

Electronic Supplementary Information

Mechanism and Origins of Ligand-Controlled Pd(II)-Catalyzed Regiodivergent Carbonylation of Alkynes

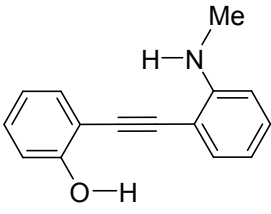
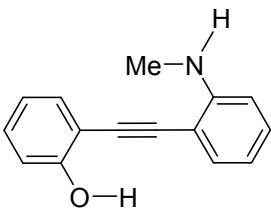
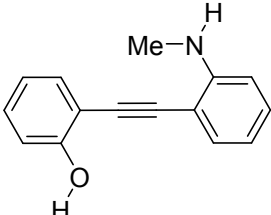
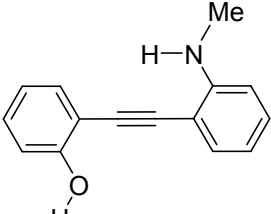
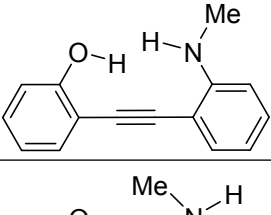
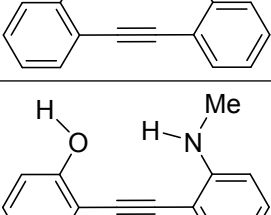
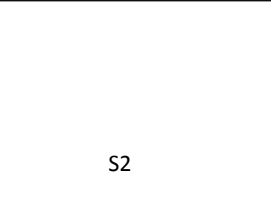
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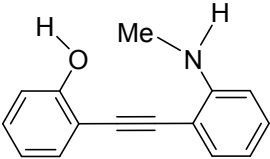
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1. Different isomers of complex 1

Table S1. Structures and relative energies of different isomers of **1**.

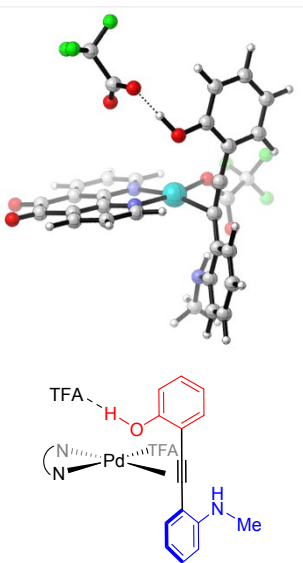
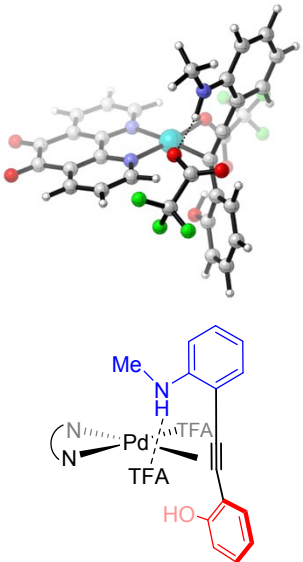
isomer	geometry	relative free energies (kcal/mol)
1		0.0
1-1		4.6
1-2		6.1
1-3		1.4
1-4		1.2
1-5		5.3
1-6		1.0

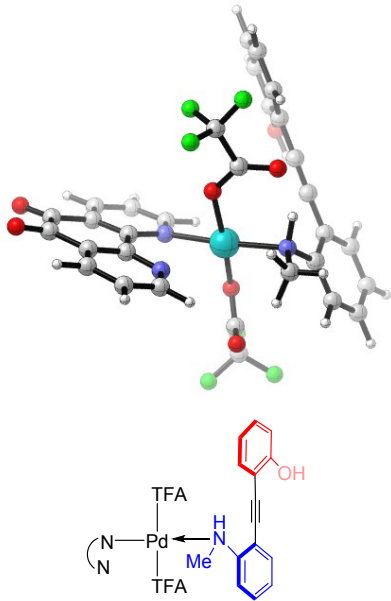
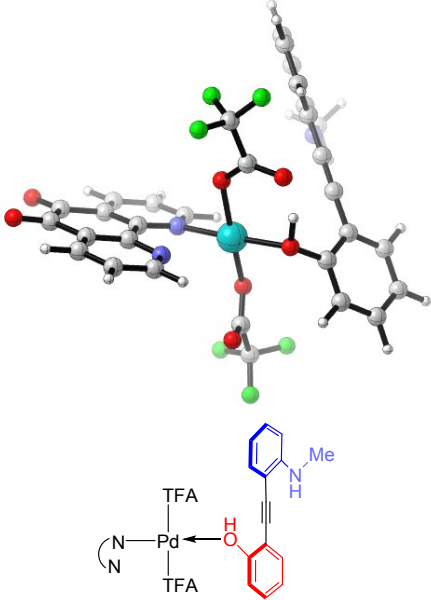
1-7		6.0
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2. Different isomers of complex 4

In complex **4**, the substrate may coordinate with the metal via O, N atom or C≡C bond, which will lead to different isomers. We have optimized all the possible isomers, and their geometries and relative free energies are listed below. Finally, the isomers with the lowest energies were used for further calculations.

Table S2. Geometries and relative energies of different isomers of **4**.

isomer	geometry	relative free energies (kcal/mol)
4		0.0
4'		2.4

4-N		5.5
4-O		16.4

3. Free energy profiles for the oxidation of Pd(0) to Pd(II) by BQ

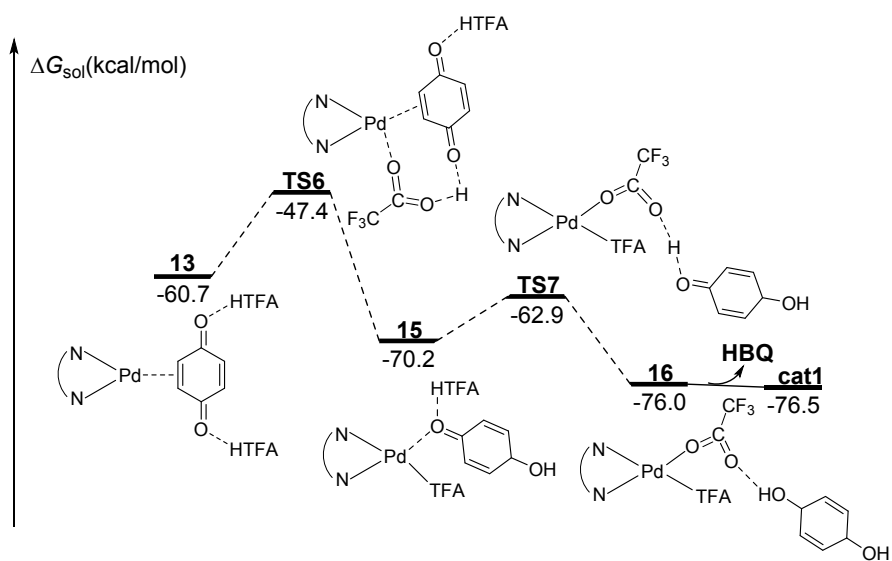


Fig. S1 Free energy profiles for the oxidation of Pd(0) to Pd(II) by BQ.

4. Calculated energies and imaginary frequencies

Table S3. Calculated energies and imaginary frequencies.

stationary point	thermal correction to Gibbs free energy at B3LYP/ ECP28MDF- AVDZ/6-31G(d,p) (in a.u.)	single-point energy including solvation energy at B3LYP-D3/ ECP28MDF-AVTZ/6- 311++G(2d,2p) (in a.u.)	imaginary frequencies
cat'	0.090882	-3541.182995	
L1	0.11841	-721.1160226	
cat1	0.153469	-1901.559228	
1	0.195799	-709.6513938	
4	0.372056	-2611.22198	
TS1	0.368942	-2611.210401	378.14 <i>i</i>
5	0.378256	-2611.244227	
6	0.351201	-2084.23648	
7	0.352449	-2197.594579	
TS2	0.351616	-2197.578137	247.64 <i>i</i>
8	0.352204	-2197.595633	
9	0.359288	-2197.622573	
TS3	0.35245	-2197.604032	740.75 <i>i</i>
10	0.357502	-2197.5984682	
11	0.328354	-1670.581028	
TS4	0.32915	-1670.572315	156.93 <i>i</i>
12	0.329824	-1670.610771	
13	0.246678	-2284.402923	
TS6	0.251959	-2284.387007	74.37 <i>i</i>
15	0.25084	-2284.422203	
TS7	0.251413	-2284.411109	102.24 <i>i</i>
16	0.250408	-2284.430998	
14	0.377663	-2611.24476	
TS5	0.373122	-2611.22523	1022.31 <i>i</i>
4'	0.376033	-2611.222072	
TS1'	0.374996	-2611.211918	134.67 <i>i</i>
5'	0.377837	-2611.261206	
6'	0.35124	-2084.253409	
7'	0.353782	-2197.614249	
TS2'	0.353036	-2197.605143	235.70 <i>i</i>
8'	0.353268	-2197.622125	
TS3'	0.358222	-2197.621356	23.93 <i>i</i>
10'	0.356454	-2197.629978	

11'	0.330374	-1670.606415	
TS4'	0.330326	-1670.57192	32.02 <i>i</i>
12'	0.327932	-1670.60692	
cat2	0.368662	-3700.201627	
4-L2	0.589598	-4409.880749	
TS1-L2	0.591143	-4409.857107	311.98 <i>i</i>
5-L2	0.590755	-4409.869384	
4'-L2	0.591893	-4409.871897	
TS1'-L2	0.594327	-4409.86694	149.70 <i>i</i>
5'-L2	0.597456	-4409.90413	

5. Cartesian coordinates of all optimized structures

cat'

Pd	0.03915500	1.63592600	0.99461300
C	-1.83331700	0.00982700	2.61506500
O	-1.44844700	1.15447000	2.27368400
O	-1.45204500	-1.12977200	2.25012500
C	1.70624000	-2.34462100	-1.42325200
O	1.33564400	-1.44756400	-2.21735400
O	1.36327100	-2.59159600	-0.24055200
C	2.75792000	-3.34767200	-1.98329400
F	3.79395900	-3.46106200	-1.13222600
F	2.19020200	-4.56426600	-2.11896200
F	3.22965000	-2.96796000	-3.17740600
C	-2.96866100	-0.02751100	3.68013600
F	-3.41786500	1.19754300	3.98068800
F	-4.00352500	-0.75974400	3.22710700
F	-2.50974500	-0.60112400	4.81081000
Pd	-0.00068200	0.05225700	-1.96672300
C	-1.98819200	-2.07529000	-1.34354700
O	-1.56525000	-2.42756900	-0.21461100
O	-1.57916700	-1.19746600	-2.14210900
C	1.83572700	-0.14886500	2.60858700
O	1.45390900	1.00840400	2.30504200
O	1.44997300	-1.27389700	2.20808200
C	2.97382900	-0.16772100	3.67119600
F	3.41968800	-1.40752200	3.90985700
F	4.01000500	0.58245200	3.25146400
F	2.52015100	0.35119200	4.82996500
C	-3.22537300	-2.89157300	-1.82380700
F	-4.17325800	-2.90643500	-0.86854300
F	-3.76066300	-2.38233000	-2.94075800
F	-2.85686500	-4.16518300	-2.07156400
Pd	-0.03888400	-1.68648000	0.90669100
C	1.98677200	2.14421400	-1.23313800
O	1.56444100	2.43581500	-0.08680200
O	1.57757400	1.30986200	-2.07691000
C	3.22326300	2.98539800	-1.67022300
F	4.17205000	2.94949800	-0.71644000
F	3.75761400	2.53675600	-2.81330900
F	2.85415100	4.27030900	-1.84922300
C	-1.70772600	2.41640000	-1.29571200
O	-1.36425900	2.59986500	-0.10164000

O	-1.33720400	1.56325700	-2.13683200
C	-2.76039500	3.44730800	-1.80055200
F	-2.19385100	4.67003800	-1.87000800
F	-3.23177800	3.13247300	-3.01353600
F	-3.79649100	3.51334200	-0.94462900

L1

C	0.74544500	-0.77779700	-0.00518700
C	1.46350600	0.43754500	0.00844400
C	2.86344200	0.39420600	0.00906800
C	3.49942200	-0.83825800	-0.00810800
C	2.70167200	-1.98647400	-0.02652200
C	-0.74543700	-0.77780300	0.00501600
C	-1.46350700	0.43753400	-0.00860700
C	-2.86344200	0.39418800	-0.00904500
C	-3.49941400	-0.83827800	0.00826000
C	-2.70165500	-1.98648900	0.02663500
H	3.42210300	1.32406000	0.02156100
H	4.58080600	-0.91957300	-0.00875200
H	3.16515100	-2.97068400	-0.04362300
H	-3.42211000	1.32403900	-0.02152700
H	-4.58079700	-0.91959900	0.00903400
H	-3.16512600	-2.97070100	0.04385600
N	-1.36445700	-1.96799700	0.02430600
N	1.36447300	-1.96799000	-0.02433500
C	-0.77311600	1.74497300	-0.02117300
C	0.77310700	1.74498200	0.02080800
O	-1.36328900	2.81214900	-0.05812800
O	1.36325500	2.81215000	0.05839400

cat1

Pd	0.34172700	0.00009200	0.00012100
O	1.75264800	1.40852700	-0.32948400
C	2.30359600	1.96156800	0.69907200
O	2.11873200	1.75892000	1.89093200
C	3.29976900	3.06146600	0.25169800
O	2.11810300	-1.75906200	-1.89103600
C	2.30321400	-1.96166300	-0.69920800
O	1.75268900	-1.40835000	0.32942800
C	3.29895900	-3.06199000	-0.25193100
C	-2.41689900	0.71667800	-0.14221800
C	-3.59930900	1.44578400	-0.29756300
C	-3.51060700	2.81423000	-0.57911500
C	-2.25489900	3.39933800	-0.69464000

C	-1.11597200	2.61188300	-0.52383000	C	4.51433200	-1.08594900	-0.01125300
C	-2.41693700	-0.71639500	0.14246400	H	4.78522800	1.04002000	0.09109100
C	-3.59939000	-1.44545400	0.29764000	H	3.97028800	-3.17939300	-0.12221000
C	-3.51078500	-2.81389800	0.57928100	H	5.58394800	-1.27765800	-0.00607700
C	-2.25511900	-3.39903800	0.69503400	O	-2.60822300	-2.23222900	0.12221600
C	-1.11614100	-2.61162700	0.52431800	H	-1.63524200	-2.19745300	0.10871300
H	-4.41848200	3.39430500	-0.70437700	N	2.21960300	1.81209400	0.13393800
H	-2.14190900	4.45445600	-0.91484800	H	1.23994800	1.94841200	-0.07305700
H	-0.11685800	3.02252600	-0.60756800	C	3.07164700	2.98114300	0.03060700
H	-4.41870300	-3.39392900	0.70442500	H	3.62837100	3.02040400	-0.91683100
H	-2.14218000	-4.45414500	0.91532000	H	2.44353600	3.87115400	0.09801400
H	-0.11705400	-3.02233000	0.60817900	H	3.79706800	3.01661000	0.85148500
N	-1.19965400	-1.29923200	0.25150600				
N	-1.19959000	1.29946500	-0.25109900	4			
C	-4.91055300	-0.76129100	0.15916900	C	-1.07753700	-2.23721900	0.09034400
C	-4.91050900	0.76164500	-0.15936900	C	-1.94937700	-3.16703100	0.66655200
O	-5.97201500	-1.34069800	0.28198000	C	-0.92477900	-2.12282200	-1.36006500
O	-5.97194000	1.34099800	-0.28271400	N	-0.35409400	-1.37465500	0.84793000
F	3.96533800	-3.58487500	-1.29150000	C	-2.08810800	-3.19044300	2.05901100
F	4.20732800	-2.58573900	0.62424200	C	-2.71394900	-4.10447300	-0.19608700
F	2.63235600	-4.06965200	0.35979400	C	-1.61044200	-2.95402200	-2.25203600
F	2.63338300	4.06954700	-0.35962200	N	-0.09578500	-1.14906800	-1.79564500
F	4.20759400	2.58496300	-0.62486900	C	-0.50585500	-1.38871100	2.18255300
F	3.96669100	3.58388700	1.29115400	Pd	0.85674800	-0.13987100	-0.24856500
1				C	-1.36355600	-2.28414700	2.82111300
C	-0.82876200	-0.04903900	-0.03843300	H	-2.76184800	-3.90635400	2.51720400
C	0.36338800	-0.31428100	-0.03785800	C	-2.52003300	-4.00676800	-1.73351000
C	-2.23664900	0.15967800	-0.02941800	O	-3.47643300	-4.93755600	0.25400300
C	-3.09469000	-0.96679800	0.05177600	C	-1.42373100	-2.76171600	-3.62602500
C	-2.80974400	1.44602900	-0.09649000	C	0.07865900	-0.96020000	-3.11290300
C	-4.48099300	-0.79269000	0.06222100	H	0.06980000	-0.66687900	2.74421700
C	-4.19042800	1.61202900	-0.08471800	C	2.04550700	0.47055500	1.47534900
H	-2.15084300	2.30643000	-0.15847900	H	-1.44839200	-2.25622600	3.90111900
C	-5.02323200	0.48923600	-0.00578900	O	-3.11462700	-4.78095000	-2.45801800
H	-5.11684700	-1.67014000	0.12491500	C	-0.57297200	-1.75139700	-4.05904200
H	-4.61683800	2.60865300	-0.13737500	H	-1.94729000	-3.39911400	-4.33048500
H	-6.10224800	0.61183500	0.00328900	H	0.74906800	-0.15851800	-3.39956100
C	1.76302600	-0.56649900	-0.03194700	C	1.40895300	1.53383100	1.28745900
C	2.68561100	0.52736400	0.04255000	C	2.80969500	-0.38340300	2.36226300
C	2.24925400	-1.88645200	-0.08959800	H	-0.40653800	-1.56574900	-5.11374700
C	4.06555500	0.23046000	0.04418900	C	0.77489000	2.77791500	1.08737200
C	3.61368100	-2.15542800	-0.07822600	C	3.54856200	-1.52765200	1.92869400
H	1.53022000	-2.69852500	-0.14445900	C	2.77953600	-0.05183000	3.73445600
				C	-0.60909000	2.91649800	1.41629100

