

Mechanistic Insight into Cp*Rh(III)-Catalyzed Lossen Rearrangement *vs*

C-N reductive Elimination for the Synthesis of Pyridones

Baoping Ling*, Jianqiao Xu, Yuan-Ye Jiang, Peng Liu, Jin Feng, Siwei Bi*

School of Chemistry and Chemical Engineering, Qufu Normal University, Qufu, 273165, PR China

Email Address of Corresponding Author: xiaoling0523@163.com and siweibi@126.com

Supporting Information

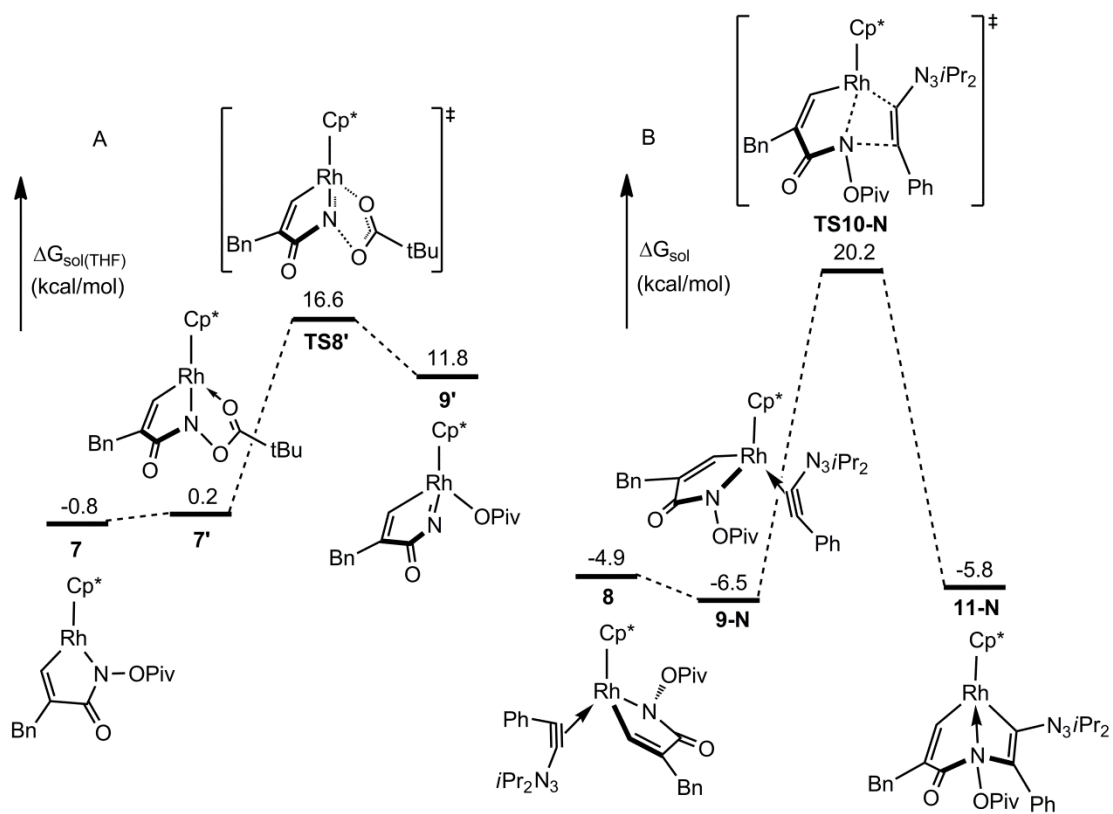


Figure S1 Gibbs free energy profiles for (A) OPiv migration from N to Rh prior to alkynyl insertion, and (B) insertion of alkynyl triazene into Rh-N bond.

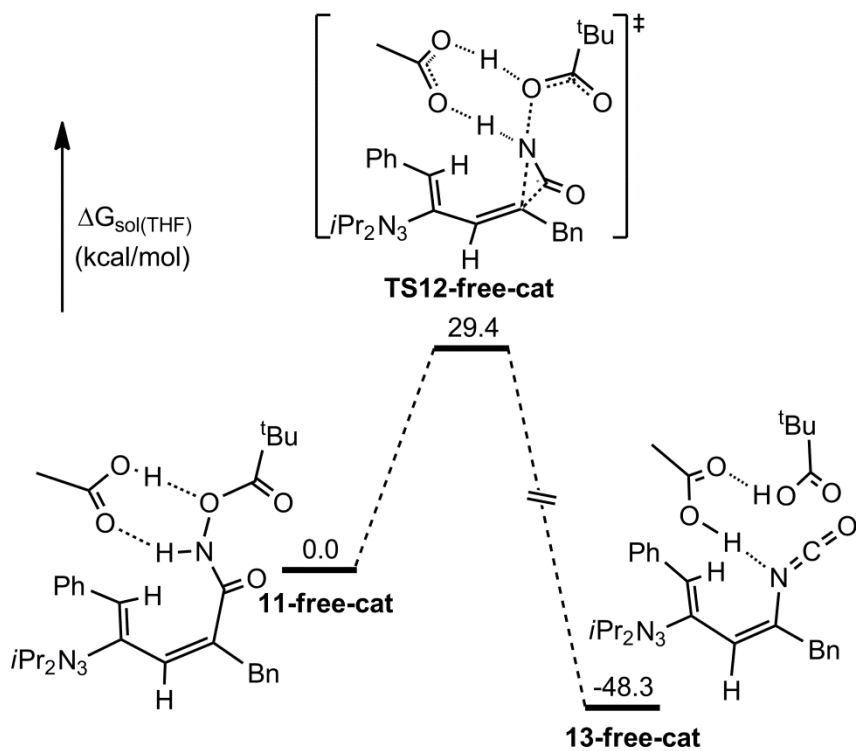


Figure S2 Gibbs free energy profile for the concerted Lossen rearrangement/OPiv migration without rhodium catalyst.

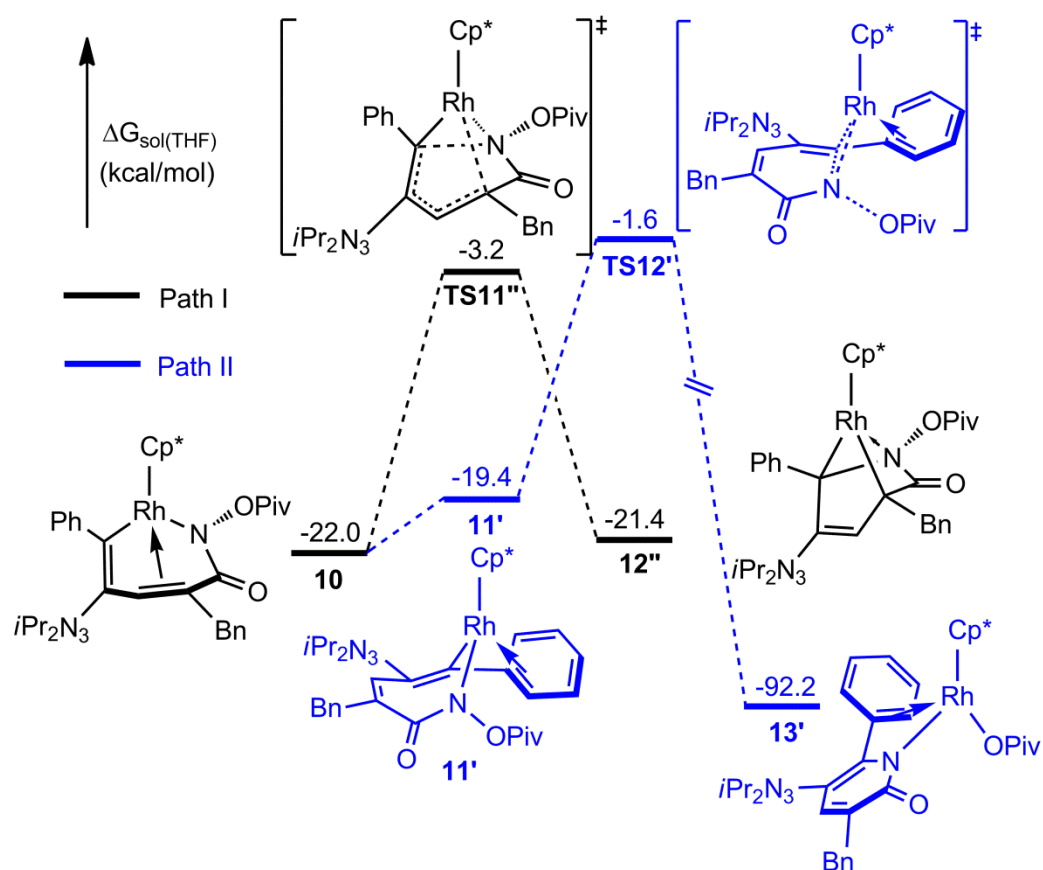


Figure S3 Gibbs free energy profiles of two pathways for C-N reductive elimination starting from **10**.

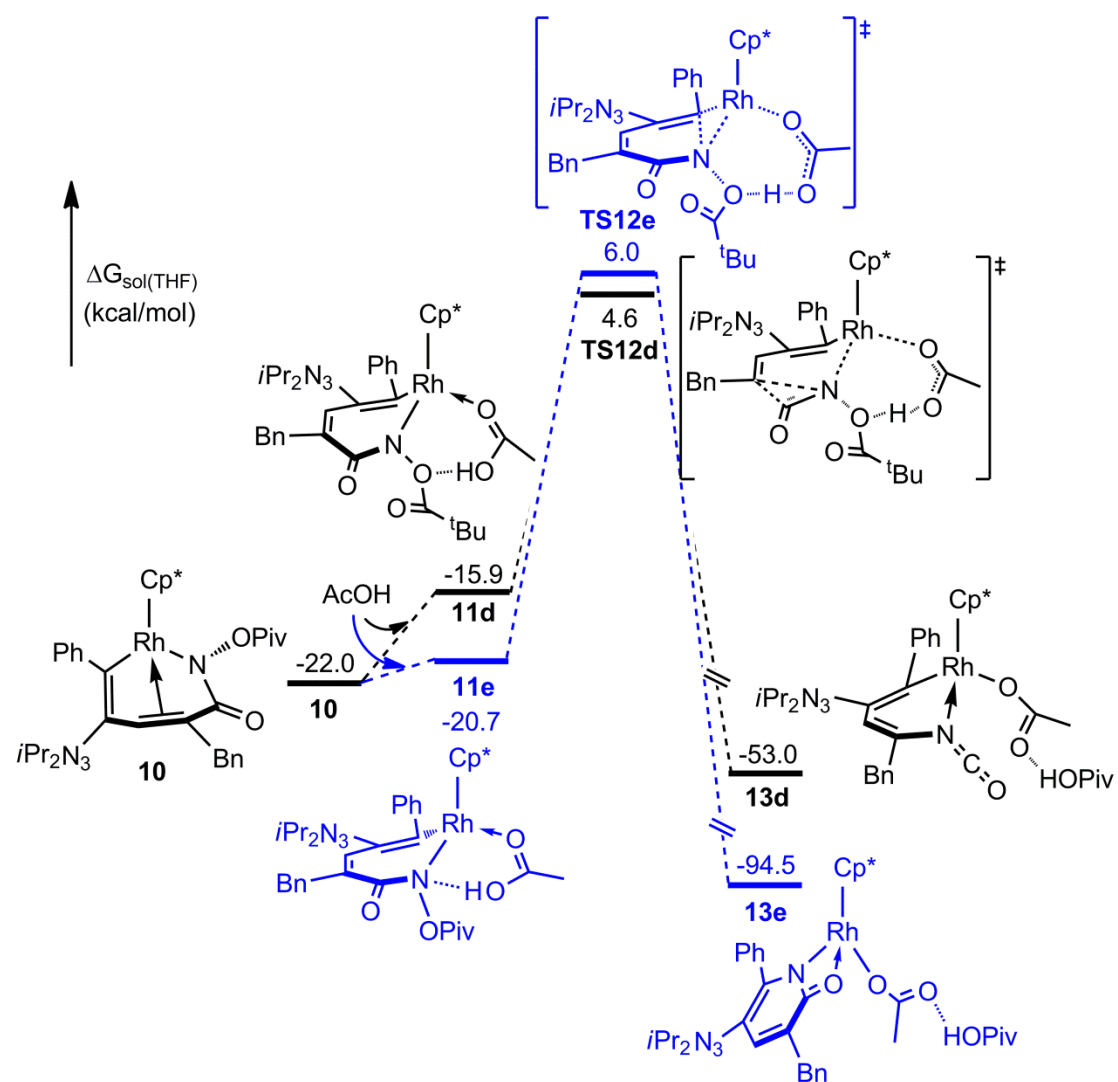


Figure S4 Gibbs free energy profile for the concerted Lossen rearrangement/N-O bond cleavage and C-N bond formation/N-O bond cleavage assisted by AcOH.

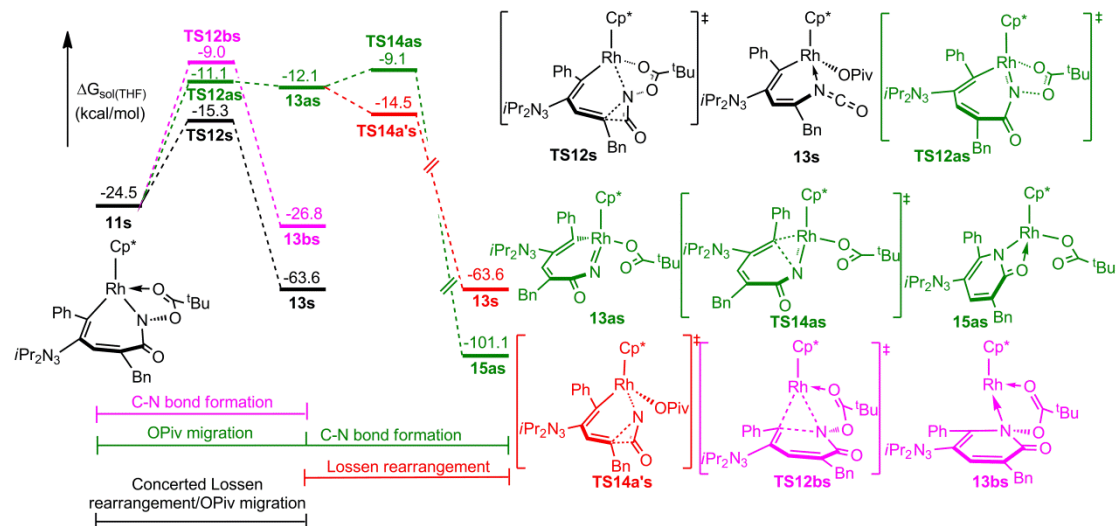


Figure S5 Gibbs free energy profiles for full optimization in tetrahydrofuran of alternative pathways starting from intermediate **11s**.

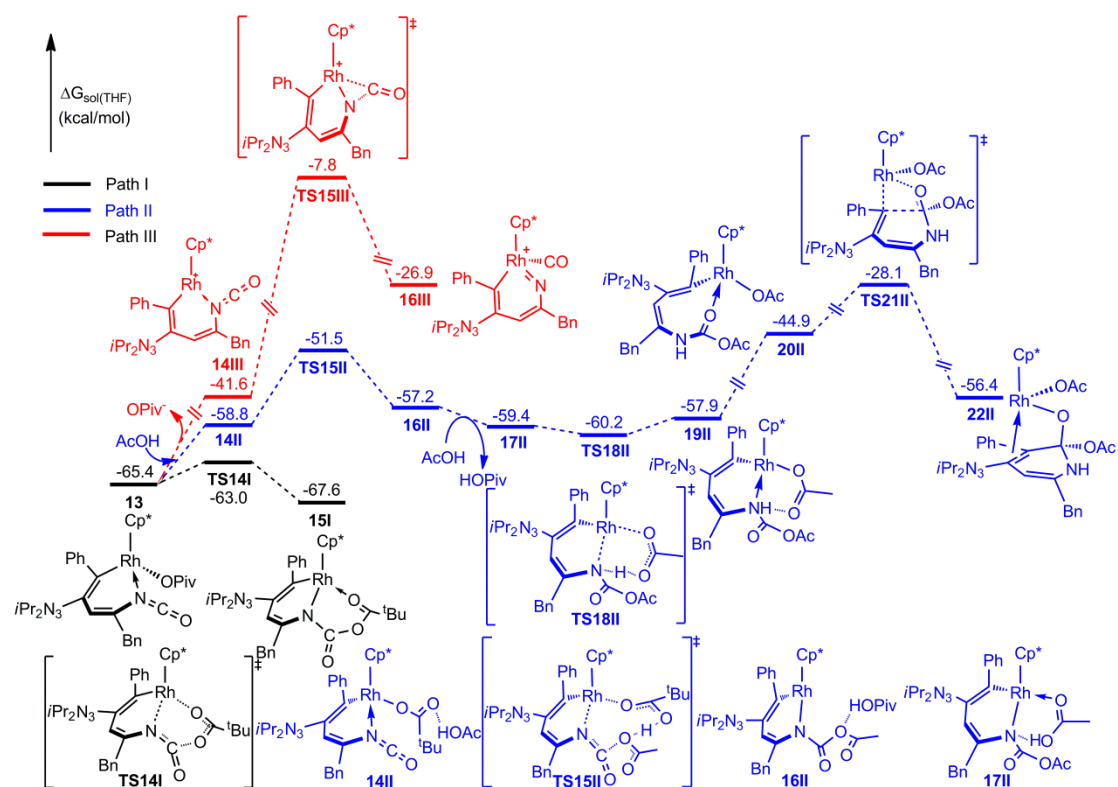


Figure S6 Gibbs free energy profiles for three pathways starting from isocyanate **13**.

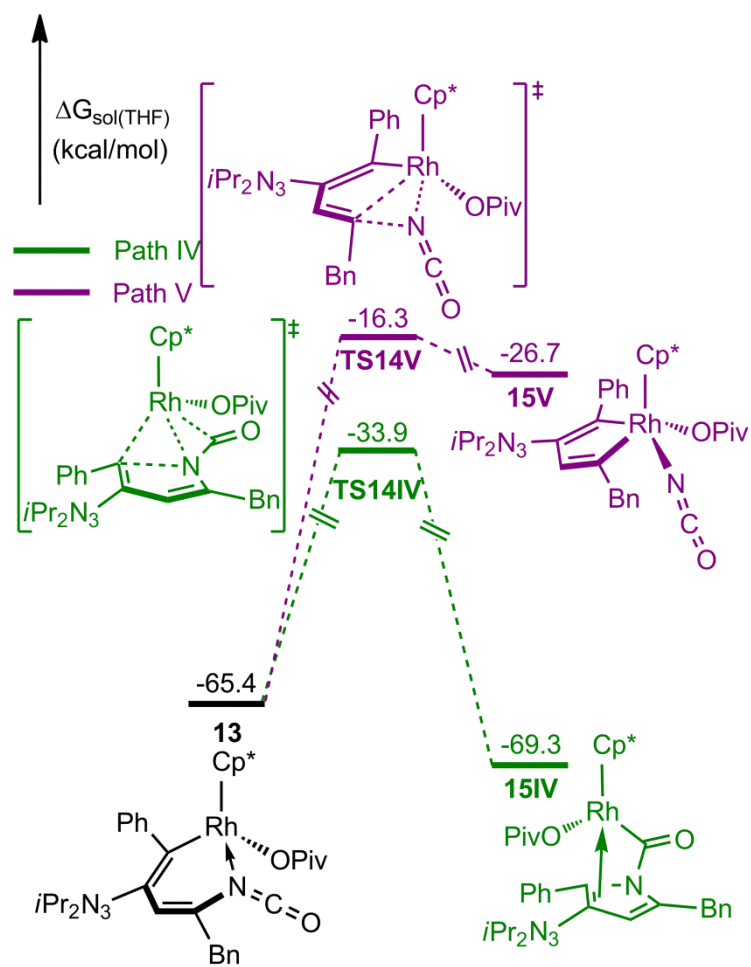


Figure S7 Gibbs free energy profiles for both pathways starting from isocyanate **13**.

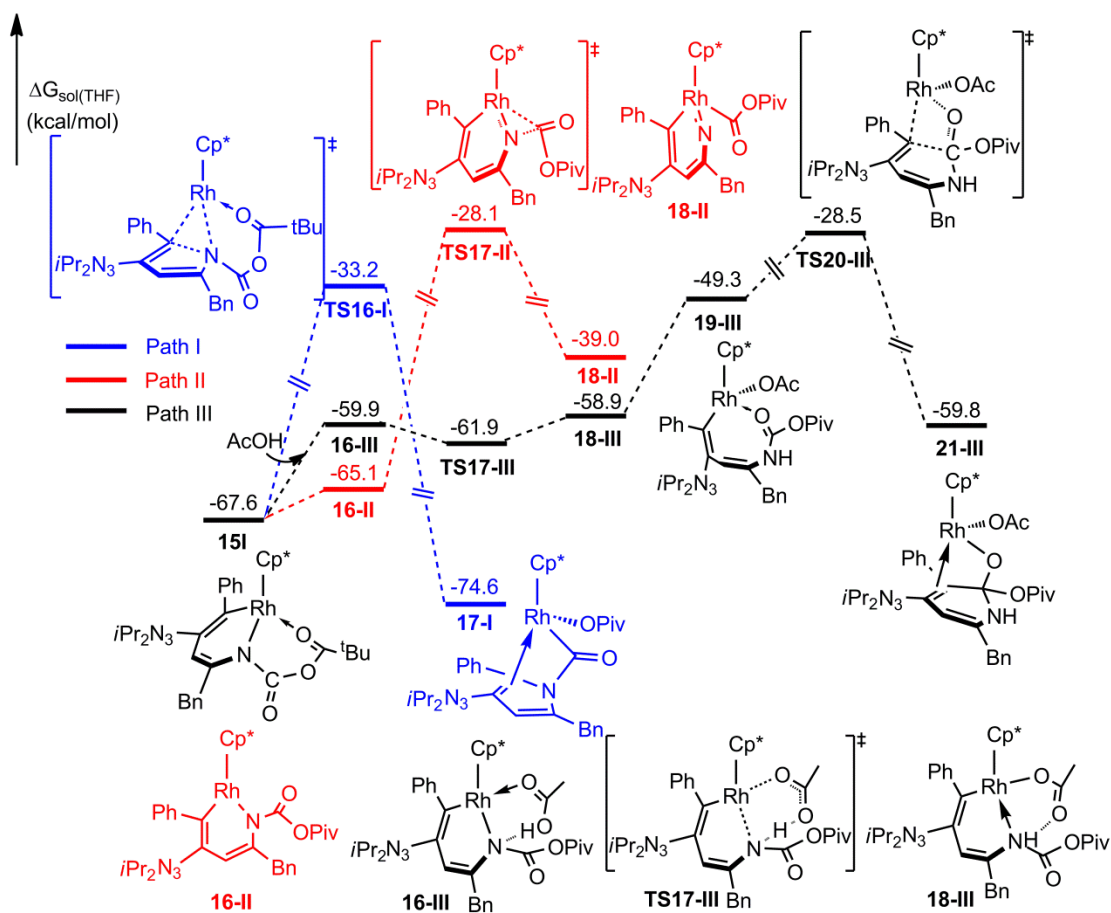


Figure S8 Gibbs free energy profiles for plausible pathways starting from intermediate **15I**.

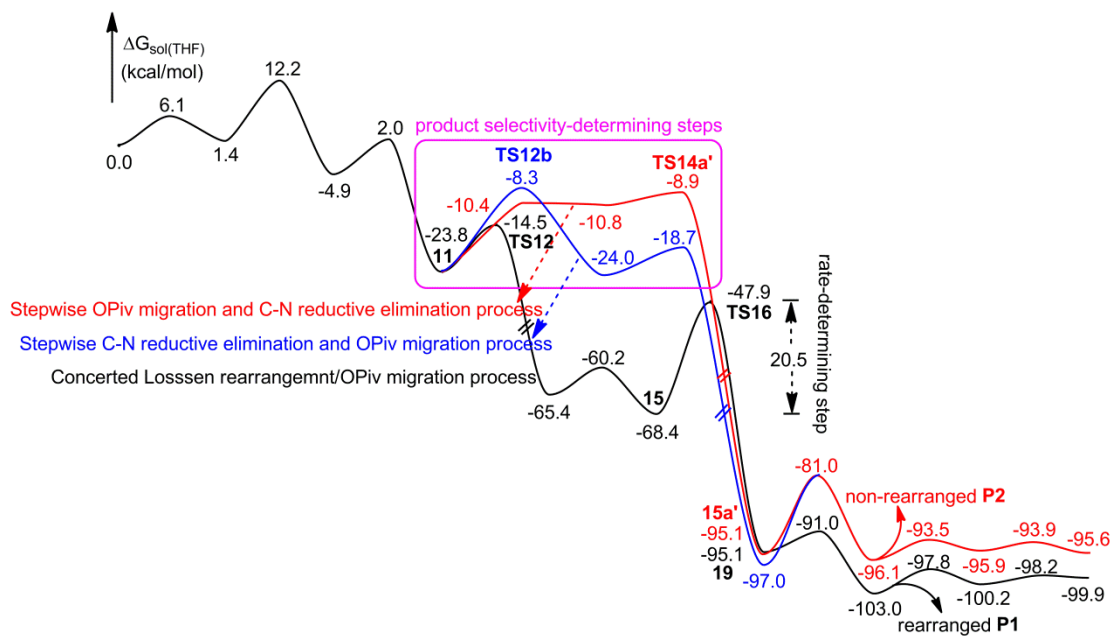


Figure S9 Summary on the free energy profiles for the formation of rearranged and non-rearranged products.

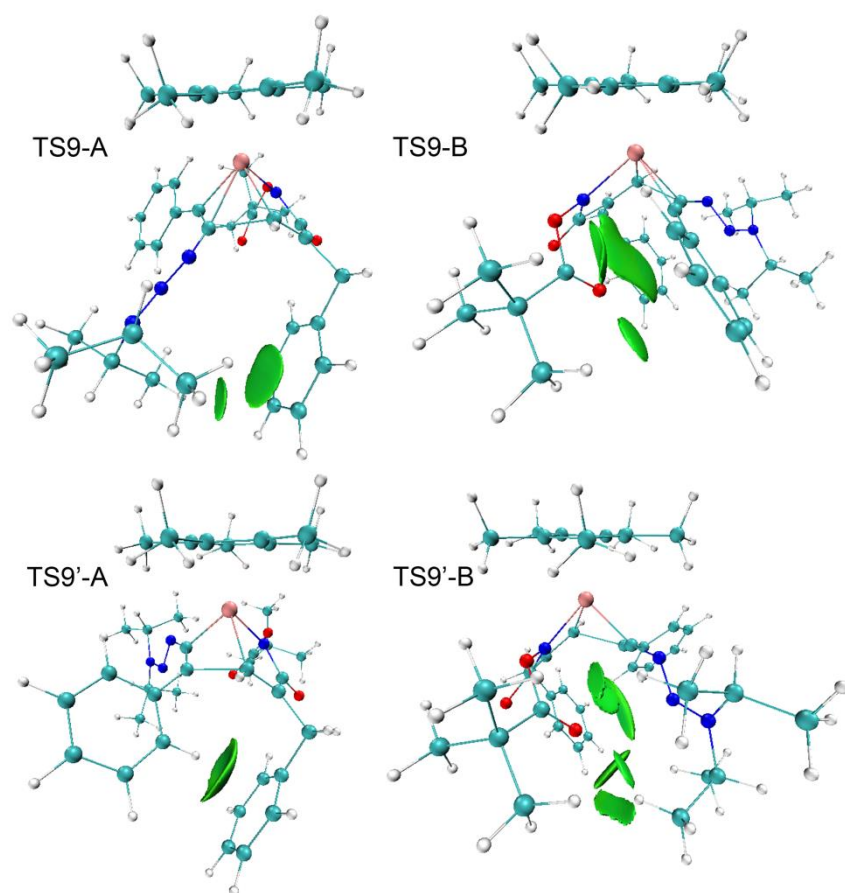


Figure S10 Intramolecular weak interactions^a for **TS9** and **TS9'**.

^a (1) T. Lu, F. Chen, *J. Comput. Chem.*, 2012, **33**, 580-592.

(2) T. Lu, Q. Chen, *J. Comput. Chem.*, 2022, **43**, 539-555.

Table S1 Electronic energies, solution-phase Gibbs free energies and solution-phase enthalpies for all species as well as imaginary frequencies of transition states.

Geometry	E(Hartree)	G_{sol}(Hartree)	H_{sol}(Hartree)	Frequency(<i>i</i> cm⁻¹)
Cat	956.7078877	-957.122133	-957.042455	
S1	-863.4735910	-862.822488	-862.752170	
S2	-709.1200824	-708.480708	-708.413402	
1	-1820.2205088	-1819.934379	-1819.814124	
TS2	-1820.2175490	-1819.934907	-1819.815480	-1075.16
3	-1820.2253840	-1819.942420	-1819.822961	
4	-1591.0826247	-1590.930838	-1590.821877	
TS5	-1591.0679124	-1590.919889	-1590.810178	-517.04
6	-1591.0946592	-1590.937878	-1590.826766	
7	-1361.9688084	-1361.935305	-1361.836789	
8	-2071.1318383	-2070.422529	-2070.285024	
TS9	-2071.1134905	-2070.411585	-2070.272665	-408.82
10	-2071.1558123	-2070.449815	-2070.308207	
AcOH	-229.0904107	-229.005295	-228.972584	
8'	-2071.1302095	-2070.420409	-2070.283348	
TS9'	-2071.1110983	-2070.403654	-2070.265845	-352.54
10'	-2071.1611144	-2070.451299	-2070.312076	
TS8'	-1361.9475758	-1361.907520	-1361.811076	-87.14
9'	-1361.9495987	-1361.917685	-1361.817736	
9-N	-2071.1318755	-2070.425115	-2070.286593	
TS10-N	-2071.0971092	-2070.382569	-2070.243796	-184.47
11-N	-2071.1424274	-2070.423994	-2070.285981	
11	-2071.1737832	-2070.452618	-2070.315458	
TS12	-2071.1494799	-2070.437865	-2070.297958	-260.06
13	-2071.2182452	-2070.514783	-2070.372374	
TS12a	-2071.1460006	-2070.431393	-2070.294208	-44.06
13a	-2071.1461357	-2070.431912	-2070.292671	
TS14a	-2071.1461086	-2070.430810	-2070.294194	-58.16
11-free-cat	-1801.7827906	-1800.334620	-1800.209641	
13-free-cat	-1801.8466877	-1800.411541	-1800.283965	
TS14a'	-2071.1388822	-2070.428929	-2070.291279	-241.18
15a'	-2071.2845001	-2070.566264	-2070.430869	
TS12c	-2071.1462948	-2070.424961	-2070.287996	
13c	-2071.2989783	-2070.577428	-2070.436600	
TS12b	-2071.1741526	-2070.452910	-2070.319175	-344.07
13b	-2071.1741526	-2070.452910	-2070.319175	
TS14b	-2071.1694657	-2070.444506	-2070.310700	-442.33
15b	-2071.2882699	-2070.569329	-2070.433532	
TS14	-2071.2162831	-2070.510686	-2070.369065	-43.70

15	-2071.2355667	-2070.523718	-2070.384313	
TS16	-2071.2000814	-2070.491036	-2070.351683	-225.16
17	-2071.2590917	-2070.547320	-2070.410947	
18	-2071.2799721	-2070.564006	-2070.423783	
19	-2300.4135256	-2299.571539	-2299.418745	
TS20	-2300.4037154	-2299.565112	-2299.412884	-160.71
21	-2300.4217106	-2299.584182	-2299.428031	
P1	-1225.7042180	-1224.659501	-1224.568941	
22	-1303.7933823	-1303.921757	-1303.823073	
TS23	-1303.7914934	-1303.925544	-1303.826045	-630.57
24	-1303.7926914	-1303.922314	-1303.822899	
HOPiv	-347.0498177	-346.802928	-346.761666	
TS14I	-2071.2269091	-2070.515133	-2070.375230	-101.10
15I	-2071.2372871	-2070.522409	-2070.383712	
TS21II	-2182.3460856	-2181.667217	-2181.529267	-375.10
22II	-2182.3788415	-2181.712343	-2181.568737	
TS15III	-1724.5206445	-1724.100381	-1723.979479	-484.00
16III	-1724.5522832	-1724.130799	-1724.009594	
TS14IV	-2071.1838151	-2070.468837	-2070.332509	-248.43
15IV	-2071.2501092	-2070.525167	-2070.392741	
TS14V	-2071.1486228	-2070.440694	-2070.301410	-384.19
15V	-2071.1642632	-2070.457237	-2070.318226	
TS16-I	-2071.1864906	-2070.467606	-2070.331115	-359.10
17-I	-2071.2533588	-2070.533652	-2070.400678	
TS17-II	-2071.1808004	-2070.459592	-2070.324891	-488.62
18-II	-2071.2001686	-2070.476877	-2070.339082	
TS20-III	-2300.3102157	-2299.465525	-2299.322053	-378.38
21-III	-2300.3464920	-2299.515368	-2299.366148	
15b	-2071.2882699	-2070.569329	-2070.433532	
15a'	-2071.2845001	-2070.566264	-2070.430869	
16a'	-2300.4052657	-2299.560338	-2299.413302	
TS17a'	-2300.3900001	-2299.549188	-2299.399630	-947.48
18a'	-2300.4126471	-2299.573139	-2299.422153	
19a'	-1303.7933823	-1303.921757	-1303.823073	
TS20a'	-1303.7914934	-1303.925544	-1303.826045	-627.69
21a'	-1303.7926914	-1303.922314	-1303.822899	
P2	-1225.7022866	-1224.652586	-1224.564185	
7'	-1361.9684687	-1361.933062	-1361.833541	
TS12-free-cat	-1801.7171244	-1800.287748	-1800.158836	-488.43
11'	-2071.1574690	-2070.445590	-2070.305940	
TS12'	-2071.1345868	-2070.417357	-2070.280110	-295.56
12''	-2071.1619916	-2070.448843	-2070.313325	
TS11''	-2071.1309839	-2070.419796	-2070.281820	-215.15

13'	-2071.2793643	-2070.561729	-2070.425811	
11d	-2300.2971736	-2299.453061	-2299.304224	
TS12d	-2300.2499182	-2299.410509	-2299.261924	-394.17
13d	-2300.4090886	-2299.570631	-2299.419436	
11e	-2300.2887607	-2299.445322	-2299.295100	
TS12e	-2300.2536613	-2299.412765	-2299.264236	-138.94
13e	-2300.3377882	-2299.504436	-2299.352708	
11s	-2071.2108933	-2070.454186	-2070.318076	
TS12s	-2071.1873557	-2070.439406	-2070.300122	-260.06
13s	-2071.2547286	-2070.516481	-2070.375950	
TS12as	-2071.1851075	-2070.432736	-2070.296129	-45.50
13as	-2071.1852354	-2070.434401	-2070.294957	
TS14as	-2071.1812376	-2070.429511	-2070.293555	-58.16
15as	-2071.3316710	-2070.576253	-2070.440272	
TS14a's	-2071.1872476	-2070.438108	-2070.299291	-50.59
13s	-2071.2543590	-2070.516727	-2070.375700	
TS12bs	-2071.1861676	-2070.429406	-2070.295197	-344.07
13bs	-2071.2133096	-2070.457771	-2070.324571	
14III	-1724.5656598	-1724.154277	-1724.034208	
TS15III	-1724.5206445	-1724.100381	-1723.979479	-484.00
16III	-1724.5522832	-1724.130799	-1724.009594	
14II	-2300.3466686	-2299.513720	-2299.360607	
TS15II	-2300.3305844	-2299.502103	-2299.350813	-292.13
16II	-2300.3456743	-2299.511215	-2299.361443	
17II	-2182.3961731	-2181.716985	-2181.575431	
TS18II	-2182.3947401	-2181.718292	-2181.576696	-850.48
19II	-2182.3971932	-2181.714616	-2181.573130	
20II	-2182.3743792	-2181.693967	-2181.553632	
TS21II	-2182.3460856	-2181.667217	-2181.529267	-375.10
22II	-2182.3788415	-2181.712343	-2181.568737	
16-III	-2300.3598398	-2299.515544	-2299.368253	
TS17-III	-2300.3588769	-2299.518713	-2299.371723	-844.64
18-III	-2300.3613058	-2299.513964	-2299.366209	
19-III	-2300.3412125	-2299.498625	-2299.352925	
21-III	-2300.3464920	-2299.515368	-2299.366148	
16-II	-2071.2384132	-2070.518559	-2070.383498	
18-II	-2071.2001686	-2070.476877	-2070.339082	

Cartesian coordinates of all calculated species (in angstrom)

Cat

C	1.09204700	-1.71538400	-0.21257600
C	1.64207000	-0.76779800	-1.14258300
C	2.19267500	0.34542500	-0.37630300
C	1.92477600	0.10469900	0.99923900
C	1.21204000	-1.16333000	1.10675300
O	-0.58465600	2.10019300	-1.00889900
O	-1.06485900	1.67262300	1.08808300
C	-1.19101000	2.41912900	0.06392600
C	-2.08134200	3.63138200	0.10925400
H	-3.09348700	3.32571700	-0.17651000
H	-2.11796700	4.03929200	1.12109000
H	-1.73570100	4.38477700	-0.60096500
Rh	0.03292200	0.20595800	-0.09655600
C	2.85409200	1.54376100	-0.98347900
H	3.83584900	1.27546400	-1.39091200
H	2.24413200	1.94714200	-1.79625200
H	2.99368100	2.33888400	-0.24925900
C	1.74066200	-0.92139300	-2.62811100
H	1.65881800	0.04707000	-3.12757100
H	2.70446800	-1.36575100	-2.90711900
H	0.94601100	-1.56395700	-3.01214500
C	0.47619100	-3.03618700	-0.54843900
H	0.12927700	-3.05903900	-1.58352200
H	1.22097100	-3.83177700	-0.42170200
H	-0.37716600	-3.23224700	0.10116000
C	0.76276800	-1.81827000	2.37379900
H	-0.25114200	-2.20169100	2.24615800
H	1.43644400	-2.64376600	2.63594600
H	0.75895300	-1.10741900	3.20268500
C	2.25303900	0.98910700	2.16233100
H	1.36698300	1.15201600	2.78187600
H	3.02557300	0.52615900	2.78705200
H	2.61702700	1.96492500	1.83622500
O	-1.84095600	-0.38081000	-0.70101600
O	-2.08904300	-1.92044500	0.94485400
C	-2.50569800	-1.27057600	-0.01696400
C	-3.93274400	-1.44466200	-0.52788200
H	-4.39997500	-2.30568400	-0.04790600
H	-4.50798700	-0.54237000	-0.29645900
H	-3.93751500	-1.56376300	-1.61481500

S1

C	0.93031100	2.50739200	0.96485400
C	1.51159900	1.28523000	1.30689500
C	2.38461100	0.64030500	0.42243600
C	2.66299400	1.24227100	-0.81090800
C	2.08381500	2.46352500	-1.15475500
C	1.21217900	3.09847600	-0.26768200
H	0.25464300	2.99589700	1.66181000
H	1.26731200	0.80998700	2.25171300
H	3.32960800	0.74198500	-1.50978000
H	2.30708200	2.91600500	-2.11675800
H	0.75521300	4.04639200	-0.53670500
C	2.94724900	-0.73567400	0.74672200
H	4.00095600	-0.80507700	0.45744900
H	2.87983100	-0.91609000	1.82474600
C	2.16067600	-1.81556100	0.03160200
C	2.67231200	-2.69006400	-0.84132600
H	2.05745800	-3.44860400	-1.31565400
H	3.73103600	-2.68639800	-1.08519300
C	0.70290700	-1.80437300	0.38488900
N	-0.14091500	-2.01689000	-0.71469600
H	0.17947400	-1.55742600	-1.56543500
O	0.29130200	-1.60973100	1.51402400
C	-1.68559400	-0.28397000	-0.67250400
C	-2.95031200	0.19731100	0.02324800
C	-4.08503200	-0.83896000	-0.08319100
H	-4.97145600	-0.45721000	0.43347100
H	-4.35638300	-1.02494800	-1.12754500
H	-3.80266300	-1.78993900	0.37294200
C	-3.37231000	1.53742700	-0.59745200
H	-4.22786000	1.94410400	-0.04917000
H	-2.55233300	2.25814700	-0.55950400
H	-3.66321100	1.41392700	-1.64538600
C	-2.54364600	0.39423900	1.50658200
H	-3.41550200	0.72594800	2.08008400
H	-2.15951100	-0.53502100	1.93365600
H	-1.75911500	1.15239100	1.59245300
O	-0.90341100	0.38666000	-1.30239900
O	-1.47023100	-1.63334000	-0.44297200

I

C	3.29302600	1.05011300	-0.91673000
C	3.84512000	-0.09875100	-0.23122900
C	3.34848900	-1.28966400	-0.89797000
C	2.43886400	-0.88413400	-1.91319600

C	2.36489700	0.57697700	-1.89481000	C	-1.14292300	-2.66708200	-0.62278500
O	1.66430500	-1.50639900	1.68825500	C	-0.17594700	-3.39281900	-0.05824300
O	-0.49739000	-1.20101600	2.28090300	H	0.81157400	-2.99813500	0.14219100
C	0.66155600	-1.58817600	2.50533600	H	-0.37362200	-4.41605900	0.25028200
C	0.99994400	-2.22852300	3.84111000	C	-0.96479600	-1.26826000	-1.13254600
H	1.48346800	-1.47412500	4.47098900	N	-0.50481200	-0.27271600	-0.20732500
H	0.09078800	-2.57295600	4.33599000	H	-0.74536400	-0.45438500	0.81825700
H	1.70411600	-3.05351400	3.70836900	O	-1.25616300	-0.97284300	-2.27459400
Rh	1.72772600	-0.15456900	0.07146100	C	-1.76666100	1.67818100	0.16521400
C	3.70589200	-2.68611300	-0.49640500	C	-2.39944400	2.88755900	-0.51809000
C	4.85143900	-0.08841800	0.87595100	C	-1.65190200	3.32151400	-1.78826700
H	5.87093100	-0.17471400	0.47944400	H	-2.16587900	4.18223500	-2.22962800
H	4.78698300	0.83498700	1.45466900	H	-0.62885400	3.60949000	-1.54058400
H	4.67484600	-0.92360500	1.55801900	H	-1.62479600	2.51969800	-2.53019200
C	3.64308400	2.47336400	-0.62888300	C	-2.42551100	4.03860500	0.50312700
C	1.49402500	1.42749000	-2.76474500	H	-2.96767500	4.89211900	0.08305700
H	1.17908600	2.30814000	-2.20386900	H	-2.91990200	3.72769400	1.42664500
H	2.02537100	1.74080800	-3.67163800	H	-1.40357300	4.34804700	0.73760700
H	0.59013000	0.88747700	-3.05404000	C	-3.83800400	2.43524600	-0.86859900
C	1.75998800	-1.78150500	-2.89998600	H	-4.37643000	3.26523200	-1.33809300
H	0.84899700	-1.33212800	-3.29405000	H	-3.82708700	1.59071300	-1.56531700
H	2.43675600	-1.97577400	-3.74101000	H	-4.37994100	2.12389100	0.02792300
H	1.48868500	-2.74041500	-2.45263500	O	-1.98729400	1.30879500	1.29360600
O	1.32308800	1.18128500	1.59811700	O	-0.95949200	0.98749500	-0.70031000
O	0.82680800	2.99833900	0.33718000	H	3.16879500	-3.42662500	-1.09153400
C	0.92966600	2.40800400	1.41949000	H	4.78080500	-2.85537200	-0.62424900
C	0.52061800	3.07825500	2.72409300	H	3.45678800	-2.84231500	0.55831200
H	0.53924600	4.16386400	2.61190600	H	3.84623000	2.61891700	0.43386800
H	-0.50167200	2.75590400	2.94613400	H	4.54979200	2.73710000	-1.18861800
H	1.16236100	2.76307500	3.54957400	H	2.83218400	3.14472000	-0.90164900
C	-5.69525200	-1.02459800	-0.61698500	TS2			
C	-4.72126200	-1.89028800	-1.11682100	C	3.40808600	0.90944500	-0.86562900
C	-3.61466100	-2.24772400	-0.33657500	C	3.87547800	-0.30347500	-0.25106400
C	-3.49117200	-1.70917300	0.95184200	C	3.25194700	-1.41968500	-0.94509500
C	-4.45673600	-0.83123000	1.44638800	C	2.37409000	-0.89701600	-1.93450400
C	-5.56465900	-0.49222300	0.66790000	C	2.41597400	0.55958200	-1.84667300
H	-6.54780300	-0.75662800	-1.23499900	O	1.59458600	-1.47277000	1.79417000
H	-4.81525000	-2.28593000	-2.12515100	O	-0.56635300	-0.99806500	2.24336000
H	-2.62390700	-1.94342500	1.56206500	C	0.57513300	-1.45836100	2.55242700
H	-4.32593500	-0.39918300	2.43327200	C	0.73520300	-2.02717900	3.94284100
H	-6.31511000	0.19226300	1.05346700	H	0.97366900	-1.19936500	4.61941600
C	-2.54546600	-3.17817700	-0.89198000	H	-0.19919200	-2.48163500	4.27684500
H	-2.64209700	-4.18255100	-0.46270000	H	1.55382600	-2.74767400	3.97370100
H	-2.68119900	-3.26987300	-1.97544700	Rh	1.74185400	-0.18305200	0.07868800

C	3.51168200	-2.85773500	-0.62032600	C	-2.32446200	2.88654200	-0.58831000
C	4.89440500	-0.43437800	0.83726700	C	-1.48846500	3.34635700	-1.79236900
H	5.88318000	-0.66317000	0.42050000	H	-1.99057400	4.19187200	-2.27551700
H	4.97408100	0.48746500	1.41612400	H	-0.49665800	3.66253900	-1.46476900
H	4.61871200	-1.23850700	1.52423500	H	-1.37956000	2.54574800	-2.52753400
C	3.86403100	2.28987400	-0.52106000	C	-2.49372800	4.03977300	0.41504300
C	1.62875800	1.51646200	-2.68358800	H	-3.03315000	4.86737100	-0.05713100
H	1.39003000	2.40135800	-2.09318900	H	-3.05165800	3.71050100	1.29481900
H	2.19075700	1.81025300	-3.57876700	H	-1.51349000	4.40204700	0.73868200
H	0.68284100	1.06802200	-2.99280500	C	-3.70248800	2.36492900	-1.06513200
C	1.59623400	-1.68781900	-2.93781400	H	-4.23123800	3.16148200	-1.59964700
H	0.69462100	-1.16346000	-3.25446500	H	-3.58165500	1.51180000	-1.74063700
H	2.22023200	-1.86448400	-3.82242300	H	-4.31332700	2.03959400	-0.21917900
H	1.28913200	-2.65638000	-2.53723900	O	-2.00537700	1.35652800	1.27718300
O	1.34234600	1.19525500	1.56783500	O	-0.83677500	1.02039900	-0.63912900
O	1.01453600	3.05488800	0.31215400	H	2.83998000	-3.52241300	-1.16567900
C	1.01438900	2.44244100	1.38448500	H	4.54278400	-3.12463600	-0.87956300
C	0.54786900	3.10638600	2.67371100	H	3.37620000	-3.03411500	0.45124400
H	0.56397000	4.19211200	2.56418600	H	4.14555800	2.35858800	0.53181200
H	-0.47820600	2.77365900	2.85933200	H	4.74499300	2.53737200	-1.12704000
H	1.16308000	2.79559200	3.52139900	H	3.07534800	3.01765500	-0.69972900
C	-5.72238500	-1.00693300	-0.67572500	3			
C	-4.73432200	-1.87788300	-1.13686100	C	3.59367300	-0.54690400	0.45255300
C	-3.64466700	-2.21727300	-0.32602800	C	3.20981100	-1.91816900	0.48190500
C	-3.55512400	-1.65549300	0.95441400	C	2.67051300	-2.26337200	-0.82884400
C	-4.53263400	-0.77073800	1.41114600	C	2.67766200	-1.09153300	-1.63417800
C	-5.62295700	-0.44912500	0.60108300	C	3.19494200	0.00363400	-0.82743100
H	-6.56055800	-0.75267600	-1.31871900	O	-0.05769700	-2.03267500	1.04130900
H	-4.80153300	-2.28898800	-2.14098600	O	-1.73832500	-0.57144000	1.52127100
H	-2.70199400	-1.87815900	1.58730500	C	-1.15675000	-1.73559000	1.54286000
H	-4.42539900	-0.31880500	2.39202500	C	-1.97456900	-2.78171300	2.24804500
H	-6.38323900	0.24109300	0.95599100	H	-2.17515100	-2.45306400	3.27169800
C	-2.55751900	-3.14839300	-0.84228800	H	-2.93819800	-2.86872800	1.73909800
H	-2.65410100	-4.14485600	-0.39434800	H	-1.44945000	-3.73600100	2.25120700
H	-2.67698500	-3.26282000	-1.92519500	Rh	1.41104300	-0.69863400	0.13783500
C	-1.15890300	-2.62459000	-0.57123600	C	2.25543900	-3.65209700	-1.20504000
C	-0.18740000	-3.36262300	-0.02841100	C	3.37580500	-2.89059700	1.60795500
H	0.80400200	-2.97371500	0.15808300	H	4.22822800	-3.55628800	1.42452600
H	-0.37836500	-4.39155300	0.26591200	H	3.54482100	-2.37581100	2.55534900
C	-0.99821000	-1.20928600	-1.05557000	H	2.48035000	-3.50895100	1.71579800
N	-0.46283200	-0.27217200	-0.14018400	C	4.25364800	0.20664700	1.56178400
H	-0.62136000	-0.53152800	1.09874100	C	3.44353700	1.39861900	-1.30342400
O	-1.41332700	-0.89778900	-2.16129300	H	3.35802600	2.09543200	-0.47069700
C	-1.70926000	1.70249300	0.15698000	H	4.44144300	1.47685100	-1.75360800

H	2.70002800	1.69029500	-2.04633600	C	-1.59261100	4.27018800	-1.43073000
C	2.21262300	-0.95239800	-3.05018000	H	-1.53476400	5.32086600	-1.73475500
H	1.60819200	-0.04983900	-3.16609700	H	-1.60612500	3.63482700	-2.32048700
H	3.07451500	-0.87731500	-3.72342000	H	-2.53095400	4.11489400	-0.88998000
H	1.60333700	-1.80151100	-3.36363000	O	-1.30897500	1.99097800	0.60794800
O	0.91126900	0.37879400	1.83966600	O	0.21018500	1.66402700	-1.03766800
O	1.93332100	2.34969900	1.38986900	H	1.85388300	-3.70126800	-2.21802100
C	1.22009800	1.61946600	2.08578800	H	3.12094000	-4.32278300	-1.15132700
C	0.54587500	2.14346900	3.34571800	H	1.49685700	-4.03190700	-0.51358200
H	1.06149600	3.03563800	3.70475600	H	3.96833900	-0.19821900	2.53496600
H	-0.48234900	2.40476900	3.07660500	H	5.34282500	0.12045500	1.46153400
H	0.51004400	1.37737500	4.12350300	H	3.97063700	1.25797500	1.53866500
C	-4.86988700	0.50811000	0.78944500	HOAc			
C	-4.15769800	0.23899500	-0.37859100	C	-0.09336300	0.12605600	-0.00007000
C	-4.07137900	-1.07022300	-0.87401100	O	-0.64469300	1.20359800	-0.00017600
C	-4.72752700	-2.09521900	-0.18063400	O	-0.77663000	-1.04713300	0.00016000
C	-5.45103300	-1.82500700	0.98423500	H	-1.71948900	-0.81158300	0.00022000
C	-5.51917400	-0.52034700	1.47595900	C	1.39603000	-0.10981800	0.00000800
H	-4.90949600	1.52578600	1.16713000	H	1.67961400	-0.69166000	0.88202200
H	-3.64211200	1.03789100	-0.90011000	H	1.67950200	-0.69367900	-0.88069200
H	-4.67625700	-3.11383400	-0.55984700	H	1.91495900	0.84777100	-0.00105400
H	-5.96144400	-2.63232700	1.50338600	4			
H	-6.07582900	-0.30701300	2.38427500	C	1.60815800	-2.80491000	0.14497300
C	-3.25920000	-1.38509400	-2.12036600	C	0.24501400	-3.17754500	0.30188900
H	-3.53469000	-2.37597600	-2.49515100	C	-0.43418700	-2.87396900	-0.94767900
H	-3.48415200	-0.65108000	-2.89949600	C	0.50426000	-2.28013000	-1.84683100
C	-1.76008500	-1.34989600	-1.87253000	C	1.77067500	-2.18852200	-1.15786200
C	-1.01921500	-2.45990500	-1.83366100	Rh	0.38122200	-0.94156500	-0.05312400
H	0.04361900	-2.42008600	-1.65918700	C	-1.82874600	-3.29635200	-1.28372600
H	-1.46542300	-3.44296200	-1.96006300	C	-0.35125500	-3.81625800	1.52026600
C	-1.19359400	0.04692000	-1.78145900	H	-0.09688100	-4.88183300	1.57573100
N	-0.13113600	0.27167000	-0.95025400	H	0.01529200	-3.31197600	2.41770100
H	-1.25142500	0.16510200	1.06444700	H	-1.44081700	-3.73390400	1.51608500
O	-1.75879300	0.94673500	-2.41985400	C	2.69738300	-2.97821500	1.15300700
C	-0.53872000	2.43942000	-0.22624900	C	3.04579300	-1.65080500	-1.72989300
C	-0.38092200	3.92470500	-0.52906800	H	3.66248400	-1.20409600	-0.94727000
C	0.93401900	4.23530500	-1.26182900	H	3.62656200	-2.44516900	-2.21508600
H	0.99645100	5.31275300	-1.44868800	H	2.83860500	-0.87404900	-2.46917700
H	1.78784000	3.93459700	-0.65127100	C	0.24649100	-1.79356300	-3.23956400
H	0.98684500	3.71701800	-2.22227400	H	0.58899600	-0.76043200	-3.35017100
C	-0.44648600	4.70670900	0.79367100	H	0.77394900	-2.41487800	-3.97226700
H	-0.44491100	5.78220700	0.58758600	H	-0.81830500	-1.81537800	-3.47962700
H	-1.35548600	4.45802700	1.34678300	O	0.90153800	-1.06592800	3.05913500
H	0.41986100	4.46533900	1.41541400	O	1.72332600	-0.01302200	1.23375200

C	1.64638200	-0.24771100	2.51865600	H	-2.48133100	-3.27552100	-0.40826200
C	2.58598600	0.64492700	3.31952800	H	2.29289900	-3.02680800	2.16364600
H	3.60825400	0.56525400	2.93754000	H	3.25217300	-3.90046200	0.94067700
H	2.26890100	1.68453000	3.19081300	H	3.39698600	-2.14099200	1.11040400
H	2.55820200	0.37198400	4.37504100	TS5			
C	-6.30945600	0.60131000	0.98312400	C	2.21995400	-2.62501400	0.84824500
C	-5.17777600	-0.07089100	0.51637300	C	1.27796000	-3.19546200	-0.05045400
C	-4.17032600	0.61607300	-0.17116500	C	1.39898400	-2.51400300	-1.32637900
C	-4.30615100	1.99590000	-0.37921900	C	2.51285300	-1.59270600	-1.22642700
C	-5.43615100	2.66612500	0.08932700	C	2.99396300	-1.62814100	0.11469300
C	-6.44168000	1.97358900	0.76913600	Rh	0.86497200	-1.00299500	0.14641400
H	-7.08307500	0.05283300	1.51341400	C	0.63544500	-2.82267700	-2.57823100
H	-5.08038800	-1.14110500	0.68584900	C	0.29932500	-4.28675500	0.25029900
H	-3.51184900	2.53570800	-0.88619300	H	0.69286300	-5.25231000	-0.08985900
H	-5.52909800	3.73613200	-0.07448300	H	0.09678800	-4.36193300	1.32064200
H	-7.31911700	2.50077500	1.13294800	H	-0.65092200	-4.11631100	-0.26146400
C	-2.95177900	-0.14442500	-0.68248100	C	2.45394500	-2.97075200	2.28720500
H	-3.05750100	-1.18927900	-0.38804900	C	4.08093100	-0.80262300	0.72963100
H	-2.91645700	-0.11096300	-1.77756400	H	3.69745900	-0.27506100	1.60877800
C	-1.65578900	0.39538100	-0.11767400	H	4.91741000	-1.43663600	1.04621400
C	-1.25571800	0.17128900	1.18369500	H	4.46237500	-0.05462200	0.03285100
H	-0.54080700	0.83701200	1.64956100	C	2.99386700	-0.71731000	-2.34319800
H	-1.83583300	-0.47510700	1.83586000	H	3.69232500	0.04118800	-1.98675700
C	-0.85412600	1.42351000	-0.91381300	H	3.50170000	-1.32046600	-3.10501100
N	0.36039400	0.83658200	-1.08626800	H	2.15638000	-0.19835500	-2.81561600
O	-1.28451700	2.49547100	-1.31218000	O	-0.99018900	0.25750300	2.39718600
C	1.75137900	2.49543700	-0.18052600	O	1.17210700	0.31212300	1.78046800
C	3.14871200	3.09937200	-0.32706600	C	0.18665300	0.68806200	2.50528400
C	4.17247200	1.94193300	-0.34825200	C	0.47506400	1.76143200	3.53031100
H	5.18972500	2.34778400	-0.34145000	H	1.51750700	1.72351000	3.85154200
H	4.04087200	1.29614800	0.52461100	H	0.28989800	2.71847100	3.03259700
H	4.04692800	1.32805300	-1.24311000	H	-0.20121000	1.66964300	4.38140200
C	3.40922600	4.01706100	0.87623700	C	-6.30474400	-0.75797700	0.67380500
H	4.39602800	4.48158900	0.77970200	C	-5.22714200	-1.22993500	-0.07941900
H	2.65512800	4.80560200	0.94066100	C	-4.34847500	-0.33689800	-0.70159100
H	3.38092400	3.45317800	1.81240300	C	-4.55583500	1.04203400	-0.55325300
C	3.22430700	3.90311900	-1.64252200	C	-5.63072800	1.51141300	0.20066500
H	4.22476500	4.33525900	-1.75269300	C	-6.50905800	0.61489900	0.81575400
H	3.02343400	3.26513000	-2.50654200	H	-6.98229000	-1.46316900	1.14765800
H	2.49702200	4.72128000	-1.64527500	H	-5.07198700	-2.30097800	-0.18838200
O	0.97433300	2.70115100	0.71719800	H	-3.85907000	1.72982600	-1.02343600
O	1.49574400	1.65364600	-1.24627300	H	-5.78097500	2.58181700	0.31096000
H	-2.27346600	-2.67278900	-2.06050400	H	-7.34520900	0.98434800	1.40290500
H	-1.81293600	-4.33005500	-1.65112100	C	-3.16023600	-0.84733800	-1.50794500

H	-3.24511000	-1.93180400	-1.63799000	C	3.68460700	-0.15791100	2.11732700
H	-3.15827800	-0.37259100	-2.49451300	H	2.81607900	-0.03128400	2.77334300
C	-1.85877300	-0.52738700	-0.81801700	H	4.45101700	-0.70796700	2.67556300
C	-1.31896800	-1.21770900	0.22379900	H	4.07846700	0.83376600	1.88595000
H	-1.04770400	-0.51920700	1.23597400	C	3.79457300	0.87350300	-0.97075300
H	-1.79285100	-2.15102200	0.53515500	H	4.01735000	1.56939100	-0.15972200
C	-1.12740400	0.70906400	-1.28469400	H	4.70355600	0.74253600	-1.57029200
N	0.17485700	0.59085800	-0.92495600	H	3.03251300	1.33743800	-1.60133500
O	-1.66119900	1.62720700	-1.90899700	O	-1.96284300	-0.36204900	1.63058000
C	0.82493600	2.74808500	-0.26758300	O	0.26692500	-0.25005800	1.97383900
C	1.95889300	3.76222300	-0.43598300	C	-0.89850200	0.01462100	2.29965300
C	3.26672800	3.05898400	-0.00419200	C	-1.20591600	0.81794700	3.52758800
H	4.09808800	3.77161200	-0.02775500	H	-0.37727800	0.75564700	4.23324300
H	3.17798600	2.65948900	1.01134900	H	-1.32104100	1.85424200	3.19520200
H	3.50008100	2.22789500	-0.67469600	H	-2.14043600	0.48844300	3.98479500
C	1.67730500	4.96369200	0.47726000	C	-5.47592200	-2.17563100	0.48059400
H	2.47753300	5.70399000	0.37476200	C	-4.46189400	-2.30223600	-0.47190300
H	0.72673000	5.43775400	0.21884000	C	-3.87871000	-1.16956200	-1.05228500
H	1.61957000	4.65574800	1.52464200	C	-4.32634600	0.10045400	-0.65754900
C	2.05605500	4.21261000	-1.90749000	C	-5.33705600	0.22653200	0.29465300
H	2.87243600	4.93434500	-2.01977800	C	-5.91636400	-0.90908300	0.86696100
H	2.24714500	3.36399200	-2.56822400	H	-5.92095800	-3.06559800	0.91783800
H	1.12777600	4.69289700	-2.23224400	H	-4.12128400	-3.29141700	-0.77031100
O	-0.06771600	2.80919800	0.54021700	H	-3.85489500	0.97743400	-1.09073200
O	0.99975600	1.71024200	-1.14977600	H	-5.67147500	1.21634900	0.59354500
H	0.52993200	-1.92786300	-3.19652900	H	-6.70440100	-0.80736300	1.60813700
H	1.14427200	-3.58997500	-3.17503900	C	-2.73327600	-1.30555100	-2.04273800
H	-0.36882600	-3.18519000	-2.34742100	H	-2.68129000	-2.33525000	-2.41137600
H	1.64203600	-3.57672700	2.69447800	H	-2.90404100	-0.64113700	-2.89636300
H	3.38848600	-3.53272100	2.40646000	C	-1.41028100	-0.92002800	-1.41211500
H	2.52883500	-2.05986000	2.88818600	C	-0.58846500	-1.72227200	-0.70856700
6				H	-1.70599300	-0.78182500	0.77334300
C	2.69089000	-2.24117000	0.89493700	H	-0.80908100	-2.78486900	-0.57808700
C	2.42129000	-2.62695800	-0.44385900	C	-1.00561100	0.53075600	-1.50249000
C	2.68288600	-1.47379900	-1.28550400	N	0.21365800	0.66804400	-0.91736200
C	3.31351400	-0.44615900	-0.45005900	O	-1.68938500	1.42488900	-2.00968900
C	3.28710500	-0.89767200	0.87658600	C	0.06550200	2.80405600	0.04772800
Rh	1.11251100	-0.90259800	0.04230700	C	0.48682100	4.25971500	-0.16477700
C	2.59357900	-1.42127400	-2.78040300	C	2.02551700	4.36887100	-0.17980400
C	1.92300200	-3.95678500	-0.91899600	H	2.31938800	5.41607500	-0.30814100
H	2.75761000	-4.57410100	-1.27284900	H	2.45653300	4.01097300	0.76214000
H	1.41667600	-4.50393100	-0.12021200	H	2.45652500	3.78624300	-0.99667600
H	1.21710300	-3.84316200	-1.74559700	C	-0.09731500	5.10977200	0.97245300
C	2.54069300	-3.06840400	2.13559300	H	0.16902300	6.16140400	0.82447900

H	-1.18613000	5.02408700	1.00292900	H	-5.05701200	1.95301100	1.65170200
H	0.28905500	4.78834600	1.94452900	H	-6.30701000	-0.01858100	2.51412400
C	-0.09221900	4.70940300	-1.52585200	C	-3.17931400	-0.47738000	-1.88814400
H	0.15578200	5.76177000	-1.70281700	H	-3.40340600	-1.41186400	-2.41283200
H	0.31424000	4.10488600	-2.33942600	H	-3.37087200	0.35097900	-2.57868400
H	-1.17999400	4.59740000	-1.54247400	C	-1.71576900	-0.45364400	-1.50027700
O	-0.72070000	2.41353600	0.87970100	C	-0.97166500	-1.48044100	-1.06944700
O	0.68843100	2.00042100	-0.86346900	H	-1.38256400	-2.48820200	-0.98384200
H	2.31539100	-0.41800800	-3.11149400	C	-1.01942800	0.87680200	-1.48696200
H	3.55402100	-1.68259300	-3.24277100	N	0.34162200	0.69635600	-1.22655900
H	1.83533800	-2.11317500	-3.15311300	O	-1.55980700	1.96140800	-1.65964400
H	1.86010900	-3.90799200	1.97797200	C	0.76331300	2.53104000	0.17479200
H	3.50878600	-3.47335500	2.45700400	C	1.32286100	3.95463200	0.18443400
H	2.14309300	-2.46354100	2.95529400	C	2.77072100	3.97163800	-0.34610400
7				H	3.15674700	4.99628100	-0.32585700
C	1.29372800	-1.50339100	1.56285800	H	3.42676000	3.35346800	0.27684100
C	1.20777400	-2.76362100	0.85068500	H	2.82232700	3.60106700	-1.37181600
C	2.25648900	-2.76832700	-0.10345100	C	1.27411900	4.49226200	1.62187800
C	3.10611300	-1.58886300	0.13255200	H	1.62188600	5.53010000	1.64153600
C	2.54258700	-0.83881700	1.16920400	H	0.25772200	4.45369400	2.02010900
Rh	0.91835600	-1.03500900	-0.47689000	H	1.91436700	3.90323600	2.28652500
C	2.56481000	-3.84398200	-1.09862100	C	0.41024100	4.79672200	-0.73809500
C	0.16909500	-3.82257800	1.06212800	H	0.75972700	5.83481800	-0.75237600
H	0.46467800	-4.49635800	1.87515700	H	0.41629700	4.40209900	-1.75637100
H	-0.79682100	-3.38337800	1.32281600	H	-0.62390200	4.78157400	-0.38217800
H	0.02549200	-4.42530700	0.16203600	O	0.16736000	1.99929700	1.08568600
C	0.39856300	-1.03561900	2.66626800	O	1.01104300	1.93335100	-1.02653900
C	3.06186900	0.42515500	1.78103100	H	2.95301000	-3.42114500	-2.02907100
H	2.24125400	1.09213900	2.04912400	H	3.32417000	-4.53140600	-0.70369000
H	3.62921400	0.20342700	2.69382100	H	1.67496700	-4.42816200	-1.34216800
H	3.72515600	0.96051100	1.09723300	H	-0.56697700	-1.54387700	2.63566700
C	4.34986500	-1.28371600	-0.64289200	H	0.86208700	-1.23784900	3.64101500
H	4.68299000	-0.25695300	-0.48011300	H	0.21755700	0.03828600	2.58061100
H	5.16484300	-1.95647600	-0.34743400	S2			
H	4.18829900	-1.41847000	-1.71651300	C	-0.70158100	-0.43792900	-0.09350000
C	-5.58455000	-1.33412400	0.96431900	C	-1.91282000	-0.31306500	-0.07124500
C	-4.78551700	-1.44768300	-0.17619800	C	-3.32340200	-0.13541900	-0.04135500
C	-4.08075700	-0.34420800	-0.67099000	C	-4.19058700	-1.24857800	-0.04320400
C	-4.18797000	0.88227300	0.00196000	C	-3.88609200	1.15835600	-0.00743300
C	-4.98390600	0.99635800	1.14126600	C	-5.57093000	-1.06927300	-0.01168000
C	-5.68582300	-0.11051100	1.62739800	H	-3.76491300	-2.24667200	-0.06921700
H	-6.12906300	-2.20040500	1.33106700	C	-5.26751300	1.32809300	0.02406700
H	-4.71188700	-2.40313200	-0.69095700	H	-3.22423600	2.01861300	-0.00598000
H	-3.63084400	1.73546900	-0.37306000	C	-6.11605000	0.21733100	0.02224300

