.81901500	1.71422200	-0.49884600
H	-1.63478700	-1.28653500	-3.41945600	C	3.52711400	-2.48718100	0.78000100
H	-1.83259000	-2.68580800	-4.47948600	C	3.24594700	-2.77142200	2.14643900
H	-2.80909000	-1.23614000	-4.75327600	C	3.22636100	-3.45566600	-0.21759000
C	-2.79007800	-3.40028500	1.96635000	C	2.67865100	-4.00764700	2.47665800
C	-1.47323700	-2.98321400	2.65282400	C	2.65505900	-4.67516300	0.16786800
C	-3.44252200	-4.56984200	2.73057900	C	2.38131900	-4.95776300	1.50241200
H	-3.47700600	-2.55043600	2.02652700	H	2.46428300	-4.23068300	3.51887900
H	-1.02076900	-2.10011900	2.18422600	H	2.42663300	-5.41788300	-0.59248100
H	-1.64933500	-2.74274500	3.70883900	H	1.94300000	-5.91206100	1.78268500
H	-0.72859800	-3.78671700	2.60989500	C	3.53751700	-1.76509400	3.25947300
H	-4.38264000	-4.88267500	2.26265000	C	4.45856100	-2.35026900	4.34885500
H	-2.78438000	-5.44579000	2.76975400	C	2.23836800	-1.22644100	3.89359300
H	-3.65988300	-4.27482900	3.76417100	H	4.05970200	-0.91445400	2.81143900
C	-3.61633600	2.68229900	0.52535200	H	5.39090300	-2.74133900	3.92644300
C	-3.26451400	3.11203400	1.83666200	H	4.71719000	-1.57740500	5.08258800
C	-3.40530100	3.55375800	-0.58296900	H	3.97305400	-3.16953600	4.89231500
C	-2.72189800	4.39145800	2.01230200	H	1.58308600	-0.75523200	3.15152100
C	-2.86243300	4.82374100	-0.34359500	H	1.66700000	-2.03229600	4.37033500
C	-2.51868700	5.24865800	0.93683000	H	2.46994000	-0.48095500	4.66471600
H	-2.45367100	4.71900500	3.01357700	C	3.53566800	-3.21338000	-1.69455700
H	-2.70914200	5.49326100	-1.18708900	C	2.26056900	-3.20798400	-2.56288800

C	4.54962200	-4.23860300	-2.24154000	C	4.61686000	-1.41120400	-1.04740800
H	4.00203400	-2.22596300	-1.77641000	C	5.25192700	-0.42235700	-0.30119300
H	1.53936100	-2.44275000	-2.24715400	H	5.08958200	0.91121500	1.37245800
H	2.51067600	-3.01193300	-3.61274300	H	5.13813000	-1.85777600	-1.89034700
H	1.74062100	-4.17188200	-2.51627600	H	6.25745800	-0.10104500	-0.55998600
H	5.47277600	-4.24255700	-1.65170600	C	2.61895200	0.39285700	2.34624600
H	4.14069400	-5.25584700	-2.22547400	C	2.39568200	1.90565800	2.14956600
H	4.81177200	-4.00195700	-3.27983000	C	3.40648000	0.13738900	3.64711300
C	3.19389400	2.92782900	-0.90103900	H	1.63646000	-0.07506200	2.46376500
C	2.90301500	3.14719100	-2.27998800	H	1.80963900	2.12729800	1.24828200
C	2.70951600	3.84185000	0.07698600	H	1.86323900	2.33278200	3.00817900
C	2.14386000	4.27198800	-2.63134300	H	3.34534200	2.44254500	2.04459600
C	1.94913200	4.94369000	-0.33555500	H	3.55656700	-0.93375100	3.82034000
C	1.66301300	5.16547200	-1.67773100	H	4.39522500	0.61046200	3.61839200
H	1.92572600	4.44633700	-3.68271300	H	2.86699600	0.54733500	4.50958100
H	1.57328000	5.63761400	0.41173800	C	2.68957900	-2.95175500	-1.58605300
H	1.07081700	6.02490400	-1.98023200	C	3.52055900	-4.25100000	-1.54108800
C	3.39579500	2.26527200	-3.43570200	C	2.47214000	-2.50980200	-3.04781100
C	2.98272800	0.78168500	-3.37042400	H	1.70663200	-3.17683500	-1.16006800
C	4.91071700	2.38614000	-3.69540400	H	3.68750800	-4.59450600	-0.51396500
H	2.89916700	2.67177700	-4.32644100	H	3.00454700	-5.05050200	-2.08590000
H	1.91075400	0.66555700	-3.15876400	H	4.50358700	-4.11489500	-2.00755900