C	1.48553200	3.87477100	0.53784900	C	5.29978400	-3.07749200	-0.75044400
C	4.20262100	-2.29827400	2.91781800	C	5.47784200	-0.67478600	0.22001200
N	3.59566100	-1.88346000	0.59997000	N	3.49446000	0.67740900	0.14140100
C	3.44095200	-0.81873400	4.68494400	C	1.23826000	-2.20478700	-1.53165300
H	2.21261300	0.82326800	4.03809500	Pd	1.43155400	0.61758900	-0.35671600
C	-1.23939900	4.15203500	1.16234600	C	1.73211200	-3.45417000	-1.90463500
C	0.85002200	5.08450300	0.31731600	H	3.48703300	-4.72036500	-1.91820100
H	2.53335400	3.74322100	0.28854200	C	6.14215000	-1.96922100	-0.06478700
C	4.14676400	-1.95155900	4.26263800	O	5.82745200	-4.13865800	-1.02505000
H	4.77014800	-3.17167800	2.61948900	C	6.18116000	0.38814400	0.79963100
C	4.45051000	-2.96079700	0.12439100	C	4.17277400	1.69496700	0.69247900
H	3.40120800	-0.54448600	5.73423000	H	0.20642500	-1.93179100	-1.70743100
C	-0.51688500	5.21003900	0.62627600	C	-1.45874000	-0.39593200	-0.27373700
H	-2.29384700	4.25760500	1.39544500	H	1.06829000	-4.16607600	-2.38136500
H	1.39769600	5.92434200	-0.09754500	O	7.30690200	-2.19153900	0.20746300
H	4.66834600	-2.56949700	4.98871300	C	5.52044100	1.58754400	1.03788600
H	4.14670400	-3.92222600	0.55148600	H	7.22877200	0.25978800	1.05025900
H	4.34269800	-3.02626900	-0.96047900	H	3.61046200	2.60863300	0.85317200
H	5.51387600	-2.80343600	0.35770700	C	-0.51239300	0.43975800	-0.80309000
H	-1.02241800	6.15492400	0.44533400	C	-1.47733200	-1.49693400	0.70018500
O	1.80515700	1.07761700	-1.56104000	H	6.02986600	2.43448200	1.48283600
C	3.05423700	0.98605500	-1.85205700	C	-1.19480300	1.21922100	-1.82375300
C	3.44365500	2.03859200	-2.92120700	C	-0.83542700	-1.42044600	1.97678500
O	3.90861900	0.21641300	-1.42665700	C	-2.17137600	-2.67195500	0.35690100
F	4.73434800	1.94313500	-3.26572300	C	-2.53156100	0.78496900	-1.85282100
F	3.22517800	3.28980400	-2.46566300	C	-0.80175900	2.22278200	-2.72667600
F	2.70027400	1.87350800	-4.03750500	C	-0.90004800	-2.55389800	2.82028100
H	3.50342000	-1.11608800	-0.06317200	N	-0.16823800	-0.28527200	2.37608100
O	-1.24266100	1.87696800	1.94525900	C	-2.23533000	-3.77370600	1.20713500
H	-2.27924200	1.96419000	1.85652700	H	-2.66078000	-2.71557600	-0.61173500
C	-4.14509400	1.62052100	0.57445800	C	-3.50008800	1.28638800	-2.71282200
O	-3.72955100	2.09043200	1.68027000	C	-1.75326700	2.74584600	-3.60197600
O	-3.55858700	0.96383700	-0.29215000	H	0.22308700	2.58111400	-2.73933200
C	-5.63339600	1.98485900	0.30726200	C	-1.58443900	-3.70536900	2.44162400
F	-6.14078500	1.35466500	-0.77074700	H	-0.42105900	-2.51987000	3.79212400
F	-5.76663400	3.31733600	0.08889800	C	0.28702300	-0.09222400	3.74145200
F	-6.42692500	1.67659100	1.35949700	H	-2.77592400	-4.66655700	0.90877800
5				C	-3.08394300	2.28690600	-3.59525400
C	3.31244800	-1.55349800	-0.70278700	H	-4.51869100	0.91324500	-2.69658200
C	3.87069900	-2.79343400	-1.04070100	H	-1.46435900	3.52302300	-4.30404500
C	4.12404500	-0.49185200	-0.09297100	H	-1.61433400	-4.55084400	3.12414700
N	2.00384000	-1.27245500	-0.93565200	H	1.08179200	-0.79990600	4.00548900
C	3.06247300	-3.75845600	-1.65180200	H	0.69558700	0.91724700	3.82050300
				H	-0.51935600	-0.19733300	4.48288600

H	-3.80167000	2.71411700	-4.28953000	C	1.37266100	2.77208800	1.06501300
O	1.20572200	2.59471400	0.06145400	H	-2.94848000	-4.67389800	0.85811200
C	0.43700500	3.11166400	0.94706500	C	2.57009600	0.55290500	-1.66176300
C	0.63086700	4.64921000	1.00223900	C	0.84852000	2.25383600	2.29080700
O	-0.35485000	2.58525000	1.72382100	C	1.36498200	4.16359500	0.86014900
F	-0.23198000	5.23772300	1.84354000	C	3.45759700	1.64544300	-1.59309100
F	0.47083000	5.21271700	-0.21379000	C	2.78221800	-0.42093500	-2.65485000
F	1.88360000	4.94539300	1.42413200	C	0.30941800	3.16897200	3.22434200
H	-0.36619200	0.57727300	1.87575800	N	0.86520300	0.90296000	2.56223000
O	-2.71545800	-0.20009000	-0.91508700	C	0.83927700	5.05226500	1.79594400
H	-4.23543900	-0.48460900	-0.07399100	H	1.78026400	4.54589600	-0.06734700
C	-6.10566200	-0.80107200	-0.29272900	C	4.54307600	1.81635800	-2.44614400
O	-5.03760700	-0.67934500	0.47592300	O	3.09196500	2.48253800	-0.58458700
O	-6.17452700	-0.66079700	-1.49199800	C	3.86261800	-0.26869200	-3.52316600
C	-7.33336200	-1.18137500	0.56326100	H	2.11608000	-1.27439600	-2.74154900
F	-8.43407000	-1.24083500	-0.19350100	C	0.30176400	4.53954800	2.97910800
F	-7.53477000	-0.27956300	1.54101500	H	-0.09304500	2.79665600	4.15954800
F	-7.14625700	-2.38431400	1.13909200	C	0.58924800	0.37994600	3.88872100
6				H	0.84417500	6.12040300	1.60124000
C	-2.71481300	0.38458100	-0.69888100	C	4.73335100	0.83376700	-3.42054400
C	-3.83798100	1.16633300	-1.00024200	H	5.20397800	2.67303200	-2.35719800
C	-2.85163300	-1.01375100	-0.27004400	H	4.03883400	-1.01327900	-4.29463800
N	-1.45329500	0.87829800	-0.80199800	H	-0.11814800	5.20864300	3.72588400
C	-3.65327800	2.48716100	-1.42350500	H	-0.45704000	0.53806500	4.17573100
C	-5.20482700	0.59999700	-0.87098600	H	0.77489400	-0.69587300	3.87195000
C	-4.10244100	-1.62856200	-0.12153700	H	1.22366700	0.82831800	4.66843900
N	-1.70287200	-1.67831700	-0.03203500	H	5.56685600	0.92374100	-4.11125300
C	-1.28769000	2.14649300	-1.21992600	O	1.24702600	-2.07014000	0.00185200
Pd	0.02527700	-0.47161300	-0.31526500	C	2.15216000	-2.18451800	0.90186200
C	-2.36052200	2.97869400	-1.53661600	C	2.76974900	-3.60683000	0.86925000
H	-4.51793500	3.09865200	-1.65785200	O	2.54844100	-1.38538800	1.74540400
C	-5.34544400	-0.87334100	-0.40663100	F	3.77628100	-3.74252800	1.74516200
O	-6.20847300	1.24315800	-1.11431800	F	3.24633800	-3.91167100	-0.35676600
C	-4.14735400	-2.96552700	0.29147000	F	1.82921200	-4.53184000	1.17841900
C	-1.75008900	-2.95947400	0.36252000	H	1.49568000	0.32609100	2.01163600
H	-0.26524600	2.49005400	-1.29805400	7			
C	1.94300800	1.92347300	0.00656500	C	-3.06555400	-0.62865700	-0.62876100
H	-2.16621000	3.99325100	-1.86481200	C	-4.24795700	-1.34631800	-0.90481500
O	-6.45619200	-1.35747000	-0.29479300	C	-4.16717900	-2.62796200	-1.45753300
C	-2.95648100	-3.63845600	0.53783200	C	-2.91975600	-3.17100100	-1.72528100
H	-5.10853300	-3.45424600	0.40986600	C	-1.79596900	-2.40491100	-1.43295900
H	-0.79192100	-3.43817700	0.53443800	C	-3.13710000	0.73335500	-0.03357600
C	1.58072900	0.75353900	-0.61717900	C	-4.38363400	1.33574500	0.24117300

C	-4.40103000	2.62428900	0.78934400	O	0.43662600	-1.85594700	0.71206700
C	-3.19918600	3.26941800	1.04286100	C	1.06112400	-1.81226100	1.83145300
C	-2.01457600	2.59252700	0.74193000	C	1.08183600	-3.21188600	2.50041000
H	-5.08218000	-3.17187900	-1.66604300	O	1.60864800	-0.87563200	2.40383500
H	-2.80445000	-4.16039400	-2.15262900	F	1.77637600	-4.08941200	1.74099500
H	-0.80141700	-2.78961300	-1.62966500	F	-0.16885800	-3.70309900	2.64398400
H	-5.35532700	3.09435900	1.00245000	F	1.65123200	-3.18218900	3.71440000
H	-3.16880600	4.26875000	1.46277600	H	1.61441000	1.04653600	1.70757900
H	-1.04997100	3.05718700	0.92375700	C	0.05034600	0.93720200	-2.00680100
N	-1.98329300	1.36021600	0.22251900	O	-0.07204900	1.72550000	-2.82710500
N	-1.85844600	-1.16891700	-0.90151800				
C	-5.66177500	0.64663000	-0.03372100	8			
C	-5.58906900	-0.77316300	-0.63044000	C	-3.01826000	-1.01641000	-0.10207300
O	-6.75232900	1.14414100	0.18784600	C	-4.25658000	-1.65147300	0.11453000
O	-6.62144000	-1.37704600	-0.86196200	C	-4.27899600	-3.01660100	0.42010900
Pd	0.20681500	-0.34739300	-0.66217500	C	-3.07962900	-3.71003000	0.50457600
C	2.88182800	1.21199500	-0.51508800	C	-1.89455600	-3.01113700	0.28042600
C	2.18043800	0.04989000	-0.69720100	C	-2.95468500	0.43255800	-0.42973600
C	3.15668800	-0.95745600	-1.06729500	C	-4.12947900	1.20667400	-0.50900100
C	4.40495200	-0.30426700	-1.06809300	C	-4.01739000	2.57051100	-0.80643000
C	3.11146500	-2.32304300	-1.39906600	C	-2.75816400	3.11689200	-1.01165100
C	5.60693400	-0.93480400	-1.37141100	C	-1.64831500	2.27399600	-0.91499600
C	4.30438400	-2.97381600	-1.71013900	H	-5.23273500	-3.50629700	0.58601700
H	2.16711900	-2.85845600	-1.41092700	H	-3.04836800	-4.76800900	0.73912000
C	5.53631100	-2.29116400	-1.69495800	H	-0.93403100	-3.51138700	0.33743600
H	6.54854900	-0.39490400	-1.35683700	H	-4.91693100	3.17357200	-0.86974700
H	4.28662200	-4.02910000	-1.96791000	H	-2.62643200	4.16814100	-1.24289700
H	6.44846200	-2.82816400	-1.93854500	H	-0.64461300	2.65966300	-1.06664500
C	2.54147300	2.60656700	-0.19080900	N	-1.74405300	0.96913200	-0.63298200
C	1.80919000	2.96398800	0.98285300	N	-1.86267700	-1.70043000	-0.01387300
C	3.02943000	3.61991900	-1.03197700	C	-5.46499200	0.61024700	-0.28575200
C	1.59854300	4.34042900	1.23691600	C	-5.53262400	-0.90118600	0.03210500
C	2.80540400	4.97054500	-0.77121000	O	-6.49965000	1.25189300	-0.34017100
H	3.59922600	3.32749500	-1.90970800	O	-6.61887300	-1.42425300	0.20680400
C	2.08268600	5.31913800	0.37332500	Pd	0.13048900	-0.68846500	-0.28192000
H	1.05674300	4.63919700	2.12721100	C	2.58137400	0.11482000	-1.27411200
H	3.18905800	5.73177100	-1.44331600	C	1.98853600	-1.12360300	-1.54336900
H	1.89816900	6.36509300	0.60509100	C	2.92680900	-2.14001400	-1.08341000
O	4.25133800	1.00751400	-0.73090800	C	4.01181900	-1.42558300	-0.55760000
N	1.32252100	2.00940900	1.84361500	C	2.95028900	-3.54036900	-1.06134500
C	0.87276700	2.32556500	3.18713100	C	5.13251900	-2.02416000	0.00097100
H	-0.05171300	2.91575000	3.18394100	C	4.06782300	-4.16552200	-0.50912200
H	0.66827000	1.38513500	3.70222900	H	2.12398000	-4.12021100	-1.46139400
H	1.62505300	2.88145100	3.76610500	C	5.14119100	-3.42067200	0.01429300

H	5.95364800	-1.43678600	0.39786300	H	-6.36197800	2.19678000	0.58954800
H	4.11243600	-5.25014700	-0.48222000	H	-4.47410000	3.83104500	0.97931800
H	5.99616900	-3.94050200	0.43556900	H	-2.14455000	2.98708700	0.87386400
C	2.23723800	1.48095600	-1.67371100	N	-2.66305200	1.03196300	0.46067700
C	2.39622200	2.59133200	-0.78372300	N	-1.95915200	-1.50339900	-0.18974700
C	1.76354600	1.69233200	-2.98083800	C	-6.10222000	-0.42311900	0.03124900
C	2.08152100	3.87751200	-1.28348000	C	-5.70241100	-1.88464300	-0.27381100
C	1.45306500	2.96619500	-3.44674600	O	-7.28176400	-0.12365900	0.07105300
H	1.67034500	0.83747200	-3.64444000	O	-6.57337000	-2.71613500	-0.45251500
C	1.62503500	4.05590700	-2.58533200	Pd	-0.61338900	0.09175300	0.26965500
H	2.19779700	4.73991600	-0.63744500	C	2.05820800	1.00430600	-1.65323900
H	1.10338100	3.10786800	-4.46416300	C	1.95613800	-0.29429200	-1.17433200
H	1.39941800	5.06170400	-2.92983300	C	2.93696300	-1.07900600	-1.91076900
O	3.80134200	-0.07081000	-0.68330900	C	3.55332900	-0.18098400	-2.79143700
N	2.83050000	2.41856600	0.50384500	C	3.34119000	-2.42388500	-1.92680200
C	2.78108600	3.47327500	1.50243000	C	4.55323800	-0.52620100	-3.69157700
H	1.77593400	3.90359600	1.61622300	C	4.34321300	-2.79827000	-2.82055900
H	3.08022600	3.04435600	2.46040200	H	2.88689900	-3.14473700	-1.25784100
H	3.47435100	4.28774300	1.26277800	C	4.94198200	-1.86646300	-3.69021000
O	0.05588900	-0.01921600	1.82653700	H	5.00049000	0.20712800	-4.35431200
C	1.12554400	0.21931500	2.46505800	H	4.67213100	-3.83307400	-2.84714200
C	0.85184200	0.93883200	3.81320700	H	5.72023600	-2.19484800	-4.37249600
O	2.30402900	-0.01167400	2.16067300	C	1.41946000	2.29391300	-1.38696400
F	0.03952700	0.20821400	4.60968200	C	0.78129800	2.62500500	-0.16180400
F	0.23891600	2.12898900	3.59722100	C	1.47403100	3.27228500	-2.40056100
F	1.97738900	1.19149500	4.50646600	C	0.24103800	3.90584000	0.00457300
H	2.82791500	1.47597100	0.87998900	C	0.91597500	4.53440700	-2.22948400
C	0.58654200	-1.33257000	-1.98761200	H	1.96147100	3.02562100	-3.33623700
O	0.05803000	-1.81076200	-2.95472900	C	0.29946100	4.85117700	-1.01939900
9				H	-0.22242100	4.17680800	0.94471600
C	-3.28179400	-1.22203300	-0.11326800	H	0.96808000	5.26296100	-3.03240100
C	-4.25619900	-2.20746500	-0.34403200	H	-0.13194900	5.83508900	-0.86096200
C	-3.85144300	-3.50961500	-0.65562200	O	3.02761600	1.07336000	-2.62495200
C	-2.49527600	-3.78862000	-0.72577100	N	0.70909800	1.64856600	0.89091300
C	-1.58479400	-2.76154700	-0.48519500	C	0.36910300	2.14768500	2.25027400
C	-3.66477700	0.16173900	0.22082500	H	-0.68164000	2.42147400	2.33248000
C	-5.01396900	0.55336800	0.26765100	H	0.60114600	1.33834400	2.94381400
C	-5.32280200	1.88832000	0.55062700	H	0.98790800	3.01641000	2.50152700
C	-4.28654400	2.78463200	0.76750800	C	1.03267600	-0.88717800	-0.19117600
C	-2.97517800	2.31234600	0.71399500	O	1.24159700	-2.01338400	0.24474700
H	-4.60186500	-4.27192700	-0.83452700	H	1.64838200	1.20102500	1.03880300
H	-2.12987800	-4.78163500	-0.96108700	O	3.11291000	0.60865200	1.72927700
H	-0.51912800	-2.94440800	-0.50955100	C	3.02544900	-0.13819900	2.74259900
				C	4.35235900	-0.90188300	3.03719000