H	-6.22514800	-1.93670400	-0.01336300	H	4.83870600	-1.55939900	0.46577800
H	-5.68484800	2.33088000	0.05019500	H	5.08034000	-2.38323400	-1.08043400
H	-7.19340000	0.35322300	0.04696500	H	4.24309100	-0.82316200	-1.02897800
N	0.60607200	-0.73321100	-0.11373100	C	-4.93117200	1.87266000	-2.77942700
N	1.38089300	0.29190200	-0.10293000	C	-3.92599300	1.07699300	-3.33378800
N	2.67451200	0.02481500	-0.15982700	C	-2.60122200	1.16892900	-2.88691500
C	3.53452500	1.20649100	0.06567100	C	-2.29905100	2.08221800	-1.86438700
H	4.55768800	0.82314300	0.07512900	C	-3.30357800	2.87632600	-1.30992600
C	3.39248200	2.20175300	-1.09153900	C	-4.62248600	2.77732600	-1.76220600
H	2.36145100	2.56043800	-1.15094300	H	-5.95257200	1.78225600	-3.14002900
H	3.64857800	1.72978900	-2.04464100	H	-4.17397100	0.36898500	-4.12169100
C	3.24751600	1.85365200	1.42742300	H	-1.28200400	2.17832300	-1.49857100
H	2.22479400	2.23800800	1.45450500	H	-3.05039800	3.57754800	-0.51953600
H	3.36348700	1.12795200	2.23768600	H	-5.39980200	3.40034300	-1.32761900
C	3.20743400	-1.35467200	-0.16089000	C	-1.52016200	0.30260200	-3.52011500
H	2.38591200	-1.96157400	-0.54685800	H	-1.98591500	-0.57426600	-3.98305000
C	4.40407500	-1.49743200	-1.10619200	H	-1.02988100	0.87797200	-4.31558000
H	4.16663000	-1.11209300	-2.10195000	C	-0.45112200	-0.12327700	-2.54074700
H	4.66057400	-2.55699200	-1.20179100	C	-0.54565000	-1.11418400	-1.65086000
H	5.29592800	-0.98055500	-0.73713800	H	-1.41296300	-1.76402600	-1.55252800
C	3.51854300	-1.81283900	1.27019700	C	0.74832800	0.75359700	-2.42005400
H	2.62856300	-1.72342700	1.89859400	N	1.59949800	0.25115300	-1.46261000
H	3.84024700	-2.85944900	1.27286300	O	0.92048100	1.78930800	-3.06518100
H	4.32205400	-1.21208800	1.71090700	C	2.04961100	2.35984400	-0.51485800
H	3.93882000	2.68371700	1.60410500	C	3.11119900	3.45874200	-0.47110500
H	4.05387500	3.06043400	-0.93903800	C	4.54275600	2.90426500	-0.37400200
8				H	5.25293400	3.73729100	-0.33384300
C	1.15274100	-3.49955700	0.48851500	H	4.67257000	2.30396000	0.53061200
C	1.08867400	-3.58682800	-0.93642400	H	4.78874600	2.28261100	-1.23754900
C	2.22672500	-2.88254300	-1.46496700	C	2.80729100	4.38216400	0.72036700
C	3.06472300	-2.48124700	-0.34555000	H	3.49021900	5.23849800	0.71069300
C	2.40917300	-2.86150500	0.84795100	H	1.78002800	4.74907100	0.66816800
Rh	1.00462900	-1.38866200	-0.36485700	H	2.92904400	3.85206000	1.66948300
C	2.59627100	-2.70027100	-2.90541000	C	2.93407800	4.22663500	-1.80481800
C	0.02634500	-4.27666800	-1.73618100	H	3.67336000	5.03320100	-1.86564000
H	0.31038300	-5.31676200	-1.93654000	H	3.05664600	3.55546700	-2.65844200
H	-0.92839400	-4.28671100	-1.20399400	H	1.93213200	4.65937000	-1.86784800
H	-0.13411700	-3.77725800	-2.69423400	O	0.89234400	2.50721400	-0.20434200
C	0.18450100	-4.08711500	1.47122400	O	2.56626300	1.19390600	-1.03676700
C	2.88491000	-2.70596800	2.26105700	H	2.96732700	-1.68522300	-3.07211000
H	2.13063100	-2.20958300	2.87838400	H	3.37764200	-3.40904500	-3.20648200
H	3.08557900	-3.68860400	2.70505100	H	1.73315400	-2.84679300	-3.55787900
H	3.79802700	-2.11259500	2.32188400	H	-0.81781000	-4.16320800	1.04360100
C	4.37794100	-1.77242200	-0.50145700	H	0.49874100	-5.09063700	1.78530900

H	0.11319700	-3.46336500	2.36637000	C	-3.49098500	2.57737200	-2.29413900
C	-0.52269100	-0.66057300	1.01689900	C	-0.74428800	4.28920800	-1.97080300
C	0.57820300	-0.14332500	1.35211900	H	-0.90982300	5.37285400	-1.93405900
C	1.41084500	0.63964100	2.21854100	H	0.32993100	4.11396400	-1.85993500
C	2.81152200	0.66178400	2.10392400	H	-1.03528600	3.93709200	-2.96257400
C	0.79803300	1.39333500	3.24157300	C	0.05680200	4.21495000	1.11117200
C	3.58057800	1.39660700	3.00335700	C	-2.19929800	2.69973700	2.72404700
H	3.27734000	0.11731900	1.29274600	H	-1.25584100	2.28450900	3.08983800
C	1.57337600	2.13000800	4.13147800	H	-2.34988600	3.67044600	3.21149300
H	-0.28511000	1.38911100	3.31359000	H	-2.99701800	2.03046500	3.04858300
C	2.96804400	2.13139500	4.02206300	C	-4.39934800	1.62895300	0.54229400
H	4.66237300	1.40272200	2.90400200	H	-4.52074700	1.39073600	1.60127500
H	1.08910300	2.70867100	4.91303300	H	-5.26930700	2.21990300	0.23183900
H	3.57030200	2.70635700	4.71919000	H	-4.40882400	0.69004000	-0.01800700
N	-1.83757200	-0.97584800	0.98892200	C	4.76628200	-1.43872500	-2.88602300
N	-2.51889100	-0.24719400	1.80531800	C	3.70232800	-0.63510300	-3.30855000
N	-3.81023600	-0.49634100	1.84468200	C	2.37754200	-1.05318100	-3.14232200
C	-4.58044800	0.49804300	2.62820100	C	2.13001800	-2.29393100	-2.53174700
H	-5.62600600	0.20283100	2.52258400	C	3.19043500	-3.09105800	-2.10417600
C	-4.19755400	0.41982600	4.11009000	C	4.51264700	-2.67029300	-2.28189700
H	-3.14228600	0.67434100	4.24006500	H	5.78891900	-1.09946600	-3.02917300
H	-4.36090800	-0.58763400	4.50443500	H	3.90581500	0.32513800	-3.77744200
C	-4.41130800	1.91079900	2.05440500	H	1.10376700	-2.62285700	-2.39739900
H	-3.37057500	2.23347900	2.14227200	H	2.98376600	-4.04737100	-1.63149800
H	-4.68325900	1.94276600	0.99692100	H	5.33603400	-3.29835100	-1.95269400
C	-4.44535100	-1.46294900	0.91715700	C	1.21739600	-0.17548300	-3.59204200
H	-3.68457500	-2.23344600	0.77126000	H	1.60592300	0.75907900	-4.01104500
C	-5.68333100	-2.11872000	1.53302300	H	0.64930500	-0.69458300	-4.37176600
H	-5.47691800	-2.50164500	2.53717700	C	0.27605600	0.11153100	-2.44590500
H	-5.98603500	-2.96051500	0.90278500	C	0.50106400	1.04266500	-1.49006100
H	-6.53695100	-1.43586500	1.58770100	H	1.32096100	1.75109400	-1.57681100
C	-4.72706000	-0.79680700	-0.43476600	C	-0.91254600	-0.77333700	-2.29647300
H	-3.82534300	-0.33354300	-0.83871500	N	-1.72692300	-0.26182600	-1.32741300
H	-5.08488800	-1.54095600	-1.15425000	O	-1.10926100	-1.79347000	-2.96608800
H	-5.49371000	-0.02161100	-0.34228300	C	-2.39133200	-2.34385000	-0.42641000
H	-5.04460100	2.61570100	2.60282200	C	-3.61675400	-3.23937900	-0.23570900
H	-4.79934900	1.12413100	4.69273400	C	-4.80429900	-2.45813200	0.35811200
TS9				H	-5.64782400	-3.13865700	0.51743300
C	-1.13643700	3.53912900	0.50296700	H	-4.53756400	-2.01576600	1.32288700
C	-1.52118400	3.59560900	-0.89232500	H	-5.13143900	-1.65840400	-0.31014200
C	-2.71968700	2.85059500	-1.03861700	C	-3.22290800	-4.39487300	0.69784300
C	-3.12823300	2.38451900	0.28601000	H	-4.06664100	-5.08373800	0.81204400
C	-2.17821900	2.86202300	1.23296700	H	-2.36921000	-4.94364800	0.29467700
Rh	-1.15844400	1.43298900	-0.26264000	H	-2.94041600	-4.01856900	1.68575100

C	-3.98172000	-3.77624200	-1.63921100	H	5.67127800	2.16736200	-0.82921100
H	-4.83676300	-4.45749400	-1.56489800	H	6.10614700	0.57115800	-0.19574800
H	-4.23917700	-2.95556600	-2.31380100	H	5.33460400	-2.70375200	1.76141000
H	-3.13862200	-4.31704200	-2.07826900	H	4.81707800	-1.70997500	4.09009700
O	-1.24968900	-2.66825500	-0.22411200	10			
O	-2.77585800	-1.11316700	-0.92190900	C	2.20128300	0.23135200	-3.13847600
H	-3.77125600	1.52170700	-2.34450700	C	3.27061800	0.68388700	-2.24977200
H	-4.40725100	3.17943100	-2.33053100	C	3.59152300	-0.37702700	-1.38671800
H	-2.90006900	2.80410500	-3.18386900	C	2.73085000	-1.51425100	-1.72010500
H	0.90260200	4.22286200	0.41867600	C	1.96057800	-1.15298700	-2.88260800
H	-0.17051900	5.25586200	1.37548900	Rh	1.33044100	0.01405900	-1.07327000
H	0.37813900	3.69919100	2.01935900	C	4.60110100	-0.38538600	-0.27912500
C	0.73847700	0.51725300	0.35513900	C	3.90373700	2.04166500	-2.28575400
C	-0.28817800	0.02663100	0.97954800	H	4.74178200	2.06250200	-2.99388000
C	-0.74459500	-0.81788600	2.03977300	H	3.19289500	2.80713200	-2.60685000
C	-2.08300300	-0.79348500	2.47717900	H	4.28540100	2.33651700	-1.30545000
C	0.15109900	-1.72309200	2.65055000	C	1.61996300	1.03304900	-4.26523500
C	-2.50883100	-1.62916500	3.50577800	C	1.09694800	-2.06878400	-3.69134300
H	-2.78198700	-0.13298600	1.97921100	H	0.25625900	-1.53497400	-4.14076700
C	-0.28267300	-2.55414000	3.67806200	H	1.68506400	-2.51578600	-4.50279400
H	1.17281500	-1.76100500	2.29101300	H	0.68688700	-2.87774100	-3.08534600
C	-1.61154800	-2.51257500	4.11384700	C	2.81845500	-2.86934800	-1.08658000
H	-3.54645600	-1.60029800	3.82739600	H	1.87427400	-3.40982900	-1.18200200
H	0.41667400	-3.24807700	4.13635400	H	3.61302300	-3.47203700	-1.54509800
H	-1.94637500	-3.16868500	4.91191100	H	3.03344500	-2.77634400	-0.01926100
N	2.05274500	0.91028300	0.53175900	C	-1.04804100	6.39143100	-0.40201600
N	2.69640100	0.09438600	1.27252500	C	-0.19901200	5.34455200	-0.76911700
N	3.94514400	0.42961400	1.56353000	C	0.34085600	4.48875100	0.19783800
C	4.71701200	-0.66866300	2.18619900	C	0.01332000	4.69239300	1.54638500
H	5.74846800	-0.30945700	2.22712700	C	-0.83422900	5.73756600	1.91186500
C	4.22840500	-0.91690200	3.61814500	C	-1.36747800	6.59074300	0.94129600
H	3.17828000	-1.22191400	3.61194000	H	-1.45659300	7.04879800	-1.16476100
H	4.31752800	-0.00977100	4.22342100	H	0.04985800	5.19526200	-1.81772000
C	4.68325500	-1.93871200	1.32625600	H	0.41933500	4.01293000	2.28991900
H	3.66753800	-2.33736000	1.26748700	H	-1.08146300	5.88569300	2.95958800
H	5.01536200	-1.73328500	0.30572900	H	-2.02768000	7.40366500	1.23067900
C	4.59548400	1.61931700	0.97710400	C	1.24699500	3.33949900	-0.21254100
H	3.77177900	2.30642300	0.77242200	H	1.48257600	3.43087800	-1.27672600
C	5.54418600	2.29109300	1.97417000	H	2.18762100	3.38384600	0.34352800
H	5.04078900	2.48737600	2.92547600	C	0.58996200	1.98576700	0.03077600
H	5.88256700	3.24644700	1.56085100	C	-0.41954700	1.57152500	-0.82313000
H	6.43771500	1.69066800	2.17299600	H	-0.64335600	2.24893600	-1.64963100
C	5.27274200	1.26486900	-0.35302300	C	1.04958500	1.29024900	1.30908400
H	4.56042400	0.79413300	-1.03437300	N	1.17525400	-0.02517200	1.01092900

O	1.36497700	1.88725000	2.33544500	C	-4.62216800	-2.59121300	0.89030000
C	1.47546900	-1.27674200	2.97842700	H	-3.63865200	-2.83572100	0.48143900
C	2.55245900	-1.85009700	3.90650700	H	-4.48379300	-2.18261400	1.89501200
C	3.39922500	-2.88537500	3.13579600	C	-5.10048600	0.90712900	0.66243900
H	4.13448800	-3.33682500	3.81044000	H	-4.50831400	1.72361300	0.24214700
H	2.77237000	-3.68891600	2.73349900	C	-6.58075400	1.19770100	0.40355900
H	3.93848300	-2.42250200	2.30573200	H	-6.80121800	1.19969900	-0.66816500
C	1.85302800	-2.52132800	5.09752200	H	-6.82869400	2.18438300	0.80718700
H	2.60110200	-2.93135800	5.78386700	H	-7.24161000	0.47392300	0.89203500
H	1.23336800	-1.80366500	5.64063800	C	-4.76783100	0.79797700	2.15699000
H	1.20082200	-3.33360400	4.76471000	H	-3.70186700	0.60084700	2.29469200
C	3.44610000	-0.68759100	4.39208300	H	-5.01452700	1.73344300	2.67024800
H	4.20007900	-1.06748400	5.09022000	H	-5.34078400	-0.00781100	2.62878800
H	3.95267200	-0.20451000	3.55357000	H	-5.20507900	-3.51492700	0.97031500
H	2.85106500	0.07409600	4.90445100	H	-6.12198800	-3.07568700	-1.39855400
O	0.28472700	-1.30987800	3.16697300	8'			
O	2.06862700	-0.70929200	1.88252000	C	-1.70252200	-3.48430100	0.40786300
H	4.13634600	-0.69312000	0.66070800	C	-1.54395800	-3.45685400	-1.01472800
H	5.41280400	-1.08784300	-0.50408900	C	-0.14090300	-3.34627300	-1.29774400
H	5.04162700	0.60237600	-0.12807300	C	0.58233100	-3.42050900	-0.03601900
H	1.53715000	2.09073300	-4.00137700	C	-0.37645400	-3.49344100	1.00269700
H	2.25091700	0.96528800	-5.16086400	Rh	-0.72713200	-1.52102200	-0.17552000
H	0.62178400	0.67699600	-4.53025100	C	0.49779000	-3.29727700	-2.65301500
C	-1.29874500	0.37306200	-0.68871600	C	-2.65457800	-3.53502800	-2.01720600
C	-0.57690200	-0.74161200	-0.87088800	H	-2.83222200	-4.57588100	-2.31524500
C	-0.92412500	-2.15754800	-0.81964900	H	-3.58555700	-3.14206000	-1.60096800
C	-1.67588300	-2.75724800	-1.84784700	H	-2.42185800	-2.95737700	-2.91432200
C	-0.50369100	-2.95784600	0.25827400	C	-3.00352600	-3.67709800	1.13157700
C	-1.99372600	-4.11384600	-1.80250500	C	-0.10927200	-3.53700500	2.47649700
H	-2.02088600	-2.14046500	-2.67124500	H	-0.77922900	-2.85609200	3.00960500
C	-0.83391300	-4.31218400	0.30618100	H	-0.26599400	-4.54698500	2.87407700
H	0.04251600	-2.49275200	1.06823400	H	0.91271200	-3.22985200	2.70410400
C	-1.57328400	-4.89865900	-0.72459100	C	2.07444200	-3.41370200	0.09902100
H	-2.57847700	-4.55707400	-2.60407200	H	2.37838300	-3.18378300	1.12226800
H	-0.51837000	-4.90959900	1.15734300	H	2.50127100	-4.38721600	-0.17351300
H	-1.82663700	-5.95425900	-0.68540400	H	2.51100900	-2.65541800	-0.55197100
N	-2.63499100	0.60888200	-0.32376000	C	-3.93800800	4.47961600	-0.95022700
N	-3.38168800	-0.40731900	-0.48382900	C	-3.80800000	3.31637500	-1.71452100
N	-4.64092200	-0.28861200	-0.07574500	C	-2.54614400	2.82993700	-2.07519100
C	-5.34612100	-1.58762200	-0.02104000	C	-1.40723000	3.54035000	-1.65969000
H	-6.32806900	-1.36993000	0.40613400	C	-1.53615300	4.69372600	-0.88643900
C	-5.54130400	-2.14807800	-1.43483400	C	-2.80104900	5.16780300	-0.52532800
H	-4.56909200	-2.36707000	-1.88387700	H	-4.92745800	4.84295800	-0.68389600
H	-6.06782200	-1.43002100	-2.07075400	H	-4.69733400	2.77276900	-2.02432000

H	-0.42283600	3.17819900	-1.94073600	H	-5.01345100	2.67401000	1.01387900
H	-0.64410600	5.22412100	-0.56408800	H	-5.56505500	-0.78170100	3.52758200
H	-2.89840000	6.06604600	0.07796800	H	-6.47207700	1.29229700	2.49711200
C	-2.40192500	1.52802200	-2.84641300	N	1.07653500	-0.13469500	2.00675100
H	-3.39232700	1.12923200	-3.08802200	N	1.46006200	1.09862500	2.04394600
H	-1.86753700	1.71157400	-3.78599400	N	2.66075500	1.30321000	2.51555900
C	-1.60605900	0.51142200	-2.05561800	C	3.12283500	2.71531200	2.52212800
C	-2.08245700	-0.40194600	-1.20455400	H	3.48678300	2.90742000	3.53858200
H	-3.14591800	-0.53399800	-1.00386500	C	4.27281300	2.93729500	1.52849800
C	-0.11966900	0.54713500	-2.20360100	H	3.92263100	2.74292900	0.51393200
N	0.45964900	-0.15425200	-1.18301000	H	5.13247100	2.29506500	1.73467500
O	0.47869200	1.13559200	-3.11118200	C	1.97122000	3.67977700	2.22919600
C	2.68640600	0.58674100	-1.39746900	H	1.59391800	3.53461500	1.21496500
C	3.95412300	0.30666900	-2.21878500	H	1.14087300	3.54573700	2.92596900
C	4.45786100	-1.13753400	-2.03437800	C	3.50401100	0.16877300	2.96549000
H	5.37479600	-1.27987800	-2.61634400	H	2.79160300	-0.53069500	3.41452200
H	4.68842300	-1.35451500	-0.98651000	C	4.14829700	-0.53914500	1.76449900
H	3.72153300	-1.86435800	-2.38366900	H	3.38689100	-0.79180500	1.02526700
C	5.04743000	1.30297700	-1.80653200	H	4.63068500	-1.46525000	2.09525600
H	5.92622500	1.17400400	-2.44681200	H	4.90495900	0.09003100	1.29040000
H	4.69168800	2.33105100	-1.90230300	C	4.51533000	0.57329000	4.03890600
H	5.35820700	1.15006500	-0.76869400	H	4.02573900	1.04519600	4.89581600
C	3.56754800	0.53491200	-3.70014900	H	5.01825000	-0.33004700	4.39717000
H	4.44561200	0.36842800	-4.33476800	H	5.28642400	1.24982300	3.66154900
H	2.76729600	-0.14301300	-4.00173200	H	2.35016200	4.70195500	2.32753500
H	3.20186200	1.55255000	-3.85510300	H	4.61300700	3.97542800	1.59981500
O	2.45430400	1.61212800	-0.80117100	TS9'			
O	1.82437800	-0.47037000	-1.48350000	C	0.66226900	3.63575600	1.23458700
H	1.34754900	-2.61147300	-2.65234400	C	0.61732400	4.03980600	-0.15478400
H	0.85314700	-4.29162500	-2.95137400	C	-0.68360600	3.74290500	-0.64441500
H	-0.20806900	-2.94838800	-3.40978700	C	-1.47995100	3.21203000	0.45807600
H	-3.73315600	-2.90503500	0.86949200	C	-0.65536800	3.19589700	1.62075800
H	-3.44251900	-4.65224100	0.88811800	Rh	0.18050400	1.78788100	0.03670800
H	-2.86275700	-3.64133300	2.21364500	C	-1.20533000	3.94424500	-2.03522900
C	-0.20271000	-0.23578000	1.58738400	C	1.76172300	4.62348200	-0.92789000
C	-1.44706300	-0.18888800	1.50632400	H	1.86335800	5.69864100	-0.73348700
C	-2.80436800	0.20263200	1.78245200	H	2.70807800	4.14721700	-0.65609200
C	-3.32114100	1.37940100	1.20747100	H	1.62377900	4.48860600	-2.00294000
C	-3.62769200	-0.57214200	2.61895500	C	1.84878300	3.79241700	2.13890500
C	-4.63426300	1.76437800	1.46829300	C	-1.08395900	2.73643800	2.98322800
H	-2.69160600	1.97594900	0.55809200	H	-0.22645300	2.60165700	3.64648700
C	-4.93998400	-0.17855800	2.87495300	H	-1.75142300	3.47131300	3.44879100
H	-3.22577200	-1.47157900	3.07225500	H	-1.61197600	1.78057500	2.91948500
C	-5.44829700	0.98845800	2.29794500	C	-2.92670800	2.82671200	0.37494200

H	-3.19991100	2.16517900	1.20026100	H	1.83532300	3.06058700	2.94915800
H	-3.57911400	3.70875800	0.41063600	C	-0.05128000	0.01614200	1.03914300
H	-3.12666700	2.29010300	-0.55528900	C	1.23687700	-0.01890500	0.91922700
C	5.47379500	-2.66823500	-1.53096400	C	2.40219600	-0.34794600	1.73598700
C	4.93441600	-1.46486800	-1.99582400	C	3.44867200	-1.12916000	1.22071000
C	3.59668000	-1.38902000	-2.39921600	C	2.46301100	0.08611300	3.07276700
C	2.80322500	-2.54657900	-2.34271500	C	4.53333100	-1.46899600	2.02756500
C	3.33973300	-3.74466200	-1.87364900	H	3.39637400	-1.47842500	0.19796900
C	4.67499600	-3.81025700	-1.46140600	C	3.55155400	-0.25267500	3.87425900
H	6.51436700	-2.70917000	-1.21956600	H	1.64450300	0.67910800	3.47007000
H	5.55483600	-0.57246500	-2.02992300	C	4.59113500	-1.02869800	3.35201900
H	1.76433600	-2.48355200	-2.65498700	H	5.32938300	-2.08014900	1.61257800
H	2.71247800	-4.63053900	-1.82443900	H	3.58942200	0.08648500	4.90580400
H	5.08823000	-4.74470400	-1.09205000	H	5.43963300	-1.29115900	3.97776500
C	2.97704500	-0.06710400	-2.81992700	N	-1.18612600	-0.46922300	1.59761000
H	3.74344100	0.71547600	-2.81884500	N	-1.19402500	-1.75296400	1.67203800
H	2.57619200	-0.15495200	-3.83542000	N	-2.26022200	-2.28247300	2.23678000
C	1.83369900	0.32040900	-1.90575200	C	-2.35061100	-3.75528800	2.09161700
C	1.97172600	0.90305900	-0.69097300	H	-2.93128100	-4.10622000	2.94891500
H	2.94982800	1.20775100	-0.32434400	C	-3.07754600	-4.13676600	0.79317000
C	0.45271400	-0.00432800	-2.36819900	H	-2.58079200	-3.66783700	-0.06019600
N	-0.43659500	0.64029500	-1.56898400	H	-4.12105800	-3.80940800	0.80634300
O	0.18719400	-0.72708700	-3.33903000	C	-0.96386000	-4.40211800	2.16803400
C	-2.29286700	-0.79758300	-1.83908500	H	-0.36209800	-4.15231900	1.29296800
C	-3.57705900	-0.91151300	-2.66613100	H	-0.42389000	-4.07084800	3.05933500
C	-4.54622800	0.24197600	-2.33712700	C	-3.39704500	-1.43474500	2.66845100
H	-5.46355400	0.13075300	-2.92524900	H	-2.92420000	-0.57899300	3.16077400
H	-4.82321600	0.24060700	-1.27754100	C	-4.20063100	-0.89861000	1.47149800
H	-4.10272000	1.21137400	-2.57573400	H	-3.53574800	-0.44983400	0.73352700
C	-4.23826000	-2.26401200	-2.36595300	H	-4.90574200	-0.13374600	1.81528200
H	-5.13328700	-2.38420800	-2.98509700	H	-4.77377900	-1.69631200	0.99226400
H	-3.55228400	-3.08786900	-2.57599900	C	-4.29006500	-2.14458800	3.68636200
H	-4.53228600	-2.33628700	-1.31536300	H	-3.71291600	-2.53124400	4.53165500
C	-3.15542300	-0.84164300	-4.15267100	H	-5.01891300	-1.42675400	4.07493000
H	-4.03461500	-0.98269700	-4.79140300	H	-4.85204800	-2.96971200	3.23739300
H	-2.69847900	0.12361900	-4.38058500	H	-1.08517700	-5.48888500	2.21536900
H	-2.41800000	-1.61441200	-4.38410400	H	-3.07147800	-5.22422900	0.66490100
O	-1.77150000	-1.68733400	-1.21307000	10'			
O	-1.78881200	0.47485100	-1.94451900	C	1.11252800	-2.30290900	-2.77588300
H	-1.77200500	3.06806100	-2.36009700	C	1.30708400	-3.37928900	-1.79909100
H	-1.86670600	4.81840200	-2.07712000	C	0.07236900	-3.62890100	-1.18607800
H	-0.39352900	4.09723000	-2.74912800	C	-0.91644000	-2.70852000	-1.76011500
H	2.78249900	3.64938800	1.58859300	C	-0.27420700	-1.98607200	-2.83185400
H	1.87570500	4.79399700	2.58637600	Rh	0.47829400	-1.36377600	-0.81584000

C	-0.23461200	-4.58241500	-0.07129500	C	-2.16657000	-2.01091100	4.57421400
C	2.61913800	-4.05399300	-1.53700500	H	-2.87400500	-2.49052600	5.25933400
H	2.87551700	-4.74410900	-2.35083600	H	-1.36921200	-2.71895500	4.33812800
H	3.43566000	-3.32852500	-1.46447500	H	-1.71630800	-1.15561500	5.08734900
H	2.60235700	-4.62500500	-0.60623400	O	-1.93929200	0.28241100	2.00579000
C	2.18413500	-1.77924100	-3.68629800	O	-0.91233600	-1.75161900	2.02158200
C	-0.96077400	-1.06341100	-3.79213100	H	-0.70210100	-4.05187000	0.76389200
H	-0.24668100	-0.41111000	-4.29970100	H	-0.92794400	-5.36262800	-0.40743100
H	-1.49454900	-1.64031000	-4.55761600	H	0.66732800	-5.06905400	0.30534200
H	-1.67996400	-0.42943600	-3.26792500	H	3.14728300	-1.71838600	-3.17218900
C	-2.38427700	-2.70139600	-1.45598500	H	2.31581000	-2.43796600	-4.55433100
H	-2.78000000	-1.68880500	-1.55737000	H	1.93998000	-0.78056900	-4.05488700
H	-2.93690900	-3.36801600	-2.13104800	C	-0.28694100	0.51263200	-0.86434500
H	-2.57079000	-3.02860500	-0.43031400	C	0.78831300	1.31154600	-0.67153900
C	6.62929100	1.15135300	0.66049400	C	1.00424100	2.76344800	-0.76940700
C	5.69312600	0.15416000	0.37206000	C	2.07394300	3.34316600	-0.06169300
C	4.56723900	-0.02317800	1.18223100	C	0.22783100	3.59517500	-1.59876700
C	4.38534200	0.81707600	2.29214500	C	2.34490900	4.70810400	-0.16421400
C	5.31825900	1.81358300	2.57685600	H	2.68795500	2.72217600	0.58556300
C	6.44277200	1.98497100	1.76296800	C	0.50037400	4.95628500	-1.69850700
H	7.49874700	1.27729200	0.02104000	H	-0.59212000	3.16533000	-2.16265700
H	5.84075700	-0.49101200	-0.49137700	C	1.55938000	5.52290500	-0.97994400
H	3.50023700	0.68377600	2.90956200	H	3.17127200	5.13289700	0.39922500
H	5.16650700	2.46014200	3.43687500	H	-0.11253700	5.57924900	-2.34478500
H	7.16598800	2.76416700	1.98681300	H	1.76808500	6.58601900	-1.05920100
C	3.52205800	-1.07556900	0.84828400	N	-1.63415200	0.72663600	-1.07997400
H	3.81827400	-1.61477000	-0.05700900	N	-2.06633500	1.80504500	-0.54473100
H	3.45184600	-1.80950100	1.65722000	N	-3.35013600	2.07096600	-0.70420300
C	2.15648400	-0.43466500	0.63800500	C	-3.81801100	3.21903700	0.10860200
C	1.97088900	0.43451600	-0.41983900	H	-4.90365400	3.23908200	-0.01572600
H	2.83304500	0.57235900	-1.07702300	C	-3.49791400	3.02954900	1.59638200
C	1.16276300	-0.64423200	1.78624100	H	-2.41791700	2.99847400	1.75077200
N	0.11580300	-1.23941200	1.20400100	H	-3.90286300	2.08826200	1.97250000
O	1.40882500	-0.39234800	2.96376200	C	-3.23458400	4.52462100	-0.44449000
C	-1.89475800	-0.86487500	2.37309200	H	-2.14430200	4.51063200	-0.36648400
C	-2.90496000	-1.55956000	3.29475400	H	-3.50304500	4.65841800	-1.49746600
C	-3.50261400	-2.78369000	2.56808400	C	-4.27904000	1.10012300	-1.31741900
H	-4.24611000	-3.26812800	3.21002800	H	-3.66607000	0.55240800	-2.03588900
H	-4.00211600	-2.48659500	1.63946100	C	-4.78411800	0.11142000	-0.25719400
H	-2.72903500	-3.51607800	2.32435200	H	-3.93648700	-0.33117400	0.26967600
C	-4.01482800	-0.55805900	3.64486800	H	-5.37349800	-0.68624500	-0.72253000
H	-4.72686400	-1.02023200	4.33645200	H	-5.41867900	0.62053800	0.47626800
H	-3.60022000	0.33723100	4.11463000	C	-5.41159300	1.78725300	-2.08391500
H	-4.55798200	-0.24299500	2.74971900	H	-5.01976600	2.53247200	-2.78253300

H	-5.96371400	1.03626000	-2.65799800	O	-0.13328000	2.83424300	2.23162600
H	-6.12948800	2.27929300	-1.42012200	C	2.74055800	0.37250900	1.90932600
H	-3.61498500	5.38067100	0.12213500	C	3.38544600	0.01082600	3.24133400
H	-3.92117800	3.85856100	2.17328300	C	4.20468400	1.20907300	3.76232000
II							
C	1.56512100	-0.26743100	-2.90663000	H	4.65103400	0.95188800	4.72813400
C	1.22934400	1.13041100	-2.78142000	H	5.01583300	1.46335800	3.07143700
C	2.45195500	1.85946500	-2.43796900	H	3.57313100	2.09058700	3.89359300
C	3.47475500	0.92481500	-2.23579000	C	4.27743500	-1.22522800	3.05250700
C	2.91155100	-0.40947100	-2.47251000	H	4.72013800	-1.50319100	4.01408500
Rh	1.70977400	0.41325900	-0.77359100	H	3.69975800	-2.07199100	2.67341500
C	2.50286500	3.34485800	-2.25620000	H	5.08830500	-1.02505200	2.34549700
C	-0.02945400	1.75757000	-3.29356200	C	2.22571900	-0.30803400	4.21674200
H	0.06303800	1.97038300	-4.36713400	H	2.63938900	-0.58224700	5.19269500
H	-0.88324800	1.09297400	-3.15061900	H	1.57145600	0.55890300	4.33846200
H	-0.24653900	2.69355400	-2.77747200	H	1.62671600	-1.14589900	3.84632100
C	0.62317200	-1.33232200	-3.38558900	O	2.83046000	-0.34933000	0.90161100
C	3.73208500	-1.66277400	-2.40058300	O	2.04906600	1.48502800	1.94698100
H	3.14271400	-2.55109200	-2.63478600	H	3.47975400	3.67700100	-1.89941900
H	4.56164000	-1.61257900	-3.11604300	H	2.28956000	3.85886800	-3.20053400
H	4.16131200	-1.79453600	-1.40233400	H	1.75378900	3.66345700	-1.52387600
C	4.89055000	1.16365700	-1.80521300	H	-0.28945700	-1.34865600	-2.78083100
H	5.14981300	0.52841300	-0.95154700	H	0.34273100	-1.14955100	-4.42955700
H	5.59506900	0.93017900	-2.61330000	H	1.07510600	-2.32506400	-3.32942600
H	5.05178400	2.20249300	-1.50925200	C	-1.19047800	-0.04922300	-0.25705900
C	-5.27231000	4.47461500	-0.25319800	C	0.05307800	-0.59236100	-0.14928100
C	-3.94248900	4.34970800	-0.66769300	C	0.30652300	-1.88477000	0.51840400
C	-2.94119400	4.00138600	0.24316300	C	1.17032600	-2.86079800	-0.00743300
C	-3.28872700	3.77263800	1.58339400	C	-0.24212500	-2.12175000	1.79722400
C	-4.61288400	3.89906900	1.99707000	C	1.46288100	-4.02781900	0.69712700
C	-5.61035100	4.25088200	1.08087100	H	1.61464700	-2.69359600	-0.98020900
H	-6.03980200	4.74531000	-0.97350800	C	0.05025800	-3.28668200	2.50415600
H	-3.68242500	4.52614300	-1.70914400	H	-0.90363900	-1.37503800	2.22531500
H	-2.50466400	3.48548600	2.27945600	C	0.90634300	-4.24944100	1.95881400
H	-4.87071300	3.72108100	3.03778000	H	2.12840800	-4.76698400	0.25879400
H	-6.64256400	4.34680500	1.40652800	H	-0.38505300	-3.44008000	3.48839400
C	-1.49374600	3.85407600	-0.19136000	H	1.13776700	-5.15550900	2.51122900
H	-1.40286400	4.11645000	-1.25306200	N	-2.37352300	-0.82446500	-0.05301400
H	-0.87837500	4.56650100	0.36731900	N	-2.35626900	-1.91504100	-0.69702100
C	-0.93723400	2.45440700	0.03841100	N	-3.37874700	-2.74456300	-0.49294800
C	-1.52558800	1.36542800	-0.49356500	C	-3.21102400	-4.05933900	-1.14091500
H	-2.43923400	1.52788200	-1.06677900	H	-4.07769600	-4.64890800	-0.82733500
C	0.10083200	2.35237300	1.12041500	C	-3.25075200	-3.91353300	-2.66667700
N	1.26003400	1.75307600	0.73164400	H	-2.41639400	-3.29115200	-3.00241400
				H	-4.18358400	-3.44128700	-2.98903400

C	-1.93683600	-4.77120800	-0.66509200	H	-1.91422400	4.05024100	2.01358600
H	-1.05092000	-4.21188100	-0.97261000	H	-4.04448800	4.82496000	3.02985500
H	-1.91080100	-4.85116200	0.42459700	H	-5.93815200	5.52841500	1.57738100
C	-4.37417400	-2.52260500	0.57461300	C	-1.27397400	3.87808300	-0.62062300
H	-4.26686000	-1.46547100	0.82418700	H	-1.33558600	3.91504900	-1.71455600
C	-5.79876600	-2.76198700	0.06491200	H	-0.46314600	4.55343100	-0.32752400
H	-6.00035400	-2.15687800	-0.82364000	C	-0.92477800	2.47578900	-0.16518500
H	-6.51912600	-2.48416300	0.84114200	C	-1.67910500	1.37159700	-0.44811900
H	-5.97850700	-3.81334500	-0.18554500	H	-2.67355200	1.54828800	-0.85753400
C	-4.04064900	-3.35566400	1.82062500	C	0.20724800	2.36264500	0.87554800
H	-3.01759900	-3.15497600	2.15033500	N	1.05405000	2.03364200	-0.07669900
H	-4.72670400	-3.10731800	2.63730700	O	0.16214300	2.65570300	2.05502700
H	-4.13368600	-4.42901400	1.62009500	C	3.12052200	0.79613000	1.52270000
H	-1.88286200	-5.77904400	-1.09078600	C	3.72491400	0.38440200	2.88490400
H	-3.16967400	-4.89326300	-3.14880600	C	4.69088300	1.46954200	3.38045300
TS12				H	5.06160900	1.21501400	4.37980200
C	1.38253600	-1.05638200	-2.68173200	H	5.55317900	1.56435200	2.71146400
C	0.99153500	0.30303300	-2.98007800	H	4.19180000	2.43963000	3.42199800
C	2.18052600	1.14187300	-2.89406000	C	4.43283500	-0.97612100	2.78983600
C	3.24123700	0.34737400	-2.41876700	H	4.83044500	-1.25935900	3.77121800
C	2.74220600	-1.01852200	-2.26390700	H	3.74136100	-1.75201400	2.45427600
Rh	1.52771900	0.26887800	-0.84968100	H	5.27180300	-0.93635500	2.08549400
C	2.18588000	2.61750300	-3.14909100	C	2.50432200	0.28082700	3.83142300
C	-0.34085400	0.72877700	-3.51580900	H	2.83875300	0.04566600	4.84864400
H	-0.38442600	0.61634900	-4.60701300	H	1.95029200	1.22410500	3.84869600
H	-1.14468900	0.12971200	-3.08048400	H	1.82362400	-0.50857400	3.49817400
H	-0.54099300	1.77622000	-3.27650100	O	2.68220700	-0.19753700	0.81804800
C	0.48170600	-2.24968500	-2.80285300	O	3.00641900	1.99598500	1.22891800
C	3.61304800	-2.15230400	-1.81303300	H	3.19744900	3.02600900	-3.11497400
H	3.08977700	-3.11033400	-1.84697800	H	1.75727300	2.84210700	-4.13165600
H	4.49806000	-2.23076900	-2.45458000	H	1.59126900	3.13405400	-2.38734000
H	3.95547400	-1.98106300	-0.78636700	H	-0.45144000	-2.09978400	-2.25067000
C	4.64268600	0.76176100	-2.08754200	H	0.23142200	-2.43048900	-3.85524800
H	4.93636900	0.35780400	-1.11401300	H	0.95437800	-3.15322000	-2.41205800
H	5.35461500	0.38678200	-2.83374800	C	-1.37019300	0.00442500	-0.12616800
H	4.73915200	1.84751400	-2.03518100	C	-0.10371800	-0.52347800	0.08732800
C	-4.86039900	5.16354800	-0.25373400	C	0.09742900	-1.66716200	0.98515500
C	-3.65619300	4.73772200	-0.82171400	C	1.06446500	-2.66228400	0.75245300
C	-2.58547300	4.34806600	-0.01138900	C	-0.62452400	-1.72911200	2.19943600
C	-2.73713700	4.37895000	1.38339200	C	1.27345900	-3.69563300	1.66151200
C	-3.93780200	4.80401700	1.94881900	H	1.65445600	-2.61375700	-0.15037100
C	-5.00312700	5.19888600	1.13310000	C	-0.40270100	-2.75054600	3.11811900
H	-5.68351300	5.46487000	-0.89587800	H	-1.35631500	-0.95735100	2.41320100
H	-3.54795900	4.71194800	-1.90363900	C	0.54193600	-3.74723800	2.85034100

H	2.01921800	-4.45617900	1.44746900	H	4.84209100	-0.28819400	-1.37754900
H	-0.96094800	-2.76469100	4.05012700	H	5.24495900	0.98687500	-2.53891000
H	0.71549800	-4.54449500	3.56721200	H	4.83173900	1.38597100	-0.84990100
N	-2.54585400	-0.79385400	0.02598000	C	-3.97659000	5.17185900	-0.42344600
N	-2.40602100	-1.94863000	-0.48444400	C	-2.65022200	4.76755300	-0.26770300
N	-3.39093600	-2.81344700	-0.28588600	C	-2.18997000	4.28280800	0.96266800
C	-3.11251400	-4.17017400	-0.79839500	C	-3.08622800	4.20721100	2.03583700
H	-3.93555200	-4.79003500	-0.43136800	C	-4.41359200	4.60982500	1.88420400
C	-3.14179100	-4.18649600	-2.33113400	C	-4.86228700	5.09353500	0.65333400
H	-2.35188000	-3.54383500	-2.72980500	H	-4.31745300	5.54878400	-1.38353900
H	-4.10298000	-3.82376100	-2.70729300	H	-1.96352000	4.82774100	-1.10832800
C	-1.79813700	-4.72731900	-0.23579900	H	-2.74069100	3.82447300	2.99278100
H	-0.94889200	-4.14341300	-0.59562000	H	-5.09628200	4.54688900	2.72672600
H	-1.78688200	-4.68390900	0.85650900	H	-5.89477300	5.40904400	0.53465900
C	-4.51195900	-2.54829300	0.64036000	C	-0.76418700	3.80947400	1.11725200
H	-4.47808600	-1.46996600	0.80345500	H	-0.10967800	4.38700800	0.44741300
C	-5.85663600	-2.90440100	-0.00152100	H	-0.41076900	4.03135700	2.13503900
H	-5.98498400	-2.37889900	-0.95220800	C	-0.55452500	2.33400200	0.83664800
H	-6.67253000	-2.61101200	0.66670400	C	-1.52061100	1.46128100	0.50087200
H	-5.95592100	-3.97957500	-0.18613000	H	-2.53206700	1.85079200	0.47250000
C	-4.28212100	-3.25510000	1.98333700	C	1.68484300	2.55543200	1.49879300
H	-3.31569200	-2.96615000	2.40519800	N	0.80917600	1.88324100	0.92477600
H	-5.07005000	-2.98248400	2.69302100	O	2.43209400	3.27386300	2.03344600
H	-4.29635300	-4.34484200	1.87057300	C	3.41180300	-0.29953300	1.38419300
H	-1.66639100	-5.76871700	-0.54726900	C	4.21264800	-1.32067800	2.22466400
H	-2.98125000	-5.20241000	-2.70636800	C	5.37284300	-0.61828500	2.94062700
13				H	5.93670400	-1.33839100	3.54479700
C	1.00313600	0.21731800	-2.80153000	H	6.05529500	-0.15660600	2.22114300
C	0.97899200	1.59241500	-2.41391200	H	5.00364400	0.17621500	3.59430600
C	2.33971700	1.97386900	-2.01569900	C	4.74581200	-2.41607100	1.27860300
C	3.15062500	0.83244700	-2.06452000	H	5.31497300	-3.16354100	1.84309700
C	2.31579300	-0.29103000	-2.49269100	H	3.91909400	-2.91567000	0.76747200
Rh	1.41597300	0.39465900	-0.60992500	H	5.41490200	-1.98908000	0.52142300
C	2.76719300	3.33455000	-1.55661800	C	3.24646100	-1.95330400	3.24805200
C	-0.18583500	2.51718900	-2.60291800	H	3.77081900	-2.70437600	3.85067100
H	-0.24376600	2.87196100	-3.64027200	H	2.84884300	-1.19293900	3.93002800
H	-1.12455900	2.01468000	-2.35763400	H	2.40512000	-2.43101200	2.73960300
H	-0.10681200	3.39365300	-1.95594700	O	2.45163500	-0.84149200	0.71002500
C	-0.15978200	-0.52104700	-3.39750800	O	3.69125500	0.91077300	1.38453000
C	2.87351200	-1.65712200	-2.76398800	H	3.48468700	3.26099800	-0.73503100
H	2.15553800	-2.29901100	-3.27777700	H	3.24090800	3.89287400	-2.37295500
H	3.76437900	-1.57862800	-3.39711000	H	1.91508500	3.92478100	-1.20936900
H	3.16282700	-2.14939200	-1.83048100	H	-0.99340600	-0.58382900	-2.68988000
C	4.59828400	0.73006000	-1.69028400	H	-0.51183000	-0.00390400	-4.29709100

H	0.11241500	-1.53942900	-3.68239100	C	2.51826400	1.93316800	-2.37426700
C	-1.39214300	0.02182800	0.27812000	C	0.59455700	-0.17795300	-3.85026200
C	-0.24082200	-0.64473200	-0.01414400	H	0.95274100	0.02790100	-4.86659300
C	-0.08753300	-2.09324500	0.21752800	H	-0.12251100	-1.00013100	-3.90064900
C	0.44641700	-2.97182500	-0.73610700	H	0.05737300	0.70136500	-3.48834400
C	-0.39173700	-2.61924000	1.48967700	C	1.68133900	-3.12516200	-3.09184900
C	0.65727100	-4.31919600	-0.44730900	C	4.13399600	-2.80848700	-1.15257200
H	0.68788700	-2.58821300	-1.71610500	H	3.46588300	-3.49703800	-0.62271100
C	-0.18025500	-3.96446800	1.78381300	H	4.62996800	-3.37851000	-1.94767300
H	-0.79218200	-1.95211300	2.24631500	H	4.89831600	-2.47093500	-0.45007600
C	0.34650800	-4.82570700	0.81599800	C	4.80382900	0.34141500	-0.85382100
H	1.06488800	-4.97521200	-1.21223400	H	5.17296400	-0.30444400	-0.05218300
H	-0.41720300	-4.34030700	2.77580400	H	5.63630900	0.51990600	-1.54700200
H	0.51716100	-5.87329700	1.04656400	H	4.52121200	1.29580800	-0.40883100
N	-2.63234100	-0.64864400	0.52926300	C	-4.22709200	5.04065900	-1.86632100
N	-2.91003400	-1.50817600	-0.35710200	C	-2.98362900	4.45637000	-2.12730600
N	-4.01219800	-2.23351400	-0.15829300	C	-2.12613700	4.10163800	-1.08113600
C	-4.16840100	-3.34400900	-1.11850100	C	-2.53406200	4.33793600	0.24076000
H	-5.04118300	-3.90500500	-0.77216600	C	-3.77225400	4.92139100	0.50105100
C	-4.46703600	-2.79852900	-2.51992500	C	-4.62453300	5.27542600	-0.55061200
H	-3.62586100	-2.19260600	-2.86872000	H	-4.88111800	5.31053100	-2.69141800
H	-5.36338800	-2.17103000	-2.51197800	H	-2.67690900	4.27759500	-3.15572100
C	-2.95365500	-4.28157500	-1.11563500	H	-1.86536100	4.04681600	1.04598100
H	-2.06706400	-3.75732700	-1.47668700	H	-4.07614300	5.10132300	1.52906000
H	-2.73102400	-4.64202900	-0.10821200	H	-5.58990400	5.72947100	-0.34376300
C	-4.74561500	-2.20219800	1.12262500	C	-0.78002400	3.45363200	-1.35433600
H	-4.48060500	-1.23726100	1.55855500	H	-0.61607300	3.40787000	-2.43762800
C	-6.26089300	-2.23602500	0.90287500	H	0.01415500	4.07379300	-0.93012300
H	-6.57251200	-1.44513900	0.21436100	C	-0.66224300	2.04680000	-0.77016700
H	-6.77277500	-2.08307800	1.85854500	C	-1.50752600	1.07755900	-1.17287200
H	-6.60292400	-3.19631800	0.50196500	H	-2.30023300	1.34836900	-1.87098400
C	-4.25417500	-3.31169600	2.06359800	C	0.25406900	1.96491500	0.42983700
H	-3.16935900	-3.25228300	2.18583600	N	1.15092700	0.94961600	0.47571100
H	-4.72470100	-3.21390300	3.04782900	O	0.17296300	2.86456400	1.28066900
H	-4.50220600	-4.30380000	1.67006000	C	2.83197500	1.94258100	1.80172300
H	-3.14048300	-5.14530300	-1.76282900	C	3.36182200	2.01612400	3.23644800
H	-4.62037600	-3.61984800	-3.22758200	C	2.20356300	2.50177400	4.13694500
11'				H	2.55731300	2.60562100	5.16875100
C	2.18784700	-1.81496400	-2.57179200	H	1.82422900	3.46819000	3.79426700
C	1.73543700	-0.51402000	-2.93946200	H	1.37083800	1.79563900	4.11387200
C	2.58319700	0.44327200	-2.25569800	C	4.52800800	3.01356500	3.27775200
C	3.64365400	-0.28327600	-1.56941000	H	4.91131300	3.09489900	4.30024500
C	3.37097900	-1.65732700	-1.73216300	H	5.34499900	2.69246200	2.62473400
Rh	1.51738600	-0.68615000	-0.73698300	H	4.20645800	4.00253700	2.94292600

C	3.83719000	0.61886800	3.68791900	H	-6.56913200	0.25289800	0.80584700
H	4.22648200	0.67345500	4.71022700	H	-6.01162800	-0.73452700	2.16832200
H	3.01766300	-0.10354700	3.66818700	H	-3.63844800	-3.41745800	3.82436200
H	4.63956300	0.24676300	3.04074100	H	-3.59217600	-5.27535000	2.03860100
O	3.19891800	2.64023900	0.88146200	TS12'			
O	1.88297600	0.97433100	1.71039000	C	1.97980200	-1.70040400	-2.66538500
H	2.67211100	2.40152500	-1.39930400	C	1.68749100	-0.33005400	-2.90846100
H	3.30136200	2.28417100	-3.05844000	C	2.70636100	0.45409000	-2.22525800
H	1.55383000	2.25779400	-2.76768600	C	3.68969500	-0.44443600	-1.67073900
H	0.63464900	-3.05607600	-3.39780500	C	3.20610100	-1.76413700	-1.88558400
H	2.26518700	-3.44749000	-3.96352900	Rh	1.60515700	-0.68518600	-0.69632800
H	1.75301400	-3.90680200	-2.33239300	C	2.81695100	1.94739600	-2.20515400
C	-1.55992200	-0.29115400	-0.63919000	C	0.54443500	0.18249300	-3.72983000
C	-0.44698700	-1.01050900	-0.45060400	H	0.68803900	-0.06946300	-4.78756000
C	-0.03178100	-2.23308100	0.18725800	H	-0.40445300	-0.25361800	-3.40114300
C	-0.20123900	-3.52993900	-0.38052000	H	0.44682900	1.26534200	-3.64822600
C	0.82955000	-2.09740000	1.32017800	C	1.21868600	-2.87720100	-3.19264400
C	0.47698000	-4.61520100	0.13517700	C	3.85978600	-3.04217700	-1.46053600
H	-0.87334000	-3.63995700	-1.22459200	H	3.13788400	-3.71665500	-0.98853600
C	1.53446100	-3.21699900	1.80630900	H	4.28291600	-3.56246900	-2.32873300
H	0.85665800	-1.16274100	1.86701500	H	4.66623800	-2.86207700	-0.74691700
C	1.37484700	-4.46031300	1.21673700	C	4.98431400	-0.04164700	-1.03358700
H	0.32476100	-5.60052800	-0.29738700	H	5.32483500	-0.79076000	-0.31380800
H	2.18645900	-3.09686700	2.66679000	H	5.77026200	0.07217400	-1.79222000
H	1.90863700	-5.32372000	1.60250500	H	4.87870500	0.90124200	-0.49813500
N	-2.89087100	-0.70917400	-0.34421800	C	-4.16080100	5.13991100	-1.50280800
N	-2.95415500	-1.73683400	0.39336600	C	-3.06784600	4.41370000	-1.98487100
N	-4.17512300	-2.19891400	0.65567400	C	-1.93169200	4.21773700	-1.19241100
C	-4.19328000	-3.20879000	1.73394200	C	-1.90659100	4.76230900	0.10108600
H	-5.24887200	-3.40551700	1.93572500	C	-2.99535400	5.48745400	0.58187200
C	-3.53703200	-4.51050200	1.25691100	C	-4.12718100	5.67969600	-0.21733500
H	-2.48492600	-4.33512600	1.01638900	H	-5.03463900	5.28352100	-2.13299100
H	-4.03758300	-4.89161300	0.36142100	H	-3.09724300	3.99775900	-2.98973100
C	-3.54405900	-2.67935600	3.02112600	H	-1.02588100	4.59813000	0.71488000
H	-2.48252500	-2.47914700	2.85334000	H	-2.96238500	5.90579400	1.58453500
H	-4.02058000	-1.75022000	3.34630600	H	-4.97414300	6.24605300	0.16026300
C	-5.38211700	-1.46954600	0.21351800	C	-0.75490500	3.40244500	-1.69830600
H	-5.08866000	-1.01960000	-0.73830300	H	-0.88338200	3.21417900	-2.77113800
C	-6.55873900	-2.41529900	-0.03874400	H	0.16642400	3.97740200	-1.57083100
H	-6.26253500	-3.25458200	-0.67524100	C	-0.59614600	2.07228700	-0.97380500
H	-7.35724900	-1.86544200	-0.54652100	C	-1.53260500	1.08675300	-1.14841500
H	-6.98262500	-2.81542400	0.88815300	H	-2.41643700	1.31969900	-1.74080900
C	-5.72814600	-0.33524100	1.18809700	C	0.39937400	2.05319900	0.09729800
H	-4.87114900	0.33148200	1.30997100	N	0.79219900	0.78378700	0.58989300

O	0.85272800	3.09011100	0.60313400	C	-4.12560900	-2.14570100	3.06691400
C	2.57102600	1.43526200	2.02974800	H	-3.11129600	-1.74256800	3.12715600
C	2.86613900	1.82031700	3.48188500	H	-4.82360300	-1.30591200	3.01059300
C	1.93842500	2.99882400	3.85456600	C	-5.20681800	-1.92202500	-0.28503600
H	2.15967700	3.33048600	4.87496900	H	-4.73588900	-1.60861700	-1.22070200
H	2.08233600	3.83896200	3.17016600	C	-6.13571400	-3.10114600	-0.58644000
H	0.88905000	2.70215600	3.79721400	H	-5.56878100	-3.97015700	-0.93394900
C	4.33834800	2.24434100	3.58166100	H	-6.84067400	-2.81347300	-1.37286400
H	4.56762000	2.54447300	4.60928600	H	-6.72902600	-3.40104800	0.28376400
H	5.00572900	1.42401000	3.30166400	C	-5.95627700	-0.71207900	0.29212700
H	4.54739700	3.08495100	2.91565300	H	-5.26049100	0.11047200	0.47446200
C	2.59089900	0.61403500	4.40471400	H	-6.72290700	-0.36563100	-0.40954700
H	2.81746300	0.88431700	5.44142100	H	-6.45338200	-0.97119600	1.23333000
H	1.54443900	0.30396100	4.35169600	H	-4.33360300	-2.70734200	3.98370500
H	3.22094000	-0.24172500	4.13582300	H	-3.45536000	-4.82394000	2.82444800
O	3.34014700	1.52482300	1.10283000	13'			
O	1.29538300	0.95013100	1.93389900	C	1.59401300	-3.91988600	-0.19984900
H	3.02417300	2.30269000	-1.19232600	C	1.06699200	-3.44061700	-1.47967500
H	3.63286000	2.27388000	-2.86155100	C	1.97399400	-2.46906200	-1.98871000
H	1.89528700	2.42190400	-2.54426900	C	3.02920600	-2.28665400	-1.00076300
H	0.17119500	-2.61875400	-3.37134800	C	2.80852600	-3.24736000	0.07083000
H	1.64540400	-3.22907900	-4.14080200	Rh	1.20149800	-1.72093800	-0.08111600
H	1.23969000	-3.71005100	-2.48561200	C	1.87736900	-1.74011300	-3.29066400
C	-1.52726900	-0.18333000	-0.50449800	C	-0.14624600	-3.98775900	-2.16113300
C	-0.34057500	-0.66873600	0.00132900	H	0.09008000	-4.93968100	-2.65359100
C	0.11213300	-1.94509900	0.49404000	H	-0.95375800	-4.16444900	-1.44825100
C	-0.34281400	-3.15781200	-0.12402000	H	-0.52031900	-3.29786200	-2.91949000
C	1.21887700	-2.02168800	1.39436200	C	0.95882900	-4.98995100	0.63111400
C	0.28007800	-4.35396500	0.14050700	C	3.68636800	-3.36948500	1.27558200
H	-1.18976700	-3.10924700	-0.79663200	H	3.33655900	-4.15050400	1.95333600
C	1.84635800	-3.26765800	1.62965100	H	4.71303400	-3.60744700	0.97746400
H	1.46333400	-1.18291700	2.02851200	H	3.69642700	-2.41747800	1.81743400
C	1.39831600	-4.41658000	1.01014000	C	4.23297300	-1.41225300	-1.11711200
H	-0.09018700	-5.26378200	-0.32384700	H	4.56745000	-1.10293300	-0.12455600
H	2.67531100	-3.30899600	2.33023200	H	5.04766600	-1.96714400	-1.60158500
H	1.87597100	-5.37143000	1.20815500	H	3.99922800	-0.51199900	-1.68156700
N	-2.79347700	-0.80425600	-0.39837300	C	1.88081600	5.73338800	0.28367800
N	-2.90191700	-1.66761700	0.51994900	C	1.19383500	4.95428200	-0.64734300
N	-4.07528000	-2.32475700	0.57194800	C	1.88450700	4.10696400	-1.52355300
C	-4.25864000	-3.05940100	1.83869900	C	3.27850700	4.04263400	-1.43559800
H	-5.27938800	-3.44868900	1.80855100	C	3.97087100	4.82544300	-0.50979600
C	-3.29107400	-4.24782300	1.90778800	C	3.27504600	5.67507900	0.35148300
H	-2.25662900	-3.89515600	1.89724800	H	1.32913400	6.38424700	0.95664700
H	-3.43337700	-4.91094400	1.04884000	H	0.10806900	4.99409900	-0.69228500

H	3.81568900	3.35783900	-2.08424900	H	-3.90640700	-3.59982100	-0.89743300
H	5.05425000	4.76161800	-0.45328200	H	-1.31814800	-3.27940900	2.52447600
H	3.81252000	6.27993300	1.07653200	H	-3.04666400	-4.53400100	1.24326300
C	1.12046800	3.27216800	-2.54000200	N	-3.17539000	1.35576900	-1.01431000
H	0.45137900	3.92424600	-3.11438200	N	-3.64324900	0.87128000	0.06253800
H	1.83392500	2.82366600	-3.23876300	N	-4.97059400	0.86209900	0.18030600
C	0.31009900	2.17177400	-1.90153600	C	-5.42269600	0.56846700	1.55611300
C	-1.05145500	2.22741200	-1.76620200	H	-6.51283200	0.63792600	1.53021900
H	-1.61168400	3.08247400	-2.13769700	C	-5.03320900	-0.86189000	1.94830700
C	1.04656000	1.01961200	-1.40479500	H	-3.94610700	-0.96971600	1.95615300
N	0.29189400	0.01649200	-0.81935900	H	-5.43908300	-1.58477200	1.23504300
O	2.28678700	0.90857400	-1.53818900	C	-4.88828400	1.59969500	2.56093600
C	1.58019100	0.35665000	2.11767000	H	-3.79613000	1.55883200	2.59270900
C	2.68046600	1.27162200	2.70005700	H	-5.18659800	2.61436000	2.28165300
C	3.04779900	2.24725400	1.55981100	C	-5.83527700	1.47057100	-0.84851900
H	3.86906200	2.90183100	1.87141900	H	-5.29769700	1.29217600	-1.78453400
H	3.34579000	1.70696000	0.65769700	C	-7.19846800	0.77872200	-0.93036700
H	2.19833600	2.88183700	1.29304500	H	-7.08615800	-0.30825300	-0.98744400
C	3.92459400	0.46789400	3.11293800	H	-7.72079200	1.11772200	-1.83052500
H	4.67818800	1.13798000	3.54243300	H	-7.84048000	1.01645400	-0.07592700
H	3.67903400	-0.29086300	3.86483900	C	-5.95369900	2.98897100	-0.65565300
H	4.36591500	-0.03766400	2.25086100	H	-4.95962200	3.44124700	-0.62391000
C	2.12235900	2.04658400	3.90278600	H	-6.51244600	3.43793100	-1.48413200
H	2.86161300	2.77217700	4.26110100	H	-6.48039900	3.22607100	0.27513600
H	1.21004800	2.57731600	3.62410400	H	-5.27506300	1.38994400	3.56364400
H	1.87791700	1.37130200	4.73056400	H	-5.41579500	-1.09950800	2.94630100
O	2.05181200	-0.68357300	1.47890800	TS11^g			
O	0.38810400	0.64451300	2.22924000	C	3.31889100	-0.79494500	-2.11569500
H	2.26920600	-0.72769900	-3.18297600	C	3.98098100	-1.07277600	-0.84494500
H	2.45451400	-2.27235200	-4.05706300	C	3.41863300	-2.25530800	-0.31001000
H	0.84154800	-1.67188100	-3.62930800	C	2.40373500	-2.73238300	-1.22230900
H	-0.12976100	-4.94620200	0.56707400	C	2.38273100	-1.84763200	-2.36203800
H	1.28072600	-5.97617500	0.27347500	Rh	1.71535100	-0.69084600	-0.58103800
H	1.24107600	-4.90085700	1.68191200	C	3.74704400	-2.90805300	1.00007500
C	-1.77829100	1.19425800	-1.12394200	C	5.08931500	-0.25613900	-0.25117400
C	-1.05938200	0.08745200	-0.68069300	H	6.06544800	-0.58838700	-0.62740100
C	-1.67056500	-1.14726100	-0.12149100	H	4.98363600	0.80136200	-0.50226300
C	-2.65335400	-1.85795300	-0.83271100	H	5.10497800	-0.33388800	0.83864600
C	-1.18687500	-1.67313100	1.09486700	C	3.68993900	0.30268600	-3.06714800
C	-3.14232400	-3.06345200	-0.34123300	C	1.55283100	-2.04111100	-3.59453600
H	-3.03422700	-1.44567400	-1.76159700	H	1.39890600	-1.09738900	-4.12306900
C	-1.68450000	-2.89588700	1.57630500	H	2.04542100	-2.73790500	-4.28430100
H	-0.55933900	-1.03040100	1.71580000	H	0.56810800	-2.44802500	-3.35137200
C	-2.65285200	-3.59565000	0.86328600	C	1.65601700	-4.02228500	-1.08804200

H	0.71018400	-3.99967400	-1.63190400	H	2.84663200	0.57757600	-3.70508900
H	2.25173800	-4.85888600	-1.47718800	C	-0.67129700	1.00044300	-1.03046700
H	1.42649300	-4.23777100	-0.04093500	C	-0.27900600	-0.35994200	-0.85313100
C	2.03343100	6.18329500	-0.23728500	C	-1.15394000	-1.50223700	-1.13938500
C	2.39925400	4.86386600	-0.51737500	C	-1.82950900	-1.53354900	-2.37763700
C	2.28100800	3.86282000	0.45461700	C	-1.27351800	-2.61423100	-0.28770800
C	1.78033300	4.20633200	1.72026400	C	-2.59774100	-2.63680200	-2.74223900
C	1.41751800	5.52305100	2.00083700	H	-1.75420000	-0.68033500	-3.04352900
C	1.54211500	6.51669000	1.02496600	C	-2.07029200	-3.70032200	-0.64483800
H	2.13343700	6.94667300	-1.00431300	H	-0.73675400	-2.62404900	0.65008800
H	2.78482800	4.60921300	-1.50254900	C	-2.73342500	-3.72320000	-1.87403500
H	1.67391200	3.42473300	2.46604200	H	-3.10401200	-2.64012500	-3.70349200
H	1.03389500	5.77541400	2.98584300	H	-2.16184200	-4.53946600	0.03952700
H	1.25687200	7.54124900	1.24739100	H	-3.34671000	-4.57497500	-2.15239800
C	2.65315400	2.42549700	0.13527100	N	-1.96747300	1.48425700	-1.33200400
H	3.18324900	2.40493600	-0.82318800	N	-2.86894000	0.78956200	-0.77114600
H	3.33545500	2.04070200	0.89796800	N	-4.13119100	1.11489300	-1.02932200
C	1.46003100	1.47658000	0.04699800	C	-5.08404100	0.43555200	-0.12358300
C	0.33033100	1.90550700	-0.74256300	H	-6.07395900	0.79677000	-0.41326000
H	0.21383600	2.95895300	-0.99497300	C	-5.03215600	-1.08077200	-0.34776400
C	1.14647700	0.76503300	1.35253400	H	-4.04413600	-1.46916700	-0.08964900
N	0.47465700	-0.41186700	1.06314400	H	-5.22849300	-1.32778800	-1.39493500
O	1.56712800	1.09553000	2.45921600	C	-4.83058700	0.80219600	1.34660500
C	-0.82899500	-0.98759100	2.89861200	H	-3.83667200	0.46967900	1.65843900
C	-0.94828600	-1.96701800	4.06815200	H	-4.89319100	1.88366500	1.49942700
C	-1.05353300	-3.40245800	3.50682200	C	-4.46552500	2.31221400	-1.82378800
H	-1.17724700	-4.11250500	4.33124900	H	-3.65731500	2.37766300	-2.55812800
H	-1.91692500	-3.50259100	2.83998800	C	-5.78915000	2.14677400	-2.57466400
H	-0.15339400	-3.67579600	2.94964100	H	-5.81910100	1.19700900	-3.11724500
C	-2.21390000	-1.61244200	4.86210500	H	-5.89693100	2.96010600	-3.29925700
H	-2.32452800	-2.29846400	5.70811500	H	-6.65567400	2.19179500	-1.90695200
H	-2.16089300	-0.58998600	5.24468300	C	-4.42917800	3.58383200	-0.96397000
H	-3.10524000	-1.68374500	4.23289700	H	-3.46724500	3.66632000	-0.45239700
C	0.30547500	-1.83575300	4.95982800	H	-4.56565500	4.47229000	-1.59014600
H	0.21340300	-2.50264400	5.82385500	H	-5.22779100	3.57189300	-0.21457000
H	1.21101700	-2.09752100	4.40780500	H	-5.57859100	0.32325200	1.98786900
H	0.42008900	-0.81066000	5.32465100	H	-5.77974000	-1.58067300	0.27702600
O	-1.59818400	-0.10390400	2.61972700	12^a			
O	0.30804200	-1.26994100	2.17109900	C	3.55806400	-1.11908300	-1.58263200
H	2.83484600	-3.13243600	1.56152400	C	4.11400600	-1.30400200	-0.25246000
H	4.28307600	-3.85208100	0.84229900	C	3.49373600	-2.45116500	0.31682800
H	4.37180900	-2.26712600	1.62532500	C	2.55149500	-2.98084800	-0.63100700
H	4.00892900	1.20194800	-2.53447700	C	2.61835500	-2.17535900	-1.82093100
H	4.51900200	-0.00497600	-3.71782300	Rh	1.88101200	-0.82290100	-0.18703800

