

Supporting Information

The underlying factors controlling Pd-catalyzed site-selective alkenylation of aliphatic amines

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I. Complete free energy profiles for the Pd(II)-catalyzed C(sp³)-H alkenylation of aliphatic amines

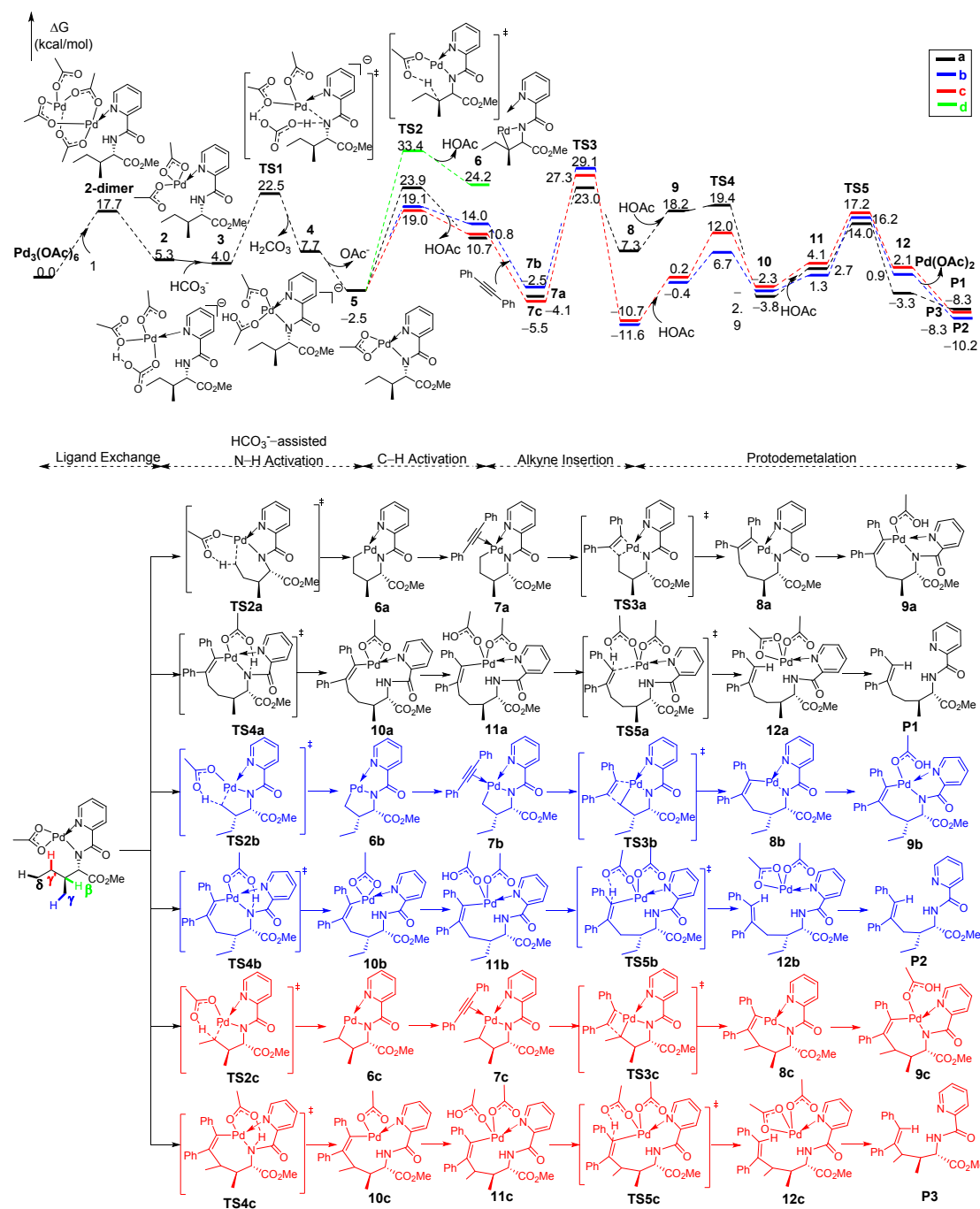


Fig. S1 Complete free energy profiles for the Pd(II)-catalyzed C(sp³)-H alkenylation of aliphatic amines. Energies are relative to **Pd₃(OAc)₆ + 1 + 2a** and are mass balanced

II. Dimeric palladium complexes

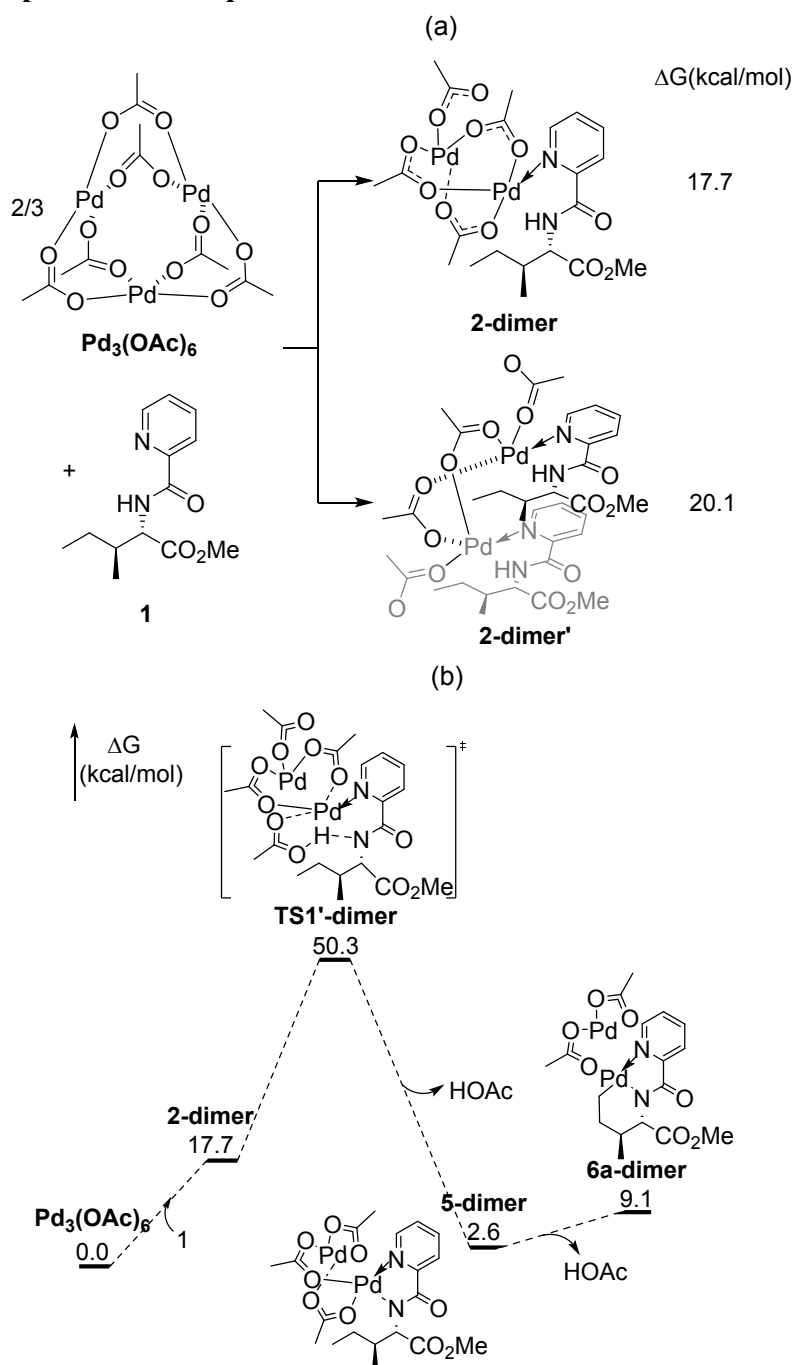


Fig. S2 (a) Two possible dimeric palladium complexes; (b) Free energy profiles for N-H activation of **2-dimer**.

III. HCO_3^- -assisted C–H activation at the δ -site.

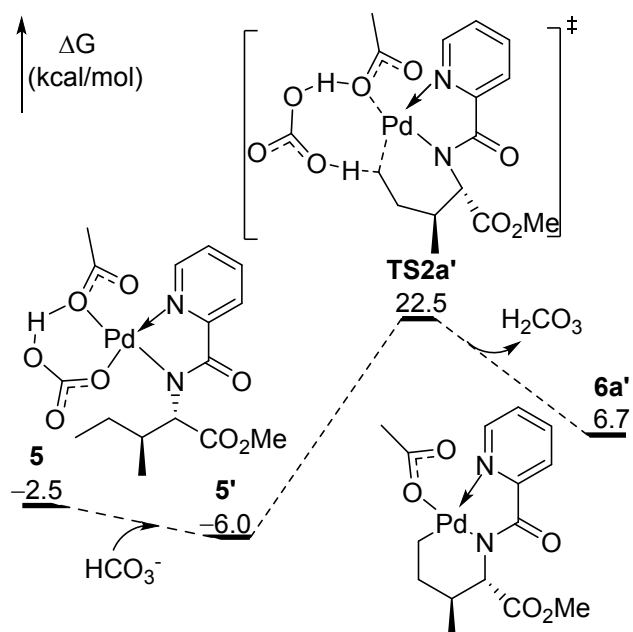


Fig. S3 Free energy profiles for the HCO_3^- -assisted C–H activation at the δ -site. Energies are relative to $\text{Pd}_3(\text{OAc})_6 + \mathbf{1} + \mathbf{2a}$ and are mass balanced.

IV. Free energy profiles for another parallel pathway of the two consecutive protonation steps.

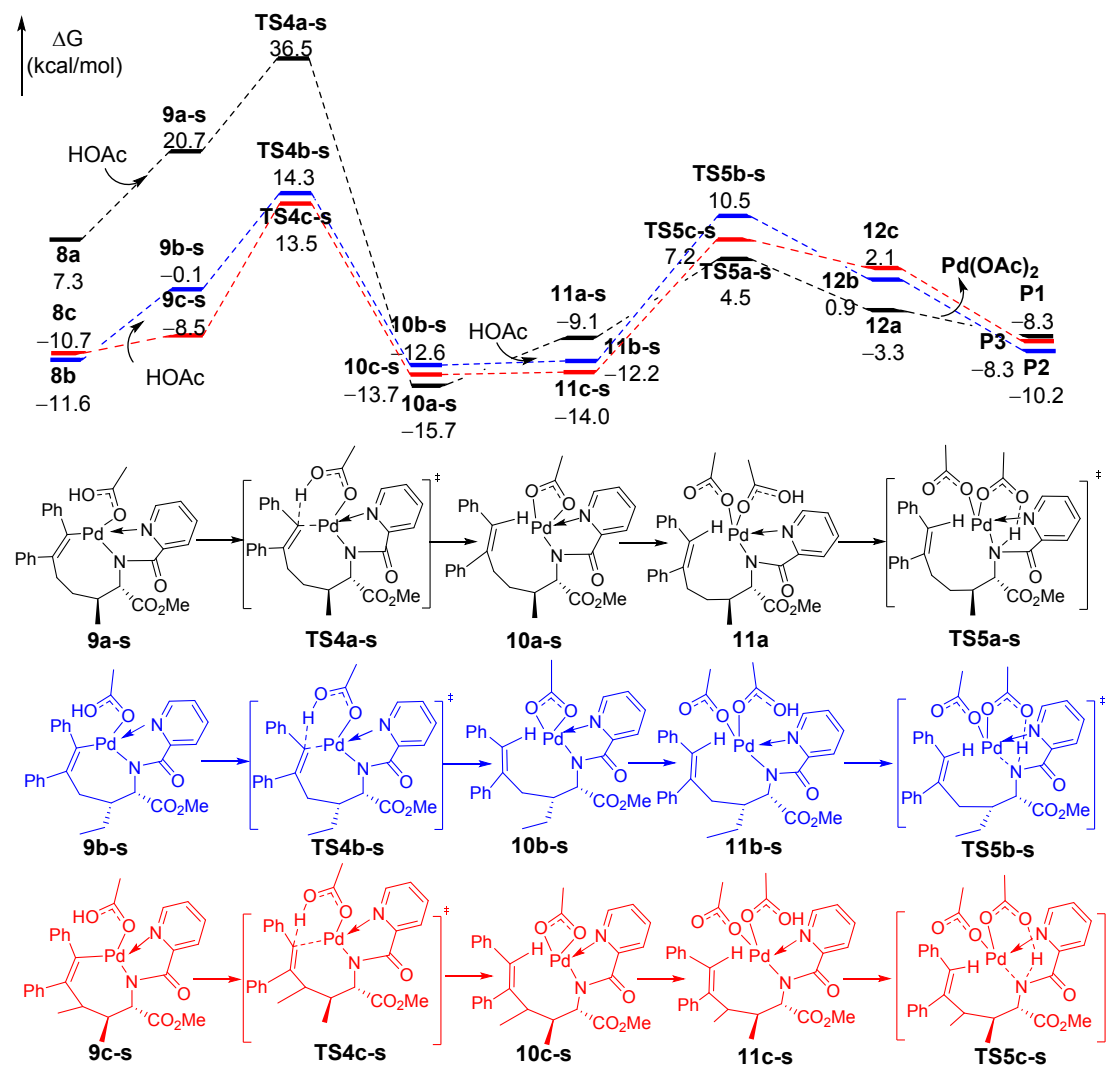


Fig. S4 Free energy profiles for another parallel pathway of the two consecutive protonation steps to afford the final products. Energies are relative to $\text{Pd}_3(\text{OAc})_6 + \mathbf{1} + \mathbf{2a}$ and are mass balanced.

V. Second insertion at 8a and two consecutive protonation steps to afford P1 using HFIP as the proton source.

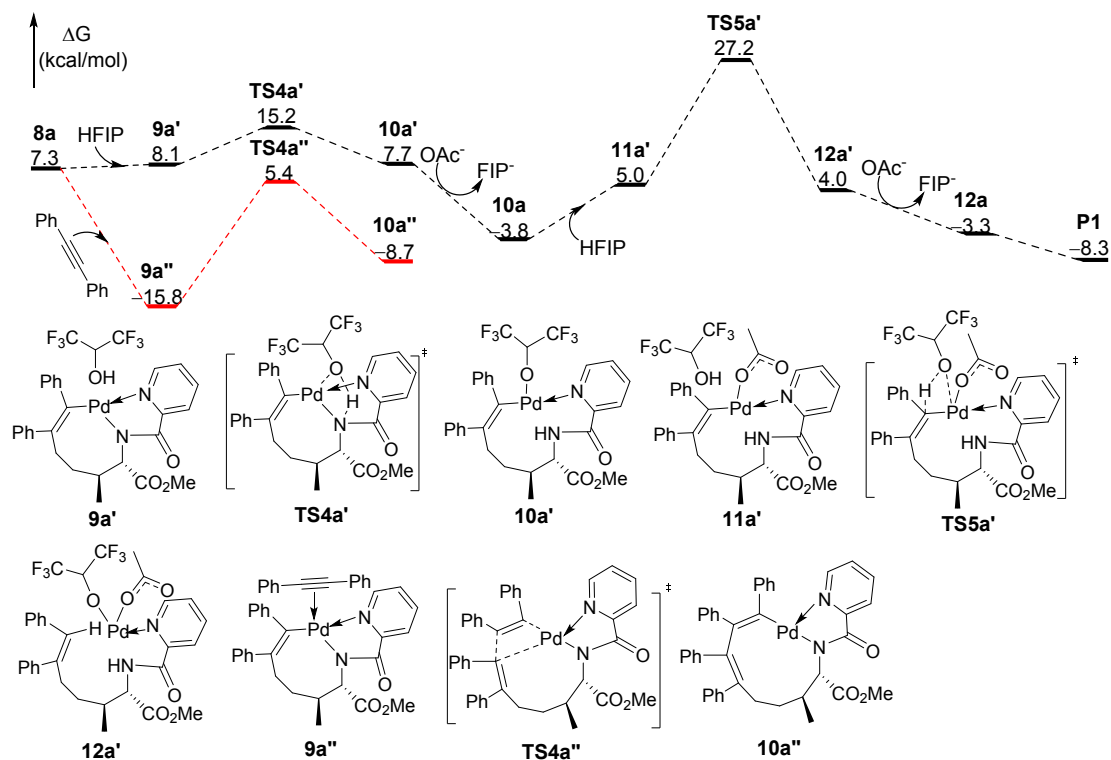


Fig. S5 Free energy profiles for the second insertion at **8a** and two consecutive protonation steps to afford **P1** using HFIP as the proton source. Energies are relative to **Pd₃(OAc)₆+1+2a** and are mass balanced.

VI. Cartesian coordinates of all the structures

Pd₃(OAc)₆

0 1

Pd	-1.04172800	-1.53165200	0.00779300
C	-2.60434900	0.23866500	1.88270000
O	-2.42849000	-0.89969000	1.35177400
O	-2.01526500	1.32040900	1.57398000
C	1.46130500	2.17792300	-1.88123500
O	2.23895600	1.33884800	-1.33280800
O	0.24102100	2.38302000	-1.59566400
C	2.05881300	3.04466800	-2.96685500
H	1.28300200	3.38386100	-3.65405400
H	2.51334000	3.92362200	-2.49711300
H	2.83767800	2.50084400	-3.50309000
C	-3.64459100	0.32342800	2.97740200
H	-3.70823100	-0.62235200	3.51685600
H	-3.41133400	1.14122200	3.66011000
H	-4.61766100	0.52547700	2.51699900
Pd	1.85769800	-0.14264300	0.00186300
C	1.50695700	2.14857200	1.87226800
O	0.44639800	2.56960500	1.31740700
O	2.15079200	1.09443700	1.57880500
C	-2.62906900	0.15721000	-1.86788400
O	-2.20187900	-0.99998300	-1.56612300
O	-2.27862800	1.25615800	-1.34062600
C	-3.68770000	0.22945700	-2.94541500
H	-3.61453200	1.17217600	-3.48905100
H	-3.59573100	-0.61669500	-3.62723100
H	-4.67206800	0.18174400	-2.46737200
C	2.03988000	2.97578000	3.02072700
H	1.49697500	2.69656100	3.93005600
H	3.10241400	2.78583000	3.17366000
H	1.86206700	4.03604000	2.83402000
Pd	-0.80173000	1.67253400	-0.01068800
C	1.16016700	-2.34214500	-1.88360600
O	0.04822700	-2.60179000	-1.33031200
O	1.95851100	-1.40377700	-1.57903000
C	1.55797900	-3.22491400	-3.04508500
H	1.06459700	-2.85023200	-3.94827900
H	2.63706400	-3.19900600	-3.19829800
H	1.21819900	-4.24769600	-2.87471400

C	1.11801400	-2.38164900	1.87833100
O	-0.11748200	-2.40068700	1.58600800
O	2.01397300	-1.66529000	1.33768000
C	1.57027700	-3.33365500	2.96282700
H	1.88996800	-4.26909000	2.49110400
H	2.41769000	-2.91628000	3.50799300
H	0.74634700	-3.55511100	3.64206600

Pd(OAc)₂

0 1

Pd	.00000100	-0.00009400	-0.01080200
O	1.74918600	1.08580800	-0.01132800
C	2.43036700	0.00020500	-0.00431400
O	1.74952500	-1.08563900	-0.01137100
O	-1.74929700	1.08565500	-0.01143100
C	-2.43036900	-0.00004400	-0.00446700
O	-1.74941700	-1.08579200	-0.01136800
C	-3.92235300	0.00015400	0.04138200
H	-4.24371600	0.00683600	1.08866200
H	-4.31431200	0.89489100	-0.44527200
H	-4.31442600	-0.90028500	-0.43443500
C	3.92236000	0.00028000	0.04130100
H	4.31447000	-0.89084500	-0.45188100
H	4.31410200	0.90420200	-0.42807600
H	4.24391800	-0.01428900	1.08843900

2

0 1

C	-1.20088800	-3.66803800	1.58926100
C	-1.37887700	-2.75112400	0.37360300
H	-0.36014300	-4.35239700	1.43530200
H	-0.99154500	-3.07777600	2.48808500
H	-2.08825700	-4.27829200	1.78574700
C	-2.54472700	-1.74676900	0.51087800
H	-0.44284600	-2.20676200	0.21718300
H	-1.54267600	-3.35324200	-0.53100700
C	-2.38634900	-0.59510100	-0.52261400
H	-2.49067200	-1.28786400	1.50736100
H	-2.25171100	-1.02375600	-1.52199800
C	-3.90369700	-2.45154100	0.37503200
H	-4.04922300	-2.83435400	-0.64111500
H	-3.96164700	-3.29784500	1.06419600
H	-4.74047500	-1.78643300	0.60470100

C	-3.66349600	0.24778300	-0.62913900	C	-2.05701400	-1.92091200	0.03283000
O	-4.52739000	0.06123000	-1.46138900	H	-0.29974200	-2.63862200	-0.99711800
O	-3.74800700	1.16782800	0.34701800	H	-1.80714000	-3.34430300	-1.56916000
C	-4.93492000	1.98538700	0.33285100	C	-1.98529400	-0.62174200	-0.84009700
H	-5.82740900	1.36631400	0.44758000	H	-1.56301900	-1.68544800	0.98355000
H	-4.83211300	2.66726900	1.17587000	H	-1.85999600	-0.91704000	-1.88886300
H	-5.00084200	2.54188100	-0.60464800	C	-3.49088000	-2.37414600	0.35683200
N	-1.22682300	0.22664600	-0.18694200	H	-4.05744800	-2.59411800	-0.55375100
H	-0.74683400	0.08473700	0.71317700	H	-3.47386100	-3.27839900	0.97085400
C	-0.90845700	1.28057400	-0.96316900	H	-4.03868200	-1.61192700	0.91958900
O	-1.52768600	1.59555600	-1.98433800	C	-3.32027700	0.13552300	-0.85291900
C	0.22021800	2.17196000	-0.48499200	O	-4.20963300	-0.07670800	-1.65357500
C	0.01262400	3.55096900	-0.54634200	O	-3.43472000	1.01399600	0.16180400
C	2.34708600	2.50429700	0.41516300	C	-4.66793600	1.75480400	0.20833800
C	1.00031300	4.41921100	-0.09203200	H	-5.51930400	1.07929900	0.31908300
H	-0.92700500	3.91248900	-0.94533700	H	-4.58595500	2.40961100	1.07516300
H	3.25744800	2.03962000	0.77315700	H	-4.79275200	2.34251400	-0.70416800
H	0.84623800	5.49257100	-0.12458700	N	-0.86104700	0.23684000	-0.42880500
C	2.18760300	3.88397000	0.40603900	H	-0.90094500	0.54115600	1.07009800
H	2.98782700	4.51553800	0.77389100	C	-0.72245800	1.32976700	-1.21644900
N	1.38660300	1.66437200	-0.02767600	O	-1.44161100	1.65945700	-2.17357300
Pd	1.91758300	-0.29839900	-0.18024100	C	0.42002800	2.24178200	-0.83295800
C	1.65726900	-0.47151400	4.09000500	C	0.38456700	3.60180800	-1.13408200
H	2.07995200	-1.46990400	4.23819300	C	2.53105100	2.47263300	0.15201700
H	2.43715200	0.25354900	4.33915500	C	1.45057700	4.41318700	-0.75530500
H	0.80067200	-0.33628200	4.75071400	H	-0.48008900	3.98597900	-1.66130100
C	2.57486700	-2.80132800	-3.14554000	H	3.36041100	1.96926000	0.63589000
H	3.62203400	-2.69516600	-3.44962500	H	1.43658200	5.47618900	-0.97214400
H	1.94118800	-2.55977000	-4.00053200	C	2.54035200	3.83984600	-0.09695800
H	2.41312100	-3.83228600	-2.82593600	H	3.39299500	4.43234500	0.21354600
C	1.23387800	-0.30603500	2.63986300	N	1.48781700	1.70136900	-0.20923300
O	2.22830900	-0.38407400	1.80031000	Pd	1.55110600	-0.28390200	0.02630000
O	0.04622000	-0.12140100	2.33627100	C	-0.09047900	0.51947000	4.29007000
C	2.30234600	-1.85978600	-2.01646200	H	0.85442000	0.29585800	4.78399600
O	1.89237300	-0.66299200	-2.22569200	H	-0.41220100	1.53630000	4.53068900
O	2.49264600	-2.19991200	-0.79599600	H	-0.86533200	-0.16368800	4.65167800
TS1				C	3.64381800	-3.40372200	-1.25887700
O 1				H	3.67649900	-4.15753700	-0.46971900
C	-0.99127400	-4.27602800	0.20718900	H	4.65314400	-3.14140000	-1.57993000
C	-1.26001200	-3.04408500	-0.66390100	H	3.10485900	-3.82709400	-2.11366000
H	-0.36630400	-4.99815000	-0.32861000	C	0.04436200	0.36638800	2.79646400
H	-0.46286900	-3.99891200	1.12633100	O	1.08457200	-0.09024300	2.28790200
H	-1.91346500	-4.79199700	0.49300200	O	-1.00332200	0.73554000	2.11318000
				C	2.91578500	-2.18505800	-0.78404900

O	3.21150500	-1.01729500	-1.19218700	H	3.72018000	-4.36688300	-0.25322100
O	1.93226500	-2.29036700	0.04051900	C	2.16704600	-2.90168500	-0.38262500
				O	0.90705900	-2.66546400	-0.33807400
5				O	2.95302900	-1.90007100	-0.26793300
0 1				TS2a			
C	-2.62523800	-0.47520300	3.73560500	0 1			
C	-1.80842400	-0.54433700	2.43909600	C	0.08489600	-2.47822800	-0.98581700
H	-1.96234800	-0.46525900	4.60726200	C	-1.25756700	-2.17192800	-1.65530100
H	-3.23205400	0.43734400	3.77026500	H	-0.05351400	-3.41814100	-0.43291300
H	-3.30088300	-1.32828500	3.84926000	H	0.86961900	-2.68774100	-1.72084700
C	-2.65476400	-0.42235100	1.15486000	C	-2.33348200	-1.64860300	-0.68441200
H	-1.06449500	0.25769500	2.45351400	H	-1.12879200	-1.46336800	-2.48135400
H	-1.24199400	-1.48659600	2.41206100	H	-1.62439100	-3.10473000	-2.10427300
C	-1.75952100	-0.41587800	-0.12142000	C	-2.27773900	-0.10058800	-0.58405400
H	-3.18800100	0.53364400	1.19174000	H	-2.12311400	-2.06456500	0.31086500
H	-1.49230900	-1.45870100	-0.33498200	H	-2.79048400	0.30949000	-1.46393900
C	-3.68081700	-1.56606600	1.05839000	C	-3.73527200	-2.10924600	-1.11479800
H	-3.17846200	-2.53992200	1.12183100	H	-3.94908800	-1.78561900	-2.14035700
H	-4.40763200	-1.51412600	1.87358300	H	-3.79796900	-3.20164300	-1.08793600
H	-4.23903400	-1.53079900	0.12068500	H	-4.51749400	-1.70523200	-0.46805100
C	-2.44543600	0.07548000	-1.41623800	C	-3.13136700	0.36262100	0.60515700
O	-1.86290900	0.14249300	-2.48270700	O	-4.31969300	0.60881400	0.53560300
O	-3.74165300	0.38546700	-1.27088900	O	-2.43980100	0.38574200	1.76079200
C	-4.41538100	0.84245100	-2.46055100	C	-3.18958500	0.77627900	2.92713800
H	-4.36977900	0.08180100	-3.24283500	H	-4.01785700	0.08524900	3.09949800
H	-5.44682100	1.02295200	-2.16098400	H	-2.48364300	0.74081900	3.75584900
H	-3.95562000	1.76366100	-2.82477900	H	-3.58461700	1.78721000	2.80386800
N	-0.48549300	0.28978300	0.00844200	N	-0.92181000	0.43862300	-0.53298800
C	-0.47954800	1.63582600	0.05691300	C	-0.86472300	1.78806100	-0.51127900
O	-1.47145300	2.38030300	0.03906900	O	-1.84073900	2.55597100	-0.56827200
C	0.91669600	2.19100500	0.13473500	C	0.52487600	2.34370800	-0.37124100
C	1.18944400	3.54783800	0.24557900	C	0.78260700	3.70986600	-0.36989700
C	3.19343000	1.66371200	0.13448000	C	2.78307900	1.84721700	-0.06094800
C	2.51954200	3.96441100	0.30607700	C	2.09751400	4.14554100	-0.20926800
H	0.35622600	4.24000400	0.27890400	H	-0.05056900	4.39188100	-0.49097500
H	3.93942900	0.87855500	0.08233500	H	3.52455400	1.06553800	0.05746900
H	2.76162200	5.01838400	0.39389600	H	2.32841800	5.20585200	-0.20541900
C	3.53529900	3.00911800	0.25031300	C	3.11251900	3.20073300	-0.05120200
H	4.58086400	3.29135100	0.29340000	H	4.14676300	3.49841200	0.07865300
N	1.90944000	1.27566300	0.08046200	N	1.51372800	1.43970000	-0.21833500
Pd	1.27710400	-0.62779500	-0.11361100	Pd	0.85637800	-0.51289900	-0.34604000
C	2.68597600	-4.29079300	-0.59159600	O	2.75903100	-1.26827100	0.02627200
H	2.64762000	-4.52631700	-1.66074500	C	2.71334500	-2.25176100	0.83977800
H	2.05667100	-5.01105100	-0.06482800				

O	1.61434900	-2.78770000	1.18452600	C	3.18702700	-1.88848700	0.19017800
C	4.00307300	-2.77576300	1.41578300	O	2.96174100	-0.66058400	-0.05870100
H	4.86071600	-2.40948000	0.85166400	O	2.26619700	-2.76548000	0.15737500
H	4.08749600	-2.43558500	2.45325600	H	1.18991600	-2.17069900	-0.31425500
H	3.98974900	-3.86754700	1.42509100	C	4.58650000	-2.31671500	0.54669500
H	0.71916100	-2.27959600	0.28777500	H	5.29435200	-1.50064200	0.40413700
TS2b				H	4.60357500	-2.63414000	1.59408500
O 1				H	4.87402000	-3.17754800	-0.06180900
C	-1.10125000	-3.91009200	1.02397200	TS2c			
C	-1.57179100	-2.46615800	0.80763400	O 1			
H	-1.32598800	-4.23620600	2.04467500	C	0.14071000	-2.34385000	-2.09489700
H	-1.60929100	-4.59791700	0.33749000	C	-0.05658700	-2.27117500	-0.57011700
H	-0.02334200	-4.02127000	0.87500800	H	1.18912400	-2.54681800	-2.33627400
C	-1.42283100	-1.97663900	-0.64787400	H	-0.45331100	-3.15789200	-2.52922100
H	-2.62648300	-2.40060300	1.09728200	H	-0.14081000	-1.41815400	-2.60473800
H	-1.02283100	-1.79125400	1.47580100	C	-1.50795800	-2.01162400	-0.07623900
C	-1.95023100	-0.53285800	-0.89068200	H	0.16318100	-3.28387700	-0.19949100
H	-2.03223400	-2.64261000	-1.27611900	C	-2.03078500	-0.63767300	-0.55901400
H	-2.12230400	-0.41929900	-1.97034500	H	-1.46293200	-1.95983900	1.01871400
C	0.03464700	-2.04131700	-1.15547900	H	-2.31916000	-0.69815700	-1.61721100
H	0.32419500	-3.09312100	-1.27221600	C	-2.46169200	-3.15702500	-0.45653000
H	0.12670300	-1.62968700	-2.16787900	H	-2.57208800	-3.24889900	-1.54174000
C	-3.32792600	-0.30713600	-0.26627600	H	-2.08463500	-4.11046400	-0.07256900
O	-4.36275800	-0.57630300	-0.84575600	H	-3.45980600	-2.99881600	-0.03792500
O	-3.27925600	0.14804300	0.99593600	C	-3.31806200	-0.26498300	0.18042800
C	-4.55451300	0.37472300	1.62515500	O	-4.43227300	-0.40789400	-0.28361500
H	-5.12266100	-0.55612300	1.69002900	O	-3.08279000	0.15029700	1.43829200
H	-4.32743600	0.75303000	2.62095700	C	-4.24865800	0.49510000	2.21003400
H	-5.13076400	1.11000200	1.05910900	H	-4.91347200	-0.36621800	2.30659300
N	-0.92618200	0.40160500	-0.45022000	H	-3.87515700	0.80090800	3.18644700
C	-1.14162400	1.73023600	-0.50034700	H	-4.78906900	1.31601900	1.73334300
O	-2.19971300	2.29540300	-0.81532300	N	-0.95505400	0.31950900	-0.37106500
C	0.08148600	2.51852500	-0.09645900	C	-1.17243900	1.63665400	-0.53048800
C	0.05785000	3.89856900	0.06057900	O	-2.25657200	2.17561300	-0.80461600
C	2.34824000	2.42743900	0.45959700	C	0.07881200	2.45189400	-0.31440300
C	1.22914900	4.55412800	0.44128100	C	0.07910000	3.83973600	-0.37520600
H	-0.87348600	4.42241100	-0.12032800	C	2.36680600	2.40466200	0.14707000
H	3.21929900	1.79562500	0.59222300	C	1.27603000	4.52382300	-0.16107000
H	1.23720900	5.63092300	0.57538700	H	-0.85498200	4.34621600	-0.58845200
C	2.39032500	3.80816300	0.64536900	H	3.23411500	1.78446100	0.34290700
H	3.32045000	4.27970400	0.94138300	H	1.30406600	5.60786900	-0.20127000
N	1.21550900	1.80515200	0.10015500	C	2.43628700	3.79616100	0.10442300
Pd	0.95308200	-0.20284300	-0.31744400	H	3.38619800	4.28942500	0.27617600

N	1.21061500	1.75579600	-0.05693200	C	-4.60732000	0.78395400	0.27368800
Pd	0.90685000	-0.29420000	-0.10294400	H	-5.39543400	1.48453600	0.52502300
C	3.13739200	-1.87125600	0.68756500	N	-2.27846600	0.39138500	-0.07683000
O	2.91715000	-0.70463600	0.22776500	Pd	-0.21955600	0.77100600	-0.18720900
O	2.20509300	-2.72325000	0.82683600	C	0.98821400	3.21952100	0.53950100
H	1.12378200	-2.18249700	0.26039300	O	-0.18696100	2.74135500	0.50606400
C	4.54238800	-2.25481900	1.07224100	O	2.01182600	2.53684000	0.20011900
H	4.56062800	-2.55165500	2.12462200	H	1.62735300	1.34533000	-0.14598600
H	4.85358200	-3.12163300	0.48233900	C	1.19969800	4.63706000	1.00163800
H	5.23377800	-1.42872500	0.90867400	H	1.79505100	4.63019000	1.91972100
				H	1.76849300	5.18673000	0.24695400
				H	0.24750300	5.13349300	1.18717100
TS2d							
0 1				6a			
C	4.30857200	-1.00473900	-0.61579400	0 1			
C	3.23748900	-0.07578300	-0.01099000	C	-0.96727900	-2.78458900	0.19912900
H	5.18668100	-1.01510900	0.03883100	C	-2.16301000	-2.27417200	-0.58008200
H	3.96133500	-2.03538400	-0.71755900	H	-1.23804800	-2.98608400	1.24720200
H	4.63989700	-0.65389300	-1.59731000	H	-0.54653000	-3.70178000	-0.24709200
C	1.89177600	-0.02852200	-0.78361200	C	-2.65690300	-0.89268100	-0.10932900
H	3.04436600	-0.37080300	1.02698300	H	-1.93763700	-2.23426500	-1.65441600
H	3.65727000	0.93181700	0.03921800	H	-3.00088700	-2.97965400	-0.47053300
C	1.15346000	-1.43897100	-0.76293000	C	-1.74491500	0.25377200	-0.62949500
H	1.46769400	-2.04476900	-1.62346400	H	-2.61448800	-0.87426000	0.98897600
C	2.08336000	0.39441900	-2.24985100	H	-1.90789700	0.35069900	-1.71201200
H	1.13508200	0.39094500	-2.79396100	C	-4.11643500	-0.67449000	-0.54414400
H	2.50574300	1.40217900	-2.31504400	H	-4.20905200	-0.72691900	-1.63548900
H	2.76588300	-0.29003200	-2.76967200	H	-4.75163400	-1.45701300	-0.11770200
C	1.45427700	-2.31965100	0.46047600	H	-4.51106700	0.29252700	-0.22537000
O	2.15818900	-3.30943600	0.42030600	C	-2.24616100	1.58453500	-0.04649100
O	0.85805600	-1.88268700	1.58394700	O	-3.03575200	2.32089700	-0.60403300
C	1.08423900	-2.68026600	2.76511600	O	-1.79824300	1.79443500	1.20687900
H	2.14942700	-2.71287900	3.00361600	C	-2.24915400	3.01010700	1.83155500
H	0.52805100	-2.18721400	3.56084300	H	-3.33866100	3.02083500	1.91185100
H	0.71579100	-3.69646700	2.61099000	H	-1.79395100	3.01962800	2.82122200
N	-0.23400500	-1.04342800	-0.82525400	H	-1.92313500	3.87772300	1.25320400
C	-1.33947100	-1.79232100	-0.66005400	N	-0.32074500	0.05535400	-0.36155700
O	-1.42830300	-3.02312600	-0.73399200	C	0.47490400	1.08960600	-0.70791700
C	-2.53859700	-0.91094000	-0.35731700	O	0.07612000	2.15313600	-1.21919700
C	-3.83278000	-1.41364700	-0.32584800	C	1.94279800	0.92198300	-0.40143700
C	-3.28369900	1.22144900	0.23476600	C	2.84702400	1.94289100	-0.68501300
C	-4.88521900	-0.55274700	-0.01034700	C	3.62684100	-0.41665300	0.47064900
H	-3.98444700	-2.46468700	-0.54332700	C	4.19243600	1.75845200	-0.36993400
H	-3.00927100	2.24736200	0.45486300	H	2.47451700	2.85111700	-1.14307300
H	-5.90604800	-0.91980100	0.01609400				

