

Electronic Supporting Information

For

**Impact of Counteranions on N-Heterocyclic Carbene Gold(I)-
Catalyzed Cyclization of Propargylic Amide**

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Table ESII. Computed relative basicity of different counteranions and their effect on relative affinity of Au(I) property among complexation to propargylic amide (in kcal/mol).^a

Anion	Basicity	Au affinity
NTf ₂ ⁻	160.8	49.9
ClO ₄ ⁻	155.9	41.0
TsO ⁻	173.1	46.3
TFA ⁻	179.3	55.7
TfO ⁻	157.5	40.9
MsO ⁻	173.6	49.1
SbF ₆ ⁻	125.2	28.2

^a The basicity is the free energy change for the reaction $HA \rightarrow A^- + H^+$ in chloroform, where HA refers to protonated counteranion (A). Au affinity is the Gibbs free energy change of the reaction $I\text{PrAuA} \rightarrow I\text{PrAu}^+ + A^-$ where L = IPr.

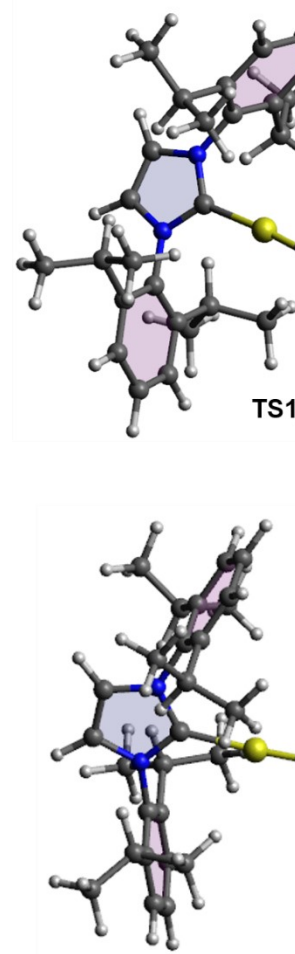


Figure ESII. Selected optimized geometries for cyclization (TS1) and protodeauration (TS2) steps of propargylic amide under 5-*exo-dig* (top) and 6-*endo-dig* (bottom) modes under effect of counteranions MsO⁻. Color codes for atoms: Gray: Carbon, white: Hydrogen, blue: Nitrogen, red: Oxygen, yellow: Gold, pale yellow: Sulphur.

Energetics for each compound examined (in Hartree)

Species	E	G
1	-630.184211	-630.033117
HNTf₂	-1826.393277	-1826.376014
NTf₂⁻	-1825.944062	-1825.936629
H⁺	-1294.284337	-1293.787688
IPrAuNTf₂	-3120.326879	-3119.803842
Int1_NTf2	-3750.532090	-3749.827422
TS1_5exo_NTf2	-3750.524226	-3749.820721
TS1_6endo_NTf2	-3750.516986	-3749.813720
Int2_5exo_NTf2	-3750.557752	-3749.854820
Int2_6endo_NTf2	-3750.556637	-3749.853747
Int2_5exo	-1924.106345	-1923.445160
Int2_6endo	-1924.095379	-1923.437948
TS2_5exo_NTf2	-3750.532127	-3749.832114
TS2_6endo_NTf2	-3750.518651	-3749.817011
2exo	-630.223501	-630.069702

2endo	-630.216956	-630.060701
HClO₄	-760.844975	-760.847968
ClO₄⁻	-760.403037	-760.416250
IPrAuClO₄	-2054.768870	-2054.269302
Int1_ClO4	-2684.984949	-2684.304640
TS1_5exo_ClO4	-2684.977985	-2684.302480
TS1_6endo_ClO4	-2684.967631	-2684.282151
Int2_5exo_ClO4	-2685.013116	-2684.333159
Int2_6endo_ClO4	-2685.006118	-2684.323760
TS2_5exo_ClO4	-2684.980140	-2684.306365
TS2_6endo_ClO4	-2684.964604	-2684.285001
TsOH	-894.632199	-894.533130
TsO⁻		
IPrAuOTs	-2188.545234	-2187.935551
Int1_TsO	-2818.761771	-2817.974408
TS1_5exo_TsO	-2818.753680	-2817.966522
TS1_6endo_TsO	-2818.735724	-2817.943284
Int2_5exo_TsO	-2818.787338	-2817.999569
Int2_6endo_TsO	-2818.783071	-2817.992329
TS2_5exo_TsO	-2818.747003	-2817.961046
TS2_6endo_TsO	-2818.750588	-2817.967631
TsOH	-894.632199	-894.533130
TsO⁻	-894.166025	-894.074145
IPrAuOTs	-2188.545234	-2187.935551
Int1_TsO	-2818.761771	-2817.974408
TS1_5exo_TsO	-2818.753680	-2817.966522
TS1_6endo_TsO	-2818.735724	-2817.943284
Int2_5exo_TsO	-2818.787338	-2817.999569
Int2_6endo_TsO	-2818.783071	-2817.992329
TS2_5exo_TsO	-2818.747003	-2817.961046
TS2_6endo_TsO	-2818.750588	-2817.967631
HTFA	-526.274963	-526.267252
TFA⁻	-526.274963	-526.267252
IPrAuTFA	-1820.185246	-1819.674730
Int1_TFA	-2450.393152	-2449.704435
TS1_5exo_TFA	-2450.384087	-2449.700790
TS1_6endo_TFA	-2450.375205	-2449.686598
Int2_5exo_TFA	-2450.420878	-2449.730223
Int2_6endo_TFA	-2450.412905	-2449.723185
TS2_5exo_TFA	-2450.400612	-2449.714007
TS2_6endo_TFA	-2450.387105	-2449.699957
HSbF₆	-839.452829	-839.465809
SbF₆⁻	-839.063073	-839.083599
IPrAuSbF₆	-2133.411748	-2132.916233
Int1_SbF6	-2763.651799	-2762.978246
TS1_5exo_SbF6	-2763.638336	-2762.967567
TS1_6endo_SbF6	-2763.628256	-2762.955986
Int2_5exo_SbF6	-2763.672392	-2762.995709
Int2_6endo_SbF6	-2763.668534	-2762.991561

TS2_5exo_SbF6	-2763.641380	-2762.965090
TS2_6endo_SbF6	-2763.621094	-2762.947266
MsOH	-663.860150	-663.829894
MsO ⁻	-663.390947	-663.370035
IPrAuOMs	-1957.774261	-1957.235984
Int1_MsO	-2587.980630	-2587.266212
TS1_5exo_MsO	-2587.976023	-2587.266287
TS1_6endo_MsO	-2587.964885	-2587.249627
Int2_5exo_MsO	-2588.010402	-2587.294464
Int2_6endo_MsO	-2588.005956	-2587.290334
TS2_5exo_MsO	-2587.985228	-2587.273604
TS2_6endo_MsO	-2587.975616	-2587.263994
TfOH	-961.295392	-961.292496
TfO ⁻	-960.851985	-960.858404
IPrAuOTf	-2255.220937	-2254.711240
Int1_TfO	-2885.439208	-2884.752129
TS1_5exo_TfO	-2885.430303	-2884.747869
TS1_6endo_TfO	-2885.426520	-2884.740066
Int2_5exo_TfO	-2885.466562	-2884.776054
Int2_6endo_TfO	-2885.460237	-2884.770319
TS2_5exo_TfO	-2885.432269	-2884.749374
TS2_6endo_TfO	-2885.424931	-2884.739753

Cartesian Coordinates:

1

N	2.26909600	-0.01513900	-0.50964100
C	1.41087200	0.92965200	-0.00275900
C	-0.03824600	0.55764600	0.01820400
C	-0.50926200	-0.76752700	-0.03536700
C	-0.98184800	1.60194000	0.13307600
C	-1.87968200	-1.05474400	-0.00250600
H	0.19297700	-1.60753900	-0.06590700
C	-2.34672500	1.33472600	0.15960600
H	-0.61467900	2.63034700	0.19660400
C	-2.80890400	0.00153200	0.08583500
H	-2.21161800	-2.09493700	-0.03288300
H	-3.08248500	2.14091000	0.23644900
O	-4.16128100	-0.15577400	0.11398500
C	-4.67754900	-1.48782200	0.01568000
H	-4.36116000	-2.10980700	0.87318900
H	-5.77207500	-1.38259200	0.02771200
H	-4.36613500	-1.97219100	-0.92793400
O	1.81410200	2.03480000	0.40450900
C	3.70935100	0.20192200	-0.53936500
C	4.45073300	-0.89272100	0.09132700
C	5.06223900	-1.82046600	0.59494300
H	5.60101400	-2.62938300	1.05802300
H	1.90373300	-0.86457900	-0.93635300
H	4.06136400	0.34421800	-1.58000200