H	3.16748300	0.29990300	-4.33844100	H	1.81471100	-1.63533700	-3.12199000
H	3.57676600	0.23703000	-2.62764900	H	3.42406100	-2.25881600	-3.53209700
H	5.21982600	3.43501200	-3.76512500	H	2.01090400	-3.32155800	-3.62398300
H	5.49442700	1.90573500	-2.90494600	C	-2.98490100	-0.49917900	0.32970100
H	5.16852100	1.89518800	-4.64215600	C	-3.36336600	0.60747600	1.14306300
C	2.99484600	3.66208300	1.56785100	C	-3.77259100	-0.84237300	-0.80429100
C	1.70805200	3.38938200	2.37317300	C	-4.49697800	1.35186100	0.79476700
C	3.74543200	4.87430000	2.15681900	C	-4.89473700	-0.06016900	-1.10901800
H	3.64436600	2.78895100	1.68223000	C	-5.25885700	1.03163200	-0.32601200
H	1.18565700	2.48868300	2.02840300	H	-4.79196000	2.19505300	1.41523100
H	1.94451800	3.25071100	3.43545000	H	-5.49976900	-0.31797400	-1.97463900
H	1.00183700	4.22451100	2.29375700	H	-6.13517500	1.62194000	-0.58090900
H	4.66510100	5.08844700	1.60167700	C	-2.57470000	0.99486200	2.39460400
H	3.12761300	5.77991600	2.13479100	C	-3.44817200	0.95339700	3.66482500
H	4.01473400	4.68449800	3.20283800	C	-1.91195400	2.38028000	2.25560800
Sr	1.90304800	0.09572500	-0.26176000	H	-1.77497400	0.26011700	2.52565000
Sr	-1.90517400	0.04980000	-0.18926100	H	-3.91581500	-0.02810000	3.79736300
7c				H	-2.84071600	1.16146200	4.55391300
C	0.89819500	-2.53342000	1.42273500	H	-4.24964900	1.70061600	3.62856000
C	-0.44244000	-2.83870100	1.75197200	H	-1.24423800	2.43366900	1.38577500
C	-1.64922200	-2.20177200	1.39194400	H	-2.66213700	3.17158100	2.13692000
H	-0.56083800	-3.68386400	2.41976200	H	-1.31602500	2.61708100	3.14530600
N	1.27043800	-1.54814200	0.60992900	C	-3.45367300	-2.05449700	-1.67919200
C	1.95837600	-3.40650100	2.07903700	C	-3.13344800	-1.66140000	-3.13547700
H	2.55842400	-3.92625300	1.32441200	C	-4.59925800	-3.08807000	-1.64659600
H	2.65489900	-2.79795200	2.66642100	H	-2.56316600	-2.53730700	-1.26393100
H	1.51249700	-4.15402500	2.73875100	H	-2.25913800	-1.00311900	-3.20170000
C	-2.91413100	-2.77625400	2.01412800	H	-2.91812800	-2.55818200	-3.72949100
H	-3.58857700	-3.15710600	1.23911400	H	-3.98269700	-1.15002900	-3.60573000
H	-2.68868200	-3.59226400	2.70409000	H	-4.84821600	-3.39038600	-0.62329100
H	-3.46889200	-2.00490300	2.55901000	H	-5.51241900	-2.68802000	-2.10360600
N	-1.74182700	-1.15481400	0.57148900	H	-4.31565400	-3.98707300	-2.20664400
C	2.64494700	-1.25587700	0.36373300	C	0.45768800	3.40070800	-1.45522500
C	3.29391100	-0.25086500	1.13542400	C	1.72135000	3.00442500	-1.93905000
C	3.32216100	-1.84763700	-0.73891000	C	2.86788600	3.70797500	-1.57208100
C	4.58978800	0.14586700	0.78349500	C	2.78267600	4.81893100	-0.72929300

C	1.53080300	5.22005700	-0.26016100	H	1.26521300	-2.92779900	-3.83636300
C	0.37408700	4.52276000	-0.61391800	C	-3.15078600	-0.07660700	0.24313500
H	1.78767400	2.16277100	-2.62635800	C	-3.47193400	1.04192300	1.06214600
H	3.83122400	3.38789500	-1.95970700	C	-3.87732600	-0.30598200	-0.95848700
H	3.67669100	5.36877500	-0.45051400	C	-4.49558600	1.90654000	0.65592600
H	1.44615200	6.08871000	0.38779000	C	-4.89243200	0.59037000	-1.31638100
H	-0.58850100	4.85388500	-0.23852100	C	-5.20274400	1.69175500	-0.52408200