H	3.88974500	-1.36635700	0.92662500				
H	4.91863500	2.53718000	-0.58018600	6c			
C	4.59072400	0.55878000	0.22062300	0 1			
H	5.62603100	0.37433800	0.48492000	C	1.53128800	-2.99045900	1.09523200
N	2.33242800	-0.23840400	0.16574100	C	1.39850300	-2.16766400	-0.18892200
Pd	0.64478400	-1.59411600	0.27314600	H	0.78784900	-3.79620100	1.12378700
				H	2.51764300	-3.47144000	1.17203900
6b				H	1.39440700	-2.38331400	1.99702700
0 1				C	2.31575400	-0.91652400	-0.28585400
C	-3.59492800	-2.25302800	1.31770100	H	1.59384600	-2.81621400	-1.05722700
C	-2.76828500	-1.00871400	0.97003900	C	1.68918400	0.23920600	0.53558500
H	-3.97993300	-2.18485400	2.34053300	H	2.28187800	-0.58896600	-1.33259100
H	-4.45521700	-2.35594800	0.64565700	H	1.87340100	0.08593300	1.60778200
H	-3.00904800	-3.17500000	1.25062000	C	3.78372900	-1.18610600	0.08057800
C	-2.28537300	-0.97060600	-0.49507800	H	3.89105100	-1.46838500	1.13297200
H	-3.38564700	-0.12531300	1.16794600	H	4.18454900	-2.00297400	-0.52888600
H	-1.90236900	-0.93786100	1.63987500	H	4.40869700	-0.30394900	-0.09087200
C	-1.55085200	0.34724800	-0.87707800	C	2.35560100	1.57342900	0.20428700
H	-3.18045200	-1.04449900	-1.13232300	O	3.20195100	2.10065600	0.90040900
H	-1.53357700	0.41854000	-1.97377700	O	1.97755500	2.05141700	-0.99567900
C	-1.30281100	-2.11483600	-0.83249300	C	2.58426800	3.29535300	-1.39035400
H	-1.61826500	-3.07765100	-0.41391100	H	3.67013800	3.19181200	-1.45178500
H	-1.19918400	-2.22899800	-1.92134000	H	2.16752500	3.52888800	-2.36937100
C	-2.29200300	1.60619000	-0.42949500	H	2.33790200	4.08200000	-0.67338900
O	-3.14571700	2.14396100	-1.10944300	N	0.25635700	0.20684600	0.25201300
O	-1.96254700	2.01468900	0.80706500	C	-0.56299200	1.19473100	0.64256300
C	-2.63886300	3.19656000	1.27365900	O	-0.21217300	2.25356000	1.19360200
H	-3.71944700	3.03797300	1.29969800	C	-2.02211700	0.93189300	0.32761700
H	-2.25568600	3.37740800	2.27716000	C	-2.98075200	1.90971600	0.57867200
H	-2.41498900	4.04393500	0.62158900	C	-3.63535000	-0.53052300	-0.47776100
N	-0.18279800	0.23479300	-0.36832700	C	-4.31620200	1.64201300	0.27962800
C	0.69782800	1.24064300	-0.53147600	H	-2.65621400	2.85278700	1.00229100
O	0.43092300	2.37081600	-0.97203200	H	-3.85164600	-1.51042000	-0.89245500
C	2.10308800	0.89147600	-0.08677700	H	-5.08226100	2.38860100	0.46355100
C	3.08713300	1.87329100	-0.01565700	C	-4.65095900	0.39996600	-0.25854700
C	3.59303600	-0.74397000	0.61913200	H	-5.67607800	0.14768000	-0.50624300
C	4.36967200	1.51620100	0.39978400	N	-2.34949500	-0.27452900	-0.19433600
H	2.82522000	2.88880500	-0.28840000	Pd	-0.51889400	-1.50168100	-0.34007300
H	3.75128000	-1.79176300	0.85545000				
H	5.15417500	2.26312700	0.46818900	6d			
C	4.62812000	0.18488600	0.72449200	0 1			
H	5.61018400	-0.13763900	1.05209400	C	4.02375900	-1.36861700	-0.60535300
N	2.35768300	-0.40193500	0.22453200	C	2.49851400	-1.38312700	-0.85291800
Pd	0.54854200	-1.57887000	-0.19364600	H	4.55669700	-1.50904100	-1.55199800

H	4.36045000	-0.42678000	-0.16487000	H	3.15458100	-1.89999400	-1.14117900
H	4.32688600	-2.17817200	0.06578500	C	3.61724500	-0.61714000	-3.45121400
C	1.61247100	-1.13166700	0.37739100	H	3.66540800	-1.70056500	-3.61410800
H	2.25193600	-0.65173900	-1.63061500	H	3.38443800	-0.14635300	-4.41152100
H	2.24152400	-2.36665800	-1.26954000	H	4.61090700	-0.28505200	-3.14267300
C	1.35203300	0.38270000	0.76620700	C	4.20116300	-0.18292800	-0.54694400
H	1.34797400	0.49295400	1.85835800	O	5.31039700	-0.64020500	-0.74288000
C	1.96692400	-1.99324900	1.58548800	O	3.99337400	1.02572200	0.01565200
H	1.23886600	-1.87417900	2.39463200	C	5.17559600	1.71657900	0.45698200
H	2.00350000	-3.05603900	1.31844200	H	5.85047700	1.90135500	-0.38211800
H	2.95305000	-1.72785500	1.99544800	H	4.82686400	2.65810100	0.87998300
C	2.37289200	1.40404100	0.27631100	H	5.69879700	1.12892300	1.21495900
O	3.38907300	1.67375400	0.89166200	N	1.82121000	-0.70176600	-0.03521300
O	2.05772400	1.94984500	-0.90972100	C	2.17163800	-1.10365700	1.20701700
C	3.00096300	2.91025700	-1.42606400	O	3.28291300	-1.56524700	1.52809900
H	3.96994900	2.43741800	-1.60174400	C	1.11933400	-0.93554700	2.27776000
H	2.57387900	3.26554500	-2.36276500	C	1.39081600	-1.28450100	3.59929200
H	3.12603500	3.73671000	-0.72330400	C	-1.02435000	-0.24094000	2.83371900
N	0.01302200	0.50221200	0.21938500	C	0.40210800	-1.09419800	4.56347800
C	-0.98170700	1.30100500	0.64404600	H	2.36596100	-1.69258000	3.83575600
O	-0.85637900	2.34701000	1.29603600	H	-1.96345000	0.17169400	2.47880000
C	-2.35346200	0.81082500	0.19567100	H	0.58699000	-1.35679500	5.60032800
C	-3.46049600	1.64756400	0.30959000	C	-0.82744500	-0.56068200	4.17610500
C	-3.66252600	-0.90410300	-0.65813700	H	-1.62351600	-0.39390100	4.89325100
C	-4.71130900	1.17744200	-0.09012800	N	-0.07129500	-0.42472200	1.90944800
H	-3.31626300	2.64367300	0.71140900	Pd	-0.14306100	-0.13930200	-0.27158500
H	-3.70103000	-1.92362400	-1.02999100	C	-2.29992400	-0.16204000	-0.41869300
H	-5.58830600	1.81267700	-0.01593700	C	-1.95098200	1.03613200	-0.29996700
C	-4.81562000	-0.12170200	-0.58449000	C	-2.03122500	2.46752600	-0.17797200
H	-5.76693900	-0.53081400	-0.90653600	C	-0.88515700	3.26266500	0.01566900
N	-2.45724100	-0.45451700	-0.28028400	C	-3.29526400	3.09250800	-0.24809800
Pd	-0.37492700	-1.36154400	-0.14152100	C	-1.00216500	4.64627700	0.13510200
7a				H	0.08707300	2.78396300	0.07024300
0 1				C	-3.40084500	4.47518700	-0.12759800
C	-0.02986200	-0.03149400	-2.30460100	H	-4.18356200	2.48670600	-0.39653900
C	1.15798700	-0.76905000	-2.90131600	C	-2.25681000	5.25688300	0.06397400
H	0.01461600	1.03790400	-2.55163700	H	-0.11083500	5.24840400	0.28371500
H	-0.97333500	-0.42865500	-2.69351500	H	-4.37838700	4.94471600	-0.18388300
C	2.53095400	-0.27045900	-2.41884600	H	-2.34418700	6.33515700	0.15664300
H	1.07666400	-1.85098100	-2.72683800	C	-3.12224600	-1.32924500	-0.59021000
H	1.12448100	-0.63867900	-3.99438400	C	-4.50145600	-1.16754800	-0.84498800
C	2.89538600	-0.83883100	-1.01964100	C	-2.59083700	-2.63101700	-0.50622200
H	2.47544600	0.82396800	-2.32803800	C	-5.31928700	-2.28199400	-1.00854000
				H	-4.91839300	-0.16794600	-0.91628000

C	-3.41848700	-3.74000300	-0.67237500	C	-2.26240100	-0.13592100	-0.44894600
H	-1.53075100	-2.75813500	-0.31193500	C	-1.97482500	0.93847600	0.12863800
C	-4.78245100	-3.57080900	-0.92330200	C	-2.11435000	2.23007300	0.74709100
H	-6.37838700	-2.14495100	-1.20536900	C	-1.05071000	2.84480500	1.43597800
H	-2.99638700	-4.73823900	-0.60575400	C	-3.35654100	2.89655600	0.67126600
H	-5.42418800	-4.43694400	-1.05305400	C	-1.22721700	4.09193700	2.03276900
7b				H	-0.09434000	2.33562300	1.49540600
0 1				C	-3.52214500	4.14205300	1.27055200
C	1.50351300	3.47775700	-2.15324700	H	-4.18067200	2.43214800	0.13926600
C	2.16545500	2.27585700	-1.46810800	C	-2.46003500	4.74439600	1.95268400
H	1.88328800	4.41526000	-1.73378800	H	-0.39924300	4.55484800	2.56133000
H	1.71569200	3.48555800	-3.22909700	H	-4.48219700	4.64515300	1.20404700
H	0.41665300	3.48145100	-2.02766100	H	-2.59350700	5.71637700	2.41781500
C	1.80822200	0.91611300	-2.10448900	C	-3.04333600	-1.17791300	-1.06229100
H	3.25156100	2.41430600	-1.51425200	C	-4.42865400	-0.97723200	-1.24664400
H	1.90064400	2.26219000	-0.40404000	C	-2.46888400	-2.39457900	-1.47883300
C	2.55001600	-0.28987900	-1.45203100	C	-5.20979800	-1.96949400	-1.83203000
H	2.12020200	0.96463500	-3.15985200	H	-4.88011700	-0.04273000	-0.92899600
H	2.51040400	-1.13159600	-2.15811500	C	-3.26003200	-3.38163300	-2.06416100
C	0.29799300	0.59515400	-2.04139500	H	-1.40466300	-2.55402400	-1.33921400
H	-0.32832600	1.44712100	-2.31575100	C	-4.62994500	-3.17410400	-2.24315700
H	0.05100300	-0.24179100	-2.70820600	H	-6.27402200	-1.80231600	-1.96890700
C	4.04347100	-0.03491300	-1.25768800	H	-2.80441100	-4.31494700	-2.38114100
O	4.87149900	-0.26358700	-2.11970700	H	-5.24294100	-3.94495100	-2.70022600
O	4.34400400	0.52720700	-0.07400200	7c			
C	5.74100900	0.78746400	0.15363000	0 1			
H	6.13221900	1.47938600	-0.59598500	C	-0.09110400	-0.01039000	-3.13050200
H	5.79986500	1.22925000	1.14760900	C	0.37438500	0.85474400	-1.95684000
H	6.31125600	-0.14346900	0.11556800	H	-1.17465000	-0.15700000	-3.10540900
N	1.81800600	-0.62574100	-0.23341100	H	0.14672100	0.46576200	-4.09227900
C	2.25051000	-1.61281300	0.57369200	H	0.37753200	-1.00089900	-3.13392100
O	3.30555600	-2.25628500	0.45187500	C	1.90804400	1.10171600	-1.88898700
C	1.30734900	-1.89906000	1.72981000	H	-0.13424700	1.82531200	-1.99997800
C	1.68973300	-2.75723400	2.75734400	C	2.62126700	-0.18428100	-1.39233300
C	-0.76400400	-1.53829800	2.71780500	H	2.06847700	1.85266400	-1.10507100
C	0.80059100	-2.99627500	3.80518100	H	2.68027800	-0.92152600	-2.20462300
H	2.67038700	-3.21579500	2.70918000	C	2.50108600	1.65396700	-3.19584200
H	-1.72734300	-1.04120600	2.65323800	H	2.45492800	0.91958200	-4.00622600
H	1.07656400	-3.65678300	4.62113900	H	1.95248000	2.54575700	-3.51683000
C	-0.44833500	-2.37609300	3.78759000	H	3.55063200	1.93686300	-3.06692800
H	-1.17056000	-2.53491600	4.58073500	C	4.07362000	0.10513600	-1.01742700
N	0.09292800	-1.30221200	1.71549100	O	5.02673400	-0.16530900	-1.72259000
Pd	-0.11787600	-0.13376100	-0.18230500	O	4.17844200	0.78256600	0.14210900

C	5.51813000	1.09906400	0.56073000	O 1			
H	6.01970500	1.71863800	-0.18626900	C	-0.15767400	-1.65382900	-1.29079600
H	5.41332800	1.64261200	1.49898400	C	0.78000100	-2.64017700	-0.59889500
H	6.09355300	0.18298800	0.71348400	H	0.34126000	-1.03842900	-2.05753400
N	1.80803300	-0.68547600	-0.29038100	H	-0.94787500	-2.15968200	-1.84189200
C	2.26432200	-1.64233600	0.53408400	C	2.28781000	-2.31403500	-0.68570600
O	3.38024000	-2.18780700	0.48419900	H	0.48905100	-2.79184400	0.44752200
C	1.27359600	-2.02472500	1.62012100	H	0.63872500	-3.61506000	-1.08261500
C	1.62650300	-2.95098300	2.59812100	C	2.76654800	-1.20281900	0.29567500
C	-0.83065300	-1.74174700	2.56025600	H	2.49717100	-1.95879200	-1.70376300
C	0.70217900	-3.27141500	3.59234100	H	2.68807500	-1.59664900	1.32038900
H	2.61415500	-3.39470600	2.55540000	C	3.08028100	-3.61568000	-0.45954800
H	-1.79134700	-1.23846600	2.50313600	H	2.87707000	-4.02696800	0.53636400
H	0.95384800	-3.98876200	4.36714600	H	2.78659900	-4.36821200	-1.19772400
C	-0.54881500	-2.65554700	3.57606800	H	4.15901700	-3.46863500	-0.54052300
H	-1.29727800	-2.87343100	4.32991700	C	4.27518900	-0.99070700	0.08291600
N	0.05708200	-1.43316600	1.60574800	O	5.14783100	-1.50757000	0.75308600
Pd	-0.09624200	-0.08165000	-0.18941800	O	4.52808300	-0.26649600	-1.02710900
C	-2.24713800	0.12222600	-0.30087400	C	5.91694300	-0.02311600	-1.30648900
C	-1.80942500	1.17187300	0.22661600	H	6.45733400	-0.96361100	-1.43772700
C	-1.77458400	2.48435200	0.81571500	H	5.93617200	0.55843500	-2.22778700
C	-0.60314900	3.00879300	1.39581600	H	6.37329100	0.54255600	-0.49044200
C	-2.95069500	3.26521400	0.82329200	N	2.01386200	0.04209400	0.17126500
C	-0.61001700	4.28020400	1.96670800	C	2.54890500	1.09458400	0.80588300
H	0.30197900	2.41014800	1.39327100	O	3.61929800	1.11815100	1.45024900
C	-2.94717900	4.53340400	1.39744800	C	1.75922400	2.37110500	0.65389100
H	-3.85727300	2.87028500	0.37579600	C	2.30205600	3.59441000	1.04007000
C	-1.77869100	5.04598900	1.97022400	C	-0.18192800	3.40927500	-0.10205800
H	0.29982500	4.67286200	2.41079300	C	1.57033400	4.76037400	0.82860600
H	-3.85818000	5.12445600	1.39636000	H	3.28795800	3.59426000	1.48899100
H	-1.78030100	6.03618300	2.41566400	H	-1.16569900	3.28606900	-0.53919700
C	-3.17759600	-0.85214400	-0.80823600	H	1.97581200	5.72577800	1.11430900
C	-4.54356500	-0.51121000	-0.91139600	C	0.30939800	4.66660800	0.23825500
C	-2.76512400	-2.14145300	-1.19717300	H	-0.29388500	5.54668300	0.04576900
C	-5.46447600	-1.43978500	-1.38842200	N	0.52540000	2.28550100	0.10710600
H	-4.87015400	0.48089600	-0.61624000	Pd	-0.03134300	0.30332600	-0.32699300
C	-3.69517700	-3.06443300	-1.67209700	C	-1.77914400	-1.03321800	-0.29769500
H	-1.71537100	-2.40556400	-1.12305000	C	-2.04574500	0.23101100	-0.42969500
C	-5.04528800	-2.71853200	-1.76986200	C	-3.18570000	1.13413800	-0.39027900
H	-6.51247300	-1.16523300	-1.46325200	C	-4.19923200	1.03074600	-1.36422900
H	-3.36382100	-4.05544400	-1.96757400	C	-3.30810800	2.11764200	0.61078900
H	-5.76711600	-3.43939600	-2.14166800	C	-5.30019100	1.88521100	-1.33329900
				H	-4.11293700	0.27850800	-2.14233500
				C	-4.41755300	2.96223500	0.64111800

TS3a

H	-2.53977100	2.19915000	1.37343900	C	-3.16369300	3.55348000	0.08912500
C	-5.41452400	2.85367700	-0.33202200	C	-0.43127700	3.57496700	0.30587200
H	-6.07244900	1.79210100	-2.09147200	C	-2.52003800	4.75871700	0.36361900
H	-4.50301900	3.70654700	1.42761100	H	-4.23870300	3.47692400	-0.02509100
H	-6.27408300	3.51679100	-0.30931500	H	0.65003400	3.53902000	0.37241300
C	-2.37511300	-2.25355200	0.25680000	H	-3.09037400	5.67392600	0.48625500
C	-3.23729400	-3.04588300	-0.52025300	C	-1.12968200	4.76895100	0.47162500
C	-2.11103100	-2.62854000	1.58553300	H	-0.58334800	5.68272700	0.67671100
C	-3.83504600	-4.18090300	0.02800200	N	-1.05388900	2.41120900	0.05365400
H	-3.44439400	-2.76312400	-1.54838600	Pd	-0.20089900	0.51930500	-0.28405700
C	-2.70635600	-3.76863600	2.12649800	C	1.64395000	-0.77126600	-0.41962600
H	-1.44565400	-2.01774100	2.18859200	C	1.79295400	0.51990400	-0.27865000
C	-3.56932100	-4.54621500	1.35030800	C	2.90020500	1.44603300	-0.08198600
H	-4.50794500	-4.78008900	-0.57831700	C	2.92564400	2.31412300	1.02738200
H	-2.49776400	-4.04706300	3.15527300	C	3.96215400	1.50054800	-1.00645700
H	-4.03319200	-5.43205900	1.77376100	C	3.98779400	3.19917000	1.21175000
TS3b				H	2.11976500	2.27055200	1.75437200
0 1				C	5.01397300	2.39711900	-0.82356300
C	-0.28171400	-4.08333600	0.73708500	H	3.95068400	0.83913300	-1.86736900
C	-1.04175600	-2.75028000	0.73459900	C	5.03226400	3.24884600	0.28479400
H	-0.12204300	-4.43415800	1.76191700	H	3.99864600	3.85172000	2.08007200
H	-0.85308600	-4.85428800	0.20741500	H	5.82372500	2.42821100	-1.54698200
H	0.69886100	-4.00587700	0.26046700	H	5.85437300	3.94422300	0.42517200
C	-1.27605700	-2.18063600	-0.68376100	C	2.50587000	-1.92561100	-0.10384600
H	-2.00603300	-2.90775700	1.22612700	C	2.87248500	-2.16380000	1.23230900
H	-0.51173200	-2.00788600	1.34197200	C	3.03475700	-2.75355200	-1.10961700
C	-2.52206000	-1.24860700	-0.82033000	C	3.73982600	-3.20838300	1.55347200
H	-1.47731000	-3.04001000	-1.34111800	H	2.46617600	-1.53041000	2.01470600
H	-2.74836700	-1.17188000	-1.89488700	C	3.90407600	-3.79530900	-0.78473700
C	-0.01900300	-1.49087700	-1.29693100	H	2.78224000	-2.56900200	-2.15009700
H	0.67325200	-2.26429200	-1.61426800	C	4.25565300	-4.02845800	0.54732500
H	-0.25551800	-0.92349600	-2.20385800	H	4.01007800	-3.38228500	2.59094100
C	-3.78131500	-1.90047500	-0.24326700	H	4.31168500	-4.42028500	-1.57381100
O	-4.45425000	-2.70007900	-0.86636000	H	4.92951400	-4.84206300	0.79857500
O	-4.04528400	-1.53904600	1.02367400	TS3c			
C	-5.23062600	-2.11757900	1.60231500	0 1			
H	-5.15623900	-3.20720900	1.62460500	C	-0.23312900	-0.82968900	-2.80768800
H	-5.28794900	-1.71792500	2.61392900	C	0.03293400	-1.45895500	-1.43150100
H	-6.11274800	-1.82847100	1.02675000	H	0.68002400	-0.38054000	-3.20655400
N	-2.19662900	0.05657800	-0.28806900	H	-0.53542400	-1.62543100	-3.50139500
C	-3.06217900	1.06964100	-0.39577900	H	-1.01527900	-0.06868100	-2.80662400
O	-4.25715100	1.02299400	-0.74174300	C	-1.17377600	-2.15487100	-0.71621200
C	-2.40839300	2.39456100	-0.05638100	H	0.72744300	-2.27496300	-1.62323200

C	-2.47968300	-1.30162600	-0.67490400	C	2.73560600	-3.43287200	2.03402800
H	-0.87106200	-2.32619000	0.32278300	H	1.47060500	-1.68653300	2.13522100
H	-2.95110300	-1.31645800	-1.66798900	C	3.66858800	-3.93175300	-0.13857800
C	-1.43062600	-3.53056100	-1.36340800	H	3.12883200	-2.58436900	-1.73045300
H	-1.68744800	-3.43378900	-2.42364000	C	3.52871400	-4.24136000	1.21670800
H	-0.54239100	-4.16438500	-1.28368400	H	2.62306300	-3.66715000	3.08867000
H	-2.25885500	-4.04818700	-0.87261700	H	4.28867400	-4.55277300	-0.77849100
C	-3.50906800	-1.96422600	0.24655500	H	4.03589000	-5.10669000	1.63301300
O	-4.42257600	-2.66708200	-0.14066800				
O	-3.25461800	-1.72997200	1.54705200	8a			
C	-4.17494200	-2.32663000	2.48054400	0 1			
H	-4.16327600	-3.41516000	2.38855200	C	0.84502100	-2.38033700	0.03421100
H	-3.83000300	-2.02325600	3.46812500	C	-0.37889000	-2.12614000	-0.89966600
H	-5.18828800	-1.96132600	2.30006700	H	0.47368600	-2.46073100	1.06462500
N	-2.14375400	0.05001900	-0.28409300	H	1.28060200	-3.35576100	-0.20295000
C	-3.07157300	1.00226800	-0.18732700	C	-1.79899800	-2.39767200	-0.30114300
O	-4.30865200	0.87968200	-0.27504500	H	-0.27000400	-1.15864800	-1.52382100
C	-2.44005000	2.36184800	0.04225600	H	-0.26238200	-2.74747700	-1.79886300
C	-3.22621300	3.49177100	0.24343500	C	-2.89062700	-1.38996600	-0.80004300
C	-0.49072400	3.63435700	0.16470900	H	-1.72844500	-2.23800400	0.78089600
C	-2.61207700	4.73131700	0.41265900	H	-3.05399800	-1.53437300	-1.87751400
H	-4.30259900	3.36531300	0.25430800	C	-2.19995000	-3.85956700	-0.55127200
H	0.59239300	3.64444200	0.12338300	H	-2.36057500	-4.04629700	-1.61914900
H	-3.20686100	5.62510800	0.57165200	H	-1.41224600	-4.53626600	-0.20573300
C	-1.22000000	4.80364000	0.36919700	H	-3.11836800	-4.12592700	-0.02054500
H	-0.69660400	5.74554700	0.48907600	C	-4.23687700	-1.71289700	-0.14323400
N	-1.08335900	2.43829500	0.00843300	O	-5.19603600	-2.16540400	-0.73541600
Pd	-0.17015800	0.56601900	-0.30722800	O	-4.20498500	-1.51124000	1.18634000
C	1.54848200	-0.79748100	-0.40322100	C	-5.43921100	-1.75880300	1.88528400
C	1.82239900	0.48831100	-0.29152200	H	-5.75570800	-2.79567800	1.75218800
C	3.00620300	1.29010300	-0.03388000	H	-5.22955500	-1.55480600	2.93447100
C	2.98632300	2.31237400	0.93666700	H	-6.22036100	-1.09116900	1.51494900
C	4.19755500	1.07188100	-0.75688600	N	-2.41800100	-0.04014100	-0.52175500
C	4.12358800	3.07877200	1.18617200	C	-3.18900600	1.02642000	-0.30956000
H	2.07964500	2.47718200	1.51088700	O	-4.42860400	1.11630000	-0.36308600
C	5.32708000	1.85092500	-0.51355000	C	-2.34588100	2.23390100	0.08329600
H	4.22347800	0.29281600	-1.51251400	C	-2.95166800	3.44849500	0.38204800
C	5.29593700	2.85560500	0.45839400	C	-0.23321800	3.12223200	0.54996600
H	4.09474900	3.85265900	1.94786900	C	-2.16551200	4.52898400	0.78053600
H	6.23549000	1.67216500	-1.08172500	H	-4.03044000	3.50846500	0.29751400
H	6.17847800	3.45960100	0.64691300	H	0.83426400	2.94313300	0.59717000
C	2.22048400	-1.99837600	0.13932200	H	-2.62234800	5.48391900	1.01981500
C	2.08594500	-2.31798500	1.50108000	C	-0.78492500	4.36107300	0.87036800
C	3.01439400	-2.82262800	-0.67641300	H	-0.13359900	5.16985200	1.18147100

N	-0.99371600	2.08506700	0.16390500	O	-2.36160500	-4.20586300	-0.91448000
Pd	-0.40205700	0.18385700	-0.43110500	O	-2.94217900	-2.83784100	0.78131400
C	1.94247100	-1.30401500	-0.02723800	C	-3.98115100	-3.76834900	1.13472900
C	1.60481400	0.00157400	-0.21813100	H	-3.56276900	-4.75692700	1.33713200
C	2.52619500	1.15303200	-0.19892500	H	-4.44912600	-3.36148200	2.03048700
C	3.22430900	1.51510400	0.97094100	H	-4.71089200	-3.84513900	0.32521300
C	2.66659500	1.97950000	-1.33257900	N	-1.54146200	-0.75997900	-0.40422800
C	4.04037800	2.64732900	0.99946800	C	-2.74909500	-0.43754700	-0.90903700
H	3.12399100	0.89676600	1.85828700	O	-3.49189500	-1.19558700	-1.56259400
C	3.49075600	3.10466700	-1.30600300	C	-3.22579000	0.95693000	-0.57741900
H	2.12289800	1.72679600	-2.23926300	C	-4.50927600	1.37430500	-0.92114800
C	4.18106200	3.44566400	-0.13879200	C	-2.75840700	3.00381700	0.42031400
H	4.56873200	2.90519700	1.91337500	C	-4.91918800	2.65810300	-0.56479100
H	3.59131800	3.71892000	-2.19671000	H	-5.15039000	0.68353200	-1.45535500
H	4.81760500	4.32533600	-0.11582700	H	-2.02644500	3.61348000	0.93966400
C	3.33551000	-1.79695200	0.19066100	H	-5.91538300	3.00760500	-0.81693000
C	3.60132900	-2.76209000	1.18114800	C	-4.03050200	3.48708500	0.12079500
C	4.41321900	-1.35295700	-0.59775700	H	-4.30872300	4.49175100	0.41897800
C	4.89304900	-3.24807500	1.38859700	N	-2.36775400	1.76544600	0.08049100
H	2.79155000	-3.12692400	1.80673700	Pd	-0.42082600	0.85507800	0.18193800
C	5.70333600	-1.84248800	-0.39494500	C	2.15679000	-0.83614600	-0.28573200
H	4.23321500	-0.62564100	-1.38215200	C	1.45168200	0.25345600	0.04143900
C	5.95173500	-2.79028700	0.60144800	C	1.68825200	1.67679700	0.18430200
H	5.07086700	-3.98565900	2.16648300	C	1.10039800	2.31502900	1.31959600
H	6.51605300	-1.48745700	-1.02283000	C	2.17183100	2.50177500	-0.87729000
H	6.95680400	-3.17110100	0.75830200	C	1.02136200	3.72709500	1.37999100
8b				H	0.88157400	1.73283400	2.21092300
0 1				C	2.10244300	3.87677300	-0.78383200
C	1.37555700	-3.16651500	2.25314300	H	2.60621400	2.02466000	-1.74994500
C	0.19378000	-2.46392400	1.57296500	C	1.51380500	4.49721900	0.34232600
H	1.28745100	-3.10071100	3.34276800	H	0.60115500	4.19781600	2.26377800
H	1.41453100	-4.22986700	1.98773700	H	2.49756000	4.49154700	-1.58731700
H	2.33461000	-2.71845700	1.97383000	H	1.46466100	5.58054300	0.39448400
C	0.18715800	-2.61630600	0.03919600	C	3.64928500	-0.78779600	-0.34940400
H	-0.74029900	-2.87803200	1.96642500	C	4.40055600	-0.03195900	0.57001700
H	0.19548500	-1.40298500	1.84156000	C	4.34946900	-1.50815800	-1.33610700
C	-1.12607600	-2.13439100	-0.65712000	C	5.79206000	0.01812400	0.49479100
H	0.16861000	-3.69646300	-0.16307900	H	3.88735400	0.50491700	1.36146900
H	-0.97985200	-2.28536000	-1.73599600	C	5.74177900	-1.45455400	-1.41371600
C	1.50121600	-2.16185000	-0.65610300	H	3.80203400	-2.10177700	-2.06166400
H	2.23980300	-2.94714100	-0.46658100	C	6.47081200	-0.69096600	-0.49959800
H	1.33216200	-2.18466900	-1.74216800	H	6.34782300	0.60346300	1.22216600
C	-2.22552100	-3.15727700	-0.31327400	H	6.25663600	-2.01095000	-2.19203000
				H	7.55476800	-0.65434500	-0.55664900

				H	0.60294400	1.71564800	2.30748200
8c				C	1.98503000	3.98934100	-0.51711200
0 1				H	2.66310200	2.18751400	-1.47141800
C	1.17299500	-1.90154500	-2.19675400	C	1.26680300	4.55288900	0.56274500
C	1.52720600	-2.01201800	-0.69759200	H	0.19923900	4.16231400	2.38570600
H	2.05320800	-1.62018200	-2.78255300	H	2.42031100	4.64175700	-1.26845100
H	0.81040300	-2.85868800	-2.58755700	H	1.15952500	5.63102900	0.63247300
H	0.40359700	-1.14384800	-2.36627400	C	3.68027700	-0.66823800	-0.13201000
C	0.33953500	-2.50827400	0.21291800	C	4.33488800	0.10771400	0.84543800
H	2.29123700	-2.79215900	-0.62134600	C	4.48461400	-1.39716400	-1.03005000
C	-1.08404300	-2.28072500	-0.37520100	C	5.72566400	0.17408900	0.90554200
H	0.37938400	-1.94201400	1.14927200	H	3.74399700	0.64616700	1.57910400
H	-1.12717000	-2.70511100	-1.38443900	C	5.87730200	-1.32872100	-0.97139200
C	0.58091400	-3.99330600	0.55450400	H	4.02495600	-2.01305700	-1.79543000
H	0.52049100	-4.62629900	-0.33797600	C	6.50686600	-0.54127000	-0.00580500
H	1.58017500	-4.11150100	0.98392000	H	6.20034100	0.77616600	1.67545400
H	-0.13574100	-4.38069600	1.28245000	H	6.47028100	-1.89398300	-1.68501400
C	-2.10433700	-3.13059900	0.40293800	H	7.59073900	-0.49288400	0.04252600
O	-2.46923300	-4.23970000	0.06755700				
O	-2.49023700	-2.54689700	1.55670600	TS4a			
C	-3.43602400	-3.29410000	2.34372900	0 1			
H	-3.01139300	-4.25359500	2.64821000	C	0.34852400	1.67423100	-1.08860200
H	-3.64674100	-2.67674200	3.21622200	C	-0.59619400	2.28716300	-0.00492100
H	-4.34930000	-3.47189600	1.77140200	H	-0.18134200	0.88833500	-1.63582400
N	-1.48711200	-0.87022600	-0.41188600	H	0.56164400	2.45572800	-1.82541700
C	-2.74918000	-0.66586500	-0.83698200	C	-2.14049500	2.21972100	-0.25642000
O	-3.52190200	-1.54463300	-1.26655500	H	-0.38118100	1.85132700	0.97553500
C	-3.25346000	0.75175300	-0.70396200	H	-0.32707800	3.34503200	0.09420600
C	-4.52765500	1.10127900	-1.14453300	C	-2.84644000	0.99267400	0.42674200
C	-2.85963800	2.90918600	0.06645100	H	-2.33243900	2.16709100	-1.33498000
C	-4.96863600	2.41129200	-0.96452400	H	-2.71583300	1.13705600	1.50660000
H	-5.13860400	0.33832100	-1.61165800	C	-2.74303500	3.53137500	0.29242400
H	-2.16125500	3.58776700	0.54548400	H	-2.51427800	3.63716600	1.36081500
H	-5.95693500	2.71015400	-1.29925600	H	-2.29901300	4.38946300	-0.22217600
C	-4.12152700	3.33185300	-0.34635300	H	-3.82382300	3.58615000	0.16667600
H	-4.42508600	4.35997500	-0.18347900	C	-4.38109200	0.89973500	0.26950700
N	-2.43811000	1.64659200	-0.10752500	O	-5.04524400	0.13408600	0.94361500
Pd	-0.47309500	0.81765200	0.17397000	O	-4.92037200	1.75043900	-0.61804100
C	2.19052100	-0.72595300	-0.19501900	C	-6.33797200	1.61832800	-0.82120800
C	1.43605500	0.32240300	0.16210300	H	-6.87920000	1.75801800	0.11718600
C	1.59236600	1.74800000	0.36301000	H	-6.60630300	2.39499200	-1.53665600
C	0.87448000	2.32989200	1.45294800	H	-6.56714500	0.63012300	-1.22694200
C	2.12929200	2.62182200	-0.63218300	N	-2.26587400	-0.33678300	0.11642800
C	0.72105700	3.73445400	1.53493200	C	-2.63374600	-0.88362200	-1.06547300

O	-3.61290600	-0.57376400	-1.76487000				
C	-1.67095600	-1.91521200	-1.61641100	TS4b			
C	-2.06983000	-2.83105000	-2.58613800	O 1			
C	0.54232000	-2.65198800	-1.75967800	C	3.19576000	3.94890000	1.01807600
C	-1.12586400	-3.69337200	-3.13936600	C	2.37021000	3.26366200	-0.07758400
H	-3.10967600	-2.83743300	-2.89019100	H	4.02488100	4.51008400	0.57496300
H	1.55976100	-2.53359500	-1.40572800	H	2.58424400	4.65644400	1.59026900
H	-1.41802800	-4.42273600	-3.88780200	H	3.63100200	3.23568000	1.72487800
C	0.20244200	-3.59773000	-2.72250100	C	1.11463300	2.53142300	0.44775100
H	0.97256600	-4.24077900	-3.13330000	H	2.05972600	4.01803400	-0.80678200
N	-0.37814500	-1.83347200	-1.21670600	H	3.00598100	2.56085700	-0.62964600
Pd	-0.14165900	-0.67268100	0.44488300	C	0.04408300	2.32022500	-0.68843900
C	1.68932100	1.11020400	-0.56589500	H	0.61699900	3.22607500	1.13865500
C	1.74339900	-0.07963200	0.09027300	H	-0.32857000	3.33441400	-0.90198200
C	2.93002600	-0.86025000	0.47719200	C	1.44848600	1.30303900	1.33633700
C	3.94179400	-1.15807700	-0.46039900	H	2.20222500	1.64117300	2.05322600
C	3.05330400	-1.40442900	1.77332500	H	0.57178000	1.06838300	1.93075600
C	5.03499200	-1.95232000	-0.11155100	C	0.63158100	1.94470900	-2.06028900
H	3.86544000	-0.75372100	-1.46517700	O	1.17764000	2.76010800	-2.77906000
C	4.15169300	-2.18816600	2.12208200	O	0.48395000	0.65637800	-2.41776200
H	2.27741000	-1.19810500	2.50420500	C	0.97329900	0.33314300	-3.73644800
C	5.14786500	-2.46932400	1.18109800	H	2.04932200	0.50769100	-3.79807100
H	5.79983800	-2.16790700	-0.85283600	H	0.74979400	-0.72244400	-3.88508300
H	4.22951600	-2.58596700	3.13043100	H	0.46475100	0.93958900	-4.48862900
H	5.99883900	-3.08747300	1.45204700	N	-1.09604400	1.49288400	-0.28049300
C	2.90235100	1.95853700	-0.79209900	C	-2.14018600	1.56301100	-1.13920900
C	3.18643200	2.49401900	-2.06245600	O	-2.21184300	2.26132600	-2.16910700
C	3.78144700	2.26552500	0.26207900	C	-3.33207700	0.68291800	-0.78804700
C	4.31203300	3.29143800	-2.27325300	C	-4.62866700	1.04051100	-1.17305000
H	2.52968700	2.27008800	-2.89864400	C	-4.09588800	-1.28788700	0.17314700
C	4.90377400	3.06792600	0.05412300	C	-5.68631800	0.19472200	-0.84403600
H	3.57363800	1.87478700	1.25333100	H	-4.77345800	1.96519200	-1.71734400
C	5.17625500	3.58374200	-1.21522000	H	-3.83460400	-2.20361100	0.69340800
H	4.51415600	3.68366700	-3.26628000	H	-6.70343500	0.45270200	-1.12086300
H	5.56320000	3.29542200	0.88735200	C	-5.41632700	-0.98925900	-0.15691600
H	6.04940900	4.20917400	-1.37734700	H	-6.20851800	-1.67742800	0.11606800
C	-0.99230900	-0.47943400	3.25712300	N	-3.07733000	-0.46911800	-0.13426500
O	-0.08027900	-0.07156300	2.51292600	Pd	-0.93977300	-0.72799500	0.26915800
O	-2.09284600	-1.05120500	2.81600200	C	1.92375600	0.00598800	0.69119200
H	-2.14698600	-1.01782200	1.80913800	C	0.99535500	-0.89687600	0.35240400
C	-0.91416200	-0.34999800	4.74806200	C	0.84023800	-2.29363800	0.00836300
H	-1.00483300	-1.34046000	5.20351800	C	1.07644700	-3.32745100	0.95789000
H	0.02852600	0.11083100	5.03838400	C	0.19266900	-2.63284300	-1.21392500
H	-1.75415200	0.25264600	5.10549400	C	0.70830400	-4.63405500	0.67986800