O	2.07542700	-0.36840400	3.50919300	C	-0.51741400	3.83303000	-0.68027900
F	5.42292100	-0.07082900	3.05981300	C	-1.20500700	4.81277900	1.42160600
F	4.59782800	-1.82962700	2.07506300	H	-2.06378800	3.44636000	2.82763600
F	4.34178800	-1.55763900	4.21713800	C	-0.66604400	4.94757700	0.13876100
10				H	-0.11246400	3.97095200	-1.67740800
C	3.33060700	-1.17216600	0.12482800	H	-1.31600100	5.67615900	2.06873700
C	4.35235700	-2.11285500	0.34490000	H	-0.36019500	5.92252500	-0.22803800
C	4.00494600	-3.44845100	0.57596100	O	-2.95864300	1.35615700	2.56162100
C	2.66473100	-3.80177200	0.57196000	N	-0.74443800	1.40872000	-1.07518100
C	1.70325000	-2.81063100	0.36976700	C	-0.32256600	1.66493000	-2.46188700
C	3.64642700	0.23771400	-0.16858800	H	0.70194400	2.06012600	-2.55251200
C	4.97193300	0.70898500	-0.12730500	H	-0.38066900	0.72387000	-3.01177400
C	5.20971700	2.06640300	-0.36320600	H	-0.99650100	2.38344000	-2.94845700
C	4.13161300	2.90137600	-0.62507800	C	-1.01738900	-0.92729000	0.38951800
C	2.85119400	2.34649900	-0.67438100	O	-1.16566300	-2.12904400	0.19460000
H	4.79887900	-4.17100000	0.74285600	H	-2.17522200	0.67267400	-1.44092000
H	2.34787600	-4.82828100	0.72639400	O	-3.09197700	0.29575100	-1.73586200
H	0.63680600	-3.02024000	0.34669700	C	-2.97249300	-0.65917000	-2.63051800
H	6.23317000	2.43058100	-0.32795900	C	-4.36112900	-1.25052800	-2.97474000
H	4.26657300	3.96567500	-0.79982100	O	-1.95839200	-1.07442800	-3.15953700
H	1.98122000	2.96464400	-0.87123700	F	-5.19126600	-0.28494500	-3.42524400
N	2.60917800	1.04437800	-0.47040900	F	-4.92367800	-1.81139000	-1.88414400
N	2.02494600	-1.51904900	0.16987900	F	-4.25775800	-2.18878100	-3.92348100
C	6.11014000	-0.20803400	0.14579100	11			
C	5.78258000	-1.70952800	0.35540200	C	2.64175200	1.09491800	0.00913300
O	7.26043900	0.17513800	0.19762500	C	3.59878800	2.07477000	-0.30091400
O	6.68650900	-2.50097600	0.53224200	C	3.26459900	3.42454000	-0.14457600
Pd	0.58274400	0.01162200	-0.26931500	C	1.99672200	3.75337900	0.31514500
C	-2.04471200	1.16421400	1.54888200	C	1.09685100	2.72641700	0.59670400
C	-1.94072600	-0.19586100	1.26102400	C	2.94884100	-0.34211200	-0.12150100
C	-2.85881700	-0.87569700	2.16287500	C	4.19171100	-0.78401900	-0.60380200
C	-3.44549500	0.13118300	2.93587700	C	4.41846000	-2.16054300	-0.72022300
C	-3.23477400	-2.20822700	2.39195400	C	3.40898800	-3.04307700	-0.35923100
C	-4.38640900	-0.09309500	3.93306700	C	2.20441100	-2.52229600	0.11569900
C	-4.17840400	-2.46135600	3.38707500	H	3.99890800	4.18645200	-0.38294600
H	-2.80319500	-3.00594300	1.80092500	H	1.69436000	4.78474600	0.45658800
C	-4.74861400	-1.42415000	4.14615500	H	0.10116600	2.93627100	0.96873500
H	-4.81324500	0.72381100	4.50442900	H	5.37532800	-2.51234600	-1.09090400
H	-4.48747900	-3.48549200	3.57586200	H	3.54020500	-4.11635000	-0.43742400
H	-5.48387900	-1.66065800	4.90837600	H	1.38793800	-3.17465300	0.40551100
C	-1.48929400	2.40941700	1.03682000	N	1.97907300	-1.20573700	0.24033700
C	-0.89224800	2.53410900	-0.26001000	N	1.40328000	1.42570400	0.44223000
C	-1.61657800	3.55778200	1.84793100				

C	5.24936900	0.18405200	-0.97524300	C	3.79961400	-2.29994500	-1.80166000
C	4.94336600	1.69129300	-0.79582200	C	2.53758900	-2.73513100	-2.18389500
O	6.33779700	-0.15391700	-1.40408300	C	1.42029900	-2.07804400	-1.66795900
O	5.80451500	2.50793000	-1.06784000	H	4.94476900	2.48851700	2.23796200
Pd	0.09161700	-0.18946400	0.86588000	H	2.73262200	3.48219900	2.93973700
C	-2.96222200	-0.47569900	-0.48843400	H	0.64292400	2.50017500	2.00127000
C	-2.66814100	0.60996800	0.33924600	H	4.70202900	-2.77441500	-2.17201800
C	-3.59983200	1.66874300	-0.02371500	H	2.40712000	-3.56674900	-2.86712100
C	-4.37648000	1.14954600	-1.06897400	H	0.41749300	-2.39065600	-1.93814900
C	-3.83453700	2.98522400	0.40230800	N	1.50711700	-1.03967600	-0.81948500
C	-5.37830800	1.85639800	-1.72072800	N	1.60587800	1.06329100	0.87419000
C	-4.83733200	3.71757100	-0.23510600	C	5.23858000	-0.74449000	-0.47994500
H	-3.25280600	3.41410900	1.21036600	C	5.29369900	0.42681800	0.53220600
C	-5.59940300	3.16431300	-1.28023700	O	6.28070800	-1.23105700	-0.88109400
H	-5.95387200	1.41307400	-2.52680200	O	6.37735100	0.81949900	0.92619600
H	-5.03634600	4.73715100	0.08286500	Pd	-0.21677800	0.11436400	-0.04014000
H	-6.37336100	3.76105800	-1.75378700	C	-2.14888400	-0.37751800	-0.61580200
C	-2.54267900	-1.85501800	-0.58286900	C	-2.20623400	0.81886800	0.18841500
C	-1.72167900	-2.48424500	0.42703300	C	-2.51391800	1.90449600	-0.75486200
C	-3.06543000	-2.64194300	-1.63836700	C	-2.63275900	1.29672700	-2.02285600
C	-1.59729000	-3.90640700	0.35680500	C	-2.71453200	3.28223300	-0.63796700
C	-2.86885400	-4.01105600	-1.70606300	C	-2.90239700	2.01458000	-3.18022300
H	-3.65852500	-2.15141500	-2.40210000	C	-3.00245600	4.02083600	-1.79243300
C	-2.14475100	-4.64256000	-0.68014700	H	-2.64879100	3.76191100	0.33291000
H	-1.02239400	-4.41982200	1.11836500	C	-3.08832600	3.39715900	-3.04490100
H	-3.28356900	-4.58553200	-2.52859400	H	-2.98333300	1.51913400	-4.14277700
H	-1.99514300	-5.71949700	-0.70348000	H	-3.16035700	5.09294800	-1.71645700
O	-4.00175000	-0.13830900	-1.33994200	H	-3.31077200	3.99029000	-3.92734500
N	-1.14551300	-1.74940300	1.41894600	C	-2.62792200	-1.64742300	-0.07921500
C	-0.62247900	-2.45702300	2.58366900	C	-2.95798500	-1.68231700	1.30466500
H	0.30533100	-3.02062400	2.39171400	C	-2.76634100	-2.80507200	-0.85881700
H	-0.40621700	-1.72984700	3.37177500	C	-3.36566800	-2.90744900	1.86345400
H	-1.36035700	-3.16724200	2.98381000	C	-3.18848500	-4.00571500	-0.29331500
C	-1.54340100	0.82450100	1.25230500	H	-2.53501500	-2.74937900	-1.91852000
O	-1.58295300	1.68280500	2.13469800	C	-3.47623100	-4.05167400	1.07327900
12				H	-3.61671600	-2.97258700	2.91432600
C	2.78333100	0.52714800	0.49711300	H	-3.28971400	-4.89430700	-0.90922200
C	4.01024600	1.02220900	0.97224500	H	-3.80152200	-4.98044200	1.53320200
C	4.00299500	2.09981400	1.86553500	O	-2.46747600	-0.06649400	-1.96759400
C	2.78611800	2.64661900	2.25084900	N	-2.89432300	-0.51685400	2.09787300
C	1.61334100	2.09902400	1.72881100	C	-3.22936900	-0.61065000	3.51923600
C	2.72977700	-0.61500800	-0.44033200	H	-2.56708200	-1.32048700	4.02401500
C	3.90505700	-1.22366800	-0.91330000	H	-3.10109100	0.37793200	3.95337100
				H	-4.26715000	-0.92989200	3.66000700

C	-2.61364100	0.76321400	1.59233000	H	1.25999700	-0.47164700	4.02451000
O	-2.72024900	1.77103900	2.30365100	C	4.76558100	-2.50569700	-1.92661500
				O	-2.66351800	-1.89433500	2.20945000
13				O	2.76237300	-1.69291200	2.25917400
C	0.62027200	2.76702600	0.04921700	C	-3.65381000	-2.25727500	-0.87959900
C	1.31907300	3.76938300	-0.63826800	F	6.05709900	-2.25924500	-1.62976800
C	2.72028300	3.73233500	-0.63955000	F	4.62204400	-3.84209100	-2.06941800
C	3.36584200	2.70704700	0.04072300	F	4.49180600	-1.93291000	-3.10618400
C	2.59992200	1.74919600	0.69972100	F	-5.80309300	-2.78835600	-1.76848200
C	-0.85200900	2.73579500	0.08365200	F	-4.23525900	-2.28415700	-3.19561500
C	-1.62794200	3.71925400	-0.54806000	F	-4.18694500	-4.20037800	-2.15951700
C	-3.02440800	3.62363200	-0.48556800				
C	-3.59389600	2.55358600	0.19422900	14			
C	-2.75889100	1.60973000	0.79406000	C	2.27082100	0.88273400	-0.16480900
H	3.27221000	4.50364300	-1.16855500	C	3.35442200	1.70301600	0.17628800
H	4.44842200	2.64196000	0.06438400	C	2.40506600	-0.17870200	-1.17095900
H	3.05953700	0.92553600	1.23562600	N	1.06097900	1.00993600	0.43924900
H	-3.63285500	4.37848100	-0.96591600	C	3.18592400	2.66953200	1.17422900
H	-4.67001900	2.43502700	0.25671500	C	4.66424900	1.53884900	-0.50357200
H	-3.15686800	0.75578300	1.32756900	C	3.60257600	-0.40199100	-1.86395700
N	-1.42053400	1.70451600	0.74852300	N	1.31421600	-0.94357300	-1.37789300
N	1.25698600	1.78045600	0.70975500	C	0.91660000	1.92874900	1.41128600
C	-0.97464900	4.84011200	-1.26707500	Pd	-0.37399900	-0.28941100	-0.26439700
C	0.58127100	4.84299200	-1.35525000	C	1.95321700	2.77545100	1.80262900
O	-1.59876700	5.74888700	-1.78822000	H	4.01942500	3.30877900	1.44444100
O	1.14584800	5.71248500	-1.99926100	C	4.78929100	0.44489400	-1.59609700
Pd	-0.03239400	0.41650200	1.74091100	O	5.63396200	2.22355300	-0.23648900
O	-3.87114600	-2.88677600	0.24227700	C	3.65334200	-1.44505200	-2.79631200
H	-3.33107000	-2.47048900	1.03754000	C	1.36699700	-1.94306400	-2.27084200
C	0.72234800	-0.94481900	3.20749100	H	-0.05683300	1.97551400	1.87938600
C	-0.70612200	-0.99860000	3.19627300	C	-2.44197200	1.73786100	0.76463900
O	-2.93799700	-1.29644400	-1.09106900	H	1.77852300	3.49969100	2.58977600
C	-4.48430100	-2.89073200	-2.02685300	O	5.84604100	0.31049800	-2.18406700
C	-1.40083500	-1.85180500	2.25775000	C	2.52134100	-2.22508200	-3.00225800
C	-0.58612500	-2.70456800	1.36529200	H	4.57391300	-1.62947000	-3.33983400
H	-1.11250100	-3.40084900	0.71952200	H	0.45583500	-2.51902300	-2.39210500
C	0.76060500	-2.65269900	1.37459400	C	-1.93158600	0.46126600	0.75116300
H	3.49565900	-2.20491400	1.10425700	C	-2.07873700	3.02385900	0.14776000
H	1.35303500	-3.30657400	0.73641000	H	2.52048200	-3.04286200	-3.71386900
O	4.09536500	-2.56877500	0.32361200	C	-2.76831600	-0.29476700	1.66888300
C	1.49921700	-1.74117100	2.27919600	C	-1.73022000	3.16304700	-1.23271900
C	3.84246000	-1.96881900	-0.81212600	C	-2.10474400	4.17222300	0.95951400
H	-1.28306300	-0.56575900	4.00459700	C	-3.71329700	0.61071000	2.19213700
O	3.02013000	-1.09879200	-1.04159200	C	-2.81433600	-1.63140900	2.10585100

C	-1.38887600	4.45183700	-1.70556900	O	1.23534200	1.04891900	1.02724700
N	-1.72289100	2.08120800	-2.08415100	O	6.55919600	0.10043400	2.24380600
C	-1.77568200	5.43605700	0.47442700	H	7.14268200	0.44582800	1.54957500
H	-2.38573600	4.05450300	2.00176400	H	4.54353600	-0.60669400	3.68870400
C	-4.68864700	0.26474300	3.12171400	C	2.55245600	0.78805400	1.28491300
C	-3.78240300	-2.00170800	3.03847500	H	0.88868000	2.27836200	0.32984100
H	-2.11684800	-2.36505700	1.71288000	C	3.55952200	1.22014600	0.40901600
C	-1.40819500	5.56352100	-0.86764100	O	0.42390700	3.13299200	-0.06915100
H	-1.12036900	4.58026600	-2.74796000	C	2.91872200	0.12698500	2.46913200
C	-1.61077700	2.22535700	-3.52422100	C	0.52033100	3.19669200	-1.37280600
H	-1.79999200	6.29982400	1.13173600	C	4.90404400	1.00528300	0.71472100
C	-4.70792500	-1.06692800	3.54188600	O	1.21197200	2.52962900	-2.11599800
H	-5.39683200	0.99665200	3.49787400	C	4.25928800	-0.09628600	2.77317300
H	-3.82849400	-3.03148000	3.38219800	C	-0.44554000	4.26503500	-1.93273000
H	-1.14245200	6.53648200	-1.27313800	H	2.14082500	-0.20851100	3.14951600
H	-0.62535200	2.60723800	-3.81716400	C	5.26026700	0.34315900	1.89607800
H	-1.73618500	1.23806200	-3.97298900	H	5.67859300	1.34901300	0.03257600
H	-2.37188100	2.89705600	-3.94914300	C	-2.76674500	-0.20385900	0.90317900
H	-5.45144200	-1.38630900	4.26650600	C	-3.96890200	0.14728000	1.52561600
O	-1.53458000	-1.80116700	-0.97969400	C	-3.95760400	1.17779600	2.47307100
C	-2.52214300	-1.63623100	-1.78101600	C	-2.75483900	1.80884600	2.76915400
C	-3.10993300	-3.00596000	-2.20687700	C	-1.59273600	1.40348600	2.11241900
O	-3.01147200	-0.60894100	-2.24207600	C	-2.68672900	-1.27318300	-0.09071100
F	-4.18979200	-2.87124700	-2.99076000	C	-3.81277600	-1.99747900	-0.49543000
F	-3.46839500	-3.74276800	-1.13375600	C	-3.65612500	-2.99555500	-1.46386100
F	-2.18695200	-3.71756800	-2.89686800	C	-2.39260400	-3.22610700	-1.99535900
H	-2.20089100	1.23804400	-1.78076400	C	-1.31305800	-2.46895400	-1.54075800
O	-3.52905700	1.84532400	1.65061200	H	-4.88169100	1.46358500	2.96408000
H	0.21128600	-2.60823900	1.75494400	H	-2.70120600	2.60683700	3.50072900
C	1.74062500	-1.88957100	2.59900100	H	-0.62713500	1.85235700	2.31334800
O	1.17440500	-2.78286600	1.79217000	H	-4.51890000	-3.56778400	-1.78744200
O	1.18574800	-1.04349900	3.25518100	H	-2.22858400	-3.98244100	-2.75396000
C	3.27584100	-2.04474600	2.56461400	H	-0.31352100	-2.61193300	-1.93276500
F	3.84027800	-1.31480200	3.52885500	N	-1.45690900	-1.52004300	-0.60074700
F	3.74294900	-1.61122200	1.37326500	N	-1.60398000	0.42386400	1.19492300
F	3.64592800	-3.32505500	2.71441100	C	-5.13809000	-1.70000500	0.10625300
				C	-5.21990100	-0.57130000	1.17260500
				O	-6.14967400	-2.30171200	-0.19817700
				O	-6.29393500	-0.31411600	1.68095900
				F	4.13109300	-1.83099000	-1.47388500
				F	2.68055300	-3.02058600	-2.58465600
				F	3.72506600	-3.88359800	-0.88197500
				F	-0.24654600	4.46284500	-3.24144800
				F	-0.30561000	5.44446300	-1.30040700
15							
Pd	0.00329200	-0.32462900	0.18735300				
O	1.50298800	-1.17361100	-0.88567400				
C	2.02372600	-2.25697900	-0.41882300				
O	1.73567100	-2.89435000	0.58615800				
C	3.15924900	-2.75940700	-1.34630800				
H	3.28209800	1.72329100	-0.51235000				

F	-1.72300600	3.85419100	-1.76073300	C	-5.32182800	0.14613200	-0.33368600
				C	-4.98010700	1.46634000	0.41454300
16				O	-6.46182600	-0.04341200	-0.71000700
Pd	-0.16657300	-0.76474700	0.54672000	O	-5.85471500	2.29241600	0.58760800
O	1.49747400	0.04878300	1.35146600	F	3.04198400	-3.77147700	-2.39483900
C	1.84178900	-0.33934100	2.53503400	F	3.16537900	-3.96941600	-0.23213700
O	1.30691200	-1.14790400	3.27992500	F	1.44600800	-4.77211300	-1.30497000
C	1.27449500	1.92894100	-2.39932500	F	2.87822800	1.74259900	3.06336200
C	2.64484700	1.79901800	-2.13660700	F	4.13486900	0.22301500	2.13210900
C	0.74635600	3.20413400	-2.64710300	F	3.52387000	0.00793200	4.20818300
C	3.47077300	2.92662900	-2.11956000				
C	1.57057600	4.32762500	-2.63154700	TS1			
H	-0.31460200	3.30540300	-2.85773500	C	3.63682900	-1.40463700	-0.62615500
C	2.93954800	4.19620400	-2.36661600	C	4.34860400	-2.57007500	-0.93396000
H	4.53283200	2.81260400	-1.91318600	C	4.29903800	-0.23507600	-0.04040300
C	3.11577100	0.41231000	2.99680100	N	2.30628900	-1.29445200	-0.87711200
H	3.06931300	0.81660600	-1.95068300	C	3.67528500	-3.63648500	-1.53993200
O	0.42215800	0.86263000	-2.43633300	C	5.79766400	-2.66572900	-0.61957000
O	3.70096600	5.33567000	-2.36271000	C	5.66297400	-0.23049100	0.27728800
H	4.62278700	5.09706200	-2.17830100	N	3.52131500	0.84880300	0.16188200
H	1.16097300	5.31459900	-2.82543900	C	1.67067500	-2.31912200	-1.47331800
H	0.89267500	0.03352800	-2.19764100	Pd	1.50242400	0.51266000	-0.33668300
O	1.69912800	-1.53246600	-1.93936000	C	2.32260600	-3.50162500	-1.82084300
C	1.57539500	-2.40505500	-1.07963700	H	4.21914200	-4.54261400	-1.78398100
O	0.88679100	-2.40927700	0.00127100	C	6.48927400	-1.43663800	0.02751400
C	2.32528400	-3.74738400	-1.26359700	O	6.45490600	-3.66258300	-0.85029400
C	-2.62938500	0.66848100	0.64818500	C	6.22038100	0.93275200	0.82154100
C	-3.58631800	1.65745200	0.89221900	C	4.05814200	1.96405400	0.67903100
C	-3.19929500	2.80748700	1.59013100	H	0.61574100	-2.18078900	-1.66810500
C	-1.88003700	2.92925400	2.01106500	C	-0.96511700	-0.77821700	0.05900300
C	-0.97632900	1.90376500	1.73207700	H	1.76130300	-4.29494700	-2.30056000
C	-2.94294300	-0.55809200	-0.07906900	O	7.67292900	-1.49728000	0.30051500
C	-4.22657900	-0.83294700	-0.55837400	C	5.40810400	2.04240700	1.02330500
C	-4.44423000	-2.03653400	-1.23904900	H	7.27525100	0.95082900	1.07393600
C	-3.38133400	-2.91559800	-1.41199400	H	3.38112100	2.80061300	0.81132600
C	-2.12567600	-2.57665600	-0.90747700	C	-0.44601500	0.07549900	-0.77170100
H	-3.92942600	3.58450600	1.78892500	C	-1.12839300	-1.72218400	1.07008300
H	-1.53792900	3.80437900	2.55107700	H	5.80207300	2.96225800	1.43957700
H	0.06340500	1.95710800	2.03165900	C	-1.21005800	0.71158000	-1.83597800
H	-5.43417700	-2.26615600	-1.61837400	C	-1.37094100	-1.31802000	2.43987700
H	-3.50752700	-3.85848200	-1.93106900	C	-1.11513400	-3.11187900	0.74619900
H	-1.27058500	-3.23326300	-1.01440600	C	-2.57819200	0.30444800	-1.86186000
N	-1.91408100	-1.42019100	-0.25827300	C	-0.72278300	1.62714000	-2.77939100
N	-1.34851500	0.79748900	1.06789000	C	-1.57925700	-2.34175400	3.40549400