C	3.75120000	-3.00767000	1.68541700	C	-0.87295600	0.16665100	5.01957400
C	5.20857700	-0.48182900	0.35975700	H	-1.19985400	-0.11382700	6.02637100
H	6.19705800	-0.88409100	0.10152100	H	0.10592100	-0.27817300	4.82646600
H	5.17253300	0.55248600	0.01032300	H	-0.76075700	1.25404200	4.98095800
H	5.13211700	-0.46157000	1.45002600	O	-1.84638000	0.98588100	1.91177000
C	4.03552300	-0.13421900	-2.60736400	O	-0.31490000	-0.66377600	2.25121900
C	1.88881500	-2.43992500	-3.10072500	H	2.84085900	-3.42924300	2.11992900
H	1.77253500	-1.52621200	-3.68891200	H	4.50114100	-3.80825000	1.64816500
H	2.43571600	-3.16765400	-3.71445900	H	4.12035600	-2.23776200	2.36732300
H	0.89221800	-2.84564900	-2.91184300	H	4.49207300	0.74126200	-2.14170800
C	1.73522200	-4.22658000	-0.47110700	H	4.79325400	-0.59251000	-3.25604500
H	0.80418400	-4.16929100	-1.03833100	H	3.21597500	0.21280400	-3.24178600
H	2.29192300	-5.10604500	-0.82090200	C	-0.56971300	0.72818500	-1.05923300
H	1.46574300	-4.39838500	0.57382000	C	-0.22935000	-0.51930100	-0.27141700
C	2.05487500	5.93413300	-1.20041100	C	-0.93959100	-1.79530500	-0.51119800
C	2.44128500	4.59223900	-1.24401700	C	-1.34558700	-2.07597600	-1.83418300
C	2.35834200	3.78133400	-0.10523200	C	-1.18592800	-2.78042400	0.46400000
C	1.87547000	4.34288800	1.08691300	C	-1.97750900	-3.27089000	-2.16096500
C	1.49072500	5.68254600	1.13213500	H	-1.16482500	-1.33875400	-2.60796700
C	1.57826700	6.48375500	-0.00990500	C	-1.83464500	-3.97172200	0.13368200
H	2.12716600	6.54708600	-2.09491000	H	-0.86344900	-2.62564000	1.48232900
H	2.81262700	4.16804800	-2.17454400	C	-2.23786500	-4.22899200	-1.17586100
H	1.79374200	3.71302000	1.96696800	H	-2.27533700	-3.45115800	-3.19028400
H	1.11928000	6.10327500	2.06282100	H	-2.01600700	-4.70658800	0.91349400
H	1.27670600	7.52687100	0.02877100	H	-2.74163900	-5.15728600	-1.42778300
C	2.74947500	2.31482600	-0.17106900	N	-1.81765600	1.02465800	-1.61872100
H	3.31021300	2.14357900	-1.09491100	N	-2.76826800	0.38236900	-1.07004100
H	3.41071000	2.06722000	0.66522200	N	-3.98612900	0.57958800	-1.57354800
C	1.56389100	1.35691500	-0.14042900	C	-5.05070400	0.03685400	-0.70426000
C	0.42206800	1.64048700	-1.05147900	H	-5.98094500	0.14818300	-1.26635600
H	0.30718900	2.62073700	-1.50472600	C	-4.82181100	-1.45865000	-0.44910500
C	1.09693200	0.99260900	1.21645800	H	-3.90659000	-1.61894200	0.12458700
N	0.28267500	-0.21393200	1.05237100	H	-4.72235100	-2.00441300	-1.39098700
O	1.39286100	1.39532200	2.32866800	C	-5.16227200	0.82379100	0.61180600
C	-1.41346500	0.10811200	2.61052300	H	-4.20514600	0.80087000	1.13962200
C	-1.91763900	-0.31758200	3.98646300	H	-5.42378200	1.87029900	0.43246000
C	-2.06569200	-1.85176500	4.05525100	C	-4.21707900	1.58839100	-2.62682200
H	-2.49165600	-2.13128500	5.02418800	H	-3.33337500	1.50778400	-3.26712300
H	-2.73258700	-2.22225000	3.26984700	C	-5.45436400	1.26319300	-3.46646200
H	-1.09979300	-2.35173100	3.95031700	H	-5.44577600	0.22070200	-3.79932200
C	-3.27358600	0.36132600	4.23189400	H	-5.46577700	1.90571800	-4.35245100
H	-3.62821200	0.11830400	5.23842500	H	-6.38668400	1.44691100	-2.92223300
H	-3.19031800	1.44662800	4.13987600	C	-4.25327100	3.01584400	-2.05978700
H	-4.02176500	0.02166000	3.50977300	H	-3.36684500	3.20383500	-1.45032200

H	-4.27233000	3.74572600	-2.87658600	O	2.63538200	0.48217800	-2.66833000
H	-5.14636600	3.17294800	-1.44634000	C	0.65415300	3.02329500	-0.69593000
H	-5.93497300	0.38576000	1.25344700	C	0.56049500	4.42844000	-1.27321800
H	-5.66643500	-1.87344400	0.11097600	C	1.92650900	4.78221100	-1.90354400
TS12b							
C	0.25600600	-0.54355700	2.77277700	H	1.87208200	5.77992500	-2.35059100
C	1.30808900	-1.18216400	2.02533200	H	2.71852400	4.79105500	-1.14719800
C	2.51802400	-0.35655100	2.13249300	H	2.20051400	4.06153600	-2.67772900
C	2.17513100	0.82068900	2.79899900	C	0.20556200	5.40914600	-0.14637000
C	0.74275300	0.74226400	3.13635800	H	0.13766000	6.42192400	-0.55503700
Rh	0.71925700	0.64022800	0.94645700	H	-0.75488600	5.15017200	0.30720400
C	3.82949800	-0.73997600	1.52661300	H	0.96504100	5.40222000	0.64018500
C	1.28413400	-2.59720600	1.54120600	C	-0.54498200	4.43375900	-2.35366100
H	1.55053600	-3.27873000	2.36021000	H	-0.63115300	5.44132200	-2.77338400
H	0.29181000	-2.87173600	1.17719100	H	-0.30844700	3.73769300	-3.16142900
H	1.99544700	-2.74984400	0.72916000	H	-1.51245100	4.15075500	-1.92971100
C	-1.10054100	-1.12727800	3.02839200	O	0.48132700	2.75498600	0.50114100
C	0.00855000	1.81511100	3.88377400	O	0.93114400	2.11033000	-1.60553600
H	-1.07082500	1.64810600	3.86737900	H	4.56935400	0.05822200	1.61413100
H	0.32979600	1.84808500	4.93254000	H	4.23617800	-1.63849800	2.00391600
H	0.20444900	2.79793200	3.44463700	H	3.71308700	-0.97503400	0.46542800
C	3.03547600	2.01209200	3.09431400	H	-1.52028100	-1.55131500	2.11321400
H	2.57103900	2.93136800	2.72110300	H	-1.04557500	-1.92014700	3.78516400
H	3.18469900	2.13608700	4.17425800	H	-1.80226700	-0.37040700	3.38757100
H	4.01854800	1.92217000	2.62680300	C	-0.84153300	-1.22696400	-0.86613000
C	5.92906800	-1.92770200	-1.14655000	C	-0.75806800	0.10758100	-0.38786500
C	4.77933000	-1.71332900	-1.90882100	C	-1.86645000	1.06177900	-0.63797800
C	3.69834600	-2.60456300	-1.83428100	C	-2.34949000	1.93726900	0.34987600
C	3.80142000	-3.71421900	-0.98430000	C	-2.43288100	1.13261100	-1.92526000
C	4.94858800	-3.92751900	-0.21709100	C	-3.38472400	2.82763400	0.07262200
C	6.01792100	-3.03276200	-0.29586100	H	-1.90723000	1.90305600	1.33926500
H	6.75742400	-1.22752200	-1.21528400	C	-3.46772100	2.02207400	-2.20405600
H	4.68970100	-0.84117700	-2.54791600	H	-2.05472400	0.46843300	-2.69618700
H	2.97376900	-4.41767100	-0.92579800	C	-3.95095700	2.87324000	-1.20516100
H	5.00897600	-4.79410000	0.43604500	H	-3.75422200	3.48420000	0.85557900
H	6.91359400	-3.19752300	0.29672200	H	-3.89309200	2.05852700	-3.20313100
C	2.42889200	-2.35234100	-2.63062100	H	-4.75505900	3.57061600	-1.42240100
H	2.69516100	-1.88275800	-3.58387700	N	-2.07177100	-1.91476200	-0.92492700
H	1.94294600	-3.30909200	-2.85082300	N	-2.91638200	-1.52028200	-0.05720200
C	1.44329000	-1.44836300	-1.91295000	N	-4.16168800	-1.99135500	-0.20889200
C	0.24096200	-1.93770000	-1.44562800	C	-5.03296000	-1.75012000	0.95264300
H	0.02780100	-2.98665300	-1.64409700	H	-6.04300000	-2.00680000	0.62508900
C	1.76771200	-0.03407400	-1.95238700	C	-4.66803100	-2.64598900	2.14756300
N	0.92821600	0.73877700	-1.12172900	H	-3.65081000	-2.42614100	2.48295200
				H	-4.71958800	-3.70580200	1.88392200

C	-5.02317600	-0.26509800	1.33818000	H	2.81139400	-4.17055200	-1.60052500
H	-4.03961900	0.03215900	1.70652900	H	4.55484900	-5.00149000	-0.04876700
H	-5.25349500	0.36271800	0.47348800	H	6.55884400	-3.60639000	0.43574200
C	-4.48691000	-2.92847700	-1.30006800	C	2.71008000	-1.77601300	-2.91576100
H	-3.86354400	-2.58439600	-2.13190800	H	3.15973400	-1.10133300	-3.65276500
C	-4.06434500	-4.36924000	-0.97367400	H	2.26663000	-2.61244600	-3.46827000
H	-3.01404600	-4.39318900	-0.67564900	C	1.61059400	-1.04044400	-2.17442600
H	-4.18827300	-5.00910500	-1.85440400	C	0.36072700	-1.62779500	-1.92200700
H	-4.67489300	-4.78691300	-0.16614000	H	0.18679500	-2.64289400	-2.27134000
C	-5.95551300	-2.83690600	-1.72158100	C	1.90073200	0.26726600	-1.74613600
H	-6.25826600	-1.79767600	-1.88227400	N	0.76556800	0.88808200	-0.98068700
H	-6.09127900	-3.38112700	-2.66142200	O	2.91633600	0.95302200	-1.87748200
H	-6.63121800	-3.28838600	-0.98732600	C	0.59688000	3.13273900	-0.28717500
H	-5.76519400	-0.07858300	2.12161900	C	0.69762300	4.58887200	-0.70810300
H	-5.35249600	-2.46742900	2.98393400	C	2.17624100	4.84685800	-1.08706600
13b				H	2.28157200	5.87506000	-1.44726300
C	-0.09922900	-0.91348800	2.63892300	H	2.83146200	4.71899900	-0.21930900
C	0.99471300	-1.42393000	1.85450600	H	2.50742600	4.15818900	-1.86817500
C	2.20108500	-0.64652400	2.17297600	C	0.26822700	5.47824000	0.46751100
C	1.81679800	0.40947800	3.00239600	H	0.36925600	6.52946400	0.18154600
C	0.36525900	0.29034100	3.23714700	H	-0.77473400	5.29096400	0.73866000
Rh	0.50713300	0.56096200	1.07186000	H	0.88640400	5.29665100	1.35033400
C	3.54426300	-0.92678500	1.57729900	C	-0.22044200	4.82756000	-1.92775400
C	1.00406800	-2.72184800	1.11000800	H	-0.17262600	5.88454600	-2.20797700
H	1.22794300	-3.54664800	1.79940800	H	0.09304200	4.22575800	-2.78305100
H	0.03838200	-2.91788200	0.63992000	H	-1.25911900	4.57484200	-1.69593600
H	1.76509600	-2.72179100	0.32842200	O	0.38765100	2.73999500	0.86045200
C	-1.45450400	-1.53693800	2.77025300	O	0.77177700	2.30254400	-1.31468900
C	-0.41637600	1.20811800	4.12919100	H	4.30486600	-0.23675300	1.94848300
H	-1.49046000	1.12012500	3.94878900	H	3.87105500	-1.94854200	1.79763000
H	-0.23097600	0.97358300	5.18552600	H	3.51616600	-0.83617900	0.48768800
H	-0.13152500	2.25166300	3.96792400	H	-1.74989000	-2.02954200	1.84305300
C	2.66079500	1.52657000	3.53746200	H	-1.46307100	-2.28344300	3.57626700
H	2.20064600	2.49772200	3.32666400	H	-2.21765600	-0.78915100	2.99926100
H	2.78000400	1.44986300	4.62566200	C	-0.70206500	-1.02963200	-1.26371000
H	3.65525100	1.52633400	3.08605200	C	-0.57982000	0.34235800	-0.76611200
C	5.92139800	-1.99153200	-0.84863500	C	-1.71590200	1.29068600	-1.07044100
C	4.93534700	-1.52330400	-1.71911500	C	-2.37010900	2.04082700	-0.08879700
C	3.80276700	-2.30078900	-1.99935800	C	-2.10043100	1.44768400	-2.41018700
C	3.68337400	-3.55605600	-1.38757100	C	-3.38005000	2.93975000	-0.43585600
C	4.66491000	-4.02447000	-0.51203400	H	-2.08419600	1.90449500	0.94791200
C	5.79034500	-3.24260400	-0.24073300	C	-3.11146200	2.34168200	-2.76016200
H	6.79263700	-1.37565400	-0.64169900	H	-1.60047100	0.85749500	-3.17277000
H	5.01303100	-0.53664600	-2.16402600	C	-3.75309000	3.09499500	-1.77298500

H	-3.88373500	3.50868500	0.34072400	H	0.19384000	-4.83589000	-1.25671100
H	-3.39725100	2.45246600	-3.80239600	H	-0.25013400	-5.27885800	-2.91018700
H	-4.54010700	3.79325400	-2.04362500	H	1.35342500	-4.60283000	-2.56735300
N	-1.85140300	-1.80636600	-1.13647000	C	4.98011100	5.00467800	-0.02988300
N	-2.79122300	-1.32328700	-0.42780800	C	4.11224400	4.31856500	-0.88354600
N	-3.91917800	-2.06848200	-0.41550400	C	4.12423900	2.92081900	-0.94632400
C	-4.98225800	-1.61393400	0.49092900	C	5.02481100	2.21511300	-0.13285500
H	-5.92863300	-1.78841800	-0.03323700	C	5.89087500	2.89891000	0.71936500
C	-5.02519100	-2.40993900	1.80829100	C	5.87283200	4.29608500	0.77470000
H	-4.08479400	-2.29762300	2.35398000	H	4.95814500	6.09083900	0.00436400
H	-5.19344000	-3.47562100	1.63371200	H	3.41771700	4.87546200	-1.50876400
C	-4.88828500	-0.11048800	0.76182400	H	5.02320400	1.12958500	-0.17342300
H	-4.00445700	0.13411400	1.35358500	H	6.58458800	2.34038600	1.34254500
H	-4.82517000	0.45720900	-0.16810100	H	6.55016300	4.82643000	1.43857600
C	-3.96899600	-3.35778400	-1.12709500	C	3.15509300	2.16708200	-1.84229900
H	-3.41786700	-3.17771900	-2.05634200	H	2.72085600	2.85658100	-2.57534200
C	-3.22239700	-4.47039700	-0.36905400	H	3.70070600	1.39426400	-2.39475200
H	-2.20855400	-4.14564800	-0.12691500	C	2.04916400	1.49751900	-1.05057800
H	-3.15252300	-5.36841200	-0.99315100	C	0.82353500	2.14016500	-0.81531100
H	-3.73801200	-4.74108300	0.55698400	H	0.68878000	3.15528500	-1.18063100
C	-5.39740700	-3.77190900	-1.48901600	C	2.29772700	0.18087000	-0.60174600
H	-5.91435400	-2.98544400	-2.04734700	N	1.14221500	-0.40835200	0.07338600
H	-5.35615100	-4.66312200	-2.12294800	O	3.29206800	-0.53933700	-0.77663900
H	-5.99719500	-4.02637700	-0.60899900	C	1.13751700	-2.40286100	1.52916600
H	-5.77942900	0.20693500	1.31357400	C	1.69216100	-3.25294900	2.67649900
H	-5.83882600	-2.04357400	2.44419700	C	3.05145900	-3.81303700	2.19901100
TS14b				H	3.49798600	-4.41463600	2.99738500
C	-1.77798300	-1.38375900	-2.47906000	H	2.92596200	-4.45221000	1.31875900
C	-0.49833400	-0.91032800	-2.96319300	H	3.73840800	-3.00351600	1.93973900
C	0.40676100	-2.05169900	-3.08267600	C	0.70808000	-4.39187600	2.98107300
C	-0.24469300	-3.16032100	-2.52040400	H	1.10787900	-5.00951800	3.79151800
C	-1.59351300	-2.73810700	-2.10425600	H	-0.26229200	-3.99477300	3.29251700
Rh	-0.20281300	-1.51703000	-0.89044400	H	0.54973400	-5.02496300	2.10478400
C	1.80790700	-1.95984700	-3.60892100	C	1.88429100	-2.36284100	3.92183000
C	-0.23096200	0.45071700	-3.52618900	H	2.26408800	-2.97341800	4.74743200
H	-0.49016900	0.48009800	-4.59239300	H	2.59678400	-1.55866800	3.72601500
H	-0.81469700	1.21416600	-3.00768200	H	0.93814900	-1.90941800	4.23149200
H	0.82271800	0.71669400	-3.42063400	O	0.17756300	-2.78349300	0.83013900
C	-3.01412000	-0.54624800	-2.36174400	O	1.76765100	-1.27758900	1.36280700
C	-2.60537400	-3.66295200	-1.49624600	H	2.28034500	-2.94335500	-3.65663900
H	-3.42896100	-3.10890000	-1.04016100	H	1.81343600	-1.53217100	-4.61827300
H	-3.02724500	-4.33729300	-2.25246400	H	2.43133500	-1.32694600	-2.96758100
H	-2.14620100	-4.28071600	-0.71898400	H	-2.78681600	0.41546700	-1.89664100
C	0.29468700	-4.54228500	-2.30698600	H	-3.45144700	-0.35813300	-3.35095100

H	-3.77349700	-1.03635500	-1.74847200	C	4.70893700	-0.73335800	-1.35423900
C	-0.25567300	1.56760000	-0.16497300	C	2.55315400	-2.12156900	-3.21549000
C	-0.11813900	0.22245000	0.39652800	H	3.26906300	-2.71271700	-3.80077700
C	-0.60926700	0.05672700	1.81758500	H	1.54547200	-2.39477600	-3.53529100
C	-1.59443100	-0.85827600	2.19732400	H	2.68985800	-1.06012400	-3.42208200
C	-0.01847700	0.86463800	2.80036600	C	1.00962300	-4.32316400	-1.46374100
C	-1.97911800	-0.97174200	3.53470000	C	2.01306200	-4.09450700	1.53150500
H	-2.05558500	-1.48052900	1.44006300	H	0.92030700	-4.12246100	1.49932500
C	-0.40172500	0.75428500	4.13642900	H	2.38624200	-5.12512600	1.49014800
H	0.74583900	1.57830700	2.50743700	H	2.30646200	-3.66066700	2.48856200
C	-1.38389200	-0.16700000	4.50898400	C	4.47974500	-1.98314900	1.58908900
H	-2.74976800	-1.68565700	3.81200200	H	4.02813000	-2.32442300	2.52256500
H	0.06867700	1.38467100	4.88560100	H	5.48046400	-2.42398300	1.51170300
H	-1.68364100	-0.25595700	5.54938700	H	4.58365900	-0.89657400	1.65019200
N	-1.39099700	2.36379200	-0.00917200	C	1.64682000	5.88413500	0.17103200
N	-2.45787500	1.74194900	0.30038300	C	1.00833700	5.22265700	-0.88042500
N	-3.52158300	2.53136700	0.53353700	C	1.56328100	4.06874500	-1.44814100
C	-4.81173600	1.83467700	0.65627500	C	2.77781600	3.58559800	-0.93762300
H	-5.40577400	2.41823600	1.36651900	C	3.41851300	4.24859700	0.10920100
C	-5.58032600	1.78260900	-0.67633700	C	2.85658200	5.39872000	0.67003700
H	-4.98550000	1.27179500	-1.43860600	H	1.19892200	6.77729800	0.59868900
H	-5.82097700	2.78303500	-1.04450400	H	0.06316100	5.60297600	-1.26130300
C	-4.64295500	0.43432600	1.25238400	H	3.18717100	2.66954500	-1.34808400
H	-4.11888000	-0.23164200	0.56459200	H	4.35842900	3.86052300	0.49313000
H	-4.06866400	0.46880300	2.17989400	H	3.35602000	5.91004100	1.48838000
C	-3.41075800	3.99621800	0.38935200	C	0.82504100	3.30671900	-2.53864100
H	-2.43423000	4.23385200	0.82526600	H	0.10230800	3.97024600	-3.02578800
C	-3.36992700	4.44776300	-1.08145700	H	1.53487100	2.95713700	-3.29363900
H	-2.60235800	3.89487100	-1.62520200	C	0.10782000	2.10956500	-1.95380100
H	-3.12545400	5.51448000	-1.13499100	C	-1.17769900	2.17146400	-1.49323100
H	-4.33438800	4.29863500	-1.57555300	H	-1.76744700	3.07789100	-1.60956800
C	-4.48971600	4.73752000	1.18179700	C	0.87439900	0.88964700	-1.77686900
H	-4.51145600	4.41870800	2.22833300	N	0.29020500	-0.12740200	-1.02352400
H	-4.26927800	5.80918800	1.15991300	O	2.03866000	0.76595100	-2.22730000
H	-5.48868100	4.60251000	0.75349000	C	1.48859300	0.42056500	1.77792000
H	-5.63307400	0.01599800	1.46138800	C	1.16230600	1.55116600	2.74364100
H	-6.52182700	1.23714900	-0.54984800	C	2.47502300	2.21560900	3.20054400
15b				H	2.25216800	3.06189700	3.85904700
C	2.00151800	-3.32718400	-0.95394600	H	3.10360600	1.50977300	3.75574200
C	2.74382100	-2.38708700	-1.75612300	H	3.03794500	2.58525000	2.34172000
C	3.74588900	-1.79027800	-0.92112400	C	0.37445900	1.01503800	3.94780900
C	3.63203800	-2.35978100	0.41222900	H	0.11202900	1.84163200	4.61676400
C	2.55098000	-3.30099700	0.38193600	H	-0.54325800	0.51788700	3.62629200
Rh	1.81429900	-1.30141700	-0.08094300	H	0.96360100	0.28764100	4.51570600

C	0.31307600	2.57150500	1.94690600	H	-6.81009200	1.99342500	2.21347500
H	0.05329000	3.41660000	2.59322800	H	-7.57438200	0.76574800	1.20707100
H	0.86710100	2.95100700	1.08653900	H	-6.11883600	-2.99449000	-0.53819500
H	-0.61306700	2.11732100	1.58127700	H	-6.80892300	-1.54717000	-2.54617500
O	0.89369300	-0.70485000	1.83199300	TS12a			
O	2.32772400	0.60570500	0.83536800	Rh	-1.38841300	-1.02122500	-0.66984900
H	5.21502100	-0.28347800	-0.49863900	N	-0.47501300	-2.32677700	0.32449900
H	5.46730600	-1.16502200	-2.01886300	C	-1.68655200	-2.43017300	-2.54731100
H	4.16505700	0.04810500	-1.89019500	C	-0.77390000	-1.32171000	-2.78108800
H	0.44230100	-3.93104500	-2.30953200	C	-1.54149600	-0.09211300	-2.75513300
H	1.53984500	-5.22086800	-1.80757500	C	-2.86223600	-0.43541400	-2.36979400
H	0.30628900	-4.62222000	-0.68706100	C	-2.95004900	-1.88727000	-2.24251300
C	-1.79151000	1.06465400	-0.85883300	O	-1.70122000	-1.16796100	2.45463400
C	-1.00737100	-0.05988300	-0.59513900	C	0.60845800	-2.46065100	1.09733900
C	-1.53653300	-1.21054400	0.18994900	C	1.74801800	-2.22521700	0.12567800
C	-1.52583200	-2.50172800	-0.34513100	C	2.03241200	-0.97026100	-0.30201400
C	-2.05123400	-1.02308000	1.48134500	O	0.78227400	-2.88575200	2.23047500
C	-2.00162300	-3.58748200	0.39513300	C	-0.09302300	0.38566100	0.05211800
H	-1.16051100	-2.64047300	-1.35558900	C	1.26695900	0.24837100	-0.09856000
C	-2.52125100	-2.10179200	2.22394200	C	-2.68927000	-0.65903100	1.93527600
H	-2.08244400	-0.02045700	1.89319600	O	-2.86960400	-0.47232600	0.65414300
C	-2.49248000	-3.39306000	1.68727200	C	-3.87523400	-0.19112100	2.82148200
H	-2.00925200	-4.58118200	-0.04568100	C	0.63944200	-1.43840500	-3.25817500
H	-2.90589900	-1.93762600	3.22668900	H	0.67338300	-1.47529900	-4.35498300
H	-2.86493900	-4.23474200	2.26430300	H	1.11493000	-2.34221600	-2.87216700
N	-3.14117600	1.23079100	-0.46826900	H	1.23289500	-0.58221300	-2.92957100
N	-3.85581600	0.20188100	-0.66459700	C	-1.26997400	-3.86609000	-2.50573300
N	-5.09504800	0.24800400	-0.16931200	H	-0.62290600	-4.04299700	-1.63738300
C	-5.96512400	-0.83177100	-0.67169100	H	-0.71306600	-4.13750100	-3.40851700
H	-6.94330000	-0.65796600	-0.21647800	H	-2.13127300	-4.53181200	-2.42255600
C	-6.12186500	-0.76841900	-2.19859600	C	-4.19505900	-2.59633500	-1.80710600
H	-5.15098500	-0.92027100	-2.67822800	H	-4.02421500	-3.66521900	-1.66633600
H	-6.51203500	0.20313900	-2.51561200	H	-5.00109600	-2.47072500	-2.54004300
C	-5.44504300	-2.19704200	-0.20711700	H	-4.54060800	-2.18005100	-0.85447000
H	-4.45007200	-2.38310800	-0.61719700	C	-4.02743700	0.47462600	-2.13385800
H	-5.36506800	-2.23303000	0.88251400	H	-4.30536300	0.45587000	-1.07367900
C	-5.60778700	1.45328700	0.50709200	H	-4.89382300	0.14451300	-2.71736100
H	-4.72024600	1.89095500	0.97328200	H	-3.80406500	1.50569400	-2.41607900
C	-6.16134500	2.47053300	-0.50005200	C	-0.99799300	1.25347100	-3.13689000
H	-5.40199400	2.70353400	-1.25054700	H	-1.73432300	2.04465700	-2.98267300
H	-6.44411400	3.39951400	0.00714200	H	-0.71980200	1.25721200	-4.19781300
H	-7.05044300	2.07730800	-1.00552100	H	-0.10975000	1.50689500	-2.55007800
C	-6.61281000	1.10303800	1.60808000	C	-4.50119600	-1.46524400	3.42401800
H	-6.21796100	0.32181200	2.26457800	H	-5.31294000	-1.19884500	4.11066600

H	-3.74778300	-2.03672500	3.97185200	H	3.01633800	-0.81701000	-0.74542300
H	-4.91740400	-2.10774300	2.63961500	C	2.63640400	-3.42285900	-0.15555200
C	-3.29429500	0.68935400	3.94427500	H	2.73815300	-3.56836300	-1.23751100
H	-4.08828800	0.97988200	4.64211700	H	2.15318000	-4.31843900	0.24791600
H	-2.84618700	1.59931500	3.53456900	C	4.01045900	-3.26168400	0.47439900
H	-2.52077200	0.14575200	4.49102800	C	4.12349500	-3.11787100	1.86556400
C	-4.92334400	0.59528200	2.02286800	C	5.16689000	-3.23825300	-0.31082000
H	-5.72375500	0.93426900	2.69086100	C	5.37728700	-2.96478000	2.45372000
H	-5.36974300	-0.02217900	1.23817800	H	3.21702200	-3.11346300	2.46606900
H	-4.47359400	1.47192900	1.54845400	C	6.42431500	-3.08327900	0.28031400
C	-0.66966400	1.57117600	0.71098100	H	5.08629900	-3.34657900	-1.39014100
C	-0.10916100	2.02570000	1.92374400	C	6.53194700	-2.94741800	1.66410900
C	-1.79993000	2.24854000	0.22073400	H	5.45507500	-2.85607700	3.53201800
C	-0.62909500	3.13494100	2.58557800	H	7.31543600	-3.06910200	-0.34139900
H	0.73983000	1.49269000	2.33731300	H	7.50774000	-2.82631700	2.12623900
C	-2.31772900	3.36222100	0.87813900	13a			
H	-2.27203400	1.89655300	-0.68474500	Rh	-1.38072800	-1.03724300	-0.68473800
C	-1.73207600	3.81734000	2.06165700	N	-0.42063600	-2.38870300	0.19005100
H	-0.18185800	3.45873000	3.52122100	C	-1.68338200	-2.35159400	-2.62918000
H	-3.18347700	3.87355000	0.46646700	C	-0.80894100	-1.20635400	-2.82075200
H	-2.13908400	4.68126300	2.57888200	C	-1.61246200	-0.00296100	-2.71669300
N	2.13732100	1.38437100	-0.02100800	C	-2.91478900	-0.40574800	-2.32634000
N	1.74212400	2.34530200	-0.74814200	C	-2.95581200	-1.86278500	-2.26883200
N	2.44231800	3.47054000	-0.68062400	O	-1.51236800	-1.05375200	2.45900300
C	1.85581000	4.59068100	-1.44238000	C	0.66186500	-2.53503000	0.96651400
H	2.48408800	5.45529700	-1.21065700	C	1.80795400	-2.21362300	0.03574700
C	1.93897600	4.32295900	-2.94963400	C	2.05718900	-0.93578400	-0.34820100
H	1.34661600	3.44051600	-3.20750000	O	0.81522800	-3.03475000	2.07265700
H	2.97334300	4.14564200	-3.25890000	C	-0.09452000	0.36384900	0.07018500
C	0.42300200	4.89410300	-0.98669700	C	1.26619800	0.25724100	-0.11242500
H	-0.23762800	4.05711800	-1.22082400	C	-2.57725100	-0.68786800	1.97560600
H	0.37768200	5.05293400	0.09381700	O	-2.83823600	-0.57985900	0.69662600
C	3.51764100	3.68075300	0.31110300	C	-3.77407100	-0.33374800	2.89786800
H	3.76331400	2.67591800	0.65884400	C	0.60011300	-1.25587400	-3.32183600
C	4.76321500	4.29048100	-0.33958900	H	0.61819700	-1.28291500	-4.41930000
H	5.09666800	3.68422200	-1.18675600	H	1.12052700	-2.14065400	-2.94987800
H	5.57535300	4.33368300	0.39305100	H	1.15975400	-0.37685200	-2.99444500
H	4.58896000	5.31221000	-0.69392400	C	-1.22636500	-3.77464200	-2.67523900
C	3.00485800	4.50029300	1.50361800	H	-0.57380400	-3.98492300	-1.81823300
H	2.12235500	4.02636200	1.94180000	H	-0.66212000	-3.97311800	-3.59220300
H	3.78056400	4.57397200	2.27295500	H	-2.06845700	-4.46837700	-2.63449400
H	2.73506400	5.51878200	1.20235300	C	-4.16876700	-2.63315100	-1.84730700
H	0.04695100	5.79102400	-1.48997900	H	-3.95555600	-3.69895100	-1.74718200
H	1.54806200	5.17713800	-3.51190800	H	-4.98741800	-2.51188300	-2.56696700

H	-4.51827500	-2.26542800	-0.87654600	H	3.68367800	2.75534100	0.65587700
C	-4.09988200	0.45581400	-2.01926500	C	4.64835500	4.36312700	-0.38865900
H	-4.33690700	0.39405500	-0.95062800	H	4.97313800	3.74057400	-1.22733900
H	-4.97618900	0.11441000	-2.58075000	H	5.47450800	4.43565400	0.32583300
H	-3.92159300	1.50238300	-2.27550800	H	4.45181500	5.37303400	-0.76484600
C	-1.11648200	1.37411600	-3.04738300	C	2.93193600	4.58655600	1.49267900
H	-1.87661500	2.13382400	-2.85602100	H	2.06211800	4.11359600	1.95651800
H	-0.84884700	1.42889700	-4.10958400	H	3.72438700	4.67398200	2.24319400
H	-0.23069900	1.63207300	-2.45889300	H	2.65015600	5.60007100	1.18578400
C	-4.29079800	-1.67221200	3.46534900	H	-0.14685900	5.77271700	-1.42817300
H	-5.11223800	-1.49364700	4.16881600	H	1.37168900	5.24186500	-3.46846400
H	-3.48820800	-2.20028500	3.98678600	H	3.03798600	-0.74217300	-0.78256800
H	-4.66465500	-2.31974400	2.66402600	C	2.74176300	-3.36697700	-0.28536400
C	-3.24127500	0.55148800	4.03953200	H	2.88365200	-3.44422500	-1.36969500
H	-4.04024300	0.75591600	4.76184100	H	2.27407200	-4.29867400	0.04856000
H	-2.87397100	1.50645800	3.65205600	C	4.08935400	-3.20377500	0.39966200
H	-2.41501500	0.05425800	4.55170300	C	4.15494200	-3.14149600	1.79985200
C	-4.89520600	0.39518300	2.14457600	C	5.26841500	-3.09900600	-0.34436600
H	-5.70577100	0.64913900	2.83754900	C	5.38473700	-2.98830900	2.43679400
H	-5.30761300	-0.22811500	1.34649900	H	3.23080500	-3.19988000	2.36972500
H	-4.52353300	1.32043100	1.69436600	C	6.50158200	-2.94426000	0.29575500
C	-0.67592400	1.52539700	0.76604700	H	5.22473800	-3.14382000	-1.43029000
C	-0.08702600	1.97208500	1.96880800	C	6.56223400	-2.88985000	1.68799900
C	-1.83672200	2.18435300	0.32524100	H	5.42557100	-2.94293100	3.52163400
C	-0.61055800	3.05611700	2.66708000	H	7.41063800	-2.86671400	-0.29454200
H	0.78446400	1.44975100	2.34693400	H	7.51910100	-2.76900600	2.18821800
C	-2.35926800	3.27341500	1.01962600	TS14a'			
H	-2.32976100	1.83747600	-0.57037600	Rh	-1.41349400	-0.87028200	-0.56559300
C	-1.74615400	3.72122300	2.19161500	N	-0.39180100	-1.99866800	0.54591900
H	-0.14180900	3.37304200	3.59447500	C	-1.20295900	-2.13796500	-2.45988100
H	-3.24966800	3.77089400	0.64527400	C	-0.79144600	-0.78156800	-2.69614200
H	-2.15629800	4.56563900	2.73784000	C	-1.94432200	0.06880000	-2.49453900
N	2.10877100	1.41472200	-0.04191300	C	-3.05982200	-0.78632000	-2.17195800
N	1.66456300	2.37733200	-0.73838400	C	-2.61456800	-2.14320100	-2.17447800
N	2.32742900	3.52356000	-0.66378600	O	-3.99272600	-1.85520700	0.92134100
C	1.70116900	4.63312000	-1.40827400	C	0.68559300	-2.67836400	0.87262800
H	2.29587100	5.51687500	-1.15994900	C	1.85217700	-2.28148000	-0.00024200
C	1.79695200	4.39523300	-2.91982900	C	2.12996500	-1.01349700	-0.38592500
H	1.24207200	3.49350800	-3.19387800	O	0.77529100	-3.59791800	1.70677900
H	2.83803800	4.26618000	-3.23048300	C	0.07724400	0.42831300	0.14469600
C	0.25767800	4.87484200	-0.94930200	C	1.41211900	0.21923600	-0.10995900
H	-0.37477000	4.02386300	-1.20906000	C	-3.65739500	-0.73542100	1.30368800
H	0.20448900	4.99988200	0.13529700	O	-2.68340100	-0.01288900	0.80801500
C	3.42326600	3.75371400	0.30048300	C	-4.39502200	0.00801900	2.44505600

C	0.53645600	-0.32166400	-3.20777200	N	1.86849300	2.31313400	-0.76186500
H	0.52102700	-0.30518500	-4.30484800	N	2.57319400	3.43379400	-0.71482900
H	1.34034000	-0.98631700	-2.88712100	C	1.98344000	4.54967200	-1.47985400
H	0.77461700	0.68105200	-2.84741500	H	2.65388000	5.39764100	-1.31443900
C	-0.33580500	-3.35706100	-2.52731000	C	1.96962400	4.23097700	-2.97950900
H	0.71992700	-3.08776300	-2.56845700	H	1.32606800	3.36811500	-3.17396300
H	-0.57627200	-3.95024300	-3.41692700	H	2.97599900	3.99711400	-3.33917600
H	-0.48614200	-3.98507500	-1.64561300	C	0.58995600	4.91838500	-0.95550500
C	-3.45856700	-3.33886000	-1.86757600	H	-0.10416300	4.08961500	-1.10948200
H	-2.87511100	-4.26023400	-1.91570600	H	0.61340100	5.12886700	0.11668400
H	-4.28733900	-3.41968600	-2.58041100	C	3.69508400	3.63953000	0.22586200
H	-3.87502000	-3.23764000	-0.86077400	H	3.90480700	2.64210200	0.61572100
C	-4.45516100	-0.32634700	-1.88833700	C	4.94224200	4.15133900	-0.50252000
H	-4.97862700	-1.05375000	-1.26772100	H	5.21880100	3.47938800	-1.32002600
H	-5.00845400	-0.18339100	-2.82473600	H	5.78201400	4.20442100	0.19760800
H	-4.44637000	0.62361500	-1.34845400	H	4.79703400	5.15564800	-0.91532800
C	-2.00103600	1.53255800	-2.81177500	C	3.26765600	4.54366800	1.39022700
H	-2.85170200	2.01410300	-2.32448100	H	2.38794800	4.13085100	1.89197500
H	-2.11374400	1.68060300	-3.89366900	H	4.08019800	4.62319000	2.11975000
H	-1.08852400	2.04319100	-2.49489100	H	3.02847100	5.55635800	1.04702100
C	-5.48578000	-0.90217900	3.02383500	H	0.20787600	5.80086600	-1.47914700
H	-6.02134600	-0.38249900	3.82649300	H	1.58478300	5.08382800	-3.54768700
H	-5.05279800	-1.82012500	3.42983400	H	3.09128000	-0.85640000	-0.87450000
H	-6.20490100	-1.19186900	2.25287700	C	2.77401600	-3.43670700	-0.36805000
C	-3.36966400	0.38803800	3.53262400	H	3.00962200	-3.40011200	-1.43759400
H	-3.87174300	0.91210100	4.35425500	H	2.25016800	-4.37465800	-0.16587200
H	-2.59168100	1.03725700	3.12558400	C	4.06166100	-3.39096300	0.43814700
H	-2.88858700	-0.50534800	3.94493600	C	4.02521500	-3.58361800	1.82724200
C	-5.02206700	1.28835300	1.85484000	C	5.28819500	-3.13176100	-0.18239600
H	-5.56304500	1.83730200	2.63387300	C	5.20102000	-3.52655600	2.57331300
H	-5.73570300	1.04673600	1.05810900	H	3.06302600	-3.76405800	2.29933800
H	-4.24721800	1.94076100	1.44518600	C	6.46653900	-3.07374200	0.56701500
C	-0.36055100	1.55524100	0.97936200	H	5.32455900	-2.98074800	-1.25911000
C	0.31094400	1.79978400	2.19679400	C	6.42552200	-3.27154600	1.94721500
C	-1.43353000	2.40033100	0.64240200	H	5.16275800	-3.67958500	3.64848400
C	-0.05171900	2.86464100	3.01780900	H	7.41305600	-2.87558900	0.07115000
H	1.12581700	1.14375000	2.48411400	H	7.33984800	-3.22636200	2.53247700
C	-1.78790800	3.47356500	1.45495000	15a'			
H	-1.99228500	2.20397200	-0.26067500	Rh	1.25726000	-1.65656500	-0.05975300
C	-1.09924900	3.71351000	2.64655600	N	0.32344600	-0.07863000	-1.06360700
H	0.47736600	3.02705500	3.95259800	C	2.20009300	-2.68562200	-1.74795600
H	-2.61170600	4.11881200	1.16305900	C	1.31530900	-3.58549400	-1.09728500
H	-1.38459600	4.54348600	3.28641900	C	1.78580400	-3.77339300	0.28087400
N	2.30550000	1.33385700	-0.08064100	C	2.94555600	-2.98660800	0.47034200

C	3.18437700	-2.24902800	-0.76562400	C	-1.45930900	-1.57201600	1.01922000
O	3.36597700	0.30957300	1.61842200	C	-2.55378000	-1.84885500	-1.12248100
C	1.11503300	0.86978600	-1.69022700	C	-2.05216700	-2.76003200	1.46657500
C	0.45030500	2.09813000	-2.09969400	H	-0.84948000	-0.97671600	1.68798700
C	-0.89088400	2.25610800	-1.87384900	C	-3.14518500	-3.02599300	-0.67025200
O	2.33137600	0.65342000	-1.89152600	H	-2.74883100	-1.48590300	-2.12700000
C	-1.00648700	0.09451100	-0.83747500	C	-2.88850200	-3.49338500	0.62634500
C	-1.66131200	1.25811600	-1.22238400	H	-1.86652300	-3.09705100	2.48260200
C	2.17366600	0.45565500	1.88609900	H	-3.80486200	-3.58513900	-1.32791800
O	1.20356400	-0.33514100	1.50244300	H	-3.35311600	-4.41031200	0.97732200
C	1.65631000	1.65292300	2.71736000	N	-3.04252300	1.49826300	-1.04941600
C	0.13204900	-4.28033800	-1.69138900	N	-3.47439300	1.07167900	0.06711700
H	0.39058000	-5.31287800	-1.95810500	N	-4.77601000	1.23659700	0.29481600
H	-0.21351100	-3.76989200	-2.59141700	C	-5.25798800	0.60893800	1.54076500
H	-0.70316100	-4.31036800	-0.98790100	H	-6.13414800	1.18576500	1.84990700
C	2.14638100	-2.22971500	-3.17168900	C	-5.68205000	-0.85138800	1.31874600
H	1.16268700	-2.40963100	-3.60969200	H	-4.83437900	-1.43477500	0.94933200
H	2.88914700	-2.77709400	-3.76502300	H	-6.49695200	-0.92817600	0.59382400
H	2.36069900	-1.16083100	-3.22206000	C	-4.21252600	0.71860600	2.65689100
C	4.34871700	-1.34760700	-0.99134600	H	-3.34700900	0.08644700	2.45115700
H	4.28832600	-0.85215100	-1.95714100	H	-3.86264500	1.74842700	2.76606000
H	5.27416900	-1.93593900	-0.92632200	C	-5.66911900	1.73174200	-0.77492300
H	4.36226100	-0.58007100	-0.21290900	H	-5.10765600	2.54728800	-1.24164600
C	3.79291300	-2.87433500	1.69775200	C	-5.91288600	0.66206800	-1.85339100
H	4.04800400	-1.82772500	1.87438300	H	-4.96373700	0.24963400	-2.20074400
H	4.71594800	-3.45278900	1.56569800	H	-6.42669400	1.10797900	-2.71163500
H	3.27499200	-3.25922800	2.57869200	H	-6.53455000	-0.15290500	-1.47134000
C	1.12769700	-4.66988400	1.28149800	C	-6.97780800	2.29614600	-0.22203300
H	1.40233400	-4.39562900	2.30171200	H	-6.79745200	3.04872400	0.55152400
H	1.43180200	-5.71062800	1.11325100	H	-7.52858300	2.77494800	-1.03745700
H	0.03977700	-4.61925700	1.19545900	H	-7.62382700	1.51498300	0.19260600
C	2.84525600	2.45716300	3.25922600	H	-4.66384700	0.39893200	3.60171400
H	2.48487600	3.32077000	3.82991500	H	-6.02562300	-1.29502900	2.25956600
H	3.47003000	2.81741600	2.44022200	H	-1.39698000	3.17280600	-2.16755700
H	3.47079800	1.84264900	3.91408500	C	1.32246800	3.18726200	-2.68323500
C	0.79998400	2.53054400	1.77802900	H	0.70495800	3.87478500	-3.27173800
H	0.41173100	3.39757000	2.32461300	H	2.05735200	2.72768800	-3.35112600
H	-0.04417900	1.96336500	1.37670900	C	2.04352300	3.95848700	-1.58661100
H	1.39300200	2.90258800	0.93964400	C	3.26260500	3.49954700	-1.06761800
C	0.78705200	1.13673900	3.88061100	C	1.46449800	5.10608100	-1.02943200
H	0.42171500	1.97995700	4.47810000	C	3.88360200	4.17592000	-0.01639700
H	1.35976700	0.47773600	4.54359900	H	3.69214400	2.58890900	-1.46901200
H	-0.07695700	0.58109000	3.50701500	C	2.08422100	5.78270200	0.02244600
C	-1.70074700	-1.10797300	-0.28656300	H	0.51489300	5.46741400	-1.41802700

C	3.29752700	5.31809500	0.53390400	H	-3.39528200	-2.32293000	3.94818200
H	4.82232200	3.80018300	0.38109500	H	-4.52588600	-2.52842100	2.59631300
H	1.61841600	6.66980400	0.44342100	C	-3.35338100	0.43935500	4.00152900
H	3.77910600	5.83789000	1.35740000	H	-4.18188100	0.58546100	4.70437300
TS14a							
Rh	-1.31444600	-1.06966900	-0.71204100	H	-3.04686100	1.41848400	3.62072100
N	-0.29177400	-2.37691000	0.21787300	H	-2.50511100	0.00374600	4.53304800
C	-1.52687500	-2.39875500	-2.63303900	C	-4.94796700	0.16191000	2.07028000
C	-0.69132300	-1.22560900	-2.83110700	H	-5.79029700	0.35738400	2.74428400
C	-1.53608900	-0.05119000	-2.74810900	H	-5.29593100	-0.48996600	1.26456400
C	-2.82777000	-0.49347800	-2.36209500	H	-4.63515800	1.11187600	1.62613800
C	-2.81985600	-1.95195900	-2.29036100	C	-0.75220300	1.52412800	0.75977600
O	-1.46221800	-0.97899800	2.45538400	C	-0.20303000	2.02123800	1.96239300
C	0.71362200	-2.47780100	1.07699700	C	-1.94157400	2.11189800	0.29473000
C	1.84142200	-2.14158200	0.11299800	C	-0.79468100	3.08384900	2.63742100
C	2.08470900	-0.84994500	-0.24600200	H	0.68850500	1.55123600	2.36163900
O	0.87657900	-2.93184800	2.19786900	C	-2.53033700	3.18267400	0.96401100
C	-0.11316100	0.37913400	0.09273300	H	-2.40359100	1.72423300	-0.60006300
C	1.26189600	0.31759200	-0.04457400	C	-1.95816600	3.67935400	2.13671700
C	-2.55601100	-0.74807000	1.95010900	H	-0.35744200	3.43873600	3.56639400
O	-2.81382300	-0.72201900	0.66895800	H	-3.44126100	3.62549300	0.57098400
C	-3.79235900	-0.48211000	2.84933800	H	-2.42067800	4.50801100	2.66498900
C	0.73079500	-1.23380900	-3.29660000	N	2.06151100	1.50572700	0.02033400
H	0.78231500	-1.25489000	-4.39303700	N	1.59282200	2.44258500	-0.69544000
H	1.26343200	-2.10731600	-2.91466300	N	2.21273900	3.61292300	-0.62699000
H	1.25892100	-0.34280000	-2.94900700	C	1.54866200	4.69276700	-1.38327500
C	-1.01976900	-3.80591700	-2.66657800	H	2.10092500	5.60216600	-1.12953200
H	-0.33214100	-3.97766000	-1.82972100	C	1.67526400	4.45529300	-2.89248500
H	-0.48060500	-4.00217800	-3.59929100	H	1.16386800	3.52961700	-3.17090900
H	-1.83447900	-4.52798400	-2.58433500	H	2.72510500	4.37094400	-3.18867400
C	-4.01300400	-2.75889900	-1.88021600	C	0.09003700	4.87224200	-0.94376300
H	-3.76783900	-3.81735100	-1.77434800	H	-0.50017500	3.99197400	-1.20486400
H	-4.82570100	-2.66594600	-2.61077700	H	0.01768100	5.00238800	0.13913400
H	-4.38505300	-2.39941500	-0.91478000	C	3.28499200	3.89368900	0.35051900
C	-4.05014000	0.32564400	-2.08470400	H	3.59019800	2.90848000	0.70679200
H	-4.31518300	0.24987600	-1.02367700	C	4.48615900	4.56522100	-0.32227400
H	-4.89786500	-0.04326300	-2.67233100	H	4.84883600	3.96420600	-1.16110200
H	-3.90248900	1.37903600	-2.33261000	H	5.30027300	4.67222600	0.40159500
C	-1.08263800	1.34208200	-3.07121900	H	4.24589900	5.56713700	-0.69417500
H	-1.86816000	2.07607900	-2.88182100	C	2.73893900	4.69715000	1.53929300
H	-0.80856700	1.41060300	-4.13094000	H	1.88621000	4.18167100	1.98912600
H	-0.21050200	1.62660100	-2.47458200	H	3.51588200	4.81888300	2.30118600
C	-4.22185800	-1.85559000	3.40614700	H	2.41344300	5.69737600	1.23205000
H	-5.07108200	-1.73995000	4.08971200	H	-0.34821200	5.74780100	-1.43406600
				H	1.22097900	5.28102600	-3.44962100

H	3.07772200	-0.63956400	-0.64343700	H	1.36701000	4.99761500	1.08308900
C	2.76544000	-3.29055300	-0.24366300	H	0.58441800	6.63990500	2.78074900
H	2.88159700	-3.35953200	-1.33156100	H	-1.66736800	7.67662600	2.56636300
H	2.30753100	-4.22567300	0.09405600	C	0.04494200	4.09451900	-1.12014700
C	4.12692900	-3.12344200	0.41241000	H	-0.57686900	4.16490400	-2.01856700
C	4.22237200	-3.07000300	1.81135100	H	1.07816800	4.31109000	-1.40507000
C	5.28796700	-3.00223900	-0.35706600	C	-0.01777800	2.67847500	-0.57083200
C	5.46462400	-2.91019500	2.42199400	C	-1.13805400	1.92913800	-0.71941400
H	3.31196400	-3.13792600	2.40207900	H	-2.00209300	2.42281300	-1.16113300
C	6.53348900	-2.84122100	0.25695700	C	1.24746200	2.20656600	0.08410200
H	5.22038300	-3.03917500	-1.44201300	N	1.18475500	0.90407000	0.52058500
C	6.62421500	-2.79623600	1.64794500	O	2.23569600	2.94367900	0.18849800
H	5.52904400	-2.87133500	3.50588600	C	2.78519400	-0.72171700	1.76232100
H	7.42858200	-2.75119200	-0.35250600	C	3.41282700	-1.45621200	2.96847100
H	7.59076200	-2.67023500	2.12780000	C	4.14702400	-0.46898400	3.88596100
TS12c				H	4.56423000	-1.00298100	4.74691200
C	0.95674300	-1.36947100	-2.80966000	H	4.96510800	0.02891600	3.35735100
C	1.26883200	0.04084500	-2.94586300	H	3.46882300	0.30669300	4.24882500
C	2.67389600	0.22597200	-2.64226100	C	4.38244800	-2.53286900	2.44772000
C	3.18165500	-1.01959900	-2.19833500	H	4.81301000	-3.08755400	3.28851500
C	2.11775300	-2.01384500	-2.30989900	H	3.86389600	-3.23687800	1.79277200
Rh	1.44143100	-0.50123800	-0.80564500	H	5.20755000	-2.08081100	1.88549500
C	3.40471800	1.53333400	-2.72015800	C	2.23790500	-2.12112700	3.71961900
C	0.37295200	1.06251300	-3.57575100	H	2.61721900	-2.67015400	4.58897200
H	0.43158600	0.99766300	-4.67020400	H	1.52513600	-1.36971000	4.07379800
H	-0.66808300	0.90996400	-3.28231800	H	1.69912900	-2.81257000	3.06773000
H	0.65547700	2.07455500	-3.28049100	O	2.26803600	-1.48481600	0.87203400
C	-0.37554800	-1.98038700	-3.13008800	O	2.78220700	0.53375400	1.75029300
C	2.29699400	-3.45822400	-1.95077400	H	4.48426200	1.38607200	-2.64561800
H	1.36510300	-4.01898300	-2.05050200	H	3.19779200	2.03138700	-3.67339800
H	3.04387800	-3.92956500	-2.60049000	H	3.10927900	2.21258400	-1.91195500
H	2.64261000	-3.55296800	-0.91596300	H	-1.18685800	-1.43246800	-2.64077700
C	4.55601400	-1.32603400	-1.68571100	H	-0.55537700	-1.96719300	-4.21193000
H	4.49075400	-1.90631900	-0.76018200	H	-0.43204700	-3.01802300	-2.79340700
H	5.12991500	-1.91490700	-2.41191600	C	-1.40162000	0.56884600	-0.28919000
H	5.11316200	-0.41339600	-1.46538000	C	-0.46941400	-0.40328800	0.02063600
C	-2.13850300	6.62060500	0.74536700	C	-0.76305500	-1.48650200	0.97744500
C	-1.69043500	5.70204000	-0.20648200	C	-0.41820800	-2.82518200	0.72373100
C	-0.42380700	5.11641200	-0.09621300	C	-1.35612700	-1.18001800	2.21838800
C	0.39047200	5.46290100	0.99201900	C	-0.69385500	-3.82692600	1.65142600
C	-0.05714000	6.37949900	1.94320400	H	0.06707500	-3.07219700	-0.21303000
C	-1.32200700	6.96209300	1.82427800	C	-1.61947600	-2.17922500	3.15313600
H	-3.12300600	7.06912000	0.64192300	H	-1.60871600	-0.14710500	2.43488100
H	-2.33014600	5.44077700	-1.04658000	C	-1.29620500	-3.51033000	2.87181800

H	-0.43091300	-4.85659200	1.42498300	H	4.23844300	-2.16958500	1.73436200
H	-2.06945500	-1.91796300	4.10710800	H	5.60437400	-2.70919600	0.74219100
H	-1.49938500	-4.28914000	3.60116300	H	5.25668000	-0.96865700	0.94192500
N	-2.78831700	0.33032600	-0.10545600	C	-0.78371200	6.16111400	0.11369100
N	-3.14872900	-0.80678400	-0.54740300	C	-1.13961300	5.16736000	-0.80110100
N	-4.39368000	-1.17638900	-0.29358900	C	-0.22058000	4.18483800	-1.18703000
C	-4.73821600	-2.52089100	-0.79787800	C	1.06807200	4.20776300	-0.63205700
H	-5.75389800	-2.71146200	-0.43991500	C	1.42542000	5.20385900	0.27741900
C	-4.75316100	-2.53264700	-2.33092100	C	0.50252600	6.18352700	0.65407700
H	-3.75509100	-2.30352000	-2.71550600	H	-1.50991700	6.91748500	0.39936300
H	-5.45254200	-1.78732000	-2.72145200	H	-2.14208700	5.15754200	-1.22343900
C	-3.80601300	-3.59265500	-0.22004100	H	1.77809000	3.43405000	-0.90845600
H	-2.78477600	-3.43688800	-0.57260800	H	2.42826500	5.21182800	0.69395000
H	-3.78421600	-3.55159400	0.87217900	H	0.78507600	6.95721800	1.36255700
C	-5.27685600	-0.44223000	0.63665500	C	-0.61789300	3.10095900	-2.17800000
H	-4.76594800	0.50834300	0.79828600	H	-1.52366400	3.40769700	-2.71186500
C	-6.64326000	-0.16336600	0.00284300	H	0.17844800	2.98147800	-2.92100500
H	-6.53039100	0.36387100	-0.94878400	C	-0.85995000	1.76159000	-1.51783000
H	-7.24027300	0.46198800	0.67424600	C	-2.10239700	1.31425900	-1.11759600
H	-7.20993000	-1.08336200	-0.17749200	H	-2.97981000	1.92978400	-1.28906600
C	-5.37682500	-1.18161900	1.97816400	C	0.24195100	0.90161500	-1.25662500
H	-4.38002400	-1.35184600	2.39437300	N	0.05493600	-0.29072900	-0.64425700
H	-5.95825500	-0.58838400	2.69154200	O	1.48383000	1.12737700	-1.55950200
H	-5.87436400	-2.15148600	1.86741100	C	3.07569700	0.88763100	1.59203800
H	-4.13835100	-4.58940800	-0.52837200	C	2.88866100	1.48537300	3.01033200
H	-5.04994900	-3.51839700	-2.70325500	C	4.13235100	1.10660800	3.83737300
13c				H	4.08702500	1.56810200	4.83045700
C	2.21559900	-2.59404700	-1.85798700	H	4.19776400	0.02038000	3.97434500
C	3.01212300	-1.59407300	-2.48726700	H	5.04049500	1.44115500	3.33050300
C	4.07002500	-1.20792100	-1.55778300	C	1.61579200	0.97216600	3.69786900
C	3.92947400	-2.00454100	-0.37888500	H	1.51401600	1.42658600	4.69052000
C	2.76276100	-2.83654200	-0.53132300	H	0.72655600	1.21584900	3.11105400
Rh	2.13676800	-0.75772500	-0.67259000	H	1.64466100	-0.11506200	3.82192000
C	5.12636100	-0.17826500	-1.80912200	C	2.81792800	3.01642800	2.84586500
C	2.80184600	-0.96761600	-3.83167800	H	2.76142200	3.50434400	3.82604600
H	3.66187900	-1.15718400	-4.48334600	H	3.70478100	3.38154200	2.32055800
H	1.90877600	-1.36122400	-4.32046400	H	1.93455100	3.30669200	2.26913100
H	2.67802100	0.11457500	-3.72566000	O	2.08829400	0.14282100	1.19183700
C	0.99826200	-3.26976700	-2.41063900	O	4.10472700	1.13836700	0.95592400
C	2.30316700	-3.89502300	0.42039400	H	5.23826400	0.45207000	-0.92450600
H	1.23693800	-4.09769300	0.31419200	H	6.08508300	-0.65700200	-2.04408500
H	2.85130200	-4.82880500	0.23889200	H	4.84997900	0.46252800	-2.64923700
H	2.47497700	-3.59824000	1.45665300	H	1.24786800	-4.27728500	-2.76446600
C	4.81100500	-1.95640200	0.82859800	H	0.22538500	-3.36131600	-1.64315200

H	0.57479300	-2.70838200	-3.24552700	C	3.27624600	-1.41722600	-2.79616300
C	-2.28119300	0.07401300	-0.45336700	C	0.47382900	-0.24916800	-3.69659000
C	-1.14609300	-0.71346600	-0.20325300	H	0.47503800	-0.59094900	-4.74028100
C	-1.16776000	-1.96413400	0.59467800	H	-0.47074900	0.26305100	-3.50337300
C	-2.01968400	-3.03320400	0.27962000	H	1.28081900	0.47736300	-3.57785700
C	-0.31650900	-2.06812400	1.70684100	C	-1.83019800	-2.19181600	-2.72696400
C	-2.02117200	-4.18825600	1.06218200	C	-0.36266700	-4.59454100	-1.00954300
H	-2.68091600	-2.94892800	-0.57543500	H	-1.43374400	-4.66385100	-1.20930500
C	-0.34052700	-3.21548600	2.50052600	H	0.11096200	-5.49384800	-1.41993700
H	0.35575000	-1.24768700	1.93800800	H	-0.21701700	-4.60627400	0.07546200
C	-1.18652100	-4.27968500	2.17988900	C	2.68445500	-4.04821400	-0.97532900
H	-2.67958200	-5.01307000	0.80392900	H	2.41419500	-4.15658100	0.08037700
H	0.30923400	-3.27953900	3.36918700	H	2.69716300	-5.05055100	-1.42084500
H	-1.19770500	-5.17416400	2.79650000	H	3.69653500	-3.64170600	-1.02046900
N	-3.51043500	-0.41353400	0.02610600	C	0.64228300	6.70258800	-0.11883600
N	-4.51492000	0.30390900	-0.26029000	C	0.45204900	5.66051300	-1.02977900
N	-5.67923300	-0.10912200	0.25398500	C	1.30166700	4.54804800	-1.03924100
C	-6.85061700	0.57634700	-0.32232900	C	2.35105800	4.49458900	-0.10786700
H	-7.72252800	0.11446800	0.14693700	C	2.53735400	5.53157000	0.80545900
C	-6.83618800	2.06506400	0.04572500	C	1.68674200	6.64055300	0.80375800
H	-5.95263000	2.54913500	-0.37842200	H	-0.02709800	7.55887900	-0.13044900
H	-6.80890000	2.19449200	1.13149500	H	-0.36746500	5.71210200	-1.74333100
C	-6.94743300	0.36255100	-1.84089400	H	3.01297500	3.63557900	-0.08808500
H	-6.07872200	0.80355000	-2.33741000	H	3.35018600	5.46902000	1.52380500
H	-6.97803200	-0.70265800	-2.08743100	H	1.83620500	7.44710200	1.51642500
C	-5.77305800	-1.37789200	1.00262200	C	1.06321200	3.40742500	-2.01789400
H	-4.80161000	-1.47068000	1.49483900	H	0.25960900	3.68547600	-2.70649600
C	-6.86056100	-1.32791100	2.07878400	H	1.96523400	3.23599200	-2.61023800
H	-6.76252700	-0.42963100	2.69532200	C	0.68878200	2.11205900	-1.30056100
H	-6.76152600	-2.20215600	2.72980900	C	-0.62208400	1.88691200	-1.04450900
H	-7.87133900	-1.35215800	1.65780700	H	-1.27734300	2.69107900	-1.37751400
C	-5.93542600	-2.57599400	0.05602000	C	1.87628600	1.29111500	-0.92907900
H	-5.14488100	-2.56894100	-0.69821500	N	1.70015100	0.29518700	0.03347300
H	-5.86967100	-3.51577700	0.61473000	O	2.97761800	1.53597900	-1.42991500
H	-6.90609200	-2.54948100	-0.45141400	C	3.78838000	0.44164200	1.14524800
H	-7.85238300	0.83474300	-2.23715100	C	5.03827000	-0.36428600	1.51528400
H	-7.72897000	2.56436200	-0.34444500	C	5.97885000	0.54222600	2.32111300
11d				H	6.86875900	-0.01982100	2.62317100
C	-0.37914600	-2.34374700	-2.37763000	H	6.29577800	1.40336400	1.72631900
C	0.65684100	-1.41112800	-2.76939100	H	5.48184700	0.92441500	3.21610400
C	1.95224700	-2.00364800	-2.42022600	C	5.73558600	-0.86628700	0.23500300
C	1.70072300	-3.15688800	-1.67008000	H	6.65584700	-1.39879000	0.49855400
C	0.24808100	-3.36818400	-1.61995100	H	5.08683800	-1.54463000	-0.32290800
Rh	0.62059900	-1.38889500	-0.60267000	H	5.99592700	-0.03203100	-0.42361900

C	4.58083200	-1.56628900	2.37325100	H	-5.61646800	2.52761500	2.84924600
H	5.45007300	-2.15981000	2.67640700	H	-6.43040900	1.10228500	2.18726500
H	4.07064000	-1.22483900	3.28069800	H	-6.50764000	-1.99338400	-0.03102600
H	3.89529200	-2.20834000	1.81367400	H	-6.81723800	-0.79105000	-2.29762900
O	3.50516700	1.54437300	1.54716500	C	0.93611400	-1.44362800	2.48519700
O	2.99468800	-0.30311800	0.32232200	O	0.91445200	-2.13749800	1.45263600
H	4.09987300	-2.04864500	-2.45817300	O	1.00462100	-0.13997300	2.50563500
H	3.34489900	-1.32776300	-3.88685400	H	1.12929600	0.23411900	1.55585900
H	3.41529500	-0.41927400	-2.37008900	C	0.82887100	-2.08864300	3.83779200
H	-2.25079300	-1.28089100	-2.28776500	H	1.37668200	-1.51443500	4.58664400
H	-1.94975000	-2.13238800	-3.81472900	H	-0.23209500	-2.09768200	4.11082100
H	-2.42177700	-3.03827300	-2.37134800	H	1.18802800	-3.11682300	3.78959600
C	-1.39575100	0.86153200	-0.35249700	TS12d			
C	-1.05167300	-0.40069700	0.03311100	C	-0.90083600	-2.20105000	-2.38457400
C	-1.86878100	-1.12438100	1.03759100	C	0.26685500	-1.42945900	-2.77299100
C	-2.29853500	-2.44985400	0.86886900	C	1.44798400	-2.21477200	-2.46180700
C	-2.16275100	-0.49925700	2.26887000	C	1.02072500	-3.36359900	-1.75256900
C	-2.99841100	-3.12382300	1.86859600	C	-0.44033500	-3.36531000	-1.72416300
H	-2.09009900	-2.94645500	-0.06638900	Rh	0.32367700	-1.54018500	-0.56809200
C	-2.85912500	-1.17077300	3.27218400	C	2.84576800	-1.83833600	-2.83570500
H	-1.83325100	0.52174700	2.42701000	C	0.23537700	-0.21326300	-3.64553200
C	-3.28222300	-2.49066300	3.08021000	H	0.12993500	-0.50757100	-4.69798800
H	-3.32634900	-4.14584900	1.69766800	H	-0.60372800	0.43447700	-3.38488700
H	-3.06814500	-0.66232800	4.20993000	H	1.15215000	0.37101800	-3.54749900
H	-3.82305000	-3.01475000	3.86285300	C	-2.31429200	-1.78389600	-2.66044300
N	-2.69947600	1.39170000	-0.04165200	C	-1.23918300	-4.45865400	-1.08554900
N	-3.63600000	0.64000800	-0.43617100	H	-2.30814300	-4.35365400	-1.28275700
N	-4.87644700	1.02616700	-0.14034200	H	-0.91932000	-5.43532500	-1.46453400
C	-5.91371900	0.04256400	-0.50363200	H	-1.08057200	-4.44706200	-0.00101900
H	-6.85142200	0.45891400	-0.12404000	C	1.86495700	-4.43666600	-1.13720500
C	-6.02311800	-0.08727600	-2.02754400	H	1.51026200	-4.65382500	-0.12543200
H	-5.07860400	-0.45542100	-2.43830800	H	1.81624000	-5.36342100	-1.72233800
H	-6.24351600	0.88102200	-2.48672400	H	2.90992800	-4.12951900	-1.06553000
C	-5.67402900	-1.31301400	0.17350300	C	2.19179200	6.47346500	-0.36539200
H	-4.75224200	-1.76418100	-0.19852400	C	1.81594800	5.42603000	-1.21021400
H	-5.57021200	-1.20147300	1.25604100	C	2.21019400	4.10962500	-0.94377300
C	-5.16076100	2.16359400	0.75674100	C	2.98610400	3.85648100	0.19862500
H	-4.22052400	2.71682300	0.79342700	C	3.35531800	4.90092200	1.04524900
C	-6.24201900	3.07777400	0.17144500	C	2.96359300	6.21326500	0.76700400
H	-5.97377700	3.39943700	-0.83901200	H	1.87693800	7.48877200	-0.59177500
H	-6.35043300	3.96834500	0.79888000	H	1.20982800	5.63521600	-2.08902600
H	-7.22105700	2.58812300	0.12848800	H	3.29701800	2.84636100	0.43975600
C	-5.49599400	1.67477600	2.17281000	H	3.94914500	4.68204500	1.92823600
H	-4.69524900	1.03565700	2.55449000	H	3.25406400	7.02403600	1.42946700

C	1.79143300	2.98514200	-1.88133600	N	-2.45295300	1.82061200	-0.05264000
H	1.14353100	3.39021700	-2.66519100	N	-3.49072700	1.22085300	-0.46139300
H	2.67845300	2.56802400	-2.36615500	N	-4.65749600	1.79330100	-0.18887700
C	1.05681600	1.86476900	-1.15745500	C	-5.82986100	1.00619600	-0.61591600
C	-0.28587700	1.93114000	-1.00610400	H	-6.69836100	1.56937400	-0.26255200
H	-0.75215300	2.82963600	-1.40741400	C	-5.89493000	0.92303300	-2.14546600
C	1.96797800	0.78546900	-0.64998700	H	-5.01500200	0.39768000	-2.52795300
N	1.36081600	-0.10536700	0.19606900	H	-5.91920800	1.92230300	-2.59029100
O	3.17039300	0.80014600	-0.95172900	C	-5.85041100	-0.38069900	0.03863300
C	3.85232600	-0.03062400	1.49296700	H	-4.99933900	-0.97338700	-0.30244700
C	5.31016200	-0.31979000	1.10206400	H	-5.78113500	-0.30531200	1.12691300
C	5.97572600	-0.88841500	2.37782800	C	-4.78532600	2.95624900	0.71367100
H	7.03691600	-1.08437100	2.18890800	H	-3.76612000	3.33343400	0.81275100
H	5.89345400	-0.17822400	3.20557700	C	-5.65278000	4.05335000	0.08800400
H	5.50516100	-1.82966900	2.68297600	H	-5.26931600	4.33855100	-0.89589200
C	5.97905000	1.01155000	0.71345400	H	-5.64538200	4.93967400	0.73039300
H	7.04577300	0.85348000	0.51923700	H	-6.69669100	3.74120400	-0.02572600
H	5.51275800	1.42229100	-0.18571500	C	-5.28209400	2.51635300	2.09769300
H	5.87227700	1.74257700	1.51842300	H	-4.62653600	1.74447700	2.51026800
C	5.42378900	-1.33305000	-0.04518500	H	-5.29170800	3.37003100	2.78339900
H	6.47999900	-1.50930400	-0.27895800	H	-6.30100700	2.11581400	2.04966000
H	4.96394300	-2.28793300	0.22403100	H	-6.77447000	-0.90889300	-0.21911800
H	4.92227800	-0.94977500	-0.93406800	H	-6.78971800	0.37777900	-2.46279200
O	3.52832700	0.92382600	2.16910000	C	0.52425000	-2.46120000	2.44376600
O	2.95922500	-0.98127600	1.09759100	O	0.18129500	-2.70565200	1.24209500
H	3.57805700	-2.47321900	-2.33561900	O	1.40626000	-1.63698800	2.81469300
H	2.98048100	-1.94602500	-3.91920200	H	2.17828600	-1.21047000	1.91652600
H	3.06793000	-0.80317500	-2.56531000	C	-0.22262400	-3.22358500	3.51632900
H	-2.54623900	-0.82764000	-2.17913200	H	0.33029800	-3.20783600	4.45608900
H	-2.46873500	-1.66823900	-3.73942800	H	-1.19417400	-2.74058100	3.65800500
H	-3.03061700	-2.52357400	-2.29669100	H	-0.40613200	-4.24981800	3.19041400
C	-1.25095200	1.08282300	-0.31890900	13d			
C	-1.13353800	-0.20585100	0.11452300	C	2.37238500	-3.21236200	-1.31006700
C	-2.02644300	-0.74556100	1.15643600	C	2.78805500	-1.99126200	-1.95777700
C	-2.73548800	-1.94837400	1.00495900	C	3.91739500	-1.46909600	-1.23357900
C	-2.15879200	-0.04876200	2.37452600	C	4.21843600	-2.37315300	-0.13752800
C	-3.58606900	-2.41446400	2.00447500	C	3.26334500	-3.43864100	-0.19003400
H	-2.62336500	-2.50924400	0.08752900	Rh	2.21212600	-1.53718600	0.07129900
C	-3.00284900	-0.51836000	3.37971200	C	4.60792500	-0.17896200	-1.54068200
H	-1.59667000	0.86833200	2.51426700	C	2.17564600	-1.35973300	-3.16726000
C	-3.73064900	-1.69893900	3.19615900	H	2.76000300	-1.61141400	-4.06091200
H	-4.13771800	-3.33831800	1.85357000	H	1.15264400	-1.71009300	-3.31558400
H	-3.08773900	0.03538300	4.31058000	H	2.14709500	-0.27538400	-3.04323200
H	-4.38966300	-2.06378400	3.97865900	C	1.32496200	-4.15957100	-1.79617200