H 3.87891000 1.15594100 -0.00774500

HNTf₂

H	-1.84671700	-0.19096700	-0.06546900
N	-0.82179300	-0.09678800	-0.03371800
S	-0.04513800	-0.84539300	1.29338900
S	-0.10625900	0.75762600	-1.32978300
O	1.19903800	1.26839900	-0.90044300
O	-1.17589100	1.59537400	-1.89087800
C	0.20162500	-0.64432200	-2.55856400
F	1.00010100	-1.55925200	-2.00192100
F	-0.97673300	-1.19306900	-2.88137600
F	0.78131600	-0.11809800	-3.64341800
O	-1.02141700	-1.80379700	1.83132300
O	1.32715600	-1.19397700	0.91335500
C	0.04481300	0.59823500	2.50948800
F	-1.20297500	0.98721700	2.80049000
F	0.66525100	0.16684500	3.61374400
F	0.72660800	1.60565000	1.95745100

IPrAuNTf₂

C	0.03360800	-1.81639700	0.01253800
C	-0.56381400	-4.00285800	-0.13393200
C	0.78083400	-3.95866300	0.12284900

H	-1.24550200	-4.83714300	-0.27592700
H	1.51829600	-4.74656200	0.25048400
N	1.12575700	-2.61293700	0.20781900
N	-1.00142600	-2.68300300	-0.19613700
Au	-0.02287400	0.15520300	0.01681400
C	-2.35196000	-2.24265300	-0.45482500
C	-3.23561600	-2.11354200	0.64000500
C	-2.70444100	-1.91369900	-1.78247200
C	-4.52468200	-1.62157200	0.36780300
C	-4.00761600	-1.42948300	-1.99776000
C	-4.90629600	-1.28130600	-0.93558100
H	-5.23483800	-1.49374700	1.19050900
H	-4.31502200	-1.15639100	-3.01231900
H	-5.91307300	-0.89436500	-1.12408100
C	2.44452000	-2.08122400	0.45696600
C	2.78024200	-1.71656900	1.77988500
C	3.31085000	-1.89831000	-0.64338600
C	4.04844800	-1.14343700	1.98435100
C	4.56653000	-1.32110300	-0.38164000
C	4.93137100	-0.94563400	0.91656800
H	4.34077900	-0.84062100	2.99501300
H	5.25930500	-1.15111300	-1.21168500
H	5.91026800	-0.48937400	1.09665300
C	-1.72757600	-2.03755100	-2.94514400
H	-0.79863000	-2.49964900	-2.56742200
C	-2.28036200	-2.95254800	-4.05251800
H	-1.53239200	-3.07383900	-4.85576000
H	-2.52950800	-3.95471400	-3.66200400
H	-3.19306100	-2.53058500	-4.50921800
C	-1.36290800	-0.64742100	-3.49935900
H	-2.25186900	-0.13669900	-3.91042700
H	-0.93555100	-0.00229900	-2.71112500
H	-0.61715500	-0.73675700	-4.30901500
C	2.90397400	-2.24781700	-2.06950500
C	3.92356100	-3.18392500	-2.74186900
H	4.06255700	-4.11328400	-2.16212000
H	3.57689000	-3.46010600	-3.75324600
H	4.91066800	-2.70094600	-2.84995100
C	1.82447600	-1.91050000	2.95053100
H	0.89928200	-2.37456700	2.56662300
C	-2.80630600	-2.42871900	2.06775400
C	-3.82808700	-3.31153600	2.80441200
H	-4.79148800	-2.79206600	2.94861700
H	-4.02611900	-4.24767800	2.25370200
H	-3.44486700	-3.57753100	3.80511800
C	1.43637300	-0.55911600	3.57852500
H	0.97383100	0.11094000	2.83267800
H	0.71193700	-0.71000300	4.39812300
H	2.31823300	-0.04357000	3.99860700
C	2.42037900	-2.86555200	4.00126200
H	1.69716800	-3.03461400	4.81851700
H	2.67335100	-3.84515800	3.55931600
H	3.34044800	-2.44954600	4.44861100
C	2.68800000	-0.96752000	-2.89850000
H	1.92415500	-0.31433200	-2.44448000
H	3.62224200	-0.38332100	-2.97882800
H	2.36033400	-1.22451100	-3.92171100
H	1.93975600	-2.78436500	-2.03251700
C	-2.53192000	-1.12358700	2.84020200
H	-2.18780200	-1.34667900	3.86601900
H	-1.75950900	-0.51610700	2.33914100
H	-3.44517300	-0.50623100	2.91298500
H	-1.85766300	-2.99253100	2.02373500

N	-0.06377700	2.24255600	0.00783300
S	-1.01407500	3.04188400	1.13698500
S	0.86538100	3.06015600	-1.12698100
O	0.43196100	4.45150200	-1.34672900
O	1.07717200	2.14005700	-2.26341900
C	2.51928600	3.14564500	-0.22553400
F	2.35824500	3.75213600	0.96109300
F	2.99959200	1.90382400	-0.03056800
F	3.38695300	3.84484500	-0.97682000
O	-1.19553800	2.12659900	2.28232900
O	-0.62238900	4.44782600	1.34204800
C	-2.66949000	3.06722400	0.23476600
F	-3.56008100	3.74339300	0.98020200
F	-2.52721700	3.66959900	-0.95637900
F	-3.10924800	1.80900700	0.04780600

Int1_NTf2

N	-1.79603200	0.34248300	-2.23224400
C	-2.08975800	1.66853800	-2.42677300
C	2.51097000	0.73563700	0.49649200
C	3.29522600	2.35620000	1.87904300
C	4.19720200	1.32879100	1.90063900
H	3.28753000	3.32134400	2.37728800
H	5.13711900	1.20066000	2.43076400
N	3.70107700	0.35008200	1.04611800
N	2.26710900	1.97312300	1.02048300
Au	1.44014900	-0.38353000	-0.80766600
C	1.15736800	2.83066600	0.67075300
C	1.20985300	3.52121500	-0.56245100
C	0.10287300	2.98209400	1.60188800
C	0.14309200	4.39082700	-0.85506200
C	-0.91856200	3.88838800	1.26835600
C	-0.90085800	4.58384300	0.05458700
H	0.13674400	4.92604500	-1.80946800
H	-1.75085000	4.03745500	1.96188100
H	-1.71875500	5.26711400	-0.19085100
C	4.38504700	-0.87686700	0.71081500
C	5.28332500	-0.85472100	-0.38074500
C	4.11599000	-2.03422200	1.47360400
C	5.94079700	-2.05770300	-0.69412900
C	4.80443600	-3.20902100	1.11801100
C	5.70589900	-3.22165700	0.04771100
H	6.64183200	-2.08076000	-1.53460300
H	4.62297400	-4.12651400	1.68683000
H	6.22901800	-4.14764200	-0.21245300
C	0.06038600	2.22227900	2.92307500
H	0.76685100	1.37617300	2.85274300
C	0.51262100	3.12687500	4.08611400
H	0.49739600	2.56699100	5.03811900
H	1.53450300	3.51468400	3.93473300
H	-0.16449200	3.99385500	4.18933700
C	-1.33149000	1.63144500	3.21069300
H	-2.06999500	2.41950200	3.44277100
H	-1.69606700	1.04645800	2.35482700
H	-1.28002700	0.95876400	4.08469400
C	3.11991400	-2.04407100	2.62522400
C	3.81423500	-2.36895200	3.96024700
H	4.61355000	-1.64217500	4.18833000
H	3.08164700	-2.34436700	4.78580700
H	4.26682200	-3.37627400	3.94178500
C	5.52533300	0.39619100	-1.21592000
H	4.97232800	1.23350300	-0.75582400
C	2.36262100	3.37658400	-1.54941900