N	-0.67440900	2.61266900	-1.77503000	H	-4.74430600	2.76415300	1.27608700
H	-0.50829100	2.03417700	-2.61216300	H	-5.45154700	0.42004100	-2.23295700
C	-2.00235000	3.23218200	-1.79623100	H	-5.99250200	2.37617000	-0.82199800
H	-2.02701100	4.14831300	-2.40362400	C	-2.73169100	1.32178000	2.36988200
H	-2.70942300	2.50878100	-2.20973400	C	-3.68861700	1.38278000	3.57708100
H	-2.33571200	3.47451700	-0.78324600	C	-1.89336900	2.61411300	2.28908900
H	-0.02257300	0.13216000	-3.01818100	H	-2.04019100	0.49187200	2.54540800
Sr	-0.03444200	0.12533200	-0.75011100	H	-4.28760400	0.46934900	3.66115100
9c-ts				H	-3.12126700	1.50288300	4.50770700
C	0.38068000	-2.65221200	1.37299600	H	-4.38274100	2.22808900	3.50228300
C	-0.99402500	-2.77133500	1.67784700	H	-1.16618000	2.58378800	1.46737500
C	-2.08876900	-1.95500500	1.32190100	H	-2.52968200	3.49156700	2.12344200
H	-1.24597700	-3.61799000	2.30551500	H	-1.33780000	2.77436200	3.22095300
N	0.90583500	-1.68749000	0.61998000	C	-3.59688200	-1.50942000	-1.85863500
C	1.29091100	-3.70967200	1.98076500	C	-3.13470600	-1.08701000	-3.26845800
H	1.94798900	-4.14774600	1.22236300	C	-4.82016500	-2.44371200	-1.95877200
H	1.94322100	-3.26689100	2.74280200	H	-2.78570700	-2.08499600	-1.40065000
H	0.71647600	-4.51131400	2.45016000	H	-2.23929200	-0.45334000	-3.24136800
C	-3.43954800	-2.36436300	1.88967600	H	-2.90244000	-1.97097100	-3.87485500
H	-4.17713500	-2.49796700	1.09133800	H	-3.91517300	-0.52200600	-3.79189600
H	-3.37153200	-3.29408800	2.45854100	H	-5.15289000	-2.78167300	-0.97126700
H	-3.83430500	-1.58481600	2.55133800	H	-5.66796700	-1.94276900	-2.44074100
N	-2.00580800	-0.87381900	0.54582500	H	-4.57573500	-3.33083700	-2.55528100
C	2.31048200	-1.60224900	0.38157800	C	1.45636600	3.22604600	-1.18951700
C	3.13940000	-0.86038700	1.26831200	C	2.59099700	2.38852800	-1.32449700
C	2.85393100	-2.12941000	-0.82290000	C	3.87958600	2.87299800	-1.11914700
C	4.48048300	-0.65392300	0.92545200	C	4.09038500	4.21150800	-0.77555900
C	4.20297400	-1.89167100	-1.11732800	C	2.98404200	5.05413000	-0.65374400
C	5.01540900	-1.15876500	-0.25722300	C	1.68811400	4.57948500	-0.85914900
H	5.11826700	-0.08368100	1.59587500	H	2.46685100	1.35254500	-1.63916800
H	4.62467600	-2.29325200	-2.03530100	H	4.72247300	2.19613800	-1.23369700
H	6.05960000	-0.98609800	-0.50388400	H	5.09560000	4.59005300	-0.61398400
C	2.60120200	-0.27420900	2.57301200	H	3.12688800	6.10089900	-0.39426500
C	2.52637800	1.26536100	2.51678800	H	0.84993600	5.26009200	-0.75209100
C	3.42309000	-0.72316100	3.79755100	N	0.18632100	2.67016400	-1.36595900
H	1.58233700	-0.64806100	2.71166600	H	0.13429400	1.79658100	-2.38001900
H	1.90715800	1.62079300	1.68372300	C	-0.93083300	3.58882400	-1.54193800
H	2.10282600	1.66549000	3.44608600	H	-0.72717700	4.36281200	-2.29880700
H	3.51862300	1.70936400	2.37819500	H	-1.80526600	3.01677300	-1.87938600
H	3.48956500	-1.81515900	3.85896500	H	-1.21250400	4.09904000	-0.60965800
H	4.44597500	-0.33025400	3.76680900	H	-0.01031500	0.95446400	-2.95172100
H	2.95878300	-0.35881500	4.72169800	Sr	-0.11543800	0.22332700	-0.63754700
C	2.01660300	-2.96993400	-1.78710000	10c			
C	2.57015700	-4.40352800	-1.91945200	C	-1.10576600	-2.51471700	1.27070500