C	3.14147300	-4.58169600	0.76658000	H	5.38497700	0.04363100	-0.80830400
H	2.08988700	-4.81149700	0.95456200	H	5.06837600	-0.22920200	-2.53427600
H	3.61715900	-5.47645100	0.34674400	H	3.87645700	0.63516900	-1.53233100
H	3.61728700	-4.35629300	1.72253400	H	0.53784200	-3.63524000	-2.33712600
C	5.32068300	-2.17990400	0.85875700	H	1.77702700	-4.89516500	-2.47409400
H	5.18895900	-2.82883200	1.72671100	H	0.85131100	-4.69594200	-0.97352400
H	6.29561400	-2.40522400	0.41096100	C	-2.01182300	-0.28775800	-0.12201800
H	5.33784100	-1.14604000	1.21348100	C	-0.88600000	-1.10725200	-0.08495200
C	-3.59962700	5.09734400	-1.07421300	C	-1.06582800	-2.57917800	0.11214700
C	-2.57164800	4.28085100	-1.55243200	C	-1.80987700	-3.28587900	-0.84850800
C	-1.47430000	3.96016600	-0.74400900	C	-0.56594300	-3.28038300	1.21712200
C	-1.42158500	4.47881000	0.55892000	C	-2.03449000	-4.65561900	-0.72144600
C	-2.44338200	5.30034700	1.03552100	H	-2.21887100	-2.74375200	-1.69522300
C	-3.53803600	5.60936500	0.22314600	C	-0.78782900	-4.65552300	1.34326000
H	-4.44502000	5.33452600	-1.71480400	H	-0.01843200	-2.74632300	1.98190400
H	-2.62293500	3.88029400	-2.56240600	C	-1.51819100	-5.34962900	0.37630500
H	-0.57002000	4.23004900	1.18645000	H	-2.61324700	-5.17979900	-1.47687900
H	-2.38704400	5.69876600	2.04516400	H	-0.40177900	-5.17979900	2.21383100
H	-4.33478200	6.24654900	0.59722900	H	-1.69323800	-6.41678200	0.48160400
C	-0.39388700	3.01834600	-1.21968200	N	-3.25582600	-0.87109500	0.19134000
H	-0.29491900	3.06529000	-2.31326600	N	-4.24284400	-0.09697000	0.01687600
H	0.57349000	3.31921200	-0.81686600	N	-5.43763300	-0.58594000	0.38247900
C	-0.62118900	1.57888700	-0.80565300	C	-6.56195300	0.22685100	-0.11605000
C	-1.84248400	1.08220400	-0.45366400	H	-7.46868800	-0.27541700	0.22993600
H	-2.71454100	1.72504500	-0.43730300	C	-6.52539200	1.63176000	0.50095000
C	0.54127800	0.70799300	-0.79462300	H	-5.62232100	2.16372400	0.19038600
N	0.35865600	-0.59710100	-0.33984500	H	-6.52931500	1.57313800	1.59329300
O	1.67378100	1.10144600	-1.16623300	C	-6.59104300	0.28566200	-1.65200900
C	2.74874300	3.47857400	0.78731300	H	-5.68343800	0.77194400	-2.02053800
C	3.16263400	4.77666800	0.08486300	H	-6.64383800	-0.71661300	-2.08689300
C	4.49137100	5.26292700	0.70434800	C	-5.57729000	-1.98555800	0.82638800
H	4.82361900	6.17630300	0.19887400	H	-4.65274500	-2.18376200	1.37581400
H	4.36957400	5.49165000	1.76884600	C	-6.75934500	-2.16515900	1.78203900
H	5.27189700	4.50474900	0.60238300	H	-6.73847600	-1.41607300	2.57915900
C	2.07346300	5.84086200	0.27471500	H	-6.70299600	-3.15702900	2.24160500
H	2.38987900	6.78250200	-0.18670100	H	-7.72585700	-2.10102900	1.27070100
H	1.12841400	5.53625900	-0.18083400	C	-5.62947300	-2.96053000	-0.35993000
H	1.88201800	6.02003300	1.33622400	H	-4.76820200	-2.80247200	-1.01231500
C	3.37023100	4.47501400	-1.41567800	H	-5.60028400	-3.99605700	-0.00364300
H	3.62488500	5.39879300	-1.94710800	H	-6.54891700	-2.82561400	-0.94025600
H	4.17842500	3.75371700	-1.55758100	H	-7.45837400	0.85776700	-1.99838800
H	2.46667500	4.05334900	-1.86470800	H	-7.39762400	2.21035600	0.17887700
O	1.71786700	3.34010700	1.43154500	C	2.03837600	-0.27656100	2.34472500
O	3.64755200	2.50806800	0.62728800	O	1.59012700	-1.45605400	2.26951400

O	2.71418700	0.15988300	1.34753100	C	-1.40999900	2.07202800	-0.12759600
H	3.24419800	1.65246400	0.93891600	N	-1.60404800	0.73965600	-0.29232000
C	1.79141700	0.62697800	3.51633800	O	-2.15691600	2.94824400	-0.59297400
H	1.45345100	1.59371900	3.12991900	C	-3.95304400	0.64702000	-0.76953000
H	1.05996200	0.18908600	4.19574700	C	-4.95724900	0.66759600	-1.92403900
H	2.73343800	0.79554600	4.04888000	C	-4.45588500	1.61237000	-3.03584400
11e							
C	-0.26501100	-1.78758100	2.71970200	H	-5.23414800	1.72996400	-3.79731200
C	-0.74447100	-0.43377800	2.90454900	H	-4.20416300	2.59351900	-2.62503800
C	-2.20622700	-0.45401900	2.81566700	H	-3.55870000	1.21795800	-3.51846700
C	-2.59503300	-1.73655500	2.41564300	C	-6.30280100	1.16021200	-1.36749200
C	-1.38152100	-2.56466700	2.32435100	H	-7.05242900	1.16174800	-2.16524300
Rh	-1.09001200	-0.91480100	0.81899400	H	-6.65290900	0.51710700	-0.55639000
C	-3.06044700	0.73970600	3.09840300	H	-6.21238300	2.17610900	-0.97317600
C	0.05871600	0.66706100	3.52151600	C	-5.10702300	-0.77307300	-2.46445700
H	0.10839400	0.52192300	4.60941300	H	-5.87377000	-0.79126500	-3.24599800
H	1.07789300	0.67688300	3.13134000	H	-4.17369200	-1.13606600	-2.90120800
H	-0.38669900	1.64267200	3.32686800	H	-5.41463400	-1.46213200	-1.67046600
C	1.15861500	-2.20662800	2.94040700	O	-4.22224900	0.70018800	0.40413500
C	-1.40878300	-4.01676400	1.95564100	O	-2.66844500	0.52374800	-1.23982500
H	-0.43298000	-4.48898100	2.08842700	H	-4.11721200	0.52684400	2.94708000
H	-2.13309300	-4.55328200	2.57847300	H	-2.90558700	1.06498400	4.13441000
H	-1.70799300	-4.13585800	0.90914800	H	-2.80185900	1.56958300	2.43566600
C	-3.97722100	-2.21988700	2.09506400	H	1.84077100	-1.63251300	2.30401200
H	-3.95329500	-2.90019500	1.23822800	H	1.44043400	-2.03015800	3.98535800
H	-4.41924400	-2.76520600	2.93893200	H	1.31001800	-3.26741100	2.73040400
H	-4.62847700	-1.38322400	1.83609600	C	1.43446900	0.52128200	0.10543400
C	2.34051700	6.45590600	0.36493600	C	0.73353200	-0.63657700	-0.05370500
C	1.63431700	5.48207600	1.07679500	C	1.25749400	-1.74663300	-0.88235200
C	0.47336500	4.90805700	0.54744700	C	1.24334100	-3.08936800	-0.46119900
C	0.02731100	5.32518600	-0.71585300	C	1.73683400	-1.48565000	-2.18447100
C	0.73024000	6.29746100	-1.42532100	C	1.73880300	-4.11299400	-1.26774500
C	1.88962900	6.86712500	-0.88909400	H	0.84467500	-3.32692900	0.51479600
H	3.23962100	6.89201900	0.79250200	C	2.22346700	-2.50775300	-2.99732600
H	1.98804400	5.16790000	2.05646000	H	1.73668600	-0.46142400	-2.54200600
H	-0.86720000	4.86568100	-1.12566000	C	2.24102600	-3.83030800	-2.54034800
H	0.37302600	6.61303700	-2.40221000	H	1.73143400	-5.13571800	-0.89987400
H	2.43512600	7.62480900	-1.44509200	H	2.58790000	-2.27105300	-3.99350100
C	-0.28047900	3.83170800	1.30960300	H	2.62730300	-4.62606400	-3.17067700
H	0.12174700	3.76772700	2.32739700	N	2.81792200	0.61204700	-0.27994400
H	-1.33434000	4.11188900	1.38550500	N	3.52505200	-0.28492800	0.26333100
C	-0.18962200	2.45834500	0.64866000	N	4.81423800	-0.31831600	-0.07364400
C	0.99070500	1.79936300	0.66970400	C	5.54152300	-1.47944800	0.47154900
H	1.81271000	2.34824500	1.13235300	H	6.55071600	-1.40990200	0.05474900
				C	5.64214100	-1.38389300	1.99856000

H	4.64223600	-1.40918000	2.44107100	H	-4.51828800	-2.07753300	3.05277400
H	6.12705200	-0.45020100	2.29878900	H	-4.65031000	-0.66523000	1.97158200
C	4.91763100	-2.80560500	0.01672600	C	3.07517200	6.43046300	0.43682600
H	3.90867000	-2.91011700	0.42115300	C	2.12056900	5.57699800	0.99802300
H	4.83961800	-2.85232700	-1.07254200	C	1.19394900	4.91488000	0.18723300
C	5.37396500	0.51641200	-1.15445500	C	1.23764600	5.11011800	-1.20150000
H	4.62305300	1.29364100	-1.30834500	C	2.18844900	5.96179800	-1.76000400
C	6.68388600	1.18263700	-0.72102900	C	3.11007100	6.62573300	-0.94351400
H	6.54419200	1.74759000	0.20507300	H	3.78838500	6.93983700	1.07919200
H	7.02028000	1.87545200	-1.49912700	H	2.09465100	5.42844300	2.07521700
H	7.48711800	0.45448800	-0.56276700	H	0.53117100	4.57264600	-1.82900100
C	5.51751300	-0.28928400	-2.45329000	H	2.21321300	6.10700100	-2.83654000
H	4.56126500	-0.74373500	-2.72577400	H	3.85079700	7.28823300	-1.38258900
H	5.84165300	0.36303000	-3.27108900	C	0.15852800	3.97715300	0.78583800
H	6.26061700	-1.08785800	-2.34788900	H	0.24124600	3.98277400	1.87889500
H	5.52435400	-3.65013600	0.36088800	H	-0.84718500	4.33385100	0.54146900
H	6.22030900	-2.22304900	2.39914700	C	0.31626900	2.55827200	0.26634500
C	-1.66315800	-2.40710700	-2.06161900	C	1.41315200	1.80266700	0.47447200
O	-1.78398700	-2.36799500	-0.83354200	H	2.26980700	2.29148700	0.93843600
O	-1.67106800	-1.33859600	-2.83771600	C	-0.79042700	2.10736400	-0.67961900
H	-1.91879400	-0.54653000	-2.29509900	N	-1.46730300	1.24052800	0.08601100
C	-1.47072500	-3.69117700	-2.81258600	O	-0.99573100	2.64310300	-1.75707600
H	-2.08002300	-3.70137300	-3.71888100	C	-4.35664500	0.95668300	-0.59713200
H	-0.41726900	-3.75040100	-3.10416500	C	-5.50821800	0.43443100	-1.49322000
H	-1.70833600	-4.53720900	-2.16909600	C	-5.28143700	0.78094300	-2.97653300
TS12e				H	-6.15605800	0.47160900	-3.55939100
C	-0.32299500	-1.53716600	2.67627600	H	-5.14542000	1.85806200	-3.11252500
C	-0.64046800	-0.13815300	2.87556600	H	-4.40622600	0.27312300	-3.38606600
C	-2.09432400	0.00874600	2.83824500	C	-6.81817600	1.07138900	-0.99715100
C	-2.63603900	-1.22657200	2.44857400	H	-7.66362000	0.67516400	-1.56989900
C	-1.53509500	-2.18831300	2.33789900	H	-6.97647200	0.86196600	0.06264800
Rh	-1.11888400	-0.53621100	0.77738000	H	-6.79810200	2.15833100	-1.12366600
C	-2.80676700	1.29842900	3.08333000	C	-5.58240300	-1.09823900	-1.31294700
C	0.31692300	0.88359400	3.40234100	H	-6.40455200	-1.49876500	-1.91606300
H	0.39725200	0.79734800	4.49405300	H	-4.65954900	-1.58312600	-1.63703800
H	1.31242100	0.74342800	2.97622900	H	-5.76530600	-1.36066400	-0.26718900
H	-0.01432800	1.89540900	3.16451600	O	-4.53986900	1.29213400	0.55974800
C	1.04636800	-2.12339300	2.85524200	O	-3.15632100	1.04131700	-1.17130200
C	-1.73904200	-3.62312700	1.96436600	H	-3.88607500	1.15903000	3.12406400
H	-0.84716800	-4.22490900	2.15254300	H	-2.46435500	1.74591800	4.02303800
H	-2.56750200	-4.05199700	2.53750000	H	-2.60837500	1.99695800	2.26366400
H	-1.98923100	-3.69442000	0.89925200	H	1.77153500	-1.66359200	2.17563500
C	-4.07213500	-1.56351900	2.19168900	H	1.38981600	-1.95361600	3.88262700
H	-4.15120000	-2.23054600	1.32857200	H	1.05288000	-3.20054000	2.67654700

C	1.64655500	0.43507300	0.02440900	13e			
C	0.72259000	-0.55811700	-0.14464200	C	-0.03010400	-0.46687700	2.79469500
C	1.04592700	-1.73932400	-0.97460400	C	-0.51957200	0.85235200	2.53626700
C	0.84895900	-3.06243100	-0.54457700	C	-1.98500900	0.78335800	2.41852800
C	1.55041600	-1.54384100	-2.27708100	C	-2.36807300	-0.55803000	2.49819500
C	1.19615100	-4.14500200	-1.35002500	C	-1.14878600	-1.35924400	2.64321900
H	0.42648200	-3.23708700	0.43381600	Rh	-0.83166600	-0.36509200	0.72504200
C	1.88714800	-2.62499200	-3.08988900	C	-2.86312000	1.97745100	2.21573300
H	1.68617800	-0.52924600	-2.63642700	C	0.27843600	2.10947100	2.69493400
C	1.72537800	-3.93460900	-2.62587500	H	0.30977800	2.41101400	3.75036200
H	1.04976000	-5.15660600	-0.98122200	H	1.30434800	1.97356000	2.34655800
H	2.27273900	-2.44411300	-4.08949900	H	-0.15829900	2.93195500	2.12686700
H	1.99173600	-4.77787800	-3.25643900	C	1.38561900	-0.80797400	3.15315200
N	3.03153600	0.23362100	-0.29402200	C	-1.18337700	-2.84628900	2.82314400
N	3.51403000	-0.77740000	0.29809300	H	-0.22151300	-3.24404800	3.15249600
N	4.77299100	-1.09205500	0.01559500	H	-1.93363600	-3.11559700	3.57459600
C	5.24543900	-2.32900600	0.66607100	H	-1.45617000	-3.33061700	1.87979700
H	6.25979000	-2.48439400	0.28729000	C	-3.73981600	-1.15263300	2.44407600
C	5.32076000	-2.14547200	2.18658300	H	-3.80139200	-1.89541700	1.64290000
H	4.32236600	-1.95702600	2.59159700	H	-3.96617900	-1.66208700	3.38943700
H	5.96226700	-1.29791300	2.44558200	H	-4.50249500	-0.39639300	2.26406100
C	4.38816300	-3.53809100	0.27157100	C	2.18518800	6.21456400	0.71389000
H	3.36721100	-3.41578500	0.63845000	C	1.12032100	5.32527900	0.55887900
H	4.33435800	-3.64635700	-0.81489700	C	0.89194700	4.69012800	-0.66724700
C	5.53891300	-0.43556100	-1.06336700	C	1.75241900	4.96310200	-1.73895900
H	4.94736900	0.44682400	-1.31345900	C	2.81824000	5.84986100	-1.58782700
C	6.91441500	0.02311000	-0.56792300	C	3.03764000	6.47826600	-0.35952700
H	6.81555100	0.66720100	0.31051600	H	2.34651200	6.70207300	1.67108800
H	7.41983900	0.59095100	-1.35565900	H	0.45697400	5.12604900	1.39646200
H	7.56243100	-0.82037600	-0.30589500	H	1.58716800	4.46971300	-2.69341100
C	5.61993700	-1.33951500	-2.30138800	H	3.47584500	6.05184700	-2.42843800
H	4.61768600	-1.63099700	-2.62731500	H	3.86608800	7.17063300	-0.24141100
H	6.11456000	-0.81003600	-3.12240000	C	-0.23854500	3.70126800	-0.82811800
H	6.19533400	-2.24945600	-2.09726500	H	-1.02982500	3.91317000	-0.09504200
H	4.80799400	-4.45635200	0.69575400	H	-0.70863300	3.84025200	-1.81381800
H	5.72280000	-3.04598600	2.66202000	C	0.16707100	2.24811700	-0.68709300
C	-2.09251300	-1.80322200	-1.96072300	C	1.40352700	1.79335300	-0.43049200
O	-1.91399400	-1.89995300	-0.70264200	H	2.19005300	2.53528500	-0.34975100
O	-2.33019800	-0.73835800	-2.59635600	C	-1.85427200	1.50617400	-1.61180500
H	-2.80135200	0.26534400	-1.85818400	N	-0.91314600	1.30342000	-0.83221100
C	-2.00344700	-3.09118200	-2.75065600	O	-2.73624200	1.72074600	-2.34279100
H	-2.55794100	-3.00468500	-3.68596300	C	-5.33555000	0.36211100	-0.20073900
H	-0.94835700	-3.27455300	-2.97512000	C	-6.17419800	-0.32476200	-1.29308300
H	-2.36906300	-3.93043300	-2.15576100	C	-5.72309000	0.16563900	-2.68651600

H	-6.36602600	-0.28142000	-3.45273700	H	5.06189700	0.36271600	-1.86304700
H	-5.81046800	1.25415200	-2.76576100	C	7.10946100	0.20900600	-1.24054700
H	-4.69186900	-0.11586000	-2.90559200	H	7.05859900	1.05202100	-0.54548400
C	-7.65282100	0.02132200	-1.06517300	H	7.50383900	0.57191700	-2.19529900
H	-8.27022800	-0.46611900	-1.82720600	H	7.82750400	-0.51874100	-0.84725500
H	-7.98669000	-0.30794700	-0.07790200	C	5.74072300	-1.59823600	-2.42021500
H	-7.81435100	1.10102000	-1.12179600	H	4.73233000	-2.00224300	-2.54519400
C	-5.96878700	-1.85311400	-1.18170200	H	6.11884300	-1.28820900	-3.40020800
H	-6.61114900	-2.36264500	-1.90794400	H	6.38915900	-2.40020400	-2.05020900
H	-4.93563800	-2.13603200	-1.39449200	H	5.44413100	-3.85500700	1.31040600
H	-6.23648500	-2.21443100	-0.18261100	H	6.31529300	-1.93941500	2.80836700
O	-5.82946500	1.01187200	0.70669000	C	-2.06272700	-2.10963200	-1.50021900
O	-4.00987800	0.20754900	-0.24146400	O	-1.48672900	-2.08057400	-0.36133100
H	-3.86385900	1.70183400	1.88131600	O	-2.72547300	-1.16886200	-2.00670600
H	-2.93741100	2.55305400	3.14726800	H	-3.62038100	-0.35788800	-0.97959800
H	-2.43315000	2.64279900	1.45966200	C	-1.89269500	-3.41018400	-2.26556400
H	2.08303300	-0.49458700	2.36935400	H	-2.49995900	-3.41184800	-3.17146300
H	1.66446000	-0.30331700	4.08548000	H	-0.83402900	-3.52619900	-2.51940300
H	1.51630100	-1.88185600	3.30111700	H	-2.16278500	-4.25413400	-1.62465900
C	1.82503000	0.39502000	-0.36178300	TS14			
C	1.01627900	-0.67470800	-0.11490200	C	-1.22118200	-1.06419400	-2.56432400
C	1.40090800	-2.04369500	-0.50902400	C	-1.26261500	-2.27064700	-1.81901700
C	1.26876100	-3.15748800	0.33453700	C	-2.64216100	-2.50310200	-1.35485400
C	1.85061300	-2.27716700	-1.82599800	C	-3.40771200	-1.39881700	-1.72247200
C	1.59178700	-4.44163000	-0.09851800	C	-2.51737400	-0.43175800	-2.39240500
H	0.90846700	-3.00721300	1.34089500	Rh	-1.64455000	-0.54317200	-0.48470300
C	2.17099500	-3.56066800	-2.26471500	C	-3.11559100	-3.68643000	-0.57035500
H	1.95128500	-1.43235400	-2.50002200	C	-0.14505300	-3.25170300	-1.67224500
C	2.04606300	-4.65415000	-1.40176800	H	-0.20947000	-4.01588300	-2.45776400
H	1.48501800	-5.28041000	0.58437100	H	0.82946400	-2.76776300	-1.73843200
H	2.51234900	-3.70853500	-3.28607800	H	-0.19823600	-3.76185400	-0.70888500
H	2.29131100	-5.65555300	-1.74340500	C	-0.06688000	-0.54812900	-3.36594700
N	3.20926100	0.25376500	-0.70048800	C	-2.95788800	0.85647300	-3.01105700
N	3.82174500	-0.50555900	0.10704700	H	-2.11856200	1.54106800	-3.14288100
N	5.09550600	-0.77520600	-0.17043100	H	-3.41629900	0.66783400	-3.99062900
C	5.69894100	-1.77745500	0.72961300	H	-3.69439200	1.36073400	-2.38154200
H	6.70313700	-1.95436000	0.33338200	C	-4.85768000	-1.17814300	-1.43098800
C	5.83132900	-1.21192300	2.14863600	H	-5.09821500	-0.11297700	-1.41082900
H	4.84068300	-0.98359700	2.55215000	H	-5.47662400	-1.64470500	-2.20780700
H	6.42330100	-0.29171500	2.14870400	H	-5.12385400	-1.60184000	-0.46130100
C	4.92433300	-3.10176400	0.70872200	C	4.07013100	-4.73679900	-0.83602700
H	3.91999800	-2.96089600	1.11267900	C	2.89931800	-4.38452700	-0.15895300
H	4.81540300	-3.48259900	-0.30998300	C	2.91469200	-3.40576300	0.84062200
C	5.72211500	-0.40441900	-1.45469300	C	4.13525000	-2.78899800	1.15454700

C	5.30590300	-3.13747000	0.48283400	H	0.91773900	2.27053300	-2.43881100
C	5.27639000	-4.11257900	-0.51858700	C	-1.98630800	4.17390700	-0.73820000
H	4.03777600	-5.50068200	-1.60788100	H	-2.07794200	2.49655600	0.61659800
H	1.96534700	-4.88199500	-0.40537400	C	-1.36597300	4.72614000	-1.86136800
H	4.15900300	-2.02159700	1.92340400	H	0.17919700	4.45135200	-3.34333600
H	6.24039500	-2.64734700	0.73958400	H	-2.79126000	4.71082400	-0.24271400
H	6.18793100	-4.38478100	-1.04269500	H	-1.68670000	5.68866200	-2.25002300
C	1.65456700	-3.00510300	1.57331100	N	2.09943700	1.55748900	-0.13295300
H	0.85802300	-3.74069500	1.39986900	N	3.26451800	1.16966000	0.17940500
H	1.83459800	-3.02682200	2.65674700	N	4.22528500	2.10338400	0.10966200
C	1.11980600	-1.62354500	1.23793700	C	5.47547900	1.68492600	0.77048000
C	1.58436900	-0.83225100	0.25691400	H	6.13094700	2.55913500	0.74727300
H	2.45654200	-1.19194000	-0.27887500	C	5.24787200	1.29001200	2.23816300
C	-0.28943200	-0.31250100	2.75230200	H	4.58041700	0.42567900	2.29296200
N	0.04672900	-1.26415800	2.07840200	H	4.78922900	2.10843100	2.80004100
O	-0.70223100	0.51809800	3.47418800	C	6.14192700	0.55538300	-0.02524700
C	-3.60724300	-0.19078600	1.63778000	H	5.48394400	-0.31660800	-0.06086100
C	-4.54329900	0.76975900	2.40625400	H	6.34598200	0.87357100	-1.05193900
C	-5.60533400	-0.03577800	3.16651900	C	3.89509500	3.51844000	-0.15651600
H	-6.28904700	0.64160500	3.69086200	H	3.03069400	3.47260400	-0.82297400
H	-6.18532900	-0.66233600	2.48406600	C	3.46232400	4.24451200	1.12495300
H	-5.13956800	-0.69682400	3.90283900	H	2.63386200	3.71135500	1.59786500
C	-5.22043700	1.67441600	1.35212800	H	3.12809500	5.26165200	0.89425900
H	-5.88583800	2.39437600	1.84182800	H	4.29330800	4.31423100	1.83589500
H	-4.47317700	2.22706500	0.77589100	C	5.03310200	4.23625600	-0.88671100
H	-5.82350800	1.08070300	0.65529000	H	5.36126900	3.66573400	-1.76085700
C	-3.73066800	1.63794900	3.38481200	H	4.68173800	5.21539500	-1.22729100
H	-4.39691100	2.33570200	3.90545600	H	5.90124900	4.41194600	-0.24247500
H	-3.22599700	1.02094800	4.13347900	H	7.08755300	0.26067100	0.44268700
H	-2.96193100	2.20985000	2.86176000	H	6.19810800	1.03134800	2.71709800
O	-2.59165000	0.41321500	1.07319300	15			
O	-3.84842500	-1.39723700	1.54988600	C	1.81330600	-0.02381200	-2.77086900
H	-3.75931000	-3.35689800	0.24712900	C	1.80675700	1.34028000	-2.33939000
H	-3.67270100	-4.37991800	-1.21266300	C	2.94138800	1.55754100	-1.44864700
H	-2.27835600	-4.23752800	-0.13606600	C	3.56409300	0.31658600	-1.25107000
H	0.88334800	-0.75165700	-2.86698100	C	2.85369500	-0.69800800	-2.02970500
H	-0.04833200	-1.02453500	-4.35383100	Rh	1.36813000	-0.01865300	-0.60889100
H	-0.13952800	0.53019700	-3.50975100	C	3.36300100	2.84550700	-0.80996000
C	1.12346600	0.52913800	-0.09003700	C	0.90583500	2.42282700	-2.85383800
C	-0.16176100	0.86069800	-0.39379700	H	1.38392700	2.94197600	-3.69409100
C	-0.54027900	2.21508600	-0.85389000	H	-0.04280800	2.01688100	-3.21257800
C	0.08969000	2.79479500	-1.97485600	H	0.68907700	3.16730400	-2.08442000
C	-1.58528200	2.93347400	-0.24234000	C	0.92696000	-0.64328000	-3.80811200
C	-0.32143800	4.02981700	-2.47528500	C	3.29710000	-2.11481100	-2.22131400

H	2.45970800	-2.76001000	-2.49168300	H	4.40107600	3.08532800	-1.06860000
H	4.05411300	-2.17819500	-3.01415700	H	2.73602100	3.67664400	-1.13478200
H	3.73494100	-2.51747400	-1.30522200	H	-0.04059000	-0.13810200	-3.85594500
C	4.75124100	0.06520500	-0.37630300	H	1.39206800	-0.58111000	-4.79983000
H	4.76935400	-0.96769100	-0.02299400	H	0.73500700	-1.69520000	-3.58617200
H	5.67964500	0.24516200	-0.93342000	C	-1.26747300	-0.52612900	-0.54687800
H	4.72963000	0.71973700	0.49665900	C	-0.19662700	-1.31515600	-0.76595800
C	0.37401600	5.72078800	-0.51644000	C	-0.13455500	-2.74247200	-1.05641700
C	0.60841800	4.64963200	0.35021200	C	-1.00118500	-3.33557400	-1.99550800
C	-0.40156700	3.72639200	0.64144500	C	0.81340100	-3.55474500	-0.40319600
C	-1.66854900	3.91891700	0.06862000	C	-0.91604300	-4.69860000	-2.27634500
C	-1.90640300	4.98345600	-0.79966000	H	-1.73975600	-2.71454200	-2.49136100
C	-0.88209200	5.88583500	-1.10138200	C	0.88500500	-4.91817100	-0.67986400
H	1.17385900	6.42331100	-0.73371700	H	1.46979600	-3.09307600	0.32689200
H	1.58582400	4.52465200	0.80522400	C	0.02694200	-5.49503700	-1.62116700
H	-2.46455200	3.21439200	0.29368300	H	-1.58764600	-5.14097700	-3.00743100
H	-2.89172400	5.10988900	-1.23970900	H	1.61406300	-5.53457300	-0.16058700
H	-1.06532000	6.71410600	-1.77976800	H	0.09108300	-6.55711400	-1.84081800
C	-0.14064600	2.58022200	1.59199000	N	-2.60179600	-0.94570700	-0.47210500
H	0.92042400	2.51951500	1.85702400	N	-3.38111200	-0.00819500	-0.11074600
H	-0.68280400	2.75024300	2.53156300	N	-4.67005700	-0.33660800	0.02519300
C	-0.54193400	1.20309100	1.10987900	C	-5.44570200	0.69851500	0.73721200
C	-0.81452600	0.85653700	-0.19302300	H	-6.44045000	0.27257000	0.88754800
H	-0.88205800	1.65574300	-0.92054900	C	-4.84520800	1.02449300	2.11431600
C	-0.93808400	-0.89033500	2.23216500	H	-3.84707400	1.45602000	2.00127800
N	-0.70030100	0.30652100	2.15823800	H	-4.75600700	0.12358100	2.72769000
O	-1.19191300	-2.00147000	2.50930200	C	-5.58494400	1.95074800	-0.13736400
C	2.46597100	-0.19170500	2.08057900	H	-4.59745300	2.36537300	-0.35832000
C	2.98682500	-0.97561000	3.31032400	H	-6.07216700	1.70841500	-1.08640500
C	3.68674500	-0.01549200	4.28132700	C	-5.10409700	-1.74777500	-0.05725600
H	4.07049100	-0.56770700	5.14684700	H	-4.45862600	-2.18245100	-0.82405600
H	4.52039300	0.49722700	3.79429800	C	-4.84179800	-2.49311300	1.25974700
H	2.99466700	0.75263000	4.63737300	H	-3.79270300	-2.40079300	1.55153100
C	3.98244700	-2.04256100	2.80920400	H	-5.07120800	-3.55774700	1.14424900
H	4.35292900	-2.64148800	3.64890600	H	-5.47228100	-2.09873600	2.06443500
H	3.50140400	-2.71035500	2.08953700	C	-6.55672800	-1.86576400	-0.52471000
H	4.84751300	-1.57689500	2.32394000	H	-6.73226800	-1.26726200	-1.42374300
C	1.80203300	-1.66902800	4.00902300	H	-6.77395400	-2.91212100	-0.76082400
H	2.15431600	-2.23425600	4.87950400	H	-7.27179700	-1.55471700	0.24421700
H	1.07216000	-0.93159100	4.36039100	H	-6.17700200	2.71536900	0.37583600
H	1.29282600	-2.35487700	3.32953000	H	-5.47808200	1.74305900	2.64531600
O	1.81546900	-0.93056300	1.22884400	TS16			
O	2.69150500	1.01981200	1.95116200	C	0.69496100	-2.07436200	1.78738300
H	3.29641300	2.75865400	0.27927000	C	1.13741800	-3.02860000	0.82664900

C	2.59992500	-2.99770200	0.78276900	C	5.18443800	2.35319500	0.48217900
C	3.04221100	-2.00178100	1.67096300	H	5.82314400	3.23276400	0.33980200
C	1.86272000	-1.34362500	2.23170200	H	4.17944100	2.68667400	0.74806100
Rh	1.71525200	-0.94649200	0.15172800	H	5.59306200	1.77772800	1.32227700
C	3.47565500	-3.81949700	-0.11105500	C	4.53608000	2.33166400	-1.95219300
C	0.28945400	-4.02095800	0.09185700	H	5.13987000	3.22731200	-2.14139200
H	0.45145200	-5.02864700	0.49300900	H	4.49909100	1.74485500	-2.87650400
H	-0.76925800	-3.77819000	0.18475100	H	3.51992100	2.64201000	-1.70112200
H	0.53440000	-4.03804200	-0.97319900	O	3.10854000	0.57479500	-0.03651300
C	-0.68445500	-1.90293200	2.34066700	O	4.60881600	-0.86214100	-0.93493800
C	1.90072500	-0.28013200	3.28457300	H	4.11554800	-3.14853000	-0.69233000
H	0.93404200	0.21933000	3.37569800	H	4.11266700	-4.49031300	0.47695600
H	2.15713000	-0.71077600	4.26090100	H	2.88628300	-4.42901500	-0.79920800
H	2.65174300	0.47428000	3.03751100	H	-1.44300500	-2.32570500	1.68282700
C	4.45391800	-1.63606900	1.99769900	H	-0.74600400	-2.40712200	3.31343600
H	4.55786000	-0.55205600	2.08818400	H	-0.92850100	-0.84909700	2.48827500
H	4.73962200	-2.08493300	2.95781600	C	-1.13451500	0.30833600	-0.09641500
H	5.13865900	-1.96914500	1.21961500	C	0.22882500	0.48458000	-0.22929900
C	-5.34774900	-3.53844200	0.52190000	C	0.71323900	1.88616800	-0.31838200
C	-4.13819000	-3.58504800	-0.17483100	C	1.17630600	2.59229000	0.80268100
C	-3.91512800	-2.75846500	-1.28255700	C	0.65353000	2.55650600	-1.54897300
C	-4.93501500	-1.88484700	-1.68322500	C	1.54567100	3.93108600	0.70176300
C	-6.14647200	-1.83688400	-0.99367900	H	1.23537400	2.08285400	1.75803200
C	-6.35525000	-2.66217400	0.11465200	C	1.03253900	3.89646200	-1.65498400
H	-5.50333300	-4.18666100	1.37971500	H	0.29975700	2.01894500	-2.42384500
H	-3.35526100	-4.26941500	0.14461200	C	1.47670600	4.59130600	-0.52926900
H	-4.76887700	-1.23085600	-2.53538100	H	1.89374700	4.46182400	1.58414000
H	-6.92478500	-1.15168800	-1.31701400	H	0.98021100	4.39578700	-2.61869900
H	-7.29688100	-2.62326100	0.65453300	H	1.77251800	5.63347800	-0.60931800
C	-2.57978700	-2.75110100	-1.98633800	N	-1.85072800	1.46849500	0.29899500
H	-2.10504300	-3.73807300	-1.91028500	N	-3.11544700	1.36194200	0.22484800
H	-2.70996200	-2.56967600	-3.06092500	N	-3.79645700	2.42206800	0.64249000
C	-1.60404100	-1.70406900	-1.47125800	C	-5.24290900	2.33953100	0.35899600
C	-1.88504000	-0.88438400	-0.42462500	H	-5.66166100	3.29840400	0.67053800
H	-2.86531600	-0.97665600	0.02158900	C	-5.51006300	2.15577900	-1.14234100
C	0.60874000	-1.03939900	-1.92229400	H	-5.09860000	1.20088700	-1.47933200
N	-0.44967300	-1.64703000	-2.22460000	H	-5.04546700	2.95733200	-1.72419400
O	1.79667900	-0.90445900	-2.14748400	C	-5.89135700	1.22775700	1.19390800
C	4.25035600	0.26696000	-0.59344800	H	-5.47939500	0.25500800	0.91406500
C	5.15447800	1.50650000	-0.80447500	H	-5.71258200	1.38896300	2.26134100
C	6.57125300	1.04974900	-1.17721100	C	-3.09796200	3.66135600	1.05511600
H	7.21263700	1.92048700	-1.35624200	H	-2.20065900	3.30592900	1.56954000
H	7.01600000	0.45289400	-0.37439000	C	-2.64056700	4.47050300	-0.16699000
H	6.55605100	0.42971500	-2.07633800	H	-2.00678200	3.85852700	-0.81187400

H	-2.05263300	5.33646500	0.15424500	C	-2.35299600	0.51687800	-1.04211200
H	-3.50177400	4.83343000	-0.73965600	H	-3.27165000	1.00246000	-0.73501300
C	-3.92972900	4.49087700	2.03494100	C	-0.09986700	-0.90251600	-1.74728000
H	-4.32002100	3.87522700	2.85131400	N	-1.31917300	-1.34377300	-2.18292200
H	-3.29265000	5.26760800	2.46875100	O	0.92109800	-1.68128400	-1.78116300
H	-4.76974700	4.99827900	1.54908000	C	3.73305700	-1.22242300	-0.09142700
H	-6.97280000	1.20496500	1.02262600	C	5.07916800	-0.50096300	-0.35383100
H	-6.58720500	2.16338300	-1.33973700	C	6.23688900	-1.48284200	-0.12396900
17				H	7.19355300	-0.99929100	-0.35387300
C	-0.79105600	-1.40209300	1.87612100	H	6.26557600	-1.82073200	0.91765400
C	-0.56313600	-2.68368700	1.28456400	H	6.12454800	-2.36800500	-0.75319100
C	0.80442200	-3.07446400	1.56269000	C	5.22583400	0.71880700	0.57355600
C	1.41627200	-2.01906400	2.31035100	H	6.18009700	1.22506100	0.38468500
C	0.45117500	-0.94987400	2.46019500	H	4.41348400	1.42881600	0.41144800
Rh	0.84457700	-1.20090800	0.35511300	H	5.21249400	0.41486500	1.62759800
C	1.45023900	-4.35900400	1.15266400	C	5.05550600	-0.03917100	-1.82512600
C	-1.55341000	-3.52515100	0.54016400	H	5.98521100	0.48683100	-2.07402600
H	-1.59811300	-4.53068100	0.97158400	H	4.95668300	-0.89727200	-2.49820800
H	-2.55570400	-3.10023500	0.57458700	H	4.21606300	0.63377900	-2.00355300
H	-1.27010300	-3.61894400	-0.51215200	O	2.73991700	-0.39821200	0.10220400
C	-2.09827000	-0.68358000	1.96676400	O	3.66579400	-2.45334200	-0.08578700
C	0.66555800	0.33398400	3.20195000	H	2.45051000	-4.15670600	0.76525700
H	0.03106100	1.12408500	2.79255600	H	1.51885700	-5.04571400	2.00598600
H	0.43434300	0.22389000	4.26928300	H	0.87235700	-4.84722700	0.36511700
H	1.70393700	0.66145100	3.11067100	H	-2.76125700	-0.94082200	1.14044800
C	2.80092800	-2.01042000	2.87290200	H	-2.59798600	-0.96151600	2.90351100
H	3.24851700	-1.01820600	2.77812400	H	-1.95984800	0.39960100	1.96591400
H	2.76572400	-2.27042800	3.93841200	C	-1.13294300	1.06617400	-0.68800600
H	3.44200100	-2.71538800	2.34613800	C	0.08735000	0.42651600	-1.12715300
C	-4.54571800	-4.57858400	-1.00219900	C	1.21432700	1.31315200	-1.55467700
C	-4.06671100	-3.56934900	-1.83902200	C	1.83516300	2.22469000	-0.68643600
C	-4.28916500	-2.22187600	-1.53167900	C	1.58472900	1.32219400	-2.90665400
C	-4.99850800	-1.90538200	-0.36496500	C	2.76607200	3.14329900	-1.16642000
C	-5.47205200	-2.91216500	0.47871600	H	1.59335700	2.19348000	0.36749800
C	-5.24710100	-4.25365600	0.16118600	C	2.52227600	2.23914500	-3.38715900
H	-4.36541500	-5.61930000	-1.25609700	H	1.13030700	0.61047700	-3.58878600
H	-3.50108900	-3.82288700	-2.73067600	C	3.10870900	3.16228800	-2.52179700
H	-5.18032700	-0.86225100	-0.11691600	H	3.23922600	3.83628200	-0.47582300
H	-6.01997600	-2.64922800	1.37935100	H	2.79123500	2.22841700	-4.43960500
H	-5.61736300	-5.03890400	0.81384300	H	3.83771300	3.87683700	-2.89306500
C	-3.71809500	-1.12357700	-2.40973500	N	-1.00077300	2.22382900	0.09283600
H	-3.55304900	-1.50307600	-3.42168100	N	-1.98327200	3.02949100	-0.01044500
H	-4.42409400	-0.28830300	-2.46908300	N	-1.95040200	4.08581800	0.77800400
C	-2.38489700	-0.62739300	-1.87375500	C	-2.96053500	5.11454500	0.44132100

H	-2.73567000	5.96494100	1.08928200	C	-1.13587100	5.77403700	1.88980500
C	-2.82953300	5.56821500	-1.01859600	C	-2.31094100	6.48033900	2.16364000
H	-3.04681200	4.73724700	-1.69431600	H	-4.37892800	6.76236200	1.62051100
H	-1.81694900	5.92389900	-1.22828900	H	-4.32772900	5.06541200	-0.18264100
C	-4.36857300	4.60577700	0.76843500	H	-0.20302500	4.25420000	0.67018200
H	-4.59920700	3.72651100	0.16048000	H	-0.23817100	5.96616400	2.47135300
H	-4.44823000	4.32758200	1.82348300	H	-2.33052100	7.22421800	2.95534600
C	-0.80625200	4.36491100	1.67683000	C	-2.22352100	3.51545200	-0.99563100
H	-0.37600200	3.38267900	1.88063300	H	-3.19141100	3.49509600	-1.50708800
C	0.25002600	5.21185400	0.95537800	H	-1.46694800	3.80012700	-1.73672100
H	0.58537300	4.70960800	0.04487200	C	-1.88022900	2.12758700	-0.48792600
H	1.11923800	5.36034400	1.60470000	C	-2.87437600	1.19716800	-0.20766100
H	-0.14826600	6.19881600	0.69526800	H	-3.92432400	1.44308700	-0.31293500
C	-1.26769900	4.97792900	3.00167800	C	-0.20619400	0.68462700	0.21917700
H	-2.06137200	4.37988700	3.45929700	N	-0.57675200	1.88107500	-0.27923400
H	-0.42077200	5.00918900	3.69385900	O	1.05353900	0.52812000	0.55922400
H	-1.62890100	6.00482000	2.88687200	C	3.85888100	0.21887600	1.40565700
H	-5.11253100	5.37956900	0.55535900	C	4.40742700	0.33940200	2.82482500
H	-3.53295800	6.38097400	-1.22465300	C	5.13657200	1.67799600	3.01086700
18				H	5.50433400	1.76305200	4.03935300
C	1.42039400	-0.25481900	-2.64828300	H	5.99251800	1.75838300	2.33316700
C	2.18368100	0.96552000	-2.72280000	H	4.46887500	2.51767700	2.80520600
C	3.59200000	0.61497900	-2.59692000	C	5.35315700	-0.84218600	3.10802800
C	3.68437500	-0.79218800	-2.37627200	H	5.69420500	-0.80951200	4.14854400
C	2.32963900	-1.32817100	-2.37293800	H	4.84484700	-1.79344900	2.93382200
Rh	2.51953000	0.11360000	-0.77909400	H	6.23721400	-0.80369200	2.46162800
C	4.71580900	1.60310400	-2.62277500	C	3.17924500	0.26590800	3.76230600
C	1.61566100	2.33090100	-2.95846300	H	3.49807600	0.38027800	4.80418300
H	1.24603400	2.42613600	-3.98680800	H	2.46178000	1.05796700	3.52693600
H	0.78943500	2.51320200	-2.26335800	H	2.67006000	-0.69594900	3.65623100
H	2.36989900	3.10330200	-2.79490500	O	3.42932700	-0.90371300	0.98532800
C	-0.05781700	-0.37058200	-2.83611100	O	3.75416600	1.24082300	0.65388600
C	1.97287000	-2.76466700	-2.15646700	H	5.65264900	1.15291800	-2.29132700
H	0.94675600	-2.87303900	-1.80315200	H	4.85796200	1.99010800	-3.63851900
H	2.08376600	-3.32963200	-3.09078200	H	4.50085600	2.44597700	-1.96080600
H	2.62408500	-3.21704700	-1.40536400	H	-0.56673200	0.55267800	-2.55744500
C	4.92089800	-1.60620700	-2.14982900	H	-0.27190700	-0.57804800	-3.89196100
H	4.78736500	-2.27599300	-1.29633500	H	-0.47593900	-1.18007400	-2.23628400
H	5.15022700	-2.21555000	-3.03214000	C	-2.49936200	-0.08614300	0.22261100
H	5.78379300	-0.97144600	-1.94035800	C	-1.13356800	-0.39410400	0.38815400
C	-3.45896600	6.22162800	1.41461100	C	-0.65651300	-1.78201300	0.60167100
C	-3.42929900	5.26393800	0.39747500	C	-1.25689100	-2.84726600	-0.10393600
C	-2.25642700	4.55618600	0.11336000	C	0.44527800	-2.08349700	1.42280400
C	-1.10730400	4.81982100	0.87374000	C	-0.78972600	-4.15532800	0.02016300

H	-2.09004400	-2.64064000	-0.76642300	H	0.24194400	-3.31878400	-0.56299700
C	0.91753800	-3.39097700	1.53798500	H	0.88027200	-4.33353800	-1.87057700
H	0.95215100	-1.28269200	1.94071900	H	1.84690100	-4.02505700	-0.41746200
C	0.30364400	-4.43512000	0.84429300	C	4.27228800	-2.98778600	-1.54071400
H	-1.27287000	-4.95316100	-0.53813600	H	4.00923900	-3.50627300	-0.61626300
H	1.78004800	-3.58530200	2.16906300	H	4.48919600	-3.74332700	-2.30623100
H	0.67532000	-5.45198700	0.93674700	H	5.16540400	-2.39487400	-1.34743800
N	-3.45089400	-1.06489000	0.58025800	C	-1.80355200	6.85467200	0.44226700
N	-4.52835000	-1.00323500	-0.08745800	C	-2.01979300	5.78571300	-0.43093200
N	-5.50203400	-1.81651500	0.31238100	C	-1.32049600	4.58185900	-0.28409000
C	-6.60510000	-1.94306300	-0.65953400	C	-0.40136500	4.46543100	0.77005700
H	-7.28135500	-2.69070500	-0.23791200	C	-0.18604900	5.53185100	1.64400200
C	-7.36247500	-0.61655200	-0.79148000	C	-0.88294400	6.73229000	1.48339200
H	-6.69328900	0.15914500	-1.17330100	H	-2.35844500	7.77962500	0.30987900
H	-7.74731200	-0.29146700	0.17944000	H	-2.74065800	5.88966000	-1.23886900
C	-6.10193800	-2.45688000	-2.01642000	H	0.13443000	3.53355800	0.91262200
H	-5.42054100	-1.72836000	-2.46409400	H	0.52545300	5.41871100	2.45782200
H	-5.56580300	-3.40332600	-1.90081400	H	-0.71427700	7.56049500	2.16593700
C	-5.32874900	-2.74673600	1.44819800	C	-1.53894600	3.44723100	-1.27963200
H	-4.56674000	-2.27056200	2.06939100	H	-2.44920100	3.64510400	-1.85529900
C	-6.61731900	-2.87610700	2.26648600	H	-0.70178700	3.43513200	-1.98948200
H	-7.01325100	-1.89238800	2.53508900	C	-1.61703200	2.07588700	-0.64343700
H	-6.40282100	-3.42257200	3.19002700	C	-2.83279700	1.46641300	-0.35661200
H	-7.39837400	-3.43154900	1.73642400	H	-3.77480800	1.95621100	-0.57205500
C	-4.78364300	-4.10369200	0.98271300	C	-0.42486100	0.32701600	0.29566800
H	-3.82838100	-3.97356600	0.46935600	N	-0.43836100	1.51287400	-0.33080500
H	-4.61921200	-4.75982200	1.84393000	O	0.75926300	-0.14375000	0.68010800
H	-5.48968100	-4.60267700	0.30896600	C	4.58490100	-0.69732100	1.00479900
H	-6.94227900	-2.61519100	-2.70006200	C	5.14492400	-0.73091500	2.44981400
H	-8.20408900	-0.72297400	-1.48343400	C	6.59463600	-1.23835700	2.41944000
19				H	7.03616300	-1.19120900	3.42161700
C	0.99224000	-1.31223400	-2.44551300	H	6.63770200	-2.27901700	2.07897700
C	1.92518900	-0.37106500	-2.95682800	H	7.19760500	-0.63893600	1.73445800
C	3.27262900	-0.86476000	-2.68023100	C	4.28576000	-1.61357400	3.36945600
C	3.14695900	-2.11604700	-1.99806300	H	4.69389400	-1.60697000	4.38712800
C	1.73877200	-2.37053300	-1.77859000	H	3.25393600	-1.25820300	3.39988700
Rh	2.24993200	-0.53591100	-0.80013500	H	4.27136600	-2.65065300	3.01688400
C	4.55239700	-0.19623000	-3.07145400	C	5.10757700	0.73181200	2.94897400
C	1.61433600	0.93296000	-3.62317200	H	5.50602800	0.79636100	3.96817100
H	1.85078500	0.88913600	-4.69276700	H	5.71535500	1.37397700	2.30253300
H	0.56052600	1.19224500	-3.50898600	H	4.08189700	1.11342500	2.95349300
H	2.20559700	1.73422000	-3.17116700	O	3.29735500	-0.87170000	0.94834500
C	-0.49734800	-1.23594500	-2.55678400	O	5.33189300	-0.46417900	0.04903000
C	1.14332500	-3.57640400	-1.12090500	H	5.25049900	-0.22447100	-2.23252700

H	4.99866900	-0.69888100	-3.93831900	H	1.54248500	0.99081400	1.27245300
H	4.37941200	0.84884800	-3.33542000	C	3.29310400	3.64023200	0.54170000
H	-0.85767500	-0.20926800	-2.46804000	H	2.47598000	4.36674200	0.47832000
H	-0.81123100	-1.62863800	-3.53181800	H	3.77946700	3.76698200	1.51216500
H	-0.98211900	-1.82862800	-1.78133500	H	4.00334500	3.80897200	-0.26694300
C	-2.83080400	0.19406400	0.24112800	TS20			
C	-1.60445200	-0.42591500	0.55766500	C	-1.28010300	-0.92442100	2.59558300
C	-1.52015100	-1.82768300	1.03498200	C	-2.25765700	0.05753700	2.91693400
C	-2.29707000	-2.82928900	0.41970800	C	-3.57649200	-0.48140500	2.57090300
C	-0.62180800	-2.21843000	2.04378400	C	-3.39009400	-1.78566700	2.03183100
C	-2.18494500	-4.16696000	0.79884100	C	-1.96406400	-2.04530800	1.96868500
H	-2.98211000	-2.55303900	-0.37452600	Rh	-2.35647600	-0.32002900	0.78100400
C	-0.51212200	-3.55578500	2.42361700	C	-4.89506100	0.20704200	2.72306700
H	0.00533300	-1.47070500	2.51090500	C	-1.98844500	1.41138400	3.49601100
C	-1.28988400	-4.53730300	1.80479400	H	-1.99356500	1.37542700	4.59218700
H	-2.79016900	-4.91952700	0.30043800	H	-1.01749900	1.78586500	3.16327300
H	0.19152200	-3.83101200	3.20427400	H	-2.74796200	2.12582800	3.17288900
H	-1.19589100	-5.57876800	2.09926600	C	0.19231700	-0.82417700	2.83339400
N	-4.01878600	-0.46227800	0.62132800	C	-1.34551600	-3.32677800	1.51243600
N	-5.00573700	-0.21691700	-0.13980000	H	-0.28236700	-3.21184600	1.30754500
N	-6.17510400	-0.70494200	0.25677000	H	-1.47225000	-4.10042100	2.28071200
C	-7.21874300	-0.66748800	-0.78745900	H	-1.81263800	-3.67828600	0.59092100
H	-8.09010100	-1.15863500	-0.34782000	C	-4.46247200	-2.73532600	1.60345300
C	-7.59196700	0.78073800	-1.12483300	H	-4.09608500	-3.41428000	0.83054000
H	-6.72245600	1.30698800	-1.52760500	H	-4.77785300	-3.34073900	2.46305300
H	-7.93287400	1.31219300	-0.23159200	H	-5.31708100	-2.19628800	1.19779300
C	-6.79392300	-1.45922300	-2.03253700	C	3.72065400	6.05752700	-0.96565800
H	-5.91854100	-0.99350200	-2.49344000	C	3.55175900	5.11370400	0.05032600
H	-6.53763800	-2.49029800	-1.77206400	C	2.30219700	4.52939800	0.28496500
C	-6.31433400	-1.49705200	1.49781000	C	1.21818900	4.90570700	-0.52124800
H	-5.49762800	-1.14528300	2.13238200	C	1.38570800	5.84629300	-1.53695900
C	-7.64303700	-1.20563300	2.20185300	C	2.63693100	6.42657800	-1.76319600
H	-7.79942300	-0.12934600	2.31890400	H	4.69785600	6.50277500	-1.13225100
H	-7.62730800	-1.65927200	3.19749900	H	4.40003300	4.82850200	0.66840300
H	-8.50251700	-1.62603900	1.66926100	H	0.24651000	4.45061800	-0.35814300
C	-6.10027500	-2.99297300	1.23210300	H	0.53650400	6.12579100	-2.15466400
H	-5.11187300	-3.16448700	0.80043700	H	2.76495100	7.16000200	-2.55442500
H	-6.16283500	-3.55511300	2.16979200	C	2.12354900	3.47838700	1.36864200
H	-6.86393200	-3.38613500	0.55148900	H	2.99916000	3.47526600	2.02624600
H	-7.60579600	-1.47905000	-2.76666500	H	1.24729400	3.72105000	1.97939400
H	-8.39138800	0.80519900	-1.87217200	C	1.91850900	2.09408900	0.78276800
C	2.71280400	2.25657300	0.44553900	C	2.99331400	1.26578800	0.48906000
O	2.87781200	1.56712100	-0.57580500	H	4.01310800	1.58829000	0.66116700
O	2.03523000	1.87603000	1.49317900	C	0.40669300	0.55450900	-0.08565400

N	0.65296800	1.74492500	0.50039300	H	8.00683900	0.33791200	-0.01390800
O	-0.83785700	0.36046700	-0.45839300	C	6.58956600	-2.13925300	2.00594300
C	-4.42120000	-0.73676000	-1.29161900	H	5.83459800	-1.52354000	2.50195900
C	-4.75087800	-0.78748500	-2.80534700	H	6.15826000	-3.12665600	1.81620200
C	-6.26227200	-0.95334300	-3.00819100	C	5.87231000	-2.20034800	-1.50359400
H	-6.50564900	-0.94804500	-4.07716400	H	5.03986200	-1.77843300	-2.07062400
H	-6.61245000	-1.89729900	-2.57903500	C	7.15610100	-2.04293000	-2.32492100
H	-6.81137200	-0.14761500	-2.51551100	H	7.38926600	-0.98710800	-2.49045900
C	-3.98891400	-1.94770000	-3.47259100	H	7.02011400	-2.52022200	-3.30030400
H	-4.19908800	-1.97335900	-4.54831600	H	8.02043100	-2.51864600	-1.84947400
H	-2.91242600	-1.83631900	-3.32611400	C	5.54389300	-3.66601300	-1.19002400
H	-4.29310700	-2.91122300	-3.04743800	H	4.58344100	-3.73840700	-0.67464000
C	-4.27373000	0.55547200	-3.40071700	H	5.47548700	-4.24521800	-2.11673300
H	-4.45212300	0.58397300	-4.48189600	H	6.32067000	-4.12029800	-0.56435400
H	-4.81808200	1.39170000	-2.94671300	H	7.44307700	-2.25741600	2.68116200
H	-3.20511900	0.69611700	-3.21473700	H	8.50582000	-0.16703300	1.61546100
O	-3.14265600	-0.81506300	-1.06597200	C	-2.99754000	2.73944800	-0.31784000
O	-5.31053300	-0.58795900	-0.44763600	O	-3.35748200	1.77315800	0.35589900
H	-5.47031100	0.08419100	1.80173400	O	-1.74983800	3.01357400	-0.63773300
H	-5.45526600	-0.22366600	3.56178400	H	-1.13612200	2.30757700	-0.30411300
H	-4.76659800	1.27457600	2.90652600	C	-3.98530000	3.73199100	-0.87263000
H	0.54048500	0.20804600	2.76706000	H	-3.62541600	4.75346000	-0.72796100
H	0.42851100	-1.20647800	3.83401700	H	-4.07545000	3.55884300	-1.95005800
H	0.75201300	-1.40990400	2.10338700	H	-4.95810100	3.58798300	-0.40401300
C	2.75248800	0.00259700	-0.08029700	21			
C	1.42712900	-0.41340000	-0.33504800	C	1.81823300	-0.04477500	-2.74016900
C	1.08922800	-1.78880600	-0.77624600	C	3.10797100	0.55494400	-2.72953000
C	1.81253000	-2.89180300	-0.27356300	C	4.06346400	-0.41640600	-2.22893800
C	0.01287100	-2.05540000	-1.64571800	C	3.34385900	-1.65347500	-1.99718300
C	1.49554600	-4.19814400	-0.64359600	C	1.96181900	-1.42192300	-2.26903800
H	2.62109400	-2.72040900	0.42714400	Rh	2.59235500	-0.08030000	-0.68415200
C	-0.30483900	-3.36426300	-2.00904600	C	5.54566300	-0.24193600	-2.13539200
H	-0.59455900	-1.23732700	-2.00732300	C	3.43364800	1.95697900	-3.13712400
C	0.43402700	-4.44241500	-1.51817800	H	3.69144700	1.98658400	-4.20291300
H	2.07057300	-5.02553500	-0.23589500	H	2.59311900	2.62503800	-2.94977700
H	-1.14404300	-3.53606800	-2.67739000	H	4.28862600	2.33315500	-2.57165000
H	0.18124900	-5.45960800	-1.80454100	C	0.54936200	0.60925100	-3.19132600
N	3.80545900	-0.83082500	-0.50658400	C	0.85592400	-2.42074800	-2.12958400
N	4.86324700	-0.72769500	0.18816900	H	-0.10752100	-1.93164500	-1.98513700
N	5.92038600	-1.38845300	-0.26920400	H	0.78953200	-3.04758400	-3.02733900
C	7.03455900	-1.47604800	0.69492000	H	1.01475400	-3.06954700	-1.26610600
H	7.77981500	-2.12000000	0.22118000	C	3.94246700	-2.93571100	-1.51195500
C	7.65699400	-0.09439000	0.92805500	H	3.22591800	-3.49126100	-0.90284600
H	6.91454800	0.58090700	1.36197900	H	4.22280600	-3.56301500	-2.36751400

H	4.82550500	-2.74077100	-0.90293600	C	-1.66406700	-0.58406800	0.25984900
C	-2.47301800	5.42152100	2.45164000	C	-1.50097500	-2.03353500	0.52373600
C	-2.65064600	4.62981700	1.31737900	C	-2.21430800	-2.97711800	-0.23830000
C	-1.61562900	4.47547600	0.38645700	C	-0.58089600	-2.50709000	1.47620300
C	-0.39555600	5.12229500	0.61072700	C	-2.02690700	-4.34532900	-0.04895000
C	-0.21734400	5.91529000	1.74691900	H	-2.90200500	-2.62831200	-1.00104100
C	-1.25363700	6.06848400	2.66917800	C	-0.39723300	-3.87641500	1.66683800
H	-3.28452500	5.53353300	3.16528800	H	0.00800900	-1.80075700	2.04728800
H	-3.59695100	4.11932000	1.15458300	C	-1.11668200	-4.80178200	0.90723500
H	0.41801800	4.97215100	-0.09094300	H	-2.58355300	-5.05385900	-0.65644900
H	0.73485900	6.41309200	1.90944400	H	0.31910900	-4.21851100	2.40813600
H	-1.11348500	6.68537900	3.55223200	H	-0.96484500	-5.86746900	1.05419200
C	-1.81471800	3.59420600	-0.83999800	N	-4.05430000	-0.74479700	0.29773400
H	-2.76032500	3.84486300	-1.33111000	N	-5.09364400	-0.32704600	-0.30914700
H	-1.00866400	3.77851200	-1.55729400	N	-6.22173800	-0.94566000	-0.00800800
C	-1.83976300	2.12641400	-0.48574800	C	-7.34376200	-0.62278100	-0.91469500
C	-2.98617200	1.39527600	-0.32929800	H	-8.16967000	-1.26235400	-0.59522400
H	-3.95500100	1.85075400	-0.48215700	C	-7.76597900	0.84181800	-0.75091900
C	-0.47696700	0.22817900	0.14177700	H	-6.94122100	1.50343600	-1.02933500
N	-0.63549300	1.53364300	-0.25760500	H	-8.04361400	1.05413800	0.28557400
O	0.67971100	-0.21535300	0.38109600	C	-6.99912600	-0.96822700	-2.36987000
C	4.30509700	-1.31037600	1.47174500	H	-6.16609800	-0.35123500	-2.71706200
C	4.30734700	-1.95458700	2.88468000	H	-6.71146100	-2.01941500	-2.46456200
C	5.74267700	-2.30286000	3.29763500	C	-6.27487900	-2.05808000	0.96805000
H	5.74933200	-2.77189300	4.28880300	H	-5.41930800	-1.88154500	1.62335700
H	6.19952500	-2.98999500	2.58032400	C	-7.55558500	-2.00820400	1.80618300
H	6.36680700	-1.40571200	3.33144500	H	-7.70890100	-1.01355300	2.23473600
C	3.44496300	-3.23261600	2.81751200	H	-7.47020300	-2.72467700	2.62862600
H	3.39229800	-3.71303900	3.80185100	H	-8.44657800	-2.28100000	1.23124800
H	2.43263500	-2.99021100	2.48480900	C	-6.07217300	-3.40862500	0.26980800
H	3.87154000	-3.95649000	2.11278800	H	-5.11517000	-3.42357800	-0.25618700
C	3.68398300	-0.96175800	3.88464200	H	-6.06585000	-4.21683300	1.00826300
H	3.64919500	-1.40141900	4.88882000	H	-6.87852900	-3.60878200	-0.44468900
H	4.27494500	-0.04081300	3.93883600	H	-7.86265500	-0.78579800	-3.01723800
H	2.67047200	-0.69413700	3.57708100	H	-8.62282900	1.06565800	-1.39394000
O	3.11100700	-0.96735900	1.10287100	C	2.54295500	2.83338100	0.01938300
O	5.34698100	-1.19748900	0.81767800	O	3.10612000	1.72309100	0.28922000
H	5.89936400	-0.65466200	-1.18958000	O	1.56233900	3.00111300	-0.75707800
H	6.03888200	-0.75102800	-2.97337800	H	0.24880900	2.07627500	-0.41014400
H	5.82173900	0.81384300	-2.17173000	C	3.11379800	4.04805900	0.73569100
H	0.55022400	1.66780300	-2.92433500	H	3.23974200	4.86695200	0.02161200
H	0.43941800	0.52299300	-4.27944200	H	2.38806900	4.37592800	1.48765700
H	-0.32430500	0.14627800	-2.72862200	H	4.06114100	3.81676600	1.22324900
C	-2.90580800	0.02485900	0.05244000				

P1

C	-5.49847000	-1.10973200	1.90206600	C	3.94192000	-0.95726300	0.89133300
C	-4.39639900	-1.37127200	1.09091700	H	3.32196500	-0.14687200	1.27924200
C	-4.45330100	-1.13192400	-0.28949800	C	4.68061700	-1.61596200	2.05987100
C	-5.63282800	-0.61691400	-0.83761800	H	3.97670400	-2.06494400	2.76662900
C	-6.73951900	-0.35101400	-0.02568500	H	5.26032300	-0.85531700	2.59174700
C	-6.67476500	-0.59795100	1.34508800	H	5.38414500	-2.38882100	1.73250200
H	-5.44070900	-1.30090500	2.96981300	C	4.89263300	-0.36883300	-0.15898000
H	-3.47631100	-1.75372000	1.52577700	H	4.32287100	0.11984300	-0.95292600
H	-5.68960200	-0.42849900	-1.90726200	H	5.54647500	0.37902700	0.30102000
H	-7.64846000	0.04824900	-0.46640100	H	5.52533400	-1.14548700	-0.60358400
H	-7.53281500	-0.39174600	1.97809900	H	3.71680300	-4.27584300	-2.08686100
C	-3.23302200	-1.38989300	-1.15599000	H	2.79612200	-5.30302700	0.08804900
H	-2.88123500	-2.41814900	-1.02618500	H	-3.31577900	1.19994700	-0.97817200
H	-3.50555600	-1.27925400	-2.21361600	22			
C	-2.08532600	-0.45755300	-0.84480400	C	2.08009700	-0.63225900	-1.41455100
C	-0.81781100	-0.86700200	-0.56656800	C	2.14611900	-1.62562000	-0.39280700
H	-0.57155900	-1.91907800	-0.53901500	C	0.85459700	-2.27912000	-0.32315900
C	-1.44921700	1.91608800	-0.58357300	C	0.04286600	-1.76810400	-1.41729100
N	-2.36140700	0.88223200	-0.85477300	C	0.77318800	-0.73808100	-2.06616000
O	-1.85696200	3.07765200	-0.57251000	Rh	0.53065300	-0.21503200	0.07026200
C	0.20284600	0.10758500	-0.30262200	C	0.47236600	-3.39141400	0.60267500
C	-0.07556300	1.47009600	-0.33852400	C	3.32111700	-1.93235700	0.47831800
C	0.95964000	2.50829500	-0.12550800	H	3.86653200	-2.78945500	0.06320300
C	2.20460700	2.43188400	-0.77522600	H	3.98520500	-1.07389800	0.55591500
C	0.71835000	3.60532100	0.71966800	H	2.99845600	-2.19190400	1.48895400
C	3.18660700	3.39779300	-0.56425600	C	3.17047900	0.33477700	-1.75423400
H	2.39215500	1.61075400	-1.45789200	C	0.30716100	0.06462800	-3.24023200
C	1.70264200	4.56931100	0.93337300	H	0.72715800	1.07176800	-3.22810500
H	-0.24814900	3.69947900	1.19907400	H	0.61342400	-0.41803200	-4.17641600
C	2.94188700	4.46930900	0.29740100	H	-0.77940300	0.16277000	-3.23919100
H	4.13991200	3.31732700	-1.07989800	C	-1.33485700	-2.23916100	-1.75872600
H	1.49803700	5.40502500	1.59702800	H	-1.93695500	-1.43687900	-2.18554400
H	3.70536900	5.22454100	0.46313000	H	-1.27728400	-3.06600700	-2.47710100
N	1.50660300	-0.26801100	0.06452700	H	-1.85078700	-2.60417900	-0.86836200
N	1.78416800	-1.48901800	-0.15644100	C	-2.43307400	0.16016200	0.19724500
N	2.97637700	-1.88829600	0.26584300	C	-3.81709200	-0.10078000	0.82414600
C	3.36702500	-3.22820900	-0.21535900	C	-4.67724500	-0.86533600	-0.20137700
H	4.39222600	-3.37445200	0.13368100	H	-5.68885600	-1.01268300	0.19215400
C	2.47830700	-4.30747800	0.41372800	H	-4.74002400	-0.31216500	-1.14112100
H	1.43783200	-4.15908700	0.11194300	H	-4.25421600	-1.85409300	-0.41346500
H	2.52903500	-4.26490400	1.50556900	C	-4.44786900	1.28159300	1.09996200
C	3.36436200	-3.29605700	-1.74904900	H	-5.45761100	1.16079500	1.50751900
H	2.35278300	-3.13758900	-2.13184100	H	-3.85363400	1.84397000	1.82839000
H	4.01625600	-2.52780200	-2.17476800	H	-4.50953200	1.86656700	0.17836500