N	-1.38191300	-0.01625400	2.78167300	C	-4.13456500	2.86653500	0.61380400
C	-1.32414500	-4.07750200	1.70500000	C	-2.88278500	3.40229900	0.88095100
H	-0.94791100	-3.38744200	-0.28985200	C	-1.75823700	2.62134800	0.60168300
C	-3.43053200	0.85231100	-2.84314600	H	-5.26533100	-2.86414000	-1.85835900
C	-1.57826600	2.15945400	-3.74388600	H	-3.06536700	-4.02794100	-2.30159300
H	0.32359400	1.91741900	-2.74881500	H	-0.96581000	-2.82294200	-1.73085600
C	-1.55625500	-3.67324700	3.03974000	H	-5.04553600	3.42094100	0.81330800
H	-1.76327100	-2.07171100	4.43866700	H	-2.76832200	4.39716500	1.29706500
C	-1.59459900	0.47740900	4.13121800	H	-0.75980600	2.99819000	0.79839500
H	-1.31678300	-5.13053100	1.44406400	N	-1.82862100	1.38819600	0.08752300
C	-2.92559600	1.76890900	-3.76449200	N	-1.90848300	-1.12585600	-1.02149100
H	-4.46780000	0.53342800	-2.87575700	C	-5.55225600	0.99748700	-0.21826100
H	-1.20288600	2.87081900	-4.47354300	C	-5.59488300	-0.42500200	-0.81639700
H	-1.72216400	-4.42834700	3.80369000	O	-6.59935600	1.58427900	-0.00594000
H	-0.82375800	0.12029300	4.82560900	O	-6.67330900	-0.93848000	-1.05638700
H	-1.55413700	1.56684700	4.09967100	Pd	0.14070900	-0.39550600	-0.57888300
H	-2.57465700	0.17803600	4.52011100	C	2.98721400	1.01012300	-0.56538000
H	-3.59227500	2.18206600	-4.51782600	C	2.16900300	-0.05381700	-0.91079100
O	1.06927300	2.45587200	0.05088400	C	3.06555700	-1.15233900	-1.25068800
C	0.19639600	2.98293600	0.82710600	C	4.36454700	-0.65439300	-1.07259600
C	0.32269800	4.52906700	0.79935400	C	2.90021100	-2.47666000	-1.68164600
O	-0.64921100	2.47257100	1.55398900	C	5.51866100	-1.39620300	-1.28797500
F	-0.61349100	5.12517800	1.55055800	C	4.04310100	-3.24214500	-1.91190200
F	0.21077900	5.00577500	-0.45815100	H	1.90778400	-2.89411500	-1.82509600
F	1.53399100	4.90771300	1.27155200	C	5.33256900	-2.71240200	-1.71560800
H	-1.14718700	0.68331400	2.07863100	H	6.50559500	-0.97265300	-1.13386200
O	-2.94278800	-0.58409200	-0.95738000	H	3.93878100	-4.27053200	-2.24533700
H	-4.13723700	-0.60453600	-0.51045700	H	6.20074500	-3.33782800	-1.90026900
C	-6.17165200	-0.84189700	-0.70485700	C	2.75459000	2.42114400	-0.23569200
O	-5.13637300	-0.64744300	0.04395800	C	2.03400300	2.83099900	0.92796800
O	-6.24677200	-0.93324000	-1.92122600	C	3.33632700	3.38698900	-1.07548800
C	-7.45435300	-0.98796000	0.15158600	C	1.90985200	4.22274200	1.16091700
F	-8.55974300	-1.01300000	-0.61042500	C	3.19624400	4.74977900	-0.83121700
F	-7.58299600	0.02772400	1.03083500	H	3.89811500	3.04689300	-1.94107400
F	-7.41959400	-2.13750300	0.86333000	C	2.47295000	5.15480800	0.29583000
TS2				H	1.37537500	4.56790000	2.03830600
C	-3.07292900	-0.49342300	-0.77736900	H	3.64163700	5.47808700	-1.50117400
C	-4.30504000	-1.10907800	-1.07685600	H	2.35315800	6.21308900	0.51333600
C	-4.31514900	-2.39298000	-1.63057100	O	4.31270500	0.65587300	-0.65955400
C	-3.10846500	-3.03271400	-1.87427000	N	1.49056100	1.92154900	1.79867500
C	-1.93122900	-2.36113200	-1.55570800	C	1.02470400	2.29032400	3.12415800
C	-3.03228600	0.86871300	-0.18488800	H	0.13626200	2.93170000	3.08410600
C	-4.22358500	1.57905000	0.07032700	H	0.75402600	1.37295600	3.65023600
				H	1.79342200	2.81305100	3.71162000

O	-0.09024500	-1.48951300	1.23644600	H	4.99843400	0.57653500	-4.34567100
C	0.79567800	-1.61859200	2.14462500	H	4.54920800	-3.60938600	-3.36038100
C	0.51851800	-2.86150100	3.03152600	H	5.63133000	-1.82677800	-4.68622800
O	1.79118800	-0.93462100	2.39379600	C	1.56391300	2.39256200	-1.05421800
F	0.57712900	-3.99198300	2.28627300	C	0.91367300	2.57345200	0.20637700
F	-0.71463800	-2.80809700	3.58262200	C	1.70922600	3.50198600	-1.91353700
F	1.40499200	-2.99216100	4.03207000	C	0.49469600	3.87813500	0.54581400
H	1.73704000	0.93967000	1.69639400	C	1.26024200	4.77003200	-1.56653000
C	0.83070400	0.34720800	-2.10443700	H	2.19455600	3.35270700	-2.87048100
O	0.93601000	0.80292800	-3.17616900	C	0.65836700	4.95523300	-0.32139000
TS3				H	0.03405300	4.05453000	1.50934300
C	-3.28861100	-1.17422500	-0.17009500	H	1.38662700	5.60012100	-2.25430000
C	-4.29572700	-2.12788800	-0.39209800	H	0.31473600	5.94022400	-0.01700000
C	-3.93466000	-3.46246300	-0.60746000	O	3.08603200	1.27949300	-2.48341300
C	-2.59004100	-3.80166000	-0.58852000	N	0.74482600	1.48296100	1.08480000
C	-1.64400500	-2.79748600	-0.38111700	C	0.25711200	1.81539700	2.44074000
C	-3.62472900	0.23457800	0.10781400	H	-0.76813900	2.20133900	2.45419600
C	-4.95348700	0.68985500	0.05668200	H	0.30035800	0.90343300	3.03784400
C	-5.21162900	2.04683600	0.27932800	H	0.90839200	2.56246200	2.91460700
C	-4.14689500	2.89871200	0.53949800	C	1.05307600	-0.91664700	-0.29956400
C	-2.86010300	2.36080600	0.59567400	O	1.22206200	-2.10140500	-0.03174700
H	-4.71329500	-4.19827300	-0.77800000	H	1.91261500	0.85302000	1.41672300
H	-2.25972000	-4.82366500	-0.73622600	O	2.90462800	0.37167200	1.76411100
H	-0.58039300	-3.00752400	-0.34736600	C	2.78051000	-0.54477300	2.67296200
H	-6.23593300	2.40207600	0.23950600	C	4.14085400	-1.22366800	2.96708100
H	-4.29616800	3.95963800	0.70569700	O	1.78320300	-0.89479800	3.28687700
H	-2.00264000	2.99281600	0.79598700	F	5.01999900	-0.32842900	3.46753000
N	-2.60004000	1.05911200	0.40269600	F	4.67932100	-1.74142200	1.84326500
N	-1.97744000	-1.50891800	-0.19100400	F	4.01432800	-2.21810800	3.85847900
C	-6.07392900	-0.24456100	-0.21456700	TS4			
C	-5.72858500	-1.73967100	-0.41228000	C	2.65343100	0.90439100	0.08402000
O	-7.23376200	0.11679300	-0.27703400	C	3.62966400	1.89198000	-0.13031700
O	-6.62506100	-2.54296200	-0.58697500	C	3.30500300	3.23112000	0.11275400
Pd	-0.56800300	0.04409600	0.27103800	C	2.02749500	3.54257500	0.55931800
C	2.13092300	1.12372100	-1.50354000	C	1.11316500	2.50689500	0.74669600
C	1.99173700	-0.22368400	-1.19379000	C	2.94684100	-0.52509800	-0.14895900
C	2.92790200	-0.94111900	-2.04835000	C	4.20298600	-0.94572700	-0.61800300
C	3.56187200	0.04031600	-2.81924400	C	4.41940300	-2.31283100	-0.82843400
C	3.28361100	-2.28515300	-2.24290600	C	3.38905000	-3.20686300	-0.56759000
C	4.53423500	-0.22095900	-3.77554000	C	2.17306300	-2.70462700	-0.10045000
C	4.25668800	-2.57613300	-3.19758200	H	4.05343300	3.99904600	-0.05079900
H	2.81510100	-3.06706000	-1.65804200	H	1.73087300	4.56544100	0.76196300
C	4.87508700	-1.56243900	-3.95321200	H	0.10637300	2.70680100	1.09502400

H	5.38524100	-2.64860000	-1.19073900	C	2.51071300	1.63559800	0.04103000
H	3.51296900	-4.27346000	-0.71772200	N	1.59568100	-0.58263000	0.20703900
H	1.34171900	-3.36780600	0.11641300	C	4.11084600	-1.71457900	0.68127800
N	1.95386900	-1.39761100	0.10562600	C	5.17343900	0.54562800	0.49505500
N	1.41136600	1.21597900	0.51432600	C	3.57720300	2.54393000	0.04254600
C	5.28403300	0.03258900	-0.87920300	N	1.23708100	2.03961100	-0.14796900
C	4.98413400	1.52897100	-0.61295400	C	1.73511300	-1.90524100	0.40877500
O	6.38671800	-0.28768600	-1.28553400	Pd	-0.15265300	0.48541500	-0.12737300
O	5.85932300	2.35300600	-0.80795600	C	2.97117800	-2.50370500	0.65263500
Pd	0.03055300	-0.40386800	0.81837100	H	5.09335900	-2.13787000	0.86025400
C	-2.98993800	-0.23173400	-0.68060600	C	4.96297700	2.06484100	0.26853300
C	-2.60432900	0.63051600	0.32664500	O	6.29942000	0.12440000	0.68114600
C	-3.15919600	1.92449200	-0.01400000	C	3.30378800	3.90073200	-0.16393000
C	-3.82271500	1.73657600	-1.24180300	C	0.97656100	3.34208800	-0.34245000
C	-3.15966400	3.20067300	0.57029400	H	0.83599300	-2.49902300	0.37276700
C	-4.48043800	2.75088400	-1.92506600	C	-1.91253500	-1.71085500	1.05442500
C	-3.81633000	4.23381200	-0.09830900	H	3.01688600	-3.57469200	0.81200700
H	-2.66868700	3.37258500	1.52269100	O	5.92569400	2.80807300	0.28585600
C	-4.46609200	4.01428300	-1.32749800	C	1.98770000	4.30266300	-0.35903900
H	-4.98131100	2.56659300	-2.86998100	H	4.11980200	4.61554700	-0.16664500
H	-3.83092500	5.22830000	0.33842400	H	-0.06542300	3.60366900	-0.48401100
H	-4.96993900	4.84000500	-1.82115900	C	-1.59892000	-1.06293400	-0.14954700
C	-2.84436600	-1.65478300	-0.76829900	C	-1.10985600	-2.22031000	2.18444700
C	-2.20321900	-2.33795200	0.31586400	H	1.73229100	5.34351200	-0.52081000
C	-3.39838000	-2.39180200	-1.83526100	C	-2.90711300	-0.92512400	-0.81769000
C	-2.23940400	-3.75417100	0.31165000	C	-0.53001800	-1.36621700	3.17091000
C	-3.37311800	-3.77881400	-1.83696100	C	-0.97204200	-3.61326100	2.29402300
H	-3.86968000	-1.85256900	-2.65088700	C	-3.85707900	-1.52374200	0.01598900
C	-2.80324300	-4.45606200	-0.74691400	C	-3.33180400	-0.41962900	-2.05465600
H	-1.78774900	-4.29971900	1.13266500	C	0.21977200	-1.97979600	4.20356400
H	-3.80543600	-4.33282000	-2.66461500	N	-0.69389900	-0.00545100	3.13009000
H	-2.79079400	-5.54277900	-0.72946800	C	-0.23077900	-4.19668300	3.31897100
O	-3.72465200	0.42967900	-1.64669600	H	-1.44300300	-4.24020500	1.54153700
N	-1.60477600	-1.61557300	1.33628700	C	-5.20934500	-1.63835500	-0.27674400
C	-1.44226100	-2.25229100	2.63796200	C	-4.68579700	-0.51458600	-2.37993600
H	-0.59105500	-2.94514600	2.67299100	H	-2.61656600	0.02397600	-2.73811000
H	-1.27567100	-1.46368400	3.37744000	C	0.36808800	-3.36150300	4.26737900
H	-2.34849600	-2.80318900	2.92391600	H	0.67758800	-1.36132200	4.96712900
C	-1.72822000	0.29935300	1.45744600	C	-0.27943000	0.87581400	4.20583500
O	-1.83684800	0.77390500	2.59555800	H	-0.12388700	-5.27510200	3.37553300
TSS				C	-5.61337500	-1.10949400	-1.50436700
C	2.70642000	0.19876200	0.24637200	H	-5.90424300	-2.11613200	0.40599800
C	3.98029700	-0.33684700	0.47508200	H	-5.03438500	-0.12326400	-3.33161200
				H	0.95156500	-3.79031400	5.07806200

H	0.80861300	0.86672800	4.34449000	O	-1.94758100	1.63699700	-2.25979600
H	-0.57572800	1.89349100	3.94319600	C	-1.39875300	-3.28265000	0.67738600
H	-0.74549000	0.61817300	5.16782900	C	3.01527200	-0.14249400	0.30555600
H	-6.65961400	-1.16673800	-1.78970000	C	4.23793200	-0.27696900	0.98004100
O	-1.64711700	1.81287500	-0.46922400	C	4.52841000	-1.49315500	1.60842800
C	-2.50316000	2.09791300	0.44411400	C	3.59704100	-2.52112400	1.54573100
C	-3.43072300	3.25368200	-0.00988100	C	2.40002600	-2.31016800	0.85943700
O	-2.64537700	1.62957600	1.57064000	C	2.64027200	1.10487400	-0.36715700
F	-4.43776100	3.45537400	0.85117100	C	3.46486800	2.23789300	-0.32915400
F	-3.96391800	3.02186400	-1.22545200	C	3.02694600	3.41840000	-0.93866600
F	-2.71778300	4.40324400	-0.09049100	C	1.78314900	3.43346200	-1.55427500
H	-1.37097700	0.38390400	2.48020700	C	1.01910500	2.26690900	-1.57145500
O	-3.24026100	-1.99623100	1.15719300	H	5.47060300	-1.61088600	2.13300900
H	-0.80751100	-1.66746600	-0.99070300	H	3.77909000	-3.47861700	2.02047000
C	0.26216000	-1.63337700	-2.89649700	H	1.63242400	-3.07047500	0.79344500
O	-0.12307400	-2.35173600	-1.90467100	H	3.65990800	4.29875900	-0.91295700
O	-0.16395800	-0.55276500	-3.29803300	H	1.39311800	4.32877700	-2.02459600
C	1.50864200	-2.21949600	-3.61201200	H	0.03631500	2.24295200	-2.03471700
F	1.58732100	-1.82452200	-4.89450800	N	1.44372200	1.12486300	-1.00488100
F	1.55071700	-3.56455700	-3.59188600	N	2.11616200	-1.14763600	0.25108500
F	2.62815800	-1.77092700	-2.98226900	C	4.78274000	2.18303400	0.35209500
TS6				C	5.19751100	0.85185900	1.02906000
O	-2.19125300	-4.09413500	0.14495200	O	5.53977000	3.13434400	0.39680400
H	-1.97029300	-4.10490400	-1.46127500	O	6.28158200	0.77681800	1.57679500
Pd	0.44300600	-0.68062400	-1.03662200	F	-2.67972600	-3.62417600	2.70869200
C	-0.72524100	-0.32042600	-2.82253100	F	-1.94655200	-1.61677700	2.29691600
C	-0.74750500	-1.73739100	-3.00126200	F	-0.56103000	-3.17620600	2.92031600
O	-0.40956600	-2.68790800	0.18483500	F	-3.60616100	3.23513200	2.86529100
C	-1.65983400	-2.93735900	2.16772300	F	-3.96414000	4.74797200	1.34206400
C	-1.75109900	-2.48408100	-2.40541900	F	-5.24562200	2.99000100	1.45488100
C	-2.86399600	-1.80953100	-1.77157800	TS7			
H	-3.66855200	-2.42353700	-1.37938300	Pd	-0.23387800	0.31878900	-0.12060400
C	-2.91898800	-0.45471600	-1.66138800	O	1.30773300	0.17850000	-1.39949200
H	-2.83096100	2.29736100	-1.28391900	C	1.73079800	-0.97315000	-1.80488400
H	-3.77630700	0.03628500	-1.21205100	O	2.62145600	2.03230700	1.31404500
O	-3.45678600	2.79551300	-0.61096100	O	1.23090900	-2.08095500	-1.67208000
C	-1.86954000	0.36902800	-2.23341500	C	1.76839500	2.73309600	0.72206100
C	-3.03043300	2.67973700	0.62112100	O	0.57030100	2.46505000	0.45231200
H	0.04905300	-2.23420300	-3.54571000	C	2.24017100	4.11569500	0.20647700
O	-2.04373400	2.10059800	1.03051000	C	3.08271000	-0.82020200	-2.54902400
H	-0.07828900	0.27948500	-3.45740400	C	1.92904900	-1.28285000	1.85856400
C	-3.97695500	3.42248300	1.59216100	C	3.29872000	-1.39178900	1.59645900
O	-1.70618800	-3.82249000	-2.39586500	H	3.85918800	-0.52576400	1.25870500