C	1.89488000	-2.31606100	-3.17895300	C	0.20371700	-3.02352400	1.40986800
H	1.00852200	-3.05096400	-1.36651300	C	1.44893800	-2.47898800	1.02174100
H	2.64370700	-4.89808600	-0.94470600	H	0.26488600	-3.98887300	1.89890300
H	1.91581500	-5.00905100	-2.55787300	N	-1.40471700	-1.36312800	0.67146000
H	3.56971400	-4.40646700	-2.37002900	C	-2.22100600	-3.36874700	1.85638900
H	1.45014000	-1.31315700	-3.13465800	H	-2.87172900	-2.76846600	2.50167100
H	2.87486000	-2.21261900	-3.65934900	H	-2.85730300	-3.78163400	1.06585100

H	-1.82306700	-4.20107400	2.44118800	H	1.83751400	1.92879100	2.11017400
C	2.67146300	-3.33314000	1.32571300	H	2.19735500	1.68872600	3.82929600
H	2.38890800	-4.31818600	1.70343300	H	3.44228900	2.30936300	2.73061300
H	3.28623200	-3.46598200	0.42933100	H	4.45290200	-1.30472000	3.42705600
H	3.31058900	-2.84981000	2.07352900	H	4.99183300	0.37064400	3.59584500
N	1.60715900	-1.29136700	0.43961000	H	3.66979400	-0.23327900	4.60335000
C	-2.74636100	-0.91385000	0.50993000	C	-0.18601200	3.00451000	-1.65830200
C	-3.53326300	-1.36045500	-0.58947300	C	-1.18140600	4.01958700	-1.83244300
C	-3.24159900	0.11522900	1.35937800	C	-1.22623700	5.13802000	-1.01049100
C	-4.78037700	-0.76642600	-0.81171400	C	-0.29979900	5.33753600	0.02550400
C	-4.49856800	0.67412900	1.09169100	C	0.71489700	4.39694200	0.19012400
C	-5.26658100	0.24435200	0.01478300	C	0.78390700	3.26292700	-0.62705300
H	-5.38424500	-1.09936100	-1.65205300	H	-1.91945300	3.91115400	-2.62026900
H	-4.88283500	1.45618200	1.74172100	H	-2.00586300	5.87901500	-1.17865500
H	-6.23772000	0.69135000	-0.17948600	H	-0.35189800	6.22003600	0.65581600
C	-3.04403900	-2.45104400	-1.54189500	H	1.49186500	4.55732300	0.93539300
C	-2.70289500	-1.87576700	-2.93098400	H	1.69276500	2.65589000	-0.60632600
C	-4.05418300	-3.60766200	-1.67755100	N	-0.12963300	1.81458200	-2.32227900
H	-2.12048300	-2.86765200	-1.12998600	C	-0.96963000	1.68729400	-3.50089500
H	-1.93958700	-1.09202600	-2.86861000	H	-0.78985200	2.49123500	-4.23480900
H	-2.32227400	-2.66371000	-3.59240600	H	-0.74355000	0.73971300	-4.00344800
H	-3.58600100	-1.43409000	-3.40775200	H	-2.05629500	1.69226300	-3.28946300
H	-4.32286600	-4.02776600	-0.70192500	Sr	-0.00337900	0.50549400	-0.23186700
H	-4.98144600	-3.28201100	-2.16328400	11c-ts			
H	-3.62944000	-4.41309700	-2.28825900	C	-0.25812600	-2.97873700	-1.86608900
C	-2.45586600	0.59904900	2.57888700	C	1.12435200	-3.26438300	-1.78530900
C	-3.17408400	0.23277500	3.89391900	C	2.16527100	-2.68508700	-1.02873300
C	-2.16611400	2.11393500	2.53658500	H	1.41710800	-4.15476900	-2.33087000
H	-1.49601400	0.06886000	2.58554400	N	-0.86309600	-1.92524000	-1.31904600
H	-3.34766000	-0.84627200	3.96479900	C	-1.06300200	-4.03839700	-2.61527700
H	-2.57469700	0.53819800	4.76003200	H	-1.23259900	-4.91227500	-1.97431100
H	-4.14721600	0.73244300	3.96627800	H	-2.03823900	-3.67187900	-2.93998800
H	-1.64255000	2.42668900	1.62234300	H	-0.50686900	-4.38737600	-3.49080100
H	-3.09075100	2.70042600	2.57698300	C	3.48248800	-3.45009900	-1.04396700
H	-1.54756600	2.41193400	3.39156300	H	3.73842500	-3.79187300	-0.03403500
C	2.90369600	-0.77335100	0.13988000	H	3.43141500	-4.32315800	-1.69783400