C	-3.69944500	-0.90233300	2.12737100	C	-1.22640300	-0.86371600	-2.71155200
H	-4.69384600	-1.06404800	2.55835500	H	-1.66518800	0.13415000	-2.73941000
H	-3.23931500	-1.87898800	1.94814600	H	-1.13583400	-1.23713400	-3.73894600
H	-3.07936900	-0.37814800	2.85795500	H	-1.92193900	-1.51566900	-2.17977100
O	-1.41760300	-0.16102400	0.89124900	C	-2.49243800	0.14845700	0.25061100
O	-2.40439500	0.68015500	-0.95554000	C	-3.85824200	-0.42291800	0.66404300
H	-0.58414000	-3.32466000	0.87274800	C	-4.68630700	-0.68877100	-0.60941100
H	0.64779200	-4.36856000	0.13562600	H	-5.68331000	-1.05038800	-0.33634600
H	1.05206500	-3.34407600	1.52632400	H	-4.79186500	0.22170600	-1.20323800
H	3.54211500	0.78702800	-0.83122400	H	-4.21429400	-1.45440300	-1.23593200
H	3.99431400	-0.17318100	-2.26920800	C	-4.55659500	0.65533700	1.52216100
H	2.80352200	1.12934700	-2.40700700	H	-5.55334100	0.31009500	1.81701800
C	2.22179500	0.71250900	2.26484400	H	-3.98534800	0.86034500	2.43382800
O	1.08113100	0.12434600	2.02672900	H	-4.65949900	1.58761800	0.96112800
O	3.11110900	0.95909900	1.44609600	C	-3.68588700	-1.71655200	1.47130100
C	2.36872000	1.11083300	3.73066400	H	-4.66607800	-2.09765100	1.77721100
H	3.40857000	1.36010900	3.94835400	H	-3.18818600	-2.48984400	0.87780900
H	1.74043000	1.98712500	3.92213400	H	-3.07837300	-1.54690800	2.36304400
H	2.02005900	0.30941400	4.38711200	O	-1.45421300	-0.38777700	0.71007000
C	0.11662000	2.78976100	-0.81585400	O	-2.52517600	1.15563300	-0.54105800
O	0.63015800	1.98081700	-0.02739800	H	-1.09320900	-2.96949700	-0.54508300
O	-0.91797800	2.55780400	-1.57053400	H	-0.13322700	-3.85778600	-1.74693100
H	-1.43877700	1.68289200	-1.30486400	H	0.42275100	-3.72857300	-0.06743100
C	0.69730400	4.17447000	-0.95571400	H	3.92083200	0.39254000	-0.20409600
H	0.84742500	4.40423400	-2.01437100	H	4.28693600	0.13511100	-1.93843300
H	-0.01683100	4.90468600	-0.56255000	H	3.39071700	1.56798700	-1.40677500
H	1.63766600	4.24209200	-0.41006600	C	2.10939000	-0.29789000	2.49474800
TS23				O	0.95305400	-0.58285400	1.96335400
C	2.25975600	-0.25257800	-1.36443400	O	3.12621100	0.06521900	1.89941300
C	1.99860800	-1.57430700	-0.85949800	C	2.09731300	-0.44959900	4.01328000
C	0.65032800	-1.92738700	-1.21428600	H	3.11926500	-0.45327700	4.39574400
C	0.11709600	-0.85804600	-2.05231700	H	1.55257500	0.39539700	4.44720100
C	1.09571200	0.16411500	-2.13972200	H	1.57364300	-1.36286000	4.30742400
Rh	0.57037500	-0.15188200	-0.00890900	C	0.16641100	2.87047300	0.13722600
C	-0.07562600	-3.19281100	-0.87686300	O	0.72794200	1.87393400	0.66067000
C	2.95281700	-2.40898700	-0.06727300	O	-0.83499500	2.83839200	-0.65678400
H	3.56205800	-3.01299800	-0.75135500	H	-1.58180000	1.88243500	-0.60040900
H	3.60314900	-1.77747800	0.53748200	C	0.71357700	4.24168000	0.47086000
H	2.42157900	-3.08630000	0.60427300	H	0.81955800	4.82488800	-0.44799200
C	3.54251500	0.50263100	-1.22108700	H	-0.00687000	4.76582800	1.10692600
C	0.97229600	1.44085500	-2.91086300	H	1.66908500	4.16094200	0.98877300
H	1.57486200	2.23256500	-2.46183200	24			
H	1.32562700	1.29230800	-3.93863500	C	2.39603000	0.36208900	-1.19237600
H	-0.05964800	1.79127300	-2.94119900	C	1.83470400	-0.88813800	-1.66573100

C	0.51060000	-0.62603100	-2.12953600	H	2.80754000	-3.35362000	3.25079900
C	0.26690300	0.81305200	-2.02460800	H	1.48920700	-2.33106000	3.88177100
C	1.42986900	1.41115100	-1.47441900	H	1.10043600	-3.65750200	2.78653400
Rh	0.62719300	-0.05717200	-0.03601800	C	0.13696300	2.31651500	1.70647300
C	-0.47104400	-1.61554600	-2.67365500	O	0.75407200	1.20580100	1.65095400
C	2.53143000	-2.21052000	-1.63230000	O	-0.77146600	2.70310200	0.91706900
H	3.16250400	-2.31641000	-2.52365900	H	-1.79565800	1.79436400	0.49803800
H	3.15317300	-2.28245400	-0.73949900	C	0.55039700	3.25871400	2.82239100
H	1.81740500	-3.03642300	-1.62055000	H	0.83733400	4.22026200	2.38569400
C	3.79272900	0.55787900	-0.69648800	H	-0.31100600	3.44347500	3.47117400
C	1.63277700	2.86713400	-1.19796500	H	1.37545200	2.84840400	3.40466600
H	2.27614200	3.00780000	-0.32670900	HOPIv			
H	2.11859400	3.34514400	-2.05708800	C	0.94271300	0.18767000	0.00002200
H	0.68530900	3.36718200	-0.99752400	O	1.52344900	1.25150100	-0.00002100
C	-0.97363100	1.52655100	-2.46473500	O	1.61267400	-0.99513500	0.00008700
H	-1.18414400	2.38002100	-1.81820600	H	2.55737200	-0.76821700	0.00009700
H	-0.85680600	1.88905400	-3.49348700	C	-0.57310300	-0.01021300	-0.00001300
H	-1.84378200	0.86816800	-2.43960700	C	-1.25185100	1.36649400	-0.00010300
C	-2.56482100	-0.02182900	0.29593600	H	-2.33977700	1.24406200	-0.00012900
C	-3.88999900	-0.78278800	0.18444900	H	-0.96561900	1.94593900	0.88163600
C	-4.53912100	-0.39355400	-1.16265000	H	-0.96556600	1.94585100	-0.88188200
H	-5.50054600	-0.90581400	-1.27233500	C	-0.96893600	-0.80607400	-1.26311000
H	-4.70829500	0.68444800	-1.22013900	H	-0.48574700	-1.78606100	-1.27985100
H	-3.90640600	-0.69042700	-2.00756300	H	-2.05399100	-0.95248400	-1.27974900
C	-4.80345300	-0.34698100	1.34953600	H	-0.68725300	-0.26676500	-2.17363800
H	-5.76857000	-0.85866200	1.27379500	C	-0.96901200	-0.80594700	1.26313900
H	-4.35730100	-0.60788100	2.31496100	H	-0.68738200	-0.26654700	2.17363000
H	-4.97511200	0.73159800	1.32991800	H	-2.05406700	-0.95235400	1.27972900
C	-3.63816700	-2.29574500	0.23852100	H	-0.48582300	-1.78593200	1.28000800
H	-4.59077900	-2.83100700	0.16909100	16a'			
H	-2.99617800	-2.62199200	-0.58417300	C	0.44660000	-1.66980100	-2.75567300
H	-3.14320700	-2.57889700	1.17072300	C	1.54031800	-0.76461800	-3.01974200
O	-1.48943900	-0.63877200	0.35801000	C	2.74242000	-1.39046900	-2.56599800
O	-2.68700500	1.27375300	0.29351600	C	2.40911900	-2.69329500	-2.01822400
H	-1.46357800	-1.44204300	-2.25090000	C	0.99187900	-2.87517800	-2.17928100
H	-0.54316500	-1.52813500	-3.76427400	Rh	1.41218600	-1.11940800	-0.86662500
H	-0.18113000	-2.63862200	-2.42903000	C	4.08517400	-0.73791800	-2.59571500
H	4.03980200	-0.22441400	0.02160200	C	1.42221500	0.53378100	-3.75138800
H	4.49678900	0.52858100	-1.53804800	H	1.45899100	0.34667600	-4.83263500
H	3.90092000	1.52367600	-0.19885400	H	0.47336200	1.02468200	-3.52358700
C	2.00574300	-1.93200500	1.83643600	H	2.22089100	1.21740400	-3.46942800
O	0.85772300	-1.55469000	1.35529000	C	-0.96350300	-1.40472800	-3.19449500
O	3.12450500	-1.58914500	1.44406400	C	0.23875200	-4.11974200	-1.83696900
C	1.84779800	-2.89236100	3.01279600	H	-0.83832800	-3.98971900	-1.95836100

H	0.55948300	-4.92989500	-2.50321500	H	3.99601900	0.27272000	-2.18861600
H	0.45358500	-4.40239300	-0.80500400	H	-1.36635000	-0.50737800	-2.71441600
C	3.36465000	-3.70863200	-1.47644900	H	-0.98170300	-1.24138100	-4.27806800
H	2.90209100	-4.24419100	-0.64673200	H	-1.63055600	-2.23791700	-2.96939900
H	3.65476500	-4.42296000	-2.25757000	C	-1.79874100	1.92683800	-0.28435600
H	4.27052100	-3.22689100	-1.10256600	C	-1.09201200	0.72761800	-0.12110700
C	2.69934000	4.63842200	2.42311900	C	-1.75042500	-0.41139500	0.59875600
C	1.77965100	4.37874000	1.40625000	C	-1.77934200	-1.73258600	0.14359900
C	2.13130400	4.54498500	0.06027000	C	-2.36154100	-0.13388200	1.83506900
C	3.43108600	4.96951100	-0.24117900	C	-2.38328900	-2.74583600	0.88739700
C	4.35435800	5.23247000	0.77286700	H	-1.30892100	-1.98154900	-0.79175800
C	3.99065700	5.06950700	2.11134900	C	-2.98099900	-1.13824900	2.57657900
H	2.40769700	4.49710600	3.46025800	H	-2.35194300	0.88408700	2.21019000
H	0.78283800	4.02626700	1.65471500	C	-2.99359700	-2.45473200	2.10724200
H	3.72381700	5.08517700	-1.28179200	H	-2.37224800	-3.76432700	0.51010600
H	5.35929100	5.55730700	0.51662000	H	-3.43808600	-0.89473100	3.53169900
H	4.70816600	5.26930800	2.90226600	H	-3.46754600	-3.24109500	2.68730000
C	1.11933800	4.29128800	-1.04983600	N	-3.18956000	2.07809600	-0.06933800
H	0.46972400	5.17014500	-1.15550800	N	-3.87583000	1.17138000	-0.63084200
H	1.66535300	4.17180200	-1.99222300	N	-5.19332600	1.21393700	-0.42822600
C	0.27246100	3.07079400	-0.80625400	C	-5.92004200	0.06463800	-0.99953400
C	-1.07563400	3.10612800	-0.57915300	H	-6.96311300	0.20328800	-0.70072500
H	-1.62589100	4.04363100	-0.61190200	C	-5.84585300	0.09351400	-2.53101500
C	0.95574300	1.79454600	-0.81607400	H	-4.80378900	0.00740400	-2.85182700
N	0.23950400	0.66267100	-0.44510700	H	-6.24970100	1.03139100	-2.92400200
O	2.16834800	1.71341600	-1.13881500	C	-5.42048000	-1.26776000	-0.42721600
C	1.13126100	-2.80935000	1.66372200	H	-4.37956600	-1.43456400	-0.71013800
C	1.09125500	-2.90020600	3.20876400	H	-5.46701100	-1.27254800	0.66445100
C	0.21443600	-4.10970000	3.58674800	C	-5.81632500	2.12000000	0.55527600
H	0.24717300	-4.27581900	4.66943000	H	-5.05341000	2.87792800	0.74169900
H	-0.82725500	-3.93402700	3.29954600	C	-7.05595800	2.80923500	-0.02437300
H	0.56474000	-5.00998800	3.07758500	H	-6.81614900	3.31253300	-0.96543300
C	0.54601600	-1.63261500	3.88310700	H	-7.42644600	3.55845100	0.68289600
H	0.43007500	-1.81106100	4.95837800	H	-7.87381300	2.10438500	-0.20988800
H	1.22306100	-0.78318800	3.76589100	C	-6.10627200	1.38405200	1.87140500
H	-0.42650700	-1.35479900	3.47284900	H	-5.19583400	0.91242300	2.25140500
C	2.54829100	-3.15000100	3.65698000	H	-6.47914400	2.08506100	2.62577200
H	2.59494600	-3.26192100	4.74610300	H	-6.86474800	0.60515400	1.73439600
H	2.94396600	-4.05712300	3.19221900	H	-6.02677900	-2.09713200	-0.80702300
H	3.19232800	-2.30883000	3.37555900	H	-6.41329500	-0.73895500	-2.95982600
O	0.94800500	-1.62289900	1.14895700	C	3.18655400	0.45805200	1.11972800
O	1.35687600	-3.82905200	1.00806800	O	3.28963200	-0.43853400	0.26743600
H	4.81197800	-1.28619300	-1.99693800	O	2.14797200	0.57052000	1.91989700
H	4.44795900	-0.67951100	-3.62888600	H	1.52956100	-0.20013300	1.72999800

C	4.22832900	1.51919500	1.28242600	O	1.15806800	2.89610900	-0.44777100
H	5.19872700	1.14044900	0.95958000	C	2.83475700	-2.21328000	1.15734200
H	3.92827900	2.33795500	0.62039600	C	2.94207500	-2.54699900	2.66714000
H	4.26501900	1.89491100	2.30480900	C	2.72459200	-4.06391800	2.82759000
TS17a'							
C	0.85470700	-0.88358900	-2.70301500	H	2.89065800	-4.36414200	3.86872000
C	1.35372800	0.47046100	-2.92014600	H	1.69888200	-4.33815400	2.55794200
C	2.76188300	0.45426000	-2.75935000	H	3.41287200	-4.61882700	2.18490700
C	3.16332600	-0.90540000	-2.42165800	C	1.93088000	-1.76793400	3.51811300
C	1.97300100	-1.73408900	-2.45170900	H	2.06099600	-2.02657000	4.57608600
Rh	1.88543900	-0.20616400	-0.86059400	H	2.05705800	-0.68974000	3.40084900
C	3.69184100	1.62341700	-2.82729300	H	0.90705200	-2.00793600	3.22977000
C	0.51844100	1.63675200	-3.34119300	C	4.38136700	-2.18139400	3.08803300
H	0.53682500	1.72490800	-4.43454500	H	4.54231600	-2.43078900	4.14300700
H	-0.51954000	1.51538400	-3.02759500	H	5.10961100	-2.72264700	2.47896700
H	0.89391800	2.56417400	-2.90723500	H	4.56273000	-1.10730300	2.96366900
C	-0.57908900	-1.28747400	-2.86692300	O	1.93770300	-1.32248100	0.86586000
C	1.95043500	-3.21697400	-2.26057600	O	3.58791700	-2.78289200	0.35865700
H	0.95458500	-3.57127200	-1.98513900	H	4.27864600	1.68415000	-1.90607400
H	2.23667800	-3.70952200	-3.19867000	H	4.37960900	1.51506400	-3.67358700
H	2.64937500	-3.49911900	-1.47245000	H	3.14360000	2.55997600	-2.93373700
C	4.56897400	-1.38200300	-2.25126500	H	-1.24162500	-0.74455900	-2.18667300
H	4.61509000	-2.11708200	-1.44635200	H	-0.90804200	-1.07918500	-3.89202800
H	4.92864700	-1.83405600	-3.18482400	H	-0.71955400	-2.35353400	-2.68151500
H	5.22909500	-0.54926800	-1.99962000	C	-2.28472300	0.77587100	-0.06723800
C	-2.60552600	6.82817200	1.33710900	C	-1.09585400	0.26628000	0.41382000
C	-2.50695800	5.93664300	0.26664400	C	-1.11760000	-1.00485300	1.20226900
C	-1.29869000	5.29044500	-0.01902800	C	-0.68864000	-2.23095300	0.68665400
C	-0.18442000	5.54922200	0.79298500	C	-1.71016200	-0.97904700	2.47274600
C	-0.28308400	6.43769600	1.86371500	C	-0.84584900	-3.40624300	1.41908600
C	-1.49230000	7.08152200	2.13965900	H	-0.22915800	-2.26359100	-0.29141700
H	-3.55054100	7.32417300	1.54190400	C	-1.87328000	-2.15411300	3.20839600
H	-3.37802700	5.74236200	-0.35532500	H	-2.06162500	-0.03298800	2.87265100
H	0.74753200	5.03510700	0.58077500	C	-1.44468600	-3.37425300	2.68026400
H	0.58778900	6.62832300	2.48516800	H	-0.50460400	-4.34848800	1.00022100
H	-1.56567900	7.77466000	2.97306600	H	-2.33041000	-2.11468300	4.19285600
C	-1.20519100	4.29701400	-1.16766400	H	-1.56774100	-4.29060100	3.25025400
H	-2.05313000	4.44250900	-1.84531900	N	-3.52228300	0.09131100	0.04980000
H	-0.28595500	4.47982700	-1.73276900	N	-3.53673400	-0.99096500	-0.61228000
C	-1.19533200	2.86561600	-0.68024000	N	-4.62056800	-1.74754300	-0.48649200
C	-2.32063700	2.10541500	-0.58053300	C	-4.60692600	-2.97788400	-1.29807600
H	-3.28684100	2.50255500	-0.88292300	H	-5.53010900	-3.50375900	-1.03765800
C	0.08645200	2.29024000	-0.29384900	C	-4.64884000	-2.63808200	-2.79328300
N	0.08943400	0.98462100	0.26422700	H	-3.75205200	-2.07797600	-3.07383600
				H	-5.52373700	-2.02532400	-3.03009100

C	-3.42025600	-3.88176200	-0.94608600	C	7.35781500	-3.78437900	0.75636300
H	-2.48120700	-3.38289100	-1.19420000	C	6.49848800	-3.20469100	-0.17954500
H	-3.39960400	-4.10651300	0.12300100	C	5.12599200	-3.47857000	-0.15849900
C	-5.66453500	-1.49293200	0.52632400	C	4.62345400	-4.34457400	0.82389000
H	-5.41043700	-0.51291400	0.93332400	C	5.48112400	-4.92226900	1.76015500
C	-7.05500200	-1.41041800	-0.11239300	C	6.85061400	-4.64583300	1.73021100
H	-7.07382100	-0.65622300	-0.90440200	H	8.42148100	-3.56419700	0.72259800
H	-7.79559600	-1.13314900	0.64468700	H	6.89880200	-2.53412500	-0.93680100
H	-7.36860200	-2.36850400	-0.54131000	H	3.55629000	-4.54147700	0.84953700
C	-5.58103300	-2.53028500	1.65491300	H	5.07898500	-5.59227100	2.51545800
H	-4.58137900	-2.53068000	2.09912600	H	7.51660100	-5.09954300	2.45894500
H	-6.30994100	-2.29356800	2.43716700	C	4.18952200	-2.82085100	-1.16141900
H	-5.80047700	-3.54090700	1.29232200	H	4.76720600	-2.45645500	-2.01739400
H	-3.48004800	-4.82137200	-1.50519500	H	3.47164900	-3.56200900	-1.52799600
H	-4.68984100	-3.55209800	-3.39450000	C	3.41287300	-1.67459800	-0.55536000
C	2.98846500	1.39526000	1.41551300	C	3.79495800	-0.36479800	-0.66465000
O	3.26799700	0.93086700	0.26660300	H	4.68845400	-0.10240000	-1.22628600
O	1.85385700	1.34698200	1.97966100	C	2.19066600	-1.99929600	0.16320100
H	0.93822400	1.01575100	1.16379700	N	1.56614900	-0.91576500	0.76909300
C	4.11118700	2.05066500	2.18728800	O	1.68811900	-3.13557400	0.23949400
H	5.03377100	2.05973300	1.60695400	C	-4.70205300	-0.13999800	0.99809500
H	3.81640000	3.07073900	2.44814700	C	-5.25976300	0.63111300	2.22015100
H	4.26435900	1.50083100	3.12100100	C	-5.15873200	2.13320200	1.87379200
18a'							
C	-1.77303000	0.33463600	-2.09287400	H	-5.52192300	2.74442400	2.70781600
C	-1.12856100	-0.94280700	-2.37793600	H	-4.12375100	2.41735100	1.66168600
C	-2.14619500	-1.90374900	-2.62313100	H	-5.76382600	2.37004200	0.99150900
C	-3.43861100	-1.23228600	-2.52075700	C	-4.42917400	0.32166900	3.47855700
C	-3.19390100	0.15330800	-2.24225600	H	-4.81733800	0.88299800	4.33657800
Rh	-2.44684600	-1.08841700	-0.61415200	H	-4.47915700	-0.74493800	3.72287500
C	-1.95921700	-3.36266300	-2.90295400	H	-3.37836200	0.57962000	3.33411500
C	0.34475400	-1.19921400	-2.38891300	C	-6.72957000	0.24863000	2.44523400
H	0.71058900	-1.21585200	-3.42275400	H	-7.14927200	0.83100700	3.27359800
H	0.89125300	-0.42077800	-1.85551300	H	-7.32074900	0.43166000	1.54537200
H	0.58522500	-2.15710600	-1.92326100	H	-6.82297500	-0.81397200	2.68923200
C	-1.08308300	1.63916900	-1.84192900	O	-3.39969400	-0.12886200	0.93967000
C	-4.23326600	1.21878400	-2.09707300	O	-5.45797300	-0.64403500	0.16311600
H	-3.90213400	1.99729400	-1.40618800	H	-2.57395600	-3.96404400	-2.22733700
H	-4.42153700	1.68638000	-3.07152100	H	-2.25382300	-3.59527100	-3.93279300
H	-5.16171200	0.79886700	-1.71098600	H	-0.91879100	-3.66277600	-2.76669700
C	-4.77791500	-1.86454200	-2.72807100	H	-0.07548700	1.50659200	-1.44321500
H	-5.46333500	-1.53837900	-1.94332300	H	-1.00302500	2.20886100	-2.77608100
H	-5.18256700	-1.58250500	-3.70800900	H	-1.64248900	2.24604600	-1.12663800
H	-4.70581900	-2.95335000	-2.68981600	C	3.04912100	0.70680500	-0.09644900
				C	1.93860300	0.40282800	0.67580000

C	1.16474500	1.38368500	1.48090500	C	2.14611900	-1.62562000	-0.39280700
C	-0.23725000	1.36428700	1.51522300	C	0.85459700	-2.27912000	-0.32315900
C	1.84635000	2.32254900	2.27629700	C	0.04286600	-1.76810400	-1.41729100
C	-0.93949000	2.27263900	2.30902800	C	0.77318800	-0.73808100	-2.06616000
H	-0.79517200	0.64530200	0.93185600	Rh	0.53065300	-0.21503200	0.07026200
C	1.14271700	3.22327900	3.07124300	C	0.47236600	-3.39141400	0.60267500
H	2.93110800	2.33985000	2.26202000	C	3.32111700	-1.93235700	0.47831800
C	-0.25594100	3.20612700	3.08761100	H	3.86653200	-2.78945500	0.06320300
H	-2.02303900	2.23132800	2.31519800	H	3.98520500	-1.07389800	0.55591500
H	1.68717400	3.93454100	3.68640800	H	2.99845600	-2.19190400	1.48895400
H	-0.80444500	3.90917000	3.70780700	C	3.17047900	0.33477700	-1.75423400
N	3.51238300	2.02697700	-0.31077100	C	0.30716100	0.06462800	-3.24023200
N	2.57688500	2.79290500	-0.70267100	H	0.72715800	1.07176800	-3.22810500
N	2.86022500	4.08307800	-0.80924300	H	0.61342400	-0.41803200	-4.17641600
C	1.71791200	4.91709800	-1.23243400	H	-0.77940300	0.16277000	-3.23919100
H	2.08623700	5.94687900	-1.20599900	C	-1.33485700	-2.23916100	-1.75872600
C	1.31848200	4.58566500	-2.67528100	H	-1.93695500	-1.43687900	-2.18554400
H	1.00746100	3.54034900	-2.74421200	H	-1.27728400	-3.06600700	-2.47710100
H	2.16005400	4.73847500	-3.35760800	H	-1.85078700	-2.60417900	-0.86836200
C	0.54194600	4.79639100	-0.25457000	C	-2.43307400	0.16016200	0.19724500
H	0.17834900	3.76765100	-0.21582700	C	-3.81709200	-0.10078000	0.82414600
H	0.84374600	5.07429400	0.75793700	C	-4.67724500	-0.86533600	-0.20137700
C	4.13102500	4.67517200	-0.34653200	H	-5.68885600	-1.01268300	0.19215400
H	4.75456700	3.81504600	-0.09611900	H	-4.74002400	-0.31216500	-1.14112100
C	4.81393400	5.46549400	-1.46797700	H	-4.25421600	-1.85409300	-0.41346500
H	4.97247200	4.83315000	-2.34612000	C	-4.44786900	1.28159300	1.09996200
H	5.78746200	5.83162700	-1.12635300	H	-5.45761100	1.16079500	1.50751900
H	4.22385300	6.33674000	-1.77284500	H	-3.85363400	1.84397000	1.82839000
C	3.90868000	5.51046200	0.92199600	H	-4.50953200	1.86656700	0.17836500
H	3.42678700	4.90827100	1.69723100	C	-3.69944500	-0.90233300	2.12737100
H	4.86705800	5.87322300	1.30720100	H	-4.69384600	-1.06404800	2.55835500
H	3.27672100	6.38355500	0.72561500	H	-3.23931500	-1.87898800	1.94814600
H	-0.27923500	5.44972200	-0.56705100	H	-3.07936900	-0.37814800	2.85795500
H	0.48687800	5.21960700	-2.99940600	O	-1.41760300	-0.16102400	0.89124900
C	-1.66363900	-2.74806700	1.18019700	O	-2.40439500	0.68015500	-0.95554000
O	-2.69342300	-2.99049400	0.48357700	H	-0.58414000	-3.32466000	0.87274800
O	-1.05846000	-1.63633600	0.98808500	H	0.64779200	-4.36856000	0.13562600
H	0.66457500	-1.15635600	1.19656000	H	1.05206500	-3.34407600	1.52632400
C	-1.10621600	-3.72093800	2.17505800	H	3.54211500	0.78702800	-0.83122400
H	-1.71283100	-4.62574100	2.21895800	H	3.99431400	-0.17318100	-2.26920800
H	-0.08187600	-3.94888700	1.86057600	H	2.80352200	1.12934700	-2.40700700
H	-1.06142000	-3.24990100	3.16150900	C	2.22179500	0.71250900	2.26484400
19a'				O	1.08113100	0.12434600	2.02672900
C	2.08009700	-0.63225900	-1.41455100	O	3.11110900	0.95909900	1.44609600

C	2.36872000	1.11083300	3.73066400	H	-4.66607800	-2.09765100	1.77721100
H	3.40857000	1.36010900	3.94835400	H	-3.18818600	-2.48984400	0.87780900
H	1.74043000	1.98712500	3.92213400	H	-3.07837300	-1.54690800	2.36304400
H	2.02005900	0.30941400	4.38711200	O	-1.45421300	-0.38777700	0.71007000
C	0.11662000	2.78976100	-0.81585400	O	-2.52517600	1.15563300	-0.54105800
O	0.63015800	1.98081700	-0.02739800	H	-1.09320900	-2.96949700	-0.54508300
O	-0.91797800	2.55780400	-1.57053400	H	-0.13322700	-3.85778600	-1.74693100
H	-1.43877700	1.68289200	-1.30486400	H	0.42275100	-3.72857300	-0.06743100
C	0.69730400	4.17447000	-0.95571400	H	3.92083200	0.39254000	-0.20409600
H	0.84742500	4.40423400	-2.01437100	H	4.28693600	0.13511100	-1.93843300
H	-0.01683100	4.90468600	-0.56255000	H	3.39071700	1.56798700	-1.40677500
H	1.63766600	4.24209200	-0.41006600	C	2.10939000	-0.29789000	2.49474800
TS20a'				O	0.95305400	-0.58285400	1.96335400
C	2.25975600	-0.25257800	-1.36443400	O	3.12621100	0.06521900	1.89941300
C	1.99860800	-1.57430700	-0.85949800	C	2.09731300	-0.44959900	4.01328000
C	0.65032800	-1.92738700	-1.21428600	H	3.11926500	-0.45327700	4.39574400
C	0.11709600	-0.85804600	-2.05231700	H	1.55257500	0.39539700	4.44720100
C	1.09571200	0.16411500	-2.13972200	H	1.57364300	-1.36286000	4.30742400
Rh	0.57037500	-0.15188200	-0.00890900	C	0.16641100	2.87047300	0.13722600
C	-0.07562600	-3.19281100	-0.87686300	O	0.72794200	1.87393400	0.66067000
C	2.95281700	-2.40898700	-0.06727300	O	-0.83499500	2.83839200	-0.65678400
H	3.56205800	-3.01299800	-0.75135500	H	-1.58180000	1.88243500	-0.60040900
H	3.60314900	-1.77747800	0.53748200	C	0.71357700	4.24168000	0.47086000
H	2.42157900	-3.08630000	0.60427300	H	0.81955800	4.82488800	-0.44799200
C	3.54251500	0.50263100	-1.22108700	H	-0.00687000	4.76582800	1.10692600
C	0.97229600	1.44085500	-2.91086300	H	1.66908500	4.16094200	0.98877300
H	1.57486200	2.23256500	-2.46183200	21a'			
H	1.32562700	1.29230800	-3.93863500	C	2.39603000	0.36208900	-1.19237600
H	-0.05964800	1.79127300	-2.94119900	C	1.83470400	-0.88813800	-1.66573100
C	-1.22640300	-0.86371600	-2.71155200	C	0.51060000	-0.62603100	-2.12953600
H	-1.66518800	0.13415000	-2.73941000	C	0.26690300	0.81305200	-2.02460800
H	-1.13583400	-1.23713400	-3.73894600	C	1.42986900	1.41115100	-1.47441900
H	-1.92193900	-1.51566900	-2.17977100	Rh	0.62719300	-0.05717200	-0.03601800
C	-2.49243800	0.14845700	0.25061100	C	-0.47104400	-1.61554600	-2.67365500
C	-3.85824200	-0.42291800	0.66404300	C	2.53143000	-2.21052000	-1.63230000
C	-4.68630700	-0.68877100	-0.60941100	H	3.16250400	-2.31641000	-2.52365900
H	-5.68331000	-1.05038800	-0.33634600	H	3.15317300	-2.28245400	-0.73949900
H	-4.79186500	0.22170600	-1.20323800	H	1.81740500	-3.03642300	-1.62055000
H	-4.21429400	-1.45440300	-1.23593200	C	3.79272900	0.55787900	-0.69648800
C	-4.55659500	0.65533700	1.52216100	C	1.63277700	2.86713400	-1.19796500
H	-5.55334100	0.31009500	1.81701800	H	2.27614200	3.00780000	-0.32670900
H	-3.98534800	0.86034500	2.43382800	H	2.11859400	3.34514400	-2.05708800
H	-4.65949900	1.58761800	0.96112800	H	0.68530900	3.36718200	-0.99752400
C	-3.68588700	-1.71655200	1.47130100	C	-0.97363100	1.52655100	-2.46473500

H	-1.18414400	2.38002100	-1.81820600	C	-5.42942300	0.43906500	0.02291700
H	-0.85680600	1.88905400	-3.49348700	C	-6.30474900	0.31089100	1.10177500
H	-1.84378200	0.86816800	-2.43960700	C	-6.50328300	-0.93253400	1.70752700
C	-2.56482100	-0.02182900	0.29593600	H	-5.96724400	-3.02195600	1.68902500
C	-3.88999900	-0.78278800	0.18444900	H	-4.41073300	-2.79463500	-0.22357500
C	-4.53912100	-0.39355400	-1.16265000	H	-5.25580200	1.40459000	-0.44167300
H	-5.50054600	-0.90581400	-1.27233500	H	-6.83468500	1.18528100	1.47015000
H	-4.70829500	0.68444800	-1.22013900	H	-7.18768700	-1.03012800	2.54572700
H	-3.90640600	-0.69042700	-2.00756300	C	-3.75745900	-0.53767200	-1.62093500
C	-4.80345300	-0.34698100	1.34953600	H	-3.59819200	-1.51486700	-2.08862100
H	-5.76857000	-0.85866200	1.27379500	H	-4.17585700	0.13491100	-2.37625200
H	-4.35730100	-0.60788100	2.31496100	C	-2.42734900	0.02384400	-1.17245200
H	-4.97511200	0.73159800	1.32991800	C	-1.36590400	-0.75717800	-0.81043600
C	-3.63816700	-2.29574500	0.23852100	H	-1.44257600	-1.84026200	-0.86896200
H	-4.59077900	-2.83100700	0.16909100	C	-2.31394400	1.47506400	-1.08871600
H	-2.99617800	-2.62199200	-0.58417300	N	-1.07792000	1.92136800	-0.60909000
H	-3.14320700	-2.57889700	1.17072300	O	-3.19276300	2.29225800	-1.37992800
O	-1.48943900	-0.63877200	0.35801000	C	-0.11783100	-0.22263700	-0.37034600
O	-2.68700500	1.27375300	0.29351600	C	0.00004300	1.14737200	-0.23756900
H	-1.46357800	-1.44204300	-2.25090000	C	1.16177800	1.87050500	0.32954500
H	-0.54316500	-1.52813500	-3.76427400	C	1.66662800	3.02115400	-0.29473300
H	-0.18113000	-2.63862200	-2.42903000	C	1.73498400	1.45076000	1.54263800
H	4.03980200	-0.22441400	0.02160200	C	2.72733500	3.72964400	0.27383300
H	4.49678900	0.52858100	-1.53804800	H	1.24391300	3.34662900	-1.24145500
H	3.90092000	1.52367600	-0.19885400	C	2.78894800	2.16133900	2.10871000
C	2.00574300	-1.93200500	1.83643600	H	1.34569300	0.56319400	2.03026500
O	0.85772300	-1.55469000	1.35529000	C	3.29158200	3.30326800	1.47630200
O	3.12450500	-1.58914500	1.44406400	H	3.11320300	4.61258600	-0.22732900
C	1.84779800	-2.89236100	3.01279600	H	3.21602800	1.82902200	3.05073600
H	2.80754000	-3.35362000	3.25079900	H	4.11571600	3.85480500	1.91880300
H	1.48920700	-2.33106000	3.88177100	N	0.91472900	-1.13635900	-0.05469000
H	1.10043600	-3.65750200	2.78653400	N	2.02478600	-0.79385800	-0.57106800
C	0.13696300	2.31651500	1.70647300	N	3.08834700	-1.50984500	-0.24196700
O	0.75407200	1.20580100	1.65095400	C	4.33850000	-1.05923600	-0.88618300
O	-0.77146600	2.70310200	0.91706900	H	5.11366500	-1.73896100	-0.51983300
H	-1.79565800	1.79436400	0.49803800	C	4.24539600	-1.20677800	-2.40943100
C	0.55039700	3.25871400	2.82239100	H	3.45140400	-0.56387000	-2.79852500
H	0.83733400	4.22026200	2.38569400	H	4.01933100	-2.24050300	-2.68777000
H	-0.31100600	3.44347500	3.47117400	C	4.69785300	0.37075400	-0.46296000
H	1.37545200	2.84840400	3.40466600	H	3.91347200	1.06628600	-0.77136200
P2				H	4.80093400	0.44464500	0.62252800
C	-5.81812600	-2.04964100	1.22702700	C	3.06910500	-2.57827500	0.77563600
C	-4.94125200	-1.92061800	0.14791900	H	2.02015800	-2.65236500	1.06859500
C	-4.73908400	-0.67925100	-0.46676200	C	3.50676500	-3.92071800	0.17860900

H	2.88291100	-4.18326900	-0.68038000	C	-0.75480500	-1.48395200	-0.34875500
H	3.41181900	-4.71246000	0.92886300	H	-1.03136900	-2.40922400	0.16302500
H	4.55225200	-3.90038200	-0.14837000	C	-1.12408300	0.43350300	-1.68648100
C	3.89772700	-2.17416600	2.00255100	N	0.27334800	0.55100500	-1.54146900
H	3.54897200	-1.21799200	2.40366000	O	-1.87028700	1.34097000	-2.04990200
H	3.80439100	-2.93357600	2.78556200	C	0.35335100	2.23515500	0.04718200
H	4.96142300	-2.07642200	1.76006500	C	0.18899200	3.71376200	0.36081500
H	5.64199100	0.67740200	-0.92477500	C	1.05851400	4.57377000	-0.57537400
H	5.19073400	-0.91767800	-2.87950800	H	0.90474900	5.63140400	-0.33894900
H	-1.03216500	2.92302400	-0.46525100	H	2.12257600	4.34864600	-0.44641100
7'				H	0.79769500	4.40908800	-1.62245000
C	2.42756000	-1.45211300	1.52052500	C	0.55067400	3.97335800	1.83078400
C	2.10385800	-2.44928300	0.56611300	H	0.36268800	5.02337100	2.07555900
C	2.49904200	-1.94069800	-0.73478200	H	-0.04319600	3.34545100	2.49837900
C	3.25392300	-0.70157700	-0.52129400	H	1.60930500	3.76393400	2.01884100
C	3.18546500	-0.39082900	0.84344300	C	-1.31365500	4.00514200	0.10637900
Rh	1.01473000	-0.60174200	0.00342900	H	-1.50327700	5.07393400	0.25002700
C	1.44619600	-3.76920500	0.82551000	H	-1.59828400	3.71637000	-0.90874300
H	2.20006900	-4.55334800	0.96529600	H	-1.94092400	3.44380200	0.80550300
H	0.82330500	-3.73685500	1.72265000	O	0.26453700	1.34540800	0.90625200
H	0.80843000	-4.06546300	-0.01104800	O	0.53978700	1.97422900	-1.24016200
C	3.70039800	0.83062500	1.54323700	C	2.18239200	-1.49133300	2.99856200
H	2.89509500	1.32345800	2.09822700	H	1.39780600	-2.20585500	3.25568000
H	4.48624900	0.57073500	2.26238100	H	3.09352200	-1.77917800	3.53869500
H	4.11334800	1.55525800	0.83827300	H	1.87296200	-0.50944200	3.36715400
C	3.86782800	0.09986000	-1.62849900	C	2.41773500	-2.67366300	-2.03928900
H	4.23367000	1.06500300	-1.27243500	H	3.32167200	-3.27349600	-2.20696200
H	4.71081100	-0.43857700	-2.07759500	H	1.55527600	-3.34293400	-2.06257800
H	3.13156400	0.29072300	-2.41536400	H	2.31643100	-1.97218300	-2.87072300
C	-5.45323200	-1.88092200	1.24756800	TS8'			
C	-4.54830900	-2.13954800	0.21415200	C	3.06892500	0.87912200	1.18508500
C	-3.98573800	-1.09329900	-0.52494000	C	3.06218600	-0.50141100	1.46979800
C	-4.34628300	0.22625000	-0.21013600	C	3.27537600	-1.20248300	0.20831300
C	-5.24874500	0.48517100	0.82032700	C	3.55549100	-0.20805500	-0.81363100
C	-5.80627300	-0.56671000	1.55418000	C	3.37186500	1.06300200	-0.22989200
H	-5.88187900	-2.70667100	1.80953200	Rh	1.33243300	-0.19620100	-0.02164300
H	-4.27806900	-3.16647100	-0.02211600	C	2.87545800	-1.16639800	2.79988200
H	-3.89954600	1.03649800	-0.77889900	H	3.84012900	-1.47689800	3.21960500
H	-5.52062800	1.51186500	1.05179400	H	2.39427600	-0.49981900	3.51922800
H	-6.51034600	-0.36225800	2.35613000	H	2.25395800	-2.06196300	2.70854700
C	-2.97248800	-1.36591200	-1.62370500	C	3.44297300	2.40558700	-0.89201400
H	-2.95715400	-2.43717100	-1.85241100	H	2.53271800	2.98044200	-0.69081400
H	-3.27053200	-0.83558600	-2.53471000	H	4.29014500	2.98858700	-0.51041800
C	-1.57741500	-0.90727800	-1.24374000	H	3.54953900	2.31705400	-1.97468100

C	3.82379900	-0.52790700	-2.25132600	C	3.47179600	-2.68123200	0.05241000
H	4.15734200	0.35395300	-2.80210800	H	4.51272900	-2.95990000	0.26200100
H	4.59474300	-1.29919600	-2.34560100	H	2.83051500	-3.24112900	0.73725400
H	2.90739100	-0.89767200	-2.73123700	H	3.23351100	-3.00064900	-0.96480600
C	-5.07021600	-0.72292300	1.71320300	9'			
C	-3.96290500	-1.56991900	1.61686900	C	3.02835000	1.18970100	0.88581700
C	-3.37769500	-1.84779100	0.37614400	C	2.79664300	-0.01133200	1.60189700
C	-3.91610100	-1.24979200	-0.77348900	C	3.13563700	-1.11827900	0.71237800
C	-5.02099400	-0.40359900	-0.67812300	C	3.63688300	-0.55801100	-0.52113500
C	-5.60403000	-0.13782600	0.56432100	C	3.52690400	0.85597100	-0.42842000
H	-5.51308000	-0.52159300	2.68479700	Rh	1.32366900	-0.18770900	-0.13582300
H	-3.55156400	-2.02366700	2.51562200	C	2.36724600	-0.14508300	3.03042100
H	-3.45646800	-1.44679500	-1.73674200	H	3.23765600	-0.18969100	3.69681500
H	-5.42833300	0.04910300	-1.57789200	H	1.74483000	0.69758200	3.34036200
H	-6.46399100	0.52199400	0.63524700	H	1.79045900	-1.06087600	3.18385800
C	-2.15802100	-2.75145100	0.27486100	C	3.85873800	1.86861700	-1.48144500
H	-2.01751800	-3.29325600	1.21591300	H	3.08030300	2.63538900	-1.53781300
H	-2.31375200	-3.49109000	-0.51943100	H	4.80412100	2.37637500	-1.25203100
C	-0.91243700	-1.96323800	-0.05433500	H	3.95159100	1.41054700	-2.46775700
C	-0.02649000	-1.42456100	0.79947700	C	4.06904500	-1.37041700	-1.69870100
H	-0.05979000	-1.56201800	1.88108300	H	4.50711800	-0.74680800	-2.48012800
C	-0.59393100	-1.64713700	-1.46036900	H	4.80902900	-2.12227100	-1.40625600
N	0.58048000	-0.79847100	-1.59368500	H	3.19948800	-1.89088500	-2.12429400
O	-1.16543600	-2.06371600	-2.45236200	C	-5.21845700	-0.62558200	1.52514200
C	-0.94745200	1.51579000	-0.54838900	C	-4.10259400	-1.46445900	1.59641200
C	-1.93451200	2.64737200	-0.16985400	C	-3.37143500	-1.78326300	0.44678900
C	-2.97563800	2.82933800	-1.28224700	C	-3.76816400	-1.23649600	-0.78255400
H	-3.67463800	3.62655800	-1.00636200	C	-4.88328500	-0.40278500	-0.85442800
H	-2.49877600	3.09525500	-2.22950600	C	-5.61344700	-0.09402200	0.29733700
H	-3.53904200	1.90690200	-1.43690400	H	-5.77514800	-0.38936800	2.42791700
C	-1.13431700	3.94679600	0.04064500	H	-3.80031700	-1.87874100	2.55562700
H	-1.81254900	4.75694800	0.33025600	H	-3.19141300	-1.45930600	-1.67391800
H	-0.38561000	3.82204500	0.82688800	H	-5.18021400	0.01095300	-1.81392200
H	-0.62331400	4.24951500	-0.88024700	H	-6.47881600	0.55984000	0.23715500
C	-2.62237200	2.22182800	1.14389100	C	-2.15487700	-2.69310300	0.52358900
H	-3.35091100	2.98436600	1.44170000	H	-2.05853200	-3.09858700	1.53618900
H	-3.15504300	1.27504600	1.02026200	H	-2.28790900	-3.53785400	-0.16317100
H	-1.88848700	2.10544300	1.94532600	C	-0.88252700	-1.98083400	0.12995900
O	-0.00718000	1.32845600	0.33283100	C	-0.12792400	-1.16161700	0.87268200
O	-1.10343700	0.87341700	-1.59365200	H	-0.30075100	-0.91188300	1.91803900
C	2.76890000	2.01490600	2.11596900	C	-0.39983100	-2.03474400	-1.26907100
H	2.60767100	1.66924800	3.13889100	N	0.85304300	-1.38273200	-1.44179500
H	3.59216000	2.73790000	2.12594800	O	-0.96254000	-2.55006600	-2.22386500
H	1.86364500	2.54028900	1.79019200	C	-0.99483700	1.51182600	-0.69986400

C	-1.92872800	2.66170200	-0.24684300	C	-4.37213300	4.24838300	-0.80085800
C	-3.00059400	2.89273200	-1.32096600	C	-3.76263300	3.36520100	-1.69415700
H	-3.69482800	3.67463100	-0.99271300	C	-2.45687300	2.90237200	-1.48013000
H	-2.54793100	3.20659900	-2.26652100	C	-1.77082000	3.33871700	-0.33670400
H	-3.56170300	1.97610800	-1.50671500	C	-2.38185800	4.21894200	0.55877300
C	-1.13209800	3.95481700	-0.00109300	C	-3.68092300	4.68046100	0.33212000
H	-1.81266000	4.76276100	0.29046000	H	-5.38514300	4.59478900	-0.98944000
H	-0.39810200	3.82104700	0.79691000	H	-4.30722500	3.03059100	-2.57482900
H	-0.60207700	4.27245900	-0.90597000	H	-0.75814100	3.00317300	-0.14257600
C	-2.58443100	2.18628800	1.06858200	H	-1.83309400	4.54656700	1.43754500
H	-3.28282600	2.94705100	1.43595600	H	-4.15020600	5.36603900	1.03244100
H	-3.14147600	1.25801700	0.91738400	C	-1.80855100	1.98593500	-2.51212700
H	-1.82410100	2.01374800	1.83646400	H	-2.59035400	1.41512500	-3.02607600
O	0.10036300	1.43958200	0.03866300	H	-1.31562300	2.61685200	-3.26315000
O	-1.29527400	0.74221500	-1.60059800	C	-0.76649000	1.04851600	-1.95142900
C	2.72904600	2.58166400	1.34632700	C	-0.97687100	-0.16854000	-1.44206000
H	2.64620400	2.63681300	2.43382100	H	-1.95407900	-0.64635200	-1.41048300
H	3.51205700	3.27566700	1.02634200	C	0.62313100	1.57465600	-1.82928700
H	1.77686700	2.91459100	0.91550300	N	1.44326700	0.60369600	-1.30650300
C	3.18290900	-2.56684600	1.09310900	O	0.96212200	2.72068900	-2.13129000
H	4.12650200	-2.79939500	1.60284300	C	2.56291300	2.08252400	0.14059400
H	2.36247700	-2.82752500	1.76567700	C	3.86376600	2.87260200	0.28628900
H	3.10428600	-3.20345800	0.20937800	C	5.10063200	2.07605300	-0.16246400
9-N				H	5.99813600	2.68733100	-0.01817400
C	0.37867400	-3.47088600	-0.73529900	H	5.21387400	1.16138100	0.42559100
C	0.05932000	-2.97106400	-2.03412000	H	5.03659100	1.80087000	-1.21739800
C	1.23401300	-2.31514700	-2.54593300	C	4.00641900	3.31163900	1.75307900
C	2.32153500	-2.54569000	-1.60373000	H	4.86734800	3.98050700	1.85858000
C	1.79804300	-3.25078000	-0.49910600	H	3.10784100	3.83640400	2.08441000
Rh	0.62125500	-1.19656200	-0.73746400	H	4.15523000	2.44901500	2.40898400
C	1.39929900	-1.64353200	-3.87469500	C	3.67437600	4.10902800	-0.62782400
C	-1.26017800	-3.09944600	-2.73218700	H	4.57747100	4.72910500	-0.59899700
H	-1.29625900	-4.02277100	-3.32270300	H	3.47524300	3.80382600	-1.65803200
H	-2.08659700	-3.12814100	-2.01665100	H	2.82354000	4.70790300	-0.29207700
H	-1.43584100	-2.25791400	-3.40586000	O	1.54460300	2.31545700	0.74538700
C	-0.52421600	-4.23866200	0.18336000	O	2.67566000	1.11843100	-0.83733000
C	2.52043600	-3.74981200	0.71610700	H	1.97032400	-0.71858200	-3.75675300
H	2.03217400	-3.40669700	1.63302800	H	1.93078600	-2.29181300	-4.58238200
H	2.52633600	-4.84650800	0.73221000	H	0.43335100	-1.38135200	-4.31059900
H	3.55455200	-3.40422300	0.74741300	H	-1.57361000	-3.99605400	0.00366300
C	3.72551800	-2.06504000	-1.82288700	H	-0.39506500	-5.32043800	0.04905000
H	4.37868600	-2.33341900	-0.98943300	H	-0.30959700	-3.99949300	1.22780300
H	4.14617800	-2.50537300	-2.73450800	C	-0.45478900	-0.88456900	1.21965600
H	3.74718300	-0.97652600	-1.93380800	C	0.77876500	-0.69170300	1.37017900

C	1.92248000	-0.41480800	2.20226500	H	1.74060500	-2.86315300	3.16112200
C	3.23768100	-0.61135400	1.75010400	H	0.06135600	-3.19552000	3.58507200
C	1.71916600	0.01886800	3.52721000	C	2.94036400	-3.23227100	0.50184700
C	4.31777600	-0.41106600	2.60755900	C	1.31677500	-3.51022900	-2.19161900
H	3.39876000	-0.90149400	0.72021300	H	1.94615400	-2.62342000	-2.31305500
C	2.80256700	0.22616100	4.37606700	H	1.94688800	-4.39504100	-2.34663400
H	0.70565700	0.19416400	3.87342100	H	0.56003400	-3.49461800	-2.97911600
C	4.10727400	0.00507400	3.92423500	C	-1.82728700	-3.86548100	-1.42682700
H	5.32837700	-0.57320700	2.24346100	H	-1.51290000	-3.83989400	-2.47276600
H	2.62906200	0.56386200	5.39386300	H	-2.33816400	-4.82055400	-1.25352300
H	4.95078900	0.16537900	4.58915200	H	-2.55581100	-3.06439200	-1.27615500
N	-1.71338200	-1.27454600	1.50990000	C	1.40798400	4.66668900	1.41247800
N	-2.64326300	-0.48518900	1.10748400	C	1.24114200	3.44887700	2.07227900
N	-3.87079800	-0.85794400	1.38261500	C	-0.01979800	3.04895000	2.53718800
C	-4.91731500	0.03956700	0.83640900	C	-1.11632300	3.89263200	2.31686300
H	-5.86472500	-0.40887200	1.14771200	C	-0.95120800	5.11622000	1.66242600
C	-4.79776400	1.43865700	1.44649700	C	0.31016200	5.50797400	1.20795900
H	-3.84356200	1.89189600	1.17101200	H	2.39303900	4.95923000	1.05856300
H	-4.86784400	1.39470200	2.53775200	H	2.09406400	2.79177500	2.22300500
C	-4.86771400	0.06955500	-0.69530400	H	-2.10189600	3.56344100	2.63027100
H	-3.93718900	0.53168100	-1.02796500	H	-1.81209500	5.75957800	1.50132700
H	-4.93853900	-0.93945700	-1.11392100	H	0.43789500	6.45804900	0.69668500
C	-4.20899500	-2.12909200	2.06004300	C	-0.20054700	1.69243600	3.19421900
H	-3.24956900	-2.52398200	2.39700600	H	0.66791900	1.46128300	3.82073900
C	-5.09473100	-1.88524000	3.28679800	H	-1.08668300	1.71349300	3.83757700
H	-4.62527100	-1.17082300	3.96863000	C	-0.36929400	0.60561200	2.15577700
H	-5.24148600	-2.82765200	3.82384000	C	0.52580500	-0.34678500	1.83652500
H	-6.08436900	-1.50401300	3.01516200	H	1.48260900	-0.41644800	2.35976500
C	-4.82456900	-3.11849200	1.06219500	C	-1.66901000	0.54489100	1.44162900
H	-4.14500200	-3.29118200	0.22204300	N	-1.55429700	-0.24595900	0.29031100
H	-5.01516300	-4.07771300	1.55399100	O	-2.70929200	1.07626000	1.82684700
H	-5.77623200	-2.75029100	0.66489900	C	-3.73430900	0.13778200	-0.60507200
H	-5.69711500	0.66779900	-1.08390600	C	-5.15376300	-0.43280900	-0.49649000
H	-5.59506700	2.08401400	1.06870200	C	-5.22173900	-1.86966700	-1.04993200
TS10-N				H	-6.25605500	-2.22849900	-1.01225900
C	1.44655700	-3.34603500	0.40784700	H	-4.88759400	-1.91405000	-2.09230600
C	0.52587300	-3.50662200	1.50548700	H	-4.60479700	-2.55271900	-0.46245000
C	-0.78454300	-3.64510900	0.95471100	C	-6.09946500	0.48425000	-1.28645600
C	-0.66359200	-3.69730900	-0.49587100	H	-7.12956800	0.12433800	-1.19406600
C	0.69705500	-3.53431800	-0.82605100	H	-6.04770600	1.50914100	-0.91250900
Rh	0.05943500	-1.62294900	0.36597000	H	-5.83264400	0.50548100	-2.34752900
C	-2.07693700	-3.80718100	1.69780800	C	-5.53256500	-0.43016600	1.00224300
C	0.89369600	-3.52396000	2.95871500	H	-6.56258200	-0.78513500	1.12165000
H	1.17809600	-4.53585900	3.27395700	H	-4.86435600	-1.07989000	1.57219200

H	-5.44949100	0.57448400	1.42352900	H	5.23959100	3.30687100	0.70624700
O	-3.45307300	1.22089500	-1.05120100	II-N			
O	-2.82627000	-0.76462000	-0.10672800	C	2.07626200	-3.29202600	-0.66909300
H	-2.86066700	-3.20134900	1.23451900	C	3.01123500	-2.65437700	-1.58462000
H	-2.41053900	-4.85325500	1.69526100	C	3.83322000	-1.79180000	-0.82778600
H	-1.98325900	-3.48647000	2.73786800	C	3.49420800	-1.96248500	0.58292200
H	3.23966900	-2.69038400	1.40338400	C	2.46454200	-2.91795200	0.68517200
H	3.42354000	-4.21836200	0.52589600	Rh	1.57085700	-1.19693400	-0.56414600
H	3.33757000	-2.68186700	-0.35464300	C	4.91656200	-0.88512300	-1.33221000
C	0.85580600	-0.18385300	-0.86154200	C	3.05369200	-2.87989100	-3.06624500
C	-0.05087800	0.65291600	-1.21527400	H	3.62982400	-3.78313000	-3.30363900
C	-0.73649300	1.70884300	-1.84129900	H	2.04934700	-3.01305700	-3.47764700
C	-1.25000400	1.55414800	-3.14871200	H	3.51614000	-2.03915600	-3.58850100
C	-0.87507100	2.94635300	-1.17564100	C	1.09282900	-4.37297800	-1.00893600
C	-1.88229600	2.61935200	-3.77430800	C	1.81480500	-3.45157100	1.92758100
H	-1.14595200	0.59452200	-3.64462200	H	0.72500800	-3.41069800	1.84218000
C	-1.50990600	4.00468500	-1.81067200	H	2.10641300	-4.49532000	2.09992900
H	-0.48723600	3.05283900	-0.17112700	H	2.10061000	-2.87405500	2.80984700
C	-2.01547000	3.84178600	-3.10426100	C	4.17281700	-1.22081600	1.69444700
H	-2.27923600	2.50374900	-4.77836200	H	3.64479000	-1.34291900	2.64265800
H	-1.61472600	4.95152700	-1.29125600	H	5.20388800	-1.56937700	1.83275400
H	-2.51839300	4.67061700	-3.59501700	H	4.21305000	-0.15021400	1.47352300
N	2.21280500	-0.23981200	-1.24917000	C	-3.91504200	1.78895900	-2.39926100
N	2.95815600	0.35466000	-0.41830500	C	-2.72890600	1.21074400	-2.84558100
N	4.27156300	0.29302000	-0.63020300	C	-1.61665500	2.00382400	-3.16042400
C	5.03835000	1.18726000	0.25963800	C	-1.71357900	3.39092100	-3.00344800
H	6.08516200	1.06358100	-0.03222600	C	-2.90113400	3.97497100	-2.55212300
C	4.64308400	2.65788400	0.05669500	C	-4.00515000	3.17634900	-2.25149500
H	3.58589400	2.79778700	0.29723800	H	-4.76488000	1.15798900	-2.15640900
H	4.80115200	2.96864400	-0.98002800	H	-2.64964400	0.13072400	-2.93714600
C	4.88191300	0.74675500	1.72048600	H	-0.84768400	4.01154300	-3.21565400
H	3.83450300	0.82532300	2.02465200	H	-2.95849100	5.05305000	-2.43056600
H	5.19799600	-0.29323800	1.84692500	H	-4.92731600	3.62833100	-1.89752800
C	4.86023400	-0.33448400	-1.82741700	C	-0.31344000	1.34894800	-3.58370900
H	4.06584300	-0.97516500	-2.21626500	H	-0.50404700	0.58827000	-4.34860400
C	5.20237600	0.71094600	-2.89749200	H	0.35326400	2.10087400	-4.01982500
H	4.31934600	1.30548800	-3.14767100	C	0.36996600	0.69235200	-2.40316200
H	5.55752000	0.22015200	-3.80968200	C	0.56818500	-0.62753200	-2.20205000
H	5.99161400	1.38817600	-2.55292700	H	0.22639600	-1.34140200	-2.95533700
C	6.05495300	-1.21960500	-1.45664000	C	0.95880100	1.60228500	-1.39587700
H	5.77574300	-1.94359800	-0.68581300	N	1.04393400	0.94754300	-0.07827500
H	6.39396800	-1.76886400	-2.34073300	O	1.43631900	2.69530900	-1.60224300
H	6.90553300	-0.63581300	-1.08936800	C	1.79744900	2.84009500	1.22745600
H	5.48617600	1.37890500	2.37875300	C	3.03246700	3.33385100	1.98841400

C	3.20633700	2.46885200	3.25654000	C	-3.15539700	-3.27243800	1.81655000
H	4.07310500	2.82066700	3.82617600	H	-2.09739200	-3.54342600	1.82334500
H	2.32440700	2.53990600	3.90166500	C	-3.49118000	-2.59532000	3.15311700
H	3.36123100	1.41756500	3.00366000	H	-2.89039000	-1.69124400	3.28097900
C	2.79250200	4.80037600	2.37787700	H	-3.28768700	-3.27395400	3.98822200
H	3.65205300	5.17774100	2.94136800	H	-4.54917600	-2.31460100	3.19594200
H	2.65501100	5.42340500	1.49006400	C	-3.97612600	-4.54091700	1.56741400
H	1.89551600	4.90040600	2.99397800	H	-3.73021000	-4.98072700	0.59646800
C	4.27612900	3.21895900	1.08199300	H	-3.75377100	-5.27758600	2.34603000
H	5.14830000	3.63134900	1.60037200	H	-5.05429200	-4.35234000	1.59732700
H	4.48639200	2.17861900	0.82331400	H	-5.72854400	-1.60593700	-1.58721700
H	4.13242400	3.77522400	0.15065700	H	-5.80614400	0.00107700	0.42714100
O	0.77257200	3.44404300	1.06749600	11s			
O	2.03538100	1.55631900	0.77068400	C	1.54584600	-0.42093800	-3.01387400
H	4.89062800	0.08205500	-0.82047000	C	1.18535000	0.97444800	-2.94844900
H	5.91132100	-1.31836900	-1.16491100	C	2.39849200	1.74093600	-2.64652300
H	4.81079500	-0.69340400	-2.40244900	C	3.43600000	0.83229800	-2.40306800
H	0.73642800	-4.27520100	-2.03768300	C	2.89689400	-0.52231300	-2.58275700
H	1.54094600	-5.37013000	-0.90285500	Rh	1.68883300	0.36318000	-0.91648500
H	0.22136200	-4.31883300	-0.35080000	C	2.43540700	3.23371900	-2.55666000
C	-0.15600700	-0.89881900	0.40920000	C	-0.08606900	1.55726900	-3.47877500
C	-0.16907700	0.43864700	0.59456900	H	-0.00420700	1.70931500	-4.56370200
C	-1.20553800	1.26284900	1.24916700	H	-0.93314500	0.89373100	-3.29468200
C	-1.61596700	0.92002200	2.54751000	H	-0.30531700	2.52283000	-3.02051500
C	-1.85994800	2.31396200	0.59029000	C	0.63091600	-1.51871100	-3.46341100
C	-2.66301800	1.60060700	3.16950500	C	3.74024300	-1.75611200	-2.48759400
H	-1.10819000	0.10772600	3.05968000	H	3.15117700	-2.66596000	-2.61439900
C	-2.90030700	2.99747300	1.21478000	H	4.50987100	-1.74213500	-3.26958300
H	-1.55684000	2.59756800	-0.40952700	H	4.25548000	-1.81398400	-1.52402200
C	-3.31001300	2.64365500	2.50342300	C	4.84836400	1.11598000	-1.99353800
H	-2.96631300	1.32171800	4.17528300	H	5.14714400	0.47932200	-1.15421000
H	-3.39710800	3.80284500	0.68245100	H	5.54416700	0.91526000	-2.81795500
H	-4.12450400	3.17819400	2.98450400	H	4.97895700	2.15719200	-1.68918800
N	-1.12627200	-1.80252400	0.81244900	C	-5.48036600	4.11423300	-0.60762700
N	-2.26833000	-1.54971300	0.31252100	C	-4.15639100	3.98697900	-1.04218100
N	-3.28177700	-2.31722800	0.69879800	C	-3.11595300	3.81520200	-0.12232700
C	-4.59365700	-1.79032700	0.25782500	C	-3.42274300	3.76794400	1.24690600
H	-5.33972700	-2.41319200	0.75877400	C	-4.74102700	3.89718700	1.68175700
C	-4.79724900	-0.33206700	0.69375300	C	-5.77630600	4.07110400	0.75539200
H	-4.07219300	0.32257200	0.20544400	H	-6.27702600	4.24482500	-1.33552700
H	-4.66886900	-0.21837500	1.77272800	H	-3.93124500	4.02094700	-2.10573900
C	-4.74796700	-1.96395900	-1.25701900	H	-2.61007500	3.61646900	1.95313100
H	-3.97566700	-1.38781300	-1.77296000	H	-4.96465100	3.86014600	2.74494100
H	-4.64511600	-3.01462300	-1.54490900	H	-6.80383100	4.16878800	1.09536400

C	-1.67634800	3.66499200	-0.58020700	N	-2.30577500	-0.98908300	0.16037500
H	-1.62788900	3.78810400	-1.66811200	N	-2.31318500	-2.14718500	-0.36138700
H	-1.07543200	4.46774600	-0.14118400	N	-3.26155300	-2.98504400	0.03542800
C	-1.05380200	2.32847100	-0.19550000	C	-3.16345800	-4.33298100	-0.56162100
C	-1.58878500	1.16013500	-0.60187500	H	-3.95948700	-4.91548500	-0.09123400
H	-2.51085000	1.21632300	-1.18314900	C	-3.43106100	-4.27778900	-2.06918400
C	0.01629500	2.40093000	0.85773500	H	-2.67068200	-3.66942100	-2.56891800
N	1.16460400	1.76882000	0.52392200	H	-4.41298100	-3.84048300	-2.27672500
O	-0.20214400	3.03069900	1.90371300	C	-1.81885500	-4.99453000	-0.23685500
C	2.78951400	0.62305700	1.75627700	H	-0.99904400	-4.45595400	-0.71789300
C	3.54899000	0.47295700	3.06915800	H	-1.63216700	-4.99700800	0.84063600
C	4.35017500	1.76190500	3.34444800	C	-4.17641500	-2.69947600	1.16127300
H	4.90583500	1.65020600	4.28108600	H	-4.02816000	-1.63964100	1.37227800
H	5.07092700	1.95797600	2.54296700	C	-5.63720800	-2.91525800	0.75554600
H	3.69166300	2.62942300	3.43661800	H	-5.89215200	-2.31117400	-0.12068200
C	4.48865500	-0.73726100	2.97312300	H	-6.29586200	-2.61857900	1.57876200
H	5.02266000	-0.85635800	3.92105300	H	-5.85004800	-3.96520500	0.52622800
H	3.93105900	-1.65595600	2.77142000	C	-3.77968900	-3.50694400	2.40386200
H	5.22802100	-0.60663300	2.17690000	H	-2.73370000	-3.32114500	2.66551300
C	2.49878100	0.24601700	4.18076100	H	-4.40589500	-3.21582600	3.25418600
H	3.00849500	0.11545000	5.14082600	H	-3.91141500	-4.58295400	2.24501600
H	1.81721100	1.09720800	4.25989800	H	-1.81153100	-6.03034100	-0.59335000
H	1.90674400	-0.65329400	3.98036100	H	-3.40270500	-5.28461600	-2.49915200
O	2.87498500	-0.19404300	0.82755100	TS12bs			
O	2.01776200	1.68906600	1.71682800	C	1.43487800	-1.10711400	-2.76700200
H	3.36289300	3.59028300	-2.10327000	C	1.16834600	0.28310800	-3.03490500
H	2.34820300	3.68141600	-3.55421600	C	2.43026500	1.02387800	-2.93342800
H	1.60004300	3.60758500	-1.95604200	C	3.40582300	0.13825100	-2.47084100
H	-0.31007800	-1.50261400	-2.90543500	C	2.77654100	-1.18578400	-2.30449000
H	0.39442700	-1.39876400	-4.52775100	Rh	1.66074800	0.08425500	-0.89468500
H	1.08461500	-2.50285800	-3.32958700	C	2.55617600	2.48701200	-3.22147700
C	-1.17356900	-0.20778400	-0.23483800	C	-0.07633300	0.82511300	-3.66164700
C	0.09906200	-0.68480400	-0.18136000	H	0.00791400	0.77960600	-4.75590500
C	0.45776800	-1.92241600	0.54337900	H	-0.95605600	0.24970300	-3.36764300
C	1.26803900	-2.92393300	-0.01955400	H	-0.24463900	1.86676400	-3.38130700
C	0.07488900	-2.07255700	1.89322400	C	0.44447100	-2.22045100	-2.91055900
C	1.67053700	-4.03339600	0.72440800	C	3.52078400	-2.42086400	-1.89752000
H	1.58029600	-2.82502500	-1.05175700	H	2.83952200	-3.21234400	-1.57544800
C	0.48001900	-3.17824200	2.64048800	H	4.11321600	-2.80871100	-2.73674300
H	-0.54700500	-1.30760700	2.34852100	H	4.21408000	-2.21388200	-1.07723200
C	1.28214800	-4.16777300	2.06042600	C	4.83739200	0.42040100	-2.13525400
H	2.28970200	-4.79598800	0.25851400	H	5.08720100	0.03559200	-1.14095700
H	0.17353300	-3.26446700	3.67998900	H	5.51090100	-0.06878000	-2.85016400
H	1.60021300	-5.02829500	2.64238900	H	5.05298200	1.49144400	-2.14542400