H	1.55716500	-3.07408900	1.89748200	C	3.30814100	-0.09592500	-0.89507600
C	-0.19882900	-3.95674800	-1.46485600	C	4.65290400	-0.14447000	-1.26263400
H	0.07592200	-1.87420700	-1.97971400	C	3.59545300	1.95488400	0.14362500
C	0.06132400	-4.95155100	-0.52829800	C	5.48718500	0.89948800	-0.88070200
H	0.91242500	-5.41723800	1.40394800	H	5.00569100	-0.99861400	-1.82947100
H	-0.68277800	-4.20283400	-2.40523300	H	3.12730800	2.77181900	0.69040700
H	-0.22665700	-5.97861600	-0.73159800	H	6.54101600	0.88095800	-1.14413300
C	3.37830800	-0.26259600	0.50013700	C	4.94978200	1.97214300	-0.16514900
C	3.84141700	-0.91672200	-0.65724900	H	5.56698700	2.80502700	0.14363200
C	4.32937100	0.11500000	1.46695800	N	2.78886600	0.94125500	-0.20934900
C	5.19674500	-1.19234800	-0.83656100	Pd	0.66236100	0.65230500	0.19392400
H	3.12902700	-1.19266200	-1.42820000	C	-2.12489700	-0.61626500	0.45930300
C	5.68527800	-0.16118000	1.28757200	C	-1.27410800	0.40851300	0.28865000
H	4.00838200	0.60803100	2.37922100	C	-1.33857500	1.85985800	0.26798500
C	6.12684500	-0.81573900	0.13526700	C	-1.67945600	2.60173700	1.44090700
H	5.52763200	-1.69305100	-1.74233600	C	-0.80594500	2.57317700	-0.84153300
H	6.39753500	0.13351000	2.05325100	C	-1.52399700	3.98335500	1.47221500
H	7.18309600	-1.02573400	-0.00531600	H	-2.07306400	2.06820500	2.29485200
C	-1.90787700	0.87731300	2.91133400	C	-0.63353100	3.96522600	-0.78320000
O	-1.49913500	-0.23585200	2.63555000	H	-0.60647400	2.04065900	-1.76162900
O	-1.88522300	1.90775100	2.05782600	C	-0.99387900	4.66619500	0.36231100
H	-1.64220000	1.71208800	1.42784700	H	-1.80601000	4.53243400	2.36232900
C	-2.49153800	1.20963000	4.25897000	H	-0.23888700	4.49219200	-1.64662200
H	-3.56587900	1.39725500	4.15944200	H	-0.87358800	5.74471000	0.40542800
H	-2.32958400	0.36726700	4.92949500	C	-3.59153700	-0.38789400	0.32887300
H	-2.03932200	2.11693200	4.66859900	C	-4.10587900	0.40206500	-0.72089700
TS4c				C	-4.51218200	-0.94759200	1.23543000
O 1				C	-5.47567800	0.63617800	-0.84210700
C	-0.79711300	-2.85979700	-0.08424900	H	-3.42315100	0.81900900	-1.44907900
C	0.19931600	-2.16682600	-1.04922200	C	-5.88198900	-0.71156900	1.11608200
H	0.71229700	-2.99453400	-1.55689200	H	-4.15248800	-1.55477800	2.06044600
C	-1.64857000	-2.00206200	0.92931100	C	-6.36915600	0.08164000	0.07706800
H	-2.55120400	-2.60862800	1.04315700	H	-5.84560900	1.24359800	-1.66356700
C	-0.58134500	-1.53562000	-2.23496100	H	-6.56518600	-1.14687100	1.84009700
O	-1.59183600	-2.02031900	-2.70094600	H	-7.43620700	0.26013400	-0.01832000
O	0.01308200	-0.45958500	-2.77541800	C	2.34380700	-0.97023600	2.60101300
C	-0.60254700	0.06257900	-3.96955200	O	1.76001700	0.10243700	2.57987300
H	-1.62110700	0.40559600	-3.76355000	O	2.27471900	-1.87149300	1.62525700
H	0.02817700	0.89157000	-4.28755700	H	1.87957700	-1.60922700	0.93606000
H	-0.63950400	-0.70692100	-4.74837900	C	3.21463000	-1.37273300	3.77404000
N	1.25670400	-1.31617600	-0.45447800	H	4.23110800	-1.60828500	3.43538400
C	2.33736300	-1.19657600	-1.29251300	H	3.23929800	-0.55876500	4.49279200
O	2.61634700	-1.89885000	-2.27537900	H	2.81067700	-2.27743900	4.24736300
				C	-1.06374500	-1.86827600	2.35518300

H	-0.20122600	-1.20582200	2.37863300	N	0.27737900	1.66483600	-1.38230200
H	-1.82331600	-1.43090200	3.01586800	Pd	-0.28926600	1.28136000	0.57719000
H	-0.78730600	-2.83610400	2.77723500	C	-1.30325400	-1.38426500	-0.14073500
H	-1.53753000	-3.26906000	-0.77652800	C	-1.64399300	-0.09573400	0.08315100
C	-0.14194600	-4.06938000	0.60073000	C	-2.99932400	0.49395600	0.03334900
H	-0.86693700	-4.62007600	1.20900700	C	-3.75229300	0.43882000	-1.15719300
H	0.24537700	-4.76303000	-0.15660200	C	-3.55023200	1.18053200	1.13606400
H	0.69302000	-3.78695900	1.25354500	C	-5.00998800	1.03638500	-1.23961000
10a				H	-3.34613800	-0.09601100	-2.01058600
0 1				C	-4.80909300	1.77274000	1.04974300
C	0.15301000	-1.82800900	-0.28463900	H	-2.98164300	1.23638400	2.05896700
C	0.96653600	-1.87526300	1.02990500	C	-5.54426700	1.70674400	-0.13734300
H	0.65245600	-1.17850500	-1.00393800	H	-5.57547200	0.97327300	-2.16559600
H	0.17908200	-2.83008800	-0.72531800	H	-5.21955900	2.28722400	1.91457000
C	2.49500900	-2.05799800	0.82493800	H	-6.52438300	2.17086000	-0.20094300
H	0.76991400	-0.97329000	1.62003200	C	-2.34109200	-2.45921400	-0.25321600
H	0.58988400	-2.71093600	1.63214300	C	-2.32584100	-3.36498600	-1.32956300
C	3.26132900	-0.69963400	0.76507300	C	-3.34207700	-2.61240800	0.72105100
H	2.66484300	-2.57752200	-0.12395800	C	-3.28259100	-4.37411900	-1.43567600
H	3.37837800	-0.34031000	1.79480100	H	-1.56687500	-3.26838300	-2.10140500
C	3.07938400	-2.91563300	1.96177700	C	-4.29631400	-3.62448600	0.61864000
H	2.86318900	-2.46381900	2.93838400	H	-3.36186500	-1.93447200	1.56815600
H	2.62789200	-3.91259400	1.95442300	C	-4.27289800	-4.50943200	-0.46076200
H	4.16088200	-3.03785100	1.87057400	H	-3.25448900	-5.05475400	-2.28245100
C	4.69938900	-0.74907800	0.20044000	H	-5.05636700	-3.72493100	1.38878400
O	5.39623900	0.23598100	0.10258500	H	-5.01549400	-5.29839000	-0.53962900
O	5.10679500	-1.98824900	-0.12392800	C	0.41302000	2.11899100	2.85757400
C	6.42665200	-2.06590100	-0.68810600	O	-0.54402800	1.28847000	2.67314200
H	7.16789300	-1.66537200	0.00763600	O	1.09226100	2.53210000	1.86396400
H	6.60419200	-3.12487400	-0.87444400	H	2.14522300	1.12178600	0.63285300
H	6.46975100	-1.49827300	-1.62045500	C	0.69833200	2.62369100	4.24845700
N	2.55081400	0.37716200	0.07337400	H	1.75833800	2.86290700	4.35319300
C	2.44087600	0.39371800	-1.27138500	H	0.12569000	3.54291700	4.41456800
O	3.04632200	-0.38243100	-2.01128400	H	0.39151500	1.88947300	4.99549800
C	1.49483200	1.39398000	-1.91214900	10b			
C	1.88353100	1.91454000	-3.14930400	0 1			
C	-0.57726500	2.43749600	-2.08969200	C	1.71403900	3.26126500	-1.89283000
C	1.01910900	2.74604700	-3.85109400	C	0.54526700	2.39316400	-1.40824100
H	2.85529100	1.63284800	-3.53619800	H	1.91776300	3.08675900	-2.95489700
H	-1.55585000	2.58580200	-1.64812800	H	1.47635100	4.32386700	-1.76966000
H	1.31450000	3.17037200	-4.80553300	H	2.63622600	3.05799100	-1.34160900
C	-0.24167900	3.00324300	-3.31320200	C	0.24276800	2.56802700	0.09477000
H	-0.96544500	3.62467800	-3.82904300	H	-0.34744800	2.66517900	-1.97538300

H	0.74208000	1.33905300	-1.62971300	C	5.55512000	0.90720000	-1.12163400
C	-1.25144500	2.34232300	0.45165900	H	3.67133000	0.00931600	-1.62846000
H	0.39929200	3.62801100	0.32146700	C	5.61261600	2.15659200	0.93922100
H	-1.33635600	2.46112700	1.53977800	H	3.78945700	2.21391500	2.06613200
C	1.17323200	1.76216300	1.09689900	C	6.26278800	1.68696000	-0.20386100
H	1.76591700	2.49276600	1.65221800	H	6.04522200	0.54495400	-2.02106600
H	0.53892700	1.26582400	1.83560000	H	6.15150500	2.76146600	1.66309100
C	-2.16542100	3.44233400	-0.11251800	H	7.30669400	1.92955200	-0.37966700
O	-1.78647600	4.43359400	-0.70304000	H	-2.20835534	0.55001744	1.04368912
O	-3.44619700	3.22460000	0.23233100	C	-0.38768330	-1.70584467	2.91559307
C	-4.39338300	4.20481900	-0.23039400	O	-1.30603538	-2.10719939	2.16176400
H	-4.39736900	4.24024400	-1.32224000	O	0.71026380	-1.16467990	2.53192096
H	-5.36227400	3.87618700	0.14335500	C	-0.56390840	-1.82640420	4.42576934
H	-4.14674800	5.19335300	0.16316600	H	0.36902904	-2.14374380	4.89790120
N	-1.77519400	0.99454000	0.20071700	H	-0.82378639	-0.84416407	4.83543669
C	-2.14821523	0.53902918	-1.02391179	H	-1.36493623	-2.52767927	4.66493188
O	-2.10391401	1.18746146	-2.07111450				
C	-2.65940574	-0.89010860	-1.03313019	10c			
C	-3.81111272	-1.19523398	-1.75618270	0 1			
C	-2.41290236	-3.09877694	-0.37053020	C	-0.30228175	0.24177355	-2.36988706
C	-4.27947054	-2.50809366	-1.75705958	C	-0.10198800	1.55536000	-1.59324100
H	-4.31793845	-0.40603365	-2.29858860	H	-1.35101141	0.12030301	-2.65815790
H	-1.81857073	-3.82201227	0.17806925	H	0.28729091	0.25178272	-3.29116643
H	-5.18120351	-2.76946410	-2.30122050	H	-0.01920513	-0.64025961	-1.79000807
C	-3.56985814	-3.47697386	-1.04861505	C	1.40705700	1.93559300	-1.38566600
H	-3.89465613	-4.51106775	-1.02259704	H	-0.47578260	2.34154143	-2.26679174
N	-1.96331581	-1.83236634	-0.35747849	C	2.39068800	0.73365300	-1.43789300
Pd	-0.18753772	-1.34794964	0.62065959	H	1.50968000	2.39814400	-0.40006100
C	2.11503200	0.70646400	0.52029900	H	2.36909800	0.31374000	-2.44896500
C	1.66559100	-0.52576500	0.25524700	C	1.78565900	2.98658000	-2.45277600
C	1.92931903	-1.70410646	-0.53141678	H	1.72610100	2.57147100	-3.46490400
C	1.53568058	-1.63660168	-1.90305111	H	1.09823200	3.83726800	-2.40594200
C	2.30252184	-2.96547589	0.01058754	H	2.79518200	3.36671000	-2.30520000
C	1.49190468	-2.80435159	-2.68580528	C	3.88947400	1.04126600	-1.19568500
H	1.38462433	-0.66417915	-2.36262976	O	4.74284000	0.18929500	-1.34411800
C	2.28542474	-4.09446551	-0.78924537	O	4.16108100	2.30570300	-0.84793800
H	2.59942817	-3.02384338	1.05246573	C	5.54759400	2.59251400	-0.58230200
C	1.86648580	-4.02151178	-2.13408775	H	6.15999900	2.37537800	-1.46001000
H	1.19778346	-2.74032070	-3.72896668	H	5.58552500	3.65378100	-0.34057900
H	2.59129998	-5.05098862	-0.37574077	H	5.89860500	1.99441100	0.26130900
H	1.85660403	-4.92062452	-2.74262222	N	2.03297100	-0.37283100	-0.54992000
C	3.54491600	1.06007900	0.25190600	C	2.33767900	-0.34840900	0.76553200
C	4.21387600	0.59830900	-0.89664000	O	2.98776700	0.55184600	1.30822000
C	4.26956200	1.85053800	1.16283200	C	1.85530200	-1.52162400	1.58087200

C	2.66669700	-2.00811000	2.60681700	0 1			
C	0.21364700	-3.08475400	2.05408800	C	0.36734400	1.76925900	-1.55181900
C	2.22225600	-3.08791800	3.36509700	C	1.33572300	0.69788000	-2.09328100
H	3.62556700	-1.53662700	2.78561100	H	0.87733400	2.35490000	-0.77709300
H	-0.76591800	-3.47470800	1.79944900	H	0.17260500	2.50144900	-2.34797000
H	2.83862400	-3.49256300	4.16132800	C	2.81656300	1.06447900	-1.82451600
C	0.97242600	-3.63945100	3.08084600	H	1.12211300	-0.28529000	-1.66520300
H	0.58428900	-4.48178000	3.64259400	H	1.18355900	0.59877300	-3.17315600
N	0.64011800	-2.04206200	1.31792900	C	3.35702300	0.44636800	-0.48491900
Pd	-1.11683419	-1.09382953	0.41788778	H	2.89053200	2.15350200	-1.74445600
C	-1.03634935	1.70356769	-0.36336211	H	3.88729500	-0.47646100	-0.75412800
C	-1.99514382	0.78467072	-0.12078937	C	3.72184500	0.61849000	-2.98398300
C	-3.47031106	0.68305965	-0.30424729	H	3.63731300	-0.46260500	-3.15198800
C	-4.34785308	1.32322101	0.60289949	H	3.43940800	1.12424200	-3.91309300
C	-4.01889154	-0.09327567	-1.35400249	H	4.77084300	0.85167800	-2.78095500
C	-5.72450175	1.19991655	0.45701290	C	4.41408100	1.29106400	0.25275000
H	-3.92391452	1.90593684	1.41462742	O	4.74359200	1.11472400	1.40272000
C	-5.39669385	-0.21123108	-1.49393712	O	4.99388900	2.20307100	-0.55577100
H	-3.35239137	-0.58640679	-2.05375854	C	6.02886100	2.98933900	0.05845500
C	-6.24984523	0.43458191	-0.59107023	H	6.83415300	2.34711700	0.42346000
H	-6.39145333	1.69433138	1.15629307	H	6.39274400	3.65767100	-0.72185600
H	-5.81070871	-0.80485533	-2.30302003	H	5.62452600	3.56021600	0.89753800
H	-7.32575038	0.33870473	-0.70294214	N	2.34879500	-0.00041300	0.46375300
C	-1.29110272	3.09372034	0.15714472	C	1.66028300	0.84181400	1.24718700
C	-1.60959423	3.29811491	1.51264298	O	1.78718000	2.07201600	1.26074600
C	-1.26659404	4.22186397	-0.68626854	C	0.67970700	0.19670700	2.20423000
C	-1.90275661	4.56991254	2.00522015	C	0.68265600	0.66016800	3.52237600
H	-1.60597165	2.44371261	2.18335797	C	-1.01999300	-1.30995700	2.70164600
C	-1.55308871	5.49485302	-0.19203126	C	-0.17799600	0.09132600	4.45361500
H	-1.03530898	4.11261753	-1.74061818	H	1.37233600	1.45477500	3.78071000
C	-1.87370870	5.67697932	1.15508132	H	-1.68616600	-2.07700400	2.32735800
H	-2.14119158	4.69511920	3.05765343	H	-0.17514000	0.42837700	5.48561000
H	-1.52718278	6.34673458	-0.86566440	C	-1.04078200	-0.92091600	4.03474700
H	-2.09180947	6.66962762	1.53757133	H	-1.73198500	-1.40084900	4.71856200
C	-1.27757146	-2.66503878	-1.24369612	N	-0.18050900	-0.76290300	1.79607500
O	-1.93175356	-1.56816495	-1.39846293	Pd	-0.36398200	-1.57577300	-0.10931300
O	-0.69777668	-3.01369625	-0.18868910	C	-0.98502000	1.42110700	-0.95961100
H	1.61168500	-1.21268800	-0.97142400	C	-1.49045100	0.15894400	-0.75347100
C	-1.21279270	-3.56560670	-2.47105249	C	-2.84516200	-0.06650700	-0.15516600
H	-0.58848398	-3.09093627	-3.23560202	C	-3.24265300	0.52831500	1.05815100
H	-0.78751574	-4.53745289	-2.21734441	C	-3.75445600	-0.94312000	-0.77949900
H	-2.20993729	-3.69606559	-2.90056107	C	-4.49385300	0.26656700	1.61524900
				H	-2.56713800	1.21311500	1.56019200
				C	-5.00742100	-1.20199000	-0.22385100

TS5a

H	-3.47793700	-1.41422000	-1.71727900	H	-2.44491700	2.51366400	1.79157200
C	-5.38465200	-0.60012900	0.97810900	H	-2.94392300	0.27776700	1.82678700
H	-4.77489400	0.74626800	2.54919800	C	-0.53024100	1.56026100	1.59173000
H	-5.69042100	-1.87611700	-0.73369500	H	-0.29072180	2.30308927	2.35929327
H	-6.36001400	-0.80177500	1.41159800	H	-0.63762310	0.60977776	2.12504702
C	-1.78568300	2.66108900	-0.69333200	C	-4.25343100	1.00917800	0.38530200
C	-1.29808400	3.64365500	0.18618800	O	-4.78790700	2.08827000	0.54635700
C	-3.00307100	2.88755200	-1.35467900	O	-4.88719200	-0.07293800	-0.08991700
C	-2.02737900	4.81201100	0.41148000	C	-6.26697800	0.12413100	-0.45798700
H	-0.36028300	3.47999700	0.71029800	H	-6.34391600	0.86331700	-1.25834800
C	-3.71800400	4.06502400	-1.14019700	H	-6.61943400	-0.84748200	-0.80118200
H	-3.38651200	2.13721200	-2.03899500	H	-6.84839900	0.46157300	0.40274200
C	-3.23558400	5.02940600	-0.25295300	N	-2.21578400	-0.38832700	0.05742600
H	-1.64529200	5.55578600	1.10528600	C	-2.03127600	-0.38814300	-1.27838600
H	-4.65461200	4.22756500	-1.66608900	O	-2.54207400	0.42191300	-2.05287800
H	-3.79648300	5.94394100	-0.08253300	C	-1.19539000	-1.52848400	-1.82650700
C	1.57885700	-3.56150800	0.83907300	C	-1.48902100	-1.95115900	-3.12428800
O	2.48498900	-2.72618600	0.67131400	C	0.47140700	-3.13823100	-1.64780800
O	0.31205700	-3.34387400	0.69585500	C	-0.78402500	-3.01173600	-3.68381400
H	2.27202200	-1.02752200	0.59143800	H	-2.27264100	-1.43379500	-3.66342400
C	1.92310500	-4.99212000	1.22821100	H	1.25305800	-3.57332900	-1.03656200
H	1.22485400	-5.36513900	1.98144100	H	-1.00862800	-3.35534600	-4.68808700
H	1.82526300	-5.63160600	0.34449300	C	0.21151500	-3.62286700	-2.92428100
H	2.94828600	-5.04737300	1.59631200	H	0.79141100	-4.45511800	-3.30623200
C	-0.86045100	-2.16343500	-2.96336000	N	-0.21022500	-2.10899600	-1.09886000
O	-0.43210000	-2.62887800	-1.86441600	Pd	0.48502046	-1.59774831	0.80054147
O	-1.34892700	-0.99854700	-3.10334000	C	0.69031310	1.47500905	0.67014186
H	-1.33160900	-0.43814400	-1.92716400	C	1.38763480	0.31949888	0.38215105
C	-0.76297400	-3.04740200	-4.18565000	C	2.67788191	0.24231057	-0.35132053
H	-1.67976600	-2.96902900	-4.77395500	C	2.74629147	-0.06049295	-1.72490522
H	0.06372400	-2.69237500	-4.80987700	C	3.88875225	0.42984639	0.34570711
H	-0.57518700	-4.08181100	-3.89833900	C	3.97546822	-0.16077177	-2.37736846
TS5b				H	1.82767375	-0.20422836	-2.28571716
0 I				C	5.11722435	0.32751968	-0.30787194
C	-1.58556400	4.36145200	0.16963800	H	3.85696959	0.66678192	1.40511662
C	-1.86781600	2.90533000	-0.22333300	C	5.16700219	0.02996631	-1.67226741
H	-1.52327200	4.99852200	-0.71903500	H	4.00212307	-0.38244179	-3.44078215
H	-2.39097300	4.75196300	0.80268800	H	6.03669864	0.48456280	0.24940480
H	-0.64490000	4.46859700	0.71716700	H	6.12306502	-0.04754529	-2.18168271
C	-1.92855100	1.96087300	0.99665000	C	1.23805396	2.79613941	0.19296813
H	-2.82243800	2.87014300	-0.75090400	C	1.37891014	3.09977544	-1.17070984
H	-1.11482800	2.55222900	-0.93253000	C	1.64172688	3.76599529	1.12819560
C	-2.81633600	0.69606400	0.81938400	C	1.90097478	4.32629222	-1.58623638
				H	1.06821767	2.37138262	-1.91242199

C	2.16859668	4.99110155	0.71565384	H	6.59330400	-0.95701200	0.72368500
H	1.55736167	3.55484081	2.19090177	H	5.57002400	-1.92546600	1.83237700
C	2.29876754	5.27802828	-0.64529215	N	1.29557500	-1.80908000	-0.04132800
H	1.99279398	4.53815588	-2.64800392	C	1.20019400	-1.34862900	1.22160800
H	2.48013317	5.71971729	1.45911571	O	2.13271400	-0.80879000	1.82338900
H	2.70464365	6.23248130	-0.96796622	C	-0.09908700	-1.62338800	1.94205900
H	-1.69402300	-1.07303800	0.59758800	C	-0.00516900	-1.98189800	3.28826000
C	-1.24173935	-3.63339366	2.16212264	C	-2.41003900	-1.83003800	2.00975800
O	-2.20156473	-2.82651149	1.98113804	C	-1.15941000	-2.28717700	4.00185900
O	-0.07706795	-3.34355333	1.69652478	H	0.97675500	-2.01968500	3.74343300
C	-1.42014078	-4.91160989	2.93791578	H	-3.34632400	-1.74406400	1.47036500
H	-0.82909593	-5.71464350	2.49212235	H	-1.10253400	-2.57684100	5.04580500
H	-1.06086630	-4.75986150	3.96168456	C	-2.38616200	-2.21698600	3.34425800
H	-2.47375297	-5.19162751	2.97562496	H	-3.31755500	-2.44680600	3.84880000
C	2.12839141	-1.15553504	3.24123552	N	-1.29157900	-1.53105600	1.31104300
O	1.22800143	-1.88062660	2.71545979	Pd	-1.76657100	-0.80385600	-0.59843600
O	2.56248558	-0.09888801	2.68629472	C	0.54585384	1.24252707	-0.93085724
H	1.92609133	0.03556415	1.55340919	C	-0.72743574	1.07316127	-0.45446573
C	2.80997252	-1.41074981	4.55931444	C	-1.41585334	2.02054821	0.46599642
H	3.88893837	-1.50666877	4.40778986	C	-1.22698847	1.98913744	1.86092024
H	2.64804749	-0.56368454	5.23206238	C	-2.32777551	2.96098944	-0.05516066
H	2.41550630	-2.32149627	5.00738251	C	-1.92089506	2.86265170	2.69953372
TS5c				H	-0.52309429	1.28209935	2.28778280
				C	-3.01957482	3.83491832	0.78420427
O 1				H	-2.48576410	3.00343907	-1.12903241
				C	-2.82243378	3.78784072	2.16696478
C	0.56431389	-0.46314881	-2.99858534	H	-1.75112300	2.82389523	3.77225136
C	1.30891500	0.42743900	-1.99211700	H	-3.71164828	4.55543465	0.35670001
H	-0.28557088	0.07424482	-3.42309978	H	-3.36062667	4.46764981	2.82115348
H	1.23068313	-0.74636313	-3.81992794	C	1.35367887	2.42378556	-0.44422026
H	0.16514154	-1.38312996	-2.56354469	C	2.03303758	2.38563688	0.78369039
C	2.64905600	-0.19477300	-1.46338300	C	1.47255417	3.57706376	-1.23739682
H	1.65203908	1.28724247	-2.58317550	C	2.80169458	3.47268040	1.20920481
C	2.49089700	-1.61590500	-0.86104400	H	1.96231789	1.49522578	1.40128341
H	3.02792900	0.46143200	-0.67562800	C	2.23428824	4.66605784	-0.81043370
H	2.38984800	-2.32985000	-1.68613300	H	0.95543869	3.62235500	-2.19274071
C	3.69389600	-0.22393300	-2.59670800	C	2.90229092	4.61719973	0.41621001
H	3.35343100	-0.83172700	-3.44231800	H	3.32154175	3.42311445	2.16223897
H	3.87373600	0.78998400	-2.96726300	H	2.30465854	5.55285681	-1.43448264
H	4.64860600	-0.62741900	-2.25557000	H	3.49668294	5.46343313	0.74901265
C	3.69009300	-2.14959600	-0.04190300	C	-2.16848781	-3.35441423	-1.14924245
O	3.69523700	-3.25991200	0.44976900	O	-2.98816606	-2.45696074	-0.71703326
O	4.71860800	-1.29706800	0.03452800	O	-0.91905634	-3.16581015	-1.02855939
C	5.85618700	-1.75557300	0.79229000	H	0.47653700	-2.21871700	-0.46992100
H	6.25042100	-2.68148100	0.36844600				

C	-2.71480045	-4.58814475	-1.81833304	H	-0.96035600	3.48583300	-3.49853000
H	-2.93113775	-4.35728189	-2.86730322	H	-1.64176100	5.45525600	0.26993200
H	-1.98291129	-5.39657946	-1.78525998	C	-1.24077300	4.63564600	-1.68816000
H	-3.64768440	-4.90014759	-1.34405697	H	-0.90165300	5.56815800	-2.12728400
C	-2.88639832	0.81323072	-2.87111262	N	-1.67861100	2.28966600	-1.97925000
O	-2.88134626	-0.24303111	-2.27180984	C	1.62630400	-0.88471800	0.50351500
O	-2.13056054	1.78212843	-2.55041573	C	2.29506500	-1.39674000	-0.55106400
H	-1.43284399	1.34685650	-1.53608033	C	3.67027400	-1.14402400	-1.02385000
C	-3.75301385	1.15308529	-4.05453807	C	4.35299100	0.07415100	-0.84749200
H	-4.37174745	2.02515523	-3.82434210	C	4.31936900	-2.15954000	-1.75097900
H	-3.12613862	1.41381251	-4.91207982	C	5.63814300	0.25234200	-1.35471900
H	-4.38689389	0.30312480	-4.30271337	H	3.86779600	0.88861100	-0.32286800
P1				C	5.60739100	-1.98413600	-2.25215500
O 1				H	3.80201900	-3.10145400	-1.91673700
C	0.17044400	-1.22392300	0.78348500	C	6.27588000	-0.77542200	-2.05310200
C	-0.54815400	-2.14187300	-0.21137700	H	6.14226800	1.20381700	-1.20949100
H	-0.38985300	-0.28733100	0.88777400	H	6.08641200	-2.78917500	-2.80242300
H	0.11631300	-1.67803700	1.78450600	H	7.27810000	-0.63143600	-2.44617200
C	-2.05207600	-2.34202200	0.11668300	C	2.24731800	0.00150000	1.53466600
H	-0.43371900	-1.74853000	-1.22842900	C	1.72164500	1.27357900	1.81349500
H	-0.05299600	-3.12038700	-0.20717500	C	3.33701400	-0.45004700	2.29731700
C	-2.97051600	-1.44898100	-0.76695100	C	2.28202700	2.07665300	2.80730500
H	-2.22597800	-2.05849300	1.15911800	H	0.87710500	1.64393600	1.23947000
H	-3.06112700	-1.93611700	-1.74603000	C	3.89210300	0.34886400	3.29551100
C	-2.44549300	-3.81899100	-0.06029400	H	3.74589400	-1.43585100	2.09902300
H	-2.23122500	-4.15891700	-1.08161600	C	3.36837700	1.61728000	3.55300900
H	-1.86921900	-4.45047400	0.62317700	H	1.86647600	3.06167000	3.00059000
H	-3.50488200	-3.98785400	0.14302400	H	4.73335600	-0.02110500	3.87480200
C	-4.42932100	-1.29085100	-0.27557900	H	3.80076400	2.24037000	4.33049600
O	-5.24867900	-0.62850100	-0.87155500	H	1.76051300	-2.11405600	-1.16960500
O	-4.70066700	-1.98461700	0.84358900	H	-2.19721500	0.14463900	-1.99648100
C	-6.03691800	-1.82327400	1.35031900	P2			
H	-6.77208100	-2.13476300	0.60468400	O 1			
H	-6.09263100	-2.45547700	2.23597000	C	-0.76204900	4.73808500	-1.39338600
H	-6.21443300	-0.77780100	1.61142600	C	0.16217700	3.86264800	-0.53678400
N	-2.45198500	-0.11615800	-1.05274700	H	-1.06366100	5.63205500	-0.83769100
C	-2.53298500	0.90218200	-0.16204700	H	-0.25619500	5.07136200	-2.30745600
O	-2.93014700	0.76983600	0.99549900	H	-1.67633200	4.21396900	-1.68666900
C	-2.07193800	2.23676900	-0.69670000	C	0.70743900	2.63760800	-1.30154900
C	-2.07814900	3.34484000	0.15300200	H	1.01558400	4.47477800	-0.22997200
C	-1.27321700	3.46979100	-2.45680000	H	-0.33985300	3.55921000	0.37966800
C	-1.65184100	4.56894700	-0.35744400	C	2.00452400	1.96809900	-0.73093100
H	-2.41555900	3.21866400	1.17498600	H	1.05348000	3.03116300	-2.26118800

H	2.45199800	1.45260100	-1.58978500	C	-4.64432100	3.31684400	0.56422300
C	-0.35196700	1.55273300	-1.72332100	H	-3.63174600	3.47699100	2.46125700
H	-1.00008400	2.04883900	-2.45434600	H	-5.38843000	2.97053400	-1.43062200
H	0.18413100	0.75616200	-2.24457900	H	-5.49668700	3.91444300	0.87376200
C	3.06939100	3.01117700	-0.36308300	H	2.34525800	0.03358000	0.04328600
O	3.33434500	3.95727000	-1.08030200	H	-1.10904300	-0.79456500	-1.21965100
O	3.70953200	2.73752000	0.77989900				
C	4.76235200	3.65513100	1.14172300	P3			
H	4.35833400	4.66019100	1.28057200	O 1			
H	5.17259800	3.27476900	2.07586600	C	0.38498400	-0.52505800	-2.92051700
H	5.53012000	3.67794200	0.36549200	C	1.53068900	0.03337900	-2.06825800
N	1.83343000	0.90682100	0.24643400	H	-0.18999000	0.28554200	-3.37465100
C	1.18104900	1.01024700	1.41555800	H	0.79036100	-1.13198100	-3.73426000
O	0.72968100	2.05045500	1.90543400	H	-0.31009400	-1.15047000	-2.35755000
C	0.99082800	-0.28938700	2.16700600	C	2.49627100	-1.08270500	-1.52107900
C	1.10407100	-0.25854300	3.55809300	H	2.17558000	0.59223800	-2.76224500
C	0.45672900	-2.55170400	2.22574700	C	1.79205300	-2.24179700	-0.75542000
C	0.90771800	-1.42367500	4.29185800	H	3.19795500	-0.60835100	-0.83290500
H	1.34631000	0.68407300	4.03340100	H	1.29350000	-2.88425200	-1.48903000
H	0.18783800	-3.43491400	1.65984700	C	3.31650000	-1.65603100	-2.69579800
H	1.00555400	-1.41862600	5.37236700	H	2.68164900	-2.17425400	-3.42217000
C	0.57863300	-2.59384100	3.60923200	H	3.83445700	-0.84823300	-3.22198900
H	0.40816700	-3.52875600	4.13053100	H	4.06919100	-2.36246500	-2.34588000
N	0.65892200	-1.42456200	1.51061000	C	2.72569400	-3.19781400	0.02957100
C	-1.29666600	0.93354700	-0.71030600	O	2.29051900	-4.12959900	0.67558000
C	-1.33652900	-0.44374200	-0.52904700	O	4.03079300	-2.92417900	-0.08859000
C	-2.36679600	-1.17193500	0.26916000	C	4.92039100	-3.79580200	0.63870400
C	-2.60574800	-0.92716800	1.62740400	H	4.78835000	-4.83093900	0.31745600
C	-3.11875500	-2.18116600	-0.36552500	H	5.92525400	-3.44619600	0.40670400
C	-3.57727900	-1.64474600	2.32706100	H	4.72569700	-3.72128200	1.71065200
H	-2.02567900	-0.17524600	2.15486500	N	0.73305900	-1.81714900	0.16318100
C	-4.09371700	-2.89435800	0.33241600	C	1.05533500	-1.22138700	1.32730100
H	-2.93610200	-2.38662100	-1.41522700	O	2.22164900	-1.03383100	1.69469500
C	-4.32914500	-2.62996400	1.68380900	C	-0.06028900	-0.73864000	2.22536400
H	-3.74536100	-1.43086600	3.37904500	C	0.19673200	-0.73099900	3.59827800
H	-4.67009500	-3.65820400	-0.18232200	C	-2.14321500	0.23540800	2.58373700
H	-5.08655400	-3.18585200	2.22875700	C	-0.75883800	-0.23737900	4.47959500
C	-2.42832100	1.77229800	-0.22746100	H	1.15031900	-1.11131300	3.94161800
C	-2.50312900	2.29537300	1.07035600	H	-3.05448500	0.61497700	2.13866700
C	-3.48065600	2.03031800	-1.12684800	H	-0.57460700	-0.23726700	5.54866200
C	-3.59832500	3.06882600	1.45507700	C	-1.95095100	0.26245400	3.95923200
H	-1.68435700	2.13156100	1.76134100	H	-2.72670400	0.66958200	4.59719700
C	-4.58566400	2.79278400	-0.72868500	N	-1.22253300	-0.25782500	1.72871300
H	-3.44556700	1.62296900	-2.13365000	C	1.14551300	1.12025300	-1.05348900

C	-0.12991200	1.46428700	-0.71638900	O	-4.49431200	1.31695800	-1.13288500
C	-0.56220000	2.59624900	0.14572800	O	-3.33741600	0.31743100	0.54077300
C	0.10183200	2.95367800	1.33357000	C	-4.40968200	0.54769900	1.48034600
C	-1.71134200	3.32554900	-0.22017900	H	-5.09738400	-0.31432900	1.45276800
C	-0.35373100	4.01605400	2.11424900	H	-3.93389400	0.65440600	2.45436000
H	0.97401900	2.39586600	1.65302000	H	-4.96258300	1.45270000	1.20369200
C	-2.16112500	4.39057200	0.56127100	N	-1.08799600	1.13864300	-0.91279000
H	-2.24125000	3.04563000	-1.12500800	H	-1.09217700	1.17659800	0.02895800
C	-1.48382400	4.74298100	1.73125400	C	-0.26608700	2.01759400	-1.55877500
H	0.17561000	4.27348300	3.02744300	O	-0.42673900	2.42219600	-2.71674800
H	-3.04359400	4.94509500	0.25417000	C	0.99384800	2.45357100	-0.81008200
H	-1.83491000	5.57072200	2.34064500	C	1.49319100	3.73156900	-1.05940500
C	2.29714400	2.01630800	-0.67592700	C	2.86748800	1.95260600	0.50643100
C	3.23264200	1.72108200	0.32767800	C	2.70407100	4.12696300	-0.49033200
C	2.46519000	3.19263300	-1.42778000	H	0.92922900	4.37179400	-1.73023600
C	4.30086900	2.58828100	0.57476900	H	3.35588200	1.19657300	1.08897600
H	3.11454100	0.82687400	0.93002900	H	3.08572000	5.13014200	-0.67543700
C	3.53410900	4.05399100	-1.17979600	C	3.40125500	3.22129200	0.30060000
H	1.74899700	3.43220300	-2.20889300	H	4.35068200	3.47457900	0.75437100
C	4.45765400	3.75428300	-0.17565400	N	1.67947600	1.58499700	-0.02337700
H	5.01120200	2.34736900	1.36076700	Pd	0.90515500	-0.19762500	0.53231700
H	3.64259900	4.95902800	-1.77066400	C	4.54911600	-2.43032500	0.19174000
H	5.29002600	4.42402600	0.01989900	H	5.33495200	-2.48297500	-0.57354500
H	-0.19921400	-2.23948800	0.05998300	H	4.04117500	-3.39924300	0.25342100
H	-0.93423800	1.07781000	-1.38384700	H	4.96827500	-2.20773800	1.16747100
3				C	0.23881400	-3.07655100	0.86687900
-1 1				O	1.01747900	-3.46951100	0.00850300
C	-0.46152100	-2.66319900	-3.07801900	O	-0.03531100	-1.81813900	1.16589600
C	-0.86727800	-1.19803500	-2.83874800	C	3.49112700	-1.40202300	-0.20169700
H	0.36420600	-2.70725100	-3.78948700	O	3.40036200	-0.94868700	-1.34610600
H	-0.11832100	-3.12452500	-2.14908300	O	2.73660800	-1.08816700	0.81335600
H	-1.28551300	-3.25380200	-3.49474100	C	-1.33798800	0.92041300	2.73918100
C	-2.01650200	-0.99068300	-1.83026200	O	-2.07640600	1.76455100	3.27928600
H	0.01001600	-0.66125200	-2.48626500	O	-0.47414300	1.11513400	1.78556900
H	-1.16273300	-0.72759400	-3.79172200	O	-1.44685600	-0.39686200	3.18002600
C	-2.24532200	0.53601400	-1.56245300	H	-0.92408100	-0.95613600	2.56773200
H	-1.71684600	-1.44621200	-0.87373400	H	-0.25208100	-3.90280700	2.80541500
H	-2.40037800	1.04993900	-2.50999500	H	-1.61202300	-3.82509600	1.68845000
C	-3.32482500	-1.65050000	-2.29989300	H	-0.35103500	-5.07302800	1.44081100
H	-3.69783500	-1.16866500	-3.22545800	C	-0.54660800	-4.04475900	1.74848300
H	-3.18334100	-2.71008500	-2.50556100	TS1			
H	-4.12348500	-1.56368300	-1.55236700	-1 1			
C	-3.49477600	0.78230600	-0.71458400	C	-0.45152100	-2.69319900	-3.09801900