C	1.21279200	-2.40686800	2.28604400	N	0.27941000	-1.70442700	-0.09054200
O	1.25344900	-0.08971500	1.71587400	C	-0.50793300	-4.37508700	-0.30121800
C	3.94781500	-2.61658400	1.76859100	C	1.86974500	-5.05256100	-0.72680000
O	3.81417600	-4.96430000	2.37630300	C	3.62251600	-3.13621700	-0.80175100
C	1.85841800	-3.63021300	2.44839100	N	2.81075400	-0.91036400	-0.41866200
H	4.75847800	-4.90048800	2.16195000	C	-1.01248900	-2.05187500	0.03995900
H	0.14982700	-2.31638200	2.49035500	Pd	1.09082200	0.17656700	0.08609300
H	1.30827900	-4.50576200	2.77965700	C	-1.43971300	-3.37731200	-0.06074100
C	3.23182900	-3.74122200	2.19295200	H	-0.79757900	-5.41734700	-0.38093300
H	1.88905900	0.69987200	1.60964400	C	3.33891400	-4.58859200	-0.90770000
H	5.01377400	-2.69541100	1.56721300	O	1.60707000	-6.23695600	-0.81478900
C	-2.94372400	-0.36185600	-0.76519800	C	4.91766900	-2.63502800	-0.97497500
C	-4.09771000	-0.76924500	-1.44193900	C	4.05329200	-0.43116000	-0.58426000
C	-3.98165700	-1.19420100	-2.76967800	H	-1.72855000	-1.25698700	0.19475200
C	-2.72697900	-1.18988500	-3.36798900	C	-0.86758800	1.93864700	-0.28505400
C	-1.61781900	-0.77205000	-2.63240800	H	-2.49471200	-3.59615700	0.04728300
C	-2.98231300	0.12196000	0.60899100	O	4.20226200	-5.41603500	-1.12950000
C	-4.16589500	0.19328100	1.34951300	C	5.13408000	-1.26629600	-0.86730800
C	-4.10735100	0.68158300	2.65952500	H	5.72958100	-3.32109600	-1.19070400
C	-2.88013300	1.08195800	3.17782400	H	4.17066100	0.64172100	-0.48375600
C	-1.73829900	0.98669300	2.38253500	C	-0.64867700	1.16149500	0.70509000
H	-4.86582100	-1.51427800	-3.31013700	C	-0.93848400	2.84619400	-1.31174800
H	-2.59052400	-1.50460100	-4.39610600	H	6.12119500	-0.83775300	-0.99608700
H	-0.62843700	-0.75499000	-3.06830500	C	-1.39518300	0.84836100	1.93180000
H	-5.01584700	0.74346000	3.24878000	C	-1.66246600	2.57616100	-2.55071100
H	-2.79261000	1.46718100	4.18696200	C	-0.23597000	4.09540900	-1.16891200
H	-0.75956700	1.28311800	2.73877500	C	-0.77763500	0.29745300	3.08151100
N	-1.79528300	0.51322900	1.12714500	C	-2.79082900	1.06134000	1.95745300
N	-1.72305900	-0.37160100	-1.35422600	C	-1.56875600	3.55324500	-3.58908300
C	-5.44484600	-0.23690400	0.72830400	N	-2.37812300	1.46064500	-2.71355000
C	-5.40883400	-0.73985500	-0.74367200	C	-0.19909200	5.01394800	-2.18234600
O	-6.50688400	-0.20759600	1.31884200	H	0.27832400	4.27866400	-0.23272100
O	-6.44521700	-1.08923000	-1.27449100	C	-1.56474500	-0.07050200	4.18255800
F	1.34873200	5.08432100	0.50084600	C	-3.56006600	0.70661600	3.05967000
F	2.36506500	4.07787800	-1.14264600	H	-3.27114900	1.48137800	1.08030400
F	3.42819800	4.48640700	0.71294600	C	-0.86859900	4.72157200	-3.40172500
F	4.04793300	-0.42224700	-1.68898800	H	-2.07573900	3.37616300	-4.52948800
F	3.47785100	-1.97562800	-3.10270600	C	-3.11543700	1.14029300	-3.92687000
F	3.00586500	0.10388000	-3.52937300	H	0.33681800	5.94973800	-2.06496700
				C	-2.94232500	0.12508700	4.17290500
4'				H	-1.06463800	-0.49470600	5.04802800
C	1.19847800	-2.67221600	-0.34832300	H	-4.63407300	0.86440300	3.04101300
C	0.83779800	-4.02002000	-0.45456000	H	-0.83422800	5.44635700	-4.21079100
C	2.58554500	-2.23669000	-0.52547000	H	-2.45054700	1.07488100	-4.79458500

H	-3.58894300	0.17032300	-3.77248700	H	6.17509200	-3.07568700	-0.52331400
H	-3.89529200	1.88127300	-4.14007500	H	4.44180900	0.87859500	-0.40861000
H	-3.53197100	-0.16568700	5.03782600	C	-1.40119200	1.17327300	0.96383600
O	2.14481400	1.91886200	0.12527700	C	-1.08501300	2.13274500	-1.06762500
C	2.44176800	2.46160600	1.24528000	C	2.12676600	3.20277700	0.28583500
C	3.36619400	3.69016100	1.05910700	H	6.48440000	-0.57395600	-0.47809300
O	2.11311200	2.13331200	2.38695000	C	-1.32605200	0.40169200	2.22368900
F	3.67754900	4.26357600	2.22768400	N	-2.60099100	1.88705700	0.62813500
F	2.77839000	4.62263300	0.28029600	C	-2.35779700	2.53786000	-0.59005800
F	4.51637100	3.31981500	0.45488200	C	-0.64954500	2.59843800	-2.32210800
H	-2.59347400	0.82637300	-1.92078500	C	3.07735500	4.31796900	-0.21974000
O	0.55904600	0.07375100	3.18074000	O	1.42160000	3.42603200	1.26859300
H	1.08157800	0.78566800	2.73711000	C	-0.24260500	0.54593400	3.12598100
C	-4.49978600	-0.30724900	-0.57671700	C	-2.34142100	-0.51641900	2.56269300
O	-5.19156500	0.71775800	-0.54981400	C	-3.48306100	2.49388200	1.63363500
O	-3.37021100	-0.53076900	-1.10236500	C	-3.17526200	3.42220900	-1.30048000
C	-5.06808300	-1.56411100	0.15134800	C	-1.46281400	3.47095900	-3.04065400
F	-5.28248300	-2.58644600	-0.71516300	H	0.31356700	2.28712400	-2.71672600
F	-6.23324200	-1.33513400	0.78849700	F	2.92932900	5.46070800	0.46559000
F	-4.19530200	-2.03174300	1.08775900	F	2.86275000	4.58796700	-1.52508500
5'				F	4.36620900	3.92442600	-0.09392200
C	1.55388300	-2.51093500	-0.41215700	C	-0.19866600	-0.23021100	4.29637100
C	1.24390200	-3.87571700	-0.48631900	O	0.78616800	1.40955500	2.95755800
C	2.94538900	-2.04208300	-0.42738000	C	-2.30100200	-1.27474300	3.72970100
N	0.58351700	-1.56280200	-0.34442900	H	-3.17497700	-0.64595300	1.88047300
C	-0.09913500	-4.26841900	-0.51090700	H	-4.45618800	2.69731700	1.18298200
C	2.32872800	-4.88894900	-0.54282500	H	-3.62738400	1.79975900	2.46047400
C	4.03009400	-2.92818000	-0.47402200	H	-3.05995500	3.42927700	2.01760200
N	3.12339800	-0.70546400	-0.40670500	C	-2.70887200	3.88495500	-2.53068600
C	-0.70348400	-1.95212600	-0.38343700	H	-4.13922200	3.73950100	-0.91490200
Pd	1.28505200	0.36842700	-0.25511700	H	-1.13155100	3.84385100	-4.00605800
C	-1.08307200	-3.29062200	-0.46667600	C	-1.21472500	-1.13054500	4.59883600
H	-0.34607500	-5.32289900	-0.57053300	H	0.64422700	-0.09200000	4.96734900
C	3.79781100	-4.39156400	-0.51700900	H	0.71414400	1.98734800	2.16513400
O	2.10859600	-6.08376500	-0.60686100	H	-3.10210600	-1.97272200	3.95300300
C	5.32679600	-2.40051000	-0.48959400	H	-3.32044400	4.57479800	-3.10544600
C	4.36699100	-0.20361700	-0.42582300	H	-1.16069700	-1.71414700	5.51368200
H	-1.43961400	-1.16181500	-0.34907900	H	-3.56152500	0.52256300	-0.19601800
C	-0.49381500	1.26287300	-0.07019800	O	-3.83558500	-0.31287300	-0.66977500
O	2.25065600	2.14970800	-0.42893400	C	-5.11590900	-0.58124400	-0.45709800
H	-2.13796600	-3.53753100	-0.49717400	O	-5.91472900	0.08585500	0.15477600
O	4.70114300	-5.20643400	-0.54069600	C	-5.48079500	-1.93313100	-1.10723800
C	5.49725200	-1.02134900	-0.46547000	F	-5.19764000	-1.92674500	-2.42146100
				F	-6.78064500	-2.19679300	-0.95068400

F	-4.77295900	-2.92938800	-0.53378300	F	-3.16897400	3.93578900	-0.32316500
6'				F	-1.76315100	4.57929300	1.21241900
C	2.77259600	-0.42502600	-0.67038000	C	-0.01187900	-2.62916900	3.39064600
C	3.86706800	-1.24050800	-0.98831700	O	-0.96462900	-0.58917600	2.76385500
C	2.95970200	0.96322100	-0.22606700	C	-0.19982200	-4.61742300	2.03010400
N	1.49462300	-0.87452900	-0.77382300	H	-1.25400800	-4.36667700	0.17700700
C	3.63473600	-2.54664800	-1.43342100	H	-3.94821200	-4.22625700	-0.34440900
C	5.25307200	-0.72380500	-0.85603900	H	-3.62460200	-3.57429100	1.27533600
C	4.23199300	1.53246500	-0.07613000	H	-5.01734300	-2.98731800	0.35205200
N	1.83590600	1.66524500	0.02200400	C	-4.86320700	-0.57359100	-3.12747700
C	1.28292700	-2.12735200	-1.21666600	H	-5.45186400	-2.30766600	-1.97855500
Pd	0.06241100	0.51077700	-0.26795700	H	-4.04565800	1.16400600	-4.12348200
C	2.32512800	-2.99019000	-1.55304300	C	0.25651900	-3.97923900	3.18838700
H	4.47669300	-3.18419600	-1.68054800	H	0.32150700	-2.12187200	4.29143500
C	5.44678400	0.73822700	-0.37416200	H	-1.52890300	-0.10070700	2.12259000
O	6.23308300	-1.39802400	-1.11169900	H	0.00397100	-5.67031200	1.86008700
C	4.32505100	2.86247600	0.35139400	H	-5.74260600	-0.60744400	-3.76499300
C	1.92960500	2.93859200	0.43250700	H	0.81752200	-4.53272800	3.93649800
H	0.24764900	-2.43016700	-1.29664700	7'			
C	-1.53665600	-0.66346900	-0.52923400	C	-3.11507500	-0.26497000	-0.87201200
O	-1.12482500	2.13070400	0.07769900	C	-4.34164500	-0.72619800	-1.39226800
H	2.09492100	-3.99083700	-1.90020200	C	-4.34128600	-1.64314800	-2.44798100
O	6.57438600	1.18167700	-0.26164900	C	-3.12998400	-2.07890400	-2.96498600
C	3.15938600	3.57354700	0.61101300	C	-1.95910800	-1.57191600	-2.40863300
H	5.30329700	3.31578600	0.47148500	C	-3.08907300	0.69554100	0.26144400
H	0.98939400	3.44815700	0.61600200	C	-4.28932600	1.19553900	0.80858600
C	-1.92736500	-1.77785700	0.20241300	C	-4.21510100	2.09751900	1.87749900
C	-2.56879200	-0.44478900	-1.51092400	C	-2.96978600	2.46401500	2.36679600
C	-2.06123900	2.22891300	0.94189400	C	-1.83495000	1.91356800	1.76409100
H	3.18880100	4.60452200	0.94428100	H	-5.28834600	-1.99399300	-2.84363800
C	-1.19925000	-2.51132200	1.26123300	H	-3.07867300	-2.78805600	-3.78325100
N	-3.16056900	-2.25757900	-0.28148100	H	-0.98786300	-1.87202800	-2.78816100
C	-3.55885400	-1.45706900	-1.32659500	H	-5.13309000	2.48761300	2.30415700
C	-2.75734400	0.50524900	-2.53520000	H	-2.86777400	3.15561900	3.19598800
C	-2.69268500	3.64402300	0.90636400	H	-0.83697300	2.15962600	2.11632900
O	-2.48570300	1.41395900	1.76060400	N	-1.89128000	1.05731900	0.73653000
C	-0.74071500	-1.88646100	2.44630900	N	-1.94569900	-0.69256400	-1.38933000
C	-0.91300800	-3.88130000	1.08736100	C	-5.61177000	0.78145500	0.29476200
C	-3.97891500	-3.32325500	0.27611700	C	-5.63940000	-0.25020300	-0.85335700
C	-4.70859600	-1.52986800	-2.12726200	O	-6.66529900	1.20823100	0.73521600
C	-3.89565200	0.43460300	-3.33186600	O	-6.71203000	-0.63642600	-1.28277100
H	-2.01699500	1.28446700	-2.69733900	Pd	0.16392600	-0.19165200	-0.78434200
F	-3.70300800	3.77212600	1.77855500	O	0.03049500	-1.68256200	0.63280800

C	0.52289400	-1.60967300	1.81036900	C	-3.02811100	0.92273000	-0.15787700
C	0.24496200	-2.90978800	2.60835700	C	-4.17136900	1.69955000	0.11512000
O	1.13809000	-0.70172900	2.36830800	C	-4.01451800	3.03096700	0.51487500
F	0.76472800	-3.98438800	1.97526800	C	-2.73489400	3.55509100	0.63131200
F	-1.08565800	-3.11628600	2.73191200	C	-1.65281400	2.72446200	0.34707900
F	0.76845700	-2.87053900	3.84277400	H	-5.47829600	-2.89540800	-1.24323100
C	0.40494300	1.03923000	-2.15673800	H	-3.34416700	-4.15964400	-1.71586000
O	0.52705300	1.78414800	-3.01825300	H	-1.17497000	-2.95515900	-1.42701700
C	2.16862000	-0.11577500	-0.57930200	H	-4.89566600	3.62763900	0.72556000
C	3.01222500	0.94377300	-0.28958000	H	-2.56448500	4.58160400	0.93554200
C	3.00008300	-1.27447600	-0.77653200	H	-0.63495400	3.08988700	0.42665100
C	2.69772200	2.37387000	-0.08129400	N	-1.79127800	1.44212500	-0.03415900
N	4.33829100	0.48825500	-0.26324900	N	-2.03441600	-1.17423000	-0.84216200
C	4.34699200	-0.85561700	-0.56157000	C	-5.53670400	1.13562300	-0.01074400
C	2.75451200	-2.62006400	-1.11510400	C	-5.67356800	-0.34039400	-0.44666500
C	1.92324400	2.81137700	1.01656400	O	-6.54286500	1.78432800	0.21591600
C	3.18430400	3.34051000	-0.98233200	O	-6.78552100	-0.82984000	-0.54537200
C	5.52745400	1.25098100	0.08482300	Pd	0.06971600	0.24267300	-0.33728700
C	5.42782700	-1.74393800	-0.66177300	C	2.92709600	0.62869800	-0.74131700
C	3.82576100	-3.50048400	-1.22200800	C	1.93499200	0.00951200	-1.53989300
H	1.73840700	-2.96233900	-1.28965200	C	2.39255300	-1.34362500	-1.81012100
C	1.65260500	4.17999400	1.17797600	C	3.62874200	-1.47912600	-1.13707700
O	1.43436700	1.98706500	1.97655400	C	1.88415400	-2.42023800	-2.55104700
C	2.91679000	4.69754100	-0.81959700	C	4.36567400	-2.66724700	-1.16288000
H	3.78025500	3.00445100	-1.82674100	C	2.61714600	-3.60345500	-2.58859300
H	6.14492800	1.45105800	-0.79795300	H	0.94061100	-2.32982200	-3.08140400
H	5.23479500	2.20086700	0.53025100	C	3.84041800	-3.72621900	-1.89973000
H	6.12534500	0.69476800	0.81281700	H	5.30927900	-2.76064900	-0.63565400
C	5.14975700	-3.06658600	-0.99316500	H	2.24089300	-4.44809700	-3.15835500
H	6.44747500	-1.41136100	-0.49207600	H	4.38692800	-4.66345500	-1.94657500
H	3.64395400	-4.53937800	-1.48385200	C	2.99162600	2.04605100	-0.32362400
C	2.14407000	5.11341300	0.27036700	C	2.95617200	2.44209600	1.03375500
H	1.06255400	4.49136000	2.03491700	C	3.09228100	3.03251900	-1.32296700
H	1.51222400	1.02785400	1.77553600	C	3.04860200	3.80856400	1.34819100
H	3.30289200	5.41988600	-1.53226800	C	3.17285000	4.38449700	-1.00119900
H	5.96721600	-3.77704000	-1.08080100	H	3.12260900	2.71769500	-2.36217100
H	1.92422300	6.16758000	0.41557500	C	3.15733000	4.76636000	0.34524000
8'				H	3.02391400	4.09469100	2.39538800
C	-3.16077900	-0.49493300	-0.58940100	H	3.25717200	5.12804600	-1.78744600
C	-4.43051800	-1.09143700	-0.72693500	H	3.22516900	5.81651500	0.61560600
C	-4.50479900	-2.42853200	-1.13657000	O	-0.14584100	-0.58034700	1.73251700
C	-3.33163200	-3.12347700	-1.39629200	C	0.83930100	-1.14265100	2.28744400
C	-2.11800600	-2.45050200	-1.23433200	C	0.41922400	-2.27869600	3.25631300
				O	2.05983500	-0.93995800	2.14942600