C	-5.36936200	4.34517100	-0.16159500	C	0.12821900	-1.21760400	1.42225700
C	-4.27537400	3.96181900	-0.94487500	C	1.08954800	-2.23807100	1.52640900
C	-2.96993600	4.04304300	-0.44439400	C	-0.69102600	-0.95523400	2.53729600
C	-2.77985500	4.51816800	0.86415000	C	1.20888000	-2.99168700	2.69285900
C	-3.86904000	4.90184700	1.64615900	H	1.73641400	-2.43793600	0.67914800
C	-5.16998500	4.81686800	1.13673500	C	-0.56979500	-1.70494200	3.70608100
H	-6.37521600	4.27407100	-0.56774300	H	-1.42850100	-0.16080000	2.47139300
H	-4.43840500	3.59555400	-1.95600400	C	0.38004000	-2.72847800	3.78874600
H	-1.76672300	4.57236300	1.25311100	H	1.94807500	-3.78632700	2.74707200
H	-3.70471200	5.26825900	2.65648200	H	-1.21137600	-1.48662600	4.55538600
H	-6.01798800	5.11521600	1.74733600	H	0.47770600	-3.31115800	4.70048400
C	-1.77918600	3.59470800	-1.27462700	N	-2.35616700	-1.08479200	-0.25558300
H	-2.10791500	3.40214900	-2.30200600	N	-1.94415300	-2.29206800	-0.21962500
H	-1.04025600	4.40114200	-1.31117100	N	-2.87143700	-3.21286600	0.05447100
C	-1.10497300	2.35221900	-0.71302700	C	-2.44063700	-4.59809400	-0.21463900
C	-1.71670100	1.11898200	-0.85659000	H	-3.25224900	-5.23235700	0.14626300
H	-2.69494100	1.11719600	-1.33599900	C	-2.25322200	-4.85848100	-1.71592900
C	0.04676700	2.57887100	0.13141900	H	-1.44784600	-4.23382900	-2.11360300
N	0.73465500	1.39077400	0.44264400	H	-3.16681200	-4.63763500	-2.27574200
O	0.39886600	3.68260300	0.58960500	C	-1.17745800	-4.94026800	0.58332500
C	2.55984700	0.79397600	1.78141800	H	-0.32186000	-4.35904500	0.23250500
C	3.30090500	0.97715600	3.09831200	H	-1.31862700	-4.72277800	1.64616300
C	3.85671000	2.41866600	3.13021300	C	-4.27948500	-2.83503200	0.28898200
H	4.41028300	2.57165400	4.06211600	H	-4.21127800	-1.85549800	0.77156600
H	4.54181800	2.59609400	2.29387000	C	-5.04978000	-2.65953500	-1.02664300
H	3.05103700	3.15592800	3.07872900	H	-4.51729600	-1.97552100	-1.69304100
C	4.44387000	-0.04428700	3.17811200	H	-6.04447600	-2.24320900	-0.83100100
H	4.97616500	0.08465400	4.12554500	H	-5.17976300	-3.61902900	-1.53875700
H	4.06090800	-1.06801200	3.13317200	C	-4.98171700	-3.79587400	1.25057400
H	5.15862500	0.08935200	2.36107000	H	-4.38034200	-3.96583900	2.14932100
C	2.30981800	0.75943600	4.26183800	H	-5.93539500	-3.35500200	1.55871500
H	2.84024500	0.88362200	5.21141100	H	-5.20549900	-4.76438500	0.79143600
H	1.48978600	1.48088500	4.22788800	H	-0.94274800	-6.00427700	0.47222800
H	1.88462000	-0.24801700	4.23472100	H	-1.99095000	-5.90788600	-1.89040400
O	2.89934000	-0.00837100	0.90220100				
O	1.51311800	1.59319500	1.65740300	13bs			
H	3.53498400	2.87591600	-2.93162600	C	-2.29556800	-1.09194800	-2.28901400
H	2.41391500	2.68669800	-4.29101900	C	-1.05205200	-0.71774600	-2.90428000
H	1.79159800	3.05770600	-2.68278900	C	-0.27544500	-1.93639200	-3.16542100
H	-0.53952700	-1.91865500	-2.54322800	C	-0.96392700	-3.01695900	-2.59936400
H	0.33777900	-2.50831200	-3.96438800	C	-2.18755000	-2.48051600	-1.98358200
H	0.75398200	-3.10554500	-2.35023000	Rh	-0.57037300	-1.48612300	-0.89656500
C	-1.31635600	-0.13109900	-0.33212000	C	1.05267300	-1.93579900	-3.85299300
C	-0.02187200	-0.38885600	0.19938600	C	-0.73072500	0.62530100	-3.47783700
				H	-1.10627600	0.69186800	-4.50765200

H	-1.18653300	1.42944900	-2.89683800	H	0.47555900	-1.94156100	4.20481500
H	0.34709800	0.79915400	-3.50205700	O	-0.36116100	-2.82827400	0.83563700
C	-3.47582800	-0.20188700	-2.04931500	O	1.44101800	-1.56159200	1.29958100
C	-3.22232200	-3.32591200	-1.30676200	H	1.55105300	-2.90475000	-3.77602600
H	-3.86017700	-2.72985200	-0.64944400	H	0.94075100	-1.69151800	-4.91686100
H	-3.86623300	-3.81109600	-2.05208300	H	1.71322300	-1.17829200	-3.41548700
H	-2.75915900	-4.11620300	-0.70933300	H	-3.17321500	0.82732000	-1.84889600
C	-0.56458500	-4.46019700	-2.55843100	H	-4.13271400	-0.19423600	-2.93038200
H	-0.65425900	-4.86276200	-1.54420400	H	-4.06979000	-0.54386300	-1.19897200
H	-1.20845800	-5.06813800	-3.20702900	C	0.13072700	1.42331000	-0.34467500
H	0.46960100	-4.60020900	-2.88291600	C	-0.02656700	0.15128800	0.37318800
C	5.73407100	4.03120000	-0.35894000	C	-0.52458400	0.21386500	1.79871400
C	4.84551800	3.34977800	-1.19714700	C	-1.66217300	-0.47345500	2.23632900
C	4.63188400	1.97344300	-1.05142700	C	0.19870100	0.98354100	2.72148100
C	5.32945100	1.28913100	-0.04167600	C	-2.06615300	-0.40301200	3.57097200
C	6.21725100	1.96597800	0.79468700	H	-2.23238000	-1.05515900	1.52036700
C	6.42396800	3.34136900	0.63954500	C	-0.20227200	1.05567200	4.05659400
H	5.88643700	5.09977500	-0.48813900	H	1.07890200	1.52516700	2.38616200
H	4.31166300	3.89340900	-1.97341800	C	-1.33472700	0.35867200	4.48694300
H	5.15630300	0.22350100	0.08114300	H	-2.95658700	-0.93644700	3.89190700
H	6.75070300	1.42075000	1.56937800	H	0.37016300	1.65439100	4.75967400
H	7.11628500	3.86796400	1.29097800	H	-1.64859200	0.41442100	5.52553100
C	3.63867400	1.23045500	-1.93054200	N	-0.86222500	2.40063300	-0.40216800
H	3.36511700	1.86353400	-2.78238600	N	-1.96050600	2.11199400	0.16973500
H	4.11866300	0.33139500	-2.33268300	N	-2.94657400	3.03154200	0.04141300
C	2.38757700	0.81664000	-1.17946400	C	-3.98727700	2.88655800	1.08070800
C	1.28680000	1.68641800	-1.05435600	H	-4.69495800	3.69922000	0.90353700
H	1.32660200	2.64311500	-1.57076800	C	-4.73824200	1.56054600	0.91370700
C	2.39415500	-0.44117500	-0.55439000	H	-4.06236600	0.71399600	1.05933500
N	1.10539100	-0.75159400	0.14218000	H	-5.17794700	1.48627100	-0.08541300
O	3.26310000	-1.32259000	-0.52541500	C	-3.41845200	3.03480100	2.50037400
C	0.62608700	-2.59556900	1.53205500	H	-2.70122700	2.23711300	2.70923900
C	1.07852000	-3.43279700	2.71672500	H	-2.90947200	3.99409100	2.62829300
C	2.36929700	-4.16558200	2.28083500	C	-2.69026000	4.32285600	-0.62763500
H	2.72938400	-4.78191000	3.11056700	H	-2.01802600	4.06962800	-1.45165000
H	2.18037600	-4.82010300	1.42330800	C	-3.97212700	4.90604000	-1.22717200
H	3.15292900	-3.45449500	2.00660600	H	-4.50531400	4.15665600	-1.82116700
C	-0.02645800	-4.43945400	3.06611000	H	-3.71531600	5.74357800	-1.88441600
H	0.30300300	-5.05818700	3.90620900	H	-4.65517100	5.29156900	-0.46281700
H	-0.94858000	-3.92755200	3.35768600	C	-1.96255700	5.32847200	0.27668300
H	-0.25169600	-5.09759700	2.22259700	H	-1.07033700	4.87584400	0.71775700
C	1.36538100	-2.51125400	3.92116400	H	-1.64978800	6.20299700	-0.30537500
H	1.66667700	-3.12672500	4.77454800	H	-2.61409300	5.67992500	1.08366700
H	2.17126700	-1.80647600	3.70442000	H	-4.22411800	2.97617400	3.24082800

H	-5.54375400	1.48795000	1.65242500	C	-3.88059600	-0.86112100	4.20638300
TS12as							
C	-1.49088800	-0.01629800	-2.71677300	H	-4.77677400	-0.60584700	4.78409400
C	-0.74300800	-1.25774600	-2.77326300	H	-3.72357300	-1.94165300	4.27424200
C	-1.67672300	-2.35817900	-2.58730500	H	-3.01942500	-0.37235300	4.67039000
C	-2.93598400	-1.80434400	-2.28237300	C	-5.25959700	-1.12722200	2.11493500
C	-2.82287500	-0.35096100	-2.35846600	H	-6.16796700	-0.91585400	2.69153500
Rh	-1.36471000	-1.00308000	-0.65599400	H	-5.41872300	-0.79129300	1.08694400
C	-1.28381300	-3.79776900	-2.61452300	H	-5.11636900	-2.21409300	2.10154800
C	0.66671400	-1.38520500	-3.25090200	C	-4.24546700	1.11062000	2.68312100
H	0.68927400	-1.39608200	-4.34885400	H	-5.14113600	1.40177100	3.24503700
H	1.27500000	-0.54343100	-2.91233500	H	-3.38802300	1.63713300	3.11361400
H	1.12799300	-2.30861700	-2.89516700	H	-4.35972200	1.44725800	1.65024000
C	-0.93035800	1.32392400	-3.08380300	O	-2.88011700	-0.49710200	0.67126600
C	-3.97612100	0.57002300	-2.12456900	O	-1.79497000	-1.29034700	2.48700700
H	-3.72514100	1.60687100	-2.35798800	H	-2.14290900	-4.45457600	-2.46410800
H	-4.82759300	0.27621200	-2.74865200	H	-0.81652500	-4.05236300	-3.57221500
H	-4.29321300	0.51377200	-1.07675100	H	-0.55487800	-4.00509700	-1.82136100
C	-4.19966600	-2.50963100	-1.90820900	H	-0.03590900	1.55703200	-2.50014400
H	-4.97313200	-2.36309000	-2.67195100	H	-0.65228100	1.32657200	-4.14493600
H	-4.04223400	-3.58253500	-1.78080400	H	-1.65734700	2.12273900	-2.92669000
H	-4.58552200	-2.10757000	-0.96520300	C	1.27641800	0.29096700	-0.00655700
C	6.55010500	-3.08322900	0.32737300	C	-0.08841000	0.39407000	0.12478000
C	5.31735400	-3.15209700	-0.32998800	C	-0.68956600	1.56804200	0.78787600
C	4.12460200	-3.22657700	0.39841300	C	-1.75582600	2.29647500	0.23243300
C	4.18225600	-3.22112100	1.80070600	C	-0.19302200	1.98520400	2.04166100
C	5.41095100	-3.15273400	2.45647500	C	-2.26521100	3.42878800	0.86508400
C	6.60029400	-3.08463100	1.72212900	H	-2.17849400	1.97652800	-0.70815700
H	7.46805700	-3.02738700	-0.25187000	C	-0.71291400	3.10687300	2.68459000
H	5.28361300	-3.15198000	-1.41699800	H	0.61528000	1.42453600	2.49966100
H	3.25173200	-3.26093400	2.36151900	C	-1.74458000	3.84489600	2.09288600
H	5.44213800	-3.15071900	3.54293300	H	-3.07562700	3.98339600	0.39974600
H	7.55675500	-3.02982300	2.23485700	H	-0.31272500	3.40570600	3.64969400
C	2.78125100	-3.31375700	-0.30967500	H	-2.14481700	4.72408700	2.58984100
H	2.93778100	-3.31305400	-1.39374400	N	2.11155100	1.45011500	0.13604100
H	2.30004300	-4.26399100	-0.05486500	N	1.72656500	2.40493100	-0.61245000
C	1.84731800	-2.17819300	0.06991000	N	2.34517400	3.56207700	-0.48711400
C	2.08002400	-0.88886000	-0.28114200	C	1.88954700	4.60543900	-1.43028100
H	3.04822100	-0.67468300	-0.73416200	H	2.47230200	5.49441500	-1.17770100
C	0.69134100	-2.53443200	0.96492500	C	2.20998900	4.21184100	-2.87607500
N	-0.40913800	-2.35188000	0.23058100	H	1.65343400	3.31417600	-3.16340500
O	0.83244500	-3.07816800	2.06229800	H	3.27849700	4.00849100	-2.99899400
C	-2.77116800	-0.78188700	1.94247600	C	0.40431600	4.92296700	-1.22891800
C	-4.04942000	-0.41458200	2.74809300	H	-0.21335900	4.06069000	-1.49210000
				H	0.19651600	5.18028800	-0.18651100

C	3.36613300	3.83874400	0.54720800	C	2.81792600	-3.29465500	-0.36006300
H	3.47274000	2.89681100	1.08705600	H	2.98829200	-3.26691600	-1.44158000
C	4.71283000	4.19479100	-0.09020700	H	2.34736700	-4.25672300	-0.13206600
H	5.04992700	3.39753700	-0.75999900	C	1.86366400	-2.17991100	0.03339600
H	5.46886300	4.32623100	0.69118700	C	2.07856500	-0.88382500	-0.30706400
H	4.65988000	5.12835400	-0.66087800	H	3.04451200	-0.65555500	-0.75812100
C	2.86346000	4.90831300	1.52327400	C	0.70904700	-2.56966300	0.91221100
H	1.91294900	4.60225100	1.97043600	N	-0.39337200	-2.38057700	0.18257500
H	3.59402500	5.04764400	2.32707800	O	0.84205500	-3.14932700	1.99307000
H	2.72114800	5.87686200	1.03204800	C	-2.67064600	-0.72397000	1.98541200
H	0.11069000	5.76705600	-1.86198800	C	-3.93784000	-0.41704200	2.83155600
H	1.93245300	5.02102300	-3.55965400	C	-3.68502400	-0.81197500	4.29259400
13as				H	-4.56890800	-0.58738200	4.90122800
C	-1.55887200	-0.01968600	-2.70940900	H	-3.46865200	-1.88080000	4.38267000
C	-0.79282600	-1.24939600	-2.78780500	H	-2.83215300	-0.26592100	4.70446900
C	-1.70573900	-2.36453000	-2.59131700	C	-5.13076000	-1.21147900	2.26805200
C	-2.96670800	-1.83155700	-2.25298800	H	-6.02547000	-1.03427500	2.87658000
C	-2.87780600	-0.37689300	-2.32403400	H	-5.34978900	-0.91424900	1.23922900
Rh	-1.37573600	-1.02232300	-0.65747200	H	-4.92809700	-2.28890600	2.27535000
C	-1.29332000	-3.79787800	-2.64044100	C	-4.22183700	1.09359500	2.73697700
C	0.61208400	-1.35156400	-3.28559000	H	-5.11504200	1.34856300	3.31995000
H	0.62071300	-1.36452300	-4.38370100	H	-3.38241500	1.67665000	3.12784500
H	1.20829800	-0.49778100	-2.95576900	H	-4.38625800	1.39737400	1.70028800
H	1.09514200	-2.26520600	-2.93344500	O	-2.86698200	-0.54469100	0.70437600
C	-1.02700800	1.33010000	-3.08490400	O	-1.62164500	-1.09109500	2.50711100
C	-4.03886100	0.52376500	-2.05371600	H	-2.14099500	-4.46852700	-2.48617800
H	-3.80403900	1.56908700	-2.26369100	H	-0.83585700	-4.03427800	-3.60740500
H	-4.89542500	0.23450600	-2.67304000	H	-0.55070800	-4.00392900	-1.85970900
H	-4.33983100	0.43872600	-1.00313200	H	-0.14184600	1.59020900	-2.49831900
C	-4.21154900	-2.55804200	-1.85656600	H	-0.74110000	1.32823800	-4.14385900
H	-5.00274300	-2.41916500	-2.60342000	H	-1.77530200	2.11208300	-2.94273300
H	-4.03535000	-3.62899800	-1.73836500	C	1.26617700	0.28713500	-0.02593100
H	-4.58364300	-2.16667900	-0.90346900	C	-0.09885400	0.38037100	0.11644300
C	6.56700900	-2.94594200	0.33709200	C	-0.70260800	1.55547600	0.77546500
C	5.34518800	-3.02722400	-0.33899600	C	-1.78044700	2.26862300	0.22301100
C	4.14994600	-3.20128200	0.36795600	C	-0.19946300	1.98917900	2.02099300
C	4.19313200	-3.28227400	1.76848300	C	-2.29537600	3.40227900	0.84898600
C	5.41100600	-3.20274900	2.44288300	H	-2.20638700	1.93736200	-0.71195700
C	6.60327100	-3.03538100	1.72944900	C	-0.72265600	3.11319100	2.65630400
H	7.48723300	-2.81250200	-0.22561500	H	0.61641000	1.43944900	2.47819200
H	5.32204600	-2.95980000	-1.42413400	C	-1.76677000	3.83595800	2.06697900
H	3.25895200	-3.39267200	2.31348800	H	-3.11506600	3.94451800	0.38530600
H	5.43137600	-3.26817500	3.52760600	H	-0.31662700	3.42529400	3.61476300
H	7.55126400	-2.97184300	2.25669500	H	-2.17011200	4.71668700	2.55871600

N	2.09442700	1.45221500	0.10945100	H	0.85536700	0.31950600	-2.90616900
N	1.69489600	2.40907000	-0.62857100	C	-0.45469600	-3.61204000	-2.29592400
N	2.31042200	3.56810200	-0.50330100	H	0.61397600	-3.39677400	-2.26543200
C	1.84370400	4.61530200	-1.43657100	H	-0.65952300	-4.19704700	-3.20058500
H	2.43539400	5.50074200	-1.19243700	H	-0.70409400	-4.23074300	-1.43042900
C	2.13768300	4.22387500	-2.88862000	C	-3.58847800	-3.40617800	-1.71012300
H	1.57037400	3.33124900	-3.17052900	H	-3.05523000	-4.35882300	-1.70127800
H	3.20269900	4.01344400	-3.02901300	H	-4.40348100	-3.47300800	-2.44043400
C	0.36410900	4.93978400	-1.20783000	H	-4.02822300	-3.23942700	-0.72237400
H	-0.26220900	4.08008700	-1.45854700	C	-4.44196000	-0.37811200	-1.92570800
H	0.17699700	5.19836700	-0.16180300	H	-4.96118000	-0.96329900	-1.16488500
C	3.34667300	3.84001900	0.51691900	H	-5.01191400	-0.44182200	-2.86131800
H	3.45598000	2.89771400	1.05554000	H	-4.42769200	0.66673200	-1.61054800
C	4.68623300	4.18896700	-0.13918000	C	-1.88260900	1.30741100	-2.93895400
H	5.00949800	3.39009100	-0.81383800	H	-2.73154600	1.86469000	-2.53842800
H	5.45404200	4.31618600	0.63136800	H	-1.94333900	1.35251300	-4.03420900
H	4.62995100	5.12288100	-0.70895100	H	-0.96041100	1.80736900	-2.63486900
C	2.86337700	4.91213400	1.49983600	C	-5.62119000	-0.59789500	2.98808300
H	1.91704200	4.61151800	1.95936400	H	-6.19630800	0.01531800	3.69158800
H	3.60532800	5.04610100	2.29408300	H	-5.21234500	-1.45404100	3.53277000
H	2.72078300	5.88211900	1.01156500	H	-6.30635900	-0.98556600	2.22841600
H	0.06207300	5.78486800	-1.83559500	C	-3.53489300	0.75008600	3.43651100
H	1.85538600	5.03745600	-3.56499300	H	-4.07593800	1.35676400	4.17240800
TS14as				H	-2.74314200	1.36110800	2.99729700
Rh	-1.43060300	-0.93290500	-0.49856700	H	-3.06470200	-0.08494000	3.96882600
N	-0.38992600	-2.00604000	0.66509700	C	-5.10517200	1.43351000	1.58690100
C	-1.26206400	-2.35427600	-2.30527300	H	-5.67324400	2.07455500	2.27133200
C	-0.78607800	-1.03940200	-2.62884800	H	-5.79022000	1.09605900	0.79996600
C	-1.90015400	-0.12231100	-2.49918100	H	-4.31690400	2.03411300	1.12662600
C	-3.05917500	-0.90167000	-2.13924200	C	-0.41308400	1.61025000	0.86679500
C	-2.67751500	-2.27380700	-2.04939800	C	0.21222400	1.92156100	2.09371100
O	-4.00911100	-1.80464800	1.11182300	C	-1.46029600	2.44465600	0.43353400
C	0.71818200	-2.62169700	1.00074600	C	-0.16866100	3.03930000	2.83318500
C	1.86415200	-2.26519900	0.09234300	H	1.01139400	1.28122300	2.45325000
C	2.11193800	-1.01444300	-0.36000300	C	-1.83205000	3.57086100	1.16407000
O	0.83818100	-3.47834100	1.90876900	H	-1.97957500	2.20224300	-0.48235600
C	0.04832500	0.43487000	0.11196500	C	-1.18867700	3.87597800	2.36723700
C	1.38720100	0.22559800	-0.11209500	H	0.32889400	3.25595600	3.77450500
C	-3.70587800	-0.63279400	1.34804500	H	-2.63101000	4.20920600	0.79710300
O	-2.71922000	0.03053400	0.80765000	H	-1.48447500	4.75001500	2.94063900
C	-4.50382000	0.23828800	2.35246100	N	2.29435300	1.32746600	-0.07294300
C	0.54966400	-0.68781600	-3.19355000	N	1.88594300	2.32753400	-0.75000400
H	0.49248900	-0.72597400	-4.28922300	N	2.58554400	3.43935200	-0.66016600
H	1.32188300	-1.38727300	-2.87227900	C	2.11450500	4.53793900	-1.53131900

H	2.75671900	5.38853300	-1.29132600	C	0.18076000	-1.96595700	-1.81850300
C	2.31070000	4.18258400	-3.00872100	C	1.49155800	-2.03873300	-1.38985700
H	1.69444200	3.31981700	-3.28066800	O	-1.75357600	-0.50559600	-1.80905100
H	3.35674300	3.93667100	-3.21692100	C	1.35068200	0.13484600	-0.34593300
C	0.66704200	4.91916700	-1.20775500	C	2.12023500	-0.99150600	-0.67471900
H	-0.01357500	4.09888800	-1.44903400	C	-2.97945100	-0.63531500	1.44863400
H	0.55233100	5.15064200	-0.14503000	O	-1.88018800	-0.05459700	1.07766700
C	3.73167100	3.61522500	0.26018300	C	-2.75469000	-1.59914500	2.64462200
H	3.85095400	2.64275200	0.73925100	C	-0.11234800	3.74464100	-1.89544000
C	5.01417700	3.94172800	-0.51103800	H	-0.14581600	4.82425000	-2.08814400
H	5.23308100	3.16627500	-1.25157700	H	0.09034200	3.23728100	-2.84099400
H	5.85722200	3.99699200	0.18547800	H	0.72314000	3.55070500	-1.21869400
H	4.94694200	4.90526900	-1.02730700	C	-2.63743400	2.44484000	-3.44047400
C	3.39876500	4.65488400	1.33642300	H	-1.66174300	2.45664600	-3.93027100
H	2.48682500	4.37506200	1.87279600	H	-3.27009600	3.20184200	-3.91977200
H	4.22005900	4.71095800	2.05875100	H	-3.09220800	1.46635000	-3.61441200
H	3.26035600	5.65474300	0.91084500	C	-4.90561900	1.86138500	-1.26228300
H	0.37169100	5.79829400	-1.79005000	H	-4.94309800	1.38739000	-2.24588500
H	2.02162000	5.02565700	-3.64482500	H	-5.66740600	2.65097100	-1.23799800
H	3.05135200	-0.86954100	-0.89292600	H	-5.14563400	1.10856100	-0.50864000
C	2.78919800	-3.42407200	-0.25473900	C	-3.82316200	2.77161800	1.57639200
H	2.99694300	-3.42018800	-1.32963200	H	-4.44045500	1.87245200	1.59448200
H	2.27720600	-4.36042000	-0.01573300	H	-4.47071800	3.65031300	1.68932400
C	4.09902500	-3.35387500	0.51408100	H	-3.14485600	2.74039600	2.43186000
C	4.10468800	-3.48585400	1.91145700	C	-0.88170200	3.99300100	1.17736100
C	5.31158200	-3.13540600	-0.15086200	H	-1.07035100	3.55514400	2.15900200
C	5.30177600	-3.41183400	2.62313400	H	-1.10489900	5.06639700	1.23758900
H	3.15474000	-3.63173600	2.41925200	H	0.18151000	3.88207300	0.95866700
C	6.51222000	-3.05966900	0.56256500	C	-4.02277000	-2.42211300	2.90471200
H	5.31852700	-3.02880700	-1.23315700	H	-3.88279500	-3.06845600	3.77944800
C	6.51085700	-3.19851900	1.95153000	H	-4.25896300	-3.05755000	2.04654900
H	5.29279500	-3.51719100	3.70498900	H	-4.88315500	-1.77204000	3.08564400
H	7.44570900	-2.89241000	0.03147300	C	-1.56833200	-2.53427300	2.34159000
H	7.44246400	-3.13885000	2.50776000	H	-1.41153600	-3.23379500	3.17204600
15as				H	-0.64825500	-1.96397000	2.19118400
Rh	-1.77800500	1.27533000	-0.52347300	H	-1.75019500	-3.12036000	1.43594600
N	0.08360300	0.21903700	-0.80558900	C	-2.43323700	-0.72895700	3.87775200
C	-2.51954300	2.72374700	-1.97681400	H	-2.26442300	-1.35897200	4.75936400
C	-1.40404600	3.29159100	-1.29385500	H	-3.26102500	-0.04661700	4.10635200
C	-1.73001800	3.35984800	0.12282500	H	-1.53532100	-0.12740000	3.70726800
C	-3.07005700	2.86367500	0.28910300	C	1.75977800	1.17807800	0.63511000
C	-3.55283900	2.43575100	-0.98931300	C	1.12790200	1.17068000	1.88978800
O	-4.10578900	-0.45035700	0.97195600	C	2.72366000	2.15492500	0.35907700
C	-0.51864600	-0.76657700	-1.51379300	C	1.49496700	2.09557400	2.86729700

H	0.34213600	0.44493600	2.07664700	H	-3.73684100	-5.91327500	0.83689800
C	3.07506200	3.09375200	1.33327200	TS14a's			
H	3.19794000	2.16970100	-0.61464600	Rh	-1.41691300	-0.56504400	-0.79734700
C	2.47207400	3.05747000	2.59302500	N	-0.63881100	-2.20196700	-0.18892400
H	1.01133100	2.07122100	3.84010500	C	-1.99157200	-1.44749000	-2.88708700
H	3.82725500	3.84502200	1.10929200	C	-0.96309300	-0.41792100	-2.94476100
H	2.75591500	3.77925300	3.35394900	C	-1.57385700	0.84897100	-2.59225600
N	3.43379100	-1.25116100	-0.21710600	C	-2.89849700	0.56718700	-2.17236900
N	4.27201900	-0.32628100	-0.46496700	C	-3.16134500	-0.85882400	-2.36735500
N	5.49145100	-0.50424800	0.03055100	O	-3.32253600	-2.30723500	1.07368700
C	6.52553500	0.38173300	-0.54832400	C	0.29088500	-2.47919600	0.71703100
H	7.47560700	-0.01449800	-0.18540900	C	1.49141500	-2.35868900	-0.19408400
C	6.53729500	0.30884200	-2.08012000	C	1.99881800	-1.12109300	-0.47673100
H	5.60411200	0.70102400	-2.49481400	O	0.27817600	-2.87111400	1.88136600
H	6.65594700	-0.72440700	-2.42137400	C	0.10577400	0.46480700	0.12026900
C	6.37790900	1.81839900	-0.03807400	C	1.44043500	0.15843300	-0.12567600
H	5.46268500	2.27489600	-0.42239000	C	-3.26369000	-1.13529600	1.44557700
H	6.34101100	1.84317700	1.05511400	O	-2.61469300	-0.16774900	0.85957000
C	5.84026500	-1.71245300	0.80922200	C	-3.97498900	-0.64574900	2.73747600
H	4.91132400	-1.98540800	1.31649400	C	0.40398000	-0.58812200	-3.52769600
C	6.24120200	-2.86328200	-0.12169000	H	0.37311400	-0.45951000	-4.61788300
H	5.44899700	-3.06025400	-0.84963000	H	0.80186400	-1.58432600	-3.31967100
H	6.41259500	-3.77842900	0.45564700	H	1.10136200	0.14900000	-3.12253800
H	7.16382200	-2.62592500	-0.66298200	C	-1.75972600	-2.88043900	-3.24109600
C	6.89838200	-1.41809500	1.87448800	H	-1.50524100	-2.97661400	-4.30294400
H	6.62037600	-0.55119900	2.48195500	H	-2.64036900	-3.49384500	-3.04134300
H	6.98142900	-2.28469100	2.53844000	H	-0.92624000	-3.28772800	-2.65858200
H	7.89059800	-1.24054500	1.44733700	C	-4.47819300	-1.50519000	-2.07524700
H	7.22691900	2.42527800	-0.37054900	H	-4.39738800	-2.59318100	-2.05109800
H	7.36777600	0.90099400	-2.47854800	H	-5.22060700	-1.23213600	-2.83612200
H	2.07680500	-2.93450500	-1.58454300	H	-4.85952100	-1.17816100	-1.10460200
C	-0.53579300	-3.09910600	-2.51906300	C	-3.92929400	1.52005900	-1.65698200
H	0.20657700	-3.77104900	-2.96186800	H	-4.19543400	1.26317400	-0.62574100
H	-1.13791100	-2.68986100	-3.33752900	H	-4.84095500	1.45759300	-2.26188400
C	-1.43809300	-3.88857700	-1.58118700	H	-3.57858800	2.55416200	-1.67695500
C	-2.76007500	-3.48411100	-1.34546100	C	-0.89900800	2.18122000	-2.71281100
C	-0.95475200	-5.02481000	-0.91777600	H	-1.50962000	2.98231700	-2.29250600
C	-3.58378700	-4.21173900	-0.48415400	H	-0.72007200	2.41301400	-3.77003000
H	-3.12861200	-2.58381900	-1.82526300	H	0.06598400	2.18538300	-2.19934300
C	-1.77505800	-5.75091000	-0.05062300	C	-4.77274100	-1.79775900	3.36044600
H	0.07053000	-5.34618000	-1.08649300	H	-5.27472800	-1.45960100	4.27462000
C	-3.09576100	-5.34923100	0.16503400	H	-4.11839300	-2.63602600	3.61554500
H	-4.60649600	-3.88525000	-0.31699100	H	-5.53358500	-2.17222700	2.66856900
H	-1.38359100	-6.63172700	0.45163100	C	-2.88582600	-0.15835700	3.71502800

H	-3.33988100	0.16809400	4.65850700	H	1.42177300	-4.46809300	-0.53334100
H	-2.32647600	0.67813300	3.28872000	C	3.42383000	-3.95030800	0.06503000
H	-2.17455500	-0.96095000	3.94197700	C	3.43379200	-4.03310500	1.46622100
C	-4.91346300	0.52334300	2.38387300	C	4.61894800	-4.15268100	-0.63482800
H	-5.43400900	0.87900000	3.28113600	C	4.61572100	-4.32260500	2.14767100
H	-5.67473200	0.21520400	1.65687200	H	2.51118500	-3.85244900	2.01253200
H	-4.34946200	1.35806500	1.95978000	C	5.80404600	-4.44352000	0.04832700
C	-0.25862900	1.54830300	1.03783300	H	4.62303900	-4.08578600	-1.72016500
C	0.46073900	1.70410000	2.24695900	C	5.80538800	-4.53094300	1.44136100
C	-1.35800000	2.40217500	0.81986200	H	4.60988400	-4.38417000	3.23274600
C	0.10489000	2.67598100	3.17737900	H	6.72363000	-4.59958700	-0.50951100
H	1.29968700	1.04672600	2.44959800	H	6.72532900	-4.75496600	1.97444800
C	-1.70178400	3.38852000	1.74035900	13s			
H	-1.93809500	2.29032400	-0.08324400	C	1.30599500	-0.14195000	-2.67021400
C	-0.97507100	3.53056200	2.92590000	C	0.96704300	1.24441100	-2.64284000
H	0.66645000	2.76446500	4.10319700	C	2.17068200	2.00018700	-2.27541200
H	-2.54562000	4.04175800	1.53594800	C	3.18712100	1.08710700	-1.96852300
H	-1.25098500	4.29156900	3.65029900	C	2.64481900	-0.26307500	-2.14651300
N	2.45525200	1.15511700	0.00401900	Rh	1.41160600	0.62349700	-0.56884300
N	2.10433200	2.27821700	-0.48827600	C	2.25132200	3.49268800	-2.22474500
N	2.91598700	3.29747200	-0.29910400	C	-0.31112300	1.83971300	-3.14816400
C	2.43556500	4.57951000	-0.86122600	H	-0.24378700	2.04285200	-4.22527600
H	3.14770600	5.32961600	-0.50960500	H	-1.15385400	1.16451500	-2.98327000
C	2.47501400	4.55108400	-2.39223800	H	-0.53531000	2.78411800	-2.64704600
H	1.78986300	3.79132500	-2.78121500	C	0.40442500	-1.23307900	-3.16470000
H	3.48260500	4.32418900	-2.75430800	C	3.48777600	-1.49757200	-2.03976000
C	1.04842100	4.94005800	-0.31854100	H	2.96967900	-2.38090400	-2.41729500
H	0.29536500	4.23288400	-0.67314400	H	4.40748000	-1.37138800	-2.62273500
H	1.03948100	4.92494700	0.77506800	H	3.77433900	-1.68891500	-1.00134200
C	4.11841000	3.23162200	0.56349600	C	4.57814000	1.38577200	-1.50322000
H	4.26361100	2.16783500	0.75392700	H	4.94685400	0.58741300	-0.85449500
C	5.35386600	3.76999500	-0.16308300	H	5.26610400	1.46760900	-2.35483500
H	5.51257200	3.24314200	-1.10901900	H	4.61510800	2.31463500	-0.93208300
H	6.23837600	3.61832000	0.46417700	C	-4.90905900	3.71828300	-2.03777600
H	5.27834500	4.84244600	-0.37119500	C	-3.55574300	3.70976200	-1.69529500
C	3.85199200	3.93977200	1.89714800	C	-3.15829700	3.76134500	-0.35219500
H	2.97283900	3.51421300	2.39007700	C	-4.14299200	3.81667900	0.64263300
H	4.71388100	3.81908200	2.56185400	C	-5.49773300	3.82567800	0.30348600
H	3.68433100	5.01301400	1.75571400	C	-5.88418600	3.77676800	-1.03828300
H	0.76585100	5.94352200	-0.65399700	H	-5.20183600	3.68104600	-3.08352100
H	2.17308400	5.52290400	-2.79640800	H	-2.79931300	3.66187400	-2.47463700
H	2.99467400	-1.08648700	-0.91771900	H	-3.84455800	3.84838700	1.68758700
C	2.13078900	-3.64558800	-0.67803000	H	-6.25002900	3.87095700	1.08619900
H	2.33120700	-3.58265300	-1.75245200	H	-6.93776900	3.78488600	-1.30335700

C	-1.69402400	3.71325600	0.01564600	N	-2.42179200	-1.07831800	0.58771000
H	-1.10187500	4.22631700	-0.75597800	N	-2.41494400	-2.15061400	-0.09316100
H	-1.53010200	4.27392100	0.94728600	N	-3.29382100	-3.08578300	0.23769100
C	-1.13113600	2.31620100	0.18418000	C	-3.24487400	-4.29779100	-0.60498700
C	-1.82380400	1.17145500	0.05305600	H	-3.98305800	-4.97900300	-0.17342300
H	-2.88609300	1.27467000	-0.14049600	C	-3.66673000	-3.97628000	-2.04289400
C	0.93007200	3.23520500	0.87058300	H	-2.95853400	-3.27885700	-2.50117600
N	0.27554500	2.26309200	0.46860700	H	-4.66145700	-3.51968500	-2.06544400
O	1.52420400	4.17449900	1.22760900	C	-1.86979100	-4.97145400	-0.54107100
C	3.27946500	0.82769100	1.73119500	H	-1.10144100	-4.32266500	-0.96763300
C	4.09981100	0.16269100	2.86763200	H	-1.58893100	-5.19137400	0.49289100
C	5.15499000	1.14088300	3.39931100	C	-4.16311500	-3.00177800	1.42953300
H	5.72136700	0.68212000	4.21862800	H	-3.99143300	-1.99889700	1.82282200
H	5.86136100	1.42529300	2.61245400	C	-5.64121600	-3.12812600	1.04690800
H	4.68947500	2.05819000	3.76971200	H	-5.91504600	-2.37663500	0.29976200
C	4.77879200	-1.11176900	2.33241600	H	-6.26764100	-2.97489100	1.93215200
H	5.36578600	-1.59507000	3.12303200	H	-5.87747400	-4.11865100	0.64311500
H	4.03516600	-1.82398400	1.96730600	C	-3.73062500	-4.02396300	2.48774900
H	5.46177600	-0.87789700	1.50651200	H	-2.67619500	-3.88585300	2.74552600
C	3.11111300	-0.21370500	3.99047600	H	-4.32836300	-3.89576200	3.39673300
H	3.64141800	-0.68050400	4.82956200	H	-3.86994300	-5.05313600	2.13920400
H	2.59352800	0.67450700	4.37257100	H	-1.88341200	-5.91107900	-1.10415500
H	2.35775200	-0.91638100	3.62305800	H	-3.69147800	-4.88899900	-2.64765300
O	2.49347700	0.00048900	1.12505900	TS12s			
O	3.38244600	2.03965200	1.48925700	C	1.44673500	-0.74378900	-2.74338600
H	3.05089600	3.83294200	-1.56301800	C	0.96282200	0.60380000	-2.95150400
H	2.44901600	3.89534600	-3.22644900	C	2.09150200	1.51571900	-2.80836800
H	1.30859700	3.93270300	-1.88635700	C	3.20291600	0.76511600	-2.37937300
H	-0.49866900	-1.31345000	-2.55190600	C	2.80014600	-0.64099600	-2.32213200
H	0.09483500	-1.02125600	-4.19451700	Rh	1.48639300	0.47116600	-0.81804800
H	0.90452300	-2.20355300	-3.15838200	C	2.00132500	2.99539600	-3.00054500
C	-1.34531000	-0.19970100	0.23189200	C	-0.38638800	0.96817500	-3.48605900
C	-0.04948700	-0.61716400	0.16763400	H	-0.38275800	0.95142300	-4.58415200
C	0.37316700	-1.91248900	0.74133600	H	-1.14894600	0.26435400	-3.14372700
C	1.12002100	-2.86267200	0.02805900	H	-0.68263100	1.97170000	-3.16958000
C	0.07998600	-2.19734400	2.09181800	C	0.63275200	-1.98300100	-2.96172900
C	1.55008400	-4.04884700	0.62403600	C	3.74477500	-1.74287200	-1.95589600
H	1.35311100	-2.67175600	-1.00929800	H	3.27795800	-2.72630000	-2.03962400
C	0.51073000	-3.37947700	2.69272000	H	4.61869300	-1.72797600	-2.61759800
H	-0.49305900	-1.47683000	2.66723200	H	4.10377100	-1.61591200	-0.92890400
C	1.25139800	-4.31578900	1.96234100	C	4.57327100	1.25203400	-2.02352300
H	2.11808100	-4.76735300	0.03813500	H	4.92695300	0.76379600	-1.11001100
H	0.27377300	-3.56726400	3.73701700	H	5.29265800	1.02303200	-2.81983000
H	1.59092500	-5.23554100	2.43045300	H	4.58491600	2.33077700	-1.85349800

C	-5.40787200	4.73587400	-0.07308100	C	0.26216300	-1.69347300	0.90741500
C	-4.18748900	4.40506400	-0.67096200	C	1.28308500	-2.60285300	0.57271100
C	-3.06764000	4.10628700	0.11333500	C	-0.39763500	-1.87843100	2.14468200
C	-3.18939600	4.13285500	1.51150600	C	1.61045900	-3.66638700	1.41071900
C	-4.40599300	4.46250800	2.10795200	H	1.81690900	-2.46979200	-0.35647800
C	-5.52005700	4.76682200	1.31776200	C	-0.05862700	-2.93019900	2.99238300
H	-6.26843000	4.96650700	-0.69548000	H	-1.17906000	-1.18320300	2.43434700
H	-4.10488900	4.38142600	-1.75493100	C	0.94404300	-3.83623000	2.62756200
H	-2.32624400	3.87582400	2.12082600	H	2.39387000	-4.35958000	1.11631200
H	-4.48692100	4.47993700	3.19161300	H	-0.57448800	-3.04097500	3.94235600
H	-6.46752500	5.02192300	1.78447400	H	1.20629700	-4.65842700	3.28734000
C	-1.73695400	3.74989300	-0.53183300	N	-2.47248900	-1.02533800	0.06951200
H	-1.83988300	3.76297700	-1.62205600	N	-2.24325700	-2.16012400	-0.46433700
H	-0.98828800	4.50718800	-0.27503600	N	-3.12131300	-3.11863000	-0.25135900
C	-1.23488100	2.39260500	-0.08006400	C	-2.78807900	-4.40749300	-0.89647000
C	-1.83621200	1.21518300	-0.41071800	H	-3.57382400	-5.09735300	-0.58001300
H	-2.82541300	1.27961500	-0.86411100	C	-2.83863200	-4.28316800	-2.42245800
C	-0.07941100	2.38672200	0.92052500	H	-2.06471900	-3.59635800	-2.77870700
N	0.85337300	2.10386200	0.02942900	H	-3.81225000	-3.90775500	-2.75308000
O	-0.14388000	2.71488200	2.09853800	C	-1.44022900	-4.94114900	-0.40009900
C	3.08982900	0.93616800	1.58915300	H	-0.62604000	-4.28354000	-0.71358900
C	3.87305100	0.44512800	2.83545200	H	-1.42201600	-5.00412000	0.69162000
C	4.77592300	1.56783000	3.36413900	C	-4.27718700	-2.98312800	0.66331600
H	5.27971700	1.24675000	4.28308800	H	-4.27230500	-1.93332900	0.95869500
H	5.54649800	1.83240800	2.63124300	C	-5.59195300	-3.28108200	-0.06312300
H	4.19501100	2.46749800	3.57962400	H	-5.71095000	-2.63263000	-0.93661300
C	4.70916400	-0.80114200	2.50662300	H	-6.43415300	-3.10107900	0.61321400
H	5.24448500	-1.13960100	3.40161800	H	-5.65075800	-4.32326200	-0.39477900
H	4.07685900	-1.61757100	2.15090400	C	-4.07685700	-3.84641600	1.91469700
H	5.45475900	-0.58417900	1.73294600	H	-3.13220700	-3.59628200	2.40722000
C	2.79519200	0.09098800	3.88453400	H	-4.89337200	-3.66662500	2.62210300
H	3.27005200	-0.25428300	4.81051900	H	-4.07149000	-4.91540600	1.67560600
H	2.17740500	0.96360600	4.12109500	H	-1.25798200	-5.94019400	-0.80996800
H	2.13628900	-0.70283400	3.51843800	H	-2.67006300	-5.25998600	-2.88774300
O	2.70755400	-0.01822900	0.80615400	TS14I			
O	2.82526300	2.14137400	1.45775700	C	-1.68782400	0.14906000	-2.79235200
H	2.94876200	3.48987500	-2.77644000	C	-1.69748800	-1.25583900	-2.51635200
H	1.72697700	3.23102400	-4.03531100	C	-2.98974300	-1.59927300	-1.91326900
H	1.23507900	3.42406500	-2.34553700	C	-3.69149300	-0.40065800	-1.71400800
H	-0.31419400	-1.93461800	-2.41674600	C	-2.87093800	0.71289200	-2.20125300
H	0.40253300	-2.09791500	-4.02797300	Rh	-1.68892800	-0.19719300	-0.60195300
H	1.16386900	-2.87904100	-2.63473900	C	-3.43139400	-2.97015000	-1.49475900
C	-1.37905500	-0.12019900	-0.09873000	C	-0.64016800	-2.23325700	-2.93385800
C	-0.06725500	-0.52726900	0.07574000	H	-0.79024000	-2.55541500	-3.97183200

H	0.35517300	-1.79142100	-2.84829400	H	-2.24237400	1.32004500	3.73607200
H	-0.65823000	-3.12434300	-2.30210900	O	-2.56059000	0.48328000	1.21192800
C	-0.64094200	0.87630100	-3.57619900	O	-3.19356900	-1.63740000	1.61637300
C	-3.31173300	2.14278100	-2.27763800	H	-3.93028300	-2.93646700	-0.52308000
H	-2.45702700	2.81934100	-2.32938800	H	-4.11939300	-3.40775300	-2.22802400
H	-3.94360700	2.30982200	-3.15970400	H	-2.58071400	-3.64943100	-1.39856100
H	-3.88743500	2.42168600	-1.39185900	H	0.35773700	0.49023900	-3.35807800
C	-5.01534400	-0.23727100	-1.03453400	H	-0.82729400	0.75426100	-4.65046200
H	-4.99940400	0.63310100	-0.37321200	H	-0.64288500	1.94229700	-3.34898900
H	-5.81516600	-0.08497800	-1.76949900	C	1.15706500	0.49940100	-0.03871500
H	-5.26111700	-1.11216100	-0.42990200	C	-0.08395500	1.01766900	-0.26299600
C	4.46421500	-3.83575600	-1.46753800	C	-0.32171500	2.46877700	-0.40582500
C	3.09728800	-3.77141900	-1.19135300	C	0.41208400	3.23666200	-1.33518000
C	2.64028400	-3.55782900	0.11434100	C	-1.32194000	3.12454500	0.33819600
C	3.58157800	-3.41153100	1.14151300	C	0.14940500	4.59314400	-1.52067700
C	4.94870700	-3.47208400	0.87016700	H	1.19660400	2.75442300	-1.90707400
C	5.39419900	-3.68319700	-0.43701500	C	-1.57239900	4.48528300	0.16141300
H	4.80266900	-4.00181000	-2.48638300	H	-1.90292700	2.54735900	1.04614800
H	2.37469400	-3.87740300	-1.99697600	C	-0.84599100	5.22752300	-0.77227200
H	3.23684100	-3.23236300	2.15671000	H	0.72681600	5.15697400	-2.24905300
H	5.66534100	-3.34923400	1.67702100	H	-2.34580500	4.96697600	0.75449500
H	6.45815900	-3.72758900	-0.65051900	H	-1.05009100	6.28512700	-0.91450000
C	1.16547900	-3.40460600	0.40162800	N	2.22545800	1.42388000	0.14818900
H	0.57934400	-4.01629900	-0.29914000	N	3.36720200	0.89228000	0.25910500
H	0.94016100	-3.80674700	1.39762600	N	4.40001900	1.73758900	0.39689400
C	0.68134600	-1.96500200	0.31971700	C	5.63489500	1.05787600	0.83212400
C	1.48202600	-0.92733100	0.02455800	H	6.36260300	1.85375700	1.01009400
H	2.52682700	-1.15809100	-0.12909400	C	5.43720100	0.27706900	2.14156000
C	-1.39267100	-2.60995800	1.17487200	H	4.72938400	-0.54139400	1.98524800
N	-0.71393700	-1.73369100	0.56449200	H	5.04810600	0.92437000	2.93262200
O	-1.64273500	-3.64722100	1.66756400	C	6.16766100	0.15181800	-0.28593900
C	-3.18664100	-0.40429000	1.88092300	H	5.45003700	-0.64399400	-0.50103900
C	-3.95504300	0.11114500	3.11508200	H	6.33584100	0.72627500	-1.20178900
C	-4.84179800	-0.99793700	3.69739800	C	4.17574200	3.18652900	0.57138100
H	-5.36063100	-0.63193700	4.59028200	H	3.28723600	3.39520800	-0.02957800
H	-5.59298100	-1.32302300	2.97111800	C	3.84696600	3.53470600	2.02998900
H	-4.24695100	-1.87306500	3.96812900	H	2.99684000	2.94051900	2.37419100
C	-4.80912500	1.32845200	2.71405200	H	3.58445800	4.59420900	2.12099100
H	-5.31956700	1.73665100	3.59313800	H	4.70496100	3.34126000	2.68382200
H	-4.18944600	2.11294400	2.27332300	C	5.34105000	4.00976400	0.01654400
H	-5.57563400	1.04613800	1.98344900	H	5.59486100	3.69581000	-1.00046100
C	-2.88828000	0.53985800	4.14755200	H	5.05615100	5.06637400	-0.01058800
H	-3.37343000	0.92423500	5.05162000	H	6.24103100	3.93447400	0.63625900
H	-2.25981200	-0.30980600	4.43580800	H	7.11347800	-0.31158400	0.01484300

H	6.38942400	-0.14678100	2.47869900	C	-5.39927900	-1.33706300	2.61208000
151				H	-6.18536800	-1.23440400	3.36676000
C	-1.65520400	0.47944800	-2.78112100	H	-5.83920100	-1.11776700	1.63363300
C	-1.52663700	-0.94581800	-2.59630900	H	-5.04833900	-2.37108800	2.61167500
C	-2.80874600	-1.45523500	-2.09951000	C	-4.75112800	1.08983600	2.92235900
C	-3.62908800	-0.34640000	-1.84781300	H	-5.53622200	1.21484400	3.67440400
C	-2.90195100	0.87401600	-2.22165100	H	-3.94269100	1.79109900	3.14391200
Rh	-1.65496200	-0.09350700	-0.62568400	H	-5.16558900	1.35682300	1.94543000
C	-3.09373300	-2.90071200	-1.82526100	C	-3.63708300	-0.71193700	4.31434400
C	-0.38109000	-1.78231100	-3.08139300	H	-4.41090800	-0.64484700	5.08576700
H	-0.39574000	-1.86696300	-4.17528600	H	-3.22689000	-1.72481700	4.31041500
H	0.57517600	-1.34829100	-2.77865100	H	-2.83420600	-0.01518500	4.57669300
H	-0.42831900	-2.79032100	-2.66455800	O	-2.67256800	0.41474600	1.27077800
C	-0.64656100	1.34712200	-3.46354200	O	-2.74869800	-1.79416500	1.76493400
C	-3.46855200	2.26133600	-2.17932300	H	-3.99912300	-3.02643700	-1.22777700
H	-2.67618700	3.00969300	-2.11931900	H	-3.22074900	-3.46328700	-2.75795800
H	-4.07756800	2.46795700	-3.06904200	H	-2.26857300	-3.35601300	-1.26874500
H	-4.10448500	2.39753700	-1.30033900	H	0.36966500	1.04834800	-3.19572800
C	-4.99912600	-0.33665700	-1.24253200	H	-0.75493300	1.25428500	-4.55142100
H	-5.04690500	0.37375700	-0.41077800	H	-0.76770000	2.39629900	-3.19368400
H	-5.74947100	-0.02548200	-1.97924000	C	1.19230900	0.53655000	-0.01672400
H	-5.28392500	-1.32060500	-0.86401800	C	-0.04366900	1.08470000	-0.19683200
C	4.29348200	-3.87983600	-1.72809600	C	-0.28881300	2.54001000	-0.24642600
C	2.92754700	-3.76311200	-1.46071000	C	0.48903000	3.38367500	-1.07014900
C	2.46445500	-3.58258800	-0.15224100	C	-1.34321700	3.13422500	0.47594800
C	3.40274900	-3.52546300	0.88823800	C	0.22265400	4.74777300	-1.16884100
C	4.76813900	-3.63679500	0.62661700	H	1.30695700	2.95076000	-1.63343800
C	5.21879800	-3.81262700	-0.68483100	C	-1.60270000	4.50187000	0.38324600
H	4.63460700	-4.01891700	-2.75036100	H	-1.96074800	2.51172900	1.11047700
H	2.21025900	-3.80149000	-2.27727200	C	-0.82710500	5.31768400	-0.44265500
H	3.05314800	-3.37331200	1.90607300	H	0.83683200	5.36832500	-1.81658200
H	5.48108600	-3.58216300	1.44456500	H	-2.41918600	4.93089100	0.95873800
H	6.28205900	-3.89710800	-0.89055700	H	-1.03520200	6.38123700	-0.51946500
C	0.99940000	-3.36386100	0.13821700	N	2.27563800	1.42488600	0.23092400
H	0.38210500	-3.83834500	-0.63848200	N	3.40054300	0.85126000	0.32133000
H	0.72236900	-3.84649900	1.07940900	N	4.45596500	1.65070200	0.52404400
C	0.61038000	-1.89239000	0.21800900	C	5.66368800	0.90275100	0.92457500
C	1.47504400	-0.89956400	-0.06363800	H	6.41735600	1.66063300	1.15346100
H	2.49596900	-1.16806600	-0.29188200	C	5.42658000	0.05291600	2.18336900
C	-1.31455300	-2.18074100	1.55100000	H	4.68864000	-0.72612300	1.97398700
N	-0.74420700	-1.58875900	0.51244300	H	5.05692500	0.66548100	3.01059200
O	-0.93697200	-2.98803400	2.37255500	C	6.17281200	0.04466500	-0.24142800
C	-3.14112500	-0.53879500	1.90295300	H	5.43522000	-0.71986400	-0.49899300
C	-4.24844300	-0.36014300	2.93762700	H	6.35799300	0.66274100	-1.12510000

C	4.27830400	3.09276000	0.78754600	H	-4.03592700	-1.90045000	1.76753200
H	3.40156400	3.36717800	0.19587800	H	-3.67702000	-2.05529000	3.49519200
C	3.94879500	3.35927500	2.26300700	H	-2.57921600	-2.75460200	2.28269300
H	3.07883800	2.77036700	2.56410400	C	-3.56918500	-0.74108900	-1.35548400
H	3.71716800	4.41861000	2.41816900	O	-2.41230800	-0.99518100	-0.87103600
H	4.79512000	3.09981400	2.90894100	C	-4.17637700	-1.87159500	-2.21694300
C	5.47400800	3.91013200	0.29208500	C	-5.41429600	-1.36275400	-2.96944800
H	5.72375100	3.65381800	-0.74194600	C	-4.57764900	-3.01074300	-1.25381500
H	5.22504500	4.97542900	0.33208500	C	-3.12059700	-2.37632500	-3.21990700
H	6.36690000	3.76433500	0.90939300	H	-6.16778000	-0.98200200	-2.27624800
H	7.10548500	-0.45893100	0.03457400	H	-5.85479900	-2.17427600	-3.55952500
H	6.35939700	-0.42702000	2.49874300	H	-5.14974200	-0.54769100	-3.64971600
14II				H	-3.71561500	-3.37311500	-0.68768200
Rh	-1.30297000	-0.05165800	0.73866400	H	-4.99955500	-3.85040200	-1.81726600
N	-0.42248600	1.14258100	-0.95535800	H	-5.33731900	-2.66991600	-0.54066900
C	-2.02743300	1.64805000	2.31879700	H	-2.78900300	-1.56458400	-3.87601800
C	-0.77685400	0.93880700	2.62017400	H	-3.54770600	-3.16744800	-3.84624100
C	-1.10100400	-0.43165000	2.88145000	H	-2.24250600	-2.77479400	-2.70802000
C	-2.46165700	-0.62006500	2.45846700	O	-3.15510500	2.47862900	-0.46366900
C	-3.05136200	0.70644600	2.21324500	H	-3.65826000	1.64245000	-0.75698000
O	-4.23831600	0.30658400	-1.17738100	C	1.02855600	3.15158100	-0.92606600
C	-1.05157200	1.19564000	-2.00658300	H	0.15002800	3.69383600	-0.55520900
C	0.86084400	1.67933000	-0.61903800	H	0.99466300	3.27425900	-2.02004000
C	1.74837900	0.84056400	-0.07321100	C	2.30945900	3.73000400	-0.37519800
O	-1.72090600	1.20270100	-2.96658500	C	2.30589800	4.46176800	0.81794100
C	0.36417500	-1.22201300	0.38607300	C	3.53398100	3.49349800	-1.01573300
C	1.55532500	-0.61139200	0.10011500	C	3.49826700	4.93887300	1.36658500
C	-4.50132800	0.94146700	1.93003200	H	1.36041000	4.66378500	1.31521400
C	-3.22928900	-1.90502400	2.50430000	C	4.72792500	3.96437900	-0.46908500
C	-2.09675200	3.13158400	2.15564900	H	3.54932800	2.92252000	-1.94068300
C	0.52600400	1.60962000	2.93052500	C	4.71310500	4.68732200	0.72686100
C	-0.22626400	-1.43603600	3.55613500	H	3.47702900	5.50768000	2.29186800
H	-4.68119500	1.97247400	1.62424500	H	5.66823000	3.76682800	-0.97579100
H	-5.10432300	0.72644300	2.82133600	H	5.64170400	5.05534000	1.15344600
H	-4.85064000	0.30117100	1.11699400	H	2.72516300	1.23574100	0.16988800
H	-1.61903900	3.45241500	1.22587600	N	2.69589300	-1.43405900	-0.10546400
H	-1.59177100	3.62076700	2.99678800	N	3.75053300	-0.79229800	-0.38916500
H	-3.12729700	3.48306400	2.11070200	N	4.85661500	-1.52750400	-0.56382800
H	0.68577800	2.47601000	2.28665800	C	5.95160600	-0.76024800	-1.18900500
H	1.36477700	0.92853300	2.77297400	C	6.44698700	0.33769000	-0.23856400
H	0.54845000	1.95065900	3.97377700	H	7.30275600	0.86231500	-0.67668700
H	0.82613000	-1.27358500	3.31777100	H	5.65344800	1.06675800	-0.05279600
H	-0.47968100	-2.45720500	3.27201700	H	6.75419100	-0.08953500	0.72049800
H	-0.34945000	-1.33939500	4.64242800	C	5.54424700	-0.18147500	-2.55350300

H	4.72284900	0.52926200	-2.42508800	C	0.31361900	1.06303000	-0.44704000
H	6.38905200	0.34006800	-3.01560100	C	1.51462000	0.48562600	-0.13766000
H	5.21049900	-0.96891000	-3.23482000	C	-4.79041300	-0.66101400	-1.43037500
H	6.76379800	-1.47486100	-1.34328300	C	-3.46910700	2.08383300	-2.20128900
C	4.79241400	-3.00383700	-0.57875700	C	-2.63301700	-3.01208500	-2.05546600
H	4.01776600	-3.24618000	0.15276000	C	-0.02586100	-1.64799000	-3.16685500
C	6.10964000	-3.63186900	-0.11683100	C	-0.63070600	1.46904500	-3.61051600
H	6.45413200	-3.18262300	0.81953900	H	-5.02727700	-1.69973900	-1.19895600
H	5.95861100	-4.70286500	0.05109800	H	-5.51390800	-0.29677400	-2.17012900
H	6.90575000	-3.53234200	-0.86229900	H	-4.93027700	-0.08035500	-0.51470200
C	4.32900400	-3.53744200	-1.94162700	H	-2.04698700	-3.37889500	-1.20831500
H	3.37861800	-3.07690900	-2.22146800	H	-2.30188900	-3.53543300	-2.95950300
H	5.07130600	-3.32697800	-2.71939200	H	-3.66920500	-3.29000400	-1.85931700
H	4.18396900	-4.62200900	-1.89655700	H	0.13468400	-2.54887100	-2.56989800
C	0.24947400	-2.68446800	0.57447400	H	0.87446200	-1.03524300	-3.08976500
C	-0.81376000	-3.40386700	-0.00462500	H	-0.15321400	-1.95183700	-4.21395500
C	1.16361500	-3.40680900	1.37278700	H	0.42931700	1.26485000	-3.44941400
C	-0.95028000	-4.77830800	0.19163300	H	-0.81773000	2.50176900	-3.31678400
H	-1.52887200	-2.86016100	-0.60564900	H	-0.83716700	1.37181500	-4.68400100
C	1.02121700	-4.77781400	1.57487100	H	-4.09256100	2.14448200	-1.30516400
H	1.98689900	-2.87896400	1.83793000	H	-4.12571400	2.21203500	-3.07171400
C	-0.03650400	-5.47515100	0.98427800	H	-2.76279400	2.91492100	-2.17316300
H	-1.77779800	-5.30369200	-0.27862900	C	-3.24506500	0.84678800	1.83873200
H	1.73804300	-5.30361600	2.20049500	O	-2.15549600	0.85368600	1.22713300
H	-0.14568800	-6.54451800	1.14226200	C	-3.64662000	2.06238200	2.68777500
C	-3.05768100	3.45127100	-1.37095900	C	-4.63954200	1.65164300	3.78847300
O	-2.21946100	4.32831700	-1.24561000	C	-4.32642100	3.06270500	1.72173700
C	-4.05653000	3.39324100	-2.51005900	C	-2.39394200	2.69983800	3.31561800
H	-4.12485300	2.37662500	-2.90449300	H	-5.54326900	1.20948600	3.36424700
H	-5.04726500	3.66589200	-2.13018200	H	-4.92174800	2.53008600	4.37862300
H	-3.76504800	4.09224200	-3.29357300	H	-4.19256500	0.91629800	4.46468100
TS15II				H	-3.64554400	3.37800800	0.92581100
Rh	-1.38285200	-0.06238900	-0.72852000	H	-4.63921800	3.95511200	2.27393700
N	-0.48834500	-1.60318600	0.46501300	H	-5.21613700	2.61980600	1.26130000
C	-2.47856200	-1.53675800	-2.22964000	H	-1.89255100	1.99433900	3.98575600
C	-1.22856600	-0.90053300	-2.67680300	H	-2.68310200	3.57838100	3.90192900
C	-1.49413800	0.50623100	-2.86327600	H	-1.67289800	3.00917700	2.55775300
C	-2.76144900	0.76584300	-2.26781300	O	-3.06696000	-2.10589400	0.90907800
C	-3.39550600	-0.52569900	-1.95305700	H	-3.67239000	-1.04034300	1.34079800
O	-4.11119600	-0.11294200	1.78365500	C	1.25376600	-3.39380300	0.38754900
C	-1.04115100	-2.09211500	1.49473800	H	0.66379600	-3.94594700	-0.35719000
C	0.90028200	-1.92015900	0.27938100	H	0.92342800	-3.77387300	1.36325200
C	1.77048400	-0.95086800	-0.03194400	C	2.72906900	-3.66136000	0.20527700
O	-1.10915400	-2.53975900	2.57571600	C	3.25673700	-3.92662600	-1.06377400

C	3.60809900	-3.55813200	1.29146900
C	4.63211100	-4.08195600	-1.24732300
H	2.58367100	-4.00066100	-1.91455600
C	4.98330000	-3.71143900	1.11315000
H	3.20885500	-3.34099400	2.27893600
C	5.49982800	-3.97064500	-0.15897000
H	5.02557800	-4.28664300	-2.23904100
H	5.65144200	-3.62329300	1.96496800
H	6.57050200	-4.08647700	-0.30018100
H	2.80125600	-1.24577700	-0.16884100
N	2.61902700	1.35395600	0.10141400
N	3.72717100	0.76126800	0.25038200
N	4.79274300	1.54443500	0.45540000
C	5.97263100	0.78958200	0.92162600
C	6.49448500	-0.12844400	-0.19155900
H	7.40791400	-0.63869700	0.13195800
H	5.74741900	-0.88798300	-0.43628300
H	6.71702000	0.44659900	-1.09535500
C	5.68310000	0.00177900	2.20932800
H	4.93768000	-0.77361200	2.01362300
H	6.59724100	-0.48038100	2.57218400
H	5.30270200	0.65768900	2.99745500
H	6.73528400	1.54188600	1.13858000
C	4.64368900	3.00129300	0.65032700
H	3.77942200	3.26760400	0.03761000
C	5.86230900	3.76784500	0.12989100
H	6.11098800	3.46351500	-0.89126400
H	5.63960100	4.83962200	0.12469800
H	6.74808200	3.62541800	0.75811000
C	4.30751100	3.34042800	2.10909300
H	3.42056700	2.78684600	2.42750800
H	5.14091300	3.08956400	2.77485200
H	4.10114700	4.41086900	2.21489700
C	0.20109000	2.51748500	-0.69697900
C	-0.88043800	3.26733000	-0.19836600
C	1.13761400	3.20078600	-1.50541700
C	-1.01274500	4.62955500	-0.46931400
H	-1.61322200	2.75698400	0.40822500
C	1.00289400	4.55890600	-1.78364800
H	1.96967500	2.64883000	-1.92542800
C	-0.07273800	5.28630900	-1.26525100
H	-1.85613700	5.17682900	-0.05514100
H	1.73800400	5.05078000	-2.41551600
H	-0.17614800	6.34577500	-1.48211200

C	-3.58140400	-3.31352200	1.09670600
O	-2.95702700	-4.33903400	0.87210600
C	-5.01648600	-3.31556600	1.60298900
H	-5.06449100	-2.80159800	2.56846100
H	-5.66369000	-2.76021300	0.91622700
H	-5.37611600	-4.33927800	1.70659900

16II

Rh	-1.49669500	0.01117300	-0.80251300
N	-0.45248900	-1.70179500	-0.19115700
C	-2.95379500	-1.16949600	-2.19821400
C	-1.90701200	-0.35950300	-2.83797900
C	-2.26018400	1.03667400	-2.65052400
C	-3.31527300	1.07143400	-1.70958500
C	-3.77865800	-0.30464400	-1.47805700
O	-3.33907900	-0.53950300	2.51003300
C	-0.90264300	-2.49675200	0.78050300
C	0.88955000	-1.90056700	-0.56989900
C	1.73259100	-0.86956000	-0.75869600
O	-0.33381200	-3.23289600	1.56116400
C	0.21060600	1.12113500	-0.68079900
C	1.44899800	0.54534700	-0.58055500
C	-4.95976500	-0.64925900	-0.62428400
C	-4.01672300	2.28633700	-1.18448400
C	-3.02083300	-2.65948300	-2.30851700
C	-0.88829000	-0.89546800	-3.79721100
C	-1.66234600	2.19727100	-3.37774400
H	-5.14055600	-1.72546000	-0.61279900
H	-5.86674600	-0.16122200	-1.00092500
H	-4.82003200	-0.31825700	0.41019800
H	-2.13696400	-3.12787100	-1.86848000
H	-3.07104100	-2.95649900	-3.36233300
H	-3.89445000	-3.07095800	-1.80097300
H	-0.50806700	-1.86047200	-3.45354200
H	-0.03814400	-0.21579300	-3.88288200
H	-1.32276500	-1.03504500	-4.79590900
H	-0.60756700	2.02999100	-3.60052400
H	-1.73388400	3.12263700	-2.80495800
H	-2.19204300	2.33703100	-4.32894600
H	-4.35735900	2.12681100	-0.15763100
H	-4.90200300	2.51452000	-1.79260400
H	-3.36114300	3.15843100	-1.18970900
C	-2.55384500	0.52753000	2.41459800
O	-1.71675600	0.65600200	1.52411700
C	-2.81042000	1.60818200	3.46435400