C	-0.84727800	-1.23803500	-2.81874800	O	3.40036200	-0.94868700	-1.25610600
H	0.35420600	-2.72725100	-3.83948700	O	2.65660800	-1.06816700	0.88335600
H	-0.07832100	-3.17452500	-2.18908300	C	-1.45798800	1.04041300	2.76918100
H	-1.28551300	-3.28380200	-3.49474100	O	-2.18640600	1.78455100	3.41928600
C	-1.96650200	-1.06068300	-1.77026200	O	-0.67414300	1.37513400	1.78556900
H	0.05001600	-0.71125200	-2.47626500	O	-1.45685600	-0.29686200	3.10002600
H	-1.16273300	-0.74759400	-3.75172200	H	-0.93408100	-0.78613600	2.43773200
C	-2.11532200	0.44601400	-1.41245300	H	-0.24208100	-3.81280700	2.79541500
H	-1.67684600	-1.58621200	-0.85373400	H	-1.61202300	-3.81509600	1.68845000
H	-2.23037800	1.00993900	-2.33999500	H	-0.32103500	-5.04302800	1.50081100
C	-3.30482500	-1.63050000	-2.26989300	C	-0.53660800	-4.00475900	1.75848300
H	-3.66783500	-1.07866500	-3.14545800				
H	-3.19334100	-2.68008500	-2.55556100	4			
H	-4.08348500	-1.58368300	-1.50236700	-1 1			
C	-3.39477600	0.73230600	-0.62458400	C	-0.44152100	-2.72319900	-3.11801900
O	-4.36431200	1.28695800	-1.10288500	C	-0.82727800	-1.27803500	-2.79874800
O	-3.32741600	0.26743100	0.63077300	H	0.34420600	-2.74725100	-3.88948700
C	-4.44968200	0.52769900	1.50034600	H	-0.03832100	-3.22452500	-2.22908300
H	-5.16738400	-0.29432900	1.41276800	H	-1.28551300	-3.31380200	-3.49474100
H	-4.03389400	0.59440600	2.50436000	C	-1.91650200	-1.13068300	-1.71026200
H	-4.93258300	1.46270000	1.21369200	H	0.09001600	-0.76125200	-2.46626500
N	-0.91799600	0.98864300	-0.72279000	H	-1.16273300	-0.76759400	-3.71172200
H	-0.99217700	1.17659800	0.36895800	C	-1.98532200	0.35601400	-1.26245300
C	-0.23608700	1.97759400	-1.41877500	H	-1.63684600	-1.72621200	-0.83373400
O	-0.55673900	2.44219600	-2.50674800	H	-2.06037800	0.96993900	-2.16999500
C	1.04384800	2.45357100	-0.78008200	C	-3.28482500	-1.61050000	-2.23989300
C	1.51319100	3.74156900	-1.02940500	H	-3.63783500	-0.98866500	-3.06545800
C	2.92748800	1.94260600	0.48643100	H	-3.20334100	-2.65008500	-2.60556100
C	2.72407100	4.13696300	-0.47033200	H	-4.04348500	-1.60368300	-1.45236700
H	0.91922900	4.39179400	-1.66023600	C	-3.29477600	0.68230600	-0.53458400
H	3.43588200	1.17657300	1.05897600	O	-4.23431200	1.25695800	-1.07288500
H	3.10572000	5.14014200	-0.63543700	O	-3.31741600	0.21743100	0.72077300
C	3.44125500	3.22129200	0.30060000	C	-4.48968200	0.50769900	1.52034600
H	4.39068200	3.48457900	0.75437100	H	-5.23738400	-0.27432900	1.37276800
N	1.74947600	1.57499700	-0.04337700	H	-4.13389400	0.53440600	2.55436000
Pd	0.90515500	-0.20762500	0.35231700	H	-4.90258300	1.47270000	1.22369200
C	4.48911600	-2.43032500	0.30174000	N	-0.74799600	0.83864300	-0.53279000
H	5.29495200	-2.47297500	-0.43354500	C	-0.20608700	1.93759400	-1.27877500
H	3.98117500	-3.39924300	0.34342100	O	-0.68673900	2.46219600	-2.29674800
H	4.88827500	-2.21773800	1.29747100	C	1.09384800	2.45357100	-0.75008200
C	0.22881400	-3.06655100	0.82687900	C	1.53319100	3.75156900	-0.99940500
O	1.02747900	-3.48951100	-0.00149700	C	2.98748800	1.93260600	0.46643100
O	-0.09531100	-1.80813900	1.02589600	C	2.74407100	4.14696300	-0.45033200
C	3.45112700	-1.39202300	-0.11169700	H	0.90922900	4.41179400	-1.59023600

H	3.51588200	1.15657300	1.02897600	H	-4.79275200	2.34251400	-0.70416800
H	3.12572000	5.15014200	-0.59543700	N	-0.86104700	0.23684000	-0.42880500
C	3.48125500	3.22129200	0.30060000	H	-0.90094500	0.54115600	1.07009800
H	4.43068200	3.49457900	0.75437100	C	-0.72245800	1.32976700	-1.21644900
N	1.81947600	1.56499700	-0.06337700	O	-1.44161100	1.65945700	-2.17357300
Pd	0.90515500	-0.21762500	0.17231700	C	0.42002800	2.24178200	-0.83295800
C	4.42911600	-2.43032500	0.41174000	C	0.38456700	3.60180800	-1.13408200
H	5.25495200	-2.46297500	-0.29354500	C	2.53105100	2.47263300	0.15201700
H	3.92117500	-3.39924300	0.43342100	C	1.45057700	4.41318700	-0.75530500
H	4.80827500	-2.22773800	1.42747100	H	-0.48008900	3.98597900	-1.66130100
C	0.21881400	-3.05655100	0.78687900	H	3.36041100	1.96926000	0.63589000
O	1.03747900	-3.50951100	-0.01149700	H	1.43658200	5.47618900	-0.97214400
O	-0.15531100	-1.79813900	0.88589600	C	2.54035200	3.83984600	-0.09695800
C	3.41112700	-1.38202300	-0.02169700	H	3.39299500	4.43234500	0.21354600
O	3.40036200	-0.94868700	-1.16610600	N	1.48781700	1.70136900	-0.20923300
O	2.57660800	-1.04816700	0.95335600	Pd	1.55110600	-0.28390200	0.02630000
H	-0.23208100	-3.72280700	2.78541500	C	-0.09047900	0.51947000	4.29007000
H	-1.61202300	-3.80509600	1.68845000	H	0.85442000	0.29585800	4.78399600
H	-0.29103500	-5.01302800	1.56081100	H	-0.41220100	1.53630000	4.53068900
C	-0.52660800	-3.96475900	1.76848300	H	-0.86533200	-0.16368800	4.65167800
TS1'				C	3.64381800	-3.40372200	-1.25887700
0 1				H	3.67649900	-4.15753700	-0.46971900
C	-0.99127400	-4.27602800	0.20718900	H	4.65314400	-3.14140000	-1.57993000
C	-1.26001200	-3.04408500	-0.66390100	H	3.10485900	-3.82709400	-2.11366000
H	-0.36630400	-4.99815000	-0.32861000	C	0.04436200	0.36638800	2.79646400
H	-0.46286900	-3.99891200	1.12633100	O	1.08457200	-0.09024300	2.28790200
H	-1.91346500	-4.79199700	0.49300200	O	-1.00332200	0.73554000	2.11318000
C	-2.05701400	-1.92091200	0.03283000	C	2.91578500	-2.18505800	-0.78404900
H	-0.29974200	-2.63862200	-0.99711800	O	3.21150500	-1.01729500	-1.19218700
H	-1.80714000	-3.34430300	-1.56916000	O	1.93226500	-2.29036700	0.04051900
C	-1.98529400	-0.62174200	-0.84009700	2'			
H	-1.56301900	-1.68544800	0.98355000	0 1			
H	-1.85999600	-0.91704000	-1.88886300	C	-1.23779500	-3.63785100	1.64673500
C	-3.49088000	-2.37414600	0.35683200	C	-1.38894200	-2.73524600	0.41680000
H	-4.05744800	-2.59411800	-0.55375100	H	-0.39098000	-4.32060400	1.52121600
H	-3.47386100	-3.27839900	0.97085400	H	-1.05312800	-3.03700300	2.54388600
H	-4.03868200	-1.61192700	0.91958900	H	-2.12741200	-4.24959000	1.82770600
C	-3.32027700	0.13552300	-0.85291900	C	-2.56223000	-1.73473200	0.51313500
O	-4.20963300	-0.07670800	-1.65357500	H	-0.45184200	-2.18781200	0.27882600
O	-3.43472000	1.01399600	0.16180400	H	-1.52616100	-3.34790000	-0.48517000
C	-4.66793600	1.75480400	0.20833800	C	-2.38197300	-0.59238300	-0.52704000
H	-5.51930400	1.07929900	0.31908300	H	-2.53586300	-1.26599000	1.50620800
H	-4.58595500	2.40961100	1.07516300	H	-2.22682200	-1.02926800	-1.51974200

C	-3.91435000	-2.44633100	0.34882100	H	-0.82693300	-3.49266100	2.02493900
H	-4.03204700	-2.83889500	-0.66722000	H	-2.21305600	-4.38805200	1.38509500
H	-3.98625500	-3.28659500	1.04399500	C	-2.19586900	-1.71815600	0.27863300
H	-4.75943600	-1.78281900	0.55085800	H	-0.30853900	-2.64211900	-0.28388600
C	-3.65591000	0.25087200	-0.66520200	H	-1.72483100	-3.44813500	-0.92578100
O	-4.50362300	0.05867200	-1.51265900	C	-1.90294500	-0.56624400	-0.74351000
O	-3.75733400	1.17858100	0.30166800	H	-1.92838000	-1.33155300	1.26911000
C	-4.94360100	1.99639500	0.26055600	H	-1.66860300	-0.98784100	-1.72411300
H	-5.83793300	1.37848300	0.36687700	C	-3.68539800	-2.10503300	0.31502900
H	-4.85404500	2.68603100	1.09872200	H	-4.04382100	-2.40956500	-0.67328100
H	-4.99412800	2.54392700	-0.68311900	H	-3.83295700	-2.94242900	1.00091800
N	-1.22856300	0.23086700	-0.17403500	H	-4.31514600	-1.28422600	0.66899400
H	-0.77587600	0.10093400	0.74025400	C	-3.14598200	0.30534600	-0.96353400
C	-0.88817400	1.27717400	-0.95174300	O	-3.94795400	0.11651400	-1.85242100
O	-1.47944100	1.58535800	-1.99080200	O	-3.27834200	1.23971100	-0.00751900
C	0.23335700	2.16608800	-0.45217700	C	-4.43067600	2.10122600	-0.12309700
C	0.02498400	3.54538500	-0.49754800	H	-5.34967000	1.51327800	-0.08311700
C	2.35518600	2.48881300	0.46472800	H	-4.37289500	2.78125200	0.72506000
C	1.00893600	4.40840700	-0.02538200	H	-4.39323600	2.65443200	-1.06394000
H	-0.91223300	3.91192100	-0.89776900	N	-0.74118100	0.26291500	-0.29650100
H	3.26482300	2.02066000	0.82026000	H	-0.81392000	0.50732600	0.76936200
H	0.85381200	5.48190400	-0.04475200	C	-0.52731900	1.44903000	-1.07969400
C	2.19394700	3.86816300	0.47282200	O	-1.16947400	1.70380600	-2.07943700
H	2.99112100	4.49581600	0.85363900	C	0.56822500	2.33655900	-0.57412200
N	1.39745300	1.65422800	0.00618300	C	0.57778600	3.70304300	-0.84144200
Pd	1.92518000	-0.30753200	-0.16249700	C	2.58026200	2.43641400	0.55900600
C	2.60237000	-2.74642900	-3.16805900	C	1.64491600	4.45778200	-0.35174500
H	3.63787800	-2.59992700	-3.49444700	H	-0.22768200	4.14749700	-1.41400200
H	1.94227400	-2.51120800	-4.00485600	H	3.35384100	1.89258200	1.09178300
H	2.48019400	-3.78668100	-2.86195800	H	1.68516300	5.52766100	-0.52669900
C	2.32494600	-1.83219400	-2.01930300	C	2.65930300	3.81736600	0.35921900
O	1.91988200	-0.62803900	-2.20320300	H	3.50362000	4.37068200	0.75503300
O	2.50350100	-2.19752600	-0.80477600	N	1.54810600	1.71863500	0.10762900
C	1.18747900	-0.33364700	2.64022200	Pd	1.18761900	-0.55837600	-0.16846000
O	2.19925300	-0.42951500	1.82890900	C	3.87181400	-2.94952100	-1.85412000
O	0.00771800	-0.10455100	2.36836500	H	4.45694400	-2.34483900	-2.55568000
O	1.52578600	-0.51160600	3.94154000	H	3.43421800	-3.78756800	-2.39892300
H	2.47825200	-0.69046800	3.97990500	H	4.54270900	-3.30966500	-1.07163300
TS1''				C	0.21772200	0.09905600	2.77603000
O 1				O	1.09122000	-0.59107000	2.17156800
C	-1.23812700	-3.96410600	1.12507200	O	-0.75921300	0.71802800	2.27854600
C	-1.32547900	-2.95688100	-0.02751100	C	2.79290200	-2.09831700	-1.26332800
H	-0.58127600	-4.79759200	0.85571000	O	1.62678900	-2.02654100	-1.75581500
				O	3.03348500	-1.37175200	-0.22196000

O	0.33589200	0.18967100	4.13254000	H	4.04853105	-1.22121861	-2.54049188
H	1.11946100	-0.32631800	4.37697100	H	4.89006559	0.22128649	-1.94288272
				C	2.18394100	-2.60663000	0.43528600
3'				O	2.86132500	-2.65425500	-0.58561000
-1 1				O	1.22441500	-1.79242000	0.74732700
C	-0.33693700	-4.08653100	-0.99876200	C	2.77371762	0.03431510	-1.40820350
C	-0.76773100	-2.71383500	-1.52861900	O	1.62017428	-0.05278791	-1.82364746
H	0.59746600	-4.39805300	-1.47514500	O	3.12579036	0.27153266	-0.16141035
H	-0.15701900	-4.04272300	0.08004400	C	-1.06131005	-0.19130291	3.19387510
H	-1.08649600	-4.86280200	-1.18761900	O	-1.91100705	-0.05111591	4.05790710
C	-1.95090000	-2.08399700	-0.76263400	O	-0.97711505	0.47021509	2.06000110
H	0.09218100	-2.04111200	-1.48432700	O	-0.04284005	-1.08923291	3.42289010
H	-1.04659600	-2.79534100	-2.59052100	H	0.45713995	-1.22739791	2.59878910
C	-2.11571500	-0.59513600	-1.19001500	O	2.36473200	-3.53716200	1.43371100
H	-1.72104500	-2.09457400	0.31060300	H	3.06057800	-4.11157600	1.09066200
H	-1.91659300	-0.51914000	-2.26383000				
C	-3.23671600	-2.90085900	-0.99054100	TS1'''			
H	-3.55233600	-2.85528000	-2.03928300	-1 1			
H	-3.06640900	-3.94868000	-0.72985400	C	-0.93784300	2.41944300	3.37801800
H	-4.07099100	-2.54382400	-0.37935700	C	-1.09279400	0.95638800	2.94446900
C	-3.56624000	-0.11034000	-1.05428500	H	-0.12953500	2.51393000	4.11106400
O	-4.41457300	-0.23833200	-1.91156100	H	-0.68160500	3.04916900	2.51994200
O	-3.80716500	0.41700300	0.16199600	H	-1.84677500	2.81570700	3.84230100
C	-5.13127000	0.91455600	0.37586100	C	-2.17956900	0.72539800	1.87330800
H	-5.87279800	0.12679200	0.21736100	H	-0.12783100	0.61694400	2.55420900
H	-5.14937500	1.25910600	1.40951300	H	-1.31529600	0.32766100	3.81752000
H	-5.34372900	1.73938800	-0.31115200	C	-2.13241200	-0.73089600	1.34909000
N	-1.17910700	0.30967400	-0.47915700	H	-1.97904400	1.39012400	1.02510200
H	-1.21767018	0.27691290	0.45948009	H	-2.28533700	-1.40961600	2.19200600
C	-1.25398400	1.60177900	-0.97487500	C	-3.58329300	1.02821600	2.42560000
O	-2.03592400	1.98270100	-1.84305000	H	-3.82813300	0.35902100	3.25960300
C	-0.26416000	2.58497100	-0.41713500	H	-3.64151100	2.05449800	2.79643600
C	-0.53700100	3.95109800	-0.40365200	H	-4.35662800	0.91754100	1.66067900
C	1.86604900	2.93541100	0.45842500	C	-3.23738800	-1.08505300	0.34401200
C	0.42749500	4.82422900	0.08930500	O	-3.83201500	-2.14498200	0.35454300
H	-1.49417400	4.28669800	-0.78410400	O	-3.45770000	-0.10883400	-0.54668400
H	2.79342600	2.46308200	0.76071000	C	-4.45197900	-0.37708400	-1.56396500
H	0.23505000	5.89215800	0.13005700	H	-5.36887200	-0.75005900	-1.10442900
C	1.64810400	4.30648500	0.52725600	H	-4.62435900	0.57859100	-2.05584800
H	2.42854700	4.95006400	0.91919200	H	-4.05688300	-1.10303900	-2.27681600
N	0.91828900	2.10048600	-0.00165300	N	-0.82993300	-1.10815800	0.73908100
Pd	1.10654000	0.11827200	0.12095700	H	-0.85841200	-1.30573700	-0.30041900
C	3.95247096	-0.14947842	-2.35695537	C	-0.01033000	-1.94597200	1.48457700
H	3.73240240	0.34311263	-3.30756458	O	-0.26245800	-2.34040400	2.61527700

C	1.29309500	-2.32201400	0.83227300	H	4.43806500	-1.45537100	1.66378000
C	1.89472200	-3.54138600	1.13093900	H	4.60543900	-0.56069800	0.15484200
C	3.06291000	-1.71763700	-0.55651600	C	2.95042900	1.22983900	-0.87658900
C	3.11495800	-3.85632800	0.53721800	O	4.04877100	1.75442900	-0.92990200
H	1.39700300	-4.21365500	1.81896500	O	2.28403500	0.82929800	-1.97422400
H	3.48119600	-0.95159800	-1.19696100	C	2.95406500	1.05333500	-3.22821500
H	3.59736400	-4.80600300	0.74243600	H	3.90466800	0.51557900	-3.25691800
C	3.70526900	-2.92917300	-0.32048100	H	2.27828500	0.67338900	-3.99326600
H	4.65393300	-3.12997800	-0.80481100	H	3.14151000	2.11939900	-3.37740700
N	1.87802900	-1.42569700	0.00821600	N	0.75491000	1.10805900	0.29476200
Pd	0.89222700	0.27952900	-0.40499900	C	0.29634800	2.35844300	0.51054200
C	4.50500500	2.56071400	-0.45931400	O	0.96558900	3.37159100	0.79382500
H	5.25097800	2.70192000	0.32390000	C	-1.19622300	2.47751400	0.38627200
H	4.08056600	3.53222700	-0.73220900	C	-1.85649700	3.68049000	0.61393800
H	4.97509900	2.14419400	-1.35422300	C	-3.19928900	1.40082400	-0.11962100
C	-0.10205200	3.04445700	-0.61221000	C	-3.24110100	3.73082800	0.46999900
O	0.57078600	3.45752300	0.32714700	H	-1.26182900	4.54189600	0.89331400
O	-0.23177700	1.82340100	-1.03816100	H	-3.67511500	0.47568200	-0.41003700
C	3.38686000	1.65034100	0.03663400	H	-3.78123000	4.65615800	0.64324900
O	3.29284900	1.32615200	1.22091200	C	-3.92101700	2.57178900	0.09466500
O	2.58093200	1.27838500	-0.92743800	H	-4.99753500	2.56303800	-0.03367500
C	-1.36371400	-0.96241600	-2.86723100	N	-1.86392100	1.35899400	0.03016700
O	-1.99806200	-1.73638700	-3.59020400	Pd	-0.67650000	-0.24286400	-0.30884100
O	-0.58932100	-1.28243500	-1.88450200	C	-3.81788400	-3.15095400	-0.67093100
O	-1.47988900	0.38144900	-3.13826900	H	-4.68078900	-3.36702200	-0.03851400
H	-1.02519800	0.89487200	-2.44105200	H	-3.17586500	-4.03790200	-0.70605000
O	-0.86611700	3.89324000	-1.36258600	H	-4.14341500	-2.93954300	-1.69292900
H	-0.73630600	4.77309500	-0.97732600	C	0.46980300	-2.93533500	-0.37771500
4'				O	-0.08571700	-3.29942600	0.66146100
-1 1				O	0.56519500	-1.75797400	-0.89009200
C	2.10275700	-1.82926200	3.17925300	C	-3.01108300	-1.98939000	-0.09705400
C	2.03190700	-0.44019000	2.53380500	O	-3.16894600	-1.62603400	1.07385600
H	1.62753300	-1.82038500	4.16644600	O	-2.18085300	-1.46623600	-0.95623900
H	1.57722400	-2.56453500	2.56065000	O	1.13803600	-3.86017200	-1.15003700
H	3.13381100	-2.17181800	3.31788400	H	1.04060900	-4.70048200	-0.67789100
C	2.63505000	-0.37031400	1.11404300	TS6c			
H	0.98201800	-0.13364800	2.48446700	0 1			
H	2.54287900	0.29664500	3.17151400	C	-0.87615300	-3.11099400	0.25257900
C	2.20524000	0.96452600	0.43617800	C	-1.60016300	-1.86500400	0.24533000
H	2.21504200	-1.18478600	0.51983500	H	0.53656700	-2.90162900	0.68399100
H	2.55003500	1.77914200	1.08254300	H	-1.06454600	-3.79329100	1.07984700
C	4.16386300	-0.52707000	1.15417400	H	-0.68316000	-3.62525600	-0.68663700
H	4.63366100	0.30341300	1.69471200	C	-2.13037600	-1.06765200	-0.96808300

H	-2.12981300	-1.61828300	1.16471500	H	-1.91253800	-2.62382800	-2.48697000
C	-1.75226400	0.42820600	-0.75883800	H	-2.09056300	-0.99162700	-3.13593900
H	-3.22618500	-1.14272300	-0.94659400	C	-2.65835700	1.08747200	0.28857000
H	-1.85552300	1.00587700	-1.68767700	O	-3.44196100	0.50439300	1.01351700
C	-1.63797500	-1.57560500	-2.32841300	O	-2.46884200	2.41746000	0.32182000
H	-0.55046400	-1.48866800	-2.42149300	C	-3.22379100	3.12836600	1.31504900
H	-1.91253800	-2.62382800	-2.48697000	H	-2.95173300	2.79112100	2.31880200
H	-2.09056300	-0.99162700	-3.13593900	H	-2.96617000	4.17883900	1.18238300
C	-2.65835700	1.08747200	0.28857000	H	-4.29597800	2.97360800	1.16954000
O	-3.44196100	0.50439300	1.01351700	N	-0.36381400	0.48666800	-0.29180900
O	-2.46884200	2.41746000	0.32182000	C	0.53580200	1.33930300	-0.81813200
C	-3.22379100	3.12836600	1.31504900	O	0.34958000	2.26991400	-1.61010500
H	-2.95173300	2.79112100	2.31880200	C	1.94837400	1.03530800	-0.32435200
H	-2.96617000	4.17883900	1.18238300	C	2.97454700	1.94762600	-0.55929000
H	-4.29597800	2.97360800	1.16954000	C	3.41118100	-0.41946200	0.74588900
N	-0.35871400	0.48666800	-0.29180900	C	4.25949400	1.65772200	-0.10802500
C	0.53580200	1.33930300	-0.81813200	H	2.72386900	2.85579400	-1.09565700
O	0.34958000	2.26991400	-1.61010500	H	3.53870600	-1.37335600	1.24649000
C	1.94837400	1.03530800	-0.32435200	H	5.07402800	2.35655400	-0.27442300
C	2.97454700	1.94762600	-0.55929000	C	4.48014500	0.45361400	0.56054100
C	3.41628100	-0.41946200	0.74588900	H	5.46461000	0.17960800	0.92824300
C	4.25949400	1.65772200	-0.10802500	N	2.16994000	-0.13994500	0.31465400
H	2.72386900	2.85579400	-1.09565700	Pd	0.34662600	-1.28732700	0.42918800
H	3.54380600	-1.37335600	1.24649000				
H	5.07402800	2.35655400	-0.27442300	TS7c			
C	4.48524500	0.45361400	0.56054100	O 1			
H	5.46971000	0.18470800	0.92824300	C	0.51543900	-2.89923400	0.54724500
N	2.17504000	-0.13994500	0.31465400	C	0.92834600	-2.28963200	-0.68228400
Pd	0.34152600	-1.28222700	0.42918800	H	-0.48068000	-2.05440700	-1.30105900
				H	0.12859600	-3.91697500	0.52007700
13c				H	1.00062400	-2.61493200	1.47728900
O 1				C	1.90055200	-1.09857400	-0.67142300
C	-0.91185300	-3.07529400	0.23727900	H	1.05795900	-2.93163600	-1.55416300
C	-1.62566300	-1.87520400	0.24023000	C	1.54753223	-0.00105873	0.39429657
H	0.94966700	-2.71292900	0.82679100	H	1.87117106	-0.62755208	-1.65970207
H	-0.94214600	-3.72699100	1.12064700	H	1.91199922	-0.35884213	1.36577762
H	-0.61176000	-3.57935600	-0.67643700	C	3.31532811	-1.67318014	-0.44278924
C	-2.13037600	-1.06255200	-0.96808300	H	3.38799168	-2.15013464	0.54113611
H	-2.12981300	-1.60808300	1.16981500	H	3.55851738	-2.42597817	-1.19948364
C	-1.75226400	0.42820600	-0.75883800	H	4.06759193	-0.88470275	-0.50193577
H	-3.22618500	-1.13762300	-0.94659400	C	2.24658015	1.33818548	0.10162022
H	-1.86062300	1.00587700	-1.68767700	O	2.70845428	1.60701914	-0.99081451
C	-1.63797500	-1.57560500	-2.32841300	O	2.23199918	2.20541907	1.13181185
H	-0.55046400	-1.48866800	-2.42149300	C	2.95246066	3.43045875	0.91947186

H	2.56844011	3.96058448	0.04496067	C	0.19479200	2.39769800	-0.08557800
H	2.80166312	4.02284116	1.82161587	C	0.19366000	3.78963900	-0.09177100
H	4.01450098	3.21756684	0.77629573	C	2.31277000	2.34187000	0.86948200
N	0.10019634	0.18558207	0.52343986	C	1.30104400	4.46963100	0.41477900
C	-0.50350562	1.13218824	-0.20476240	H	-0.67219600	4.30294600	-0.49322700
O	-0.00379335	2.13642262	-0.76063638	H	3.13007400	1.72656200	1.23309500
C	-1.99472889	0.90317841	-0.40247747	H	1.32281300	5.55478000	0.42614200
C	-2.85831399	1.97588375	-0.62451420	C	2.37975000	3.73440700	0.90583700
C	-3.73572297	-0.61559636	-0.73311400	H	3.26033700	4.22170400	1.30950500
C	-4.20552473	1.73107581	-0.87560105	N	1.24607400	1.68757400	0.38817200
H	-2.44929081	2.97883216	-0.59866979	Pd	0.86255100	-0.45329200	0.06979700
H	-4.02944436	-1.65829124	-0.79358571	C	3.55691100	-1.59003400	-0.33265200
H	-4.89528124	2.55422455	-1.03348411	O	2.74477600	-1.31381400	0.56206700
C	-4.65402086	0.40953855	-0.93196927	O	3.30244600	-1.35733800	-1.61118300
H	-5.69131315	0.17084422	-1.13854386	H	2.39746700	-0.96390100	-1.66581000
N	-2.43695206	-0.37779068	-0.46622238	C	4.88970000	-2.21292000	-0.06335500
Pd	-0.98114500	-1.52969900	0.15755900	H	5.04359200	-2.31856000	1.00912000
13b				H	4.93166800	-3.19464700	-0.54475400
0 1				H	5.67985600	-1.59766000	-0.50204700
C	-1.71683700	-3.68089600	1.64370400	TS6b			
C	-1.98318900	-2.26235900	1.12401100	0 1			
H	-2.13829800	-3.80794600	2.64642500	C	3.60934400	-2.15081500	-1.90504800
H	-2.17738700	-4.43369200	0.99265900	C	3.04778600	-0.97194600	-1.09919700
H	-0.64787000	-3.90618300	1.70844100	H	4.30600000	-1.78862600	-2.66801400
C	-1.53996200	-2.03935000	-0.33723300	H	4.15713800	-2.84698500	-1.25900000
H	-3.05779900	-2.06588800	1.20614800	H	2.82940300	-2.71835900	-2.42080200
H	-1.48441000	-1.53106700	1.77218200	C	2.19263500	-1.40205800	0.11593500
C	-1.90639500	-0.63037500	-0.89462200	H	3.89729200	-0.37747700	-0.74682800
H	-2.07070400	-2.78386900	-0.95164900	H	2.46093200	-0.31843300	-1.75605200
H	-1.84816000	-0.67911600	-1.99152900	C	1.74459600	-0.21817700	1.05892600
C	-0.01384500	-2.19714700	-0.53269900	H	2.83693600	-2.05002200	0.73145100
H	0.38522600	-3.07095500	-0.00883000	H	1.74560600	-0.57884300	2.09157900
H	0.21737600	-2.31061500	-1.60139100	C	0.94996700	-2.21548000	-0.30920500
C	-3.35377500	-0.22883800	-0.61492100	H	1.17696500	-2.92735400	-1.10995700
O	-4.27077100	-0.49583000	-1.36922700	H	0.51755400	-2.76463000	0.53334700
O	-3.52521500	0.38022600	0.57101000	C	2.74273400	0.93866000	1.05158000
C	-4.87250400	0.78408100	0.87457300	O	3.59702700	1.07476200	1.90451000
H	-5.53989900	-0.08059800	0.89716500	O	2.63499900	1.72761200	-0.02974700
H	-4.82447600	1.25381900	1.85627300	C	3.54597800	2.84242400	-0.08472200
H	-5.23193400	1.49667700	0.12852300	H	4.58036900	2.49228100	-0.08362900
N	-0.90219800	0.29955800	-0.38389800	H	3.31836100	3.36083300	-1.01492800
C	-0.99347600	1.61957200	-0.61764900	H	3.38466700	3.50206500	0.77056000
O	-1.93268800	2.20673500	-1.18247300	N	0.34597800	0.16749000	0.70175700

C	-0.11736600	1.48703600	0.82043200	H	-3.81912400	1.07434600	-3.06540700
O	0.41034000	2.35481700	1.49923800	N	-0.53648800	-1.38523000	-1.24013000
C	-1.38506100	1.76181100	0.04079100	C	0.39798200	-2.33141600	-0.93085000
C	-2.09837800	2.93093500	0.29694200	O	0.15397900	-3.53202300	-0.83065100
C	-2.88287900	1.13191300	-1.61302200	C	1.79005500	-1.83735900	-0.62570600
C	-3.25176500	3.19504400	-0.44118500	C	2.87039200	-2.66507500	-0.93396400
H	-1.73682000	3.60711100	1.06244100	C	3.19305200	-0.33692800	0.45142600
H	-3.15772800	0.39430500	-2.36015000	C	4.15378200	-2.29393700	-0.54903000
H	-3.82648700	4.09729900	-0.25998600	H	2.67547300	-3.58914700	-1.46456900
C	-3.65093400	2.28022500	-1.41314400	H	3.28280900	0.59069700	1.00450300
H	-4.53960000	2.44348700	-2.01259100	H	5.00739500	-2.91792400	-0.79155200
N	-1.77325100	0.87383300	-0.90730000	C	4.31369800	-1.10746200	0.16554400
Pd	-0.47270400	-0.92117600	-0.89866700	H	5.28774100	-0.77404000	0.50481300
C	-2.13568100	-2.07007700	1.36551300	N	1.94353200	-0.67775900	0.05973800
O	-2.14432100	-2.28675400	0.12193100	Pd	0.60607200	0.91382200	0.43878300
O	-1.36203500	-1.25583700	1.98338200	C	0.76662500	3.42010100	0.10955300
H	-0.41434400	-0.50072000	1.27667300	O	1.77475100	2.76408700	-0.27857200
C	-3.11747500	-2.83789100	2.24083700	O	-0.23444800	2.79813100	0.63554800
H	-3.78332300	-3.45655200	1.63786400	H	-0.18798000	-0.42767500	-1.24541100
H	-2.56156000	-3.47391400	2.93734900	C	0.68406400	4.91653900	-0.04277800
H	-3.70517200	-2.13705600	2.84106900	H	-0.03449700	5.15859900	-0.83292600
				H	0.32197500	5.37099500	0.88297500
				H	1.65804300	5.32917500	-0.30814800
14b							
0 1							
C	-2.71945100	-1.78315000	3.26419700	TS7b			
C	-2.93153200	-1.58446400	1.75886400	0 1			
H	-3.66264300	-2.04847600	3.75234800	C	-2.20581200	1.13146600	0.91024600
H	-2.00500300	-2.59136100	3.45982200	C	-0.68446100	1.31118200	0.92175800
H	-2.34185300	-0.87738800	3.74830900	H	-2.61350500	1.12494000	1.92888600
C	-1.62646100	-1.31813600	0.96975900	H	-2.71048700	1.96605700	0.40939300
H	-3.40444100	-2.48425000	1.34465600	H	-2.81725700	-0.15040600	1.01385400
H	-3.63751500	-0.76373700	1.58865900	C	-0.21386100	1.46953500	-0.52614600
C	-1.83827800	-1.49129200	-0.57406100	H	-0.41315000	2.17659500	1.54207400
H	-0.93397600	-2.12990200	1.22832000	H	-0.20697000	0.43236200	1.37342500
H	-2.23518700	-2.49196400	-0.75400200	C	1.33372700	1.60966400	-0.69161700
C	-0.98948900	0.01996100	1.36466400	H	-0.63289100	2.40402100	-0.92065000
H	-1.72044600	0.83375600	1.27346600	H	1.54498100	1.66978500	-1.76345200
H	-0.65255400	-0.02568000	2.40665700	C	-0.78282600	0.29728200	-1.31752200
C	-2.85346900	-0.51643600	-1.15435600	H	-0.78877000	0.47083000	-2.40372800
O	-4.05462700	-0.66548800	-1.05047400	H	-0.24257900	-0.63415600	-1.09815800
O	-2.28084100	0.53896300	-1.75692800	C	1.78540600	2.93699500	-0.08537500
C	-3.18444300	1.52593200	-2.30046400	O	1.42754400	4.01517400	-0.51662600
H	-3.80850200	1.94321700	-1.50787900	O	2.57486200	2.78406500	0.99003700
H	-2.54800000	2.29525800	-2.73406000	C	3.00825700	4.00118400	1.63357900

H	2.14681500	4.56609600	1.99594200	C	-0.85132300	4.46888300	-0.88799100
H	3.63668800	3.68438500	2.46432500	H	0.13293700	4.79409300	-1.23196300
H	3.57694200	4.61684400	0.93394800	H	-1.57732200	4.52259700	-1.69781800
N	2.08121700	0.47849100	-0.18339500	H	-1.16519300	5.09293000	-0.04881100
C	2.64655500	-0.44941800	-0.99439900	N	-1.06791500	0.56828600	0.28675700
O	2.52334700	-0.46831500	-2.22243200	C	-1.89612400	-0.18875700	1.04641600
C	3.45781600	-1.49382900	-0.26467600	O	-1.74651500	-0.39296300	2.25460800
C	4.06392500	-2.51874700	-0.99318400	C	-3.05373200	-0.78907400	0.28231500
C	4.27689200	-2.29651100	1.72353500	C	-3.97411500	-1.59247500	0.95794000
C	4.81091500	-3.47083800	-0.30092800	C	-4.16273200	-1.03750900	-1.71250900
H	3.94051400	-2.54866900	-2.06904800	C	-5.03601100	-2.13465900	0.23547900
H	4.34288300	-2.18049900	2.80303600	H	-3.84214700	-1.77254800	2.01808600
H	5.29713500	-4.28321300	-0.83214100	H	-4.21004800	-0.79789300	-2.77249700
C	4.92131300	-3.35957900	1.08474000	H	-5.77242600	-2.76385400	0.72578500
H	5.49218100	-4.07724800	1.66431400	C	-5.13427700	-1.85373300	-1.12692500
N	3.55740700	-1.37819600	1.07020900	H	-5.94322700	-2.25446700	-1.72852200
Pd	-2.67857100	-0.15832000	-0.80856600	N	-3.14032900	-0.51181600	-1.02961200
C	-4.67712000	-1.25780000	0.92772200	Pd	3.26971800	-1.53479700	-0.08957400
O	-4.66520900	-0.90892000	-0.29424800	H	-1.34291300	0.69582100	-0.67953400
O	-3.71362100	-1.02131300	1.72626900				
H	2.31304300	0.41388300	0.80049500	16b			
C	-5.87631700	-2.01428900	1.45747300	0 1			
H	-6.75406500	-1.83654400	0.83475800	C	-0.70986900	1.90566700	-2.12675800
H	-5.65058700	-3.08628000	1.44160300	C	-2.01997400	1.66401200	-1.33706800
H	-6.07885500	-1.73143100	2.49222200	H	-0.66673000	1.29109800	-3.03764300
				H	-0.62999400	2.95661200	-2.43738700
15b				C	-1.75762600	1.81026600	0.18225400
0 1				H	-2.81464500	2.35145800	-1.65947300
C	3.03558900	0.02060500	-1.35638200	H	-2.39967600	0.66011000	-1.55938500
C	1.67754300	0.69549900	-1.13199800	C	-2.03006300	0.49231500	0.97852300
H	3.17417500	-0.35171700	-2.37951300	H	-2.45495700	2.52988400	0.63592100
H	3.86242100	0.69874500	-1.10307900	H	-1.68636200	0.64780600	2.00481300
C	1.44706300	0.71050700	0.38145900	C	-0.31838700	2.32299300	0.38124000
H	1.64140100	1.70048600	-1.57878200	H	-0.28152100	3.40384600	0.19906600
H	0.88729100	0.10297400	-1.61131200	H	0.07059400	2.12003300	1.38488900
C	0.06583100	1.28704300	0.83018200	C	-3.53612700	0.25535900	1.05960700
H	2.19765200	1.36915400	0.83605800	O	-4.28257700	0.95261800	1.71587000
H	0.00040900	1.19640900	1.91803200	O	-3.94852100	-0.76857100	0.29235800
C	1.68369600	-0.72486400	0.87061000	C	-5.36977000	-1.02273300	0.28726000
H	1.84872500	-0.78789100	1.95411800	H	-5.90941600	-0.14548400	-0.07495200
H	0.84466000	-1.37757100	0.59478500	H	-5.51311300	-1.86752200	-0.38428100
C	0.02742700	2.78000400	0.51147700	H	-5.71202400	-1.26942900	1.29425600
O	0.72605000	3.59757400	1.07777100	N	-1.34056200	-0.67880900	0.46343100
O	-0.81187800	3.08155000	-0.49426600	C	-0.14038000	-1.08960400	0.88663700

O	0.47580300	-0.55770100	1.83450400	N	-1.20309200	-0.03692900	0.28295900
C	0.40964300	-2.28860000	0.15647300	C	-1.78251900	-1.18065000	0.71556700
C	1.62772200	-2.84774000	0.54756800	O	-2.59437100	-1.22502600	1.64409800
C	0.12735300	-3.83898100	-1.51434900	C	-1.35669700	-2.42201300	-0.03038700
C	2.09910600	-3.95969600	-0.15132100	C	-1.89126900	-3.65648200	0.34246200
H	2.18053700	-2.41904800	1.37441200	C	-0.09581000	-3.37123600	-1.69933700
H	-0.49398500	-4.20986400	-2.32597000	C	-1.48883000	-4.79269400	-0.35783900
H	3.04216100	-4.42180300	0.12300800	H	-2.60033400	-3.69981900	1.16049100
C	1.33720200	-4.46689200	-1.20200800	H	0.61788400	-3.22387500	-2.50659000
H	1.66494900	-5.33039800	-1.77071600	H	-1.88252200	-5.77007600	-0.09651400
N	-0.33225200	-2.77244700	-0.85439800	C	-0.57284100	-4.64995400	-1.39956400
Pd	0.93760500	1.53826700	-0.99883700	H	-0.23190500	-5.50584400	-1.97237100
H	-1.74696200	-1.21364800	-0.29611000	N	-0.47449700	-2.27403300	-1.03387800
C	3.50444500	0.88341700	1.02410900	Pd	2.22005200	1.23699900	-0.59110300
O	2.91455700	1.27649600	0.01290800	H	-0.56682900	-0.11645800	-0.50082400
O	2.94613400	0.19537000	1.99922400	C	2.89222900	-1.01966900	1.08420400
H	1.97889100	-0.03852300	1.83265800	O	3.42733000	-0.43354800	0.09348300
C	4.96609300	1.16181800	1.25475200	O	1.83548000	-0.59483700	1.65161600
H	5.08338200	1.75580700	2.16619400	H	1.46074000	0.62252500	1.05722000
H	5.50317000	0.22142200	1.40677300	C	3.51480500	-2.29998900	1.59672100
H	5.38618300	1.70087200	0.40676500	H	3.37751900	-2.38794100	2.67585700
TS8b				H	3.00884100	-3.14830800	1.12266200
0 1				H	4.57459500	-2.34462200	1.34179600
C	1.14231300	2.74376400	-1.38823300	17b			
C	-0.31615800	2.60308500	-0.96704400	0 1			
H	1.28313100	2.66308400	-2.47596300	C	2.03603700	1.64966100	-0.86624100
H	1.59696800	3.67771900	-1.03332900	C	0.51281900	1.68378200	-0.79089100
C	-0.41360700	2.30561700	0.55010200	H	2.40560600	1.52635300	-1.88862100
H	-0.89575100	3.50276100	-1.22183900	H	2.49528800	2.53859200	-0.41294000
H	-0.77364700	1.78865700	-1.54093600	C	0.01341800	1.67328300	0.66303100
C	-1.49112100	1.24355400	0.88917300	H	0.14563000	2.58077300	-1.31216400
H	-0.74299600	3.20796100	1.07984700	H	0.09837100	0.81797300	-1.32319100
H	-1.51064800	1.11027900	1.97649900	C	-1.53545800	1.59626500	0.78282100
C	0.96810600	1.91981800	1.12153500	H	0.30188500	2.61636400	1.14166300
H	1.62169800	2.79402500	1.19095800	H	-1.78524500	1.59917900	1.84921800
H	0.86832300	1.58940700	2.16537500	C	0.67747200	0.51349000	1.41821200
C	-2.88250600	1.79662500	0.54925800	H	1.77159500	0.76294400	1.59513500
O	-3.40630300	2.68103900	1.19832300	H	0.32977300	0.39229400	2.44828100
O	-3.43058300	1.23695100	-0.53797400	C	-2.15256700	2.86711600	0.19565300
C	-4.73760200	1.72760300	-0.90184400	O	-1.85949100	3.97881000	0.58832700
H	-4.69512700	2.79563100	-1.12610600	O	-3.01897200	2.62326400	-0.79761800
H	-5.02696700	1.16152000	-1.78591800	C	-3.62331600	3.78464300	-1.40756800
H	-5.44564000	1.55724900	-0.08815200	H	-2.85534400	4.42135400	-1.85150200