F	-0.14065500	-3.29749700	2.55682700	C	-4.35308200	-1.91121800	-0.03819700
F	-0.50012100	-1.85369200	4.14954700	C	-3.66208700	-1.84136800	-2.36501700
F	1.45243400	-2.78780200	3.94857300	C	-0.78036100	0.04741300	2.36743200
H	2.55126800	0.66515300	1.84058200	C	-1.74378100	-1.94033900	3.38342900
C	0.70138300	0.67973800	-2.04157100	C	-4.63817800	-1.67971700	2.42565700
O	0.32381400	1.14914300	-3.08074800	C	-5.64578500	-2.32583100	-0.37877200
N	3.92680400	-0.26880800	-0.51026500	C	-4.94541300	-2.25466700	-2.71265700
C	5.13655700	-0.04556700	0.27342600	H	-2.90874300	-1.66011000	-3.12180400
H	5.27101300	1.02241000	0.43767400	C	-0.07611500	0.27606600	3.56342200
H	5.06771200	-0.55915600	1.23642700	O	-0.59625600	0.88388700	1.31851900
H	5.99778100	-0.42877500	-0.27802100	C	-1.01153400	-1.72492000	4.54882000
O	2.83910200	1.58776600	2.07145600	H	-2.37690500	-2.81859100	3.30973100
10'				H	-4.78299300	-2.69745000	2.80060700
C	3.43325100	-0.71515100	-0.82997500	H	-4.17228600	-1.07429900	3.20061400
C	4.53468000	-1.35374000	-1.42167100	H	-5.61314300	-1.24964900	2.18586700
C	3.62178200	0.37953200	0.13956000	C	-5.92812600	-2.49362600	-1.73183300
N	2.16061000	-1.06730300	-1.13489500	H	-6.39888500	-2.51777200	0.37836400
C	4.31154300	-2.38771400	-2.33758800	H	-5.19493900	-2.39721500	-3.76059000
C	5.92045100	-0.94011500	-1.09022600	C	-0.18914400	-0.59806100	4.64228700
C	4.89910100	0.85571200	0.47617700	H	0.57344000	1.14375900	3.61974200
N	2.50611900	0.91038000	0.67281400	H	-1.63931300	1.67167600	0.73036300
C	1.96006800	-2.05328900	-2.02678900	H	-1.08631100	-2.42623600	5.37416300
C	3.00507600	-2.74076100	-2.64270300	H	-6.91991700	-2.81835300	-2.03338000
H	5.15926000	-2.88745200	-2.79379600	H	0.37355800	-0.40462800	5.55171100
C	6.11370100	0.24164700	-0.10761500	O	-2.40487100	2.25531500	0.30054800
O	6.90116500	-1.48550800	-1.56233800	C	-1.97178800	3.00756800	-0.67551200
C	5.00179400	1.92510300	1.37407600	C	-3.15167900	3.74530700	-1.35074400
C	2.61213700	1.93850100	1.52592000	O	-0.83252500	3.16112300	-1.07264100
H	0.92595300	-2.26949600	-2.25961300	F	-3.84093600	4.48041200	-0.45523400
H	2.78064000	-3.53156900	-3.34930200	F	-4.00791700	2.85976300	-1.90146000
O	7.24106200	0.62183700	0.15104000	F	-2.72147700	4.56489200	-2.31926500
C	3.84257700	2.47995800	1.90130900	11'			
H	5.98339700	2.30318900	1.63938800	C	2.88348000	-1.05200600	0.21718700
H	1.67787500	2.32937300	1.91415800	C	3.87004900	-1.86795600	0.79337500
H	3.87795200	3.31353600	2.59360500	C	3.50608500	-3.11939100	1.30263900
Pd	0.64563400	-0.06883600	-0.03721100	C	2.18056700	-3.51917000	1.21048500
C	-0.92099200	-0.87193300	-0.94003500	C	1.25652000	-2.65882100	0.61869500
C	-2.16604400	-1.24515100	-0.27784900	C	3.22409100	0.26609300	-0.34839000
O	-0.82493000	-0.94792500	-2.16924400	C	4.54334600	0.74671400	-0.36032800
C	-2.49405900	-1.28692700	1.09239900	C	4.80147200	1.98670600	-0.95740700
C	-3.35082400	-1.66305000	-1.00497800	C	3.74975500	2.69791600	-1.52141500
C	-1.66998300	-1.05525100	2.28989800	C	2.46498100	2.15658700	-1.45258800
N	-3.81488400	-1.66901200	1.21909100	H	4.26329500	-3.75262000	1.75235500

H	1.85088200	-4.48188700	1.58418900	C	2.77135300	-0.55542100	-0.44980600
H	0.21807300	-2.93850000	0.49712600	C	4.01418700	-1.14880600	-0.73294400
H	5.81745900	2.36656300	-0.97404300	C	4.04583600	-2.30579300	-1.52043100
H	3.90828800	3.65554100	-2.00434700	C	2.85128000	-2.82810400	-1.99894300
H	1.60633300	2.67244600	-1.86848800	C	1.66066000	-2.17909700	-1.66882900
N	2.20825900	0.97665100	-0.87171600	C	2.67627100	0.67556000	0.36615100
N	1.59005100	-1.44824000	0.13775000	C	3.82945300	1.30179200	0.87156500
C	5.63999500	-0.04202500	0.24601900	C	3.68950000	2.47596400	1.61997100
C	5.28216500	-1.41794000	0.86167100	C	2.41697800	2.98743100	1.83623900
O	6.79552100	0.34064200	0.27779400	C	1.32340300	2.30255700	1.30570300
O	6.16239200	-2.08454900	1.37485700	H	4.99986400	-2.77132600	-1.74420400
Pd	0.23263500	-0.01111900	-0.64151600	H	2.82881300	-3.71949800	-2.61580900
C	-3.12284900	0.65734800	0.26942400	H	0.70507200	-2.55370900	-2.02082100
C	-2.73221700	-0.60713800	-0.21893800	H	4.57405500	2.96498700	2.01376400
C	-3.93235100	-1.42123300	-0.28755500	H	2.26000700	3.89734300	2.40457300
C	-5.00438400	-0.59993200	0.13366900	H	0.31439000	2.67177700	1.45280000
C	-4.20454200	-2.74661200	-0.67110400	N	1.44132100	1.16861800	0.59392600
C	-6.32848500	-1.05094600	0.17890100	N	1.61606800	-1.07190600	-0.91104100
C	-5.51945700	-3.20406800	-0.62812400	C	5.17618900	0.73550300	0.62186400
H	-3.39718200	-3.39319800	-0.99228300	C	5.27291400	-0.56486900	-0.21403500
C	-6.57140400	-2.36650200	-0.20912300	O	6.19817600	1.24453100	1.04652000
H	-7.13684500	-0.40761800	0.51084200	O	6.36809300	-1.05777600	-0.41836800
H	-5.73905700	-4.22721500	-0.92107400	Pd	-0.25795000	-0.05866600	-0.16717700
H	-7.58688600	-2.75135400	-0.18237400	C	-2.26896800	0.40152500	0.34064300
C	-2.33224300	1.84390900	0.62204600	C	-2.23212100	-0.81936100	-0.44570500
C	-1.25487000	2.27972000	-0.20977400	C	-2.58169400	-1.92191700	0.45388300
C	-2.63311500	2.57239800	1.79106300	C	-2.81086600	-1.34231100	1.73067800
C	-0.62731400	3.50732700	0.11352900	C	-2.73300800	-3.29712100	0.26807700
C	-1.96040300	3.74652900	2.11980200	C	-3.13892500	-2.14274100	2.83154600
H	-3.40401800	2.20206500	2.45986400	C	-3.07671800	-4.09625700	1.36415600
C	-0.96984200	4.22596100	1.25417800	H	-2.58323200	-3.72969900	-0.71601900
H	0.15372000	3.86833300	-0.54843400	C	-3.26778900	-3.52095800	2.62884500
H	-2.21173400	4.28373300	3.02921700	H	-3.31838900	-1.71284000	3.81173700
H	-0.45224400	5.15573200	1.47809100	H	-3.19565300	-5.16818100	1.23470400
C	-1.41082300	-1.10821700	-0.57715400	H	-3.53375800	-4.15374700	3.47137200
O	-1.27395400	-2.27405300	-0.96873600	C	-2.66211100	1.65376700	-0.33072500
O	-0.86956800	1.59111900	-1.28206200	C	-2.81844200	1.59726400	-1.73467500
N	-4.49485400	0.65229800	0.45249000	C	-2.88268900	2.89842000	0.29001700
C	-5.37016900	1.78953900	0.72500900	C	-3.14544300	2.72788300	-2.48262500
H	-5.71551900	1.79076200	1.76335000	C	-3.21671100	4.03043000	-0.45180700
H	-4.84471100	2.72047600	0.52199200	H	-2.78381600	2.98619100	1.36468100
H	-6.23859200	1.72924200	0.06450200	C	-3.34321100	3.94990900	-1.84171800
				H	-3.25360400	2.62918900	-3.55839600
				H	-3.37869300	4.97538400	0.05847100

12'

H	-3.60169200	4.82895500	-2.42434700	O	-0.88426400	-3.59064700	1.15350200
C	-2.45357200	-0.80914700	-1.87846500	C	0.63618200	-1.16341200	3.48227800
O	-2.47967000	-1.77773500	-2.62141500	C	2.06284700	0.70148900	2.73805100
O	-2.66382800	0.43224600	-2.46265700	C	4.51557300	-2.37369000	0.95198500
C	-2.55209000	0.88764200	2.84016700	C	3.53164400	-3.03687000	-1.75355600
H	-1.71309000	1.57906900	2.72579900	C	1.64086400	-3.00760000	-3.27981300
H	-3.46538700	1.46267900	3.02864800	H	-0.08527900	-1.89377600	-2.61614600
H	-2.34997400	0.26862400	3.71692600	F	-2.15737700	-5.72738700	0.23922600
N	-2.66930100	0.03912700	1.66295000	F	-1.90749200	-4.81584200	-1.72035700
TS1'				F	-3.66852700	-4.35832000	-0.51990700
C	-1.84006700	2.35728200	-0.27595600	C	0.77694100	-0.69992600	4.80148600
C	-1.75327800	3.75398800	-0.27687100	O	-0.13530200	-2.23664500	3.29795700
C	-3.13499800	1.67157700	-0.31377400	C	2.19642700	1.12804700	4.04399000
N	-0.73029900	1.57265500	-0.25915100	H	2.56906900	1.20936500	1.92333800
C	-0.48866100	4.35374700	-0.27823100	H	5.43302500	-2.22638400	0.36482400
C	-2.98734900	4.58055400	-0.27730900	H	4.67681100	-1.94066000	1.94322000
C	-4.35004900	2.36789400	-0.32393000	H	4.34028900	-3.44715400	1.06535100
N	-3.09281100	0.32357600	-0.35144400	C	2.93126200	-3.43226600	-2.95212200
C	0.48292700	2.15556100	-0.27777000	H	4.54666500	-3.34640000	-1.52799000
Pd	-1.14214500	-0.43603200	-0.25034300	H	1.18587800	-3.31029000	-4.21804800
C	0.63675600	3.54298600	-0.28794100	C	1.54608000	0.42096000	5.07456800
H	-0.41044800	5.43555400	-0.27778900	H	0.27308800	-1.24343700	5.59421300
C	-4.35730000	3.85110600	-0.29235500	H	-0.23911400	-2.53322800	2.35880700
O	-2.96359900	5.79642300	-0.26636800	H	2.79935300	1.99987800	4.27644800
C	-5.54190000	1.63456800	-0.36738500	H	3.48567900	-4.06352500	-3.64110900
C	-4.23508900	-0.37825500	-0.39873000	H	1.64624600	0.75572100	6.10319800
H	1.35539300	1.51030900	-0.28156900	H	3.47480500	-0.69982100	0.29289900
C	0.79341800	-1.11225200	-0.10950900	O	3.50106400	1.05189300	-0.12776700
O	-1.85642200	-2.32119000	-0.47454000	C	4.59611200	1.46977000	-0.60974100
H	1.63648500	3.95854100	-0.29906600	O	5.70061900	0.92208600	-0.68624400
O	-5.38084300	4.50777800	-0.28349000	C	4.47431300	2.91256100	-1.18543300
C	-5.48259100	0.24638200	-0.40687600	F	3.52579300	2.97928100	-2.15499300
H	-6.49113000	2.15950100	-0.37262900	F	5.61915100	3.37786800	-1.72150300
H	-4.13023300	-1.45692600	-0.43203000	F	4.10193700	3.79989500	-0.22109300
C	1.17888500	-0.89988100	1.09925100	TS2'			
C	1.50144100	-1.83274000	-1.16400200	C	-3.14322200	-0.40344200	-0.86233800
C	-1.59488000	-3.39448200	0.16935400	C	-4.36653300	-0.89712700	-1.35900400
H	-6.38244400	-0.35653000	-0.44367200	C	-4.36058900	-1.94509400	-2.28456000
C	1.28776700	-0.45428900	2.42274500	C	-3.14649100	-2.47542700	-2.69617600
N	3.35157100	-1.73050800	0.35347200	C	-1.97862100	-1.93392100	-2.16637700
C	2.83715000	-2.21373500	-0.85913400	C	-3.12038200	0.69813100	0.13376900
C	0.92759100	-2.20742200	-2.38558700	C	-4.32195600	1.26023700	0.61266800
C	-2.34069900	-4.60004900	-0.45991500	C	-4.25142000	2.28201600	1.56782200

C	-3.00780700	2.69981600	2.01834600	C	5.25674300	-2.82976400	-1.18887000
C	-1.87091600	2.08409500	1.48724700	H	6.45217400	-1.12678600	-0.59520700
H	-5.30466100	-2.32267800	-2.66231600	H	3.84568000	-4.36124800	-1.76593500
H	-3.09054200	-3.28786900	-3.41171400	C	1.83484800	5.16103000	0.11863700
H	-1.00713000	-2.31196800	-2.46470300	H	0.89421800	4.54034500	1.96123600
H	-5.17040500	2.72184300	1.94055100	H	1.52235800	1.09367100	1.80808300
H	-2.90795500	3.48138700	2.76362800	H	2.87085200	5.47332700	-1.75729500
H	-0.87664000	2.36441900	1.82174000	H	6.11240600	-3.49273500	-1.27975000
N	-1.92308200	1.11583800	0.56414300	H	1.56572700	6.20593100	0.24658000
N	-1.97039400	-0.92677100	-1.27230200				
C	-5.64183000	0.80009100	0.13184400	TS3'			
C	-5.66523700	-0.33797900	-0.91133200	C	3.26020900	-0.50652600	-0.80298200
O	-6.69690500	1.27311200	0.51812700	C	4.43124100	-1.24226900	-1.04324800
O	-6.73598400	-0.74287300	-1.32828500	C	4.35595900	-2.42478700	-1.78825200
Pd	0.08353300	-0.32511700	-0.66775400	C	3.11993100	-2.82042000	-2.28565100
O	-0.13779600	-1.51914500	1.08189100	C	1.99711900	-2.03705900	-2.00794500
C	0.62300500	-1.44925700	2.09784100	C	3.29979000	0.76772400	-0.06395500
C	0.48321700	-2.69871900	3.00586800	C	4.51067800	1.30008700	0.41344600
O	1.42575100	-0.57442000	2.44319600	C	4.48341000	2.53874200	1.06949800
F	0.92019300	-3.80185900	2.35227100	C	3.27177500	3.20064300	1.21874400
F	-0.80624000	-2.91659200	3.34454100	C	2.11141100	2.59425100	0.72252900
F	1.19100800	-2.59549800	4.14233400	H	5.26209200	-2.99079600	-1.97000300
C	0.82759200	0.39424400	-2.18547200	H	3.01111600	-3.71682800	-2.88551400
O	1.07331200	0.79477500	-3.24934100	H	1.01423100	-2.28042500	-2.40376400
C	2.11545400	-0.05867600	-0.74112700	H	5.41597100	2.95258200	1.44187600
C	2.90655500	1.03809000	-0.38859900	H	3.20791200	4.16313700	1.71292000
C	3.01646300	-1.16594100	-0.96730200	H	1.13840200	3.07365000	0.80220000
C	2.51661000	2.44995900	-0.18478700	N	2.12918500	1.40664700	0.10798200
N	4.23437600	0.65112500	-0.35342600	N	2.05403000	-0.91593600	-1.27037500
C	4.32679100	-0.68647400	-0.70275700	C	5.79471900	0.57674600	0.23204400
C	2.84439100	-2.50616200	-1.35518900	C	5.74906600	-0.77429300	-0.52999700
C	1.78246800	2.87407800	0.94482600	O	6.85580800	0.99755700	0.65022800
C	2.90196600	3.41068800	-1.14034300	O	6.77622100	-1.40457200	-0.69528300
C	5.38043600	1.47117100	0.01845100	Pd	0.37576500	0.20267700	-0.57645100
C	5.45703900	-1.50688900	-0.80354500	O	-0.93238500	1.95725000	-0.43606800
C	3.96495000	-3.32397000	-1.46567500	C	-1.70264100	2.26490300	0.51513700
H	1.85008500	-2.89352000	-1.56068500	C	-2.23960800	3.71516400	0.42334800
C	1.44963800	4.23320600	1.08016900	O	-2.01443800	1.61136200	1.53189000
O	1.38463400	2.06125100	1.95107300	F	-2.60596900	4.04501500	-0.82476300
C	2.56616700	4.75433700	-1.00328400	F	-1.23504200	4.55890300	0.79315000
H	3.47203800	3.08018900	-2.00439800	F	-3.27811300	3.93719400	1.23762900
H	5.98918600	1.71315200	-0.85868300	C	-1.04218500	-0.84925400	-1.43631900
H	5.03175600	2.39594900	0.47540900	O	-0.89059200	-1.17334500	-2.60244900
H	5.99731700	0.93049000	0.74114500	C	-2.31609900	-1.03742700	-0.71834300