C	3.03424600	4.73369600	-1.82989400
H	2.34358600	5.43161500	-2.33450000
H	3.37985800	5.21349000	-0.89766800
H	3.90901500	4.59330200	-2.48920700
C	4.97707400	0.21248300	-2.64363400
H	3.89819800	-0.02312400	-2.62740200
H	5.12123200	1.13673400	-3.23069900
H	5.49659500	-0.60851200	-3.16917800
C	7.01398700	0.78580700	-1.23691300
H	7.15367500	1.72304800	-1.80363200
H	7.40477100	0.94099100	-0.21617900
H	7.63004600	0.00776600	-1.72109700
C	1.96603000	-3.02268700	2.34252400
H	1.45242000	-2.77817900	1.39845200
H	2.32765400	-4.06432900	2.27643300
H	1.21573400	-2.97632500	3.15015800
H	2.68275000	-1.03457900	2.71289200
C	1.89119200	2.70962700	-2.85441600
H	2.72314800	2.64640100	-3.57810300
H	1.52572500	1.68606600	-2.65721600
H	1.06463900	3.26911900	-3.32373500
H	3.12822000	2.71959500	-1.10097800
C	-3.05488900	2.27628600	-1.46218800
C	-3.38786100	1.69596800	-0.22559000
C	-3.62560100	3.52220300	-1.79930700
C	-4.26709100	2.33120000	0.65905700
H	-2.94289700	0.74789100	0.08462000
C	-4.50556500	4.16495600	-0.93319500
H	-3.35597100	3.97586600	-2.75736900
C	-4.82884100	3.57503100	0.30956900
H	-4.50136700	1.85625300	1.61347700
H	-4.95637500	5.12825400	-1.19070500
O	-5.68438500	4.28527200	1.09874100
C	-6.02968400	3.72028500	2.36788400
H	-5.13754500	3.58726600	3.00808100
H	-6.71253700	4.44263000	2.83840300
H	-6.54604100	2.74964400	2.25176000
O	-1.58405100	2.32681700	-3.35782700
C	-0.89245000	-0.34609200	-3.12847000
C	0.07427800	-1.18491300	-2.40037900
C	0.73432900	-2.11512100	-1.89215200
H	1.11438700	-3.09451500	-1.63230900
H	-2.29832700	-0.24345300	-1.55217200
H	-1.44063300	-1.02353700	-3.81401400
H	-0.38954200	0.42454800	-3.73812700
N	-2.64546600	-1.90662000	-0.39535800
S	-2.91019000	-3.14360300	-1.44174100
S	-1.82291700	-2.09506100	1.01013000
O	-0.92777900	-0.92176900	1.17946000
O	-1.31313800	-3.45237600	1.31829600
C	-3.17698400	-1.78306800	2.28285400
F	-3.78145100	-0.59540700	2.06152900
F	-4.10551800	-2.75502100	2.24440300
F	-2.61426000	-1.75786300	3.50822800
O	-3.43017300	-2.50971800	-2.67708100
O	-1.83145500	-4.15510900	-1.53741700
C	-4.38107100	-4.07706100	-0.72836800
F	-4.83709000	-4.94893600	-1.64894400
F	-4.01131100	-4.75622100	0.37314900
F	-5.36618100	-3.21786800	-0.40815300

TS1_5exo_NTf2

N	-2.42402600	-0.92933700	-1.68925200
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C	-2.87175600	-2.22084500	-1.76326800
C	3.34266700	0.43858500	-0.13758800
C	4.39621500	2.45306700	-0.13859600
C	5.29887100	1.51496900	0.28526700
H	4.48503900	3.52612200	-0.28441400
H	6.33814800	1.59771800	0.59178800
N	4.63382100	0.29090600	0.27767800
N	3.20718100	1.77553500	-0.38978000
Au	1.95352200	-0.98862000	-0.46197200
C	1.93947500	2.35961400	-0.76040200
C	1.55195400	2.32756200	-2.11742100
C	1.11522700	2.85598100	0.27738900
C	0.25748900	2.78825100	-2.42352700
C	-0.16901100	3.29702200	-0.08479100
C	-0.59903800	3.24921300	-1.41710500
H	-0.08363300	2.77391900	-3.46378500
H	-0.84755400	3.66940000	0.68616300
H	-1.61326300	3.57174600	-1.66908300
C	5.17860300	-0.96831700	0.72526000
C	5.86458000	-1.77826400	-0.20653900
C	4.96217600	-1.33819400	2.07247800
C	6.34185400	-3.01877900	0.25413700
C	5.45907300	-2.59021800	2.47769700
C	6.13994000	-3.42084500	1.57986500
H	6.87113600	-3.68083400	-0.43803500
H	5.30578300	-2.91862000	3.51023800
H	6.51533200	-4.39273100	1.91648300
C	1.61499500	2.96663600	1.71362100
H	2.49841900	2.31224400	1.81892600
C	2.07498400	4.41351200	1.98592800
H	2.49291000	4.49993200	3.00461600
H	2.84885900	4.73841100	1.26842500
H	1.22608800	5.11594900	1.90601100
C	0.58985500	2.50818900	2.76111400
H	-0.31588400	3.13901300	2.76589600
H	0.27410600	1.46899100	2.58443900
H	1.03730600	2.57174000	3.76892400
C	4.19797600	-0.45021800	3.04753500
C	4.97675300	-0.22786900	4.35592100
H	5.98306700	0.18316100	4.16290400
H	4.43342400	0.48422500	5.00121300
H	5.09628900	-1.16578900	4.92643400
C	6.03666900	-1.36456800	-1.66273600
H	5.77434800	-0.29521100	-1.74712900
C	2.48460100	1.84770900	-3.22360500
C	2.85576400	3.01660000	-4.15619700
H	1.96332100	3.41495700	-4.67037100
H	3.32128700	3.84595600	-3.59573400
H	3.57004600	2.68118000	-4.92868800
C	5.06247700	-2.15363600	-2.55992000
H	4.01655200	-2.01339200	-2.23096300
H	5.14206900	-1.81667600	-3.60889600
H	5.28471600	-3.23528600	-2.52933100
C	7.48734900	-1.52158000	-2.14988000
H	7.58244400	-1.14129900	-3.18202700
H	8.19186500	-0.96017900	-1.51204300
H	7.80468400	-2.57910300	-2.15800300
C	2.79519100	-1.02455200	3.32573800
H	2.21262700	-1.12795100	2.39237200
H	2.86024500	-2.02010500	3.80008000
H	2.23344900	-0.35837500	4.00412000
H	4.06088500	0.53880200	2.57597800
C	1.88474000	0.67410700	-4.01795600

H	2.59143200	0.33725600	-4.79699800	C	4.96803200	-1.27089200	0.35323600
H	1.67539500	-0.18574200	-3.35754200	C	5.43255900	-1.60054400	-0.93917100
H	0.94424900	0.96121300	-4.52046700	C	4.87733000	-2.20538700	1.40889600
H	3.41638900	1.48570900	-2.75529900	C	5.82666100	-2.93274300	-1.15895800
C	-4.27617200	-2.49129100	-1.38357600	C	5.28258800	-3.52417300	1.13371700
C	-5.24275600	-1.47348800	-1.28253000	C	5.75204300	-3.88435500	-0.13505100
C	-4.63611900	-3.81347200	-1.03969800	H	6.18688700	-3.22722300	-2.14989500
C	-6.53520400	-1.75122000	-0.82742300	H	5.22240400	-4.27878400	1.92460800
H	-5.00031100	-0.44310100	-1.55494500	H	6.05893600	-4.91738400	-0.32850300
C	-5.91851200	-4.10371900	-0.58825600	C	1.88368700	2.17319000	3.33041500
H	-3.88061900	-4.60088500	-1.11464600	H	2.79863200	1.59745200	3.10715500
C	-6.87736200	-3.07109200	-0.46850700	C	2.24707300	3.21625700	4.40287300
H	-7.25807200	-0.93651200	-0.74722700	H	2.62037400	2.71647400	5.31419300
H	-6.20541400	-5.12051700	-0.30417900	H	3.03029200	3.90804600	4.04591300
O	-8.09672500	-3.45156600	-0.00016400	H	1.36919900	3.82172000	4.68962200
C	-9.08440000	-2.42822500	0.17531900	C	0.83086900	1.17776500	3.85408900
H	-9.34174900	-1.94678600	-0.78587100	H	-0.11032300	1.69103400	4.11818600
H	-9.97187400	-2.93927300	0.57585700	H	0.58959100	0.41355200	3.09701100
H	-8.74490700	-1.66090900	0.89439800	H	1.20619900	0.66889200	4.75998400
O	-2.07512900	-3.12350400	-2.12386100	C	4.32810600	-1.83274500	2.78042700
C	-1.01002400	-0.75046600	-1.97903500	C	5.30408000	-2.20216200	3.91114400
C	-0.19827000	-1.85088000	-1.42301600	H	6.28636100	-1.71886300	3.76939700
C	0.65056000	-2.59628800	-0.86032500	H	4.89890400	-1.87478700	4.88459800
H	0.87669300	-3.63274400	-0.62675600	H	5.46830400	-3.29241000	3.96903600
H	-2.84178300	-0.26753100	-1.00821900	C	5.47332100	-0.58341200	-2.07213500
H	-0.83599200	-0.70050600	-3.07024400	H	5.20598900	0.40429200	-1.65798200
H	-0.68825900	0.20761600	-1.54033700	C	2.27713400	2.99324100	-1.74540600
N	-3.12369500	0.75391500	0.58826800	C	2.66216000	4.33125700	-2.40196300
S	-2.30988000	0.07177300	1.85013500	H	1.76874400	4.93036700	-2.65032200
S	-4.52461400	1.58451300	0.82534300	H	3.30153900	4.93791300	-1.73713900
O	-5.31874500	1.20424000	2.01605400	H	3.21545400	4.15093400	-3.34052200
O	-5.18205500	1.69325400	-0.49976700	C	4.42520300	-0.92886800	-3.14699300
C	-3.94294600	3.34496900	1.17549600	H	3.41325000	-0.98553300	-2.70693700
F	-3.02070800	3.37108600	2.15615200	H	4.41624300	-0.15740200	-3.93727400
F	-3.40778700	3.88936000	0.06088000	H	4.64257400	-1.90225600	-3.62179200
F	-5.00273000	4.08623200	1.55009200	C	6.88118800	-0.46260300	-2.68186900
O	-0.94304800	-0.21633400	1.35069800	H	6.89008900	0.31379800	-3.46683800
O	-2.49659200	0.72216400	3.16660000	H	7.62894700	-0.18668200	-1.91800100
C	-3.08538800	-1.64990700	2.05142200	H	7.20550800	-1.41025600	-3.14656300
F	-2.52246600	-2.51169500	1.18039900	C	2.94610300	-2.47820600	2.99964300
F	-2.84031800	-2.08141700	3.30314700	H	2.23929600	-2.17873000	2.20470000
F	-4.41179000	-1.61610300	1.84747700	H	3.01575400	-3.58071400	2.99748100