C	-3.40700800	1.00647400	4.74860800	C	5.85187500	3.74211300	0.05216500
C	-3.81853900	2.59807900	2.83036500	H	6.22901400	3.43260000	-0.92725100
C	-1.48670000	2.33148900	3.77415000	H	5.65342900	4.81820400	0.02004900
H	-4.36038600	0.50981100	4.55454800	H	6.64210500	3.58173100	0.79323100
H	-3.57331800	1.80228900	5.48168300	C	4.05172600	3.33678200	1.81421500
H	-2.72773400	0.27194500	5.19164500	H	3.11899400	2.80347000	2.01303600
H	-3.40944300	3.05735800	1.92609600	H	4.79027600	3.05912500	2.57438800
H	-4.04422300	3.39606000	3.54489100	H	3.85956200	4.41147400	1.90493600
H	-4.75783900	2.09681800	2.57354700	C	0.05798200	2.59056400	-0.73820500
H	-0.75944900	1.64288800	4.21513500	C	-0.91380100	3.27819600	0.01269300
H	-1.67093400	3.13856000	4.49039500	C	0.85010300	3.35994500	-1.61967500
H	-1.04095000	2.75752600	2.87387300	C	-1.08523500	4.65864700	-0.10249700
O	-2.37654900	-2.42555200	0.92012300	H	-1.53070800	2.70993200	0.69323500
H	-3.01595800	-1.21547900	1.85445700	C	0.67960300	4.73683300	-1.73828100
C	1.34817000	-3.33019100	-0.87345300	H	1.59980600	2.85607100	-2.21896600
H	1.29658000	-3.48793600	-1.95914700	C	-0.29204300	5.39884900	-0.98117100
H	0.66110500	-4.04550000	-0.41768900	H	-1.84101100	5.15618000	0.50091900
C	2.75612200	-3.59108000	-0.38099200	H	1.30220300	5.29595700	-2.43209200
C	3.83224600	-3.70962200	-1.26584000	H	-0.42679500	6.47267200	-1.07541900
C	3.00553800	-3.64897200	0.99900100	C	-3.02767800	-3.64022000	0.86838000
C	5.13648800	-3.87779700	-0.78889900	O	-2.60489400	-4.58155000	0.24948600
H	3.65062600	-3.66118600	-2.33711700	C	-4.30264500	-3.61330600	1.67289500
C	4.30375400	-3.81812600	1.47633000	H	-4.04110900	-3.62692300	2.73641500
H	2.16754700	-3.54505700	1.68210000	H	-4.87377900	-2.70034800	1.49051100
C	5.37587300	-3.92956600	0.58400700	H	-4.90081900	-4.49208100	1.43404300
H	5.96170600	-3.96399000	-1.49073400				
H	4.48298200	-3.85941700	2.54743400	17II			
H	6.38821900	-4.05495300	0.95804700	C	1.74438700	-2.50222600	-1.83432400
H	2.75163500	-1.10997000	-1.03227000	C	2.49866400	-1.32143400	-2.16454600
N	2.54354900	1.40951500	-0.29145300	C	3.63868800	-1.22716400	-1.25221100
N	3.62828600	0.78985300	-0.07815400	C	3.47178600	-2.22942200	-0.28414300
N	4.69294400	1.54383500	0.20843200	C	2.28535800	-3.02178800	-0.61063400
C	5.81344700	0.75062800	0.75695800	Rh	1.49497700	-0.99869400	-0.25930400
C	6.38549400	-0.17949900	-0.32048500	C	4.77247600	-0.25635100	-1.37385100
H	7.25488400	-0.72051300	0.06762900	C	2.27982400	-0.44457600	-3.35855800
H	5.63495100	-0.91470200	-0.62137300	H	2.86676000	-0.80983600	-4.21095100
H	6.69337400	0.39071600	-1.20232700	H	1.22618300	-0.43172100	-3.64511800
C	5.40022300	-0.03414500	2.01233500	H	2.58237900	0.58447500	-3.15116300
H	4.64330900	-0.77987300	1.75540800	C	0.63920900	-3.08337400	-2.65937100
H	6.26636600	-0.55370200	2.43594500	C	1.90846000	-4.30043200	0.07308400
H	4.98842200	0.63128900	2.77675400	H	0.87026400	-4.57211300	-0.12142600
H	6.58133000	1.47736900	1.03383200	H	2.55233800	-5.12059800	-0.27106900
C	4.55946800	3.00167800	0.40437500	H	2.02193700	-4.21498400	1.15627600
H	3.78420300	3.29751900	-0.30705200	C	4.29513900	-2.46344500	0.94373900
				H	3.66428300	-2.37902000	1.83514000

H	4.72903000	-3.46989000	0.93472800	N	-2.78415100	-0.69762600	-0.50145400
H	5.10675100	-1.73918900	1.03212100	N	-3.54195300	0.30142800	-0.67058000
C	-1.97056400	4.92780200	0.51637300	N	-4.84813400	0.07399300	-0.46639300
C	-1.64054700	4.04979300	-0.51391400	C	-5.61915300	1.32238900	-0.30507800
C	-0.31681400	3.93591800	-0.96389400	H	-6.64608400	1.01287300	-0.09744600
C	0.67448400	4.70921500	-0.35104900	C	-5.11198600	2.16413000	0.87759000
C	0.34713500	5.58077000	0.69182300	H	-4.07624600	2.47049600	0.70576600
C	-0.97356500	5.69723900	1.12508500	H	-5.14705000	1.59592200	1.81129000
H	-3.00254100	5.00619100	0.84871400	C	-5.61551500	2.12479400	-1.61246600
H	-2.40962700	3.42755700	-0.96466100	H	-4.59679500	2.42887300	-1.86709700
H	1.70786600	4.60907900	-0.66354700	H	-6.01041800	1.52411200	-2.43715500
H	1.13367100	6.15966000	1.16745500	C	-5.30921400	-1.23755300	0.03571000
H	-1.22658900	6.37683200	1.93443300	H	-4.67545700	-1.95977200	-0.48639900
C	0.02739700	2.91515500	-2.04203800	C	-5.05392900	-1.40650800	1.54110600
H	-0.75010200	2.91791000	-2.81151100	H	-4.00187000	-1.22190600	1.76839700
H	0.97408500	3.16782700	-2.51661600	H	-5.29351800	-2.42938700	1.85148800
C	0.05381500	1.52704200	-1.41599100	H	-5.67615600	-0.72002200	2.12567200
C	-1.06409400	0.77128500	-1.48483500	C	-6.76665100	-1.50867400	-0.34421300
H	-1.87506900	1.16591100	-2.08496100	H	-6.94232900	-1.31318900	-1.40650600
C	2.30571700	1.79508200	-0.61685100	H	-6.99955500	-2.55963200	-0.14571300
N	1.09510900	1.17646600	-0.51895500	H	-7.47081400	-0.90724900	0.24051400
O	2.82164200	2.42665200	-1.51827200	H	-6.22994300	3.02506400	-1.50918100
C	3.61773000	2.53811400	1.26953600	H	-5.72717300	3.06229800	0.99807100
O	3.39043200	3.70575500	1.08298100	C	0.98881800	0.25641700	2.56380700
O	3.06503900	1.50997700	0.55512100	O	1.52904300	-0.68162000	1.94653100
H	5.26122000	-0.09213800	-0.41138600	O	0.43105000	1.28723400	2.00357100
H	5.52457200	-0.64215200	-2.07394300	H	0.59886200	1.25724600	0.97915800
H	4.44258400	0.71546600	-1.74505300	C	0.91377600	0.23692200	4.06756300
H	-0.02634500	-2.29931500	-3.02745200	H	1.09251200	1.23579300	4.47091800
H	1.05602600	-3.61709800	-3.52235100	H	-0.09940200	-0.06383500	4.35605700
H	0.04011100	-3.78477800	-2.07913900	H	1.62585600	-0.48277600	4.47143700
C	-1.40226600	-0.42713100	-0.72296900	C	4.52656200	1.96689700	2.33152100
C	-0.52331600	-1.30404300	-0.15970600	H	5.41161700	1.53461200	1.85308500
C	-0.98538800	-2.56188200	0.46953800	H	4.83026500	2.75732500	3.01714500
C	-1.81334900	-3.45161700	-0.25148700	H	4.02006200	1.16014700	2.86836200
C	-0.60123200	-2.95112500	1.76661400				
C	-2.22888600	-4.66378200	0.29362400	TS18II			
H	-2.13818500	-3.16685200	-1.24541200	C	1.53358900	-2.70137400	-1.79265800
C	-1.02780100	-4.16031300	2.31809800	C	2.39554600	-1.60416600	-2.12318700
H	0.05275200	-2.30619000	2.33761800	C	3.50752500	-1.57962800	-1.16786500
C	-1.83945600	-5.02768100	1.58648300	C	3.22748300	-2.53916000	-0.18458200
H	-2.86211100	-5.32588700	-0.29145200	C	1.98235900	-3.22859800	-0.53137300
H	-0.71662300	-4.42717000	3.32500100	Rh	1.36532600	-1.15718500	-0.23590700
H	-2.16392300	-5.97223100	2.01379600	C	4.72538500	-0.71585800	-1.27809000
				C	2.29904500	-0.74513400	-3.34557700

H	2.92940500	-1.15214300	-4.14663100	C	-2.16398600	-3.28587600	-0.31457400
H	1.27069400	-0.69670200	-3.70910600	C	-0.95822900	-2.89981200	1.73388400
H	2.63145500	0.27363800	-3.13507800	C	-2.71091900	-4.44929800	0.22139900
C	0.40765700	-3.21455800	-2.63513000	H	-2.43380400	-2.97297300	-1.31672100
C	1.48129300	-4.45659900	0.16332700	C	-1.51761900	-4.05810200	2.27570600
H	0.43244000	-4.65112700	-0.06233700	H	-0.25233800	-2.32129400	2.31469400
H	2.07058700	-5.33074700	-0.14391400	C	-2.39272600	-4.84365300	1.52466900
H	1.56712700	-4.35605800	1.24750900	H	-3.39140700	-5.04803700	-0.37866600
C	3.98633700	-2.81004000	1.07675000	H	-1.25970500	-4.35101000	3.29037600
H	3.34212400	-2.62249000	1.94267700	H	-2.82036400	-5.74939900	1.94521500
H	4.31255900	-3.85543500	1.11830900	N	-2.86797200	-0.44217300	-0.52729500
H	4.86708500	-2.17130500	1.16358600	N	-3.51831400	0.63298000	-0.67649300
C	-1.24257400	5.12996900	0.65516100	N	-4.84256400	0.53746200	-0.48542100
C	-1.09688800	4.20362000	-0.37500500	C	-5.48237400	1.85504100	-0.30473900
C	0.15973500	3.96377400	-0.95012600	H	-6.54143600	1.65092700	-0.13053700
C	1.27163600	4.65768200	-0.46224700	C	-4.92095000	2.60635500	0.91388600
C	1.12902600	5.57809300	0.58058400	H	-3.85338100	2.80111500	0.77627700
C	-0.12615100	5.82088400	1.13796400	H	-5.04301000	2.02226800	1.83017500
H	-2.22405200	5.30674600	1.08743300	C	-5.36083300	2.68832500	-1.58700500
H	-1.95747600	3.63972400	-0.72718600	H	-4.31038900	2.89872900	-1.80450600
H	2.25583000	4.45831000	-0.87182000	H	-5.78670200	2.15103600	-2.43951800
H	2.00666700	6.09521200	0.95783400	C	-5.44114000	-0.73077400	-0.01750700
H	-0.23638900	6.53716800	1.94764200	H	-4.88356100	-1.50214900	-0.55618600
C	0.30119400	2.89832400	-2.03023500	C	-5.21338600	-0.96400800	1.48384700
H	-0.50164900	3.00713600	-2.76554800	H	-4.15029200	-0.88752100	1.72122800
H	1.25086300	3.01225600	-2.55222600	H	-5.55199500	-1.96716300	1.76461300
C	0.15997500	1.52617200	-1.39402100	H	-5.77090500	-0.23716500	2.08461600
C	-1.01274700	0.87068000	-1.47908400	C	-6.91675400	-0.83752900	-0.40842400
H	-1.77464100	1.32963300	-2.09831500	H	-7.06548000	-0.59424700	-1.46496300
C	2.43373800	1.56269500	-0.57562000	H	-7.25840100	-1.86373800	-0.24086400
N	1.14564100	1.09737400	-0.44849200	H	-7.55721500	-0.18313300	0.19234300
O	3.00758700	2.01305000	-1.54460200	H	-5.88866200	3.64084400	-1.47383500
C	3.93231200	2.31932500	1.16532400	H	-5.43712900	3.56348200	1.04451300
O	4.02091100	3.44312900	0.74843600	C	0.88552300	0.14898200	2.51074500
O	3.11477600	1.34501100	0.63634400	O	1.35800300	-0.86107200	1.91397100
H	5.22390500	-0.60259000	-0.31288600	O	0.46843200	1.20992700	1.94174900
H	5.44267400	-1.16818000	-1.97490600	H	0.73943400	1.17578500	0.77012800
H	4.48858300	0.28174000	-1.65178500	C	0.76688900	0.08051100	4.01621500
H	-0.17114200	-2.39190100	-3.06093000	H	0.78589400	1.08118500	4.45034600
H	0.80187200	-3.82224000	-3.45886100	H	-0.19532300	-0.38388200	4.26047300
H	-0.27315800	-3.83171400	-2.04912900	H	1.55942200	-0.54412800	4.43228300
C	-1.46488000	-0.30469500	-0.73583800	C	4.64557000	1.74968100	2.36567400
C	-0.67740200	-1.27280000	-0.18885600	H	5.22103400	0.86666100	2.07262600
C	-1.27150900	-2.48102200	0.42724500	H	5.30228600	2.50659600	2.79285500

H	3.90867000	1.42716400	3.10738700	O	3.03078800	1.45271400	0.73186300
19H				H	5.09859800	-0.42552000	-0.25463600
C	1.56613600	-2.67603000	-1.86209400	H	5.53532200	-1.15157800	-1.81005000
C	2.42476700	-1.57471700	-2.16839300	H	4.50780000	0.28564500	-1.75250300
C	3.52359100	-1.55069700	-1.19551200	H	-0.11930000	-2.36001500	-3.15637300
C	3.25061600	-2.53528200	-0.23600600	H	0.83464700	-3.81162800	-3.52058500
C	2.00844400	-3.22099700	-0.60122600	H	-0.25449400	-3.78107700	-2.12241600
Rh	1.38276700	-1.17606900	-0.25875700	C	-1.45896900	-0.33402100	-0.72552500
C	4.72661500	-0.65955400	-1.25496400	C	-0.65924500	-1.30215400	-0.19581600
C	2.33229300	-0.69350100	-3.37537000	C	-1.24387300	-2.52024400	0.40843700
H	3.00261200	-1.05817300	-4.16412100	C	-2.13907500	-3.31683700	-0.33827200
H	1.31516400	-0.67708300	-3.77171600	C	-0.91144400	-2.95777800	1.70376300
H	2.61908500	0.33238000	-3.13448100	C	-2.67329900	-4.49249200	0.18415600
C	0.44242800	-3.18406500	-2.71090200	H	-2.42104100	-2.98889500	-1.33243100
C	1.51063400	-4.46447900	0.06667900	C	-1.45993600	-4.12710900	2.23221500
H	0.46145600	-4.65592600	-0.16013500	H	-0.19597900	-2.38644400	2.27974600
H	2.10109500	-5.32934100	-0.26379200	C	-2.33924900	-4.90499300	1.47765400
H	1.60141500	-4.38756500	1.15214900	H	-3.35628100	-5.08585800	-0.41837300
C	4.00217100	-2.81913800	1.02620200	H	-1.18917300	-4.43574400	3.23880500
H	3.37079300	-2.57406900	1.88814300	H	-2.75742200	-5.81978700	1.88810100
H	4.26967500	-3.87961800	1.08966600	N	-2.85908300	-0.46916500	-0.50269700
H	4.91768500	-2.22838900	1.09186900	N	-3.50628800	0.60874900	-0.64833300
C	-1.25363200	5.14878100	0.57840500	N	-4.82929900	0.52073700	-0.44530500
C	-1.10670000	4.18834400	-0.41941300	C	-5.46049700	1.84203800	-0.26106000
C	0.13979900	3.97199200	-1.02543800	H	-6.51959400	1.64360200	-0.08071800
C	1.24002800	4.72237400	-0.60091500	C	-4.88829000	2.59116400	0.95384000
C	1.09699000	5.67777200	0.41010700	H	-3.82015900	2.77895200	0.81131700
C	-0.14840800	5.89734600	0.99752600	H	-5.00896200	2.00932000	1.87157100
H	-2.22636000	5.30638600	1.03670400	C	-5.34289900	2.67418500	-1.54451900
H	-1.95587700	3.57910900	-0.71980100	H	-4.29314600	2.88190000	-1.76796000
H	2.21729500	4.53915700	-1.03398500	H	-5.77498900	2.13783500	-2.39449400
H	1.96683600	6.23764600	0.74090500	C	-5.42918200	-0.74280100	0.03383900
H	-0.25928600	6.63938100	1.78344700	H	-4.88054800	-1.51900600	-0.50713500
C	0.28654800	2.87393300	-2.07195400	C	-5.18834900	-0.97077300	1.53391100
H	-0.50703200	2.96178800	-2.82026400	H	-4.12310000	-0.89628800	1.76208700
H	1.24196800	2.97008200	-2.58821700	H	-5.52772300	-1.97171600	1.82155200
C	0.13338800	1.52364100	-1.40225500	H	-5.73837900	-0.24011600	2.13686500
C	-1.02024600	0.84142400	-1.48052400	C	-6.90889200	-0.84387800	-0.34293500
H	-1.78241700	1.27072000	-2.12156900	H	-7.06630900	-0.60445400	-1.39911600
C	2.41497100	1.60457500	-0.50747000	H	-7.25394000	-1.86762400	-0.16759400
N	1.11460800	1.12811400	-0.41910700	H	-7.54045000	-0.18375100	0.26095900
O	2.99778000	2.00685700	-1.48686300	H	-5.86719300	3.62835000	-1.42896500
C	3.70226300	2.51183500	1.31985600	H	-5.39781700	3.55170800	1.08566700
O	3.84439700	3.59169800	0.81553400	C	0.98047500	0.01200700	2.55682400

O	1.44089600	-0.96654700	1.86068600	H	1.92358900	-3.23675800	-1.68157400
O	0.47738900	1.06398500	2.10770600	H	1.10634800	-3.97150700	-0.30373300
H	0.75124100	1.15220900	0.60271600	C	1.22307800	-1.83845200	-0.23732200
C	1.05775000	-0.19281800	4.06192300	C	1.13595800	-0.78671000	-1.06106000
H	0.90589100	0.75290200	4.58424700	H	1.53538500	-0.90535600	-2.06681900
H	0.26896100	-0.89160200	4.36209600	C	-0.42035200	-1.69720300	1.51362400
H	2.01647900	-0.63866700	4.33825500	N	0.86678000	-1.67579100	1.15144300
C	4.14738000	2.08373800	2.69234100	O	-1.34256900	-2.14376600	0.83246400
H	4.65506700	1.11692400	2.64650300	C	-0.02959600	-0.16515100	3.37123600
H	4.79774800	2.84517100	3.12117800	O	1.16558500	-0.02021100	3.24668900
H	3.25545900	1.95845500	3.31494100	O	-0.75076100	-1.17197000	2.75165600
20II				H	-4.70908600	-2.82106000	-0.20828800
C	-1.99316400	-0.39541500	-2.72115500	H	-4.79314700	-3.56898600	-1.83169000
C	-2.20253800	-1.72436600	-2.27627200	H	-3.35620700	-3.77062100	-0.81536200
C	-3.54513600	-1.82227500	-1.68470000	H	-0.10290500	-0.60127100	-3.73445200
C	-4.12093300	-0.54732500	-1.71985300	H	-1.26931600	0.45401600	-4.53883600
C	-3.12973300	0.38273000	-2.26847400	H	-0.41078300	1.01539300	-3.09230500
Rh	-2.17203100	-0.36556800	-0.50271800	C	0.70036900	0.56927700	-0.65226500
C	-4.14038100	-3.06771600	-1.10582900	C	-0.54949600	0.88549100	-0.19096900
C	-1.29233900	-2.89965800	-2.44185100	C	-0.75831100	2.17177200	0.50892600
H	-1.76030500	-3.65419100	-3.08485800	C	-1.91090000	2.95870500	0.32934100
H	-0.33597400	-2.61279600	-2.88002900	C	0.17966900	2.61585100	1.46639900
H	-1.09431000	-3.35562000	-1.46823500	C	-2.09413700	4.15159700	1.02418300
C	-0.87833100	0.14630500	-3.56153000	H	-2.68078800	2.61169000	-0.34432400
C	-3.40790700	1.79394400	-2.68648400	C	-0.00932300	3.80018500	2.17715100
H	-2.49613500	2.39521500	-2.68559000	H	1.05051100	2.00576200	1.67105800
H	-3.82167500	1.80635000	-3.70399700	C	-1.14344400	4.58308700	1.95297700
H	-4.13756800	2.27236300	-2.02939300	H	-2.99227400	4.73932900	0.85262500
C	-5.48209900	-0.13963800	-1.25534300	H	0.73117600	4.10709800	2.91137000
H	-5.43042600	0.78821700	-0.67915600	H	-1.29297900	5.50701200	2.50478500
H	-6.13323600	0.03783100	-2.12126100	N	1.66660600	1.59733600	-0.78893500
H	-5.92571900	-0.89748300	-0.61271000	N	2.86062700	1.18526900	-0.92184500
C	5.34122700	-2.57972400	0.72884500	N	3.76905300	2.14236400	-1.18481800
C	4.09382900	-2.37355000	0.13972500	C	5.16029700	1.70634100	-0.97293100
C	3.15089200	-3.40933800	0.08359400	H	5.77562000	2.58675100	-1.17429400
C	3.47759900	-4.65046400	0.63922800	C	5.41580400	1.27086200	0.47957700
C	4.72607200	-4.85918300	1.23012400	H	4.79440300	0.41080300	0.73925700
C	5.66243400	-3.82482300	1.27524800	H	5.18096500	2.07759500	1.17914300
H	6.05894600	-1.76512700	0.76413200	C	5.54967500	0.61852300	-1.98224400
H	3.83320400	-1.40076900	-0.26773300	H	4.93578500	-0.27447400	-1.84578600
H	2.75044500	-5.45850300	0.61086700	H	5.40868700	0.97739400	-3.00604500
H	4.96399600	-5.82842600	1.65959700	C	3.38660200	3.56806900	-1.22546700
H	6.63214100	-3.98584000	1.73751100	H	2.35499000	3.55643000	-1.58554200
C	1.80563900	-3.17762000	-0.59261100	C	3.38541500	4.20829200	0.16973100

H	2.73925800	3.64364900	0.84415000	C	3.46359300	-2.83772300	-1.53913500
H	3.00346600	5.23344400	0.11532500	C	3.93970200	-4.15242000	-1.54778500
H	4.39752300	4.24701900	0.58762400	C	5.07609200	-4.50225700	-0.81398700
C	4.24247700	4.34979300	-2.22711300	C	5.74548600	-3.53899700	-0.05877300
H	4.28218800	3.83940900	-3.19408800	H	5.78194000	-1.47113500	0.55420800
H	3.80325700	5.34073500	-2.37937700	H	3.75101800	-0.86042700	-0.73474800
H	5.26793800	4.50368000	-1.87435800	H	3.41911300	-4.90702800	-2.13213600
H	6.59966400	0.33630600	-1.85292800	H	5.43277800	-5.52823200	-0.82921100
H	6.46697500	0.99430300	0.61584600	H	6.62679500	-3.81065300	0.51502300
C	-3.94614700	-0.15698200	1.82174000	C	2.23688000	-2.44034900	-2.35363300
O	-2.91596300	0.42583500	1.27056500	H	2.54460000	-1.82250800	-3.20487600
O	-4.54399900	-1.14906500	1.40487400	H	1.75466400	-3.33742700	-2.75649500
H	1.51364700	-1.20148100	1.77763700	C	1.25803400	-1.65788500	-1.51656500
C	-4.38936800	0.51483300	3.12121700	C	1.09646800	-0.30914900	-1.64574200
H	-3.94134200	-0.01874600	3.96597500	H	1.62493800	0.18109700	-2.45617000
H	-4.07719700	1.56065100	3.16236700	C	-0.52276000	-1.94004900	0.05962300
H	-5.47453400	0.43550600	3.21683000	N	0.69998600	-2.35171800	-0.45499900
C	-0.95778700	0.70275800	4.15717100	O	-1.53469600	-1.92643900	-0.71502200
H	-1.59152200	0.09341100	4.80615100	C	0.15011500	-2.56003400	2.34467500
H	-0.38864800	1.43115700	4.73242200	O	1.32613500	-2.78570700	2.13063100
H	-1.60613300	1.20326700	3.43013700	O	-0.79020700	-2.38991100	1.37324600
TS21H							
C	-2.17457400	1.71621800	-2.01232000	H	-5.02243600	-1.62993800	-1.79315500
C	-2.56368800	0.52868800	-2.70313600	H	-5.49768600	-0.75559800	-3.27851500
C	-3.85831100	0.10718900	-2.19020300	H	-4.03196700	-1.74877100	-3.25174700
C	-4.22306100	1.00842800	-1.15229700	H	-0.22509500	2.05708500	-2.86527500
C	-3.16002400	1.98206200	-0.99353800	H	-1.31897800	3.44835900	-2.91063800
Rh	-2.32314100	0.00534100	-0.55693500	H	-0.53756100	2.96772800	-1.39148500
C	-4.65144900	-1.07394100	-2.65669100	C	0.64814500	0.50356400	-0.54052300
C	-1.81603100	-0.16123800	-3.80284200	C	-0.35915200	0.16527500	0.35989900
H	-2.28544800	0.02651500	-4.77600300	C	-0.21209800	0.66964200	1.74459300
H	-0.77885100	0.17576400	-3.85034500	C	-1.23481900	1.32929600	2.44994300
H	-1.80215200	-1.24130000	-3.63243100	C	1.00978500	0.44992000	2.41945900
C	-0.99681800	2.59017400	-2.30738200	C	-1.03953900	1.76099800	3.76099600
C	-3.18980600	3.18531600	-0.09970000	H	-2.18905400	1.48095800	1.96650700
H	-2.18334400	3.46101200	0.22520300	C	1.20072200	0.86791600	3.73498400
H	-3.62821800	4.04929000	-0.61671000	H	1.80572000	-0.07932400	1.90573800
H	-3.78870900	2.99631600	0.79435100	C	0.17455500	1.52986800	4.41398000
C	-5.47944800	0.97424400	-0.34058600	H	-1.84518600	2.27308200	4.28057200
H	-5.26638000	1.21423600	0.70438500	H	2.14781100	0.67090400	4.23007800
H	-6.19316000	1.71562400	-0.72209400	H	0.31657200	1.85578700	5.44064200
H	-5.93075000	-0.01625600	-0.36247000	N	1.37978200	1.69124900	-0.28359400
C	5.27003000	-2.22502700	-0.03720800	N	2.61903500	1.61367800	-0.56663100
C	4.13543700	-1.87659200	-0.76846900	N	3.31295600	2.73627000	-0.43102500
				C	4.77632700	2.52256800	-0.41729700

H	5.21693200	3.51791500	-0.33232000	C	-2.70775000	3.09958100	0.80691300
C	5.20828000	1.69046000	0.80025700	H	-1.64190500	3.16509400	1.04065200
H	4.74122900	0.70278900	0.76543800	H	-3.06913800	4.10971200	0.57458300
H	4.91190200	2.17157600	1.73585700	H	-3.22386400	2.75795500	1.70698100
C	5.24843800	1.90100200	-1.73692200	C	-5.15423200	1.02959900	0.47691900
H	4.84104900	0.89506800	-1.86093100	H	-4.81272000	1.19439100	1.50140900
H	4.93049200	2.51113000	-2.58738500	H	-5.98132500	1.72198800	0.27566700
C	2.67193700	3.97522300	0.06913000	H	-5.51570400	0.00335200	0.40649500
H	1.66356400	3.93853500	-0.35091300	C	5.38588100	-1.42770700	-0.20722400
C	2.54497500	3.97096800	1.59917800	C	4.33167800	-1.08154000	-1.05001400
H	2.03901600	3.06668300	1.94335400	C	3.83658700	-2.00159900	-1.98679000
H	1.96033900	4.83750700	1.92593700	C	4.41302700	-3.27308700	-2.05537600
H	3.52996800	4.03362200	2.07423800	C	5.47158400	-3.62073400	-1.21189400
C	3.37051600	5.22861000	-0.46319200	C	5.96097500	-2.69951700	-0.28647300
H	3.52493700	5.17069200	-1.54496600	H	5.75541400	-0.70567700	0.51578000
H	2.74236900	6.09988300	-0.25431200	H	3.86700500	-0.10285000	-0.96628300
H	4.33748800	5.40729800	0.01831200	H	4.02905600	-3.99901500	-2.76746000
H	6.34061800	1.83182100	-1.74712500	H	5.90513200	-4.61462300	-1.27448200
H	6.29549600	1.56196200	0.80701800	H	6.77991200	-2.97075700	0.37344100
C	-3.94898200	-1.49297100	1.37651000	C	2.65927900	-1.62557200	-2.88015500
O	-3.01365100	-0.58904300	1.31504000	H	2.92964200	-0.79418400	-3.53946500
O	-4.63599900	-1.92014700	0.44675100	H	2.38342100	-2.47389300	-3.51477100
H	1.33389000	-2.82813700	0.18830100	C	1.48909300	-1.20768500	-2.02106100
C	-4.13952800	-2.04753100	2.78762900	C	1.22797000	0.13222000	-1.76364800
H	-3.59860600	-2.99800900	2.84925900	H	1.75222600	0.89290900	-2.32530300
H	-3.74261200	-1.37081100	3.54714300	C	-0.31557200	-1.82019700	-0.53700400
H	-5.19748500	-2.25268900	2.96712800	N	0.85298900	-2.17964300	-1.35910500
C	-0.48279000	-2.44529900	3.70183200	O	-1.39312000	-1.64727800	-1.29071900
H	-1.35077300	-3.10584200	3.76830600	C	0.23513900	-3.92060700	0.79175700
H	0.24933100	-2.69096500	4.47019300	O	1.26068100	-4.26237800	0.21550700
H	-0.83957200	-1.41889300	3.82735100	O	-0.56895000	-2.91235200	0.44582900
22II				H	-5.01711400	-1.21486300	-1.57704500
C	-2.13309400	2.08719300	-1.54180800	H	-5.77263700	0.01932000	-2.62967300
C	-2.69536900	1.09270500	-2.39404500	H	-4.38662300	-0.92448700	-3.20647800
C	-3.89354400	0.57783100	-1.76095700	H	-0.20893200	2.47972300	-2.43307500
C	-4.04389300	1.25723200	-0.50039100	H	-1.36431300	3.81779500	-2.50943100
C	-2.93929300	2.15810900	-0.33567000	H	-0.54639800	3.43310000	-0.98832800
Rh	-2.17252000	0.09249800	-0.49033600	C	0.65577500	0.45265800	-0.50716500
C	-4.82515500	-0.44526700	-2.32858200	C	-0.06102000	-0.50990700	0.25397600
C	-2.14860600	0.61687600	-3.70524700	C	0.23553000	-0.52348100	1.72554100
H	-2.79863600	0.91507500	-4.53586000	C	-0.49874000	0.20734800	2.66790900
H	-1.14972600	1.01863400	-3.88557300	C	1.36720700	-1.23261900	2.16202800
H	-2.06849100	-0.47437600	-3.69942400	C	-0.11696600	0.22354700	4.00903500
C	-0.99554000	2.99756200	-1.88064100	H	-1.37634600	0.75013500	2.34227200

C	1.74134500	-1.22934600	3.50776300	O	-1.59019800	-1.11466100	0.00010200
H	1.96364600	-1.78510000	1.44056900	C	0.53068000	0.01424900	0.00000300
C	1.00019500	-0.49801800	4.43780400	C	1.10047000	1.43611800	-0.00017100
H	-0.70037300	0.79668300	4.72502000	H	2.20278300	1.43397100	-0.00011200
H	2.61743600	-1.78985900	3.82288500	H	0.74672400	1.98710200	0.87653900
H	1.29025000	-0.48919800	5.48486600	H	0.74682900	1.98685300	-0.87708200
N	0.93177100	1.64579100	0.17966300	C	0.99356300	-0.74977700	1.25146300
N	1.88874900	2.32251000	-0.31830400	H	2.08588300	-0.89451400	1.27035400
N	2.18739100	3.43609600	0.32953400	H	0.49834300	-1.72468400	1.27473900
C	3.44259100	4.06651200	-0.13593400	H	0.71202400	-0.20794300	2.16396200
H	3.60921400	4.91598200	0.52912100	C	0.99365600	-0.75012500	-1.25120800
C	4.63689200	3.10872500	-0.01181100	H	2.08597900	-0.89486100	-1.26997900
H	4.51197300	2.25702200	-0.68556500	H	0.71218300	-0.20855100	-2.16388200
H	4.73171100	2.72797600	1.00886400	H	0.49844000	-1.72504000	-1.27424600
C	3.27091400	4.59092300	-1.56595000				
H	3.06736600	3.76067300	-2.24775300	14III			
H	2.43732400	5.29702100	-1.62441500	C	3.92755800	-0.04556700	1.28680700
C	1.55541700	3.75482200	1.63466000	C	4.27540000	-1.27142200	0.59263900
H	0.53333700	3.38448100	1.53804500	C	4.28569200	-0.99655700	-0.79289900
C	2.22769500	2.97050600	2.76987300	C	3.97993300	0.42109100	-0.97625400
H	2.20608900	1.89845000	2.56208700	C	3.84122000	1.02153600	0.31826200
H	1.69086600	3.13815700	3.70864500	Rh	2.18591100	-0.41298900	-0.00934800
H	3.26513200	3.29462400	2.90765400	C	4.59679700	-1.94872900	-1.90515200
C	1.50462900	5.26137400	1.89119400	C	4.58294500	-2.56959900	1.27425000
H	1.09641900	5.79895000	1.02973300	H	4.61606400	-3.40475700	0.57464500
H	0.85486200	5.45123400	2.75075500	H	5.56036900	-2.50780200	1.76686500
H	2.48646500	5.68210400	2.13106600	H	3.84554100	-2.80145800	2.04890300
H	4.18211500	5.09795200	-1.89815500	C	3.86358200	0.12086400	2.77040300
H	5.56449200	3.62618500	-0.27603900	C	3.85168900	2.48228100	0.62753700
C	-3.58458700	-1.91461300	1.19590300	H	3.33278300	2.70279100	1.55967400
O	-2.66381900	-0.99616800	1.20238600	H	4.89340600	2.81106200	0.73130000
O	-4.42490700	-2.12583200	0.31904100	H	3.38298600	3.07340900	-0.15873000
H	1.29106000	-3.08596600	-1.17908300	C	4.00709800	1.15107800	-2.27942400
C	-3.58904200	-2.74011300	2.48281500	H	3.41037100	2.06321300	-2.23088200
H	-3.86286800	-3.77211300	2.24984900	H	5.03912400	1.43260000	-2.52577700
H	-2.61928100	-2.70037500	2.98088600	H	3.62861800	0.53137200	-3.09538100
H	-4.35024200	-2.33909500	3.16161800	C	-4.67672200	-3.49973100	1.30400300
C	-0.28663400	-4.60041700	2.03308700	C	-3.28571900	-3.59853000	1.24353800
H	-1.36129700	-4.77433000	1.94772300	C	-2.62868000	-3.63756700	0.00746800
H	0.24990400	-5.53486500	2.19730600	C	-3.38690500	-3.57985600	-1.16839300
H	-0.12771400	-3.92447400	2.87990600	C	-4.77802600	-3.48265100	-1.11098700
OPIV				C	-5.42532200	-3.43862000	0.12619900
O	-1.61079600	1.16043100	-0.00017700	H	-5.17491200	-3.47541200	2.26844600
C	-1.06524100	0.02978500	-0.00003500	H	-2.70561900	-3.63950800	2.16202100
				H	-2.88574800	-3.60653600	-2.13277500

H	-5.35519900	-3.44522400	-2.02991000	H	-4.86710100	3.40146400	-2.02278700
H	-6.50751000	-3.36453800	0.17214100	H	-4.18791600	4.91679600	-1.41415100
C	-1.11810400	-3.65046400	-0.05598800	H	-5.48953600	4.13307800	-0.52611000
H	-0.70799100	-4.21007900	0.79715600	C	-3.19251500	3.87081400	1.02251600
H	-0.78554000	-4.18159100	-0.96023400	H	-2.38331200	3.34123700	1.52958900
C	-0.50738300	-2.26026500	-0.05826200	H	-2.86974600	4.90285100	0.85453700
C	-1.20907600	-1.11730700	-0.00866400	H	-4.07628300	3.88872400	1.66913800
H	-2.28287900	-1.23219400	0.03266100	H	-6.41085300	0.27810800	1.61194000
C	1.65423200	-3.17749400	-0.31298900	H	-6.69983700	0.07330700	-0.96148100
N	0.90965400	-2.20120900	-0.12598900	TS15III			
O	2.40305900	-4.05351600	-0.48422200	C	3.33930800	-0.67576500	1.71277300
H	4.00891300	-1.72188600	-2.79823600	C	3.91267000	-1.64677000	0.81154700
H	5.65525400	-1.86964200	-2.18208200	C	4.44269500	-0.94007600	-0.29979600
H	4.40463500	-2.98580100	-1.62465200	C	4.25493000	0.48717400	-0.07827300
H	3.51182700	-0.78883100	3.26189700	C	3.60064000	0.64596800	1.17798600
H	4.86390400	0.34622600	3.16313900	Rh	2.13648100	-0.49093000	-0.18899500
H	3.20201100	0.94343300	3.04895700	C	5.15848200	-1.52848300	-1.47769200
C	-0.74873000	0.25914500	-0.03427700	C	3.86181500	-3.13300000	0.99729600
C	0.57128100	0.72370300	-0.01935400	H	4.62160400	-3.63477900	0.39476600
C	0.73540100	2.19878100	-0.01844100	H	4.03373300	-3.39884600	2.04381200
C	0.67606400	2.92611500	1.18136900	H	2.87954800	-3.52520400	0.70301800
C	0.92248100	2.90006100	-1.22062100	C	2.73805300	-0.98835700	3.04750100
C	0.80741900	4.31490400	1.18007100	C	3.36923800	1.93136900	1.90539800
H	0.51642100	2.39257300	2.11455500	H	2.46444000	1.89422000	2.51427100
C	1.05409700	4.29009500	-1.22174200	H	4.21545800	2.12806200	2.57486300
H	0.94340600	2.34791400	-2.15604000	H	3.27491700	2.77478100	1.22097000
C	1.00015100	5.00299500	-0.02082200	C	4.85411600	1.56718300	-0.92529500
H	0.75655400	4.86169100	2.11735800	H	4.38015700	2.53160500	-0.74122700
H	1.19229600	4.81723000	-2.16154700	H	5.92335300	1.66834900	-0.70086200
H	1.10330500	6.08369600	-0.02146700	H	4.76444500	1.33973500	-1.99073300
N	-1.71753300	1.26962600	-0.08812200	C	-4.07940000	-3.50262700	1.62759000
N	-2.93131700	0.85308400	-0.00746400	C	-2.75350500	-3.55822900	1.19778200
N	-3.85148800	1.77093300	-0.10747200	C	-2.44628600	-3.60813400	-0.16962300
C	-5.23429700	1.26884700	0.09518100	C	-3.49402800	-3.60648100	-1.09831300
H	-5.86240300	2.16016300	0.12913600	C	-4.82324300	-3.55510500	-0.67117200
C	-5.66216000	0.39506100	-1.09019300	C	-5.11838700	-3.49765700	0.69262600
H	-5.03082500	-0.49612800	-1.14839300	H	-4.30267700	-3.46960900	2.68986500
H	-5.58560000	0.94273600	-2.03376600	H	-1.94700700	-3.55908600	1.92715200
C	-5.36168900	0.53192200	1.43405200	H	-3.26936600	-3.64552000	-2.16125700
H	-4.78145300	-0.39417600	1.42518800	H	-5.62584900	-3.56453900	-1.40263700
H	-5.01350400	1.15775800	2.26081200	H	-6.15110300	-3.45857600	1.02561000
C	-3.50885000	3.20357900	-0.32231200	C	-1.00351400	-3.57213400	-0.62149700
H	-2.58961500	3.17550800	-0.91270700	H	-0.39482900	-4.29804800	-0.07435200
C	-4.58721000	3.94352300	-1.11505400	H	-0.92008900	-3.83881100	-1.68372000

C	-0.34264000	-2.19709900	-0.45101400	H	-3.25466100	5.10239600	0.03759000
C	-1.17372700	-1.05225900	-0.44660100	H	-4.31796200	4.16744700	1.10185700
H	-2.23345800	-1.22369500	-0.58247100	H	-5.98722700	0.51781000	2.26101700
C	1.76440800	-1.49824900	-1.79978500	H	-6.81530000	-0.00156600	-0.14287100
N	0.97492600	-2.21016500	-0.35989300	16III			
O	1.80781800	-1.96400900	-2.85929900	C	3.05950600	-1.03350700	1.47744100
H	4.92033800	-0.99130600	-2.39892100	C	3.86516700	-1.67591600	0.45617300
H	6.24256800	-1.45859600	-1.32772500	C	4.49881300	-0.65480400	-0.28672300
H	4.90544100	-2.57992300	-1.62398400	C	4.18267000	0.63553600	0.33471800
H	2.20228900	-1.93979800	3.02470600	C	3.33931600	0.38663400	1.44672800
H	3.52711700	-1.06585300	3.80654300	Rh	2.16170200	-0.32712600	-0.47970000
H	2.04318900	-0.20969700	3.36795700	C	5.46005100	-0.83604300	-1.42320700
C	-0.77713200	0.27719300	-0.32391700	C	3.90806700	-3.14896900	0.22524800
C	0.60188500	0.71204500	-0.22670700	H	4.65402600	-3.42209100	-0.52305100
C	0.84766000	2.15516200	-0.11277800	H	4.14724700	-3.67568700	1.15458000
C	0.28561500	2.91236000	0.93679700	H	2.92178100	-3.48950100	-0.11809400
C	1.66931900	2.80729800	-1.05058500	C	2.27795200	-1.76571700	2.52406800
C	0.56668200	4.27002700	1.05684700	C	2.88377100	1.37261700	2.47460600
H	-0.35082300	2.42117800	1.66463100	H	1.87400000	1.15150300	2.82583100
C	1.91231500	4.17656900	-0.95080800	H	3.55303900	1.33130800	3.34240100
H	2.09332900	2.23324100	-1.86770500	H	2.88735700	2.39383500	2.09251200
C	1.37315400	4.90959700	0.10945800	C	4.83255800	1.93530600	-0.03143500
H	0.14988800	4.83402600	1.88576300	H	4.28061800	2.78808700	0.36588600
H	2.52722100	4.66945700	-1.69778000	H	5.84979800	1.97478000	0.37717100
H	1.57660800	5.97235400	0.19625500	H	4.91423100	2.05616000	-1.11493300
N	-1.72687100	1.30074800	-0.35711900	C	-2.99567800	-3.36098200	2.08975600
N	-2.89908900	0.90161000	0.00021800	C	-1.87200200	-3.37008800	1.26448700
N	-3.87216000	1.74937700	-0.13724300	C	-1.99775400	-3.59092600	-0.11548400
C	-5.17286200	1.29128600	0.42141700	C	-3.27470000	-3.79789700	-0.65103400
H	-5.78847500	2.19170900	0.48085000	C	-4.40260800	-3.79107400	0.17348800
C	-5.83220900	0.28422400	-0.52830200	C	-4.26632800	-3.56877000	1.54499900
H	-5.21932700	-0.61890300	-0.60364600	H	-2.88216300	-3.19565800	3.15719400
H	-5.96514800	0.70520200	-1.52813800	H	-0.88503600	-3.20121900	1.68911600
C	-5.00137900	0.72342600	1.83436700	H	-3.38737300	-3.97134900	-1.71837700
H	-4.43280500	-0.20923300	1.81313800	H	-5.38535200	-3.96081500	-0.25617100
H	-4.48635400	1.43599300	2.48521800	H	-5.14221200	-3.56331400	2.18655400
C	-3.67991100	3.11280000	-0.70158200	C	-0.77054000	-3.53058800	-1.00539400
H	-2.76477000	3.03849000	-1.29137300	H	-0.02188600	-4.27354700	-0.71756900
C	-4.83339100	3.51833300	-1.62183400	H	-1.04729100	-3.73028700	-2.04748700
H	-4.99054000	2.78252100	-2.41490100	C	-0.11769400	-2.14417400	-0.92123200
H	-4.58301900	4.47313900	-2.09272200	C	-1.03483500	-1.02802500	-1.06362500
H	-5.77440900	3.65933500	-1.08230100	H	-2.03460700	-1.25887200	-1.41773100
C	-3.44425800	4.10472300	0.44476000	C	2.12863700	0.06087900	-2.34055300
H	-2.57494700	3.80560900	1.03547100	N	1.13428900	-2.06602300	-0.66494300

O	2.11623300	0.27669300	-3.46561300	C	0.63847500	-0.30282600	2.74568500
H	5.39325000	-0.01718300	-2.14360100	C	-0.13759000	-1.46479700	2.34498600
H	6.48877000	-0.85315600	-1.04344600	C	0.77011900	-2.57468800	2.17411400
H	5.28321900	-1.77214300	-1.95565400	C	2.09403600	-2.07091600	2.28681000
H	1.78555600	-2.63964700	2.09136200	C	2.00016800	-0.65552300	2.66915400
H	2.94485100	-2.11300400	3.32294600	Rh	1.07652800	-1.03786300	0.54708800
H	1.51626100	-1.12738300	2.97656700	C	0.38830900	-3.99738000	1.89102400
C	-0.80049500	0.27985800	-0.67992100	C	-1.63471400	-1.54009800	2.35386800
C	0.49041400	0.74035900	-0.26781100	H	-1.99767800	-1.95065500	3.30473200
C	0.60147700	2.09321000	0.26435800	H	-2.07605800	-0.55066100	2.21902400
C	-0.23718100	2.51009000	1.32414500	H	-2.01510100	-2.17251700	1.54757800
C	1.55256900	3.00313400	-0.24107200	C	0.04509400	1.02548100	3.10135300
C	-0.09452800	3.77774500	1.87847700	C	3.18341200	0.20042100	2.99826500
H	-0.97438900	1.82205500	1.72157200	H	2.90644100	1.25294200	3.09988200
C	1.64835100	4.29102400	0.27854500	H	3.62395500	-0.12311500	3.95017600
H	2.18975600	2.70146000	-1.06455900	H	3.93906300	0.10473800	2.21597400
C	0.83741700	4.67728000	1.35006200	C	3.35809500	-2.87183500	2.22694600
H	-0.72141800	4.07222200	2.71437100	H	4.15483900	-2.28080000	1.77546200
H	2.36008100	4.99163900	-0.14701900	H	3.66268700	-3.18854700	3.23367800
H	0.92779900	5.67479400	1.76850800	H	3.21883000	-3.76883200	1.61795800
N	-1.84919300	1.22528700	-0.69627200	C	-5.06881000	-4.22665200	0.11157700
N	-2.96357600	0.68195500	-0.36507300	C	-3.71838100	-4.02513600	-0.17694300
N	-4.03614900	1.41847300	-0.46041700	C	-3.32133900	-3.47570000	-1.40249300
C	-5.25299800	0.79929600	0.12680600	C	-4.30696900	-3.13483200	-2.33743700
H	-5.99697100	1.59843600	0.15012500	C	-5.65882000	-3.33332500	-2.05263100
C	-5.75945000	-0.33676500	-0.76848900	C	-6.04364200	-3.87867300	-0.82582100
H	-5.01923300	-1.14103600	-0.80748900	H	-5.35898600	-4.65794100	1.06546200
H	-5.95346500	0.01642700	-1.78504600	H	-2.96209100	-4.30346800	0.55315700
C	-4.99551400	0.33228200	1.56438500	H	-4.00983200	-2.70774300	-3.29200500
H	-4.27683400	-0.49071100	1.58000200	H	-6.41073900	-3.06494400	-2.78933000
H	-4.60935900	1.15130500	2.17891100	H	-7.09521200	-4.03565700	-0.60397400
C	-4.00501300	2.81300000	-0.96812600	C	-1.86232800	-3.20963900	-1.68923200
H	-3.11353100	2.85295000	-1.59810400	H	-1.23016100	-3.90334300	-1.12117500
C	-5.23065900	3.13134500	-1.82811300	H	-1.63518400	-3.40876300	-2.74383400
H	-5.37284800	2.38331700	-2.61288400	C	-1.43455900	-1.79001600	-1.36417900
H	-5.07946300	4.10190700	-2.30918500	C	-2.23422300	-0.77054300	-0.92836700
H	-6.15096300	3.20176300	-1.24095600	H	-3.31299400	-0.84331000	-0.90037400
C	-3.82134300	3.78974700	0.19997200	C	0.83466000	-2.32742500	-0.97395500
H	-2.89899200	3.56802800	0.74251000	N	-0.09571100	-1.47002600	-1.43000800
H	-3.76030100	4.81567000	-0.17603500	O	1.28676700	-3.40601200	-1.25371400
H	-4.66610700	3.73453800	0.89498000	C	3.75260600	-0.37361900	-0.78002100
H	-5.93135000	-0.01873200	2.00900400	C	4.50539000	0.09993300	-2.05138200
H	-6.68902300	-0.74812800	-0.36383500	C	5.35539600	-1.09362900	-2.53287400
TS14IV				H	5.96302300	-0.80608400	-3.39907600

H	6.01917300	-1.43439500	-1.73378800	C	-4.83468200	4.58485000	0.06377300
H	4.71640100	-1.93291000	-2.82963000	H	-5.30487100	3.86693800	0.74184900
C	5.42870500	1.26279000	-1.64072500	H	-5.54493000	4.81917700	-0.73553000
H	6.04421100	1.58082900	-2.49034500	H	-4.64871600	5.51143000	0.61727600
H	4.84087500	2.12544200	-1.30773000	C	-2.85513000	4.96969300	-1.51071900
H	6.08413900	0.95686100	-0.82177000	H	-1.94774600	4.51299600	-1.91548900
C	3.54483700	0.55241300	-3.16000800	H	-3.52307700	5.21926400	-2.34160200
H	4.11442000	0.87628500	-4.03978500	H	-2.57617500	5.90565400	-1.01418900
H	2.87649700	-0.26005800	-3.45595200	H	-0.20369800	5.47317500	2.02252900
H	2.92027000	1.38462100	-2.82529000	H	-2.09200000	4.78662700	3.66470700
O	2.46652800	-0.41557000	-0.91485800	15IV			
O	4.39811600	-0.66229000	0.23366700	C	-0.78496000	-0.08525000	2.62653100
H	1.02561100	-4.43014200	1.11570000	C	-2.03381200	-0.12809000	1.85915200
H	0.48350700	-4.60904400	2.79606300	C	-2.37002000	-1.51004000	1.65695200
H	-0.64819500	-4.06725000	1.55071100	C	-1.23267600	-2.27693200	2.07084200
H	-0.60073100	1.39732500	2.29888200	C	-0.30055500	-1.38167600	2.76830300
H	-0.56295700	0.94867100	4.01156900	Rh	-0.64553800	-1.01752400	0.35727800
H	0.81889200	1.77514100	3.28071700	C	-3.65505000	-2.07971800	1.13857000
C	-1.57221000	0.42737800	-0.54121700	C	-2.93399000	1.05795100	1.68388600
C	-0.17941900	0.49923700	-0.42913400	H	-3.38834400	1.34208600	2.64260700
C	0.56033100	1.68700600	-0.85432700	H	-2.37917000	1.92271300	1.31067800
C	1.66086800	2.17510100	-0.12223000	H	-3.74109000	0.85678000	0.98092000
C	0.17458400	2.38553900	-2.01815100	C	-0.19400700	1.18399600	3.14641900
C	2.31541500	3.34082000	-0.50647800	C	0.90033100	-1.84893400	3.52696800
H	1.99840700	1.62557700	0.74782600	H	1.52470700	-1.01204300	3.84669300
C	0.84323600	3.54011600	-2.41561400	H	0.58880200	-2.40559400	4.42080500
H	-0.65979900	2.00883200	-2.60078100	H	1.52752000	-2.49043800	2.90729200
C	1.91234100	4.02700400	-1.65586700	C	-1.11719000	-3.76858300	2.04333800
H	3.15369300	3.70479300	0.08000700	H	-0.07613000	-4.07560100	1.92625800
H	0.53847100	4.05646900	-3.32146200	H	-1.49513000	-4.20406300	2.97812000
H	2.43776100	4.92522200	-1.96721000	H	-1.68805600	-4.19036000	1.21316700
N	-2.38711400	1.57204800	-0.42352200	C	-6.29190400	0.33053800	-0.31120200
N	-1.99614900	2.39075000	0.46902600	C	-5.25275400	0.22583800	-1.23996900
N	-2.61407800	3.56013800	0.50912900	C	-4.50205300	1.35277100	-1.59408700
C	-2.07378700	4.50162800	1.51114700	C	-4.81581000	2.58657400	-1.00945000
H	-2.56563800	5.45540100	1.30021200	C	-5.84763500	2.69167500	-0.07722100
C	-2.45751900	4.06304000	2.92907600	C	-6.58865900	1.56095100	0.27681100
H	-2.01558200	3.08932600	3.15529300	H	-6.86364500	-0.55363200	-0.04375400
H	-3.54360000	3.98071200	3.03214300	H	-5.00277200	-0.73598500	-1.67648700
C	-0.56095400	4.69175500	1.34414400	H	-4.24375200	3.46973000	-1.28208700
H	-0.02834200	3.76559900	1.56600600	H	-6.07551100	3.65480600	0.37053900
H	-0.31183300	4.97612800	0.31833800	H	-7.39323000	1.64056700	1.00198800
C	-3.55362900	4.00428700	-0.54245400	C	-3.36218300	1.23266100	-2.59186300
H	-3.80718200	3.09098900	-1.08266800	H	-3.44671200	0.29476100	-3.14263200

H	-3.43389700	2.04870000	-3.32165300	N	2.71334100	3.08290600	0.72129000
C	-1.98456100	1.30711700	-1.98993300	C	3.48208400	2.66395700	1.91858000
C	-1.32433700	2.39675700	-1.43429200	H	4.48574600	3.07106300	1.76233400
H	-1.68100500	3.41738600	-1.42171600	C	2.89426000	3.30709900	3.18294500
C	-1.69564700	-1.06595800	-1.29781000	H	1.86951800	2.96654700	3.34076800
N	-1.18699600	0.20060100	-1.88573200	H	2.88493300	4.39749500	3.10873100
O	-2.59596700	-1.69537900	-1.78925100	C	3.60414900	1.14027500	2.03605300
C	1.87333100	-2.50875700	0.02982200	H	2.63394600	0.64281400	2.07303300
C	2.69951300	-3.70203400	-0.51597300	H	4.15197000	0.71997000	1.18972100
C	2.24539700	-4.94535300	0.27923900	C	3.22511300	4.13307700	-0.19316900
H	2.80912900	-5.83031900	-0.03845200	H	2.38675200	4.34588500	-0.85768800
H	2.41351200	-4.80616100	1.35363000	C	3.59581200	5.41810000	0.55144700
H	1.18112600	-5.14040900	0.11520700	H	2.74399500	5.80805800	1.11567600
C	4.19435700	-3.44630500	-0.27395400	H	3.89925600	6.17798100	-0.17538900
H	4.78484900	-4.31196500	-0.59636700	H	4.43325100	5.27246200	1.24141300
H	4.53100300	-2.57188700	-0.83877200	C	4.38218000	3.56521700	-1.02685700
H	4.38841300	-3.25497900	0.78377300	H	4.06948000	2.65685700	-1.54830100
C	2.42956800	-3.91861200	-2.01412900	H	4.70150200	4.30253000	-1.77035400
H	3.00684000	-4.77602400	-2.38145100	H	5.24897000	3.32557300	-0.40087700
H	1.36878300	-4.10401200	-2.19431000	H	4.15773400	0.89476300	2.94748600
H	2.71717500	-3.03673500	-2.59248600	H	3.48898000	3.02820200	4.05851900
O	0.69217900	-2.40978800	-0.49100800				
O	2.33248300	-1.78259200	0.92397700	TS14V			
H	-3.48159200	-2.76289100	0.30355200	C	-1.15485100	-0.75859200	-2.56172000
H	-4.16705000	-2.62807400	1.93864600	C	-1.18792700	-2.12497200	-2.13715200
H	-4.32064300	-1.29310600	0.78454900	C	-2.51440100	-2.42973700	-1.62353200
H	0.02389800	1.87442500	2.32701900	C	-3.28038600	-1.26889300	-1.72941400
H	-0.89259500	1.68309900	3.82949800	C	-2.42035200	-0.18256200	-2.22435000
H	0.73586200	0.99850700	3.68596300	Rh	-1.36950600	-0.54210300	-0.32484900
C	-0.08488300	1.95949000	-0.92126400	C	-2.97901500	-3.72407500	-1.02767500
C	0.05974200	0.54923700	-1.21659800	C	-0.09911300	-3.09021700	-2.47183300
C	1.29486000	0.09374100	-1.93423800	H	0.02614800	-3.13103500	-3.56090300
C	2.55555100	0.15063300	-1.32886900	H	0.85751300	-2.76570600	-2.04845500
C	1.21788600	-0.29504500	-3.28254200	H	-0.31750600	-4.10098700	-2.12472400
C	3.71068600	-0.12763500	-2.05777800	C	-0.02861700	-0.14602000	-3.33406600
H	2.61382400	0.34820400	-0.27237800	C	-2.92224600	1.19199000	-2.54238400
C	2.37383200	-0.58653300	-4.00665600	H	-2.11654000	1.85494800	-2.85813300
H	0.24969500	-0.35593600	-3.76621700	H	-3.67544600	1.14863500	-3.33850800
C	3.62947600	-0.49054300	-3.40410000	H	-3.38126200	1.63613100	-1.65451200
H	4.67577200	-0.08463900	-1.56011700	C	-4.73756500	-1.11210600	-1.45118300
H	2.29002300	-0.88320000	-5.04851200	H	-4.95246000	-0.12252400	-1.04170500
H	4.52953900	-0.71536800	-3.96900400	H	-5.29818800	-1.20489200	-2.39171200
N	0.88993300	2.82506400	-0.49112200	H	-5.09773200	-1.85796500	-0.74407100
N	1.62669600	2.39173900	0.46552900	C	3.75598500	-4.98398200	-0.19790300
				C	2.43657200	-4.52295000	-0.22712300

C	1.96852200	-3.63301400	0.74446400	C	-1.31333200	3.08236700	0.26783300
C	2.84928200	-3.21486200	1.75408000	C	-0.27596500	4.40313400	-1.96111500
C	4.16738400	-3.66622000	1.78275300	H	0.82668200	2.59117600	-2.32289400
C	4.62621500	-4.55243700	0.80301500	C	-1.68728500	4.39719000	-0.00466800
H	4.10172800	-5.67734400	-0.95951900	H	-1.70521400	2.56928900	1.13341100
H	1.76624000	-4.86132800	-1.01196900	C	-1.18198800	5.06112300	-1.12494500
H	2.49530100	-2.51841400	2.50960400	H	0.14127000	4.91550000	-2.82409600
H	4.83613400	-3.32943800	2.56985600	H	-2.37419700	4.90613100	0.66626800
H	5.65318500	-4.90556100	0.82401000	H	-1.48024300	6.08390400	-1.33766700
C	0.54968600	-3.09377700	0.71790200	N	2.31633500	1.55033000	-0.19437200
H	-0.06940700	-3.68334800	0.03844300	N	3.46248900	1.02468700	-0.05670600
H	0.09180600	-3.19813100	1.70464400	N	4.50212500	1.86047400	-0.06881900
C	0.51290900	-1.63001200	0.34776700	C	5.75705000	1.22332700	0.37864200
C	1.52953200	-0.81584300	0.02041200	H	6.48338200	2.03534900	0.46725700
H	2.54170300	-1.19882800	-0.03378100	C	5.60515000	0.55742800	1.75522300
C	-0.52499900	-0.15700900	2.47053300	H	4.90288300	-0.27843700	1.69599800
N	-0.78767800	-1.03244700	1.66369400	H	5.22926000	1.26905900	2.49568400
O	-0.30511300	0.62888700	3.32898700	C	6.25729900	0.23206600	-0.67918100
C	-3.66407100	-0.03306200	1.33998300	H	5.52642800	-0.57068100	-0.81259300
C	-4.55519100	0.89477600	2.20079500	H	6.40175800	0.73091700	-1.64209100
C	-5.79278900	0.11399900	2.66589100	C	4.31157600	3.32569500	-0.08299300
H	-6.41576800	0.74537900	3.30932400	H	3.37256600	3.47019100	-0.62198000
H	-6.39719700	-0.20835100	1.81176000	C	4.13208200	3.87172000	1.34008500
H	-5.50246200	-0.78114000	3.21976500	H	3.30436400	3.36045300	1.83832000
C	-4.98244200	2.13445400	1.39271700	H	3.90763400	4.94322200	1.31304700
H	-5.60330100	2.79100200	2.01275500	H	5.04321500	3.73192900	1.93268200
H	-4.11640500	2.69887300	1.04193300	C	5.43040400	4.03063300	-0.85418400
H	-5.57526800	1.84787700	0.51579100	H	5.56706100	3.58439700	-1.84377200
C	-3.71201400	1.32569500	3.42071900	H	5.16918100	5.08539400	-0.98577200
H	-4.30287200	1.97885000	4.07291100	H	6.38905300	3.99902900	-0.32554500
H	-3.39720400	0.45503800	4.00477300	H	7.20848700	-0.21347100	-0.36995300
H	-2.81074100	1.86277900	3.11573000	H	6.57230400	0.17646600	2.09969300
O	-2.76273000	0.63240700	0.64896500	15V			
O	-3.80278200	-1.25354300	1.34097000	C	1.02724800	0.83093300	-2.42950800
H	-3.41215500	-3.53044700	-0.04097200	C	1.26430100	2.22213100	-2.07374500
H	-3.74263700	-4.20473600	-1.65019600	C	2.63097400	2.38822100	-1.67364000
H	-2.15686300	-4.43335200	-0.90576800	C	3.25585200	1.14555300	-1.82167000
H	0.93129200	-0.33114100	-2.84349900	C	2.24735100	0.14826300	-2.21877200
H	0.01327200	-0.58093900	-4.34087500	Rh	1.23100000	0.58770100	-0.18181400
H	-0.15603900	0.93120100	-3.43392800	C	3.28068700	3.62355000	-1.13081200
C	1.27377500	0.60053200	-0.18779500	C	0.27679500	3.28763600	-2.39123100
C	-0.02085300	1.00824600	-0.32234700	H	0.17968200	3.35359700	-3.48312600
C	-0.42340700	2.39581200	-0.57850300	H	-0.71338800	3.02975100	-2.00050100
C	0.10157400	3.08955100	-1.68938600	H	0.57262300	4.26812400	-2.01673800

C	-0.18748400	0.35524300	-3.16446000	O	3.98226100	1.12303700	1.04354300
C	2.60140800	-1.25932900	-2.57295600	H	3.73082200	3.38495600	-0.16132500
H	1.73947900	-1.82475600	-2.92330900	H	4.07050700	3.99389200	-1.79438100
H	3.36708900	-1.26180400	-3.35832000	H	2.55930500	4.43120700	-0.98574700
H	3.00781900	-1.77199900	-1.69615000	H	-1.10311000	0.66275300	-2.65323500
C	4.71177200	0.85070900	-1.74144700	H	-0.20112200	0.78121800	-4.17583000
H	4.88712400	-0.15380900	-1.35000700	H	-0.19747800	-0.73077700	-3.25218600
H	5.13571200	0.87983000	-2.75595000	C	-1.40286600	-0.55094300	-0.17223100
H	5.23776900	1.56668500	-1.11210300	C	-0.10121700	-0.96464900	-0.21388900
C	-3.55153000	5.20578600	0.12153600	C	0.31616100	-2.35840500	-0.38132500
C	-2.27874000	4.64719200	-0.02057900	C	-0.14698800	-3.10273500	-1.48610400
C	-1.81684600	3.67664500	0.87540300	C	1.12809400	-3.00799800	0.56598100
C	-2.65924600	3.27797100	1.92428200	C	0.21423600	-4.43716300	-1.65457600
C	-3.93287200	3.82762600	2.06624300	H	-0.81069400	-2.62495100	-2.19867500
C	-4.38448800	4.79373000	1.16246700	C	1.48424600	-4.34497700	0.39710900
H	-3.89062100	5.96236100	-0.58083900	H	1.46184100	-2.45821300	1.43407900
H	-1.63594800	4.97496700	-0.83349300	C	1.04155500	-5.06194300	-0.71692000
H	-2.30869600	2.52381300	2.62422300	H	-0.15240300	-4.99100300	-2.51471900
H	-4.57112900	3.50618000	2.88466900	H	2.10759600	-4.82893200	1.14374700
H	-5.37548600	5.22466700	1.27289000	H	1.32720800	-6.10197700	-0.84723800
C	-0.45836900	3.02716200	0.71227500	N	-2.43612100	-1.50256100	-0.20241100
H	0.21339600	3.67175300	0.13774100	N	-3.59409800	-0.97943500	-0.17741600
H	0.02426400	2.90655200	1.68899800	N	-4.61711600	-1.83011100	-0.22344900
C	-0.52475600	1.63743200	0.12481900	C	-5.91362900	-1.19702800	0.09110400
C	-1.62423800	0.87331500	0.00369000	H	-6.63882100	-2.01358500	0.12381400
H	-2.62841900	1.26007200	0.13654000	C	-5.89561400	-0.51009900	1.46524800
C	0.83527900	0.00364600	2.63126600	H	-5.18986800	0.32507900	1.46362000
N	1.13529500	0.89742600	1.86781700	H	-5.59590000	-1.21059600	2.24987300
O	0.58969400	-0.82448700	3.45347800	C	-6.31926800	-0.22863000	-1.02655900
C	3.78575200	-0.09210800	1.05360300	H	-5.58535800	0.57807800	-1.10709400
C	4.72509800	-1.05296900	1.82487400	H	-6.36991100	-0.74593000	-1.98930800
C	6.09508500	-0.38020300	1.99841000	C	-4.40169300	-3.29248900	-0.18358600
H	6.75774900	-1.02349700	2.58811700	H	-3.44825500	-3.43793000	-0.69691900
H	6.57112900	-0.20073700	1.02801800	C	-4.24132600	-3.78702000	1.26045000
H	5.99319800	0.58361800	2.50066900	H	-3.43642800	-3.24110500	1.75859500
C	4.88242500	-2.39157300	1.08360500	H	-3.99143400	-4.85314700	1.27215200
H	5.53918400	-3.05989400	1.65207300	H	-5.16899100	-3.65023800	1.82738600
H	3.91929600	-2.88331700	0.94000800	C	-5.48916000	-4.04715900	-0.95216700
H	5.33375400	-2.24503700	0.09489100	H	-5.63288600	-3.62507300	-1.95142700
C	4.07227400	-1.28423200	3.20566800	H	-5.18873500	-5.09380000	-1.06231500
H	4.70154300	-1.94829700	3.80938000	H	-6.45259700	-4.04191100	-0.43173200
H	3.95814800	-0.33765800	3.74281700	H	-7.29868100	0.21250000	-0.81508300
H	3.08108500	-1.73534500	3.11513100	H	-6.89095200	-0.12362600	1.70795600
O	2.79200200	-0.70267600	0.45661500				

TS16-I

C	-1.08532900	-0.64108200	3.10964800	H	-5.52023000	1.52614500	-1.87168800
C	-0.56421400	0.70152600	3.00714400	H	-4.51423500	1.61120900	-3.33374300
C	-1.69045100	1.64134800	3.05890700	C	-5.41208100	-1.22364300	-1.50365800
C	-2.86192500	0.89253600	2.97851700	H	-6.28862000	-1.48881300	-2.10272300
C	-2.49070900	-0.53773400	2.94992100	H	-4.91740300	-2.14725800	-1.19082500
Rh	-1.55878900	0.23613700	1.06550500	H	-5.75455800	-0.70196200	-0.60622800
C	-1.55555700	3.13142600	3.15389900	C	-4.00917400	-1.10850200	-3.60393600
C	0.86653100	1.08505900	3.24410300	H	-4.88901500	-1.38029800	-4.19605000
H	1.04825100	1.23771300	4.31709400	H	-3.35222700	-0.49415400	-4.22284900
H	1.55296000	0.31127800	2.89483400	H	-3.47589600	-2.02691600	-3.34186800
H	1.12957600	2.01292400	2.73033800	O	-3.16465100	-0.19794300	-0.29973700
C	-0.26221700	-1.88103400	3.29563200	O	-2.31731600	0.66147500	-2.23147200
C	-3.49309500	-1.65546800	2.97765600	H	-2.48617600	3.64160400	2.89204600
H	-3.02440800	-2.62208000	2.77546500	H	-1.28460900	3.44069700	4.17266400
H	-3.98232100	-1.72372900	3.95875200	H	-0.77305600	3.50741400	2.48850700
H	-4.27960200	-1.50487700	2.23168300	H	0.58702100	-1.90765900	2.60506300
C	-4.27747500	1.38969600	2.95906100	H	0.13785900	-1.93675100	4.31684800
H	-4.87034400	0.88230600	2.19099800	H	-0.85409100	-2.78446100	3.12675300
H	-4.77611800	1.20753200	3.92060100	C	1.27654700	-0.37252500	0.01241400
H	-4.32716900	2.46355800	2.76103600	C	-0.09937100	-0.58080000	-0.24501900
C	4.03976900	5.15541800	-0.56782000	C	-0.51361600	-1.71977800	-1.11433000
C	2.84628200	4.61218700	-0.08312900	C	-1.42128600	-2.69951100	-0.68067000
C	1.97060500	3.93018900	-0.93445300	C	0.06314200	-1.86545200	-2.39019900
C	2.31295400	3.79996100	-2.28908300	C	-1.72896400	-3.79777300	-1.48473600
C	3.50035900	4.34354000	-2.77527500	H	-1.86953000	-2.59478200	0.30135800
C	4.36957300	5.02303300	-1.91595100	C	-0.26058200	-2.94947700	-3.20507800
H	4.70751000	5.68199100	0.10877000	H	0.77675800	-1.12149500	-2.73199800
H	2.59088300	4.72458300	0.96831600	C	-1.15416300	-3.92349200	-2.75246400
H	1.63600500	3.27019000	-2.95292400	H	-2.41489500	-4.55807200	-1.12060000
H	3.74918800	4.23930100	-3.82802200	H	0.19173100	-3.03963500	-4.18881300
H	5.29518600	5.44583700	-2.29664400	H	-1.39805500	-4.77551600	-3.38115300
C	0.66880700	3.34439100	-0.41598400	N	2.12162100	-1.47263400	0.08793300
H	0.48373100	3.73364800	0.59503500	N	3.33409800	-1.19050400	0.35637400
H	-0.15662400	3.69852900	-1.03727000	N	4.16371100	-2.25433000	0.49383100
C	0.66137500	1.83245900	-0.38352200	C	5.58572100	-1.86969900	0.51388400
C	1.64919700	1.00989300	0.05319800	H	6.14290600	-2.81069200	0.53865400
H	2.63149700	1.35558700	0.34406300	C	6.00995900	-1.09341900	-0.74507200
C	-1.14964100	1.38357100	-1.86566000	H	5.46557100	-0.14777600	-0.80794000
N	-0.53552600	1.08875000	-0.66940800	H	5.80323900	-1.66651900	-1.65354300
O	-0.78162000	2.16734000	-2.70807500	C	5.91423500	-1.08697100	1.79371100
C	-3.24914000	0.02997900	-1.49943800	H	5.33596500	-0.15988800	1.82590200
C	-4.46812500	-0.34600400	-2.34048500	H	5.66729600	-1.67529300	2.68254700
C	-5.17748100	0.96829600	-2.74977200	C	3.72198300	-3.62412000	0.17413900
H	-6.05431300	0.73112600	-3.36064900	H	2.64962600	-3.60979600	0.38093400