C	-2.54028800	-1.51479900	0.56910000	H	-4.58196000	-3.93909000	-0.64782300
C	-3.60429700	-0.75868500	-1.30495300	H	-2.21314400	-3.34095100	-1.14780600
C	-1.59333100	-2.14632100	1.51477500	N	-2.38966200	-1.37339400	-0.55032400
N	-3.90555600	-1.52695100	0.80808500	N	-1.27244700	1.06113200	-0.09467600
C	-4.56913000	-1.04996500	-0.31080900	C	-5.42132900	0.41698500	0.76065300
C	-4.02431700	-0.26813000	-2.55212300	C	-4.80868700	1.82758600	0.93143800
C	-0.45734400	-1.47059000	2.00395300	O	-6.59208300	0.23977000	1.04861600
C	-1.78193300	-3.48646900	1.89983800	O	-5.52016600	2.73968600	1.31451000
C	-4.57484900	-1.81238200	2.06707200	Pd	-0.22997800	-0.73383300	-0.94407900
C	-5.93903800	-0.85180200	-0.52338300	C	3.13064700	-0.33324700	0.50742000
C	-5.38402700	-0.08041400	-2.77103500	C	2.56899500	0.27134500	-0.61705000
H	-3.29503900	-0.05113000	-3.32859900	C	3.01525600	1.63226700	-0.65201400
C	0.45442200	-2.13172000	2.83334900	C	3.84272700	1.80639300	0.49227800
O	-0.18475400	-0.17702100	1.65432700	C	2.81205700	2.70786400	-1.53682100
C	-0.87883400	-4.14238600	2.73087200	C	4.45149400	3.03767700	0.77245600
H	-2.64465300	-4.02547700	1.51109300	C	3.42173400	3.92580700	-1.26029700
H	-5.24690000	-2.67175400	1.96994900	H	2.19567700	2.57458200	-2.41983100
H	-3.83116100	-2.02912700	2.83281500	C	4.23011900	4.08723400	-0.11502400
H	-5.15971900	-0.93775900	2.37918000	H	5.07509900	3.18156500	1.64848400
C	-6.33103300	-0.36564300	-1.76560900	H	3.27749500	4.76606000	-1.93367100
H	-6.67254100	-1.07126000	0.24938300	H	4.69296400	5.05051200	0.08010500
H	-5.72410900	0.29431400	-3.73284600	C	2.93297200	-1.74243100	0.79798700
C	0.24919700	-3.46106400	3.19364500	C	2.22970200	-2.48891500	-0.18619400
H	1.31407400	-1.57275500	3.19691100	C	3.36822300	-2.43757100	1.94662400
H	-1.01460700	0.42189300	1.64910900	C	2.03405300	-3.86689600	-0.04205100
H	-1.04754700	-5.18128100	3.00547200	C	3.15366500	-3.80386000	2.09655300
H	-7.38640500	-0.20403000	-1.96528800	H	3.87306100	-1.90433100	2.73945900
H	0.96346800	-3.95739600	3.84023600	C	2.49456800	-4.52470500	1.09424400
TS4'				H	1.50824500	-4.40055300	-0.82808400
C	-2.58996100	0.92303100	0.16348700	H	3.50282200	-4.30541900	2.99384300
C	-3.36906600	1.99994900	0.62669800	H	2.33199500	-5.59327000	1.20071600
C	-2.76240900	3.24719900	0.81290700	C	1.70287300	-0.41698800	-1.57173000
C	-1.40779400	3.38225200	0.53914600	O	1.54968000	-0.11422800	-2.77543300
C	-0.70328700	2.26441900	0.09297400	O	1.72960400	-1.92815300	-1.33297200
C	-3.19208300	-0.41147900	-0.05689000	N	3.90665700	0.60112400	1.18100000
C	-4.54509600	-0.65790700	0.24247700	C	4.75087900	0.38281200	2.34976500
C	-5.06149000	-1.94162800	0.03252900	H	4.15197200	0.20529500	3.24764600
C	-4.22508200	-2.93089300	-0.46891100	H	5.42484600	-0.46136800	2.18613200
C	-2.89887300	-2.60009400	-0.74858500	H	5.35940700	1.27104300	2.51350500
H	-3.35808700	4.08089700	1.16923300	cat2			
H	-0.89302000	4.32747000	0.67095900	Pd	0.00224500	0.32406700	-0.10871100
H	0.35766900	2.32702300	-0.12251300	O	1.51663100	1.83311300	0.19617200
H	-6.10302300	-2.13899400	0.26309000	P	1.12225300	-1.25698900	1.07527600

P	-1.29947500	-1.55110100	-0.14889100	C	-5.31094800	-1.91728500	0.69458000
C	-0.15062000	-2.58565600	0.87366700	H	-6.21655200	-2.20885800	0.17333500
H	0.22033000	-3.46898100	0.35082600	C	-4.09029700	-1.91388700	0.01601800
H	-0.59263800	-2.88526500	1.82712600	H	-4.05267500	-2.21316200	-1.02851800
C	1.34343600	-0.89069500	2.84562400	S	2.46121300	2.67187900	-0.65516400
C	1.50637200	0.43751000	3.27084300	O	1.83891700	3.84805800	-1.27899500
H	1.49398700	1.25151900	2.55373600	O	3.75888600	2.86291200	0.02920900
C	1.69330600	0.70967300	4.63043600	C	2.88068500	1.54026400	-2.08844500
H	1.81546800	1.73195200	4.96118300	F	3.70451000	0.55530800	-1.68100100
C	1.72045200	-0.33350300	5.55671300	F	3.49844400	2.24943800	-3.04346800
H	1.86087500	-0.12623800	6.61391500	F	1.78212800	0.96904600	-2.63384500
C	1.56443600	-1.66105000	5.12820500	O	-1.11545000	1.76204300	-1.23677900
H	1.58396300	-2.47113000	5.85007800	S	-2.51023000	2.32400000	-1.01872300
C	1.37379300	-1.94501900	3.77814500	O	-2.77815400	3.46852100	-1.89280900
H	1.24711600	-2.96944600	3.45271100	O	-3.55635300	1.29289900	-0.90046100
C	2.70468400	-1.83787700	0.38082200	C	-2.39005000	3.05839500	0.69530000
C	2.70571600	-2.46524200	-0.88551300	F	-2.05728300	2.12499800	1.60495500
H	1.77428900	-2.59817900	-1.43849800	F	-3.56452200	3.59381100	1.04717600
C	3.90365400	-2.90230900	-1.43895300	F	-1.45385000	4.02044800	0.72760800
H	3.90491200	-3.38674300	-2.41225100				
C	5.10903500	-2.71714400	-0.74873000	4-L2			
H	6.04725600	-3.05384300	-1.18359800	Pd	-1.14517900	0.06372100	-0.04889900
C	5.11047000	-2.07795700	0.49773900	C	1.03596300	-1.37943500	-0.01981300
H	6.04165300	-1.93128400	1.03863200	C	0.75131200	-0.56480500	-0.94286300
C	3.91543000	-1.63987100	1.06824300	C	1.25090900	-2.30052800	0.99858100
H	3.92065000	-1.16175000	2.04113400	C	1.33370000	-0.01391500	-2.15527100
C	-1.46997600	-2.30262700	-1.79900100	C	0.79080300	-3.66921100	0.87039000
C	-1.62865600	-3.69147600	-1.91999900	C	1.97667900	-1.90977300	2.16455400
H	-1.64042900	-4.32863700	-1.04399200	C	2.72506600	-0.19239200	-2.38494700
C	-1.76433800	-4.25958600	-3.18949400	C	0.57111600	0.68665800	-3.10533000
H	-1.88574600	-5.33769200	-3.28821000	C	1.06630400	-4.55968200	1.94385500
C	-1.74638400	-3.45094800	-4.32720000	N	0.13148000	-4.08051500	-0.22939400
H	-1.85754300	-3.89999700	-5.30870900	C	2.23271500	-2.80304400	3.17964500
C	-1.59974600	-2.06503300	-4.20368600	H	2.33004700	-0.88578400	2.22141500
H	-1.58439000	-1.43839900	-5.08745600	C	3.31195500	0.36454700	-3.53246900
C	-1.45761100	-1.49176800	-2.94214700	C	1.15700300	1.21840000	-4.25128500
H	-1.34177200	-0.41396800	-2.84956800	H	-0.49412400	0.79593200	-2.93310400
C	-2.91758500	-1.54090500	0.69191800	C	1.76377400	-4.13129900	3.05630600
C	-2.98124100	-1.15231800	2.04225100	H	0.73085900	-5.58811200	1.88235600
H	-2.07872600	-0.85182200	2.56948000	C	-0.39402500	-5.42133000	-0.42590400
C	-4.19946300	-1.15316900	2.71068000	H	2.78880300	-2.49774600	4.05961400
H	-4.23950000	-0.85910500	3.75052100	C	2.53292800	1.06185100	-4.45343100
C	-5.36817000	-1.53797400	2.03800700	H	4.37842800	0.23587200	-3.69093100
H	-6.32014200	-1.53186300	2.56557900	H	0.55010200	1.75153100	-4.97648500

H	1.96038000	-4.84145200	3.85501000	C	-1.01235900	3.43818000	-1.37246100
H	-1.11307200	-5.69296200	0.35591600	H	-1.48062900	2.52454700	-1.72217500
H	-0.90403500	-5.44271000	-1.38882400	C	1.16096700	1.98556200	1.90093600
H	0.40624600	-6.17019000	-0.43597100	C	1.17471200	1.99267500	3.30426600
H	3.00436100	1.48000000	-5.33868700	H	0.25178700	2.01710800	3.87304800
H	-0.07464800	-3.40540700	-0.95809900	C	2.39300500	1.98407700	3.98757200
O	3.42297000	-0.90804800	-1.48695400	H	2.39604500	1.99469500	5.07351000
H	4.40210800	-0.83474600	-1.63993700	C	3.59660700	1.96776500	3.28026400
P	-2.95192600	0.98324200	1.13400200	H	4.54144700	1.95806300	3.81600800
P	-0.38911100	1.98296400	0.94595800	C	3.58839600	1.96494100	1.88161300
C	-1.84894300	2.14678700	2.07868500	H	4.51877200	1.95302300	1.32283400
H	-2.21001700	3.16507400	2.23464700	C	2.37646700	1.97005700	1.19256600
H	-1.61756900	1.68452600	3.04151300	H	2.38029200	1.96954900	0.10696900
C	-3.83173200	-0.06434700	2.34765700	O	-2.19044100	-1.70751600	-0.72770900
C	-4.29376300	-1.32732800	1.94129300	S	-2.35278100	-2.07651300	-2.19098800
H	-4.10499300	-1.67977500	0.93276600	O	-2.79131500	-0.96211400	-3.04676900
C	-4.99735400	-2.13177100	2.83893800	O	-1.25565500	-2.92543000	-2.69828800
H	-5.35121000	-3.10818100	2.52105700	C	-3.82076800	-3.21358000	-2.06613600
C	-5.23879100	-1.68631000	4.14093100	F	-3.53000600	-4.26688000	-1.29308100
H	-5.78254000	-2.31651600	4.83869000	F	-4.15673400	-3.64738600	-3.28516900
C	-4.77972000	-0.43059300	4.54695500	F	-4.86566200	-2.56376100	-1.53463100
H	-4.96788000	-0.08081400	5.55779900	O	6.07045000	-0.69388200	-1.72707100
C	-4.07675200	0.38238200	3.65623400	S	6.71177200	0.26779500	-0.77007300
H	-3.72853100	1.35704700	3.98443400	O	8.17675900	0.35799600	-0.90544600
C	-4.20370700	1.95828600	0.22914300	O	5.98554800	1.54621600	-0.61659700
C	-4.89325800	3.00124400	0.86907300	C	6.45916700	-0.57826500	0.86527500
H	-4.67219300	3.25578100	1.90161500	F	5.15847700	-0.85623900	1.06280100
C	-5.86952500	3.71516800	0.17473900	F	6.87457900	0.20827200	1.87311700
H	-6.39919600	4.52325900	0.67066300	F	7.14544100	-1.73020600	0.92180900
C	-6.16494900	3.39149500	-1.15335300				
H	-6.92606800	3.95035600	-1.69020800	5-L2			
C	-5.48314100	2.35233700	-1.78974000	Pd	-1.03246700	0.05481000	-0.15391000
H	-5.71049000	2.10034700	-2.82149900	C	1.86631100	-0.65330900	-0.38370000
C	-4.50065800	1.63398800	-1.10365900	C	0.85024700	0.05254900	-0.94779000
H	-3.96967800	0.82970300	-1.60476900	C	2.02288400	-1.39761000	0.87834800
C	-0.36602400	3.46077600	-0.12761300	C	1.36695600	0.54579800	-2.21814800
C	0.24646700	4.64331200	0.32081500	C	2.15799900	-2.81876600	0.87857300
H	0.75390000	4.67270800	1.27974800	C	2.03619900	-0.70110400	2.09476200
C	0.20519100	5.78946300	-0.47311600	C	2.68972800	0.07952900	-2.34050400
H	0.68095200	6.70082400	-0.12326800	C	0.84065200	1.31675300	-3.26842100
C	-0.44187300	5.76472300	-1.71199100	C	2.32886800	-3.47027500	2.11868500
H	-0.46792500	6.65898300	-2.32782400	N	2.13763700	-3.51553800	-0.31603700
C	-1.05065800	4.59056900	-2.15997500	C	2.19430900	-1.36098000	3.31521800
H	-1.55075500	4.56651000	-3.12359700	H	1.93930600	0.38015300	2.07154000

C	3.51344800	0.33288900	-3.42909800	H	-4.10382100	-0.50620800	-1.55304900
C	1.64577000	1.58962100	-4.37438700	C	-1.73290500	3.41332000	-0.73606100
H	-0.17555000	1.69332700	-3.21880800	C	-1.71918300	4.79391100	-0.47788300
C	2.34890300	-2.74918100	3.31187600	H	-1.29907500	5.17684500	0.44717000
H	2.43705600	-4.54855200	2.14836600	C	-2.24645800	5.68278200	-1.41523800
C	2.02406300	-4.96570300	-0.34271300	H	-2.23139900	6.74934500	-1.21064600
H	2.20885100	-0.80092400	4.24521000	C	-2.78877000	5.20448900	-2.61168300
C	2.96397300	1.10610200	-4.45508900	H	-3.19457600	5.90068300	-3.33998700
H	4.52948700	-0.04392600	-3.47576600	C	-2.80471100	3.83266000	-2.87207000
H	1.24835200	2.18573200	-5.19106200	H	-3.22112400	3.45626900	-3.80187000
H	2.48186000	-3.28457400	4.24864100	C	-2.27627000	2.93779300	-1.93890100
H	1.14515400	-5.34298000	0.20143900	H	-2.28135600	1.87116300	-2.14241800
H	1.94618000	-5.28346600	-1.38432400	C	0.29101800	3.05871400	1.35056200
H	2.91578800	-5.43630100	0.08468100	C	0.17885300	3.56183200	2.65602200
H	3.56733800	1.33414700	-5.32883100	H	-0.74758800	3.46716300	3.21211900
H	1.61084200	-3.06402300	-1.05703300	C	1.26521900	4.20743500	3.25212300
O	3.02028700	-0.65975200	-1.22939900	H	1.16839600	4.59518900	4.26195300
H	4.48449700	-1.09879600	-0.67244000	C	2.46414100	4.35678600	2.55340600
P	-3.09946600	0.34972200	1.03870600	H	3.30709000	4.85748600	3.02074500
P	-1.10665300	2.22983800	0.51522500	C	2.57857900	3.86261100	1.25049900
C	-2.48360400	1.96920400	1.73784900	H	3.51021800	3.97322400	0.70425300
H	-3.20140700	2.78826200	1.81670600	C	1.49978600	3.21471500	0.64920600
H	-2.04927900	1.76460500	2.72038500	H	1.59864300	2.83454600	-0.36262900
C	-3.52983800	-0.71848900	2.46433500	O	-1.18970300	-2.07349500	-0.52116000
C	-3.41903700	-2.11028200	2.30948700	S	-1.32679900	-2.64561600	-1.91748400
H	-3.06740400	-2.52752700	1.37095400	O	-2.22987800	-1.87969900	-2.79545600
C	-3.76022400	-2.96015600	3.36373800	O	-0.05163900	-3.09894300	-2.50704700
H	-3.67170200	-4.03544800	3.23787500	C	-2.24651900	-4.21357200	-1.51906900
C	-4.20494200	-2.42923000	4.57678800	F	-1.52548000	-4.98391400	-0.69429800
H	-4.46486500	-3.09160400	5.39749800	F	-2.49063600	-4.89506100	-2.64453700
C	-4.31249200	-1.04466700	4.73616800	F	-3.41605400	-3.92986000	-0.92581000
H	-4.65772000	-0.62914400	5.67850300	O	5.33775600	-1.38280900	-0.21662900
C	-3.97782600	-0.18929000	3.68524300	S	6.42134300	-0.21919500	-0.18254900
H	-4.06493700	0.88457200	3.82074300	O	7.66285700	-0.79847100	0.30493600
C	-4.66857100	0.69693400	0.15512300	O	6.37461000	0.58443900	-1.39950900
C	-5.67037100	1.50294900	0.72099600	C	5.73521600	0.85391700	1.17950600
H	-5.52428400	1.95812000	1.69665500	F	4.52413200	1.29036100	0.82102400
C	-6.86205000	1.72320200	0.03031200	F	6.55000100	1.89247600	1.35616200
H	-7.63203300	2.34973000	0.47136300	F	5.64231300	0.15643500	2.30809400
C	-7.06520100	1.13906400	-1.22435300				
H	-7.99462000	1.31279400	-1.75925600				
C	-6.07385500	0.33464600	-1.78930300				
H	-6.22779900	-0.11924800	-2.76422700				
C	-4.87566300	0.11346700	-1.10481300				
				TS1-L2			
				Pd	1.04997800	-0.13808500	-0.06482400
				C	-1.52657200	1.24022800	-0.22813800
				C	-0.77802900	0.39031200	-0.89947200