TS1_gendo_NTf2

N	-2.16367800	-1.54666700	-1.99569800	H	4.18919200	-0.73826400	2.80864800
C	-2.47970300	-2.79977300	-1.54512500	C	1.40008200	2.14330300	-2.68354200
C	3.22114200	0.47879400	0.44347300	H	1.90147900	1.99442300	-3.65660800
C	4.50540000	2.22777900	1.12010600	H	1.21167900	1.15033100	-2.23558700
C	5.32430000	1.13568800	1.01308900	H	0.42145600	2.62025900	-2.86662200
H	4.70622400	3.25567500	1.41030400	H	3.21041300	2.43063000	-1.56646300
H	6.38850800	1.00920300	1.19376400	C	-3.88877200	-3.01103500	-1.12022000
N	4.52089000	0.08016600	0.59535900	C	-4.93792000	-2.14943500	-1.49383500
N	3.22671100	1.80675100	0.76856900	C	-4.17733800	-4.11110700	-0.28278700
Au	1.70270100	-0.65004700	-0.26907400	C	-6.24073300	-2.35813800	-1.02895800
C	2.04935100	2.64496900	0.80082700	H	-4.75671400	-1.30407100	-2.16494600
C	1.58166200	3.20953700	-0.40688500	C	-5.46764800	-4.32910600	0.18763000
C	1.40781300	2.83912300	2.04512800	H	-3.36166000	-4.78292700	-0.00015200
C	0.41446600	3.99209700	-0.33993100	C	-6.51151900	-3.44807800	-0.17691300
C	0.25994200	3.64922200	2.05616800	H	-7.03210500	-1.67110900	-1.33644000
C	-0.23686700	4.21412100	0.87752600	H	-5.69886600	-5.17176200	0.84618700
H	0.00198200	4.41950400	-1.25901400	O	-7.73652900	-3.73928800	0.34039300
H	-0.27383400	3.80945400	2.99813000	C	-8.82281300	-2.86985800	-0.00120900
H	-1.15277900	4.81077100	0.90535000	H	-9.01452600	-2.87189100	-1.08986500
				H	-9.70088200	-3.27211500	0.52467000

H	-8.63296000	-1.83552100	0.33871400
O	-1.62633300	-3.72520400	-1.47964800
C	-0.80340100	-1.17063000	-2.32565100
C	0.15001200	-1.63034700	-1.25183000
C	0.24712300	-2.69079100	-0.57178600
H	0.48810500	-3.50388500	0.09645800
H	-2.72387000	-0.74914000	-1.64188800
H	-0.48455300	-1.64938700	-3.26934400
H	-0.77924800	-0.08127500	-2.45955900
N	-2.98975900	0.92416500	-0.80620200
S	-2.52950700	1.10566800	0.76172700
S	-4.19788700	1.79162100	-1.49047400
O	-5.23790800	2.32895900	-0.58414800
O	-4.59808700	1.05328900	-2.71417300
C	-3.27473500	3.29404900	-2.14763600
F	-2.78303900	4.03142700	-1.13320200
F	-2.25215800	2.90208600	-2.93804400
F	-4.11807700	4.05319500	-2.87368000
O	-1.11147700	0.68546900	0.84269900
O	-2.98452200	2.34361100	1.43350100
C	-3.46264700	-0.28748600	1.62094700
F	-2.90433100	-1.47492800	1.31012300
F	-3.38324400	-0.10711600	2.95429200
F	-4.75609200	-0.29313400	1.25176900

Int2_5exo_NTf2

N	2.45198600	1.10110200	-0.45309500
C	2.59091400	2.41512500	-0.44055700
C	-3.68140300	-0.55399300	-0.00087000
C	-4.48343200	-2.69184000	-0.01213600
C	-5.51525100	-1.86765100	0.34638400
H	-4.43290800	-3.76971400	-0.14253500
H	-6.55215100	-2.07457200	0.59825700
N	-5.00489200	-0.57121100	0.34693600
N	-3.37520500	-1.87362300	-0.21469200
Au	-2.36942500	0.99308800	-0.15682600
C	-2.06830600	-2.31859400	-0.63998600
C	-1.75418100	-2.24284700	-2.01551400
C	-1.15435400	-2.77140000	0.34110200
C	-0.45876900	-2.63484200	-2.40164200
C	0.12851200	-3.14436900	-0.09977900
C	0.47240200	-3.07615400	-1.45586200
H	-0.17856200	-2.58855000	-3.45914300
H	0.87652300	-3.48011600	0.62380300
H	1.47600700	-3.36825600	-1.77337200
C	-5.76618500	0.61704000	0.64415200
C	-6.45360900	1.25013000	-0.41588200
C	-5.76872200	1.10435400	1.96971600
C	-7.16906400	2.42159900	-0.10967900
C	-6.50243500	2.27828700	2.22128400
C	-7.19421200	2.93025700	1.19437400
H	-7.70667500	2.94596800	-0.90596400
H	-6.52310200	2.68890700	3.23581400
H	-7.75566800	3.84503300	1.41104200
C	-1.51744800	-2.79558600	1.82127000
H	-2.61846600	-2.84374000	1.89828800
C	-0.95070300	-4.02037200	2.55753200
H	-1.32905700	-4.04089100	3.59447200
H	-1.24417200	-4.96481900	2.06698600
H	0.15130100	-3.99091900	2.61277400
C	-1.05861500	-1.49034100	2.50383300
H	0.04269300	-1.41435100	2.49814300
H	-1.46632700	-0.60385500	1.98514400

H	-1.39952700	-1.46543600	3.55457000
C	-4.99073100	0.42622300	3.08968900
C	-5.89789000	0.06643200	4.27942400
H	-6.73692100	-0.57939300	3.96664900
H	-5.31841800	-0.47318000	5.04907900
H	-6.32282600	0.96812800	4.75488800
C	-6.38965800	0.72819200	-1.84593400
H	-5.94444200	-0.28198900	-1.82320400
C	-2.74594900	-1.74786800	-3.06075100
C	-3.04494300	-2.83528700	-4.10895800
H	-2.13921800	-3.10688800	-4.67968600
H	-3.43435200	-3.75427200	-3.63719800
H	-3.79920300	-2.47412800	-4.83043500
C	-5.46446200	1.62054900	-2.69602500
H	-4.45005800	1.66743400	-2.26138500
H	-5.38388500	1.22575300	-3.72453600
H	-5.85638800	2.65169700	-2.75624100
C	-7.78440100	0.60077200	-2.48231400
H	-7.70245300	0.15601900	-3.48957300
H	-8.44690800	-0.04198800	-1.87677200
H	-8.27549200	1.58335900	-2.59425200
C	-3.80945100	1.30951300	3.53499200
H	-3.14061500	1.53488600	2.68482500
H	-4.16553700	2.26833000	3.95223600
H	-3.21766200	0.79817400	4.31464200
H	-4.57206400	-0.51594600	2.69648400
C	-2.24143200	-0.45334000	-3.72451000
H	-2.98810800	-0.07016900	-4.44236400
H	-2.05726300	0.32855600	-2.96539400
H	-1.29972800	-0.62395200	-4.27641000
H	-3.69507400	-1.50824900	-2.55139000
C	3.81838700	3.17616300	-0.40047600
C	5.07451400	2.53043900	-0.44171400
C	3.76517600	4.59071300	-0.31333700
C	6.25321700	3.27104300	-0.39454900
H	5.14915700	1.44227600	-0.52191800
C	4.93628200	5.33194700	-0.26529000
H	2.79655100	5.09596400	-0.28050600
C	6.19280300	4.67983700	-0.30124200
H	7.21025500	2.74704500	-0.43474600
H	4.91282100	6.42282700	-0.19501400
O	7.27280200	5.49204000	-0.24282400
C	8.57455600	4.88400200	-0.25771900
H	8.74337500	4.32622000	-1.19569200
H	9.28777600	5.71779600	-0.19325300
H	8.71067900	4.21263400	0.60846400
O	1.42026200	3.05615100	-0.46752900
C	1.03889000	0.71902900	-0.47891100
C	0.35373400	2.06876400	-0.41456400
C	-0.93168800	2.42584100	-0.30592300
H	-1.12998900	3.50772200	-0.28160500
H	3.21552600	0.39936800	-0.29720700
H	0.80929500	0.15787700	-1.40319200
H	0.80879300	0.07146200	0.38224900
N	4.29878700	-0.94086700	0.22566800
S	3.64109300	-1.77921100	1.48292000
S	5.43546700	-1.58858700	-0.77412700
O	6.29164400	-2.63780000	-0.17985900
O	6.04679400	-0.44660300	-1.49560100
C	4.40813400	-2.45873200	-2.08914000
F	3.85786000	-3.58220800	-1.59209400
F	3.42584400	-1.64040000	-2.52126300
F	5.20206900	-2.77954300	-3.12688900