C	3.42850900	-0.89079000	-1.17641400	H	4.30963000	-2.81649400	-1.37645000
C	3.60214200	-0.00616100	1.11453600	N	2.06248400	-1.57122600	-0.30043500
C	4.63286100	-0.24513900	-1.48372300	C	-2.28670600	-1.84643100	-1.27175000
C	4.79891400	0.62320600	0.75157700	C	-3.01307700	-2.58869600	-0.29888400
C	5.31734100	0.50924400	-0.53566500	C	-2.97233300	-0.93277900	-2.12138200
H	5.03982600	-0.33405200	-2.48774500	C	-4.39613500	-2.39655600	-0.19336800
H	5.33560900	1.21270700	1.49073600	C	-4.35716800	-0.78333100	-1.97445400
H	6.24783900	1.00552500	-0.79771800	C	-5.07027700	-1.50240000	-1.01887900
C	2.72324400	-1.70608500	-2.25911200	H	-4.95596000	-2.96064100	0.54864100
C	3.56559800	-2.92185200	-2.69605600	H	-4.89054100	-0.09387000	-2.62102600
C	2.35076300	-0.84272600	-3.48233000	H	-6.14465300	-1.36943600	-0.92328400
H	1.79429000	-2.09417300	-1.82731500	C	-2.33336200	-3.58361500	0.64349100
H	3.80762900	-3.57288000	-1.84861900	C	-2.97431800	-4.98451500	0.57757500
H	3.01963100	-3.51936900	-3.43606900	C	-2.32461200	-3.07396000	2.09839100
H	4.51098900	-2.60749200	-3.15421300	H	-1.29004400	-3.68801600	0.33476700
H	1.74914400	0.03052500	-3.20245900	H	-2.99706500	-5.36705200	-0.44817100
H	3.24666500	-0.47300100	-3.99577100	H	-2.40670200	-5.69307200	1.19272200
H	1.78052400	-1.43802700	-4.20644700	H	-4.00500500	-4.97770300	0.95081800
C	3.07595700	0.15510100	2.54098900	H	-1.82014300	-2.10353700	2.18004200
C	2.61096500	1.59984900	2.81730800	H	-3.34361700	-2.94926400	2.48437600
C	4.10892900	-0.27910800	3.59959000	H	-1.80199800	-3.78050700	2.75503100
H	2.20368200	-0.49625700	2.65105900	C	-2.23508500	-0.16694700	-3.22141800

C	-2.83920400	1.21391600	-3.53122800	C	-2.44933900	3.06213500	2.74141900
C	-2.14451600	-0.99541700	-4.52081000	C	-2.40750200	1.48066300	2.72834400
H	-1.20106000	-0.01213000	-2.88204300	C	-1.28661400	3.71169100	3.50078800
H	-2.96286000	1.82298200	-2.63013200	H	-1.28149000	4.78358200	3.28093500
H	-2.18393200	1.76018800	-4.21855100	H	-1.39629400	3.58388800	4.58325600
H	-3.81606800	1.12864200	-4.02140300	H	-0.32106500	3.30398900	3.19652200
H	-1.61557000	-1.93912600	-4.36567800	C	-1.68769700	0.85048400	3.91675000
H	-3.14776100	-1.22579100	-4.89997400	H	-2.19915200	1.10785500	4.85116800
H	-1.61050800	-0.43290100	-5.29607000	H	-1.69400400	-0.24079400	3.82777600
C	3.17208700	-1.10693300	0.47392800	H	-0.65068000	1.18615900	3.99176900
C	4.14843100	-0.24318500	-0.09620300	C	-3.78622700	0.83652700	2.53774000
C	3.23032700	-1.41715300	1.86048700	H	-3.66376900	-0.23342600	2.34711700
C	5.12965900	0.30735900	0.73745100	H	-4.41031100	0.96003000	3.42885100
C	4.23387100	-0.83965200	2.64874400	H	-4.31229500	1.26890900	1.68154500
C	5.17717000	0.02315200	2.09955500	C	-3.77128100	3.65775900	3.23136100
H	5.87330800	0.97391900	0.30821100	H	-3.96493500	3.38123500	4.27420600
H	4.28153800	-1.07738700	3.70888100	H	-3.71599600	4.74929500	3.17554800
H	5.94832500	0.46440000	2.72543300	H	-4.61517100	3.33322000	2.61897900
C	4.16875000	0.09975800	-1.58569900	Sr	0.13422200	0.03574500	-0.00988200
C	5.50161800	-0.29772900	-2.25343800	12c			
C	3.88091600	1.59342300	-1.83310400	C	-0.85267500	2.99928700	-1.64899900