H	-4.29145700	3.39634800	-2.17436200	C	-3.03784900	2.63759800	2.01913000
H	-4.18143300	4.35455600	-0.66239900	H	-4.10156300	2.39775500	2.08245400
N	-2.10263200	0.38214800	0.23422800	H	-2.58679900	2.63898300	3.01036700
C	-2.56527000	-0.62182500	1.02325300	H	-2.91609600	3.61231000	1.54133200
O	-2.45477800	-0.64257200	2.25192000	N	-0.50857400	0.37427700	-0.34806000
C	-3.23436100	-1.74338600	0.26693300	C	0.14800900	1.53604300	-0.72329800
C	-3.72839700	-2.84252000	0.97134800	O	-0.40473500	2.52230600	-1.20995600
C	-3.91932600	-2.60580400	-1.74659700	C	1.64194900	1.54180500	-0.50434400
C	-4.34682800	-3.86468200	0.25266200	C	2.32824000	2.74657800	-0.36658500
H	-3.62132800	-2.87389700	2.04898800	C	3.60422100	0.31988100	-0.33245600
H	-3.98015400	-2.48214000	-2.82547400	C	3.71115700	2.71432000	-0.19097800
H	-4.74404800	-4.73602800	0.76392400	H	1.77297900	3.67615700	-0.40201200
C	-4.44526800	-3.74635700	-1.13325500	H	4.06769200	-0.66154900	-0.33565700
H	-4.91806900	-4.51720000	-1.73247900	H	4.27226600	3.63560200	-0.07313300
N	-3.32402000	-1.61952800	-1.06795900	C	4.36076500	1.48033600	-0.17263900
Pd	2.76548900	0.09702300	0.18382900	H	5.43469400	1.40900800	-0.04136000
H	-2.32649000	0.31318700	-0.75135100	N	2.27306400	0.34908200	-0.49436000
C	4.78519700	-1.35339300	-0.34311100	Pd	0.86376300	-1.30607700	-0.77077800
O	4.18385000	-1.65882000	0.72139000	H	-0.24442200	-0.02233300	0.83434800
O	4.35826800	-0.36586000	-1.05981800	C	0.72868900	-1.40196800	2.25305300
H	0.51418000	-0.44606900	0.91453400	O	-0.01158600	-0.37390300	2.01241100
C	5.99967500	-2.10569700	-0.82287900	O	1.30221000	-2.11333400	1.39086600
H	5.79766400	-2.54153200	-1.80599000	H	-4.34969200	-0.71271200	-1.70761400
H	6.84062600	-1.41532800	-0.93663100	C	0.89369800	-1.74408100	3.72328600
H	6.26302800	-2.89512600	-0.11848500	H	1.51666400	-2.62980300	3.85042000
				H	1.34650900	-0.89696400	4.24762900
				H	-0.08932900	-1.91556900	4.17208000
TS9b							
0 1							
C	-0.58593000	-2.65451200	-1.01165600	7a'			
C	-1.92891200	-2.09393200	-1.44522200	0 1			
H	-0.66410000	-3.20442800	-0.06577600	C	0.20223800	-1.88049800	-1.62942500
H	-0.14954300	-3.31129300	-1.78347000	C	-1.22436500	-2.28240900	-1.97071700
C	-2.56372400	-1.05102800	-0.49212700	H	0.62826600	-2.56667900	-0.88478600
H	-1.85968000	-1.66132000	-2.45331700	H	0.84062400	-1.91452200	-2.51960000
H	-2.63519900	-2.93428300	-1.53197700	C	-2.20089100	-2.24805900	-0.78197200
C	-1.93371100	0.35437100	-0.71591000	H	-1.62095200	-1.66461600	-2.78849300
H	-2.35571300	-1.35073600	0.54396900	H	-1.20688100	-3.31413800	-2.35546300
H	-2.03049200	0.60510400	-1.77791700	C	-2.69599600	-0.80614600	-0.48765800
C	-4.08911600	-1.02568200	-0.69017700	H	-1.65855300	-2.59920700	0.10773200
H	-4.49753700	-2.02820600	-0.53199300	H	-3.38919000	-0.51513200	-1.28954300
H	-4.59222600	-0.34773800	0.00328200	C	-3.38459100	-3.19730800	-1.03495600
C	-2.72756400	1.45419300	0.00126400	H	-3.92750800	-2.90814300	-1.94297700
O	-3.64152800	2.07001500	-0.50984300	H	-3.02014700	-4.21968600	-1.17643100
O	-2.33467200	1.62423100	1.27440200	H	-4.10088500	-3.20430100	-0.21041000

C	-3.56850000	-0.83009200	0.77575800	H	0.35874000	-3.23940000	1.06643000
O	-4.77646700	-0.96672500	0.77495700	C	-2.74052600	-2.07729400	0.16298400
O	-2.83331700	-0.79902200	1.90685800	H	-1.22625000	-2.84417500	-1.19673600
C	-3.58208100	-0.84858700	3.13414000	H	-1.62658700	-3.90181900	0.13446100
H	-4.16126100	-1.77299700	3.19599100	C	-2.82115600	-0.67795800	-0.51708700
H	-2.84262100	-0.80824800	3.93323200	H	-2.80299700	-1.91655200	1.24796000
H	-4.26140100	0.00459400	3.19964700	H	-2.92840900	-0.83343500	-1.60133000
N	-1.61109000	0.17044000	-0.38860900	C	-3.93373000	-2.95391100	-0.26182100
C	-2.02283800	1.40369500	-0.02302300	H	-3.89141700	-3.17382200	-1.33527100
O	-3.20332800	1.73416700	0.19986800	H	-3.91176300	-3.90687600	0.27575600
C	-0.93386200	2.43420600	0.16068600	H	-4.89498300	-2.47664300	-0.06184700
C	-1.24531600	3.72641500	0.57924900	C	-4.14497100	-0.01785300	-0.09624500
C	1.33265400	2.92927100	0.10682500	O	-5.17319800	-0.05636400	-0.74397800
C	-0.21149700	4.64247200	0.76658500	O	-4.07702500	0.49923600	1.14815500
H	-2.28541300	3.97694600	0.74885600	C	-5.27802200	1.13177500	1.62147800
H	2.33497800	2.56543500	-0.09627600	H	-6.10489500	0.41830300	1.65508200
H	-0.42592700	5.65503400	1.09363700	H	-5.04712500	1.49391800	2.62291600
C	1.10238300	4.23745200	0.52948500	H	-5.54985600	1.96503000	0.96880600
H	1.93741900	4.91563100	0.66624100	N	-1.66661200	0.17385000	-0.24275300
N	0.33642200	2.05050900	-0.07273700	C	-1.81319900	1.45255900	-0.61678100
Pd	0.38533300	-0.00600300	-0.84876100	O	-2.82971000	1.97326900	-1.12496900
C	2.32031800	0.20148500	-1.83075200	C	-0.61251600	2.32149400	-0.33583900
C	2.53806500	-0.28392200	-0.70424200	C	-0.69499300	3.70743500	-0.45155600
C	3.24904600	-0.83462000	0.42548400	C	1.60319200	2.45733700	0.36135400
C	2.59503300	-1.16608200	1.62594800	C	0.41638300	4.48408400	-0.13342200
C	4.64049600	-1.04128600	0.32284500	H	-1.63332000	4.13534800	-0.78299100
C	3.31643100	-1.69237700	2.69703900	H	2.49526700	1.91999000	0.66040300
H	1.52443000	-1.00833400	1.70650200	H	0.37377600	5.56595100	-0.20958000
C	5.35238700	-1.56661800	1.39812900	C	1.58401000	3.84742300	0.28885800
H	5.15093800	-0.78877100	-0.60136500	H	2.47263500	4.40918700	0.55412200
C	4.69420800	-1.89422100	2.58786000	N	0.52999400	1.71014700	0.05009800
H	2.79987900	-1.94522800	3.61816800	Pd	0.35465600	-0.39029300	0.10128100
H	6.42330000	-1.72213500	1.30714900	C	1.55015800	-2.19551200	-0.29530300
H	5.25297200	-2.30472000	3.42349400	C	2.23250200	-1.14620100	0.02540700
C	2.44084300	0.74245000	-3.19119600	C	3.60781700	-0.67105400	0.07561500
H	2.01740100	1.74973400	-3.25712400	C	4.51217400	-1.22509200	1.00351300
H	3.49553700	0.79050200	-3.48402000	C	4.06766700	0.33377600	-0.79787900
H	1.91222800	0.10981600	-3.91174700	C	5.83545400	-0.78844900	1.04998200
TS3a'				H	4.16730800	-1.99737500	1.68448400
O 1				C	5.39504200	0.75980100	-0.75127200
C	-0.21614200	-2.39865000	0.68400200	H	3.38238100	0.76287600	-1.52256700
C	-1.43471300	-2.85138000	-0.11970400	C	6.28282700	0.20448000	0.17389600
H	-0.48181100	-1.83760700	1.59358800	H	6.51943600	-1.22732600	1.77075200
				H	5.73611000	1.52701200	-1.44046500

H	7.31443300	0.54135200	0.21117200	C	1.86631100	-1.31153800	0.02704600
C	1.67206500	-3.46150500	-1.06974200	C	3.21683800	-0.71607800	0.05982200
H	0.96322800	-3.49070000	-1.90340800	C	3.89967700	-0.49784500	1.27353400
H	2.68355200	-3.51837100	-1.48455500	C	3.83862500	-0.28486600	-1.13013300
H	1.49825000	-4.35032700	-0.45379500	C	5.15594000	0.11287500	1.29459600
8a'				H	3.43499200	-0.81306700	2.20384500
0 1				C	5.09504400	0.32037300	-1.10923100
C	0.14391000	-3.14153300	0.28223900	H	3.32378400	-0.43208500	-2.07608700
C	-0.83896900	-2.40020600	-0.67354800	C	5.76032700	0.52349200	0.10407800
H	-0.27090700	-3.10777500	1.30010000	H	5.66274300	0.26671500	2.24351300
H	0.17315300	-4.20492700	0.01743700	H	5.55604900	0.63561200	-2.04142900
C	-2.20669200	-1.93262800	-0.07530800	H	6.73711500	0.99806200	0.12059400
H	-0.28513700	-1.64422200	-1.34793400	C	2.60219400	-3.63790500	0.73942900
H	-1.05728100	-3.05262000	-1.53088300	H	3.61209300	-3.22648300	0.77859700
C	-2.75344300	-0.61452000	-0.72424800	H	2.36348600	-4.04557500	1.73122200
H	-2.03566400	-1.69032000	0.97993000	H	2.60175600	-4.48961100	0.04590400
H	-2.99174100	-0.80070600	-1.78109800	9a'			
C	-3.22181400	-3.08331100	-0.15136600	0 1			
H	-3.47508200	-3.31582400	-1.19202400	C	0.10906100	-0.24802600	2.49070900
H	-2.80851400	-3.98846800	0.30446400	C	-0.87765200	-1.38009600	2.06192300
H	-4.14905900	-2.84355300	0.37664300	H	-0.21492700	0.70173200	2.05366100
C	-4.08567700	-0.22485000	-0.07415400	H	0.02409000	-0.11562900	3.57684500
O	-5.16052900	-0.25961600	-0.63887500	C	-2.34964300	-0.97482100	1.71640400
O	-3.93285400	0.08625000	1.22583000	H	-0.46128600	-1.93832800	1.21816600
C	-5.12528700	0.51212900	1.91070600	H	-0.92095500	-2.10264700	2.88505100
H	-5.89150900	-0.26516100	1.87042300	C	-2.59863000	-0.74635100	0.18209900
H	-4.82317800	0.69837900	2.94051600	H	-2.60697700	-0.04933800	2.24557500
H	-5.51158300	1.42661700	1.45484000	H	-2.43014800	-1.72031200	-0.29447200
N	-1.72627900	0.41062800	-0.59390200	C	-3.26418500	-2.10997700	2.22485700
C	-1.94543400	1.72133600	-0.49579400	H	-2.98757600	-3.06154100	1.75257300
O	-3.02002200	2.34213600	-0.58917300	H	-3.13921900	-2.23410600	3.30529400
C	-0.65170100	2.46704100	-0.18927800	H	-4.31938000	-1.92411400	2.02725600
C	-0.65137800	3.85063600	-0.05583400	C	-4.04164700	-0.39418900	-0.24320500
C	1.63519000	2.37643000	0.29325900	O	-4.38577800	-0.41854300	-1.41067200
C	0.53469900	4.51040700	0.26363700	O	-4.88607000	-0.11449700	0.76265900
H	-1.59010400	4.37195500	-0.20289300	C	-6.21363700	0.27306800	0.36807700
H	2.50944900	1.74919700	0.42127000	H	-6.68482100	-0.51040600	-0.22965200
H	0.55246200	5.59009900	0.37228600	H	-6.76284200	0.42816600	1.29620600
C	1.69539000	3.76035300	0.44440300	H	-6.17782800	1.19770600	-0.21284600
H	2.63981600	4.22792800	0.69863300	N	-1.67262800	0.20184500	-0.48387400
N	0.49146700	1.74527400	-0.01764100	C	-1.94954200	1.51435500	-0.31235800
Pd	0.17449700	-0.27637900	-0.37777500	O	-3.02348300	2.01328900	0.06644000
C	1.57740200	-2.60515600	0.31752700	C	-0.77363400	2.44643600	-0.52011600

C	-0.96343400	3.80298300	-0.76956300	H	-0.90378000	-2.29178200	2.64441000
C	1.54216400	2.74103600	-0.40920000	C	-2.72999800	-0.79371600	0.13182800
C	0.14473900	4.64228200	-0.85929300	H	-2.72678500	-0.29467200	2.24554600
H	-1.97782700	4.16789800	-0.87733800	H	-2.64806300	-1.73551500	-0.42697900
H	2.50631300	2.27324100	-0.24839200	C	-3.29754800	-2.36716600	2.04240900
H	0.01920800	5.70028500	-1.06514600	H	-2.98228700	-3.26330800	1.49249500
C	1.41771600	4.10210000	-0.67183300	H	-3.16368800	-2.57416800	3.10925500
H	2.30780700	4.71895700	-0.72290500	H	-4.36167900	-2.21161700	1.86100600
N	0.46791800	1.93245300	-0.33985000	C	-4.15960700	-0.30662100	-0.18535000
Pd	0.48918200	-0.10460900	-0.34442900	O	-4.53945800	-0.11076100	-1.32484200
C	1.59409000	-0.47607700	2.14637700	O	-4.96384600	-0.17633300	0.88405900
C	2.06428200	-0.35188600	0.88277200	C	-6.29056000	0.30472600	0.60763700
C	3.46330800	-0.39731000	0.42639300	H	-6.80831300	-0.36166600	-0.08606400
C	4.43164700	0.47666800	0.96463000	H	-6.80204700	0.32662800	1.56946000
C	3.86988700	-1.27219700	-0.60404900	H	-6.24665400	1.30786100	0.17683500
C	5.74975700	0.46748400	0.50256700	N	-1.76033700	0.12644900	-0.50783800
H	4.14063000	1.16540000	1.75277800	C	-1.91085300	1.42238000	-0.17052300
C	5.18686400	-1.28431900	-1.05881400	O	-2.87897700	1.91569200	0.43952400
H	3.13781400	-1.94608800	-1.03850100	C	-0.75735500	2.37320000	-0.45333000
C	6.13460100	-0.41291800	-0.51007000	C	-1.01882300	3.72459300	-0.68064200
H	6.47529100	1.15110000	0.93536500	C	1.54606600	2.79199900	-0.42679800
H	5.47705400	-1.97466400	-1.84644200	C	0.03970300	4.61897600	-0.80933400
H	7.15907600	-0.42008300	-0.87072400	H	-2.05215600	4.04456300	-0.73559900
C	2.46232900	-0.87525800	3.32517900	H	2.53750000	2.37260100	-0.29931000
C	-0.17764300	-2.41894200	-2.03870500	H	-0.14878300	5.67004000	-1.00231700
O	0.52568800	-2.14026000	-1.04929800	C	1.34566500	4.14577600	-0.66871800
O	-1.09997500	-1.61742200	-2.52940500	H	2.20039700	4.80861600	-0.74192500
H	-1.23590300	-0.80681900	-1.94379700	N	0.51787900	1.92359100	-0.33621100
C	-0.03292400	-3.71870400	-2.77088500	Pd	0.70619800	-0.08823900	-0.54362600
H	0.19750400	-3.51951900	-3.82150700	C	1.45215400	-0.53028000	2.14161200
H	0.75638100	-4.31926000	-2.32185000	C	2.02272600	-0.38310600	0.92976300
H	-0.98241800	-4.26090900	-2.74121700	C	3.44603900	-0.41477500	0.55727900
H	3.48762400	-1.10768500	3.03116400	C	4.34660000	0.53054800	1.09066300
H	2.49403200	-0.07673100	4.07867700	C	3.94364300	-1.35755400	-0.36768100
H	2.03960200	-1.75697200	3.82482300	C	5.69359300	0.52693500	0.72155000
TS4a'				H	3.98082800	1.26381200	1.80378100
0 1				C	5.28852300	-1.36014100	-0.73064100
C	-0.04834600	-0.33098400	2.36930800	H	3.26023600	-2.08437000	-0.79572700
C	-0.94692300	-1.50082200	1.88586500	C	6.17016700	-0.41674700	-0.19013700
H	-0.36117800	0.59312200	1.87842900	H	6.36967800	1.26288000	1.14803900
H	-0.22531400	-0.17849600	3.44152300	H	5.65292200	-2.10020000	-1.43792300
C	-2.44198900	-1.15327100	1.62709700	H	7.21728800	-0.41916300	-0.47836400
H	-0.52157300	-1.93952700	0.97803700	C	2.24620200	-0.93751200	3.36880300
				C	-0.16566100	-2.23784500	-2.20195700

O	0.70078600	-2.06822600	-1.30657600	C	1.29387500	3.99132300	-0.92770400
O	-1.12406600	-1.39664700	-2.46238400	H	2.15065700	4.62639000	-1.12191000
H	-1.31199500	-0.62541100	-1.69554300	N	0.45879500	1.76292000	-0.55717000
C	-0.13582000	-3.47093400	-3.06028600	Pd	0.95159700	-0.24746000	-0.75181500
H	-0.08352500	-3.17866400	-4.11298900	C	1.07988700	-0.56448600	2.18865300
H	0.71739000	-4.09755700	-2.80398500	C	1.78427000	-0.36794800	1.05909300
H	-1.06627400	-4.02967300	-2.92287000	C	3.25776700	-0.28274000	0.94051500
H	3.29498300	-1.13876800	3.14289000	C	3.94774300	0.84843100	1.42332500
H	2.20285300	-0.15321600	4.13586600	C	4.01011100	-1.29859200	0.31380200
H	1.81100200	-1.83940600	3.81840900	C	5.33308200	0.95862100	1.28885300
10a'				H	3.38640500	1.63680000	1.91707900
0 1				C	5.39410400	-1.18658900	0.18251300
C	-0.44347700	-0.50081900	2.24556900	H	3.49647800	-2.17506700	-0.06811800
C	-1.19721100	-1.66997500	1.57078900	C	6.06220800	-0.05706800	0.66608700
H	-0.77122100	0.44574200	1.81333400	H	5.84298500	1.83716500	1.67494000
H	-0.75551500	-0.46114500	3.29673600	H	5.95434200	-1.98518200	-0.29635400
C	-2.71650100	-1.42158000	1.37255800	H	7.14004000	0.02773000	0.56193300
H	-0.72951900	-1.90368600	0.60837300	C	1.75062100	-0.85929800	3.51837800
H	-1.06755200	-2.56505100	2.19126900	C	0.64595900	-2.04821500	-2.52087400
C	-3.04301600	-0.80925400	-0.02569800	O	1.26142400	-2.23394700	-1.41138600
H	-3.06044900	-0.71795200	2.13791700	O	0.11994800	-0.91584100	-2.76562500
H	-3.02534200	-1.62873000	-0.75394400	H	-1.40140500	-0.15611300	-1.23186400
C	-3.49206600	-2.74093100	1.53742500	C	0.58668900	-3.16279200	-3.53210500
H	-3.11840500	-3.49818000	0.83689600	H	-0.33492900	-3.09853900	-4.11368400
H	-3.35920600	-3.13309800	2.55050200	H	1.43109000	-3.05889600	-4.22256500
H	-4.56308400	-2.61391700	1.36478700	H	0.66197500	-4.13535800	-3.04280700
C	-4.44326900	-0.17806400	-0.18593900	H	2.83584400	-0.93944900	3.43382100
O	-4.81634200	0.32762900	-1.22488500	H	1.52013200	-0.07585000	4.25267500
O	-5.21099300	-0.28747300	0.90606000	H	1.36774700	-1.79967200	3.93649500
C	-6.53205100	0.27994400	0.79970100	11a'			
H	-7.08770300	-0.19415200	-0.01206100	0 1			
H	-7.01149900	0.08564200	1.75796700	C	0.65135200	-1.18980600	-2.26604700
H	-6.46602400	1.35404900	0.61428500	C	1.33136300	-1.96237500	-1.11590500
N	-2.06115700	0.15547900	-0.52619600	H	1.15228000	-0.22375400	-2.39493100
C	-1.97114600	1.40274600	-0.02079100	H	0.86197900	-1.73635000	-3.19342800
O	-2.80394300	1.86896700	0.76224300	C	2.85351700	-1.68287900	-1.04497900
C	-0.79203900	2.26960000	-0.42035800	H	0.87086800	-1.71577600	-0.15449700
C	-1.03929400	3.63984800	-0.53088500	H	1.17373900	-3.03611200	-1.27165700
C	1.47779000	2.62090100	-0.78793100	C	3.20205800	-0.55552700	-0.01619000
C	0.00755600	4.51322600	-0.80544000	H	3.18565100	-1.35209500	-2.03404100
H	-2.05333100	3.99166700	-0.38762400	H	3.38528000	-1.04929800	0.94668500
H	2.46479500	2.17903000	-0.85169000	C	3.63591100	-2.95591300	-0.68234600
H	-0.17454100	5.57776300	-0.90781700	H	3.28455900	-3.36931700	0.27128200

H	3.49778500	-3.72368000	-1.45041800	H	1.27429800	0.38657000	5.43196500
H	4.70761300	-2.75833700	-0.59362500	C	-1.62804000	-3.20209100	0.85669200
C	4.50195100	0.22456900	-0.29624100	O	-1.40286000	-2.12415900	1.42912500
O	4.83775500	1.20801900	0.33096000	O	-1.72678900	-3.32641200	-0.44967600
O	5.25624500	-0.33627300	-1.25471200	H	-1.58031800	-2.43650000	-0.88419000
C	6.51122900	0.31916800	-1.52554000	C	-1.81127900	-4.47827400	1.62100600
H	7.13323200	0.33984600	-0.62806300	H	-2.77112200	-4.92971500	1.35540900
H	6.98652200	-0.27080700	-2.30795300	H	-1.02555800	-5.18429200	1.33572500
H	6.33776700	1.34150400	-1.86790000	H	-1.76738200	-4.28566900	2.69154600
N	2.13150200	0.39107200	0.27328600	H	-1.35616500	-2.07659800	-3.96265400
C	1.81162100	1.38920300	-0.56354100	H	-2.55522600	-0.81723900	-3.59916100
O	2.39240200	1.61881600	-1.63294600	H	-0.99205700	-0.39479100	-4.32035300
C	0.68303000	2.30320200	-0.13348400				
C	0.87929300	3.67396400	-0.31963200	TS5a'			
C	-1.44494400	2.69604500	0.71805400	O 1			
C	-0.11360500	4.57313300	0.05278400	C	-0.72905400	1.01583500	-2.39529500
H	1.81625400	4.00464700	-0.75071700	C	-1.35690400	1.88043900	-1.28436700
H	-2.35876500	2.26623500	1.10810100	H	-1.29192300	0.07695900	-2.48683700
H	0.03351400	5.64081700	-0.07208400	H	-0.90123800	1.51830700	-3.35591300
C	-1.29916400	4.07127200	0.58683400	C	-2.87531100	1.61315900	-1.13157900
H	-2.10896400	4.72404200	0.89196700	H	-0.85825400	1.72303200	-0.32469800
N	-0.47721400	1.81932500	0.36928000	H	-1.20503900	2.93495000	-1.53670100
Pd	-0.96032300	-0.16160800	0.77157100	C	-3.18720200	0.54624400	-0.02715400
C	-0.84777500	-0.89991600	-2.22453500	H	-3.25264700	1.23087000	-2.08526300
C	-1.54621900	-0.45678100	-1.14926000	H	-3.35589300	1.09724300	0.90679000
C	-2.95278600	0.03464200	-1.24847500	C	-3.63535100	2.90975900	-0.80710000
C	-3.22450700	1.25458100	-1.90156500	H	-3.24114400	3.37333200	0.10571000
C	-4.03775400	-0.64690000	-0.66127200	H	-3.52864000	3.63248100	-1.62227000
C	-4.52099700	1.76656200	-1.96950100	H	-4.70261600	2.72280900	-0.66074900
H	-2.40501800	1.79644700	-2.36525300	C	-4.48386300	-0.26249000	-0.22957000
C	-5.33489800	-0.13704200	-0.73280200	O	-4.77843000	-1.23156600	0.43888300
H	-3.86981700	-1.59067300	-0.15199900	O	-5.28451200	0.26010200	-1.17172800
C	-5.58363200	1.07409300	-1.38387100	C	-6.54395200	-0.41454300	-1.36611800
H	-4.70066900	2.70643100	-2.48446700	H	-7.12571700	-0.41001400	-0.44189100
H	-6.15324800	-0.68947800	-0.27925000	H	-7.05828700	0.14538900	-2.14583800
H	-6.59314200	1.47097300	-1.43682400	H	-6.37563300	-1.44625000	-1.68169500
C	-1.49055500	-1.05138200	-3.59516000	N	-2.09920900	-0.36823800	0.29641300
C	0.36913100	0.22564000	3.46775100	C	-1.76873200	-1.40230500	-0.49127400
O	1.48793300	0.07942200	2.92705100	O	-2.35605400	-1.69648500	-1.54123500
O	-0.75851900	0.24458800	2.85214000	C	-0.61261800	-2.26535200	-0.03176200
H	1.72657900	0.33418600	1.22604500	C	-0.76765200	-3.64703900	-0.16687600
C	0.28185200	0.40088800	4.97958600	C	1.52122600	-2.56158300	0.84262600
H	-0.21331600	1.34829400	5.21430100	C	0.25035000	-4.50144500	0.24231100
H	-0.32858000	-0.39880300	5.41050400	H	-1.69356000	-4.02117400	-0.58607700

H	2.41794700	-2.09048900	1.22388500	H	-1.89007000	-2.48805200	-1.99797500
H	0.13557000	-5.57696900	0.15749800	H	-2.51824300	-3.66494100	-0.87902100
C	1.41672800	-3.94466300	0.76345000	C	0.01421100	-3.05991000	-0.04847200
H	2.24301300	-4.56090000	1.09871100	H	-0.96674500	-1.11653600	-0.17962400
N	0.53206800	-1.72807100	0.45245700	H	-1.63291500	-2.19078200	1.04444100
Pd	0.96050800	0.27756700	0.80286000	C	1.25716700	-2.33648900	0.54139500
C	0.72073500	0.58418900	-2.36148000	H	0.23699600	-3.26726400	-1.09747900
C	1.53539100	0.57585100	-1.24987300	H	1.04305700	-2.08439900	1.58502700
C	2.93532300	0.04577800	-1.31367900	C	-0.22522800	-4.39131200	0.68511100
C	3.20696600	-1.27772900	-1.71427400	H	-0.32490800	-4.23825300	1.76574800
C	4.02760800	0.84736700	-0.92624600	H	-1.14656800	-4.86004300	0.32895000
C	4.51116000	-1.77433700	-1.73755600	H	0.58426000	-5.10816600	0.51971200
H	2.38450000	-1.92121800	-2.01285300	C	2.48126800	-3.26602300	0.53898500
C	5.33154700	0.35117800	-0.94946700	O	3.18273900	-3.48590300	-0.42710000
H	3.85160900	1.87264600	-0.61755000	O	2.67791800	-3.81391200	1.75027500
C	5.58130100	-0.96272600	-1.35405200	C	3.77990000	-4.73997900	1.85073500
H	4.68989300	-2.79766100	-2.05632500	H	4.71922400	-4.23923100	1.60698500
H	6.15499300	0.99538000	-0.65353800	H	3.78414800	-5.07871000	2.88563600
H	6.59640100	-1.34839300	-1.37184900	H	3.63254700	-5.58280200	1.17178600
C	1.20643400	0.19592400	-3.73942700	N	1.64049500	-1.07737100	-0.10532800
C	-0.28371400	-0.13017100	3.46314400	C	1.65840100	-0.82557800	-1.43350900
O	-1.40199700	0.04266600	2.93909500	O	1.15119200	-1.51052600	-2.32296300
O	0.84096400	-0.16742200	2.83055700	C	2.44527100	0.41006200	-1.85150400
H	-1.68189500	-0.25935700	1.23661300	C	3.22549600	0.28492200	-3.00336200
C	-0.16426100	-0.30561100	4.97059600	C	3.17883100	2.60767000	-1.56900900
H	0.45648000	-1.17527500	5.20268500	C	4.01278300	1.34990500	-3.42761300
H	0.32978900	0.57230900	5.39949300	H	3.19926000	-0.65624500	-3.53781100
H	-1.14987100	-0.42015300	5.42312400	H	3.11620300	3.51093900	-0.97494000
C	1.55279100	3.19207600	0.69860900	H	4.63032700	1.25802500	-4.31487300
O	1.34049900	2.19024700	1.45387700	C	3.99470900	2.53274800	-2.68978200
O	1.63338300	3.11821700	-0.56539500	H	4.59083900	3.39217100	-2.97370500
H	1.49136000	1.82746500	-0.89281500	N	2.41314900	1.57173300	-1.15938800
C	1.69022500	4.54644900	1.35362700	Pd	1.09935300	2.02514300	0.34065600
H	2.45532500	5.13357000	0.84233400	C	-3.64828200	-1.87124300	-0.96836300
H	0.73738500	5.07783300	1.25688100	C	-3.98866400	-1.00235100	0.00495700
H	1.92910200	4.44322600	2.41215800	C	-5.23718700	-0.22911900	0.16747200
H	1.06908100	1.03966000	-4.42622200	C	-5.94396400	0.34911000	-0.90496100
H	2.24970200	-0.11179700	-3.76259500	C	-5.72776600	-0.00554400	1.47006700
H	0.59097700	-0.62329500	-4.13354800	C	-7.10879200	1.08680100	-0.68428500
12a'				H	-5.56472700	0.24619500	-1.91581800
0 l				C	-6.89195000	0.72799300	1.69086100
C	-2.31171300	-2.58952500	-0.98687300	H	-5.18747300	-0.42452400	2.31556000
C	-1.23845700	-2.15799900	0.02015400	C	-7.59285100	1.27483900	0.61185800
				H	-7.63261100	1.52511600	-1.52937500

H	-7.25139400	0.87593600	2.70550200	H	-5.72281900	-3.03374900	1.43696700
H	-8.49826300	1.85040600	0.78102100	H	-5.98430000	-1.32154400	0.97563600
C	-4.54987700	-2.27099400	-2.11301300	N	-1.90520900	0.07548000	-0.83019400
C	3.37579600	1.47344900	2.04846500	C	-2.26652200	0.94240900	0.14277600
O	3.27290500	0.27281400	1.75757900	O	-2.92697800	0.62110500	1.13519700
O	2.62698800	2.43026700	1.57834200	C	-1.79607100	2.35987600	-0.07532600
H	2.19953000	-0.46401400	0.50541100	C	-2.11468400	3.33788000	0.86791700
C	4.43110800	1.95785000	3.02831700	C	-0.66746800	3.86302300	-1.39150000
H	5.05431000	2.72396300	2.55824500	C	-1.67377000	4.64098300	0.64385500
H	3.94662700	2.41708500	3.89517000	H	-2.69219000	3.06362000	1.74236800
H	5.05302200	1.12431600	3.35522500	H	-0.09436500	4.03991300	-2.29864100
C	-1.30707400	2.38063200	0.49693500	H	-1.90195100	5.42984400	1.35361300
O	-0.53204700	2.56410900	1.50178700	C	-0.93562900	4.91142200	-0.50737700
O	-0.76063900	1.95320300	-0.58143700	H	-0.57240000	5.91062200	-0.72222100
H	-3.28013700	-0.85785200	0.81787600	N	-1.08522200	2.60944000	-1.18797100
C	-2.76632400	2.69318800	0.56511100	C	2.02576400	-0.63077400	1.06736700
H	-3.33600900	1.98547800	-0.03918200	C	2.88769500	-1.04654600	0.11739600
H	-3.11164300	2.67484400	1.59978100	C	4.31315200	-0.70854800	-0.06508300
H	-2.92834800	3.69834300	0.16003300	C	4.85780900	0.56208500	0.20202300
H	-4.45810400	-3.34660700	-2.30535100	C	5.17651200	-1.69161100	-0.58868700
H	-5.60050300	-2.04635300	-1.92074300	C	6.21227600	0.82347700	-0.00971100
H	-4.26078300	-1.76417000	-3.04327900	H	4.21215900	1.36147600	0.54790900
P4				C	6.52937300	-1.43261300	-0.79816600
O 1				H	4.77449700	-2.67386800	-0.82427200
C	0.57179700	-1.06390000	1.08645000	C	7.05681500	-0.17244700	-0.50354100
C	0.06751300	-1.93819800	-0.06694800	H	6.60522300	1.81419800	0.20118000
H	-0.04317500	-0.15774900	1.16093800	H	7.17236200	-2.21333300	-1.19479000
H	0.38909100	-1.59512900	2.03353500	H	8.11011500	0.03376900	-0.66903500
C	-1.44392800	-2.28094300	0.01948900	C	2.39219200	0.27320100	2.22123700
H	0.28874200	-1.45861500	-1.02863100	H	2.51716800	-1.75805300	-0.61705800
H	0.63277700	-2.87739700	-0.06429500	H	-1.39955400	0.47019700	-1.61312400
C	-2.31120800	-1.32601700	-0.84885300	H	3.46615200	0.29537200	2.41438000
H	-1.76976100	-2.17750600	1.05968700	H	2.06142900	1.30484600	2.04181600
H	-2.19761500	-1.64108900	-1.89304600	H	1.88602900	-0.05933400	3.13501800
C	-1.67746900	-3.73585700	-0.42491900	7a''			
H	-1.30153900	-3.89346500	-1.44341400	O 1			
H	-1.13970600	-4.42339700	0.23520500	C	-0.14251100	-2.35159400	-0.49589500
H	-2.73430500	-4.00959500	-0.40436200	C	0.90426600	-2.89579500	0.46393000
C	-3.83589200	-1.37874300	-0.59929500	H	0.10151400	-2.63130300	-1.53030800
O	-4.62565800	-0.73997800	-1.26439500	H	-1.13357500	-2.75594900	-0.26283500
O	-4.19801800	-2.21939800	0.37951400	C	2.33118400	-2.37065600	0.22552800
C	-5.61296000	-2.29387600	0.64569800	H	0.61399500	-2.70569700	1.50664100
H	-6.15560200	-2.60398400	-0.24956100	H	0.93201300	-3.99137800	0.35538400

C	2.53180100	-0.95578800	0.83257400	H	-0.92856200	0.49805300	-3.71655300
H	2.48236300	-2.28987600	-0.86065100				
H	2.57450000	-1.05922700	1.92609300				
C	3.36501100	-3.36082600	0.78848800	TS3a''			
H	3.21413800	-3.50797200	1.86478000	0 1			
H	3.25544700	-4.33454500	0.30071500	C	-0.15767400	-1.65382900	-1.29079600
H	4.39309000	-3.02190500	0.64262900	C	0.78000100	-2.64017700	-0.59889500
C	3.92767200	-0.44247600	0.44794800	H	0.34126000	-1.03842900	-2.05753400
O	4.92629000	-0.59080200	1.12500200	H	-0.94787500	-2.15968200	-1.84189200
O	3.95239900	0.09958800	-0.78747300	C	2.28781000	-2.31403500	-0.68570600
C	5.23528200	0.57758400	-1.22944900	H	0.48905100	-2.79184400	0.44752200
H	5.96020500	-0.23913700	-1.26545500	H	0.63872500	-3.61506000	-1.08261500
H	5.07109500	0.98518300	-2.22639800	C	2.76654800	-1.20281900	0.29567500
H	5.60449700	1.35440400	-0.55571700	H	2.49717100	-1.95879200	-1.70376300
N	1.47881200	-0.01039500	0.46255700	H	2.68807500	-1.59664900	1.32038900
C	1.69838500	1.24550800	0.90809200	C	3.08028100	-3.61568000	-0.45954800
O	2.67608500	1.60793000	1.59025700	H	2.87707000	-4.02696800	0.53636400
C	0.67691500	2.27912600	0.49600400	H	2.78659900	-4.36821200	-1.19772400
C	0.83248500	3.61453100	0.86274300	H	4.15901700	-3.46863500	-0.54052300
C	-1.28121100	2.75678900	-0.65469000	C	4.27518900	-0.99070700	0.08291600
C	-0.11647500	4.54464900	0.44142700	O	5.14783100	-1.50757000	0.75308600
H	1.69095300	3.88767000	1.46419300	O	4.52808300	-0.26649600	-1.02710900
H	-2.10170000	2.36582100	-1.24837800	C	5.91694300	-0.02311600	-1.30648900
H	-0.01889400	5.59132700	0.71184900	H	6.45733400	-0.96361100	-1.43772700
C	-1.19231600	4.11025900	-0.33349300	H	5.93617200	0.55843500	-2.22778700
H	-1.95222000	4.79970900	-0.68432700	H	6.37329100	0.54255600	-0.49044200
N	-0.36635800	1.86498500	-0.24909500	N	2.01386200	0.04209400	0.17126500
Pd	-0.32266700	-0.32215400	-0.48010400	C	2.54890500	1.09458400	0.80588300
C	-2.43967200	-0.51179300	-0.95292200	O	3.61929800	1.11815100	1.45024900
C	-1.83310200	-0.44924600	-2.03948600	C	1.75922400	2.37110500	0.65389100
C	-1.47659600	-0.41533000	-3.46490400	C	2.30205600	3.59441000	1.04007000
C	-3.51536100	-0.62850700	0.00215600	C	-0.18192800	3.40927500	-0.10205800
C	-4.82408300	-0.86769200	-0.46622100	C	1.57033400	4.76037400	0.82860600
C	-3.29638400	-0.50392600	1.38627600	H	3.28795800	3.59426000	1.48899100
C	-5.88152400	-0.97674700	0.43307800	H	-1.16569900	3.28606900	-0.53919700
H	-4.99922500	-0.96715700	-1.53296200	H	1.97581200	5.72577800	1.11430900
C	-4.36171400	-0.61551600	2.27927200	C	0.30939800	4.66660800	0.23825500
H	-2.28973100	-0.32134100	1.74852500	H	-0.29388500	5.54668300	0.04576900
C	-5.65505600	-0.85128800	1.80753400	N	0.52540000	2.28550100	0.10710600
H	-6.88481300	-1.16155000	0.06080600	Pd	-0.03134300	0.30332600	-0.32699300
H	-4.17972600	-0.51794400	3.34536500	C	-1.77914400	-1.03321800	-0.29769500
H	-6.48244000	-0.93790200	2.50534400	C	-2.04574500	0.23101100	-0.42969500
H	-0.84407400	-1.26859000	-3.73000400	C	-3.18570000	1.13413800	-0.39027900
H	-2.38350500	-0.45505300	-4.07838100	C	-2.37511300	-2.25355200	0.25680000