O	2.42457400	-1.02771200	1.87656700
O	3.57809900	-3.24994100	1.32086000
C	4.84920600	-1.46298000	2.89166000
F	5.00885200	-0.13707900	3.05715100
F	4.33878600	-1.99154700	4.02071100
F	6.04036200	-2.02524600	2.63640100

H	-6.71748200	-1.14165000	-3.91546500
H	-7.73840200	-0.56940900	-2.56497400
H	-7.26049800	0.55352300	-3.86715700
C	-3.98206900	2.83909000	2.54973100
H	-3.16342200	2.57594800	1.85617100
H	-4.21509000	3.91015800	2.41186600
H	-3.61762300	2.69975700	3.58296000
H	-4.93146100	0.91561100	2.46401200
C	-1.73795400	-2.48036600	-2.49405100
H	-2.28454800	-2.61536300	-3.44453100
H	-1.72414100	-1.40213700	-2.25195600
H	-0.69392600	-2.80501900	-2.64997900
H	-3.43313000	-2.88425700	-1.23819100
C	3.78238100	2.99327500	-0.84275300
C	4.91800900	2.20801400	-1.14363900
C	3.96302200	4.32714100	-0.39980600
C	6.20303400	2.72538600	-0.98687400
H	4.80850300	1.19018400	-1.53000500
C	5.23961500	4.84855000	-0.24397100
H	3.08943000	4.94062200	-0.16558900
C	6.37310600	4.05111700	-0.53025400
H	7.06323800	2.09952300	-1.23221200
H	5.39382400	5.87308400	0.10570300
O	7.57260200	4.65058600	-0.34107400
C	8.75617700	3.88827500	-0.62407800
H	8.79639600	3.59480200	-1.68812100
H	9.59751800	4.55758300	-0.39536500
H	8.81613800	2.98885400	0.01414000
O	1.44179300	3.33058900	-1.02691400
C	0.85603500	0.58285300	-1.22636800
C	-0.23227000	1.55441200	-0.81811300
C	0.10905500	2.84948800	-0.76489000
H	-0.51320400	3.70943500	-0.51593200
H	2.94642300	0.46253600	-0.76701100
H	0.76028100	0.29793700	-2.29268200
H	0.81482100	-0.34792300	-0.64067200
N	3.80119900	-1.00256500	-0.26848900
S	3.76509200	-1.36100800	1.33624800
S	4.44772000	-1.97894100	-1.41608000
O	5.50840200	-2.90602400	-0.96466900
O	4.66224000	-1.11893100	-2.60525900
C	2.99827700	-3.07997500	-1.90248200
F	2.70565600	-3.94255900	-0.91162400
F	1.90895100	-2.32482300	-2.16522600
F	3.32204400	-3.77481400	-3.00846700
O	2.71559100	-0.50212600	1.93060000
O	3.83516600	-2.80111200	1.67624000
C	5.38780500	-0.61891900	1.93372100
F	5.39090800	0.70891200	1.70623600
F	5.51272900	-0.83909200	3.25654500
F	6.42732200	-1.17860900	1.29086800

Int2_gendo_NTf2

N	2.19277000	1.15502300	-1.00216200
C	2.43835600	2.44701700	-0.96910400
C	-3.58604900	-0.41593600	0.33446700
C	-4.70736500	-2.21988800	1.16606900
C	-5.63704000	-1.26357200	0.85571900
H	-4.80947500	-3.21836300	1.58313900
H	-6.72013000	-1.25283600	0.94560500
N	-4.93123900	-0.17316400	0.35048500
N	-3.46599000	-1.68397800	0.83965800
Au	-1.99647000	0.69691100	-0.27339900
C	-2.18257600	-2.32406900	1.01450700
C	-1.65802500	-3.08587000	-0.05372800
C	-1.47630800	-2.08948600	2.21576700
C	-0.36507700	-3.61617600	0.10766200
C	-0.18744400	-2.64181300	2.32268300
C	0.36713500	-3.39065900	1.27902200
H	0.08583500	-4.18982500	-0.70707200
H	0.40258300	-2.45863700	3.22601000
H	1.38645800	-3.77554500	1.37195400
C	-5.51957200	1.06624200	-0.09375000
C	-5.87901900	1.19013600	-1.45434200
C	-5.68228300	2.10522500	0.84932100
C	-6.42963200	2.41807000	-1.86441600
C	-6.24057100	3.31079700	0.38697200
C	-6.61210700	3.46545100	-0.95368300
H	-6.71111500	2.55625100	-2.91322700
H	-6.37594200	4.14112300	1.08736800
H	-7.04032600	4.41402000	-1.29391100
C	-2.04026200	-1.23754900	3.34564200
H	-3.07368100	-0.95222400	3.08164600
C	-2.10246200	-2.02309100	4.66779100
H	-2.56069300	-1.40398500	5.45922500
H	-2.70268600	-2.94368500	4.56230200
H	-1.09461500	-2.31409500	5.01219400
C	-1.22572500	0.06050000	3.50439000
H	-0.17578600	-0.15673800	3.76892000
H	-1.22159300	0.63926000	2.56348700
H	-1.65726200	0.69252600	4.30109400
C	-5.22602200	1.96602500	2.29597500
C	-6.35124100	2.29390100	3.29258400
H	-7.23897800	1.66021900	3.12182100
H	-6.00324700	2.12448600	4.32672900
H	-6.66878000	3.34896300	3.21811600
C	-5.63869600	0.07143200	-2.45977800
H	-5.32820000	-0.82919900	-1.90221400
C	-2.41104400	-3.28311100	-1.36379600
C	-2.53705200	-4.77119900	-1.73502000
H	-1.54911600	-5.22924000	-1.91728700
H	-3.03389000	-5.34622900	-0.93426400
H	-3.13146000	-4.88419000	-2.65870800
C	-4.48603200	0.44752500	-3.41099300
H	-3.56614000	0.68158700	-2.84549000
H	-4.26611700	-0.38632100	-4.10112600
H	-4.74587600	1.33289900	-4.01853300
C	-6.91355500	-0.28838200	-3.24266300

Int2_Sexo

N	-3.91866100	1.21278700	-2.26059800
C	-3.63117300	0.15538600	-1.57257700
C	2.21193300	-1.56511300	0.13864300
C	4.08720600	-2.70983700	0.77720300