H	3.37316900	-0.47435800	-2.07095000	C	-2.21482100	2.64594100	-1.76742500
H	5.74319100	-1.35498300	-2.09761600	C	-2.96491500	1.58849000	-1.20693200
H	5.45068200	-0.11845000	-3.33395500	H	-2.81545300	3.38053200	-2.29429100
H	6.33823500	0.29267200	-1.86157800	N	0.07372100	2.27498500	-1.02344800
H	2.92260400	1.89964800	-1.40466100	C	-0.49747900	4.35348700	-2.25486100
H	4.66010300	2.22594800	-1.39049500	H	-0.70094700	5.15945700	-1.53892500
H	3.85276900	1.80646600	-2.90842700	H	0.55776500	4.41889300	-2.52716100
C	2.24050600	-2.38343800	2.50972000	H	-1.10566500	4.54822900	-3.14284800
C	1.36660000	-1.68321800	3.56828100	C	-4.47605500	1.78604200	-1.29809900
C	2.94643700	-3.60759900	3.12615800	H	-4.74791200	2.27144000	-2.24009000
H	1.57643800	-2.75511900	1.72293000	H	-5.03210800	0.85182400	-1.20778000
H	0.81996700	-0.82921900	3.14616900	H	-4.80974000	2.44745600	-0.48832600
H	0.62896000	-2.37673200	3.99005900	N	-2.45529300	0.51745400	-0.59477800
H	1.97236800	-1.29319100	4.39466200	C	1.38255700	2.79406100	-0.79007700
H	3.55220700	-4.13371900	2.38060300	C	1.61530100	3.69698500	0.28479700
H	3.61084500	-3.31883800	3.94899700	C	2.47720000	2.30493200	-1.55623500
H	2.21015100	-4.31563900	3.52582100	C	2.93062400	4.08230700	0.56961500
H	-1.86945500	2.23828900	-0.52289800	C	3.77124100	2.73289100	-1.23408400
N	0.67785800	2.46090900	0.00941900	C	4.00463400	3.61047600	-0.17935700
C	0.73526100	3.42798700	-0.98142900	H	3.11746100	4.76759000	1.39265200
C	1.39356400	4.67944300	-0.85714500	H	4.61215400	2.37099000	-1.81771800
C	0.10745300	3.17618900	-2.23131800	H	5.01773300	3.92485700	0.05685900
C	1.40170100	5.60376600	-1.90251800	C	0.47757800	4.25297400	1.14254700
H	1.90591600	4.93333300	0.06453300	C	0.49853300	5.79298100	1.21464800
C	0.11852200	4.10412800	-3.26495700	C	0.48828000	3.65546900	2.56357100
H	-0.39340000	2.22180400	-2.38265100	H	-0.46972500	3.96170900	0.68143900
C	0.76545100	5.33617700	-3.11473000	H	0.50039700	6.24216500	0.21565200
H	1.91966100	6.55071300	-1.76145100	H	-0.38375200	6.16091500	1.75216300
H	-0.37915300	3.86211200	-4.20221600	H	1.38333900	6.16328600	1.74531400
H	0.77799700	6.06083300	-3.92392700	H	0.37784800	2.56460500	2.54199300
C	1.48007100	2.74031200	1.18873900	H	1.42573700	3.87998900	3.08605000
H	1.19150000	3.66619300	1.71475500	H	-0.33648700	4.06240500	3.16173100
H	1.36738300	1.92235500	1.92195800	C	2.26351800	1.37211000	-2.74907800
H	2.56011100	2.82086400	0.97551200	C	3.34749700	0.28856800	-2.88826100
B	-1.80259900	2.33004500	0.65867600	C	2.13659000	2.16812500	-4.06538700
O	-2.31318900	3.39737700	1.33559500	H	1.30010000	0.86309900	-2.60511900
O	-1.65023400	1.19961000	1.49820800	H	3.49428100	-0.26244400	-1.95420900

H	3.05799700	-0.43238200	-3.66020600	H	1.78017200	-3.51980700	4.79864100
H	4.31149100	0.71667900	-3.18782700	H	0.82104300	-3.60898300	3.30639800
H	1.30221700	2.87517200	-4.03429800	C	0.90188400	-0.88215500	4.35882300
H	3.05399200	2.73653700	-4.26142800	H	1.45498700	-0.96305300	5.30189100
H	1.97300800	1.48841600	-4.91052000	H	0.41695700	0.10042700	4.34431100
C	-3.31972900	-0.46326100	-0.01706900	H	0.12222400	-1.64772700	4.34879600