C	-2.23729400	-3.04588300	-0.52025300	H	-4.55279700	2.64447600	0.14979900
C	-2.11103100	-2.62854000	1.58553300	H	0.24293700	3.61458800	0.41421400
C	-3.83504600	-4.18090300	0.02800200	H	-3.82106100	4.99667500	0.73720000
H	-3.44439400	-2.76312400	-1.54838600	C	-1.72778000	4.48089800	0.62299300
C	-2.70635600	-3.76863600	2.12649800	H	-1.35342000	5.46798700	0.86927100
H	-1.44565400	-2.01774100	2.18859200	N	-1.22554900	2.20433600	0.06727100
C	-3.56932100	-4.54621500	1.35030800	Pd	-0.08181500	0.53534900	-0.43522200
H	-4.50794500	-4.78008900	-0.57831700	C	2.59296100	-0.22428800	-0.08564600
H	-2.49776400	-4.04706300	3.15527300	C	1.88911800	0.93387700	-0.20942900
H	-4.03319200	-5.43205900	1.77376100	C	2.49330300	2.30946900	-0.11410200
H	-2.92232155	2.06142036	-0.85469177	C	4.07058400	-0.28468700	0.15742500
H	-4.00800103	0.69364726	-0.91438674	C	4.58093400	-0.92291500	1.30256800
H	-3.46516129	1.31155427	0.62723014	C	4.99001800	0.24682400	-0.76408400
8a''				C	5.95582600	-1.01074500	1.52689000
O 1				H	3.89302500	-1.34600300	2.02989400
C	1.90160600	-1.59703200	-0.09665800	C	6.36580200	0.16186800	-0.54084800
C	0.60142800	-1.67627400	-0.95112800	H	4.61877800	0.72106400	-1.66819200
H	1.65201700	-1.88685800	0.93361600	C	6.85506500	-0.46617800	0.60672200
H	2.61308600	-2.35120800	-0.44840900	H	6.32453300	-1.50283000	2.42285100
C	-0.65251200	-2.33120400	-0.28703600	H	7.05553600	0.58014000	-1.26895400
H	0.41776900	-0.70430700	-1.54610800	H	7.92514800	-0.53451300	0.78018400
H	0.82244800	-2.23236700	-1.87343700	H	3.58538900	2.30001500	-0.03833200
C	-2.00632000	-1.71131200	-0.77335600	H	2.22422200	2.92556100	-0.98135800
H	-0.60206600	-2.11558900	0.78669500	H	2.11892200	2.83359100	0.77553400
H	-2.14857300	-1.93583700	-1.84013700	9a''			
C	-0.60447500	-3.85439800	-0.47992300	O 1			
H	-0.72021100	-4.12049300	-1.53680100	C	-1.25920500	-0.59206900	-1.35233700
H	0.35470500	-4.25356100	-0.13570800	C	-0.39855600	-1.81101300	-0.88831300
H	-1.39283000	-4.36112800	0.08377100	H	-0.60548200	0.26110800	-1.55752400
C	-3.17884800	-2.39352200	-0.06018900	H	-1.71902500	-0.85002000	-2.31262700
O	-3.97041600	-3.13885700	-0.60193700	C	1.08856200	-1.89201900	-1.37157700
O	-3.18079000	-2.13183200	1.25944900	H	-0.41538300	-1.88562600	0.20318700
C	-4.27040800	-2.70277700	2.00760200	H	-0.90721900	-2.71647600	-1.23910800
H	-4.27319500	-3.79107900	1.91494700	C	2.12316700	-1.31632700	-0.33790900
H	-4.10370300	-2.40751400	3.04271300	H	1.19794000	-1.33615000	-2.31084200
H	-5.22168400	-2.30582000	1.64590900	H	2.04549100	-1.95663500	0.54978800
N	-1.94724000	-0.27357300	-0.54550400	C	1.39801400	-3.38153700	-1.63652100
C	-3.00098400	0.51616900	-0.34699300	H	1.24127200	-3.97101700	-0.72383900
O	-4.21104300	0.22715200	-0.38157300	H	0.71686300	-3.77417600	-2.39827600
C	-2.55982000	1.93470200	-0.01065700	H	2.41856200	-3.54793900	-1.97986000
C	-3.50827300	2.92309900	0.22577400	C	3.61701600	-1.42266400	-0.71667700
C	-0.82517600	3.44973400	0.37346500	O	4.49725000	-1.22864900	0.10161700
C	-3.09337500	4.21400900	0.54846900	O	3.86450100	-1.78551600	-1.98560600

C	5.25113400	-1.80245400	-2.36539400	TS4a''			
H	5.81936900	-2.48651100	-1.73115200	O 1			
H	5.26859400	-2.13865000	-3.40163500	C	-1.12642300	-0.91549500	-1.09793700
H	5.67295800	-0.79797300	-2.28279100	C	-0.35680700	-1.97975200	-0.27112500
N	1.85635100	0.06647200	0.12834300	H	-0.43554700	-0.13615400	-1.42455200
C	2.24522700	1.05745000	-0.70542400	H	-1.50090300	-1.39306900	-2.01009600
O	3.06883700	0.98245400	-1.63350100	C	1.09294900	-2.30022500	-0.73935900
C	1.49956300	2.36616400	-0.53491000	H	-0.33287400	-1.67912100	0.78093100
C	2.01511900	3.55746500	-1.03890500	H	-0.94091400	-2.90764600	-0.29810700
C	-0.49441500	3.42641000	0.06036300	C	2.17074500	-1.45663400	0.01843900
C	1.24940000	4.71872800	-0.96678700	H	1.18321000	-2.08824800	-1.81085700
H	3.00113900	3.53995900	-1.48737000	H	2.19366200	-1.84588500	1.04498300
H	-1.48325200	3.31986900	0.48854400	C	1.35124500	-3.80287700	-0.50926400
H	1.63784700	5.65935500	-1.34343100	H	1.19277600	-4.06161300	0.54571600
C	-0.02977900	4.64943500	-0.41361000	H	0.64918600	-4.39961000	-1.10078400
H	-0.66772800	5.52363600	-0.34964000	H	2.36297700	-4.10175500	-0.78570400
N	0.25793800	2.31080500	0.00800600	C	3.62823900	-1.61816300	-0.46284000
Pd	-0.09934800	0.55406200	0.98628200	O	4.56310600	-1.10267300	0.12168600
C	-2.37309100	-0.16358000	-0.36821200	O	3.78809500	-2.41713700	-1.53209100
C	-2.08639600	0.50496200	0.77690700	C	5.13676200	-2.54601600	-2.01416000
C	-3.03922300	1.04460900	1.80388000	H	5.78990900	-2.95031700	-1.23741400
C	-3.77250000	-0.54365400	-0.74623800	H	5.08250200	-3.22976100	-2.86078400
C	-4.29924900	-0.19227900	-2.00360900	H	5.51793900	-1.57319100	-2.33380000
C	-4.59542000	-1.27625700	0.12741000	N	1.87229300	-0.01021400	0.15300300
C	-5.59894000	-0.54651800	-2.36621700	C	2.09730000	0.70866800	-0.96419600
H	-3.68729500	0.37533500	-2.69970400	O	2.70845500	0.31892200	-1.97761700
C	-5.89645800	-1.63368300	-0.23416600	C	1.45877300	2.08537800	-1.07498400
H	-4.20295100	-1.57922300	1.09379100	C	2.05809000	3.05712400	-1.87702500
C	-6.40511700	-1.26911100	-1.48214400	C	-0.41120900	3.45634500	-0.76094700
H	-5.98378000	-0.25575800	-3.34001700	C	1.40652700	4.26653200	-2.09864400
H	-6.50930600	-2.20402500	0.45869800	H	3.01829800	2.83115700	-2.32413100
H	-7.41600300	-1.54794600	-1.76540700	H	-1.39166300	3.55749100	-0.31201800
C	0.90665500	-1.13814000	3.16221800	H	1.86792500	5.03659500	-2.70815700
O	-0.13961800	-0.94683900	2.51300000	C	0.14241600	4.46458300	-1.54038200
O	2.07873800	-0.64665500	2.82050100	H	-0.41301700	5.38129100	-1.70268600
H	2.04271700	-0.18815900	1.92107300	N	0.23856300	2.29864200	-0.51965900
C	0.91820200	-1.95856400	4.41614900	Pd	-0.20330700	1.02985800	1.00390800
H	1.25309100	-1.33540900	5.25089200	C	-2.30181300	-0.27125900	-0.34845000
H	-0.07701500	-2.34982500	4.62059700	C	-2.11636100	0.69638200	0.57559800
H	1.63438000	-2.77818100	4.31126400	C	-3.13848500	1.47210000	1.35486200
H	-4.08806300	0.96179600	1.49536200	C	-3.66890100	-0.79526700	-0.67285900
H	-2.92639100	0.51803200	2.75994600	C	-4.13578600	-0.80303400	-2.00031100
H	-2.83128400	2.10232200	2.01070000	C	-4.51118900	-1.31428600	0.32541300
				C	-5.40183800	-1.29739900	-2.31459200

H	-3.50457600	-0.40728300	-2.79152400	O	-2.44763800	0.94824700	-1.95147200
C	-5.77810000	-1.81200000	0.01210900	C	-1.41110800	-1.17998400	-1.91067800
H	-4.16155900	-1.33861600	1.35345700	C	-1.96035800	-1.54507900	-3.14191500
C	-6.22983100	-1.80388200	-1.30887200	C	0.23380200	-2.80790700	-2.13208600
H	-5.74311500	-1.28502600	-3.34611900	C	-1.40125800	-2.59005000	-3.86927200
H	-6.40858300	-2.21230600	0.80138200	H	-2.81348200	-0.98735300	-3.50729900
H	-7.21440400	-2.19168200	-1.55385600	H	1.11518300	-3.27177500	-1.70729300
C	0.90758200	-0.17506300	3.32740900	H	-1.82739800	-2.89050300	-4.82058700
O	-0.23594100	-0.03532600	2.82179500	C	-0.27465400	-3.22848100	-3.35482700
O	2.01943500	0.08228000	2.70385400	H	0.21476500	-4.03741600	-3.88498000
H	1.94460500	0.20411200	1.60858900	N	-0.32355800	-1.81385300	-1.40401500
C	1.05346500	-0.66188900	4.74119300	Pd	0.42373700	-1.63948000	0.53008400
H	1.63337700	0.06525500	5.31671200	C	2.09828900	0.66250000	-0.22416300
H	0.07681100	-0.80832100	5.20049100	C	2.08032800	-0.66709500	0.00757000
H	1.61380700	-1.60152600	4.74411000	C	3.27392500	-1.58871600	0.05493300
H	-4.15958400	1.23596200	1.03353600	C	3.38538800	1.42183900	-0.36437200
H	-3.06386000	1.26309800	2.42870500	C	3.65271500	2.16951400	-1.52608300
H	-2.98953900	2.55196300	1.23333100	C	4.34491700	1.43660000	0.66246400
10a''				C	4.83903800	2.89123300	-1.66180000
0 1				H	2.92767900	2.17467800	-2.33586500
C	0.82082200	1.49283900	-0.35773100	C	5.53209100	2.16087800	0.53025400
C	0.10723900	1.80157600	0.97871200	H	4.15071000	0.88168400	1.57591300
H	0.13663800	0.98475700	-1.03658800	C	5.78519800	2.89020600	-0.63309700
H	1.06149500	2.44681800	-0.83998800	H	5.02551500	3.45368600	-2.57269300
C	-1.31611800	2.40344600	0.83409800	H	6.25600600	2.15913600	1.34068700
H	0.06321700	0.89228600	1.58931000	H	6.70736800	3.45481200	-0.73661000
H	0.73004300	2.50873700	1.54001300	C	-0.29418900	-2.32840000	2.86633800
C	-2.42464700	1.30561500	0.82550500	O	0.82912400	-1.77222800	2.58700200
H	-1.37467800	2.95035600	-0.11292800	O	-1.14000500	-2.53527700	1.94059800
H	-2.58136400	0.98855200	1.86340500	H	-1.77731000	-0.72512700	0.65582400
C	-1.58721700	3.38690400	1.98694000	C	-0.57194500	-2.75825800	4.28269600
H	-1.46090400	2.88808100	2.95597000	H	-1.64467800	-2.73569100	4.48264200
H	-0.87727000	4.21882800	1.94803000	H	-0.22216700	-3.78821100	4.41463200
H	-2.59578400	3.80364400	1.94517800	H	-0.03772600	-2.12370100	4.99206500
C	-3.82315900	1.74389400	0.33918000	H	4.20271600	-1.07137700	-0.20891700
O	-4.76673800	0.98104200	0.29403400	H	3.40392400	-2.02870900	1.05102800
O	-3.90107400	3.04330600	0.02474800	H	3.15065100	-2.42511400	-0.64474100
C	-5.19249300	3.50069000	-0.42410200	11a''			
H	-5.94879900	3.32450200	0.34364700	0 1			
H	-5.07600400	4.56721200	-0.61072900	C	-1.03671000	1.74689400	-0.36572100
H	-5.47830300	2.97951300	-1.34017900	C	-0.21166800	1.40235800	-1.62407600
N	-2.07008300	0.07832700	0.10914200	H	-0.36138900	1.92874700	0.47408600
C	-2.02257100	0.03485600	-1.23823200	H	-1.52063000	2.71184000	-0.55070100

C	1.07242800	2.26196700	-1.74083200	H	-6.83013500	3.22882000	1.09297400
H	0.05718700	0.34081000	-1.63152500	C	2.40634900	-2.95034800	-0.67868900
H	-0.83598100	1.57313600	-2.50932500	O	2.80972600	-1.84305000	-1.10008600
C	2.32019000	1.54345900	-1.13233500	O	1.29804300	-3.14688700	-0.05875700
H	0.91277700	3.19165100	-1.18569400	H	2.18747400	-0.40901800	-0.31572700
H	2.76048800	0.93156400	-1.92955900	C	3.25471400	-4.19630400	-0.90295500
C	1.36097100	2.62392300	-3.20727700	H	3.38699600	-4.73600800	0.03923600
H	1.45663500	1.71844400	-3.81941800	H	2.73663800	-4.87036200	-1.59321500
H	0.54380800	3.22247500	-3.62242700	H	4.22821900	-3.93468900	-1.31960700
H	2.28402400	3.20103900	-3.30681400	C	-1.70857000	-2.09186100	-2.61336500
C	3.46878300	2.46570300	-0.67667800	O	-0.88847500	-2.45550800	-1.75538300
O	4.45763600	2.06006600	-0.10110900	O	-2.47359100	-1.02906000	-2.48664000
O	3.29611100	3.74648400	-1.03915700	H	-2.30328500	-0.59315500	-1.60386200
C	4.36169500	4.64660000	-0.67620900	C	-1.89500600	-2.84473100	-3.89540800
H	5.30257400	4.32830400	-1.13035700	H	-2.94932700	-3.10758800	-4.01660800
H	4.06295100	5.62236700	-1.05671700	H	-1.61824400	-2.19834000	-4.73389700
H	4.47726200	4.67709400	0.40926900	H	-1.27760800	-3.74129800	-3.89921400
N	2.03204600	0.58527500	-0.07014000	H	-2.60657300	-1.84915500	1.93769400
C	1.74692000	0.98431400	1.17774800	H	-3.90737600	-0.94358100	1.15505100
O	1.75809200	2.16728000	1.54548900	H	-3.16258500	-2.33312200	0.34582800
C	1.40194200	-0.07957900	2.19931100				
C	1.93711500	0.09385700	3.47905300	TS5a''			
C	0.26904400	-1.98208700	2.90734200	O 1			
C	1.63987000	-0.81536800	4.48687600	C	-1.16482300	1.25198800	-1.53627500
H	2.57958100	0.94813000	3.65290600	C	0.16836700	0.83706200	-2.19146900
H	-0.40332400	-2.78935700	2.64526000	H	-0.99079600	2.08155300	-0.83854300
H	2.06105300	-0.69719600	5.47967800	H	-1.81302100	1.69483100	-2.30589500
C	0.78578300	-1.87669200	4.19187000	C	1.23342100	1.95898500	-2.11281000
H	0.51281500	-2.61465300	4.93740900	H	0.56624000	-0.07741400	-1.74281900
N	0.56544900	-1.10723900	1.91885300	H	-0.01716900	0.60234700	-3.24479500
Pd	-0.22486900	-1.65489800	0.07984600	C	2.15491000	1.82913300	-0.84970400
C	-2.11530600	0.75692000	0.09184600	H	0.71247300	2.91941400	-2.05197200
C	-1.90126800	-0.55669900	0.36113300	H	3.05253900	1.28508000	-1.17038100
C	-2.95837800	-1.45799100	0.97495600	C	2.11414400	1.98215000	-3.37281700
C	-3.44446500	1.41192900	0.37147500	H	2.60703300	1.01341900	-3.52182400
C	-3.54342800	2.38167300	1.38489600	H	1.51010600	2.19124300	-4.26141900
C	-4.59413300	1.12141900	-0.38045000	H	2.88848600	2.75129600	-3.30364900
C	-4.75246300	3.02773500	1.64594500	C	2.70271200	3.15593200	-0.28827400
H	-2.66515900	2.62678400	1.97638800	O	3.26671200	3.24988300	0.78204700
C	-5.80475400	1.76977100	-0.12261700	O	2.55803900	4.18035700	-1.14359900
H	-4.54284000	0.38593400	-1.17855100	C	3.11142800	5.43953800	-0.71035700
C	-5.88942400	2.72436800	0.89230800	H	4.18350300	5.34188400	-0.52662800
H	-4.80605500	3.76811400	2.43940300	H	2.92352300	6.13732300	-1.52507500
H	-6.68016600	1.52934500	-0.71959800	H	2.61746900	5.77510600	0.20384200

N	1.63188700	1.02101200	0.24413000	H	-2.85790900	-1.58072600	1.34151400
C	0.69797800	1.46531300	1.09786700	H	-3.77487700	-1.80205600	-0.14447600
O	0.19694700	2.59780200	1.06709600	H	-2.49331300	-2.94015700	0.27468000
C	0.26079300	0.50148100	2.18092100	12a''			
C	0.08641700	1.02847100	3.46293300	0 1			
C	-0.38246700	-1.60411600	2.92845900	C	3.30529400	-0.98539300	-0.23894000
C	-0.31426600	0.19880800	4.50426600	C	1.82003200	-0.96322700	-0.62366500
H	0.27591900	2.08408900	3.61360300	H	3.40251400	-1.45850600	0.74919100
H	-0.56996400	-2.63939400	2.67228100	H	3.86284900	-1.64207700	-0.92010200
H	-0.44046400	0.59315600	5.50705200	C	1.14240700	-2.33967700	-0.45785900
C	-0.54941300	-1.14745600	4.22955700	H	1.30507400	-0.23601100	0.00816100
H	-0.86460600	-1.84075400	5.00080100	H	1.70445000	-0.62126200	-1.66193600
N	0.01201400	-0.80195200	1.91468000	C	-0.39823400	-2.23905200	-0.65101500
Pd	0.18539600	-1.79053300	0.09671000	H	1.31442400	-2.67863900	0.56704500
C	-2.02677700	0.27046400	-0.77159000	H	-0.59381700	-1.97631000	-1.69552300
C	-1.74334300	-1.03386300	-0.45645400	C	1.71564900	-3.38367300	-1.43271400
C	-2.77358300	-1.88255400	0.29125200	H	1.54870300	-3.08641100	-2.47496200
C	-3.34295200	0.88863900	-0.39331400	H	2.79214200	-3.49718100	-1.28510800
C	-3.40570000	1.80968000	0.66445600	H	1.26734000	-4.37106300	-1.29249900
C	-4.51411400	0.59303000	-1.10795900	C	-1.06493100	-3.59859700	-0.38677300
C	-4.62124100	2.40407200	1.01146500	O	-1.29021100	-4.05503900	0.71521100
H	-2.49966100	2.06933000	1.20499700	O	-1.36956900	-4.22492200	-1.53640700
C	-5.72575300	1.19380500	-0.76203600	C	-1.97656500	-5.52722100	-1.40222200
H	-4.47396400	-0.10475900	-1.93991600	H	-2.92227500	-5.45004800	-0.86171600
C	-5.78405900	2.09745400	0.30171900	H	-2.14480400	-5.87784200	-2.41933800
H	-4.65572200	3.11274400	1.83415600	H	-1.30860700	-6.20625200	-0.86774200
H	-6.62328700	0.95669300	-1.32615700	N	-1.09681400	-1.22803500	0.15019100
H	-6.72739700	2.56337400	0.57107700	C	-0.85089200	-0.91545800	1.44157500
C	2.99263100	-2.31604000	0.91292700	O	0.10458000	-1.29832700	2.11818400
O	3.29133300	-1.15449600	0.57149400	C	-1.88589900	-0.02709400	2.12069500
O	1.80484900	-2.82174900	0.89298700	C	-2.13029200	-0.29660500	3.46980900
H	2.12162600	0.12538000	0.41654100	C	-3.45957900	1.69500600	2.16404100
C	4.07712900	-3.27410600	1.38538100	C	-3.07668800	0.44437200	4.16852400
H	3.76046900	-3.79029400	2.29545100	H	-1.56684400	-1.09320100	3.93867900
H	4.24391400	-4.03660300	0.61726200	H	-3.95513300	2.48002700	1.60673200
H	5.00995500	-2.73822000	1.56440900	H	-3.27878100	0.23379900	5.21341200
C	-0.20690000	-2.93215900	-2.61358400	C	-3.75931500	1.45827800	3.49866900
O	0.53069400	-2.92875300	-1.57645400	H	-4.50810400	2.06664100	3.99243300
O	-1.26213800	-2.23825700	-2.73230600	N	-2.53814100	0.97479100	1.48548000
H	-1.41245500	-1.57994400	-1.59946600	Pd	-2.18339900	1.67566700	-0.41182200
C	0.22478100	-3.79202600	-3.77802400	C	4.03537600	0.34986400	-0.19630900
H	-0.64847500	-4.23362100	-4.26143200	C	3.44720000	1.52499600	-0.47680400
H	0.73039000	-3.15521700	-4.51175200	C	4.06709200	2.89396600	-0.41322600
H	0.91653100	-4.56838300	-3.45113600	C	5.48150000	0.24114400	0.17567000

C	5.86836100	-0.28753700	1.41949400	H	1.88350300	-4.32563900	0.32571600
C	6.49094700	0.62612400	-0.72250500	H	3.44905500	-3.50857500	0.24968100
C	7.21628900	-0.41317300	1.75869900	C	3.83780500	-0.68477500	-0.18817600
H	5.10697900	-0.58892600	2.13383600	O	4.62016200	0.22051300	0.01719500
C	7.84048300	0.49809000	-0.38671400	O	3.98177000	-1.58133300	-1.17411400
H	6.21104500	1.02113000	-1.69499500	C	5.12389500	-1.38750000	-2.03264300
C	8.20840900	-0.02169800	0.85603100	H	6.04882600	-1.42528900	-1.45361400
H	7.49171900	-0.81536900	2.72976600	H	5.08886900	-2.20270300	-2.75357000
H	8.60355800	0.80107300	-1.09845400	H	5.05309600	-0.42328800	-2.53986800
H	9.25761600	-0.12221300	1.11870200	N	1.89311500	0.32851600	0.85555300
C	-4.42328000	0.02479000	-1.13052700	C	1.54295300	1.10981000	-0.19052700
O	-3.66550300	-0.95134200	-1.03306100	O	1.73502700	0.80003000	-1.37043100
O	-4.09046200	1.25980500	-0.87846400	C	0.88071100	2.41059500	0.19413800
H	-2.01497600	-0.97151200	-0.23837400	C	0.45498900	3.28332100	-0.80863200
C	-5.86292100	-0.13530600	-1.58683000	C	0.15418600	3.81613100	1.85627400
H	-6.53920200	0.37989300	-0.89966100	C	-0.15146700	4.48011200	-0.42981600
H	-5.98462800	0.32384600	-2.57300700	H	0.60591000	3.01288800	-1.84669600
H	-6.12365300	-1.19216500	-1.64621500	H	0.04952700	3.99931000	2.92310800
C	-0.41480800	2.86201600	-1.60594100	H	-0.49587300	5.18511800	-1.17977800
O	-1.54178600	2.58372900	-2.15120600	C	-0.30559900	4.75425300	0.92819400
O	-0.24723300	2.47416100	-0.39724200	H	-0.77099700	5.67299200	1.26846300
H	2.39457400	1.51620400	-0.75024500	N	0.73596300	2.66467400	1.50579100
C	0.65439900	3.58360300	-2.36239500	C	-2.18054800	-1.45881500	0.64900400
H	1.29994600	4.13443500	-1.67673100	C	-2.48081900	-1.80499900	1.91283200
H	1.26502900	2.85035600	-2.90050300	C	-3.80556400	-1.67552300	2.61183200
H	0.20641400	4.25843000	-3.09404100	C	-3.20404900	-0.92904000	-0.30595800
H	5.08360200	2.87683600	-0.01509500	C	-3.04984900	0.33424700	-0.90265900
H	4.10257500	3.36220000	-1.40594500	C	-4.32550900	-1.69598900	-0.66356500
H	3.46258200	3.55640900	0.21961400	C	-3.99072800	0.81914500	-1.81159400
P5				H	-2.19350300	0.95031400	-0.64308700
O 1				C	-5.26645000	-1.21425200	-1.57545400
C	-0.78416300	-1.59231600	0.05965700	H	-4.45172300	-2.68277900	-0.22783400
C	0.32073300	-2.11353000	0.98555300	C	-5.10309900	0.04628800	-2.15273400
H	-0.48728000	-0.62402200	-0.36028400	H	-3.85512500	1.80249000	-2.25300500
H	-0.84777500	-2.25731900	-0.81509400	H	-6.12435300	-1.82698300	-1.83781100
C	1.71862300	-2.15649200	0.31292200	H	-5.83361100	0.42206900	-2.86316100
H	0.36129900	-1.50873600	1.89902800	H	-1.68258800	-2.20713100	2.53325100
H	0.05649600	-3.12762300	1.30734300	H	1.72498600	0.71523200	1.77555900
C	2.60266200	-0.93671500	0.70729800	H	-4.20738700	-2.65973200	2.88639300
H	1.58477000	-2.13187800	-0.77301000	H	-3.68839100	-1.11910100	3.55041400
H	3.02334600	-1.14416000	1.69879600	H	-4.55436600	-1.16496100	2.00319500
C	2.44835800	-3.45956800	0.68436100	9a			
H	2.54165100	-3.55283800	1.77340900	O 1			

C	0.34852400	1.67423100	-1.08860200	C	5.14786500	-2.46932400	1.18109800
C	-0.59619400	2.28716300	-0.00492100	H	5.79983800	-2.16790700	-0.85283600
H	-0.18134200	0.88833500	-1.63582400	H	4.22951600	-2.58596700	3.13043100
H	0.56164400	2.45572800	-1.82541700	H	5.99883900	-3.08747300	1.45204700
C	-2.14049500	2.21972100	-0.25642000	C	2.90235100	1.95853700	-0.79209900
H	-0.38118100	1.85132700	0.97553500	C	3.18643200	2.49401900	-2.06245600
H	-0.32707800	3.34503200	0.09420600	C	3.78144700	2.26552500	0.26207900
C	-2.84644000	0.99267400	0.42674200	C	4.31203300	3.29143800	-2.27325300
H	-2.33243900	2.16709100	-1.33498000	H	2.52968700	2.27008800	-2.89864400
H	-2.71583300	1.13705600	1.50660000	C	4.90377400	3.06792600	0.05412300
C	-2.74303500	3.53137500	0.29242400	H	3.57363800	1.87478700	1.25333100
H	-2.51427800	3.63716600	1.36081500	C	5.17625500	3.58374200	-1.21522000
H	-2.29901300	4.38946300	-0.22217600	H	4.51415600	3.68366700	-3.26628000
H	-3.82382300	3.58615000	0.16667600	H	5.56320000	3.29542200	0.88735200
C	-4.38109200	0.89973500	0.26950700	H	6.04940900	4.20917400	-1.37734700
O	-5.04524400	0.13408600	0.94361500	C	-0.99230900	-0.47943400	3.25712300
O	-4.92037200	1.75043900	-0.61804100	O	-0.08027900	-0.07156300	2.51292600
C	-6.33797200	1.61832800	-0.82120800	O	-2.09284600	-1.05120500	2.81600200
H	-6.87920000	1.75801800	0.11718600	H	-2.14698600	-1.01782200	1.80913800
H	-6.60630300	2.39499200	-1.53665600	C	-0.91416200	-0.34999800	4.74806200
H	-6.56714500	0.63012300	-1.22694200	H	-1.00483300	-1.34046000	5.20351800
N	-2.26587400	-0.33678300	0.11642800	H	0.02852600	0.11083100	5.03838400
C	-2.63374600	-0.88362200	-1.06547300	H	-1.75415200	0.25264600	5.10549400
O	-3.61290600	-0.57376400	-1.76487000				
C	-1.67095600	-1.91521200	-1.61641100	9b			
C	-2.06983000	-2.83105000	-2.58613800	0 1			
C	0.54232000	-2.65198800	-1.75967800	C	-2.59822800	-4.54338200	0.17247300
C	-1.12586400	-3.69337200	-3.13936600	C	-1.97731100	-3.49616500	-0.76028100
H	-3.10967600	-2.83743300	-2.89019100	H	-3.32978700	-5.15544900	-0.36547000
H	1.55976100	-2.53359500	-1.40572800	H	-1.83472700	-5.21682800	0.57943000
H	-1.41802800	-4.42273600	-3.88780200	H	-3.12115600	-4.08532200	1.01921800
C	0.20244200	-3.59773000	-2.72250100	C	-0.91247500	-2.61026100	-0.07008000
H	0.97256600	-4.24077900	-3.13330000	H	-1.51032200	-4.01941600	-1.60513900
N	-0.37814500	-1.83347200	-1.21670600	H	-2.75792600	-2.86549700	-1.19235000
Pd	-0.14165900	-0.67268100	0.44488300	C	0.14710600	-2.07909300	-1.06740700
C	1.68932100	1.11020400	-0.56589500	H	-0.33092000	-3.28470900	0.57501600
C	1.74339900	-0.07963200	0.09027300	H	0.66599900	-2.96458700	-1.45930100
C	2.93002600	-0.86025000	0.47719200	C	-1.51715400	-1.57795600	0.92221200
C	3.94179400	-1.15807700	-0.46039900	H	-2.31821800	-2.09759700	1.45355500
C	3.05330400	-1.40442900	1.77332500	H	-0.75674000	-1.36552500	1.67729100
C	5.03499200	-1.95232000	-0.11155100	C	-0.42017400	-1.39580800	-2.32577300
H	3.86544000	-0.75372100	-1.46517700	O	-1.59064100	-1.27815400	-2.62971200
C	4.15169300	-2.18816600	2.12208200	O	0.58074300	-0.98298000	-3.13419700
H	2.27741000	-1.19810500	2.50420500	C	0.17716300	-0.38421300	-4.37953300

H	-0.37542100	0.54146100	-4.19997700	H	1.47306100	-1.58770700	1.51827900
H	1.10111400	-0.17502800	-4.91726700	C	2.20604900	-1.96186100	4.65002000
H	-0.45067000	-1.07171000	-4.95045800	H	3.13581100	-2.52073900	4.50922100
N	1.17575100	-1.22442300	-0.44916100	H	2.32037300	-1.24830000	5.46500300
C	2.46680800	-1.50416800	-0.79047200	H	1.42411300	-2.68642100	4.89616100
O	2.88490300	-2.55058700	-1.30467800				
C	3.44806600	-0.39188700	-0.48758000	9c			
C	4.82085400	-0.62611300	-0.51909100	0 1			
C	3.77851600	1.86014900	-0.02172400	C	-0.79711300	-2.85979700	-0.08424900
C	5.69234700	0.43476100	-0.27890400	C	0.19931600	-2.16682600	-1.04922200
H	5.17064600	-1.62847900	-0.73501600	H	0.71229700	-2.99453400	-1.55689200
H	3.31953100	2.82592900	0.16283300	C	-1.64857000	-2.00206200	0.92931100
H	6.76630300	0.27872200	-0.29136200	H	-2.55120400	-2.60862800	1.04315700
C	5.16271400	1.70071900	-0.02622700	C	-0.58134500	-1.53562000	-2.23496100
H	5.80359200	2.55501900	0.16122800	O	-1.59183600	-2.02031900	-2.70094600
N	2.93980500	0.83594700	-0.24597800	O	0.01308200	-0.45958500	-2.77541800
Pd	0.77956300	0.77928500	-0.11417900	C	-0.60254700	0.06257900	-3.96955200
C	-2.04793400	-0.23286900	0.43041800	H	-1.62110700	0.40559600	-3.76355000
C	-1.17374400	0.72779800	0.08554400	H	0.02817700	0.89157000	-4.28755700
C	-1.13309500	2.17715400	0.07608700	H	-0.63950400	-0.70692100	-4.74837900
C	-1.50330600	2.94304700	1.22012400	N	1.25670400	-1.31617600	-0.45447800
C	-0.40551400	2.83342200	-0.95942500	C	2.33736300	-1.19657600	-1.29251300
C	-1.19407400	4.28861700	1.29991100	O	2.61634700	-1.89885000	-2.27537900
H	-2.03896800	2.44849000	2.02406000	C	3.30814100	-0.09592500	-0.89507600
C	-0.07553500	4.19875900	-0.84636100	C	4.65290400	-0.14447000	-1.26263400
H	-0.22159000	2.31609300	-1.89687800	C	3.59545300	1.95488400	0.14362500
C	-0.46662300	4.92098200	0.27108700	C	5.48718500	0.89948800	-0.88070200
H	-1.50378000	4.86160100	2.16910700	H	5.00569100	-0.99861400	-1.82947100
H	0.46171800	4.68537100	-1.65489500	H	3.12730800	2.77181900	0.69040700
H	-0.22285400	5.97589600	0.35246100	H	6.54101600	0.88095800	-1.14413300
C	-3.51321400	0.03539600	0.44344800	C	4.94978200	1.97214300	-0.16514900
C	-4.10337400	0.82357500	-0.56394600	H	5.56698700	2.80502700	0.14363200
C	-4.35265600	-0.47255300	1.45405700	N	2.78886600	0.94125500	-0.20934900
C	-5.46904700	1.10417200	-0.55406400	Pd	0.66236100	0.65230500	0.19392400
H	-3.48269100	1.19776300	-1.37158200	C	-2.12489700	-0.61626500	0.45930300
C	-5.71908300	-0.19078500	1.46413400	C	-1.27410800	0.40851300	0.28865000
H	-3.93440600	-1.07156400	2.25695400	C	-1.33857500	1.85985800	0.26798500
C	-6.28551400	0.59883300	0.46083900	C	-1.67945600	2.60173700	1.44090700
H	-5.89828700	1.70899100	-1.34817500	C	-0.80594500	2.57317700	-0.84153300
H	-6.34126300	-0.58703700	2.26188900	C	-1.52399700	3.98335500	1.47221500
H	-7.35032200	0.81278600	0.46678300	H	-2.07306400	2.06820500	2.29485200
C	1.84584600	-1.23574900	3.37780300	C	-0.63353100	3.96522600	-0.78320000
O	1.69155600	-0.02948300	3.28810000	H	-0.60647400	2.04065900	-1.76162900
O	1.70900600	-2.08018500	2.34221600	C	-0.99387900	4.66619500	0.36231100

H	-1.80601000	4.53243400	2.36232900	C	3.15465200	2.47509500	-2.59014200
H	-0.23888700	4.49219200	-1.64662200	H	3.11553700	1.64038300	-3.30115400
H	-0.87358800	5.74471000	0.40542800	H	2.65465800	3.33174600	-3.05338400
C	-3.59153700	-0.38789400	0.32887300	H	4.20350300	2.74152300	-2.43526300
C	-4.10587900	0.40206500	-0.72089700	C	4.51593400	1.45592600	0.24753700
C	-4.51218200	-0.94759200	1.23543000	O	5.18078000	0.72184700	0.94931800
C	-5.47567800	0.63617800	-0.84210700	O	4.81183900	2.74827300	0.03744900
H	-3.42315100	0.81900900	-1.44907900	C	5.98111900	3.24055700	0.72189700
C	-5.88198900	-0.71156900	1.11608200	H	6.86643800	2.67785300	0.41801500
H	-4.15248800	-1.55477800	2.06044600	H	6.07231200	4.28590900	0.43031800
C	-6.36915600	0.08164000	0.07706800	H	5.85146500	3.15335400	1.80261100
H	-5.84560900	1.24359800	-1.66356700	N	2.51839500	0.04573800	0.25703100
H	-6.56518600	-1.14687100	1.84009700	C	2.07131000	0.36835900	1.47925600
H	-7.43620700	0.26013400	-0.01832000	O	2.29176500	1.45040400	2.04040400
C	2.34380700	-0.97023600	2.60101300	C	1.25850500	-0.67709400	2.21422800
O	1.76001700	0.10243700	2.57987300	C	1.52819300	-0.83694300	3.57590200
O	2.27471900	-1.87149300	1.62525700	C	-0.43172600	-2.26973300	2.33569100
H	1.87957700	-1.60922700	0.93606000	C	0.80766300	-1.76251700	4.32207400
C	3.21463000	-1.37273300	3.77404000	H	2.30530600	-0.22680100	4.01941500
H	4.23110800	-1.60828500	3.43538400	H	-1.21513200	-2.80396500	1.81306300
H	3.23929800	-0.55876500	4.49279200	H	1.01869400	-1.90599000	5.37658200
H	2.81067700	-2.27743900	4.24736300	C	-0.19280800	-2.49467300	3.68543800
C	-1.06374500	-1.86827600	2.35518300	H	-0.79171900	-3.22524900	4.21695100
H	-0.20122600	-1.20582200	2.37863300	N	0.27833300	-1.38317400	1.60237600
H	-1.82331600	-1.43090200	3.01586800	Pd	-0.23867300	-1.36715000	-0.41356000
H	-0.78730600	-2.83610400	2.77723500	C	-1.31227300	1.51585900	-0.19854700
H	-1.53753000	-3.26906000	-0.77652800	C	-1.52475500	0.17376800	-0.11905600
C	-0.14194600	-4.06938000	0.60073000	C	-2.80343700	-0.42386200	0.36290900
H	-0.86693700	-4.62007600	1.20900700	C	-3.26316100	-0.14292100	1.66571600
H	0.24537700	-4.76303000	-0.15660200	C	-3.54418700	-1.34209200	-0.40849300
H	0.69302000	-3.78695900	1.25354500	C	-4.41962300	-0.73994100	2.16767000
11a				H	-2.70763800	0.55876200	2.28024000
0 1				C	-4.70650100	-1.93143700	0.09038600
C	0.05820800	2.17658300	-0.38770700	H	-3.21016000	-1.59636500	-1.40929300
C	0.99384800	1.67538900	-1.50831300	C	-5.14990300	-1.63522400	1.38191500
H	0.58477100	2.11744500	0.56959600	H	-4.75235400	-0.50191600	3.17433100
H	-0.10248600	3.24599100	-0.55797100	H	-5.26451000	-2.62581600	-0.53167100
C	2.46505000	2.09797200	-1.26863100	H	-6.05205100	-2.09770600	1.77138300
H	0.94016400	0.58648400	-1.60207800	C	-2.43112700	2.49738400	0.02438400
H	0.65281100	2.09098700	-2.46380500	C	-2.28301500	3.53731500	0.96039900
C	3.29165600	0.97612200	-0.55742800	C	-3.62694800	2.43818300	-0.71070200
H	2.46614600	2.98035500	-0.62104100	C	-3.30135500	4.46837100	1.16825900
H	3.71734400	0.34450700	-1.34750900	H	-1.36832800	3.61062300	1.54171800
				C	-4.64205800	3.37492200	-0.51126400