C	3.90340900	-3.97326200	-1.31257000	H	1.25165600	2.93897400	-3.18193900
H	3.39192300	-3.23989800	-1.94124300	C	1.10738800	1.57017700	-1.57919600
H	3.47705500	-4.95977300	-1.52696600	C	2.03633500	0.64934600	-1.11378900
H	4.96246600	-3.99948700	-1.59304200	H	3.10670500	0.78544000	-1.10205600
C	4.37408600	-4.65910300	1.09869100	C	-1.16321000	1.83031400	-0.67651000
H	4.25072700	-4.37933300	2.14910900	N	-0.16092600	1.04375500	-1.48760300
H	3.89951800	-5.63439100	0.94695500	O	-1.37423900	2.99956900	-0.85540400
H	5.44387400	-4.78866300	0.90107300	C	-3.69365400	0.15310200	-0.97239700
H	6.97927400	-0.83380700	1.82911400	C	-5.13079600	-0.39354200	-1.20204400
H	7.08316600	-0.87548500	-0.71561900	C	-6.09173000	0.51337300	-0.40071900
17-I				H	-7.12998000	0.19631000	-0.55421700
C	-0.54999000	-0.27188200	2.92708100	H	-5.87799200	0.46152300	0.67181100
C	0.09373500	0.98730400	2.53298800	H	-6.00449400	1.55731600	-0.71923000
C	-0.91021400	2.00996200	2.50294900	C	-5.26332300	-1.84685400	-0.71283300
C	-2.17773900	1.36917300	2.69048800	H	-6.28591300	-2.20616100	-0.88080300
C	-1.92636500	-0.04100800	3.02207300	H	-4.57805400	-2.50951000	-1.24979000
Rh	-1.32259600	0.55742300	0.82263400	H	-5.04044900	-1.92855700	0.35344600
C	-0.70054400	3.48244500	2.30437600	C	-5.47185000	-0.31029200	-2.69904700
C	1.57974400	1.19897000	2.48935100	H	-6.50148100	-0.64598700	-2.87117400
H	1.96504000	1.43752900	3.49036800	H	-5.36536000	0.71244800	-3.06596500
H	2.09998700	0.30344400	2.14163000	H	-4.80163000	-0.94519400	-3.28663100
H	1.85928400	2.01775100	1.82196500	O	-3.13355500	-0.24072700	0.13135700
C	0.18569600	-1.55595400	3.17723900	O	-3.18610700	0.92982400	-1.78752600
C	-3.01862500	-1.02337700	3.31064100	H	-0.99618900	4.03584600	3.20376300
H	-2.62485400	-2.01943200	3.52552200	H	0.35032800	3.70864500	2.10817700
H	-3.61725800	-0.70339600	4.17195700	H	-1.28645500	3.85729400	1.45990200
H	-3.68533800	-1.09956500	2.44439600	H	0.87221000	-1.78940200	2.35737800
C	-3.51405700	2.04260300	2.77007200	H	0.77896800	-1.49384300	4.09931900
H	-4.28964200	1.42106500	2.31562600	H	-0.50377900	-2.39668900	3.28385500
H	-3.80151700	2.23104100	3.81360000	C	1.33703900	-0.50018500	-0.69451900
H	-3.50478700	3.00050200	2.24462600	C	-0.06966700	-0.30535200	-0.92947900
C	4.02034600	4.83741200	-0.11368900	C	-0.85745500	-1.40826700	-1.56750800
C	2.79450400	4.29137500	-0.49582000	C	-1.02377200	-2.64229200	-0.91813300
C	2.67115000	3.56554000	-1.68896500	C	-1.34934200	-1.26662700	-2.87406600
C	3.80561900	3.40794400	-2.49538000	C	-1.64421700	-3.70956800	-1.56447100
C	5.03463800	3.95226400	-2.11642400	H	-0.66964000	-2.75739100	0.09962500
C	5.14594300	4.66706600	-0.92271500	C	-1.97534600	-2.33623500	-3.51605400
H	4.09491200	5.40297900	0.81104200	H	-1.25067100	-0.31278700	-3.37776300
H	1.91651600	4.43929400	0.12820700	C	-2.12133300	-3.56464400	-2.86979300
H	3.72347500	2.85997600	-3.43110100	H	-1.76484600	-4.65516200	-1.04218700
H	5.90259700	3.82325800	-2.75716700	H	-2.34583000	-2.20540600	-4.52921000
H	6.09999200	5.09547600	-0.62906900	H	-2.60593100	-4.39658900	-3.37312400
C	1.33792200	2.96791400	-2.08716500	N	1.84162400	-1.71726100	-0.26068500
H	0.50625100	3.59398200	-1.74742600	N	3.10919300	-1.68970300	-0.07407700

N	3.67773300	-2.82808600	0.26693100	C	2.32558800	-3.22021900	-1.36881100
C	5.13157400	-2.73345300	0.52938500	C	2.33535500	-4.25084500	-0.42145200
H	5.43261300	-3.74385600	0.82032200	C	3.50949600	-4.59412100	0.25255100
C	5.90197700	-2.33991300	-0.73800200	C	4.69619400	-3.90734600	-0.00752300
H	5.59771400	-1.34529100	-1.07425900	H	5.62341800	-2.35569200	-1.18797900
H	5.71662000	-3.04903400	-1.54970200	H	3.55629600	-1.77802300	-2.39753000
C	5.42217800	-1.78582100	1.70068300	H	1.41057300	-4.77261700	-0.19414300
H	5.11616900	-0.76632600	1.45203700	H	3.49330100	-5.39501200	0.98647800
H	4.88584600	-2.09709700	2.60193800	H	5.60763800	-4.16824500	0.52253500
C	2.94646800	-4.11445800	0.36909200	C	1.03556200	-2.82082600	-2.06510100
H	1.92984300	-3.86899200	0.06009000	H	1.23771700	-2.66613400	-3.13193000
C	3.51624600	-5.15225800	-0.60749100	H	0.31606700	-3.64316400	-2.00914100
H	3.50427700	-4.77279400	-1.63295000	C	0.38131100	-1.53738900	-1.53801500
H	2.90246300	-6.05787900	-0.57474000	C	1.02104800	-0.34146900	-1.68172700
H	4.54197100	-5.44190300	-0.35527400	H	1.97896500	-0.33254800	-2.18234400
C	2.91691800	-4.61989100	1.81777700	C	-1.14276700	-2.68810600	-0.14295400
H	2.47422100	-3.87485300	2.48477300	N	-0.86899400	-1.62607900	-0.97642100
H	2.31375200	-5.53144500	1.87852200	O	-2.03680900	-3.49349500	-0.16592300
H	3.91896500	-4.86293400	2.18820600	C	-0.24751000	-1.94610300	1.95100600
H	6.49378600	-1.78047900	1.92339400	C	1.06474500	-1.79182500	2.71443500
H	6.97747800	-2.32290700	-0.53552200	C	1.59347200	-3.17820700	3.13233200
16-II				H	2.54246100	-3.06013900	3.66559700
C	-3.94533400	1.26554400	-0.39750100	H	0.88859500	-3.68517400	3.80011500
C	-4.03229700	0.42799000	-1.57205200	H	1.76756600	-3.81005500	2.26112000
C	-4.24553000	-0.94753700	-1.13781900	C	0.81153300	-0.91804600	3.95234300
C	-4.19050600	-0.96592900	0.26819700	H	1.74160700	-0.80696000	4.51893900
C	-3.96086700	0.39717800	0.73256500	H	0.46072200	0.07667400	3.66478700
Rh	-2.18734800	-0.09279900	-0.57794400	H	0.05689800	-1.36384600	4.60658800
C	-4.43401100	-2.13032600	-2.03968400	C	2.07422700	-1.09260800	1.77375100
C	-4.10637300	0.91565200	-2.98555100	H	3.01322000	-0.92930400	2.31246300
H	-5.15140000	1.08098300	-3.28094300	H	2.28292700	-1.69532000	0.88928000
H	-3.56806100	1.85835700	-3.10408400	H	1.69742100	-0.12114700	1.43982000
H	-3.67320900	0.19054200	-3.67854700	O	-1.27937900	-1.36668200	2.22087500
C	-3.98318700	2.76185900	-0.38118000	O	-0.13743600	-2.79438700	0.88654000
C	-3.90721100	0.77905900	2.17756100	H	-3.93691600	-3.01023800	-1.62764100
H	-3.56022700	1.80423800	2.30970500	H	-5.50018300	-2.35357500	-2.17240800
H	-4.90562500	0.69045100	2.62592900	H	-4.00907700	-1.94042400	-3.02840500
H	-3.23226400	0.11229900	2.71981000	H	-3.45278600	3.18750800	-1.23460400
C	-4.35946500	-2.13787900	1.18107300	H	-5.02445500	3.10663400	-0.42312900
H	-3.50978300	-2.21365200	1.86371700	H	-3.52244900	3.17058700	0.51885200
H	-5.27118500	-2.01622700	1.77996800	C	0.61869000	0.87716100	-1.05311700
H	-4.42866700	-3.07340100	0.62702600	C	-0.64457200	1.15748600	-0.54044700
C	4.70427300	-2.89019700	-0.96471000	C	-0.81909200	2.44558900	0.17483600
C	3.53188000	-2.56000000	-1.64471300	C	-0.81572000	3.68556700	-0.48755500

C	-0.98355600	2.44069300	1.57075400	C	3.57231900	-2.98349400	-1.03210200
C	-0.98422100	4.87575900	0.21818300	C	3.82316600	-1.74391300	1.95074900
H	-0.66927800	3.70265100	-1.56329500	H	3.39509000	-2.74067200	1.84046800
C	-1.14489100	3.63254100	2.27994400	H	4.83340200	-1.84990300	2.36785900
H	-0.99138200	1.48501300	2.08714300	H	3.21853300	-1.19366700	2.67723000
C	-1.15087200	4.85676600	1.60660300	C	4.48418600	1.26340200	1.70945700
H	-0.98400600	5.82285400	-0.31543800	H	3.64307100	1.21141400	2.40613500
H	-1.26631200	3.60359400	3.35986300	H	5.38467000	0.92074000	2.23519200
H	-1.28136100	5.78487400	2.15588400	H	4.61372100	2.30613500	1.42311600
N	1.59217200	1.89477900	-0.85454500	C	-3.64852900	4.15058600	-0.52928400
N	2.79061800	1.48563300	-0.93197700	C	-2.81037900	3.58676400	-1.49356800
N	3.72484700	2.41371200	-0.72864300	C	-1.41679900	3.69322800	-1.38831900
C	5.07027100	1.83779700	-0.52875700	C	-0.87804300	4.38495300	-0.29419000
H	5.72389600	2.68175300	-0.29789300	C	-1.71316500	4.95540500	0.66681800
C	5.10106800	0.85322100	0.65048000	C	-3.10123000	4.83778100	0.55580900
H	4.47941100	-0.01821000	0.42980100	H	-4.72645800	4.05565100	-0.62840700
H	4.72426100	1.32198600	1.56399900	H	-3.24303400	3.05589100	-2.33844200
C	5.56557600	1.18072100	-1.82319600	H	0.20018000	4.45241200	-0.18311700
H	4.90937400	0.34882000	-2.09331200	H	-1.27774100	5.48888200	1.50731000
H	5.56995300	1.89842600	-2.64875600	H	-3.74935100	5.27838300	1.30796300
C	3.34645400	3.78354400	-0.31205900	C	-0.50181000	3.00738400	-2.38668300
H	2.44390300	3.99914000	-0.89008800	H	-1.03176800	2.84997600	-3.33360200
C	2.96582000	3.83511700	1.17492200	H	0.38051400	3.61918400	-2.58870900
H	2.17673500	3.11163900	1.38966900	C	-0.02625800	1.65780000	-1.83168600
H	2.58611800	4.82967900	1.43108700	C	-0.99101000	0.64646700	-1.70498600
H	3.83411400	3.62601300	1.80982200	H	-1.99316700	0.85332800	-2.06349900
C	4.42000400	4.80854600	-0.68185300	C	1.46717600	1.86577100	0.37445200
H	4.73588700	4.69702300	-1.72372400	N	1.24132900	1.58702600	-1.45681100
H	4.00939100	5.81504400	-0.55531900	O	2.19486600	2.77505100	0.66222600
H	5.30502100	4.73965600	-0.04055600	C	0.12635600	1.10334900	2.17922700
H	6.58120200	0.79356600	-1.69050900	C	-1.27456500	1.13947400	2.79549500
H	6.12561500	0.51237800	0.83383400	C	-1.33039900	2.43122200	3.64577000
TS17-II				H	-2.30333300	2.49934400	4.14399900
C	3.74507600	-1.54261600	-0.66430200	H	-0.54856400	2.43284000	4.41173100
C	3.97889300	-0.45233100	-1.60256000	H	-1.20668700	3.31462700	3.01294900
C	4.32585200	0.72374800	-0.85003000	C	-1.44174500	-0.09959100	3.69043700
C	4.22770800	0.38707900	0.52429000	H	-2.41445200	-0.06583800	4.19171500
C	3.87447500	-1.01279700	0.64456900	H	-1.39364800	-1.01826600	3.09629300
Rh	2.09221800	0.03177500	-0.52341300	H	-0.65528400	-0.14753700	4.44705000
C	4.60515800	2.07436200	-1.44039300	C	-2.37410600	1.17802900	1.72110500
C	4.02068000	-0.57075600	-3.09565900	H	-3.35315400	1.22652900	2.20979600
H	5.03421000	-0.82475000	-3.43514400	H	-2.27364600	2.04655700	1.06845800
H	3.34366100	-1.35073800	-3.45188600	H	-2.35137800	0.28171800	1.09929500
H	3.73218200	0.37075700	-3.56817700	O	1.09243400	0.56856200	2.68934200

O	0.18389400	1.78948200	1.01542000	C	-3.86562900	0.77608600	-1.12190800
H	5.08737700	2.73062700	-0.71339700	C	-3.93802500	-0.60297000	-1.54742800
H	5.26088800	1.99337300	-2.31340300	C	-4.12199200	-1.42831300	-0.38286800
H	3.66755700	2.55175700	-1.75007800	C	-4.08661200	-0.57732200	0.75103200
H	2.99790800	-3.09903900	-1.95436600	C	-3.94630900	0.79386100	0.29829900
H	4.55281500	-3.45199500	-1.18793200	Rh	-1.96461000	-0.43475200	-0.36166100
H	3.04905600	-3.53816600	-0.25209500	C	-4.23826200	-2.92075100	-0.41504600
C	-0.78863500	-0.57579200	-1.06625400	C	-3.95721600	-1.11654300	-2.95525200
C	0.45778900	-1.01023400	-0.53299800	H	-4.98399900	-1.34551100	-3.26923100
C	0.48571200	-2.38125200	0.03518100	H	-3.54729800	-0.38749800	-3.65829600
C	0.28679700	-3.50981500	-0.78304100	H	-3.36647600	-2.03332800	-3.03032500
C	0.68958400	-2.58222600	1.40951900	C	-3.81573700	1.96962900	-2.02752500
C	0.30674800	-4.79504300	-0.24746500	C	-4.10736400	1.99193000	1.18491000
H	0.11195100	-3.36324700	-1.84449300	H	-3.81786700	2.91167100	0.67389200
C	0.68874500	-3.87090300	1.94870400	H	-5.15751800	2.09690500	1.48866700
H	0.84659500	-1.72152000	2.04957800	H	-3.50585100	1.89655400	2.09144300
C	0.50355800	-4.98272800	1.12501300	C	-4.25673800	-0.97480300	2.18532300
H	0.16313900	-5.65270200	-0.89942200	H	-3.61195800	-0.37172900	2.82847600
H	0.83968200	-4.00252800	3.01688100	H	-5.29778200	-0.82620400	2.50009400
H	0.51269400	-5.98465400	1.54475100	H	-3.99297300	-2.02216500	2.33893100
N	-1.86527400	-1.48058600	-0.85889200	C	3.78289300	-4.80298400	-0.36942700
N	-3.01766000	-0.99360100	-1.07619100	C	2.84047500	-4.39883800	-1.31933700
N	-4.03061600	-1.82599100	-0.87858800	C	1.52155800	-4.11764700	-0.94476100
C	-5.34874400	-1.15774800	-0.89013100	C	1.16079100	-4.24166300	0.40630000
H	-6.07611200	-1.93672800	-0.65350900	C	2.09906800	-4.64693900	1.35414100
C	-5.43772700	-0.06179300	0.18219500	C	3.41401500	-4.92821000	0.97043700
H	-4.73636600	0.74698000	-0.03982700	H	4.80255700	-5.01798600	-0.67785300
H	-5.19414900	-0.45951000	1.17131100	H	3.13286800	-4.29918000	-2.36226800
C	-5.65787600	-0.61275600	-2.28973300	H	0.14902000	-3.99242100	0.71450700
H	-4.92049400	0.14525800	-2.56767200	H	1.80435500	-4.73395400	2.39619000
H	-5.62758000	-1.41240500	-3.03567100	H	4.14498600	-5.23949800	1.71150200
C	-3.79662900	-3.18698100	-0.33902800	C	0.50643800	-3.60502600	-1.95004800
H	-2.86443400	-3.50804200	-0.81124600	H	0.95794000	-3.56066600	-2.94887400
C	-3.55895000	-3.14662400	1.17760000	H	-0.36722200	-4.26057300	-2.00301700
H	-2.74175900	-2.46261100	1.41526900	C	0.02362000	-2.21425900	-1.52197900
H	-3.28032700	-4.14157700	1.53972400	C	1.05515700	-1.20707600	-1.43073200
H	-4.46244900	-2.82725600	1.70843300	H	2.06641900	-1.50491100	-1.69025100
C	-4.90822300	-4.15944100	-0.73643600	C	-1.12211400	-1.18123100	1.31432900
H	-5.12028300	-4.10731900	-1.80878000	N	-1.22436700	-2.05222600	-1.25351300
H	-4.58639000	-5.17866300	-0.50210600	O	-1.39005600	-2.23081000	1.82045300
H	-5.83909400	-3.98145500	-0.18779900	C	-0.33209300	0.57903600	2.74135900
H	-6.65188500	-0.15467100	-2.30886600	C	0.89208600	1.25808800	3.37011400
H	-6.45068200	0.35273500	0.21494000	C	0.86239500	0.88755200	4.87026600
				H	1.69134700	1.37924500	5.39043000

18-II

H	-0.07793700	1.20705200	5.32766100	C	3.49340400	3.52746000	0.00691600
H	0.96551500	-0.19369800	5.00975200	H	2.57840800	3.09602400	0.41599900
C	0.72612000	2.78212700	3.20850200	H	3.28813200	4.57005700	-0.25754600
H	1.52926700	3.30146800	3.74162100	H	4.26991400	3.51728000	0.77885000
H	0.77091000	3.07483400	2.15513600	C	5.19244600	3.35257000	-1.88286300
H	-0.23486900	3.10950000	3.61287500	H	5.54708200	2.74278900	-2.71950100
C	2.20750800	0.79422200	2.73084900	H	4.94569600	4.34669600	-2.26768600
H	3.04728300	1.32420700	3.19255900	H	6.01255500	3.47760900	-1.16828400
H	2.36019200	-0.27957700	2.86583800	H	6.63254500	-1.00047900	-0.90653000
H	2.21946800	0.99518100	1.65797200	H	6.25875300	0.04119700	1.41509800
O	-1.47834300	0.92853300	2.97269400	16-III			
O	-0.01560400	-0.45315200	1.94959700	C	0.66292400	-2.95950700	-1.94080000
H	-4.35601600	-3.33387300	0.58862100	C	1.59241400	-1.97034600	-2.41382900
H	-5.09865200	-3.23580200	-1.01714300	C	2.84198700	-2.10992400	-1.66054300
H	-3.33175000	-3.35277300	-0.85707500	C	2.59814600	-3.02383000	-0.62734300
H	-3.26691800	1.75070700	-2.94684200	C	1.23365900	-3.54162300	-0.75907700
H	-4.82833400	2.28493200	-2.31039500	Rh	0.90842700	-1.39235300	-0.43272600
H	-3.32097900	2.81627900	-1.54763700	C	4.12849200	-1.43331600	-2.01794700
C	0.85477600	0.11285700	-1.09972100	C	1.42042900	-1.09736600	-3.61815500
C	-0.45057800	0.65871700	-0.83204400	H	1.76929300	-1.61677000	-4.52004000
C	-0.60745100	2.11922400	-0.96043900	H	0.37121800	-0.82758400	-3.75667100
C	-0.26571800	2.77253000	-2.16226800	H	1.99212300	-0.17260100	-3.51083100
C	-1.11526400	2.88918300	0.09890000	C	-0.62076300	-3.33743000	-2.61012500
C	-0.45058900	4.14465200	-2.30284000	C	0.69177900	-4.69619100	0.02669700
H	0.13786400	2.18859400	-2.98299100	H	-0.39492200	-4.75688200	-0.04273500
C	-1.26240700	4.27081400	-0.03184500	H	1.11639000	-5.63964300	-0.34151800
H	-1.38555400	2.39742000	1.02386300	H	0.94446000	-4.60464000	1.08578900
C	-0.94113700	4.90303200	-1.23421400	C	3.51203900	-3.41908700	0.49059300
H	-0.20212000	4.62751200	-3.24387800	H	3.06515300	-3.14841700	1.45346200
H	-1.63936900	4.84852900	0.80741100	H	3.67498900	-4.50298200	0.49429700
H	-1.07113000	5.97615500	-1.34061500	H	4.48253400	-2.92561000	0.41864200
N	1.92682500	1.04546000	-1.09553300	C	-1.08203500	5.19502900	0.23066400
N	3.05407200	0.50746800	-0.86325000	C	-1.05510400	4.18969300	-0.73348100
N	4.10675700	1.30661900	-0.94642500	C	0.15559400	3.78935600	-1.31819500
C	5.35646500	0.68958400	-0.45160400	C	1.34164700	4.40578900	-0.90838200
H	6.14768600	1.40898200	-0.67069200	C	1.31803200	5.40499100	0.06924100
C	5.30743600	0.45419500	1.06420100	C	0.10887600	5.80662300	0.63672700
H	4.51028900	-0.25378300	1.30574200	H	-2.02961500	5.49566700	0.67033800
H	5.11442200	1.38437500	1.60520700	H	-1.97534800	3.68916100	-1.02394000
C	5.65914500	-0.60647700	-1.21527700	H	2.28900100	4.08030600	-1.32297500
H	4.89858800	-1.36349500	-1.00793300	H	2.25187500	5.85873200	0.38871600
H	5.68347700	-0.42489300	-2.29390300	H	0.09146100	6.58526600	1.39459300
C	3.94331300	2.74950600	-1.23850000	C	0.16624400	2.64459500	-2.32371800
H	3.12424700	2.78344900	-1.96342700	H	-0.65598700	2.77171500	-3.03426700

H	1.09882600	2.64291100	-2.88597700	N	-5.03282900	1.06033600	-0.16671800
C	-0.05748400	1.33139500	-1.58868400	C	-5.48763800	2.45885600	-0.03703900
C	-1.31057000	0.83120100	-1.53146100	H	-6.53618700	2.40344800	0.26513100
H	-2.06559400	1.35631900	-2.10379500	C	-4.70574900	3.22087900	1.04586100
C	2.25465100	1.15983400	-0.95404000	H	-3.64484500	3.26590100	0.78411500
N	0.95051300	0.82186100	-0.72837000	H	-4.79412900	2.72847900	2.01826700
O	2.81337900	1.55057200	-1.96100700	C	-5.41695800	3.17150000	-1.39345000
C	3.90320700	1.84555700	0.66222400	H	-4.38175200	3.22413200	-1.74048100
C	4.83566800	1.26999000	1.73206500	H	-6.00334400	2.63373700	-2.14429200
C	3.99858100	0.66970800	2.88037900	C	-5.73191400	-0.08087800	0.46016300
H	4.66477000	0.32573500	3.67870100	H	-5.31082100	-0.95731100	-0.03970900
H	3.31914900	1.41603200	3.30552300	C	-5.41060200	-0.20575900	1.95675800
H	3.40906900	-0.17933400	2.53048200	H	-4.32955600	-0.24179700	2.10754900
C	5.72922200	2.40385900	2.25489000	H	-5.84153100	-1.12844100	2.36022500
H	6.41383900	2.01620400	3.01613300	H	-5.82552200	0.63712900	2.52016100
H	6.31705300	2.84532700	1.44618700	C	-7.23699200	-0.04263500	0.18451400
H	5.12885100	3.20230300	2.69912300	H	-7.44020500	0.11853100	-0.87856600
C	5.69154100	0.15929400	1.08874500	H	-7.67999800	-0.99957900	0.47794200
H	6.38938500	-0.24578400	1.82928500	H	-7.74896700	0.73784100	0.75744900
H	5.05615400	-0.65242400	0.72999600	H	-5.80594000	4.19139300	-1.30935500
H	6.27382800	0.54288500	0.24462500	H	-5.08571300	4.24359800	1.14260800
O	3.91263500	2.98525600	0.27125200	C	0.75069600	-0.00187600	2.35302400
O	3.02224300	0.88928400	0.21086600	O	1.13495600	-1.02401700	1.74535900
H	4.91164700	-1.64974200	-1.29001200	O	0.41419500	1.11177900	1.78424600
H	4.47301400	-1.79570700	-2.99475400	H	0.57652900	1.03659200	0.74862000
H	4.02498100	-0.34827700	-2.09730400	C	0.61461300	-0.03246900	3.85159100
H	-1.12776600	-2.45875200	-3.01515700	H	0.69682100	0.97020200	4.27236100
H	-0.41646500	-4.02780500	-3.43813900	H	-0.37803700	-0.43223400	4.08869100
H	-1.30216500	-3.82858700	-1.91570700	H	1.36342800	-0.70009500	4.27947000
C	-1.82909400	-0.22963800	-0.67192300	TS17-III			
C	-1.11429100	-1.26734800	-0.15022300	C	0.63545600	-3.01801500	-1.92306600
C	-1.77761100	-2.37757700	0.57089700	C	1.59406100	-2.06257000	-2.39529500
C	-2.87770500	-3.04383300	-0.01662300	C	2.81796300	-2.19736500	-1.59807000
C	-1.33893800	-2.85012000	1.82293400	C	2.53197500	-3.07859700	-0.54824100
C	-3.50494300	-4.11416600	0.61577500	C	1.16124900	-3.57487500	-0.70514800
H	-3.24169600	-2.69770400	-0.97677000	Rh	0.87067000	-1.43051100	-0.42688700
C	-1.97533000	-3.91502300	2.46258700	C	4.12435800	-1.55142700	-1.93780700
H	-0.47460800	-2.39300400	2.28396400	C	1.48346600	-1.22465600	-3.63119800
C	-3.06034500	-4.55675000	1.86547400	H	1.95410100	-1.73766600	-4.47997600
H	-4.34570400	-4.60439100	0.13157100	H	0.43941400	-1.03026200	-3.88433700
H	-1.61207800	-4.24902500	3.43129700	H	1.98560000	-0.26395700	-3.49358100
H	-3.55043800	-5.39010500	2.36085000	C	-0.64015200	-3.39234200	-2.61055200
N	-3.20647300	-0.16653500	-0.31276300	C	0.57876500	-4.69759100	0.09661900
N	-3.73458700	0.97002800	-0.49026400	H	-0.50569500	-4.74722700	-0.00584600

H	1.00353500	-5.65621200	-0.22965400	H	4.03772400	-0.46875800	-2.05785700
H	0.79902900	-4.57480600	1.15954400	H	-1.13174800	-2.51544400	-3.03785600
C	3.40180500	-3.44947800	0.61216100	H	-0.43038100	-4.09885900	-3.42327200
H	2.93379900	-3.12085200	1.54678200	H	-1.33920100	-3.86371800	-1.91993300
H	3.53322400	-4.53602000	0.66886800	C	-1.84125300	-0.20099800	-0.69458600
H	4.38778800	-2.98643200	0.54734200	C	-1.15429100	-1.25941400	-0.18012300
C	-0.88924400	5.22933100	0.22167200	C	-1.85454900	-2.34781300	0.53940400
C	-0.91162300	4.21635200	-0.73417600	C	-2.94849800	-3.00311100	-0.06963500
C	0.27349100	3.78530400	-1.34849300	C	-1.46046200	-2.80244200	1.81216800
C	1.48374000	4.37762800	-0.97660900	C	-3.61302900	-4.05118900	0.56232000
C	1.50977800	5.38471300	-0.00708500	H	-3.27853600	-2.66502800	-1.04512800
C	0.32582400	5.81723000	0.58966400	C	-2.13541300	-3.84368700	2.45108600
H	-1.81698700	5.55379500	0.68583900	H	-0.60100100	-2.35062100	2.28760200
H	-1.85023800	3.73335300	-0.99426900	C	-3.21306100	-4.47780800	1.83244800
H	2.41182200	4.02770000	-1.41446000	H	-4.44851100	-4.53501700	0.06281300
H	2.46183500	5.81971600	0.28320700	H	-1.80818000	-4.16557000	3.43654800
H	0.34651200	6.60112200	1.34194000	H	-3.73250100	-5.29324800	2.32778800
C	0.23110000	2.63252000	-2.34366200	N	-3.21672300	-0.10468800	-0.33816600
H	-0.58831300	2.78484500	-3.05265400	N	-3.71021300	1.04969600	-0.49931700
H	1.15983600	2.58860400	-2.91155300	N	-5.00431700	1.17523100	-0.16979800
C	-0.04115500	1.33815500	-1.59719000	C	-5.41442400	2.58546700	-0.01961200
C	-1.29680500	0.85489400	-1.54776200	H	-6.46330500	2.55896700	0.28517700
H	-2.03773300	1.38292400	-2.13673600	C	-4.60610600	3.30884600	1.07040400
C	2.27441200	1.10117700	-0.93642800	H	-3.54519200	3.32597900	0.80523100
N	0.94883700	0.82625700	-0.69895700	H	-4.70512600	2.80602500	2.03633600
O	2.83114700	1.41051400	-1.96976500	C	-5.32530700	3.31322100	-1.36688300
C	3.94627000	1.80124100	0.64858600	H	-4.28982300	3.33789000	-1.71636700
C	4.82253500	1.23522200	1.76757400	H	-5.93033500	2.80395900	-2.12280300
C	3.93581500	0.67108500	2.89626100	C	-5.73226100	0.04812000	0.45046500
H	4.56937200	0.33156300	3.72251400	H	-5.34588500	-0.83436800	-0.06661200
H	3.25412400	1.43531900	3.28304300	C	-5.39793800	-0.10899200	1.94132100
H	3.34328800	-0.17416300	2.54231600	H	-4.31708300	-0.18066700	2.07981700
C	5.71833800	2.36409900	2.29734100	H	-5.85255700	-1.02429800	2.33546800
H	6.36894900	1.97987100	3.08935200	H	-5.78099800	0.73723300	2.52200800
H	6.34126500	2.77905100	1.50107800	C	-7.23852500	0.13870000	0.19435300
H	5.11745800	3.18104000	2.70630700	H	-7.44983500	0.32277500	-0.86344000
C	5.68037200	0.09728400	1.17379200	H	-7.70833400	-0.80802500	0.47902500
H	6.34188400	-0.30702600	1.94717800	H	-7.71772700	0.92601800	0.78592700
H	5.04304700	-0.70950400	0.80666500	H	-5.68185500	4.34363600	-1.26842400
H	6.30115900	0.45479600	0.34578300	H	-4.95522500	4.34092300	1.18283000
O	4.02709900	2.90873900	0.18413300	C	0.70213400	-0.00422000	2.29703500
O	3.01866200	0.86527300	0.23602400	O	1.07032900	-1.06404700	1.71144900
H	4.88235200	-1.75357900	-1.17975900	O	0.40967300	1.09089900	1.71421900
H	4.49215400	-1.95177100	-2.89109900	H	0.63261100	0.99678700	0.54692600

C	0.56269900	-0.04468000	3.80018500	O	2.84032400	1.31686600	-1.94360300
H	0.65125200	0.95633900	4.22376100	C	3.98665900	1.77821700	0.66097100
H	-0.43309600	-0.43779800	4.03507300	C	4.81615100	1.20330800	1.80719500
H	1.30467200	-0.71876600	4.23120400	C	3.89581200	0.63442500	2.90515700
18-III							
C	0.59558200	-3.04191400	-1.95730600	H	4.50594200	0.29481500	3.74867500
C	1.58190100	-2.11248700	-2.40974300	H	3.19668200	1.39244000	3.27073600
C	2.78090400	-2.25861300	-1.57489400	H	3.31716500	-0.21094200	2.52987300
C	2.45579100	-3.12751900	-0.52691200	C	5.70667800	2.32248000	2.36628700
C	1.07812800	-3.59658800	-0.71572200	H	6.33523300	1.92687500	3.17016000
Rh	0.82423600	-1.46724000	-0.43879800	H	6.35082600	2.74021900	1.58872100
C	4.10612400	-1.63446800	-1.88078900	H	5.10115400	3.13882300	2.77024700
C	1.51642500	-1.27331800	-3.64828200	C	5.68185800	0.06363400	1.22401200
H	1.97519400	-1.80299700	-4.49321500	H	6.31691600	-0.35281200	2.01276600
H	0.48261800	-1.03963100	-3.91090200	H	5.04904700	-0.73597800	0.83269800
H	2.05112200	-0.33150700	-3.50582800	H	6.32902200	0.42396800	0.41778100
C	-0.66808200	-3.40794000	-2.67041400	O	4.14349000	2.84638000	0.13285700
C	0.45689000	-4.70702600	0.07276500	O	2.99102800	0.88429600	0.29033800
H	-0.62490500	-4.74079900	-0.05890100	H	4.84340700	-1.85925200	-1.10866800
H	0.87642900	-5.67175700	-0.24211900	H	4.48653200	-2.03281500	-2.82985900
H	0.65216600	-4.58439700	1.14029000	H	4.04341300	-0.54955000	-1.99310200
C	3.27896800	-3.48153900	0.67175700	H	-1.09433500	-2.54835000	-3.19235200
H	2.80663900	-3.06789800	1.57080300	H	-0.46149900	-4.18916600	-3.41268400
H	3.34748400	-4.56805500	0.79379100	H	-1.41957100	-3.78710900	-1.97761400
H	4.29069700	-3.07722000	0.60402700	C	-1.85856500	-0.16312200	-0.70507900
C	-0.69933900	5.28794400	0.19911300	C	-1.19781900	-1.24725200	-0.20981400
C	-0.77444300	4.26604100	-0.74415100	C	-1.93516400	-2.32401600	0.48987700
C	0.38261800	3.79522100	-1.38213900	C	-3.03797400	-2.94290200	-0.13960500
C	1.61823400	4.35574100	-1.04640300	C	-1.56744500	-2.79920200	1.76245100
C	1.69710100	5.37198400	-0.08927300	C	-3.73856400	-3.97825100	0.47463900
C	0.54084100	5.84427600	0.53074200	H	-3.34750500	-2.58529500	-1.11514400
H	-1.60528100	5.64304000	0.68309600	C	-2.27990600	-3.82551300	2.38404700
H	-1.73260500	3.80737700	-0.97553600	H	-0.69802800	-2.37735300	2.24669300
H	2.52509200	3.97619000	-1.50387700	C	-3.36678600	-4.42464200	1.74639000
H	2.66790800	5.78240800	0.17305000	H	-4.58054700	-4.43499300	-0.03917200
H	0.60234800	6.63433200	1.27413300	H	-1.97431000	-4.16447900	3.37068900
C	0.28158700	2.63375500	-2.36288500	H	-3.91476600	-5.22920800	2.22864700
H	-0.53630800	2.80992100	-3.06814300	N	-3.22828700	-0.02969300	-0.34174200
H	1.20256300	2.54397800	-2.93917500	N	-3.68474700	1.14199200	-0.48644200
C	-0.03906000	1.36283500	-1.60241600	N	-4.97105800	1.30699800	-0.14299200
C	-1.29392400	0.88873300	-1.55326100	C	-5.33127500	2.72882800	0.02501100
H	-2.02492600	1.41738700	-2.15525400	H	-6.37757800	2.73502600	0.33936600
C	2.28776200	1.08013600	-0.89256500	C	-4.48886800	3.41451900	1.11345600
N	0.94005000	0.84518000	-0.67567800	H	-3.43048200	3.39878200	0.83833700
				H	-4.59455600	2.90607600	2.07558600

C	-5.23062700	3.46565700	-1.31656200	C	5.72435800	-3.12462500	-0.77197700
H	-4.19810200	3.45933300	-1.67572300	C	4.35531000	-3.21255500	-1.02659900
H	-5.85909400	2.98360200	-2.07123300	C	3.43391100	-3.27823300	0.02573500
C	-5.72636900	0.19891200	0.47984000	C	3.91257600	-3.24677900	1.34224900
H	-5.38369600	-0.69063600	-0.05583100	C	5.28100700	-3.14889800	1.60042000
C	-5.36793000	0.01049300	1.96158700	C	6.19135700	-3.08960800	0.54342100
H	-4.28798500	-0.10113300	2.07838500	H	6.42444100	-3.07570300	-1.60093500
H	-5.84727200	-0.89348700	2.35257900	H	3.99525700	-3.22276600	-2.05226100
H	-5.70957300	0.86151500	2.56076800	H	3.20590500	-3.29368500	2.16630900
C	-7.23327300	0.34756500	0.25708300	H	5.63530300	-3.12218800	2.62692300
H	-7.46042700	0.55453700	-0.79321600	H	7.25643200	-3.01668900	0.74315400
H	-7.73107600	-0.58560700	0.53881100	C	1.94114800	-3.30661300	-0.25671300
H	-7.67041600	1.14282800	0.87014200	H	1.75198600	-3.73292400	-1.24650600
H	-5.55190400	4.50637200	-1.20568300	H	1.43326100	-3.94184700	0.48011100
H	-4.80250000	4.45647300	1.23891400	C	1.35368200	-1.91982700	-0.19683400
C	0.69051800	-0.14097100	2.33590800	C	0.86841100	-1.21980400	-1.22145500
O	1.05203800	-1.18169400	1.66708600	H	0.88773300	-1.68317700	-2.20673700
O	0.36746400	0.96455800	1.85256400	C	0.20948500	-1.01465000	1.69065500
H	0.65734500	0.96590800	0.36902200	N	1.38020400	-1.28831400	1.09492800
C	0.64030600	-0.33267200	3.84205700	O	-0.86017400	-1.55535600	1.43834100
H	0.71593400	0.62947000	4.35045600	C	1.18816800	0.91309700	2.85791900
H	-0.32449200	-0.78624400	4.09667000	C	0.61328900	2.14866100	3.53069900
H	1.42924500	-1.01030400	4.17445800	C	1.76309900	3.09023000	3.91645200
19-III				H	1.35294300	3.99619400	4.37271200
C	-2.74342000	-1.43277700	-2.27514800	H	2.43923700	2.61754700	4.63543000
C	-2.57733000	-2.56792600	-1.43352100	H	2.35051200	3.37800000	3.04172400
C	-3.68143000	-2.60571000	-0.46495700	C	-0.20641600	1.75135500	4.77569100
C	-4.45552400	-1.45881200	-0.65564600	H	-0.62891600	2.65400300	5.22801700
C	-3.83100100	-0.65193600	-1.71359300	H	-1.02544400	1.07989400	4.51501600
Rh	-2.29769500	-0.70979300	-0.25728300	H	0.42311300	1.26047200	5.52558800
C	-3.87877400	-3.64497900	0.59590400	C	-0.30991900	2.81008100	2.47580200
C	-1.55278100	-3.65263700	-1.56000900	H	-0.76281300	3.70782500	2.90965200
H	-2.03427000	-4.60160000	-1.82440300	H	0.25097500	3.10980200	1.58524300
H	-0.81187000	-3.41987900	-2.32566400	H	-1.10068700	2.12517200	2.16387300
H	-1.02553800	-3.79198800	-0.61215000	O	2.33070500	0.78379600	2.47161400
C	-1.99161800	-1.09897100	-3.52664500	O	0.21257200	-0.04969900	2.69049600
C	-4.40939900	0.59808700	-2.30132300	H	-3.95878800	-3.15378800	1.56920400
H	-3.64121000	1.19445800	-2.79675200	H	-4.79035300	-4.22662900	0.41421800
H	-5.19049900	0.35507900	-3.03370800	H	-3.03764100	-4.34079200	0.62852600
H	-4.85405500	1.22317700	-1.52385000	H	-1.00343100	-1.56185200	-3.54206600
C	-5.67862600	-1.05682000	0.10363900	H	-2.54721300	-1.45944400	-4.40157000
H	-5.67670900	0.01928100	0.29602400	H	-1.85890600	-0.02084100	-3.63138900
H	-6.57744000	-1.28877200	-0.48258800	C	0.41539100	0.20134900	-1.15829300
H	-5.72742400	-1.56351600	1.06622600	C	-0.87182400	0.60226300	-0.94860100

C	-1.30333300	1.95891600	-1.36086500	C	2.37206400	-1.94005000	-2.40880400
C	-0.93890500	2.42293600	-2.64618900	C	3.70314400	-1.40353700	-2.16870000
C	-2.14869000	2.78353500	-0.59250600	C	4.09806700	-1.80604500	-0.86480200
C	-1.38142800	3.65215400	-3.13091400	C	3.02121300	-2.57724300	-0.27258000
H	-0.29349500	1.80559800	-3.26189400	Rh	2.24359000	-0.56470500	-0.67019500
C	-2.57920900	4.01920300	-1.07515900	C	4.50222200	-0.55717800	-3.11081600
H	-2.47797300	2.43086800	0.37466600	C	1.58709700	-1.74885100	-3.66990100
C	-2.20241300	4.46355600	-2.34424500	H	1.98559100	-2.37177800	-4.47987700
H	-1.08399300	3.97599400	-4.12507800	H	0.53605300	-2.00351300	-3.52353300
H	-3.22307700	4.63692100	-0.45387400	H	1.62789400	-0.70406900	-3.98949200
H	-2.54808200	5.42339300	-2.71820800	C	0.78957400	-3.59622800	-1.13509300
N	1.40736300	1.19666300	-1.33273900	C	3.06985600	-3.30350400	1.03821000
N	2.59003100	0.74402000	-1.40643400	H	2.07412600	-3.38408200	1.48128800
N	3.55881900	1.66980800	-1.51194700	H	3.46947700	-4.31858400	0.91221300
C	4.89458000	1.12271900	-1.19570800	H	3.71040400	-2.78259100	1.75390900
H	5.56087300	1.98823000	-1.14783800	C	5.39974700	-1.50081100	-0.19369500
C	4.93104500	0.40738300	0.16451100	H	5.24535000	-1.29577100	0.86909500
H	4.35620500	-0.52015400	0.12100300	H	6.07531300	-2.36154400	-0.27822300
H	4.51511700	1.03367700	0.95724300	H	5.87041800	-0.62300200	-0.63410100
C	5.36631700	0.20660400	-2.33074500	C	-5.23199400	1.96401600	-0.99231300
H	4.67418200	-0.63264400	-2.43512400	C	-4.13405900	1.30093800	-1.53868300
H	5.40301000	0.74992200	-3.27973700	C	-3.48463000	1.81461000	-2.67146500
C	3.24841400	3.10511200	-1.35528900	C	-3.94558800	3.00990300	-3.23232500
H	2.24466800	3.21223400	-1.77181200	C	-5.04548400	3.67496600	-2.68441900
C	3.18985100	3.50630400	0.12640700	C	-5.69272200	3.15276200	-1.56415800
H	2.52823800	2.82937400	0.67109000	H	-5.72587600	1.55501700	-0.11546600
H	2.81090300	4.52856500	0.23263700	H	-3.76090300	0.38898900	-1.08015500
H	4.18253700	3.46289000	0.58857200	H	-3.44135200	3.42315200	-4.10242600
C	4.20484200	3.98015800	-2.16898000	H	-5.39059100	4.60350200	-3.13034300
H	4.24900000	3.64723400	-3.21022200	H	-6.54493000	3.67155600	-1.13482900
H	3.85070500	5.01596700	-2.15332100	C	-2.29598200	1.07023000	-3.27216900
H	5.22221300	3.98005700	-1.76335700	H	-2.64603700	0.16511600	-3.78137500
H	6.36140600	-0.19548800	-2.11384700	H	-1.80707400	1.70122200	-4.02199600
H	5.96080200	0.14465900	0.42633200	C	-1.30968800	0.67470200	-2.20368100
C	-3.39352700	0.14486600	2.32995700	C	-1.18704100	-0.60711800	-1.75459300
O	-2.73988300	0.62502600	1.30758400	H	-1.75003200	-1.37470300	-2.27481500
O	-3.78910800	-1.01236400	2.47379700	C	0.50860400	1.53246600	-0.90001800
H	2.18632000	-0.72656400	1.36379100	N	-0.71028500	1.72967600	-1.53426000
C	-3.71282000	1.18808100	3.40177600	O	1.50544500	1.15622300	-1.59890500
H	-3.51836600	0.76456800	4.39041900	C	-0.09322200	3.17197600	0.84873800
H	-3.15043300	2.11361500	3.27139900	C	0.60803700	3.94807800	1.96029300
H	-4.78333300	1.41554000	3.35025800	C	-0.44779800	4.71718600	2.76606000
TS20-III				H	0.04094400	5.27469300	3.57136600
C	1.99379500	-2.71955100	-1.27192800	H	-0.99751000	5.42208300	2.13600600

H	-1.17252600	4.02920600	3.20988300	H	-2.05549400	-2.26048500	2.91710500
C	1.60214900	4.92899900	1.29572900	H	-2.05293400	-3.91074600	3.56553900
H	2.11503500	5.50482700	2.07306900	H	-3.57498700	-3.01337000	3.46295700
H	2.34865500	4.39298500	0.70597900	C	-3.61559300	-5.08259300	1.56154500
H	1.08453000	5.63528200	0.63723500	H	-3.83764300	-5.42334700	0.54566500
C	1.37009600	2.96155900	2.87113200	H	-3.00652600	-5.84757600	2.05257800
H	1.98754800	3.52817100	3.57684600	H	-4.55493900	-5.01343800	2.11965500
H	0.67566700	2.34393900	3.44440900	H	-6.54240100	-2.28236400	-0.77217800
H	2.00898800	2.29710600	2.28934700	H	-6.31836600	-1.03445300	1.46619000
O	-1.29180400	3.19058900	0.63104200	C	4.10040900	1.41750900	0.45156100
O	0.81223900	2.49589800	0.08864900	O	3.07457900	0.69103900	0.79633400
H	4.90566900	0.30353300	-2.57304900	O	4.62623100	1.47364800	-0.66180700
H	5.32607400	-1.13347000	-3.55026400	H	-1.33011900	2.42834500	-1.12110700
H	3.87933700	-0.18449100	-3.92705200	C	4.66463400	2.25521100	1.60073300
H	0.00960200	-3.33243100	-1.85123100	H	4.23569900	3.26130400	1.55814800
H	1.07601000	-4.63995200	-1.31651300	H	4.42161100	1.82341700	2.57382500
H	0.35431000	-3.52795100	-0.13627300	H	5.74644900	2.34660800	1.47990100
C	-0.73349900	-0.89618800	-0.41509100				
C	0.30526200	-0.25522000	0.25712200	21-III			
C	0.17373000	-0.17396400	1.73009500	C	-2.17880400	-1.41157800	-2.17084200
C	1.17181300	-0.59993800	2.62365800	C	-1.04717800	-1.78790900	-2.94708400
C	-1.02246500	0.33936500	2.27842900	C	-0.62241000	-3.10706400	-2.51879600
C	0.96398400	-0.56004300	4.00160500	C	-1.51137100	-3.52788300	-1.46376100
H	2.11582400	-0.94443700	2.22579700	C	-2.44177100	-2.46971400	-1.20817000
C	-1.22568700	0.39162400	3.65611300	Rh	-0.38625900	-1.73499600	-0.83587200
H	-1.79061400	0.70874200	1.60694300	C	0.49341400	-3.90848800	-3.11082600
C	-0.23451700	-0.07004900	4.52719300	C	-0.35602800	-0.96613800	-3.99198100
H	1.74771300	-0.90510400	4.67079800	H	-0.40095400	-1.45460900	-4.97160100
H	-2.15581200	0.79449600	4.04821800	H	-0.80688700	0.02466300	-4.07759600
H	-0.38838600	-0.03383900	5.60206200	H	0.69483900	-0.83205100	-3.71470000
N	-1.49420900	-1.84836800	0.31238900	C	-3.03456100	-0.20525000	-2.39126800
N	-2.74290700	-1.82026700	0.06762200	C	-3.56427700	-2.46867200	-0.21575900
N	-3.46647600	-2.76732300	0.65042800	H	-3.67562700	-1.47760400	0.23157400
C	-4.91756100	-2.48201000	0.64693400	H	-4.51797600	-2.74001000	-0.68690300
H	-5.38499600	-3.33550400	1.14202300	H	-3.37644400	-3.17886200	0.59269000
C	-5.23839600	-1.21363400	1.45300100	C	-1.43503800	-4.83964400	-0.74787100
H	-4.74716400	-0.34680300	1.00332200	H	-1.78293000	-4.74668300	0.28349300
H	-4.88946300	-1.30104200	2.48525900	H	-2.06280700	-5.58268000	-1.25526800
C	-5.45513500	-2.40682600	-0.78699800	H	-0.40554100	-5.19900300	-0.72562500
H	-5.02156500	-1.55842500	-1.32115100	C	2.84848900	5.97657200	-0.15201700
H	-5.21738500	-3.32169300	-1.33767500	C	1.91926000	5.17393300	-0.81198700
C	-2.84016800	-3.76291600	1.55151100	C	2.34299700	4.16271600	-1.68430900
H	-1.85951900	-3.94394400	1.10406300	C	3.71499300	3.96657300	-1.87884700
C	-2.61878500	-3.19463800	2.96014100	C	4.64813500	4.76537600	-1.21371000
				C	4.21701500	5.77308400	-0.35071000

H	2.50634100	6.75907000	0.51947500	H	1.48883800	1.42743500	2.40079800
H	0.85502000	5.32317700	-0.64633600	C	-0.39669700	-0.13042200	4.76326100
H	4.05725600	3.18081400	-2.54780100	H	-1.95889300	-1.55687200	4.33510500
H	5.70942000	4.59677600	-1.37057100	H	1.20744400	1.30852600	4.85239700
H	4.94135000	6.39633700	0.16560800	H	-0.52546500	-0.18322400	5.84091900
C	1.32342300	3.25581100	-2.34752200	N	-2.13137100	1.03806100	0.45358200
H	0.45767100	3.83197300	-2.68627800	N	-2.89858700	1.97687900	0.06598200
H	1.76716800	2.78377800	-3.23344300	N	-4.10118600	1.98590100	0.61393600
C	0.84646900	2.15600500	-1.42225900	C	-4.92625900	3.15409000	0.24603700
C	-0.49630200	1.91090900	-1.19684300	H	-5.84227000	3.05748800	0.83506900
H	-1.24409700	2.52875200	-1.67322100	C	-4.23571100	4.46894800	0.63180400
C	1.45352500	0.12782700	-0.24121100	H	-3.30384100	4.58338800	0.07211100
N	1.79062000	1.44702000	-0.78998600	H	-3.99916800	4.48630100	1.69941700
O	1.41304100	-0.80301400	-1.20169200	C	-5.29188300	3.10181600	-1.24176700
C	3.77875400	-0.19941000	0.44430100	H	-4.38671800	3.16246900	-1.85236600
C	4.60889800	-1.06993100	1.38945600	H	-5.80721900	2.16726400	-1.48259600
C	5.98259100	-0.40845800	1.59324900	C	-4.49255000	1.06266400	1.70602800
H	6.62785500	-1.06666700	2.18428900	H	-3.71654400	0.29708400	1.70722700
H	6.46389300	-0.21113400	0.63278500	C	-4.44366200	1.77765800	3.06173400
H	5.88754300	0.54331500	2.12748100	H	-3.44279400	2.17874500	3.24221200
C	4.77975200	-2.42213200	0.65241900	H	-4.67330600	1.06891800	3.86347000
H	5.34914200	-3.11188100	1.28560700	H	-5.17008500	2.59608800	3.11683800
H	3.81780700	-2.88242700	0.41196800	C	-5.84464500	0.40613000	1.41355400
H	5.32900300	-2.28012000	-0.28311200	H	-5.83478900	-0.09395200	0.44043200
C	3.90417300	-1.28182600	2.73960100	H	-6.05810600	-0.34445300	2.18087900
H	4.51763200	-1.93051500	3.37428800	H	-6.66941400	1.12655800	1.42224100
H	3.75629400	-0.33221600	3.26384200	H	-5.94602200	3.93874000	-1.50520700
H	2.92342200	-1.73873900	2.60961000	H	-4.88701600	5.31914400	0.40629300
O	4.25804900	0.40572000	-0.50333700	C	1.24849600	-3.62084800	0.81180200
O	2.47330200	-0.20510000	0.76117800	O	0.40669200	-2.63496900	0.85321600
H	1.11444100	-4.32173300	-2.31309700	O	1.73107900	-4.14905000	-0.19461500
H	0.09635600	-4.72417500	-3.72865500	H	2.78132400	1.57029200	-0.98610500
H	1.12675800	-3.28043000	-3.74119700	C	1.60440300	-4.15829100	2.19865500
H	-2.43729700	0.68232000	-2.60903300	H	2.68948900	-4.25893800	2.28068000
H	-3.69825100	-0.38270100	-3.24682000	H	1.22386400	-3.51658300	2.99490100
H	-3.65760300	0.01366700	-1.52476000	H	1.17402900	-5.16038700	2.30246100
C	-0.86407300	1.03444800	-0.14229100	11-free-cat			
C	0.08128100	0.17296300	0.47938900	N	1.68886200	-0.65841200	-1.12965700
C	-0.05399300	-0.00724000	1.96484900	O	2.15711600	-1.92638800	-0.72560000
C	-1.02690100	-0.84158000	2.53605000	C	2.24295000	0.38283700	-0.40842800
C	0.73814000	0.76914500	2.82366400	C	1.61829900	1.71857000	-0.66840700
C	-1.20104300	-0.89905500	3.91702500	C	0.34640500	2.03729600	-0.36520300
H	-1.63584800	-1.45592300	1.88535600	O	3.25496900	0.24282100	0.26677500
C	0.57557000	0.70196100	4.20902200	C	-0.42261200	0.31796400	1.24887500

C	-0.69808900	1.22339000	0.27254000	C	-5.87576500	2.49972400	-0.37838500
C	3.40055500	-2.26942700	-1.26828600	H	-5.96420100	2.03674000	0.60881800
O	3.93098900	-1.62358800	-2.12560900	H	-6.15028000	3.55522700	-0.28665200
C	3.91962700	-3.54348100	-0.60283600	H	-6.60517700	2.03039200	-1.04639300
C	5.39568200	-3.70624800	-1.00112600	H	-5.75742300	-1.91403500	-0.83771800
H	5.79195500	-4.63114800	-0.57058500	H	-4.55120400	-1.59533400	-3.06586600
H	5.99362800	-2.86716800	-0.63503800	H	0.01280600	3.04251500	-0.62271200
H	5.50779500	-3.74682500	-2.08713500	C	2.58451700	2.76240900	-1.22073600
C	3.79077100	-3.42343000	0.93174000	H	2.12206800	3.24391200	-2.08950200
H	4.30166700	-4.26782900	1.40534700	H	3.48649100	2.25704600	-1.58029700
H	2.74684400	-3.43746800	1.25459400	C	2.96707300	3.82182000	-0.19964800
H	4.24143000	-2.49346300	1.28946000	C	3.61413500	3.45755600	0.99058000
C	3.09617500	-4.74468800	-1.12298900	C	2.67349400	5.17049500	-0.42534400
H	3.48247000	-5.66689500	-0.67693800	C	3.96131300	4.42824400	1.92848400
H	3.17660500	-4.83428000	-2.21099900	H	3.82849700	2.40777300	1.16950800
H	2.03856500	-4.66302500	-0.85964000	C	3.02158400	6.14426700	0.51507100
C	-1.30095100	-0.53150300	2.05891000	H	2.17095500	5.46351300	-1.34436000
C	-2.67039400	-0.29045200	2.29815700	C	3.66717700	5.77538600	1.69487000
C	-0.71827000	-1.65115300	2.68655700	H	4.46282100	4.13362600	2.84644400
C	-3.41982700	-1.15385000	3.09222100	H	2.78692500	7.18790500	0.32372700
H	-3.14723300	0.57964100	1.86809000	H	3.93856100	6.52953500	2.42832600
C	-1.47175300	-2.52155800	3.47190800	H	0.63061700	0.21323700	1.49896300
H	0.33787300	-1.85114100	2.53139100	H	0.68366700	-0.73829800	-1.29781300
C	-2.83202400	-2.28234400	3.67445500	C	-1.00201200	-2.90789900	-0.44393000
H	-4.47265800	-0.94353400	3.25953900	O	-0.90455600	-1.99071500	-1.24422200
H	-0.99434000	-3.38635600	3.92351400	O	0.05262800	-3.42808900	0.20316100
H	-3.42486100	-2.95704900	4.28503500	C	-2.29394200	-3.56377800	-0.04408600
N	-1.98139000	1.63034500	-0.17146900	H	-2.15525200	-4.63804800	0.09456200
N	-2.72224600	0.67494500	-0.55346700	H	-2.60559700	-3.13930700	0.91627100
N	-3.95947900	0.99859400	-0.90036300	H	-3.05889500	-3.36380800	-0.79291200
C	-4.73076100	-0.11085700	-1.49957400	H	0.85130600	-2.92538700	-0.07101600
H	-5.60966200	0.35715600	-1.95217700	TS12-free-cat			
C	-3.93682400	-0.81254600	-2.60874400	N	1.97677000	0.64957700	-0.82026600
H	-3.02248500	-1.25852100	-2.21082300	O	3.19095100	-1.11179300	-0.33806200
H	-3.65549300	-0.09869700	-3.38938800	C	2.04761300	1.28689900	0.31875800
C	-5.19588700	-1.07937000	-0.40504900	C	0.95046200	2.10713300	-0.43371100
H	-4.33085600	-1.47489800	0.13155400	C	-0.39126100	1.87159800	-0.20277200
H	-5.83861600	-0.57018800	0.31967600	O	2.62168600	1.43466500	1.35981400
C	-4.44285600	2.39413400	-0.90854200	C	-0.49861600	-0.21503100	1.14120900
H	-3.77711300	2.91659800	-0.21789700	C	-1.09197600	0.76048400	0.38272300
C	-4.27108800	3.00876800	-2.30352700	C	4.47024000	-0.83308300	-0.40908000
H	-3.22538800	2.94468200	-2.61608700	O	4.91936700	0.30013300	-0.51367200
H	-4.56746700	4.06291300	-2.29778900	C	5.39907500	-2.08104400	-0.35839900
H	-4.88897100	2.48800600	-3.04362000	C	6.85721400	-1.61854500	-0.23951000

H	7.52983000	-2.48421800	-0.22603900	H	-3.97818200	-2.46301100	-3.44423200
H	7.00926300	-1.04344500	0.67816400	H	-1.06217600	2.65539700	-0.55626500
H	7.12772000	-0.97120200	-1.07685500	C	1.43637800	3.36936400	-1.12489600
C	5.02091100	-2.96172100	0.84832200	H	1.01258500	3.41920000	-2.13405300
H	5.68948700	-3.82861200	0.90634800	H	2.52219600	3.29931500	-1.24368100
H	3.99463600	-3.32965000	0.77123800	C	1.06533000	4.60935000	-0.33189400
H	5.11222600	-2.40188900	1.78532500	C	1.55005900	4.77722300	0.97437800
C	5.19978300	-2.87272400	-1.66831700	C	0.22370400	5.58518600	-0.87528300
H	5.85645200	-3.75056900	-1.68189700	C	1.20349300	5.90664700	1.71344600
H	5.44526900	-2.25437100	-2.53847000	H	2.18802800	4.01261100	1.41065800
H	4.16846000	-3.22017300	-1.77456100	C	-0.12325600	6.71835700	-0.13431800
C	-1.08966200	-1.36092700	1.81610000	H	-0.15739200	5.46220500	-1.88636000
C	-2.42560800	-1.42748100	2.26800100	C	0.36673100	6.88159400	1.16120900
C	-0.24452000	-2.46593700	2.05751800	H	1.58633100	6.02683700	2.72290000
C	-2.89561600	-2.56560700	2.91254800	H	-0.77478800	7.47018400	-0.57081800
H	-3.08146200	-0.57774900	2.12428400	H	0.09854700	7.76121300	1.73934200
C	-0.73083200	-3.61612200	2.67465200	H	0.57523700	-0.15677200	1.27241100
H	0.78833000	-2.42801300	1.72233600	H	1.31816300	-0.17071100	-1.02446100
C	-2.05849400	-3.67100000	3.10475400	C	0.62091000	-2.59099200	-1.22615100
H	-3.92244000	-2.59553200	3.26585700	O	0.37463200	-1.39725200	-1.45926700
H	-0.06965000	-4.46359500	2.82829800	O	1.74574000	-3.04307900	-0.74012900
H	-2.43760000	-4.56290800	3.59481600	C	-0.42028900	-3.66158900	-1.44493300
N	-2.48968800	0.80597200	0.10761900	H	0.04285100	-4.57191000	-1.83104600
N	-2.86676400	-0.25602100	-0.47967300	H	-0.86913800	-3.89836200	-0.47415500
N	-4.15466400	-0.39178300	-0.71902800	H	-1.19848200	-3.30463500	-2.11800800
C	-4.48215900	-1.59320500	-1.51834300	H	2.44381300	-2.25226300	-0.57665000
H	-5.55448500	-1.52500200	-1.72233400	13-free-cat			
C	-3.72703600	-1.57644300	-2.85371300	N	0.38926600	1.48394300	-1.10994100
H	-2.64859100	-1.56112200	-2.67503100	O	3.09558600	1.28014000	0.38609800
H	-3.98836800	-0.68793100	-3.43665700	C	1.26521800	2.07178100	-1.72164100
C	-4.21104200	-2.86414100	-0.70513500	C	-0.69701000	1.89860000	-0.30568500
H	-3.15481700	-2.91245000	-0.43149000	C	-1.25577000	1.04834000	0.56834500
H	-4.79854300	-2.87152000	0.21725400	O	2.14279400	2.50821100	-2.36877000
C	-5.16631800	0.62123900	-0.35561100	C	0.47469000	-0.59007100	1.20872600
H	-4.62926700	1.32338700	0.28548700	C	-0.80872000	-0.33682800	0.82848700
C	-5.65672300	1.37174000	-1.60000300	C	4.28270600	1.88640500	0.63819100
H	-4.81566400	1.83034600	-2.12738200	O	4.31383300	2.81636300	1.41116200
H	-6.35670400	2.16272100	-1.31244600	C	5.52158800	1.32766500	-0.08553900
H	-6.17639900	0.70203000	-2.29391000	C	6.75197800	2.11317300	0.39152500
C	-6.30667900	-0.01018000	0.45085000	H	7.65001300	1.73861900	-0.11119000
H	-5.91773400	-0.53460100	1.32872000	H	6.88683700	2.01367500	1.47176800
H	-6.99279900	0.77095400	0.79239600	H	6.64435600	3.17817900	0.17163000
H	-6.88828700	-0.72177800	-0.14461300	C	5.68986500	-0.17017700	0.25892700
H	-4.46594500	-3.75425400	-1.28887000	H	6.60668400	-0.54890100	-0.20555200

H	4.85839500	-0.77638600	-0.10758400	C	-2.48947700	3.65541500	0.10049200
H	5.77854400	-0.31507600	1.34148500	C	-2.53439500	4.31252100	1.33487700
C	5.34692200	1.50584500	-1.61108900	C	-3.69352100	3.25739800	-0.49720900
H	6.25279600	1.16041200	-2.12118100	C	-3.75653800	4.57105000	1.95969200
H	5.19274500	2.55880200	-1.86637700	H	-1.60612900	4.61758300	1.81104700
H	4.50367000	0.93414800	-2.00269900	C	-4.91575000	3.51327700	0.12373000
C	1.17260200	-1.85566800	1.43248500	H	-3.66770600	2.73512000	-1.45047200
C	0.59205700	-3.13825700	1.31961800	C	-4.94983600	4.17126300	1.35638100
C	2.55001200	-1.78475200	1.73677200	H	-3.77485200	5.08319200	2.91737900
C	1.35929800	-4.28621100	1.50639300	H	-5.83997500	3.19894100	-0.35261200
H	-0.45836800	-3.21086600	1.07627100	H	-5.90073000	4.37169100	1.84144200
C	3.31571900	-2.93418900	1.91130000	H	1.10353600	0.28819400	1.31561000
H	3.01859800	-0.80923100	1.81583800	H	0.52672200	-0.46205400	-1.53692500
C	2.72444200	-4.19530400	1.79846100	C	2.00971200	-1.61773200	-1.72884000
H	0.88891200	-5.26199100	1.41622000	O	0.70260900	-1.38541900	-1.82877700
H	4.37545800	-2.84404100	2.13281900	O	2.82766900	-0.74721200	-1.45464400
H	3.31782200	-5.09474000	1.93624900	C	2.37500200	-3.05685500	-1.95304500
N	-1.73453600	-1.37806800	0.66126300	H	3.39981900	-3.12065200	-2.31915200
N	-2.84228600	-0.96642600	0.18129300	H	2.31422800	-3.56497500	-0.98435800
N	-3.76766300	-1.89230200	-0.02723000	H	1.67965000	-3.54040800	-2.64112500
C	-4.93616700	-1.37627200	-0.77280100	H	3.13865800	0.56186500	-0.27897200
H	-5.61416800	-2.22356600	-0.89001300				
C	-5.65071600	-0.29030000	0.04095000				
H	-4.99200700	0.56833700	0.19325500				
H	-5.95042200	-0.67336400	1.02085500				
C	-4.53049900	-0.87146700	-2.16565900				
H	-3.82864500	-0.03840500	-2.06719000				
H	-4.04585100	-1.66078500	-2.74745200				
C	-3.45861600	-3.32933100	0.14243000				
H	-2.84225600	-3.36763200	1.04547900				
C	-4.71501000	-4.16654100	0.38826000				
H	-5.34068000	-3.72724500	1.17106000				
H	-4.41541700	-5.16718800	0.71409600				
H	-5.32012500	-4.28960800	-0.51584500				
C	-2.62213600	-3.85580000	-1.03496000				
H	-1.73367500	-3.23784300	-1.18592500				
H	-2.29846200	-4.88352100	-0.83778300				
H	-3.21303100	-3.85943700	-1.95720100				
H	-5.41047600	-0.52620400	-2.71793700				
H	-6.54707400	0.04846200	-0.48891700				
H	-2.15094600	1.38376000	1.07931700				
C	-1.17141400	3.32055700	-0.55655000				
H	-1.25055200	3.45942700	-1.64339200				
H	-0.38672100	4.01181400	-0.21837100				