C	-3.61913100	-1.65462000	-0.73932100	C	2.77988000	0.19501000	3.09656700
C	-3.79585800	-0.30443900	1.31237000	H	2.18271600	1.10306900	2.95939800
C	-4.39229400	-2.64235100	-0.11701600	H	3.35660800	0.31244800	4.02016700
C	-4.55583000	-1.32994700	1.88976500	H	3.47818700	0.11977000	2.25892600
C	-4.85859700	-2.49054200	1.18663400	C	4.01509300	-2.34642000	3.78444200
H	-4.63462900	-3.55118900	-0.65878900	H	3.93753700	-2.09327100	4.84907600
H	-4.92052300	-1.21261400	2.90721100	H	4.48849600	-3.33117500	3.70655300
H	-5.45379100	-3.27340300	1.64902800	H	4.67258800	-1.62285800	3.29713500
C	-3.14629000	-1.85403900	-2.18133200	Sr	-0.03745400	-0.03030800	-0.00286800
C	-4.13838500	-1.26417400	-3.20687600	13c-ts			
C	-2.86996600	-3.32561800	-2.54027800	C	2.74065300	-2.34504100	1.21382800
H	-2.20799400	-1.29477800	-2.29611600	C	1.83922000	-3.42976000	1.23405800
H	-4.25997900	-0.18572500	-3.08661800	C	0.50408400	-3.53682100	0.78340300
H	-3.78363900	-1.44871300	-4.22828900	H	2.25667200	-4.35209500	1.62013400
H	-5.12481800	-1.73261700	-3.10269400	N	2.44261900	-1.11326900	0.79890200
H	-2.23070500	-3.82045900	-1.80216100	C	4.15392200	-2.65295000	1.68934600
H	-3.79750200	-3.90402100	-2.62205700	H	4.87541600	-2.53453300	0.87269000
H	-2.37133600	-3.38562100	-3.51437700	H	4.46125400	-1.96222700	2.48112400
C	-3.50726400	0.95169200	2.13329600	H	4.23549500	-3.67349200	2.06963400
C	-2.60364900	0.64154800	3.34314400	C	-0.10747500	-4.92869200	0.86998000
C	-4.79928400	1.65244700	2.59833700	H	-1.03179400	-4.91717200	1.45661000
H	-2.96789000	1.65578200	1.49217900	H	-0.37599600	-5.29686800	-0.12697100
H	-1.66490800	0.16274000	3.03994500	H	0.58224400	-5.64287500	1.32474300
H	-2.35406000	1.56041900	3.88760200	N	-0.21830900	-2.53351500	0.28728700
H	-3.09720900	-0.04010000	4.04603600	C	3.44136800	-0.10150400	0.69810300
H	-5.45472500	1.88679000	1.75299400	C	4.18231200	0.03660400	-0.51038900
H	-5.36885400	1.02707800	3.29584000	C	3.60321000	0.85413700	1.74003300
H	-4.56118000	2.59000200	3.11516600	C	5.01311500	1.15139100	-0.67318800
H	2.53370300	-0.94421800	0.23284700	C	4.44568000	1.95272400	1.52191300
N	0.97489700	-2.49901500	-0.08890500	C	5.13808100	2.11509200	0.32509600
C	1.59693800	-2.92125600	-1.31851200	H	5.57702700	1.26508700	-1.59584600
C	2.91922300	-3.39420000	-1.35440300	H	4.56868000	2.68862200	2.31241600
C	0.87424500	-2.86712100	-2.52091000	H	5.78536300	2.97576000	0.17819300
C	3.49946500	-3.77984600	-2.56434200	C	4.11063700	-1.01345300	-1.62051200
H	3.48114200	-3.45571600	-0.42825500	C	5.50580500	-1.54122100	-2.01040200
C	1.45265200	-3.26320800	-3.72838200	C	3.37516600	-0.49318500	-2.87108500
H	-0.15640800	-2.52043600	-2.50421400	H	3.53641000	-1.86262700	-1.24033000
C	2.77244900	-3.71817100	-3.75525600	H	6.04773100	-1.92172500	-1.13779900
H	4.52642600	-4.13667700	-2.57375700	H	5.41464800	-2.35844400	-2.73596900
H	0.87208100	-3.21282500	-4.64638000	H	6.12411900	-0.76077600	-2.46920000
H	3.22794300	-4.02389100	-4.69336400	H	2.34466200	-0.19241400	-2.64119100
C	0.14454100	-3.57826300	0.48431200	H	3.88273800	0.37862900	-3.30125200
H	0.75494700	-4.43513600	0.80302100	H	3.32604200	-1.26919000	-3.64460800
H	-0.39154300	-3.19749100	1.35899300	C	2.94376000	0.68057100	3.10891900