H	-3.76351100	1.65541800	-1.45031500	H	5.03031900	4.49330300	0.02693700
C	-4.48612100	4.39254600	0.43218400	N	1.84684700	1.10675800	0.12775400
H	-3.16696000	5.25487300	1.90572700	C	1.42147400	1.02413200	1.40045800
H	-5.55406600	3.31033900	-1.09821900	O	0.95382800	1.94659400	2.07333000
H	-5.27634600	5.12102500	0.58876600	C	1.56230900	-0.34709200	2.02515800
C	2.00851600	-3.35641400	-0.88770500	C	1.98918700	-0.42493400	3.35178200
O	2.83931100	-2.42096000	-0.88553100	C	1.35461100	-2.66058200	1.91690500
O	0.75037300	-3.23450300	-0.65621100	C	2.11770000	-1.66838200	3.96158600
H	2.46960500	-0.92688900	-0.10114200	H	2.21489100	0.49598500	3.87564700
C	2.47593800	-4.77751800	-1.17867900	H	1.08022400	-3.51850300	1.31611800
H	2.24070000	-5.42442100	-0.32766400	H	2.45937500	-1.74697000	4.98838900
H	1.93937300	-5.17491200	-2.04566400	C	1.79684800	-2.80873800	3.22601100
H	3.54958600	-4.80278700	-1.36909100	H	1.87544000	-3.80217300	3.65252400
C	-1.15361400	-0.85042400	-3.35298100	N	1.23566700	-1.45451400	1.32164200
O	-0.65863700	-1.58178400	-2.48150300	Pd	0.54183500	-1.52128700	-0.64066400
O	-1.67308700	0.33297600	-3.10002600	C	-1.46302600	0.73671000	-0.51616000
H	-1.59783500	0.52864100	-2.12558200	C	-1.13792300	-0.52101600	-0.10912800
C	-1.19618400	-1.25516300	-4.79485900	C	-1.97736200	-1.35444200	0.80122300
H	-2.20636200	-1.11937600	-5.18899800	C	-1.94811100	-1.17835900	2.19814800
H	-0.52802500	-0.60270300	-5.36605000	C	-2.77217800	-2.39980900	0.29021000
H	-0.87862300	-2.29075100	-4.90415800	C	-2.69301900	-2.00061300	3.04461500
11b				H	-1.33213300	-0.39190500	2.62210800
0 1				C	-3.52224500	-3.21770400	1.13637000
C	-1.49083000	4.57815000	-0.68553300	H	-2.81013900	-2.57217300	-0.78140300
C	-0.40256400	3.70156200	-0.05193100	C	-3.48583700	-3.02362100	2.51917500
H	-1.92355700	5.25550300	0.05833200	H	-2.65623500	-1.83685300	4.11818600
H	-1.07601400	5.19309100	-1.49311500	H	-4.13495700	-4.00840900	0.71219900
H	-2.30915700	3.98365100	-1.10180200	H	-4.06752700	-3.66111500	3.17848800
C	0.25385000	2.74243300	-1.06742700	C	-2.78647900	1.35013800	-0.12556800
H	0.36793700	4.36049100	0.35778600	C	-3.06817700	1.76291200	1.18597300
H	-0.80232500	3.14505300	0.79531100	C	-3.78971100	1.51005300	-1.09825200
C	1.70726200	2.26785900	-0.73294800	C	-4.30823900	2.31416300	1.51502200
H	0.41055400	3.33863700	-1.97509700	H	-2.30484300	1.66673000	1.94992300
H	2.11770500	1.92639300	-1.69204100	C	-5.03334900	2.05255300	-0.76964100
C	-0.63721600	1.54118800	-1.53129500	H	-3.60278200	1.19751300	-2.12261700
H	-1.34744700	1.94862400	-2.26049900	C	-5.29728400	2.45858300	0.54026100
H	0.01014500	0.85319100	-2.08520900	H	-4.49920800	2.63184700	2.53626200
C	2.62044600	3.44631100	-0.36613400	H	-5.79445800	2.15628200	-1.53791900
O	2.56047500	4.52572200	-0.92413000	H	-6.26261100	2.88469400	0.79762800
O	3.52993500	3.14168000	0.56881300	H	2.38322300	0.31872300	-0.26968800
C	4.45504400	4.19498900	0.90608700	C	3.37880400	-2.04542900	-1.24732200
H	3.91793000	5.06180200	1.29704200	O	3.54759700	-0.82322900	-1.03928400
H	5.11017700	3.77538700	1.66802500	O	2.25834100	-2.67107600	-1.13894600
				C	4.56028300	-2.90820500	-1.67355500

H	5.48555800	-2.33074900	-1.66867800	H	-1.01359100	-2.55466700	5.10994600
H	4.65787000	-3.76767300	-1.00358800	C	-2.33243400	-1.76088500	3.59185600
H	4.38331600	-3.30063700	-2.68015400	H	-3.23735000	-1.80844600	4.18671500
C	-0.99790400	-1.71012500	-3.34958100	N	-1.30935800	-1.18275500	1.49309100
O	0.02198300	-1.85534100	-2.66064000	Pd	-1.76085200	-0.33504800	-0.35965700
O	-2.08674400	-1.10671000	-2.91459800	C	0.78612200	1.27320000	-0.73260300
H	-1.92107400	-0.76393600	-1.99488200	C	-0.39790700	1.13770900	-0.07457600
C	-1.08561500	-2.21641400	-4.75640800	C	-0.79573000	2.01074900	1.07366800
H	-1.31987600	-1.38699100	-5.42955500	C	-0.15823700	1.90097800	2.32530500
H	-0.14667300	-2.68451900	-5.04648300	C	-1.86964300	2.91668900	0.96643200
H	-1.90348100	-2.93952600	-4.82837200	C	-0.57039400	2.66889600	3.41523100
11c				H	0.66614600	1.20604300	2.44157800
0 1				C	-2.27499500	3.69190900	2.05394600
C	0.35387800	-0.27973200	-2.83426100	H	-2.39064300	3.02701100	0.02048700
C	1.35055300	0.44845400	-1.91631000	C	-1.62949100	3.57041000	3.28658900
H	-0.30664400	0.43273300	-3.33156300	H	-0.05666800	2.56462500	4.36716200
H	0.89618100	-0.80218600	-3.62858900	H	-3.09896900	4.39036300	1.93574500
H	-0.26593400	-1.01783100	-2.31956700	H	-1.94689000	4.17031200	4.13449900
C	2.57303300	-0.46108700	-1.52274600	C	1.72621300	2.40046700	-0.36035700
H	1.81054400	1.21851200	-2.54973800	C	2.69509400	2.25280700	0.64512700
C	2.17235900	-1.88087800	-1.03583800	C	1.67315100	3.61618500	-1.06184400
H	3.11031200	0.02824500	-0.70850900	C	3.57538700	3.29562300	0.94561200
H	1.88260800	-2.47709800	-1.90819000	H	2.75795700	1.31668300	1.19165500
C	3.53598000	-0.56398900	-2.72283900	C	2.54750200	4.66090100	-0.75692100
H	3.04370100	-0.99688300	-3.60062400	H	0.93956100	3.74827500	-1.85347300
H	3.89604500	0.43151600	-3.00086200	C	3.50327700	4.50365600	0.24953500
H	4.40541100	-1.17946200	-2.48894700	H	4.31731000	3.16167200	1.72813600
C	3.29356700	-2.70673900	-0.35949500	H	2.48202400	5.59561100	-1.30693100
O	3.09942000	-3.82402900	0.07530900	H	4.18606600	5.31436000	0.48712900
O	4.48744500	-2.09938500	-0.32992600	C	-2.57402300	-3.05781100	-0.98138000
C	5.54986200	-2.84284400	0.29964500	O	-3.12321100	-1.94199800	-0.64078000
H	5.70963800	-3.79292100	-0.21456700	O	-1.34303300	-3.25176000	-1.09657600
H	6.43360600	-2.21117700	0.22244800	H	0.13385900	-2.32985500	-0.48057000
H	5.30543300	-3.03492300	1.34651700	C	-3.54770400	-4.19601600	-1.25980900
N	1.01454400	-1.91355800	-0.14484100	H	-3.01217300	-5.11588200	-1.49763100
C	1.12686000	-1.51204900	1.13145600	H	-4.18981500	-4.35898700	-0.38885400
O	2.18431000	-1.13059700	1.65115800	H	-4.19977700	-3.92711700	-2.09700300
C	-0.11853500	-1.59334200	1.97634900	C	-2.64478000	1.58178300	-2.64926200
C	0.01899900	-2.07734200	3.27906500	O	-2.74349000	0.50948700	-2.03634600
C	-2.39484100	-1.27022800	2.29362800	O	-1.67555600	2.45133900	-2.43528900
C	-1.09999800	-2.17145700	4.09860000	H	-1.06057200	2.09132400	-1.73892500
H	1.00447100	-2.37245900	3.61784100	C	-3.62616700	1.99068800	-3.70429200
H	-3.32987000	-0.93236300	1.86618900	H	-4.38422500	1.21981900	-3.83107600
				H	-4.09526900	2.93555200	-3.41448100

H	-3.09840700	2.16129000	-4.64693900	C	-6.23823900	-2.51966900	-0.49556600
12a				H	-5.35941400	-1.04779800	0.79332000
0 1				C	-5.25460800	-2.75261500	-2.68488100
C	-2.18421800	1.96032500	0.10027000	H	-3.59809300	-1.44957000	-3.11032800
C	-0.91046200	1.64273400	-0.69211200	C	-6.21124000	-3.14441900	-1.74572900
H	-1.92311900	2.03643600	1.16544800	H	-6.96642500	-2.82814400	0.24961400
H	-2.55479600	2.96057300	-0.16455500	H	-5.21395900	-3.23504200	-3.65751200
C	0.13665700	2.77588100	-0.61178100	H	-6.92020400	-3.93309600	-1.98029000
H	-0.47899200	0.70972600	-0.31252600	C	-4.53769200	1.39941600	0.80363300
H	-1.15013500	1.47342900	-1.75057900	C	-4.45579100	1.42633900	2.20578400
C	1.53679700	2.23700000	-1.02490400	C	-5.73217400	1.81994500	0.19520500
H	0.21797300	3.11131300	0.42466400	C	-5.54399100	1.83938700	2.97723400
H	1.44100100	1.77751800	-2.01366100	H	-3.53962300	1.10848400	2.69631000
C	-0.26708200	3.96952000	-1.49419100	C	-6.81682700	2.24103700	0.96525900
H	-0.24322900	3.70633400	-2.55766800	H	-5.80436200	1.81512400	-0.88839900
H	-1.28205600	4.29683500	-1.25404000	C	-6.72778500	2.24951600	2.35968500
H	0.38967300	4.83166400	-1.34555300	H	-5.46509400	1.84253000	4.06074800
C	2.56812200	3.36888600	-1.15950600	H	-7.73104600	2.56501200	0.47575900
O	3.20318400	3.84981100	-0.24385100	H	-7.57240900	2.57594800	2.95953500
O	2.68416700	3.76206600	-2.44008300	C	4.00518300	-1.59060400	-1.81901300
C	3.60015800	4.84963200	-2.68381000	O	3.79124600	-0.37024600	-1.77632600
H	4.60930200	4.57244200	-2.37190000	O	3.40656900	-2.48904800	-1.08959600
H	3.56637400	5.02590600	-3.75787400	H	2.71618400	0.53932800	-0.65125000
H	3.28598500	5.74245500	-2.13863500	C	5.02861900	-2.17625000	-2.77738800
N	2.09827000	1.19903000	-0.15682600	H	5.74943700	-2.78916800	-2.22906500
C	2.17186700	1.24153700	1.19346100	H	4.52564100	-2.82873400	-3.49760900
O	1.58061600	2.02140800	1.94104200	H	5.54787300	-1.37855000	-3.30892600
C	3.15342700	0.25822800	1.81725000	C	-0.39423900	-2.65058100	0.39417100
C	3.95444300	0.75143200	2.84956800	O	0.30883400	-2.98193200	-0.62533200
C	4.21320200	-1.81654900	1.95626200	O	0.17516500	-1.90501700	1.26893800
C	4.91933500	-0.06579300	3.42905000	H	-2.46519700	-0.16673900	-1.49684600
H	3.80518000	1.77531900	3.16847300	C	-1.79119400	-3.14604000	0.57903900
H	4.26731000	-2.82972800	1.57727700	H	-2.37170100	-2.43173200	1.16405800
H	5.55357400	0.31132000	4.22435600	H	-2.26628300	-3.31803300	-0.38770700
C	5.05798500	-1.37323200	2.96501400	H	-1.75566300	-4.09627300	1.12372800
H	5.79685800	-2.05028100	3.37763200	12b			
N	3.27324300	-1.02188800	1.39804200	0 1			
Pd	1.94020600	-1.98319900	0.18330600	C	-3.42913000	4.20042200	0.16274100
C	-3.36103200	1.00391600	-0.03047100	C	-2.20283200	3.28459000	0.25539900
C	-3.35102700	-0.04726900	-0.87724500	H	-3.66373200	4.62657300	1.14373800
C	-4.36985200	-1.08621100	-1.12861200	H	-3.24704100	5.03421500	-0.52535400
C	-5.33145400	-1.50604200	-0.18812300	H	-4.32130500	3.66885300	-0.18126000
C	-4.34336900	-1.74345500	-2.37504200	C	-1.74187000	2.72583100	-1.10598300

H	-1.37257500	3.85127500	0.68437100	C	-5.27920300	0.93759700	-0.11361600
H	-2.40771400	2.46403900	0.95037000	C	-4.46739100	-0.14222200	2.32419000
C	-0.30493700	2.14633800	-1.08083600	H	-2.59959100	-0.55916400	1.34077900
H	-1.66435000	3.58443000	-1.78483300	C	-6.15654500	0.92729500	0.97284000
H	-0.12699400	1.66568700	-2.05124200	H	-5.61010100	1.35001100	-1.06274100
C	-2.74043900	1.75663900	-1.80892000	C	-5.75292700	0.39063300	2.19710900
H	-3.68168500	2.30362100	-1.93806400	H	-4.14228800	-0.55930900	3.27321500
H	-2.36051700	1.57533700	-2.82111400	H	-7.15537700	1.33940400	0.86090300
C	0.76823100	3.24939400	-1.00877900	H	-6.43264900	0.38829600	3.04414500
O	0.54510400	4.43774200	-1.11737400	H	-0.11603000	0.14253600	-0.44529900
O	1.99503200	2.72029400	-0.91816200	C	5.05711000	-0.07961700	0.92088700
C	3.09534600	3.65132400	-0.83717900	O	4.97053000	0.89836900	0.17861000
H	2.92356100	4.36289600	-0.02693000	O	4.15702400	-1.03138400	1.02658800
H	3.97000500	3.03587700	-0.63586700	C	6.25819300	-0.30591100	1.82854400
H	3.20024800	4.19350800	-1.78013200	H	6.96623700	0.51673600	1.72284200
N	-0.06300000	1.08959600	-0.09579300	H	5.93332500	-0.38035000	2.87064200
C	0.39574800	1.29565100	1.15729400	H	6.75005000	-1.24869700	1.57050700
O	0.55525900	2.40137300	1.67391900	C	2.18998900	-1.06387500	-2.60358400
C	0.64726600	0.04997500	1.98542800	O	3.36438200	-1.05078000	-2.10289300
C	0.05178500	-0.00645500	3.24729000	O	1.20614700	-1.01380100	-1.77855100
C	1.64984400	-2.02373300	2.33262700	H	-1.80180700	-0.56968200	-2.51191600
C	0.24419700	-1.12515700	4.05153900	C	1.96478900	-1.16569900	-4.07868000
H	-0.55427000	0.83050200	3.57230300	H	1.08466500	-0.58760800	-4.36726900
H	2.31904900	-2.78012000	1.94275900	H	2.84525500	-0.81894800	-4.62130800
H	-0.22483200	-1.18827200	5.02771800	H	1.78313700	-2.21439700	-4.33823800
C	1.05496600	-2.15663500	3.58011900				
H	1.24153500	-3.04855300	4.16684400	12c			
N	1.44719600	-0.94646600	1.54209000	0 1			
Pd	2.56571500	-0.93190300	-0.18517600	C	0.38498400	-0.52505800	-2.92051700
C	-3.05189400	0.40795000	-1.16909900	C	1.53068900	0.03337900	-2.06825800
C	-2.51258900	-0.71462000	-1.69789600	H	-0.18999000	0.28554200	-3.37465100
C	-2.72860900	-2.13704800	-1.36026200	H	0.79036100	-1.13198100	-3.73426000
C	-3.95654400	-2.65640000	-0.90735800	H	-0.31009400	-1.15047000	-2.35755000
C	-1.66706000	-3.03996500	-1.57003200	C	2.49627100	-1.08270500	-1.52107900
C	-4.10385500	-4.01855600	-0.64788800	H	2.17558000	0.59223800	-2.76224500
H	-4.80353000	-1.99342400	-0.77331900	C	1.79205300	-2.24179700	-0.75542000
C	-1.81345700	-4.40129300	-1.30173000	H	3.19795500	-0.60835100	-0.83290500
H	-0.71772500	-2.65901200	-1.93694600	H	1.29350000	-2.88425200	-1.48903000
C	-3.03306600	-4.89742500	-0.83525700	C	3.31650000	-1.65603100	-2.69579800
H	-5.06325400	-4.39686800	-0.30581600	H	2.68164900	-2.17425400	-3.42217000
H	-0.97692400	-5.07539200	-1.46542900	H	3.83445700	-0.84823300	-3.22198900
H	-3.15258900	-5.95769100	-0.63201600	H	4.06919100	-2.36246500	-2.34588000
C	-3.98607500	0.39830900	-0.00245800	C	2.72569400	-3.19781400	0.02957100
C	-3.59575500	-0.14154000	1.23536200	O	2.29051900	-4.12959900	0.67558000

O	4.03079300	-2.92417900	-0.08859000	O	-3.26975100	-1.59834800	0.41693800
C	4.92039100	-3.79580200	0.63870400	O	-1.75872800	-3.24764500	0.11789700
H	4.78835000	-4.83093900	0.31745600	H	-0.19921400	-2.23948800	0.05998300
H	5.92525400	-3.44619600	0.40670400	C	-4.01399300	-3.82140000	0.73611900
H	4.72569700	-3.72128200	1.71065200	H	-3.59320900	-4.77033000	1.07095900
N	0.73305900	-1.81714900	0.16318100	H	-4.67953700	-3.41006800	1.49759100
C	1.05533500	-1.22138700	1.32730100	H	-4.60677800	-3.99933000	-0.16755600
O	2.22164900	-1.03383100	1.69469500	C	-2.11660330	-0.01386849	-2.26904440
C	-0.06028900	-0.73864000	2.22536400	O	-1.08987428	0.46507016	-1.62017155
C	0.19673200	-0.73099900	3.59827800	O	-3.09310184	-0.56877603	-1.75468232
C	-2.14321500	0.23540800	2.58373700	H	-0.58988605	1.80451672	-2.03148458
C	-0.75883800	-0.23737900	4.47959500	C	-2.00946601	0.18452543	-3.77447965
H	1.15031900	-1.11131300	3.94161800	H	-1.13554534	-0.35193637	-4.15624955
H	-3.05448500	0.61497700	2.13866700	H	-2.90958885	-0.18499908	-4.26665396
H	-0.57460700	-0.23726700	5.54866200	H	-1.86919411	1.24441004	-4.00562240
C	-1.95095100	0.26245400	3.95923200				
H	-2.72670400	0.66958200	4.59719700	9a-s			
N	-1.22253300	-0.25782500	1.72871300	0 1			
Pd	-1.87905100	-0.28592200	-0.23334900	C	-0.09001500	-1.13772200	-1.48171700
C	1.14551300	1.12025300	-1.05348900	C	0.81148300	-2.12872400	-0.67460100
C	-0.00350920	1.85336374	-1.08513309	H	0.46548100	-0.21428300	-1.66358600
C	-0.36227440	3.00812265	-0.21952578	H	-0.26023700	-1.58538600	-2.46569200
C	-0.09561785	3.04435454	1.16150432	C	2.36498500	-1.95848000	-0.75778300
C	-1.03336898	4.10457106	-0.79721662	H	0.53215800	-2.13262500	0.38094900
C	-0.46625224	4.14677516	1.93152967	H	0.57654300	-3.13873200	-1.03054800
H	0.39748384	2.20551300	1.63806312	C	2.97369700	-0.97878400	0.31237900
C	-1.39838198	5.20747396	-0.02416194	H	2.63678600	-1.57774200	-1.74975700
H	-1.26007608	4.07793366	-1.85823829	H	2.76491400	-1.41076300	1.29939200
C	-1.11504076	5.23563012	1.34357851	C	2.98089400	-3.36205600	-0.58046700
H	-0.24968206	4.15195978	2.99617296	H	2.68163300	-3.79407900	0.38382700
H	-1.90599364	6.04592630	-0.49308240	H	2.62469400	-4.03768000	-1.36525000
H	-1.40080423	6.09319426	1.94582176	H	4.06962200	-3.34325600	-0.62360900
C	2.29377619	1.54839618	-0.17604575	C	4.51106100	-0.83385100	0.28505500
C	2.67458748	0.89160674	1.00427128	O	5.13127000	-0.36546000	1.21511800
C	3.05943261	2.64347263	-0.61404198	O	5.09559200	-1.28613900	-0.84388100
C	3.78735965	1.32907871	1.72853183	C	6.48204600	-0.94759500	-0.97992800
H	2.09002706	0.05395946	1.36898854	H	7.06340200	-1.32536500	-0.13516400
C	4.17077484	3.07516979	0.11023525	H	6.81005900	-1.41079200	-1.91117800
H	2.77647911	3.15982422	-1.52715867	H	6.58601800	0.13883100	-1.03476900
C	4.53948791	2.41818016	1.28644812	N	2.36880000	0.35778600	0.32211000
H	4.06297390	0.81314095	2.64409145	C	2.81202700	1.27954200	-0.54587800
H	4.74589247	3.92551196	-0.24493363	O	3.85323400	1.28801100	-1.22352900
H	5.40372126	2.75325124	1.85254696	C	1.82935400	2.41862300	-0.73282500
C	-2.89790300	-2.84813200	0.40008600	C	2.20571100	3.59518200	-1.37587800

C	-0.37835900	3.16627100	-0.55162500	C	-1.00447000	1.62385100	-1.60939100
C	1.25538800	4.58828100	-1.59139200	C	-0.16996900	2.68190500	-0.81691800
H	3.23894800	3.67899700	-1.69298200	H	-1.71228000	2.15770300	-2.24841900
H	-1.38498000	2.94078900	-0.21948300	C	1.34302900	2.31151000	-0.74832500
H	1.52917500	5.51773600	-2.08169800	H	1.70856400	2.43753100	-1.77665500
C	-0.05902200	4.36883700	-1.17321200	C	2.06594300	3.44118200	0.00078800
H	-0.83502500	5.11074000	-1.32736900	O	2.28255900	4.52875200	-0.49920600
N	0.54992600	2.21457900	-0.33725600	O	2.32961500	3.15712300	1.29163000
Pd	0.31834800	0.54358600	0.80051700	C	3.01081500	4.18955400	2.02558600
C	-1.47190000	-0.76949700	-0.88090000	H	2.42499900	5.11170200	2.03324000
C	-1.57481500	0.12940800	0.15166200	H	3.12766700	3.80392800	3.03788800
C	-2.80127500	0.80838100	0.62789100	H	3.98838600	4.38849800	1.57953900
C	-3.82333700	1.22791100	-0.25173700	N	1.76526900	0.97278600	-0.30792400
C	-2.93210500	1.16054300	1.98788100	C	3.11295500	0.85652600	-0.41741100
C	-4.93139800	1.93326300	0.21501100	O	3.88771100	1.78351600	-0.72852300
H	-3.74310100	0.99555800	-1.30797500	C	3.69923400	-0.50059400	-0.15649900
C	-4.04904200	1.84938400	2.45662200	C	5.07389800	-0.68981100	-0.03271400
H	-2.12974900	0.90556400	2.67432600	C	3.28911100	-2.76983300	0.13081100
C	-5.05737300	2.23921700	1.57210600	C	5.55541600	-1.97842200	0.18997500
H	-5.70019200	2.24579600	-0.48660600	H	5.72551100	0.17128500	-0.11685200
H	-4.12407200	2.09713500	3.51196600	H	2.53996200	-3.55220200	0.18000200
H	-5.92299600	2.78685900	1.93334700	H	6.62078100	-2.15687600	0.29549000
C	-2.65482000	-1.42005400	-1.53563900	C	4.64872400	-3.03682200	0.27350600
C	-2.79838900	-1.40956600	-2.93573500	H	4.98202300	-4.05440300	0.44414000
C	-3.64422700	-2.07557800	-0.78151800	N	2.83287700	-1.52496200	-0.07990600
C	-3.89175700	-2.01632000	-3.55369700	Pd	0.81387700	-0.85652500	-0.18068100
H	-2.05675000	-0.90338200	-3.54708600	C	-1.77313300	0.65492500	-0.71838100
C	-4.73243700	-2.69092100	-1.39871000	C	-1.13065300	-0.31326600	-0.02441400
H	-3.56114700	-2.10876300	0.30027100	C	-1.78610200	-1.20380900	0.97711100
C	-4.86358600	-2.66292700	-2.78817100	C	-1.30613700	-1.23118200	2.30172100
H	-3.98272400	-1.98350100	-4.63593800	C	-2.85077300	-2.06514600	0.64673600
H	-5.47731200	-3.19701300	-0.79089800	C	-1.87496800	-2.07314800	3.25899200
H	-5.71110100	-3.14258300	-3.26907900	H	-0.48314000	-0.57739300	2.57754600
C	-0.43354400	-1.69964700	2.82169900	C	-3.41400700	-2.91198000	1.60183400
O	0.33429900	-0.80432100	2.44711400	H	-3.24466700	-2.06268800	-0.36486500
O	-1.49524100	-2.07669400	2.13702800	C	-2.93023700	-2.92082700	2.91301900
H	-1.55608300	-1.52108600	1.31306900	H	-1.49148300	-2.06669400	4.27568100
C	-0.21406900	-2.45521600	4.09899700	H	-4.23680800	-3.56422600	1.32147200
H	-1.10823100	-2.38596200	4.72507900	H	-3.37104600	-3.57960700	3.65555900
H	-0.05549600	-3.51387900	3.87140400	C	-3.24772800	0.91163100	-0.59247800
H	0.65040700	-2.05325000	4.62511900	C	-3.88307500	1.08023700	0.65027100
				C	-4.03882400	1.00386400	-1.75255300
9b-s				C	-5.25400300	1.32608900	0.73023400
0 1				H	-3.29508300	1.02866600	1.56024800

C	-5.41244600	1.23951500	-1.67423100	H	-1.25103900	1.43168700	3.73717500
H	-3.57619400	0.87642000	-2.72781200	H	0.38861000	1.54669900	4.44862500
C	-6.02697900	1.40327100	-0.43092200	H	-0.50884100	3.03081900	3.99454800
H	-5.71813500	1.46213200	1.70323600	N	1.48221600	1.44684700	0.04697200
H	-6.00088700	1.29598000	-2.58585700	C	2.78046800	1.81507300	0.13198600
H	-7.09450100	1.59344100	-0.36760900	O	3.21886500	2.97393600	0.25474700
C	-0.46965000	-3.30752000	-1.37113400	C	3.75724100	0.66632500	0.07203200
O	0.23792000	-2.91845100	-0.42983600	C	5.13107800	0.88401800	0.13368300
O	-1.12470000	-2.47981100	-2.16571300	C	4.06271000	-1.63488000	-0.07353400
H	-1.02570700	-1.55959700	-1.81329700	C	5.99010300	-0.21295100	0.08850400
C	-0.66718800	-4.75710100	-1.68682600	H	5.48769900	1.90345600	0.21700200
H	-1.68597300	-5.04140000	-1.40354200	H	3.58586000	-2.60597600	-0.15331600
H	-0.56220600	-4.92448200	-2.76128100	H	7.06528300	-0.07210400	0.13497600
H	0.04642300	-5.36392300	-1.13187300	C	5.44786400	-1.49480000	-0.01507800
H	-0.32690100	1.08178200	-2.27814400	H	6.07979400	-2.37522300	-0.04986600
H	-0.13787400	3.57633700	-1.45261800	N	3.24104600	-0.57496300	-0.03264300
C	-0.81852800	3.14661800	0.50664700	Pd	1.11091300	-0.53118700	-0.11625600
C	-2.00637400	4.09328100	0.28219500	C	-1.61104800	0.52746600	-0.89389800
H	-0.07784200	3.67548500	1.11273400	C	-0.91351800	-0.33658100	-0.11055300
H	-1.12861300	2.28318700	1.10288700	C	-1.54698500	-1.28499200	0.85373500
H	-2.45812800	4.38554500	1.23607800	C	-1.09046100	-1.34291000	2.18612700
H	-1.67936100	5.00830500	-0.22543300	C	-2.55756700	-2.18996000	0.47165700
H	-2.79101100	3.63491400	-0.32552100	C	-1.63671600	-2.24315100	3.10181400
9c-s				H	-0.29983800	-0.66665000	2.49478400
0 1				C	-3.09554300	-3.09886100	1.38400600
C	0.00415900	0.86266600	-2.90252900	H	-2.92987400	-2.17620800	-0.54757200
C	-0.94382900	1.51038300	-1.87126500	C	-2.64195000	-3.12886900	2.70507400
H	-0.51443800	0.05344000	-3.43013600	H	-1.27189700	-2.25579600	4.12546200
H	0.30729900	1.59265900	-3.65853200	H	-3.87437000	-3.78439400	1.06057900
H	0.90944100	0.45111300	-2.45043800	H	-3.06344400	-3.83535600	3.41433400
C	-0.36927300	2.76279200	-1.12409100	C	-3.10770700	0.65555400	-0.82472400
H	-1.76022700	1.92988100	-2.47050100	C	-3.77249900	0.97524600	0.37054200
C	0.49978000	2.51406100	0.14194600	C	-3.88237700	0.48135700	-1.98651200
H	-1.24282700	3.30518500	-0.74751900	C	-5.16209800	1.10446600	0.40475400
H	1.07935700	3.43823200	0.28936200	H	-3.19157300	1.14507600	1.26945800
C	0.36808300	3.70540900	-2.09076700	C	-5.27235700	0.59926500	-1.95111200
H	1.33928000	3.30161100	-2.39387900	H	-3.39230600	0.23747300	-2.92591100
H	-0.22200300	3.88223400	-2.99654600	C	-5.91932400	0.91204900	-0.75293800
H	0.54704200	4.67572700	-1.61572700	H	-5.65347700	1.36106700	1.33947200
C	-0.33206800	2.46210700	1.42740400	H	-5.84898700	0.44760600	-2.85955500
O	-1.42288700	2.98568200	1.56461100	H	-7.00079500	1.01014800	-0.72378200
O	0.33422700	1.89659000	2.45378400	C	0.38257000	-3.22160200	-1.30977100
C	-0.31091200	1.98751600	3.73929000	O	1.03010700	-2.64357000	-0.42376800
				O	-0.49845700	-2.60532400	-2.07570300

H	-0.60777600	-1.67429900	-1.75684100	C	-1.50375400	0.16112200	-0.72893700
C	0.53099400	-4.68469800	-1.58936700	C	-2.85857000	-0.09193100	-0.14040400
H	-0.39334600	-5.19578700	-1.30208600	C	-3.25690100	0.45685100	1.09415100
H	0.67802700	-4.84545800	-2.66033000	C	-3.76675700	-0.94471800	-0.79908200
H	1.36677000	-5.09297200	-1.02362500	C	-4.50955800	0.17522100	1.63950500
TS4a-s				H	-2.58024200	1.11809200	1.62521400
O 1				C	-5.02160100	-1.22348700	-0.25567300
C	0.33247200	1.81532300	-1.48771600	H	-3.49096300	-1.38085200	-1.75392400
C	1.29999500	0.77321400	-2.08426000	C	-5.40031500	-0.66620100	0.96794800
H	0.84269800	2.36751700	-0.68853400	H	-4.79027000	0.61638800	2.59208900
H	0.13543200	2.58304400	-2.24832500	H	-5.70456000	-1.87669100	-0.79194900
C	2.78210800	1.14519100	-1.83198800	H	-6.37617100	-0.88362500	1.39225900
H	1.10387700	-0.22675700	-1.68794800	C	-1.83741000	2.65601700	-0.61884400
H	1.12836000	0.71198100	-3.16359900	C	-1.37245100	3.62044100	0.29217800
C	3.35667800	0.47101700	-0.53666200	C	-3.04980000	2.88603600	-1.28876300
H	2.84518700	2.23002600	-1.70325400	C	-2.11793100	4.77387400	0.54232900
H	3.86502700	-0.44680800	-0.85878900	H	-0.43799300	3.45519300	0.82116700
C	3.66515700	0.76176400	-3.03047100	C	-3.78199600	4.04900800	-1.05001000
H	3.58334800	-0.31061700	-3.24721400	H	-3.41589700	2.15255900	-2.00035400
H	3.35737200	1.30944800	-3.92682800	C	-3.32181900	4.99455200	-0.13014100
H	4.71732100	0.99139900	-2.84028800	H	-1.75322300	5.50229500	1.26099400
C	4.45249300	1.26916500	0.19655200	H	-4.71377300	4.21528500	-1.58298800
O	4.85309700	0.99556000	1.30872700	H	-3.89605400	5.89676000	0.05908100
O	4.96971200	2.25123900	-0.55826600	C	1.61396600	-3.57889200	0.81947800
C	6.05181800	2.99504300	0.03788100	O	2.52578500	-2.74210500	0.67209200
H	6.88346100	2.32990800	0.28003700	O	0.35608400	-3.36319700	0.61894300
H	6.35108900	3.72665400	-0.71120900	H	2.28446600	-1.02171900	0.53609300
H	5.71189000	3.49416000	0.94763400	C	1.94261400	-4.99829900	1.26032900
N	2.37112400	0.00400100	0.42947100	H	1.31669900	-5.28448900	2.11012700
C	1.71169000	0.82834000	1.25666200	H	1.72189300	-5.69300400	0.44355900
O	1.87817500	2.05481200	1.31058300	H	2.99595800	-5.08107800	1.53002100
C	0.72808200	0.17333400	2.20214500	C	-0.89256200	-2.10312900	-3.00496100
C	0.73701600	0.61330200	3.52731800	O	-0.46595600	-2.59432400	-1.91326900
C	-0.97316800	-1.33634300	2.68266800	O	-1.36120500	-0.92641200	-3.11272000
C	-0.12153300	0.03259000	4.45477700	H	-1.34198400	-0.39553200	-1.91836800
H	1.42968400	1.39897900	3.80306600	C	-0.81731300	-2.96132500	-4.24452800
H	-1.64824500	-2.09252400	2.30319600	H	-1.73109500	-2.84761200	-4.83121400
H	-0.11305900	0.35369800	5.49109000	H	0.02010000	-2.61447600	-4.85907400
C	-0.98815100	-0.96941500	4.02274200	H	-0.65734500	-4.00715000	-3.98338900
H	-1.67824500	-1.45843100	4.70054300	TS4b-s			
N	-0.13599900	-0.77979900	1.78019900	O 1			
Pd	-0.34899200	-1.56700400	-0.13715500	C	-0.76204900	4.73808500	-1.39338600
C	-1.01625000	1.43502500	-0.90859200	C	0.16217700	3.86264800	-0.53678400

H	-1.06366100	5.63205500	-0.83769100	H	-4.67009500	-3.65820400	-0.18232200
H	-0.25619500	5.07136200	-2.30745600	H	-5.08655400	-3.18585200	2.22875700
H	-1.67633200	4.21396900	-1.68666900	C	-2.43392100	1.76669800	-0.23306100
C	0.70743900	2.63760800	-1.30154900	C	-2.50312900	2.29537300	1.06475600
H	1.01558400	4.47477800	-0.22997200	C	-3.48625600	2.03031800	-1.12684800
H	-0.33985300	3.55921000	0.37966800	C	-3.59832500	3.06882600	1.45507700
C	2.00452400	1.96809900	-0.73093100	H	-1.68435700	2.12596100	1.75574100
H	1.05908000	3.03676300	-2.26118800	C	-4.58566400	2.79278400	-0.72868500
H	2.45199800	1.45260100	-1.58978500	H	-3.45116700	1.62296900	-2.13365000
C	-0.34636700	1.55833300	-1.71772100	C	-4.64432100	3.31684400	0.56422300
H	-0.99448400	2.04323900	-2.45994600	H	-3.63174600	3.47699100	2.46125700
H	0.19533100	0.76736200	-2.24457900	H	-5.39403000	2.97613400	-1.43062200
C	3.06939100	3.01117700	-0.36308300	H	-5.49668700	3.91444300	0.87376200
O	3.33434500	3.95727000	-1.08030200	H	2.34525800	0.03358000	0.04328600
O	3.70953200	2.73752000	0.77989900	C	3.25816500	-2.49370200	-0.34700100
C	4.76235200	3.65513100	1.14172300	O	3.52460100	-1.27709700	-0.30426800
H	4.35833400	4.66019100	1.28057200	O	2.06646200	-2.99481000	-0.39897200
H	5.17259800	3.27476900	2.07586600	C	4.37463800	-3.52711000	-0.35760500
H	5.53012000	3.67794200	0.36549200	H	5.33636600	-3.05447300	-0.15533700
N	1.83343000	0.90682100	0.24643400	H	4.17786100	-4.30679600	0.38320100
C	1.18104900	1.01024700	1.41555800	H	4.41044200	-4.01056800	-1.33933100
O	0.72968100	2.05045500	1.90543400	C	-0.41462200	-1.91597100	-3.35477600
C	0.99082800	-0.28938700	2.16700600	O	0.52227100	-2.18563500	-2.53448700
C	1.10407100	-0.25854300	3.55809300	O	-1.44153800	-1.24209700	-3.04648400
C	0.45672900	-2.55170400	2.22574700	H	-1.27144300	-0.86736500	-1.74605100
C	0.90771800	-1.42367500	4.29185800	C	-0.29270900	-2.45425900	-4.76083600
H	1.34631000	0.68407300	4.03340100	H	-0.60755200	-1.69434400	-5.47888000
H	0.18783800	-3.43491400	1.65984700	H	0.72731500	-2.77704500	-4.96805000
H	1.00555400	-1.41862600	5.37236700	H	-0.96641000	-3.31130800	-4.86441300
C	0.57863300	-2.59384100	3.60923200				
H	0.40816700	-3.52875600	4.13053100	TS4c-s			
N	0.65892200	-1.42456200	1.51061000	0 1			
Pd	0.47338200	-1.68373900	-0.54628300	C	0.43851100	-0.40671500	-2.88059600
C	-1.29666600	0.91114700	-0.71590600	C	1.38581000	0.40450400	-1.98701800
C	-1.30852900	-0.45494200	-0.52344700	H	-0.25039500	0.25569100	-3.40423300
C	-2.36119600	-1.17193500	0.26356000	H	1.01673000	-0.93565200	-3.64317900
C	-2.60574800	-0.92716800	1.62740400	H	-0.14700900	-1.14864000	-2.33425000
C	-3.11875500	-2.18116600	-0.36552500	C	2.63370200	-0.43587100	-1.51629000
C	-3.57727900	-1.64474600	2.32706100	H	1.83669400	1.16341800	-2.64275400
H	-2.02567900	-0.17524600	2.14926500	C	2.25790500	-1.81508900	-0.90501900
C	-4.09371700	-2.89435800	0.33241600	H	3.16008900	0.13332800	-0.74922300
H	-2.94730200	-2.39782100	-1.41522700	H	1.95664600	-2.48557600	-1.71705700
C	-4.32914500	-2.62996400	1.68380900	C	3.59885900	-0.61508500	-2.70518900
H	-3.74536100	-1.43086600	3.37904500	H	3.13528100	-1.16786600	-3.52901300