C	-1.77361800	2.03348900	0.93277700	C	4.52326200	-1.32799700	0.20077300
C	-1.28244400	0.05393500	-2.23068400	C	5.54299300	-2.04952700	0.84480700
C	-1.44405500	3.43323900	0.95547500	H	5.41898900	-2.37542300	1.87381500
C	-2.36216600	1.43567800	2.07113100	C	6.72315500	-2.34381800	0.16343400
C	-2.47404500	0.74769300	-2.50753300	H	7.50917000	-2.90167600	0.66416900
C	-0.75223000	-0.79691400	-3.20717100	C	6.89546200	-1.91946600	-1.15869100
C	-1.71141200	4.15290300	2.14745900	H	7.81730200	-2.14913300	-1.68550300
N	-0.91043600	4.04372600	-0.13565400	C	5.88599500	-1.19961900	-1.79950600
C	-2.60621100	2.16027400	3.22685800	H	6.01852500	-0.86683500	-2.82504200
H	-2.61905700	0.38377600	2.01984200	C	4.69877500	-0.90100400	-1.12396000
C	-3.16060000	0.61286000	-3.70721300	H	3.91828300	-0.33565500	-1.62462900
C	-1.42991400	-0.94929600	-4.41967100	C	0.65619700	-3.49030200	-0.90881900
H	0.17142300	-1.33371100	-3.01661800	C	-0.49059800	-4.20165400	-1.29351100
C	-2.27564300	3.52552200	3.24832000	H	-1.42017600	-4.08584900	-0.74704300
H	-1.47203400	5.20858700	2.19892900	C	-0.44068600	-5.07289700	-2.38401400
C	-0.41885500	5.41062700	-0.13181700	H	-1.33302700	-5.62214100	-2.66960600
H	-3.05116800	1.68374100	4.09423900	C	0.74741900	-5.24127000	-3.09689200
C	-2.62198200	-0.25597800	-4.66358600	H	0.78354700	-5.92152600	-3.94281300
H	-4.07669100	1.16376700	-3.89371300	C	1.89183400	-4.53367100	-2.71786400
H	-1.02766700	-1.61153100	-5.18043100	H	2.82084300	-4.66226200	-3.26561900
H	-2.46530900	4.11094400	4.14439200	C	1.84984100	-3.65864300	-1.63264900
H	0.34540100	5.58010800	0.63878000	H	2.74882100	-3.11745400	-1.35557300
H	0.02473000	5.61263900	-1.10742100	C	-0.83459400	-2.79604500	1.52285100
H	-1.23265000	6.12655200	0.03045300	C	-0.66678000	-3.75196800	2.53987000
H	-3.13770200	-0.38513700	-5.61060200	H	0.30847600	-4.18267700	2.74335900
H	-0.56546500	3.45639900	-0.88677600	C	-1.76383800	-4.16657600	3.29551600
O	-2.83530900	1.58546600	-1.47991600	H	-1.62527100	-4.90300900	4.08151800
H	-3.84013100	1.47350800	-1.16566900	C	-3.03257600	-3.64116400	3.03879200
P	2.96299600	-0.93791000	1.07579200	H	-3.88413800	-3.96668200	3.62930100
P	0.59643200	-2.31149600	0.49509500	C	-3.20686800	-2.70121600	2.02090700
C	2.13695600	-2.55532700	1.50866900	H	-4.19030800	-2.29428600	1.81160200
H	2.71098500	-3.44954400	1.25701600	C	-2.11229400	-2.27366400	1.26563500
H	1.87783100	-2.57953700	2.56956500	H	-2.26164000	-1.54301000	0.47906100
C	3.41859100	-0.09076200	2.63218800	O	1.81208100	1.85073600	-0.45262500
C	3.50616400	1.31202900	2.60667300	S	2.04024700	2.38052900	-1.85622500
H	3.28940500	1.85400700	1.69057500	O	2.67100700	1.41408300	-2.77104300
C	3.87239500	2.01047200	3.75828700	O	0.90037100	3.15337800	-2.38922300
H	3.93656900	3.09442800	3.73215400	C	3.35405700	3.64708500	-1.49233900
C	4.14600600	1.31821900	4.94067100	F	2.88590300	4.57639800	-0.64976100
H	4.42453000	1.86373500	5.83771600	F	3.73342400	4.24334000	-2.62781000
C	4.05787000	-0.07590800	4.97034700	F	4.42104600	3.05821500	-0.93504600
H	4.27111700	-0.61707600	5.88764800	O	-5.20788900	1.36137400	-0.79017800
C	3.69628700	-0.78261100	3.82161100	S	-5.79235600	-0.02537700	-0.61427500
H	3.63635300	-1.86569200	3.86156200	O	-7.02701500	-0.24039800	-1.38226200

O	-4.77411500	-1.09150000	-0.65082200	H	-6.53596800	4.34485300	-0.22843100
C	-6.35182800	0.02297800	1.15536000	C	-6.47264800	2.65190900	-1.56563700
F	-5.32201400	0.28576800	1.97444500	H	-6.16862600	0.85899300	-2.72885900
F	-6.86665600	-1.16811000	1.49959000	H	0.37624500	6.56274100	-1.63825600
F	-7.28937700	0.96167400	1.33489000	C	-0.84692100	5.29340200	-2.88419900
				H	-2.04001900	3.80741800	-3.89824400
4'-L2				H	2.45179200	3.16079800	4.42370400
Pd	-1.17087700	0.08971400	-0.09089700	C	3.57828400	2.92216900	2.59853800
P	-2.94588800	1.13036900	0.99637500	H	4.42598400	2.61692100	0.63733700
P	-0.46929400	2.18340700	0.51851900	H	-5.20156000	-1.70785200	5.40432400
C	-1.90567600	2.52915400	1.63620800	H	-7.30753800	2.99736700	-2.16830900
C	-3.63856000	0.22876600	2.42606300	H	-0.95019900	6.03243500	-3.67336400
C	-4.32002700	1.77066500	-0.01789400	H	4.53919300	3.09342900	3.07468600
C	-0.57003200	3.38765000	-0.85385700	F	6.68943100	1.68463100	-0.05427300
C	1.10498100	2.47180800	1.37544100	C	7.04217600	0.39209000	-0.20811200
H	-2.31608500	3.53771900	1.56178600	S	5.99565100	-0.72201600	0.84869300
H	-1.64505600	2.31223600	2.67477200	F	6.91697700	0.08709800	-1.51268000
C	-3.85849700	-1.15439300	2.32567700	F	8.34226200	0.28326300	0.11799600
C	-3.98378100	0.91223900	3.60368700	O	6.21782700	-0.19762200	2.21329300
C	-4.96546400	2.97544400	0.30257600	O	6.55413600	-2.06633200	0.57877300
C	-4.75678100	1.00723500	-1.11276500	O	4.63146800	-0.49138800	0.30419300
C	0.04150100	4.64652000	-0.72584200	H	3.28420600	-1.34412300	-1.09795900
C	-1.32090500	3.09142300	-2.00178100	N	3.22838000	-1.74771200	-2.02852200
C	1.16953900	2.72761500	2.75413100	C	2.31420300	-1.18222400	-2.88578900
C	2.28638100	2.43573300	0.61306200	C	4.51904400	-2.22491000	-2.50345600
H	-3.58895000	-1.68691600	1.42035100	C	1.07582300	-0.64839600	-2.39524400
C	-4.42389100	-1.84591100	3.39828500	C	2.53159900	-1.14706900	-4.28194200
C	-4.54609000	0.21023200	4.67049400	H	5.11390500	-1.44174300	-2.99516400
H	-3.81986800	1.98159300	3.69654300	H	5.08273600	-2.58883100	-1.64371800
H	-4.63852600	3.57228500	1.14866000	H	4.38885700	-3.05076300	-3.21052300
C	-6.03891300	3.41138700	-0.47526000	C	0.76075600	-0.75104100	-0.99299700
C	-5.83388700	1.45044500	-1.88175300	C	0.15021000	-0.09475700	-3.29807500
H	-4.25926800	0.07440100	-1.35854400	C	1.58997300	-0.60248800	-5.14891400
H	0.62242300	4.89227800	0.15677600	H	3.45470900	-1.54571300	-4.68555500
C	-0.09996000	5.59229300	-1.74153500	C	0.94810100	-1.19157300	0.16031000
C	-1.45917200	4.04481200	-3.01196800	C	0.39201900	-0.06408100	-4.66653400
H	-1.79613000	2.12162600	-2.10178800	H	-0.77856100	0.29542800	-2.89748000
H	0.27281400	2.76196100	3.36240300	H	1.80053100	-0.59154800	-6.21511600
C	2.40733000	2.95565500	3.35837100	C	1.18231100	-1.65389500	1.47805600
C	3.51678300	2.66342100	1.22581900	H	-0.34021500	0.36293300	-5.34426600
H	2.24591600	2.23506800	-0.45307500	C	0.56917200	-2.84549900	1.96563000
H	-4.59075100	-2.91597000	3.31728800	C	2.06719900	-0.94038300	2.32998500
C	-4.76576400	-1.16640400	4.56977900	C	0.82486500	-3.25810200	3.28258300
H	-4.81140000	0.74108600	5.57998200	O	-0.25889500	-3.61813900	1.24500900

C	2.31674100	-1.37036600	3.62155500	H	3.31012300	-1.40418200	4.78766500
H	2.56336300	-0.06451800	1.93270200	H	3.47345400	-2.12958800	-4.79987600
C	1.68254200	-2.53027400	4.09663100	H	1.20389300	-2.22921400	5.85421400
H	0.34626800	-4.16453000	3.63923100	H	3.57495300	-1.70449000	0.12696300
H	-0.35160300	-3.35930800	0.30154800	O	7.32213800	-0.11064000	0.52951700
H	3.00247300	-0.81859100	4.25602700	S	6.11523500	-0.50541600	-0.21615700
H	1.87103500	-2.87356100	5.10992800	O	6.31921100	-1.29945300	-1.44277900
O	-1.03120200	-3.55428100	-1.37183400	O	5.00287400	-1.00887100	0.65993400
S	-2.25115800	-2.76163600	-1.65585300	C	5.42498900	1.10378900	-0.83853800
O	-2.42660700	-1.58648000	-0.71589300	F	5.27225700	1.98509600	0.16602300
O	-2.53214900	-2.46591800	-3.06476400	F	4.22158200	0.91781000	-1.41298800
C	-3.66859000	-3.82631600	-1.08629400	F	6.24430400	1.64835600	-1.74920100
F	-3.68333700	-4.96788400	-1.78107800	O	-1.11993700	-3.70540100	-0.67465800
F	-4.82670400	-3.18351600	-1.27686400	S	-2.10862500	-3.01347700	-1.53315000
F	-3.54274800	-4.11173700	0.21626200	O	-2.32292500	-1.56379800	-1.15667800
5'-L2				O	-2.01540400	-3.25062700	-2.97853500
Pd	-1.11636200	-0.06442800	-0.13416800	C	-3.74854500	-3.74099600	-1.03565000
C	0.66793700	-1.03674100	-0.39898000	F	-3.76825800	-5.04770000	-1.32040200
C	1.48220400	-1.62647500	0.51224000	F	-4.74466900	-3.13694700	-1.69437300
C	1.26469100	-1.23792200	-1.73019100	F	-3.95015800	-3.58622600	0.28218300
C	1.39803600	-1.80475300	1.97213800	P	-2.96451200	1.38595300	0.34992000
N	2.69968900	-2.21808200	-0.17967900	P	-0.24493600	1.86669000	0.72075900
C	2.47300700	-1.92938600	-1.59905800	C	-1.86865400	2.55289600	1.30882300
C	0.84249900	-0.87777300	-3.01530800	H	-1.99424200	3.62252100	1.12886200
C	0.22567700	-2.30836600	2.58994300	H	-2.00486600	2.34989500	2.37395200
C	2.50006900	-1.50052700	2.79849600	C	-4.32870400	0.89931500	1.47110600
C	2.93072100	-3.67652500	0.10307700	C	-4.74285500	-0.44084300	1.48746300
C	3.29808400	-2.26194600	-2.65829300	H	-4.24608800	-1.17085800	0.85784600
C	1.64844800	-1.21037500	-4.10854600	C	-5.79351600	-0.83858900	2.31800400
H	-0.09802600	-0.35791800	-3.16260500	H	-6.10758800	-1.87834800	2.32568500
C	0.16774200	-2.43553300	3.98559900	C	-6.42921100	0.09597700	3.13745500
O	-0.88350200	-2.69943800	1.91207300	H	-7.24384200	-0.21414400	3.78558600
C	2.44501000	-1.65239400	4.18080100	C	-6.01578900	1.43224000	3.12737300
H	3.40986200	-1.12354000	2.34275900	H	-6.50796600	2.16012700	3.76598200
H	3.82427600	-3.99100500	-0.43560900	C	-4.96992100	1.83669000	2.29765600
H	3.08202300	-3.80041500	1.17442300	H	-4.65570700	2.87634600	2.29732000
H	2.05952700	-4.23870200	-0.23234100	C	-3.71208100	2.31267900	-1.04198900
C	2.86180800	-1.88755000	-3.93631900	C	-4.12530800	3.64938300	-0.92494400
H	4.24222000	-2.77334900	-2.50947200	H	-3.99038300	4.18954600	0.00744900
H	1.32743300	-0.93862600	-5.11002700	C	-4.71293100	4.29542400	-2.01354500
C	1.26541300	-2.11141400	4.77595500	H	-5.02754800	5.33070900	-1.91814700
H	-0.74582600	-2.82349100	4.42627800	C	-4.89628700	3.61479500	-3.22101400
H	-0.71809800	-2.85741300	0.96008200	H	-5.35365900	4.12203600	-4.06562700
				C	-4.48959200	2.28418500	-3.34169700

H	-4.62827200	1.75248600	-4.27869500	C	-4.04715800	-0.26453400	2.47299000
C	-3.89585600	1.63332800	-2.25794100	C	-5.55341300	0.90645700	0.97051900
H	-3.57495200	0.60002200	-2.35630800	C	-3.81141900	3.93903100	-0.05065100
C	0.35394400	3.03429100	-0.55467100	C	-3.42310300	2.42041700	-1.90956200
C	0.68429700	4.35115700	-0.18783200	C	0.89614600	4.17635200	1.17226500
H	0.61899100	4.66627100	0.84942700	C	1.00139900	2.95731600	-0.92602900
C	1.10325100	5.25898700	-1.15907700	C	0.43413200	0.51792400	3.81494600
H	1.35904400	6.27435500	-0.87079000	C	2.34347600	1.35903100	2.57090400
C	1.19573100	4.86426900	-2.49819500	C	0.36194300	-3.69385900	1.52844800
H	1.52553300	5.57459900	-3.25083700	C	2.33757800	-2.36137900	2.11925200
C	0.86523600	3.55956600	-2.86626000	C	3.52091200	-3.77280400	-1.68557000
H	0.93553900	3.24850200	-3.90446600	C	2.80714500	-1.81948800	-3.80312900
C	0.44358500	2.64496900	-1.89712400	C	1.16839000	-0.17160000	-4.49869600
H	0.18722200	1.63075200	-2.17978400	H	-0.16743700	0.53305700	-2.96016700
C	0.97042200	1.95974600	2.08397900	H	-3.04025700	-0.49723200	2.80857900
C	0.56681900	1.89485800	3.42701700	C	-5.13857300	-0.86961200	3.09376500
H	-0.47729900	1.76420900	3.69007900	C	-6.64133700	0.29079600	1.59404500
C	1.51380100	2.00241100	4.44677300	H	-5.72505000	1.59462700	0.14975000
H	1.19045700	1.96502200	5.48278000	H	-3.79181000	4.15603300	1.01330900
C	2.86668700	2.15952000	4.13726200	C	-4.26553200	4.90880400	-0.94488300
H	3.60031200	2.24673200	4.93344000	C	-3.88265400	3.39562100	-2.79712400
C	3.27590900	2.19505600	2.80227700	H	-3.09798200	1.45418500	-2.28338300
H	4.32705400	2.29982500	2.55364800	H	0.63808600	4.22311300	2.22634600
C	2.33520900	2.09494100	1.77695500	C	1.46442200	5.28703500	0.55131800
H	2.66621500	2.13238400	0.74483600	C	1.57062600	4.07526400	-1.54198700
TS1'-L2				H	0.82395700	2.05410400	-1.49798100
Pd	-1.02737700	0.05530600	-0.19376800	H	-0.62648700	0.30219100	3.89750400
C	0.71675200	-1.00040400	-0.81722100	C	1.27534700	0.20619500	4.88314000
P	-2.79522400	1.39190900	0.60262300	C	3.17762400	1.04107300	3.64349700
P	-0.11451100	1.57004500	1.25570300	H	2.76756200	1.80826200	1.68077300
C	1.09615000	-1.85840100	0.05933700	C	0.55047500	-4.43954700	2.70274100
C	1.23345400	-0.90459300	-2.18607900	O	-0.67980500	-4.03431200	0.75770100
C	-1.73921200	2.17757200	1.91881200	C	2.51937600	-3.12286200	3.25842700
C	-4.25004500	0.63774800	1.41408100	H	3.03254400	-1.57008700	1.86207600
C	-3.38545800	2.68994500	-0.53156500	H	4.48529100	-3.64724600	-2.19705800
C	0.66334200	3.00299400	0.43260100	H	3.70718100	-4.27564000	-0.73242700
C	0.96357800	1.11235900	2.65690600	H	2.87869600	-4.41052700	-2.29869400
C	1.25556000	-2.61918800	1.23187400	C	2.22345100	-1.03457300	-4.80184800
N	2.85220900	-2.50252800	-1.41366800	H	3.64141600	-2.47063600	-4.04298100
C	2.33310900	-1.75027700	-2.48985000	H	0.71823700	0.43794100	-5.27656900
C	0.67540900	-0.10817000	-3.19388100	H	-4.97440700	-1.56091800	3.91517400
H	-1.81558000	3.26266800	2.01606100	C	-6.43733600	-0.59309500	2.65512800
H	-1.96114700	1.71872500	2.88537300	H	-7.64817900	0.50807700	1.24962600
				H	-4.59247200	5.87438800	-0.57047200

C	-4.30043500	4.63864200	-2.31627800
H	-3.90937100	3.18388000	-3.86197500
H	1.64396600	6.19079000	1.12611800
C	1.80191900	5.23766100	-0.80563100
H	1.83256400	4.03260000	-2.59506500
H	0.85733500	-0.24146400	5.77985400
C	2.64534100	0.47136900	4.80212200
H	4.24212000	1.24063400	3.56652100
C	1.61358500	-4.15899400	3.54960900
H	-0.14328400	-5.24565500	2.91865400
H	-0.73758200	-3.54459300	-0.09238800
H	3.35343300	-2.92192900	3.92248500
H	2.60445900	-1.09300100	-5.81752800
H	-7.28623100	-1.06845100	3.13783300
H	-4.65316400	5.39755600	-3.00861300
H	2.24493000	6.10568900	-1.28523500
H	3.29512800	0.23083400	5.63846500
H	1.74806800	-4.75665800	4.44677200
H	3.43382600	-1.91680200	-0.79979100
O	4.68234700	-0.92911100	0.28947000
S	5.82906000	-0.21658200	-0.34803800
O	7.05414600	-0.16560400	0.47455000
O	6.01850300	-0.52278200	-1.78108800
C	5.24199700	1.54469800	-0.35819200
F	5.10392700	2.01790300	0.89652800
F	4.04729500	1.65138500	-0.97221800
F	6.11085700	2.33932500	-1.00352700
O	-1.50251700	-3.31779700	-1.73083800
S	-2.56172600	-2.34620200	-2.08596500
O	-2.24679800	-0.91824800	-1.70518600
O	-3.12864500	-2.45456900	-3.43366800
C	-3.96393000	-2.75376000	-0.93103500
F	-4.41204000	-3.99007300	-1.17223400
F	-4.96909400	-1.88502100	-1.09860000
F	-3.54892900	-2.68721200	0.34389300