C	3.01991600	-3.28899500	1.40632500
H	5.14989200	-2.93697300	0.79924700
H	2.95340200	-4.12810100	2.09402500
N	1.89066100	-2.57761800	1.00610000
N	3.57399100	-1.66664000	0.01033400
Au	0.97500000	-0.22641900	-0.77085200
C	4.36395500	-0.76455800	-0.78942800
C	4.62954400	-1.10805000	-2.13366000
C	4.81463200	0.43453600	-0.19378500
C	5.38061400	-0.19424500	-2.89488100
C	5.56485700	1.31134100	-0.99816400
C	5.84447800	1.00173800	-2.33413900
H	5.59706600	-0.42087200	-3.94370300
H	5.92507200	2.25312800	-0.57112300
H	6.42483300	1.70068300	-2.94549500
C	0.55454500	-2.84864200	1.47511700
C	-0.25001100	-3.74774000	0.74139700
C	0.11472500	-2.20439600	2.65366400
C	-1.53883200	-4.01374000	1.23908500
C	-1.18576900	-2.49709300	3.10189300
C	-2.00190900	-3.39791200	2.40786400
H	-2.18918700	-4.70574400	0.69386000
H	-1.56412700	-2.00775900	4.00490700
H	-3.01103900	-3.61225800	2.77496600
C	4.49083400	0.79673100	1.25011300
H	3.92446700	-0.03923900	1.69533800
C	5.77054400	0.98590100	2.08442000
H	5.51314400	1.21577800	3.13347100
H	6.39463100	0.07491400	2.07728800
H	6.38568900	1.81909000	1.70051200
C	3.58826100	2.04244200	1.31191100
H	4.10006900	2.93086700	0.90054800
H	2.66033800	1.88294900	0.73465000
H	3.31204700	2.26516600	2.35799700
C	0.98031800	-1.19380000	3.39548100
C	1.09418400	-1.51378100	4.89601900
H	1.48170700	-2.53372900	5.06478000
H	1.78287200	-0.80152400	5.38348400
H	0.11880700	-1.43278100	5.40771100
C	0.21905300	-4.38324800	-0.56050700
H	1.27469000	-4.10276900	-0.71833900
C	4.09175200	-2.38746800	-2.76217200
C	5.19489100	-3.19452800	-3.46814700
H	5.61355900	-2.64774200	-4.33129800
H	6.02596600	-3.43022700	-2.78062500
H	4.78403600	-4.14649300	-3.84807200
C	-0.58821600	-3.82463900	-1.74814800
H	-0.52087100	-2.72325800	-1.78868700
H	-0.20230300	-4.23005300	-2.70065300
H	-1.65623100	-4.09677500	-1.67051900
C	0.15065000	-5.91946700	-0.50589100
H	0.54253600	-6.35253500	-1.44317200
H	0.74739000	-6.32040600	0.33223100
H	-0.88737500	-6.27619100	-0.38365800
C	0.44656300	0.23331500	3.16582300
H	0.40541600	0.46990900	2.08776600
H	-0.57216300	0.34730700	3.57813800
H	1.10000000	0.97461000	3.65998200
H	1.99813600	-1.23715300	2.97007100
C	2.93091700	-2.06621200	-3.72334500
H	2.50639400	-2.99731200	-4.14016100
H	2.12371400	-1.52150400	-3.20120300
H	3.27534200	-1.43975400	-4.56560100

H	3.68565300	-3.02049200	-1.95420800
C	-4.56938800	-0.86831000	-1.10493100
C	-5.93383600	-0.77797400	-1.44230000
C	-4.13067500	-1.95840400	-0.32054000
C	-6.84792500	-1.74614400	-1.01759300
H	-6.27354700	0.06638000	-2.04934200
C	-5.03374200	-2.92821800	0.10807300
H	-3.07658600	-2.04045500	-0.04377300
C	-6.39909300	-2.83277600	-0.23706600
H	-7.89975200	-1.65192400	-1.29651200
H	-4.70439400	-3.77555600	0.71700900
O	-7.19888500	-3.83393400	0.22907300
C	-8.59089300	-3.77381100	-0.09870500
H	-8.75126200	-3.81090700	-1.19202600
H	-9.04424800	-4.66137700	0.36638600
H	-9.06483200	-2.86323100	0.31189400
O	-2.30913400	-0.05024200	-1.24128800
C	-2.63815600	1.90295100	-2.47718900
C	-1.58306700	1.02870300	-1.80928700
C	-0.24400700	1.10632000	-1.69954700
H	0.17553800	1.99632200	-2.19656200
H	-2.45131800	2.03338000	-3.56055900
H	-2.67710800	2.92079600	-2.04180400

Int2_6endo

N	2.94951000	-2.73678200	0.61903700
C	3.86568200	-2.48958000	-0.24715400
C	-1.03904700	2.25258400	0.33956800
C	-2.07398800	4.25190500	0.73640700
C	-3.05216400	3.30865000	0.58201100
H	-2.12346000	5.31885300	0.93748600
H	-4.13613600	3.37901300	0.61787900
N	-2.40134700	2.10012700	0.34412300
N	-0.85858200	3.58868700	0.58451500
Au	0.38492600	0.81926900	0.05288400
C	0.43404600	4.22527400	0.64286400
C	1.09980800	4.29186400	1.88667600
C	0.97261700	4.75165000	-0.55275200
C	2.36009100	4.91675000	1.90932300
C	2.23559700	5.36543600	-0.47440400
C	2.92175300	5.44882100	0.74299400
H	2.90948500	4.97928500	2.85414800
H	2.68865200	5.77624400	-1.38225100
H	3.90526700	5.92848100	0.78188300
C	-3.06869900	0.84758100	0.08784900
C	-3.43293100	0.03939900	1.18843900
C	-3.32239900	0.48774400	-1.25441900
C	-4.08085500	-1.17685300	0.90685800
C	-3.97347200	-0.73884000	-1.47976300
C	-4.35070700	-1.56116100	-0.41219600
H	-4.36957500	-1.83528800	1.73206200
H	-4.18043000	-1.05388800	-2.50766400
H	-4.85487100	-2.51299200	-0.60935400
C	0.25121500	4.62723100	-1.88889300
H	-0.76777400	4.24935200	-1.69450900
C	0.10934300	5.98420300	-2.60039900
H	-0.47066900	5.86508300	-3.53252000
H	-0.41182600	6.72113700	-1.96462100
H	1.09185300	6.40791000	-2.87358100
C	0.96165300	3.59509000	-2.78559300
H	1.99385400	3.91402700	-3.01713200
H	1.01289300	2.61054800	-2.28723100
H	0.42035600	3.47403100	-3.74082700

C	-2.88985000	1.35734600	-2.42822600	Au	0.94993400	-0.21648400	-0.83741600
C	-4.08279700	1.75106600	-3.31697300	C	4.28761100	-0.60614900	-0.78671700
H	-4.85765200	2.28503600	-2.73931900	C	4.69508300	-1.11621100	-2.04022000
H	-3.74759300	2.41462200	-4.13356600	C	4.56144100	0.71473100	-0.35847700
H	-4.55535800	0.86630400	-3.77900500	C	5.43497200	-0.25874100	-2.87491500
C	-3.08689400	0.42766800	2.62051200	C	5.30612500	1.52668700	-1.23286000
H	-2.79457300	1.49231500	2.62400700	C	5.74311600	1.04534000	-2.47292500
C	0.51415000	3.68368100	3.15449900	H	5.76320700	-0.61456600	-3.85614200
C	0.40947900	4.71500200	4.29155500	H	5.54071800	2.55431600	-0.94146100
H	1.40310400	5.08529600	4.59987000	H	6.31936800	1.69808600	-3.13698100
H	-0.19819100	5.58683800	3.99213700	C	0.54858800	-2.82426900	1.49329800
H	-0.06413900	4.25715500	5.17790400	C	-0.23399000	-3.61300200	0.61957600
C	-1.87080300	-0.38517300	3.10782600	C	0.08861500	-2.38749800	2.76021800
H	-1.00209600	-0.23284800	2.44205300	C	-1.51808800	-3.98650900	1.05965600
H	-1.58259900	-0.07839300	4.12937800	C	-1.20070700	-2.79285000	3.14882800
H	-2.09939500	-1.46585600	3.12556400	C	-1.99379800	-3.58818900	2.31279600
C	-4.27996500	0.27542500	3.57862600	H	-2.15124100	-4.59610600	0.40708500
H	-4.00658100	0.64477800	4.58256600	H	-1.59407600	-2.47381300	4.11829000
H	-5.15594800	0.84912700	3.22906900	H	-2.99267300	-3.89535800	2.64053400
H	-4.58711700	-0.77933100	3.68927600	C	4.08998100	1.23003700	0.99699300
C	-1.78979500	0.65111800	-3.24199600	H	3.15476000	0.70108300	1.24779700
H	-0.92811900	0.39981500	-2.59801000	C	5.12579900	0.89674400	2.08970700
H	-2.16460700	-0.28534500	-3.69230400	H	4.76613100	1.23818100	3.07662000
H	-1.43475400	1.30260500	-4.06021100	H	5.31487800	-0.18903600	2.15414700
H	-2.45488300	2.28824700	-2.02513900	H	6.08933000	1.39773200	1.88474600
C	1.33339300	2.45274500	3.58686900	C	3.75705300	2.72996300	0.99422200
H	0.87488600	1.97366700	4.47050800	H	4.66056300	3.35737900	0.89063000
H	1.38130400	1.70634300	2.77422200	H	3.06110200	2.98876800	0.17952500
H	2.36836500	2.73433700	3.85108900	H	3.27427200	3.00083900	1.94801200
H	-0.50915600	3.33810200	2.92677900	C	0.94505100	-1.52726200	3.68364600
C	5.11194800	-3.28647100	-0.31382700	C	1.75255000	-2.40181100	4.66596600
C	5.32444500	-4.32444700	0.61371000	H	2.41722900	-3.11281100	4.14938900
C	6.10512300	-3.04169700	-1.28813200	H	2.37850000	-1.76585200	5.31683900
C	6.48656200	-5.10036000	0.58584400	H	1.07205500	-2.98541000	5.31191300
H	4.55422400	-4.51387700	1.36680300	C	0.26023500	-4.06819200	-0.74788600
C	7.26613400	-3.81278000	-1.33184000	H	1.26821700	-3.65018200	-0.90835000
H	5.96087000	-2.23872300	-2.01528400	C	4.27534100	-2.50300200	-2.51611700
C	7.46854700	-4.84811600	-0.39494700	C	5.39224300	-3.25208900	-3.26016100
H	6.62022700	-5.89464200	1.32380100	H	5.64835800	-2.76512200	-4.21731900
H	8.03779000	-3.62958100	-2.08577200	H	6.31352900	-3.31904000	-2.65546500
O	8.63652600	-5.54342400	-0.52032800	H	5.06308000	-4.27935300	-3.49526600
C	8.88349500	-6.59264200	0.42028600	C	-0.64331900	-3.52941800	-1.87167500
H	8.11434500	-7.38478900	0.35758900	H	-0.69502600	-2.42689500	-1.83900600
H	9.86174800	-7.01331100	0.14474000	H	-0.24639200	-3.82725500	-2.85826600
H	8.92955500	-6.20664800	1.45549300	H	-1.67279200	-3.92143100	-1.78896800
O	3.84466900	-1.48907900	-1.20016700	C	0.38078300	-5.60201800	-0.80995300
C	1.71776100	-1.93602800	0.60147800	H	0.78007100	-5.91532800	-1.79095500
C	1.79309700	-0.63680900	-0.18721100	H	1.05867900	-5.98429600	-0.02665500
C	2.83547200	-0.51561800	-1.03140400	H	-0.60107400	-6.09015200	-0.67594700
H	3.05688400	0.33613200	-1.67994100	C	0.12120900	-0.50051800	4.47923600
H	0.89812900	-2.57705900	0.20933800	H	-0.57420600	0.05681800	3.83573300
H	1.43549400	-1.73802500	1.65409200	H	-0.46348500	-0.98253300	5.28299900