H	3.90435400	0.36276500	-3.09022300	H	4.21991500	3.29448300	1.61027100
H	4.49896600	-1.15257700	-2.40672400	H	2.30825800	5.60892900	-1.47034200
C	3.39805700	-2.57064400	-0.17865200	H	4.01614400	5.41965900	0.33328600
O	3.21559100	-3.64310600	0.36080600	C	-2.32259300	-3.35266200	-0.29732200
O	4.58822800	-1.95872400	-0.22628400	O	-2.93746100	-2.22806700	-0.11194100
C	5.66670800	-2.63737700	0.44875000	O	-1.10159100	-3.47697200	-0.51495100
H	5.82079300	-3.63036700	0.02146500	H	0.26455400	-2.30426500	-0.22724200
H	6.54539700	-2.01263200	0.29566000	C	-3.22376600	-4.57736000	-0.25772400
H	5.44300000	-2.73166200	1.51337800	H	-2.62771300	-5.48620100	-0.16640100
N	1.11586800	-1.77128900	0.00670100	H	-3.93366700	-4.50740000	0.57012800
C	1.25428700	-1.23462300	1.22969800	H	-3.80352900	-4.62498500	-1.18578600
O	2.32464500	-0.79187000	1.66985900	C	-2.77732300	0.71048500	-2.82844600
C	0.03682500	-1.18719400	2.11736700	O	-2.79182400	-0.34253600	-2.11498900
C	0.23863900	-1.41484200	3.48102600	O	-2.02677800	1.70563400	-2.59213700
C	-2.22157700	-0.79338500	2.48310000	H	-1.26782700	1.35907700	-1.52274900
C	-0.83654300	-1.34474800	4.35889600	C	-3.67182200	0.74706900	-4.04459800
H	1.24143000	-1.64172100	3.82068500	H	-4.50020900	0.04672300	-3.93648200
H	-3.17874900	-0.53297800	2.04985300	H	-4.04278400	1.76033800	-4.20749500
H	-0.69747100	-1.53066700	5.41864800	H	-3.07961800	0.45850400	-4.91977900
C	-2.09266000	-1.02412500	3.84666600				
H	-2.96584600	-0.94617900	4.48407900	10a-s			
N	-1.18069100	-0.87398000	1.62487700	0 l			
Pd	-1.78233600	-0.52530600	-0.33768500	C	0.93287200	-1.49050500	-1.38804900
C	0.76109900	1.27255400	-0.88129600	C	-0.02776700	-0.63533800	-2.22285300
C	-0.54913800	1.25763800	-0.44623100	H	0.43705000	-1.80075000	-0.46056500
C	-1.04253600	2.21957400	0.59556300	H	1.11967200	-2.43462700	-1.92205200
C	-0.43577400	2.33408200	1.86104200	C	-1.42773600	-1.28075700	-2.40586700
C	-2.18805800	3.00282800	0.34918400	H	-0.13761100	0.35686000	-1.77117300
C	-0.94077200	3.20176300	2.82967000	H	0.41799900	-0.47345800	-3.21166100
H	0.43731600	1.73433600	2.09157900	C	-2.47816400	-0.68212900	-1.42205800
C	-2.68920100	3.87610400	1.31587100	H	-1.35190700	-2.35322600	-2.20104000
H	-2.68236600	2.93577800	-0.61425900	H	-2.78702500	0.28513000	-1.83881900
C	-2.06916000	3.98080200	2.56279800	C	-1.90896600	-1.08938200	-3.85556500
H	-0.44858700	3.26839200	3.79618200	H	-1.93447500	-0.02365500	-4.11555100
H	-3.56733000	4.47558000	1.09145900	H	-1.22254400	-1.58280000	-4.55124300
H	-2.46005500	4.65803400	3.31663900	H	-2.90611900	-1.50469800	-4.01704000
C	1.67741700	2.40312600	-0.47780600	C	-3.79671000	-1.47503300	-1.28549800
C	2.64399100	2.30401500	0.53442700	O	-4.71599000	-1.10306300	-0.58026900
C	1.57467500	3.60609800	-1.19754000	O	-3.85311400	-2.58098400	-2.04039500
C	3.47923500	3.38744300	0.82088000	C	-5.07255200	-3.34385500	-1.94686800
H	2.73668200	1.38555200	1.10491300	H	-5.92938100	-2.73458500	-2.24261900
C	2.40828700	4.68621900	-0.90588200	H	-4.94520500	-4.18294600	-2.62940700
H	0.83357500	3.69554900	-1.98717500	H	-5.21724400	-3.70005500	-0.92472600
C	3.36559400	4.58029900	0.10562500	N	-1.98709400	-0.37790500	-0.07730400

C	-1.82334000	-1.37917300	0.80834300	H	-1.90502900	5.25565500	-1.75490200
O	-1.98701100	-2.58987800	0.59177000				
C	-1.40093400	-0.87515700	2.16150800	10b-s			
C	-1.12190400	-1.71497200	3.23159500	0 1			
C	-0.95343300	1.02446000	3.44675600	C	-2.07694800	4.34584300	0.98748100
C	-0.74294100	-1.14971500	4.44989300	C	-1.97793300	2.96556000	0.32493500
H	-1.21196600	-2.78495600	3.08484900	H	-2.28616700	5.11690300	0.23822800
H	-0.90762200	2.10741000	3.47386800	H	-2.88886500	4.37137100	1.72443800
H	-0.51886700	-1.78192200	5.30270100	H	-1.15332000	4.63472200	1.49773500
C	-0.65752600	0.23872600	4.55863300	C	-1.79139400	1.81498900	1.33549300
H	-0.36816400	0.71706600	5.48714600	H	-2.89674300	2.78026200	-0.23477700
N	-1.31387200	0.46828300	2.27956000	H	-1.17295100	2.96220900	-0.41382800
Pd	-1.78918400	1.48337800	0.60655500	C	-2.16885700	0.39258100	0.81690500
C	2.28033700	-0.88639000	-1.02164300	H	-2.53247500	1.98944000	2.12624200
C	2.64883800	0.35110400	-1.41890800	H	-2.00697300	-0.26885800	1.67916700
C	3.86630000	1.12795600	-1.10888800	C	-0.43714800	1.81888300	2.11172000
C	4.59542500	1.00584300	0.09026700	H	-0.37882700	2.78974300	2.62160600
C	4.29228000	2.09602000	-2.03947800	H	-0.51620600	1.07276200	2.91089000
C	5.71520200	1.80081500	0.33122300	C	-3.66788400	0.17899300	0.51099000
H	4.27469200	0.29437500	0.84249900	O	-4.10204600	-0.78193400	-0.09427900
C	5.41675600	2.88584100	-1.80215400	O	-4.45889300	1.11020400	1.06979600
H	3.73231100	2.22186200	-2.96311000	C	-5.87771000	0.91408200	0.90093800
C	6.13718900	2.73977900	-0.61451700	H	-6.18766600	-0.03323400	1.34738800
H	6.25748000	1.69085500	1.26643700	H	-6.35095200	1.75102900	1.41256700
H	5.72663300	3.61846800	-2.54224300	H	-6.13808500	0.91628900	-0.15951000
H	7.01034800	3.35673000	-0.42288100	N	-1.36078500	-0.18569500	-0.25248700
C	3.16397300	-1.81181200	-0.24804100	C	-1.57356800	0.16116600	-1.54144100
C	2.76418500	-2.33436100	0.99361900	O	-2.33541900	1.03773800	-1.96975900
C	4.39263400	-2.23409900	-0.78387600	C	-0.74098700	-0.66216600	-2.48936200
C	3.57774300	-3.23192400	1.68797100	C	-0.65211500	-0.39294500	-3.84914600
H	1.81655500	-2.02723500	1.42734800	C	0.67823200	-2.50800000	-2.69359400
C	5.20223100	-3.13725200	-0.09466300	C	0.14329600	-1.21472300	-4.64757500
H	4.70804000	-1.84911200	-1.74896400	H	-1.20876700	0.44793500	-4.24590300
C	4.79927200	-3.63770900	1.14621200	H	1.17029200	-3.33016300	-2.18616100
H	3.25504200	-3.61594700	2.65174400	H	0.23368700	-1.02535600	-5.71211800
H	6.14693700	-3.45281500	-0.52864800	C	0.81940300	-2.28591000	-4.06133900
H	5.42953800	-4.34031100	1.68369000	H	1.44648700	-2.94808600	-4.64698300
C	-2.01574300	3.79156800	-0.20340700	N	-0.08519400	-1.70507400	-1.93519000
O	-2.24786700	2.78200700	-0.95989800	Pd	-0.44737300	-1.93944100	0.03107200
O	-1.65273000	3.54867800	0.99821100	C	0.88885400	1.59662300	1.39503000
H	1.96146700	0.88159000	-2.07377600	C	1.62754500	0.50396300	1.69493100
C	-2.19477800	5.19132500	-0.70422900	C	2.98979300	0.12119500	1.26844800
H	-3.25333800	5.46260400	-0.62674800	C	3.30775700	-1.25027800	1.19885300
H	-1.61080800	5.88915000	-0.10253400	C	4.01701100	1.04452100	0.99107400

C	4.58092800	-1.68384900	0.82836000	C	-3.19508200	-1.64980400	-1.25111700
H	2.53917800	-1.98317400	1.42805200	O	-3.86585400	-2.01954100	-2.19447600
C	5.29231700	0.61127900	0.62983700	O	-3.55560800	-1.84083000	0.03336100
H	3.82023000	2.10703000	1.07252700	C	-4.84901600	-2.43820600	0.23468600
C	5.58101300	-0.75324100	0.53759400	H	-4.89535500	-3.42592300	-0.22999800
H	4.79253000	-2.74836900	0.77484300	H	-4.97219000	-2.51866900	1.31412300
H	6.06779900	1.34498600	0.42711600	H	-5.62923800	-1.80371200	-0.19213900
H	6.57574100	-1.08578700	0.25526100	N	-1.67127500	0.14304100	-0.48030200
C	1.35297900	2.64910500	0.44066600	C	-2.62463000	1.08432000	-0.53918400
C	1.60066000	2.33704300	-0.90715600	O	-3.67371000	1.04370800	-1.21163800
C	1.55224500	3.97393000	0.86434100	C	-2.35485500	2.28867600	0.34438600
C	2.03070300	3.31685200	-1.80202800	C	-3.32540400	3.27354300	0.51076300
H	1.45102400	1.31771100	-1.24858800	C	-0.88392700	3.42022200	1.74545400
C	1.99140400	4.95367800	-0.02876100	C	-3.05040100	4.36407800	1.33473400
H	1.38070600	4.23638100	1.90467500	H	-4.26871200	3.15885600	-0.00941900
C	2.22900000	4.62974600	-1.36636100	H	0.09716300	3.43620800	2.20828900
H	2.21124200	3.05496200	-2.84098100	H	-3.79215800	5.14262400	1.48291900
H	2.14832700	5.96981300	0.32217900	C	-1.80913200	4.43912500	1.96653600
H	2.56538600	5.39267400	-2.06238700	H	-1.55331700	5.26795000	2.61712100
C	-0.09594300	-3.55597300	1.86026200	N	-1.14913000	2.37105700	0.95115600
O	0.38089700	-3.77502800	0.69557200	Pd	0.07217035	0.82408643	0.30549404
O	-0.74950000	-2.46564700	2.03257400	C	1.45138941	-1.27528617	0.04784596
H	1.15819300	-0.22851300	2.35111700	C	2.64495714	-0.58631105	0.11932565
C	0.11814700	-4.51341500	2.99271000	C	4.08301880	-0.95505424	0.24623963
H	0.89688700	-4.11659700	3.65292900	C	5.09251856	-0.01530533	-0.07576700
H	-0.79868300	-4.61148400	3.57836200	C	4.47160439	-2.21795497	0.76088348
H	0.43488500	-5.48678400	2.61632000	C	6.43512393	-0.33995702	0.07309653
10c-s				H	4.79371861	0.96052568	-0.44615526
0 1				C	5.81595095	-2.52442950	0.93817342
C	0.92236048	-0.57175510	-2.40071282	H	3.70454572	-2.93963378	1.02421695
C	0.78332800	-1.63930500	-1.30324800	C	6.79872334	-1.59179818	0.58562580
H	1.96850818	-0.41621182	-2.67296985	H	7.20177493	0.38174199	-0.19135014
H	0.39416348	-0.89085443	-3.30404692	H	6.10374554	-3.49049092	1.34129781
H	0.50895019	0.39405661	-2.09476766	H	7.84824117	-1.83758854	0.71719591
C	-0.71295900	-2.10336600	-1.10950600	C	1.50139209	-2.34095766	1.11561559
H	1.31103592	-2.52525410	-1.67971986	C	2.02929701	-2.05826042	2.39483703
C	-1.80351000	-1.00727900	-1.36781700	C	1.08264915	-3.66323985	0.87339316
H	-0.83129200	-2.40385900	-0.06299100	C	2.12680510	-3.04148616	3.37635545
H	-1.74678000	-0.69019600	-2.41790000	H	2.35459538	-1.04787107	2.61863309
C	-0.97449000	-3.34393300	-1.98718200	C	1.17761300	-4.64805869	1.85976435
H	-0.91662800	-3.10500900	-3.05443800	H	0.68220635	-3.94662217	-0.09205477
H	-0.23150400	-4.12029800	-1.77977300	C	1.69770541	-4.34642019	3.11763198
H	-1.96039000	-3.77710100	-1.80509400	H	2.53767953	-2.78492906	4.34896550
				H	0.84269730	-5.65697415	1.63533974

H	1.76928235	-5.11301790	3.88342298	H	2.70052600	-3.64129600	4.13168400
C	0.98520785	1.92033777	-1.34923368	N	2.18326600	-1.25862700	1.83065600
O	0.42951299	2.51631534	-0.44873807	Pd	2.48443500	-0.69456700	-0.07042700
O	1.32153080	0.75173961	-1.25092193	C	-3.84263300	0.52295300	-0.39362800
H	2.89306602	-0.00922489	-0.64586293	C	-3.46401800	-0.75836000	-0.58580500
C	1.34538404	2.49049173	-2.69541978	C	-4.26185800	-2.00083500	-0.58007300
H	2.42514465	2.41710319	-2.85371886	C	-5.44060500	-2.18104600	0.16988700
H	0.85868920	1.91278774	-3.48644146	C	-3.78257800	-3.09895800	-1.32132700
H	1.03204864	3.53197664	-2.74980565	C	-6.11957800	-3.39876000	0.15448800
11a-s				H	-5.81758500	-1.36881400	0.78044100
0 1				C	-4.46527800	-4.31459700	-1.34263300
C	-2.84471400	1.67308700	-0.37448500	H	-2.86337800	-2.98933900	-1.89204300
C	-1.35974800	1.31109600	-0.48591600	C	-5.64163700	-4.46996900	-0.60577400
H	-3.00196000	2.23963900	0.55536400	H	-7.02347500	-3.51388600	0.74651000
H	-3.13159500	2.36847500	-1.17505300	H	-4.07560400	-5.14121700	-1.93031200
C	-0.41620300	2.51873200	-0.30968200	H	-6.17398900	-5.41671000	-0.61478900
H	-1.12198000	0.56335200	0.27591800	C	-5.26463200	0.96237900	-0.25067800
H	-1.16125500	0.83870000	-1.45862300	C	-5.70561800	1.63503500	0.90138900
C	1.06194500	2.04506200	-0.28890700	C	-6.17815500	0.76752700	-1.30036400
H	-0.63232000	2.98685700	0.65370000	C	-7.02488800	2.07956900	1.00943800
H	1.31479000	1.74269300	-1.30989900	H	-5.01641400	1.79727500	1.72567200
C	-0.59927600	3.55562300	-1.43197500	C	-7.49425600	1.21868300	-1.19657400
H	-0.44060500	3.09853700	-2.41681600	H	-5.84734400	0.25906800	-2.20104900
H	-1.60817800	3.97628400	-1.41964600	C	-7.92364400	1.87439800	-0.03982700
H	0.09753800	4.39181700	-1.32864200	H	-7.34928500	2.58738200	1.91344600
C	2.09951300	3.11912400	0.06682500	H	-8.18417900	1.06030200	-2.02079000
O	3.29733400	2.97579300	-0.18434800	H	-8.94855800	2.22461900	0.04193000
O	1.63513900	4.18355900	0.70009400	C	3.67731600	0.47347100	-2.61985700
C	2.60466500	5.18244200	1.09902600	O	2.74241500	-0.15154700	-2.07698300
H	3.13757100	5.56022400	0.22489700	O	4.25871100	1.52946600	-2.12208200
H	2.02389400	5.97274300	1.57054100	H	3.84240900	1.88807300	-1.27752100
H	3.31539900	4.75048600	1.80548600	C	4.21430100	0.03065100	-3.94730300
N	1.37344900	0.87690000	0.54659500	H	5.01010800	-0.69287400	-3.73959300
C	1.09761600	0.91437000	1.86976500	H	3.43277200	-0.46958400	-4.51984900
O	0.55314300	1.83144600	2.50147000	H	4.63539500	0.86729000	-4.50509300
C	1.52126200	-0.34726800	2.57675200	H	-2.40867200	-0.93424500	-0.78119500
C	1.25529500	-0.57137100	3.92140200	C	4.70493000	-2.39151500	-0.91523800
C	2.59794800	-2.41326600	2.37773700	O	3.46645200	-2.43067300	-0.50283900
C	1.67726500	-1.76666800	4.50298900	O	5.38063000	-1.36487800	-1.05083600
H	0.72725400	0.19651300	4.47437400	C	5.27696300	-3.76716500	-1.23619100
H	3.12211200	-3.08875900	1.71258300	H	4.70576000	-4.22707400	-2.04888400
H	1.48080300	-1.96760200	5.55101500	H	6.32410200	-3.68429100	-1.52956500
C	2.35611600	-2.69996000	3.71901000	H	5.18943100	-4.42459000	-0.36595600

11b-s				C	-1.87319000	-5.02161300	-1.26629300
0 1				H	-3.11300000	-3.27592600	-1.38965200
C	-4.29071700	2.87196200	-0.60651800	C	-0.57860900	-5.54363000	-1.34066300
C	-2.92746900	2.47402100	-0.02538100	H	1.50174500	-5.07518100	-1.67469400
H	-4.99051100	3.12581500	0.19701100	H	-2.71569300	-5.68382700	-1.08592700
H	-4.19999200	3.75146500	-1.25560600	H	-0.40818600	-6.60845400	-1.21042300
H	-4.75042000	2.07056200	-1.19246000	C	-3.19793800	-0.83784800	-0.50342400
C	-1.85601700	2.20377600	-1.10193900	C	-2.87952000	-1.27403200	0.79407200
H	-2.56976200	3.28281900	0.61311400	C	-4.55246100	-0.77837000	-0.87233400
H	-3.04304700	1.60362400	0.62635300	C	-3.88203100	-1.63722700	1.69372000
C	-0.37197300	2.25986600	-0.61972700	H	-1.83691100	-1.32048200	1.09164200
H	-1.91717000	3.04793600	-1.80124700	C	-5.55637500	-1.14984300	0.02478400
H	0.21829300	2.00931900	-1.50753300	H	-4.82270500	-0.45854700	-1.87499200
C	-2.13315600	0.96990600	-2.01650600	C	-5.22517700	-1.57792400	1.31218600
H	-3.11873900	1.13850400	-2.47076000	H	-3.61446800	-1.96684000	2.69395700
H	-1.41813900	1.01082200	-2.84611900	H	-6.59706300	-1.10575600	-0.28400000
C	0.14653400	3.66546700	-0.25060700	H	-6.00596200	-1.86227800	2.01163400
O	1.24902800	3.86704000	0.22357900	C	4.19786900	-1.32714000	0.23265400
O	-0.69093100	4.65846600	-0.59483500	O	4.73320600	-0.20258000	0.04904800
C	-0.21997100	5.99549400	-0.33397100	O	2.94209400	-1.56808900	0.12886800
H	0.70612000	6.18897800	-0.87969400	H	-0.41486800	-0.90372200	-2.55561400
H	-1.01297000	6.65760500	-0.67919100	C	5.06839100	-2.49789900	0.63964000
H	-0.04431600	6.13354100	0.73493200	H	5.06124700	-2.57736600	1.73272500
N	0.05177100	1.29839700	0.39981100	H	4.67519900	-3.43156600	0.23325700
C	-0.22208000	1.56924600	1.69551200	H	6.09684100	-2.34086600	0.31276300
O	-0.83610400	2.54795200	2.14519300	C	2.82664000	1.07334400	-2.34166200
C	0.28693500	0.50368100	2.62847800	O	1.84803300	0.46909500	-1.83485400
C	-0.05324100	0.46275700	3.97501600	O	3.96645300	1.25958200	-1.76523300
C	1.55917800	-1.44684400	2.82233600	H	4.15283400	0.67075600	-0.89661700
C	0.42956900	-0.58299900	4.76089200	C	2.70290200	1.64858600	-3.72577700
H	-0.68685400	1.24856400	4.36885100	H	2.89295800	2.72518400	-3.68431000
H	2.19220700	-2.16044900	2.30991400	H	3.46635400	1.20697100	-4.37231500
H	0.17571000	-0.64180300	5.81419500	H	1.71135300	1.46079200	-4.13473900
C	1.24137700	-1.55453600	4.17376200				
H	1.63179700	-2.38740600	4.74721600	11c-s			
N	1.08800000	-0.43338200	2.07705400	0 1			
Pd	1.52812300	-0.06099300	0.14867300	C	1.64705700	-2.46978700	0.51723900
C	-2.12012400	-0.44904800	-1.46283900	C	0.18937600	-2.07714200	0.04836200
C	-1.18940200	-1.32083800	-1.91339900	H	0.28172400	-1.63606900	-0.94601700
C	-1.03087600	-2.77031400	-1.67817200	C	2.74035800	-2.07080000	-0.53085900
C	0.26421000	-3.31834800	-1.77642300	H	3.68440700	-2.38481700	-0.06293300
C	-2.09906600	-3.65564700	-1.43346000	C	-0.76725300	-3.26170200	-0.14393600
C	0.49085900	-4.68349700	-1.60065600	O	-1.76555200	-3.49323900	0.50632900
H	1.10137800	-2.65702400	-1.98260900	O	-0.38841900	-4.01690600	-1.19949500

C	-1.19899100	-5.18033700	-1.46574600	O	-2.56362500	2.17064500	-0.44364300
H	-2.22425900	-4.88676400	-1.70095200	H	1.98923700	-0.51688300	-2.57297100
H	-0.73608600	-5.67012800	-2.32137100	C	-4.51543900	3.48444300	-0.77820200
H	-1.20431700	-5.84678000	-0.60065400	H	-4.93365000	3.64950500	0.22140200
N	-0.44339000	-1.04941400	0.86778100	H	-3.82290600	4.29970300	-0.99407300
C	-0.49914400	-1.18218400	2.20996400	H	-5.33781600	3.47986500	-1.49473900
O	-0.05183200	-2.10935200	2.90088200	C	-2.16974900	-0.76552000	-2.58375900
C	-1.14686500	0.00465400	2.87537900	O	-1.31039700	-0.22857400	-1.83886200
C	-1.21648800	0.13453400	4.25680100	O	-3.44655600	-0.68948800	-2.41946100
C	-2.19610700	2.06934400	2.56467400	H	-3.77990400	0.04527500	-1.71862200
C	-1.79505500	1.28085800	4.79978100	C	-1.69383600	-1.58669000	-3.75095400
H	-0.81269200	-0.66557300	4.86577600	H	-2.52463700	-1.87495900	-4.39369000
H	-2.56283200	2.79118900	1.84581300	H	-0.95416300	-1.01773400	-4.31933000
H	-1.85978600	1.40803600	5.87543200	H	-1.19614600	-2.48190000	-3.36496900
C	-2.28624000	2.26442000	3.94027300	C	1.80118500	-3.92629800	0.98188300
H	-2.73763200	3.17389500	4.31986500	H	1.08748100	-4.13404900	1.78271800
N	-1.63950200	0.95781400	2.05470300	H	1.64439100	-4.64692900	0.17577100
Pd	-1.52522500	0.46968100	0.10509900	H	2.80931800	-4.08219200	1.38100800
C	2.84145900	-0.54899800	-0.67250400	H	1.83491200	-1.85370100	1.39787400
C	2.43925100	0.09131700	-1.79166700	C	2.64357900	-2.83175900	-1.86052700
C	2.50703200	1.52626200	-2.14047500	H	3.44403100	-2.52006000	-2.53848100
C	1.50124400	2.06163700	-2.96899600	H	2.74442900	-3.90718300	-1.69322700
C	3.55603800	2.37783900	-1.74521300	H	1.68987600	-2.67758200	-2.37347800
C	1.51948600	3.40172600	-3.35627100				
H	0.69141900	1.41571900	-3.29844400	TS5a-s			
C	3.57939100	3.71503500	-2.14035500	0 1			
H	4.36400900	1.98630700	-1.13737500	C	-1.88470500	2.08295600	-0.68536600
C	2.55927000	4.23714300	-2.94080600	C	-0.45122000	1.54497500	-0.60274700
H	0.72554000	3.79077800	-3.98792200	H	-2.01786300	2.85885400	0.08270300
H	4.40355400	4.35059000	-1.82803900	H	-2.04657400	2.60357100	-1.63867300
H	2.58124000	5.27921500	-3.24637300	C	0.61873700	2.65478600	-0.59365700
C	3.37718400	0.16311800	0.52922600	H	-0.37367700	0.95031900	0.31196600
C	2.60342000	1.12433000	1.20309300	H	-0.25693000	0.85730400	-1.43631600
C	4.65482300	-0.13388500	1.03374500	C	2.07144800	2.11204100	-0.41952800
C	3.09501500	1.77321000	2.33623700	H	0.40743600	3.31411800	0.25444200
H	1.60958500	1.35453500	0.83242800	H	2.44836400	1.84897700	-1.41411300
C	5.15027300	0.52019700	2.16372300	C	0.56094200	3.48875600	-1.88915900
H	5.27568000	-0.86820400	0.52775200	H	0.62912100	2.83612200	-2.76830700
C	4.37161200	1.47535400	2.82049800	H	-0.37642700	4.04638600	-1.95768100
H	2.47931600	2.51176100	2.84258400	H	1.37547100	4.21360900	-1.93600600
H	6.14548900	0.28304300	2.52924600	C	3.07859300	3.15025800	0.13426800
H	4.75477500	1.98153600	3.70182900	O	4.20052600	2.86029100	0.49480500
C	-3.79840900	2.15026500	-0.78847700	O	2.60604000	4.40442700	0.12932200
O	-4.44534800	1.11478100	-1.09707000	C	3.51245900	5.41700400	0.61356000

H	4.42351200	5.43294700	0.01197800	H	3.38163500	0.48840200	0.09710100
H	2.97352700	6.35857000	0.51971500	C	5.15982300	-0.64317900	-2.74401300
H	3.77027600	5.22398100	1.65690900	H	5.61125500	-1.62824400	-2.58224900
N	2.23244100	0.85649200	0.37978100	H	4.72534600	-0.62985400	-3.74465400
C	1.84524800	1.00440500	1.73080500	H	5.93938700	0.11353500	-2.64966800
O	1.82281000	2.07616600	2.31477700	H	-1.74638600	-0.58551200	-0.62435800
C	1.32112400	-0.24079300	2.38513100	C	2.12065000	-3.85086500	-0.81158600
C	1.07561200	-0.29587700	3.75230600	O	1.20408000	-2.91556200	-0.88415700
C	0.40503700	-2.36264400	2.06091800	O	3.24347800	-3.70741500	-0.32249300
C	0.47951500	-1.44036700	4.28232400	C	1.66667400	-5.17652400	-1.40806600
H	1.34430600	0.55520100	4.36665600	H	1.55385600	-5.06881300	-2.49179900
H	0.16911100	-3.13966100	1.34414700	H	2.39980400	-5.95627400	-1.19845300
H	0.28296500	-1.51404400	5.34642900	H	0.69129200	-5.46365300	-1.00548700
C	0.13206100	-2.48182100	3.42297700				
H	-0.34246400	-3.38361500	3.79237200	TS5b-s			
N	0.99250400	-1.26467100	1.56203200	0 1			
Pd	1.73093300	-1.05512100	-0.30554500	C	-0.92632600	4.91249700	-0.67366800
C	-3.00766000	1.06699000	-0.52401600	C	-0.31004600	3.69682400	0.03152800
C	-2.77594400	-0.26261800	-0.48708000	H	-1.36274800	5.60041600	0.05791000
C	-3.70567600	-1.39337600	-0.29452500	H	-0.16455600	5.46431900	-1.23695100
C	-4.92031300	-1.31360500	0.41461600	H	-1.72158200	4.63298700	-1.37018700
C	-3.32451800	-2.65143500	-0.80293200	C	0.34927500	2.70459900	-0.95537000
C	-5.72556900	-2.43948000	0.58238000	H	0.44850900	4.05635300	0.73288100
H	-5.22787100	-0.36978800	0.84921700	H	-1.06180800	3.19798600	0.64558500
C	-4.13348500	-3.77567600	-0.64121100	C	1.59323900	1.91603600	-0.41998900
H	-2.38233700	-2.74014700	-1.33869100	H	0.84848700	3.34125300	-1.69576000
C	-5.34235900	-3.67441700	0.05111500	H	2.04411200	1.47983500	-1.31741700
H	-6.65539200	-2.35285000	1.13794900	C	-0.62665300	1.87112100	-1.84386300
H	-3.81758100	-4.73048700	-1.05238900	H	-1.10726700	2.60494900	-2.50529300
H	-5.97393600	-4.54804400	0.18383200	H	-0.01539400	1.24463700	-2.50326400
C	-4.36981300	1.68271300	-0.48789800	C	2.65992600	2.89166500	0.12225800
C	-4.73911800	2.56376600	0.54240200	O	3.21295900	2.81330900	1.19695100
C	-5.29055700	1.43873400	-1.52051100	O	2.94382300	3.83625800	-0.79396500
C	-5.99914100	3.16514600	0.55198000	C	3.95569200	4.79290900	-0.41642000
H	-4.04179400	2.76681200	1.35083400	H	4.90436600	4.28675800	-0.22593200
C	-6.54661500	2.04644800	-1.51640300	H	4.04660900	5.47116200	-1.26350400
H	-5.01378200	0.76796300	-2.32850700	H	3.64954800	5.33696800	0.47951200
C	-6.90680900	2.90974200	-0.47847700	N	1.46685900	0.74977900	0.50697400
H	-6.27024900	3.83412300	1.36391900	C	0.76423000	0.93945500	1.71774000
H	-7.24365700	1.84693800	-2.32548700	O	0.59404300	2.01109100	2.26947800
H	-7.88517600	3.38144500	-0.47425700	C	0.13166100	-0.30809500	2.27468600
C	4.09253400	-0.43698600	-1.69975300	C	-0.46099600	-0.31310800	3.53305400
O	2.91083900	-0.84146000	-1.97895700	C	-0.56345700	-2.49814200	1.86343600
O	4.41799800	0.10734100	-0.59677300	C	-1.12083100	-1.46454100	3.96264900

H	-0.40175200	0.58283300	4.13934500	H	5.90174900	0.09430300	-1.33048600
H	-0.56674600	-3.32173900	1.16094700	H	5.66970000	-1.65760500	-1.19656500
H	-1.58642100	-1.49753800	4.94178700	H	5.09393800	-0.82167400	-2.64777000
C	-1.17916900	-2.56759400	3.11183100				
H	-1.68959200	-3.47854000	3.40260600	TS5c-s			
N	0.07958600	-1.39020800	1.46474400	0 1			
Pd	1.27129700	-1.22525100	-0.15038900	C	-1.65042500	-2.22161500	0.49172900
C	-1.75073600	1.00568600	-1.28083000	C	-2.11281200	-0.94589100	-0.31013000
C	-1.76383000	-0.31685500	-1.56888800	H	-1.54833000	-0.91737500	-1.24496400
C	-2.80221500	-1.34908400	-1.37015100	C	-0.66485800	-3.14687200	-0.30833500
C	-2.39071200	-2.69766200	-1.33308900	H	-0.58520000	-4.03806500	0.32682900
C	-4.18449100	-1.08343200	-1.29839000	C	-3.59551800	-0.97321700	-0.71990400
C	-3.31525800	-3.73290200	-1.19270600	O	-4.46916300	-0.25949700	-0.27854300
H	-1.33167100	-2.93114400	-1.40619100	O	-3.79862300	-1.89336900	-1.68003700
C	-5.10713800	-2.12052300	-1.16739500	C	-5.15699600	-2.02669500	-2.14799700
H	-4.54264500	-0.06362600	-1.36539200	H	-5.50140200	-1.08717000	-2.58498000
C	-4.68009800	-3.44985300	-1.10568100	H	-5.13003000	-2.81241600	-2.90152000
H	-2.96871800	-4.76245200	-1.16125800	H	-5.81767800	-2.30697000	-1.32494000
H	-6.16770400	-1.88829700	-1.12277600	N	-1.79970800	0.36446500	0.34858300
H	-5.40304400	-4.25418400	-1.00437000	C	-2.10694900	0.46797700	1.72613600
C	-2.87723400	1.68786800	-0.57119500	O	-2.98437300	-0.15545800	2.29600700
C	-3.19729600	1.36316800	0.75802800	C	-1.17024100	1.34409000	2.51245100
C	-3.65495000	2.66044000	-1.22268100	C	-1.42007900	1.65493200	3.84475700
C	-4.25436000	1.99230800	1.41605700	C	0.91617000	2.38803400	2.58833100
H	-2.61162900	0.61039500	1.27598900	C	-0.45874500	2.36605600	4.56218900
C	-4.71978900	3.28366500	-0.56851400	H	-2.35054900	1.32436900	4.29069600
H	-3.44106000	2.91563000	-2.25691200	H	1.80953700	2.65116300	2.03553800
C	-5.02111600	2.95515500	0.75485300	H	-0.63020300	2.62654600	5.60106800
H	-4.47995100	1.72934800	2.44572500	C	0.72901900	2.72721200	3.92697500
H	-5.31409000	4.02514000	-1.09495800	H	1.50676300	3.27085600	4.45090400
H	-5.84584800	3.44355500	1.26551200	N	-0.02164000	1.71693800	1.90224900
C	1.92883900	-4.01700800	-0.27454500	Pd	-0.05968400	1.42543000	-0.08789800
O	2.82490500	-3.76543000	0.53467300	C	0.75510600	-2.57226900	-0.37089000
O	1.04362400	-3.15430700	-0.71217800	C	1.25745800	-2.05995200	-1.51657100
H	-0.87131100	-0.70465000	-2.05889600	C	2.61593100	-1.57006700	-1.83042800
C	1.75629300	-5.40599500	-0.87456900	C	2.75283200	-0.54298300	-2.78408900
H	0.71413400	-5.72900600	-0.80220600	C	3.78923500	-2.12783600	-1.28839400
H	2.01659600	-5.37738900	-1.93778800	C	4.00948300	-0.06300600	-3.15351500
H	2.40419200	-6.12070900	-0.36583800	H	1.85971900	-0.11122700	-3.22830800
C	3.89664300	-0.53568800	-0.88664400	C	5.04552200	-1.65417000	-1.66457700
O	2.86133100	-1.02440200	-1.45394300	H	3.71656100	-2.94707200	-0.58177100
O	3.87078400	0.08599400	0.22649100	C	5.16337600	-0.61492100	-2.59228400
H	2.66700000	0.40302600	0.58313300	H	4.08645100	0.73741400	-3.88409800
C	5.22591500	-0.72772100	-1.56909900	H	5.93727500	-2.10541800	-1.23817700

H	6.14380800	-0.24883100	-2.88301400
C	1.51782600	-2.62253000	0.91565100
C	2.09559000	-1.46190500	1.46148500
C	1.65672700	-3.82590500	1.63046500
C	2.78365000	-1.50159100	2.67434700
H	2.00650100	-0.52526600	0.92202100
C	2.35293400	-3.86887300	2.84006200
H	1.23832900	-4.74448300	1.22900200
C	2.91560100	-2.70615500	3.37015100
H	3.21790000	-0.58974200	3.07512700
H	2.45616600	-4.81344200	3.36661600
H	3.45251000	-2.73846200	4.31372500
C	1.47959200	3.77379500	-0.65145800
O	0.41220800	4.38927400	-0.57733800
O	1.62639700	2.49115200	-0.42998200
H	0.58084700	-2.00330900	-2.36655800
C	2.78152000	4.46948500	-1.02601300
H	3.57231100	4.21116500	-0.31632100
H	3.10582700	4.12666200	-2.01394700
H	2.64017600	5.55071200	-1.04912200
C	-1.69312900	1.77226200	-2.38075400
O	-0.49324800	1.43314400	-2.10975300
O	-2.64139800	1.78758900	-1.52662000
H	-2.32036600	1.18438500	-0.44218000
C	-1.99911200	2.20211000	-3.79227200
H	-3.02472500	1.94211500	-4.05769200
H	-1.89693400	3.29151400	-3.84796800
H	-1.29181600	1.75585900	-4.49228800
C	-2.81117300	-3.04775100	1.07696500
H	-3.48088500	-2.41523400	1.66149300
H	-3.39465000	-3.54286400	0.29635100
H	-2.41171200	-3.82397200	1.73731700
H	-1.07382900	-1.84269100	1.34115500
C	-1.20452200	-3.64399400	-1.65790800
H	-0.48482100	-4.32869000	-2.11619000
H	-2.14623100	-4.18105000	-1.52309300
H	-1.39888900	-2.83786700	-2.37010900