H	-0.59199900	-3.93271700	-0.24471400	C	1.99761400	1.84073300	3.47547000
B	1.93909900	-1.79685900	0.92309800	C	4.00736100	0.49552700	4.21256800
O	2.81977200	-2.62199700	1.71536400	H	2.34420700	-0.23494200	3.07213000
O	1.06595500	-1.07664300	1.94822700	H	1.16027900	1.92357900	2.77281400
C	2.63659900	-2.39317900	3.11204000	H	1.57405500	1.67828200	4.47434700
C	1.84565800	-1.02542500	3.16424600	H	2.52895400	2.80045400	3.49518700
C	1.83813000	-3.56946000	3.70486900	H	4.69313100	-0.32822300	3.98579100
H	2.34231600	-4.50234600	3.43201700	H	4.61093700	1.40225900	4.33986000

H	3.52473400	0.28029300	5.17323000	C	-6.11645200	1.61088300	0.78092600
C	-1.54566800	-2.76175200	-0.18724900	H	-5.22129800	0.75044900	-0.95971600
C	-2.65729000	-2.59737100	0.68451400	C	-4.69241900	2.95787800	2.16542600
C	-1.76066800	-3.03562500	-1.56667300	H	-2.65229700	3.15578700	1.52920700
C	-3.94975800	-2.68980600	0.15200000	C	-5.95111200	2.40370500	1.91419500
C	-3.07361300	-3.12294000	-2.04543500	H	-7.08348000	1.16366000	0.56273300
C	-4.16573800	-2.94870600	-1.19914500	H	-4.53501000	3.57096000	3.04957600
H	-4.80325800	-2.55828700	0.81160500	H	-6.78170600	2.58415700	2.59095400
H	-3.24435300	-3.33383500	-3.09846400	C	-2.91909600	0.78845500	-1.83703900
H	-5.17801400	-3.01900800	-1.58863100	H	-3.70151600	1.15795200	-2.51601400
C	-2.48421500	-2.34607500	2.18251000	H	-2.00115700	0.70017900	-2.41974900
C	-3.18443100	-3.42978300	3.02855200	H	-3.22020800	-0.20713700	-1.49082200
C	-2.97618400	-0.94501800	2.59806300	B	-1.47520700	2.48087800	-0.68098500
H	-1.41402300	-2.40022700	2.40647800	O	-1.40928700	3.82939000	-0.40223800
H	-2.85319400	-4.43887200	2.75770100	O	-0.33533300	2.05287900	-1.43106100
H	-2.96693500	-3.27652500	4.09217700	C	-0.11492700	4.33275600	-0.79766100
H	-4.27353600	-3.39462100	2.90742800	C	0.34631700	3.27626600	-1.87801600
H	-2.42824400	-0.14261300	2.09107800	C	-0.31124700	5.74752700	-1.34775700
H	-4.04031900	-0.80932600	2.37304500	H	-0.65965300	6.40144800	-0.54233700
H	-2.84142500	-0.80328700	3.67761200	H	0.63211000	6.15519900	-1.72985700
C	-0.59557500	-3.25011500	-2.53251200	H	-1.05662800	5.77436500	-2.14581500
C	-0.49921900	-2.11838100	-3.57563400	C	-0.18828300	3.57237000	-3.28573100
C	-0.66872500	-4.61778700	-3.24020000	H	0.30051500	4.44766700	-3.72561400
H	0.32790000	-3.23595100	-1.94586000	H	0.00744300	2.71152700	-3.93382900
H	-0.38207600	-1.13436000	-3.10169900	H	-1.26780300	3.75034800	-3.27117500
H	0.36008900	-2.27107900	-4.23975000	C	1.84933200	3.02807200	-1.92942800
H	-1.40092300	-2.06935900	-4.19753500	H	2.08245100	2.26739900	-2.68158600
H	-0.72277600	-5.43853100	-2.51679800	H	2.37410500	3.94619400	-2.21741600
H	-1.54738100	-4.69182900	-3.89166700	H	2.25536700	2.70290000	-0.96833000
H	0.21962900	-4.77431100	-3.86401200	C	0.78226700	4.38192300	0.44566300
H	-0.66808000	1.57202000	1.22731600	H	1.76921900	4.79831600	0.21648100
N	-2.69826500	1.71126700	-0.72459100	H	0.30369300	5.02331200	1.19254800
C	-3.78483000	1.94249300	0.14879100	H	0.89603200	3.39191900	0.89231800
C	-5.05164900	1.37785300	-0.09303300	Sr	0.28068200	-0.05969500	0.02644300
C	-3.62225100	2.73277300	1.30572800				