TS2_5exo_NTf2

N	-3.76854100	0.71956900	-3.05994100
C	-3.60031300	0.00208800	-2.00228100
C	2.17162000	-1.45326000	0.19069200
C	4.08928600	-2.48091700	0.87842800
C	3.04289300	-3.10590700	1.49757900
H	5.16061400	-2.65930900	0.91577200
H	3.01285500	-3.95192700	2.17780700
N	1.88200100	-2.45697300	1.07836400
N	3.53701700	-1.47742400	0.08623800

H	-6.17888800	-0.31916300	-2.65104100
C	-5.15545300	-2.33476200	0.52135700
H	-3.19001100	-1.50384300	0.24610600
C	-6.48306000	-2.40295200	0.04477000
H	-7.87517900	-1.70725800	-1.48842700
H	-4.88688500	-2.90617000	1.41461800
O	-7.32514500	-3.19780600	0.75852100
C	-8.68606400	-3.29076300	0.31948800
H	-8.75305900	-3.70365400	-0.70355600
H	-9.17627400	-3.97883200	1.02323200
H	-9.18968200	-2.30752800	0.35678800
O	-2.30008900	-0.01170800	-1.46834700
C	-2.46291400	1.31624900	-3.34998400
C	-1.53162500	0.79709100	-2.27647400
C	-0.22067100	1.05305300	-1.97704100
H	0.26086200	1.69365300	-2.73279400
H	-0.28658600	1.94353000	-0.83790700
H	-2.12179100	1.04478300	-4.36672400
H	-2.51246200	2.42182900	-3.31528200
N	-0.37685900	2.91540800	-0.00405600
S	-0.44406100	2.59458900	1.63894500
S	-0.81524400	4.38019800	-0.68042900
O	-1.75496300	5.17180600	0.13253500
O	-1.07683400	4.12033200	-2.11090600
C	0.84669300	5.26300900	-0.62203700
F	0.69151100	6.52044700	-1.06648800
F	1.31350800	5.28265700	0.63770700
F	1.72025800	4.61260200	-1.41153600
O	0.65079400	1.65990600	1.96015100
O	-0.67394800	3.80640300	2.44616200
C	-2.03761000	1.56790800	1.73813400
F	-2.95307600	2.04617000	0.88176800
F	-1.76423800	0.28583300	1.44270500
F	-2.51275700	1.64056000	2.99379300

TS2_6endo_NTF2

N	-2.84560000	2.07331500	0.76673800
C	-3.27780900	2.20330400	-0.43202400
C	0.38199800	-2.39296400	0.50299700
C	-0.13685100	-4.43014500	1.38679800
C	1.03785300	-4.56547300	0.69741700
H	-0.72825200	-5.14581000	1.95177800
H	1.68507500	-5.42293600	0.53313000
N	1.33668200	-3.31131100	0.16495700
N	-0.51951800	-3.09948600	1.25439900
Au	0.09623300	-0.44260700	0.06622600
C	-1.70399500	-2.48622200	1.81011000
C	-1.61207800	-1.88945500	3.08763300
C	-2.87540300	-2.44690000	1.02016400
C	-2.75947500	-1.24105200	3.57895000
C	-3.99165300	-1.78125900	1.55785100
C	-3.93502900	-1.18363200	2.82174100
H	-2.72219800	-0.75807200	4.56055500
H	-4.91001200	-1.71125100	0.96606400
H	-4.81182300	-0.65957300	3.21596900
C	2.50199400	-3.01822200	-0.63542900
C	3.67287400	-2.57740200	0.02115200
C	2.41171300	-3.17873400	-2.03621500
C	4.79105900	-2.29249400	-0.78349400
C	3.56225800	-2.88900700	-2.79178400
C	4.73927100	-2.45185700	-2.17327300
H	5.71181400	-1.93394300	-0.31375800
H	3.52961600	-2.99409200	-3.88058400

H	5.62167600	-2.22380900	-2.78033600
C	-2.94441500	-3.04943100	-0.37742300
H	-1.97058100	-3.51979100	-0.59920400
C	-4.01991300	-4.14778900	-0.46349700
H	-4.02576200	-4.59910600	-1.47142500
H	-3.83719500	-4.95174700	0.27097100
H	-5.02841100	-3.73906900	-0.27401000
C	-3.18045500	-1.95346200	-1.43372500
H	-4.15467200	-1.45470800	-1.28635100
H	-2.39419900	-1.18015900	-1.38005900
H	-3.17317100	-2.38895000	-2.44881500
C	1.10930100	-3.57411100	-2.72038900
C	1.30764700	-4.65858800	-3.79198600
H	1.81514900	-5.54803700	-3.37981900
H	0.32917900	-4.97719800	-4.19193600
H	1.90609500	-4.28940800	-4.64325000
C	3.71677200	-2.35477600	1.52774300
H	2.84436300	-2.86490100	1.97310900
C	-0.31947200	-1.88391900	3.89395100
C	-0.51557200	-2.50034500	5.29052800
H	-1.22283300	-1.90932400	5.89892200
H	-0.90406000	-3.53196000	5.22639400
H	0.44535600	-2.53052700	5.83361800
C	3.58326300	-0.85192000	1.84470000
H	2.65274000	-0.43781500	1.41943800
H	3.56290800	-0.68640600	2.93637600
H	4.43157700	-0.28083400	1.42986200
C	4.97747900	-2.94947700	2.17694000
H	4.92436900	-2.83692000	3.27390300
H	5.08494700	-4.02408700	1.94752500
H	5.89485400	-2.43602400	1.83934300
C	0.43036000	-2.32305000	-3.31487800
H	0.23377800	-1.56942900	-2.53079000
H	1.07033700	-1.85658500	-4.08518700
H	-0.53285000	-2.59113300	-3.78471000
H	0.43090600	-3.98631900	-1.95276800
C	0.25131700	-0.45581500	3.98606600
H	1.21589600	-0.45777800	4.52427400
H	0.41921900	-0.03003100	2.98219700
H	-0.43826800	0.21432600	4.53000400
H	0.42177000	-2.50282400	3.35935100
C	-4.70266300	2.15135400	-0.79976000
C	-5.67367700	1.98227500	0.20825600
C	-5.13001800	2.23256500	-2.14428400
C	-7.03279900	1.89329800	-0.10259900
H	-5.34141500	1.91208100	1.24803600
C	-6.48320100	2.14966000	-2.46575800
H	-4.39153000	2.35715400	-2.93991400
C	-7.44688700	1.97835100	-1.44923100
H	-7.76085900	1.76126600	0.70108300
H	-6.82108700	2.21135300	-3.50451700
O	-8.74227900	1.90462900	-1.86693000
C	-9.74982800	1.72196200	-0.86689900
H	-9.77231400	2.56731900	-0.15479800
H	-10.70387400	1.68006600	-1.41247600
H	-9.60380200	0.77640400	-0.31281800
O	-2.44163000	2.34605100	-1.55891700
C	-1.38819600	2.14539400	0.94456600
C	-0.63435700	1.48683300	-0.21182300
C	-1.22053700	1.70943100	-1.42104500
H	-0.83690900	1.40219800	-2.39836500
H	0.86603600	1.96661600	-0.29276100
H	-1.09585400	3.21376200	1.01941900

H	-1.13464500	1.68450400	1.91165700
N	1.91963100	2.51034400	-0.31989700
S	2.61800900	2.90491800	1.15532800
S	2.66312300	2.66218200	-1.81771600
O	3.70891500	3.69761000	-1.81047900
O	1.57551200	2.64490200	-2.81294900
C	3.54815100	1.00575000	-2.00613500
F	4.44710300	0.84867500	-1.02582500
F	2.64295500	0.01667700	-1.96441000
F	4.16939900	0.99469900	-3.19716900
O	1.82791300	2.20153300	2.18214700
O	4.08888700	2.84196300	1.11638400
C	2.15931300	4.72917300	1.31515700
F	0.82274400	4.85302100	1.36972000
F	2.70123100	5.19395800	2.45238100
F	2.63286800	5.41901400	0.26985100

2exo

N	2.09522400	1.50227500	-0.00043000
C	1.50096100	0.35613500	-0.00050600
C	0.06177100	0.10250100	-0.00085700
C	-0.83610000	1.18875800	-0.00081200
C	-0.45514000	-1.21295500	-0.00100500
C	-2.21676200	0.98054200	-0.00068000
H	-0.43661000	2.20711700	-0.00080500
C	-1.83006600	-1.43133300	-0.00086900
H	0.23048800	-2.06436800	-0.00108100
C	-2.72317800	-0.33747900	-0.00051800
H	-2.89006700	1.84024800	-0.00063400
H	-2.24157200	-2.44485900	-0.00082200
O	-4.04638100	-0.65664200	0.00006500
C	-4.98839400	0.42136700	0.00240900
H	-4.88499500	1.04925400	-0.90159300
H	-5.98094100	-0.05214000	0.00543400
H	-4.87976500	1.04984100	0.90536000
O	2.31351500	-0.77635700	-0.00002400
C	3.53411200	1.21296500	0.00029600
C	3.62843800	-0.30380300	0.00045600
C	4.67379300	-1.14127100	0.00094300
H	5.69113900	-0.74307200	0.00135000
H	4.53840700	-2.22588300	0.00099700
H	4.01831200	1.66259200	-0.88720000
H	4.01736700	1.66268800	0.88827000

2endo

N	-2.16399600	-1.24354300	-0.00002100
C	-1.58832700	-0.09674800	0.00007400
C	-0.11881500	0.04785800	0.00005800
C	0.69391500	-1.10273600	-0.00000100
C	0.50533200	1.31590000	0.00010300
C	2.08734500	-1.00710800	-0.00001700
H	0.21146900	-2.08425300	-0.00003500
C	1.89428700	1.42487500	0.00009200
H	-0.10664000	2.22113300	0.00014500
C	2.69869400	0.26536500	0.00003200
H	2.68820400	-1.91951500	-0.00006700
H	2.38338800	2.40362400	0.00013000
O	4.04494100	0.47861700	0.00003100
C	4.89630800	-0.67142200	0.00001400
H	4.74034900	-1.28980600	-0.90311800
H	5.92429800	-0.28018000	0.00006200
H	4.74029400	-1.28988300	0.90308300

O	-2.21545900	1.14893200	0.00017600
C	-3.62510100	-1.34198400	0.00006000
C	-4.31923500	-0.00639700	-0.00027100
C	-3.60313400	1.12435800	-0.00020300
H	-5.41177500	0.04814200	-0.00061700
H	-4.00631800	2.13970900	-0.00045200
H	-3.93037800	-1.94781200	-0.87917300
H	-3.93031000	-1.94736500	0.87963000

HClO₄

O	0.41832100	0.78170400	-1.23729000
O	0.41826900	0.78124100	1.23762100
O	0.67247300	-1.36286900	-0.00022500
Cl	0.15239200	0.01377800	0.00001700
O	-1.53926100	-0.30022200	-0.00008500
H	-1.96280300	0.60187800	-0.00001000

IPrAuClO₄

C	-0.01134500	-0.85951400	0.46873800
C	0.69175400	-2.49232900	1.88414300
C	-0.67700300	-2.50186900	1.89145300
H	1.42250900	-3.09896600	2.41235400
H	-1.39376800	-3.11928500	2.42626400
N	-1.08708200	-1.49641900	1.02163100
N	1.07900500	-1.48206300	1.00942500
Au	-0.02986300	0.63045200	-0.81145500
C	2.44344900	-1.11242500	0.71697100
C	3.09023100	-1.74315300	-0.36829600
C	3.05500100	-0.12383700	1.51954500
C	4.41507700	-1.35580300	-0.63772600
C	4.38137200	0.22452400	1.20663000
C	5.05476200	-0.38487600	0.14157700
H	4.94602300	-1.81538500	-1.47743500
H	4.88682000	0.99207000	1.80158700
H	6.08504500	-0.09473900	-0.08864200
C	-2.45841200	-1.14900800	0.73544000
C	-3.10076000	-1.79582100	-0.34303300
C	-3.07977500	-0.16250100	1.53305700
C	-4.43054900	-1.42591900	-0.61260300
C	-4.41001000	0.16964800	1.21861500
C	-5.07884100	-0.45509500	0.15956300
H	-4.95828700	-1.89875500	-1.44698900
H	-4.92302200	0.93599400	1.80835100
H	-6.11251700	-0.17750400	-0.07093800
C	2.32587100	0.56054100	2.66852800
H	1.30009000	0.15555300	2.71477500
C	3.00466500	0.25516700	4.01637300
H	2.44937100	0.73340900	4.84236000
H	3.04181000	-0.83104800	4.21194600
H	4.04017600	0.63832700	4.04021900
C	2.21072200	2.07681600	2.42809900
H	3.20397100	2.55981100	2.41587700
H	1.71713000	2.29683200	1.46550600
H	1.61883200	2.54689700	3.23350600
C	-2.35356200	0.54733100	2.66896300
C	-3.09429300	0.37748100	4.00769300
H	-3.22858300	-0.68792100	4.26409300
H	-2.52344900	0.85746300	4.82186800
H	-4.09342700	0.84696900	3.97936300

C	-2.39042000	-2.81963300	-1.21912500	H	0.13383700	4.70183800	3.16770700
H	-1.39289900	-3.01130100	-0.78717700	H	1.91165200	4.88171200	3.16961000
C	2.38912100	-2.76727400	-1.25123800	H	0.93741000	5.52791100	1.81754300
C	3.15617400	-4.09990400	-1.30496700	C	-0.07253300	3.12685400	0.87343400
H	4.15606800	-3.97549000	-1.75673500	H	-0.10335000	3.89043700	0.07847500
H	3.29090200	-4.52919900	-0.29676400	H	-0.03926600	2.13863400	0.38113200
H	2.60250700	-4.83273700	-1.91793400	H	-1.01781600	3.18975500	1.44118500
C	-2.17632500	-2.25733100	-2.63707900	C	-1.48877100	-0.58759300	2.75451400
H	-1.61407400	-1.30695600	-2.60504800	C	-1.60599400	-0.69133200	4.28749100
H	-1.60691200	-2.97487100	-3.25432600	H	-0.64150300	-0.95414900	4.75629200
H	-3.14019800	-2.06446300	-3.14088300	H	-1.94346300	0.26953900	4.71536000
C	-3.14112800	-4.16214700	-1.25636300	H	-2.34051800	-1.46632200	4.57138000
H	-2.58075600	-4.89442500	-1.86387500	C	2.29320900	-3.44060300	0.75028900
H	-3.26716900	-4.58279300	-0.24340000	H	2.84444900	-2.52100000	1.01454900
H	-4.14411000	-4.05450500	-1.70561400	C	4.99235600	0.35704100	0.18426200
C	-2.13826100	2.03599600	2.33647000	C	6.40653500	0.43379400	0.78835800
H	-1.56647100	2.16318900	1.40084600	H	7.05865700	1.10699800	0.20416000
H	-3.10159400	2.56256300	2.21644900	H	6.37964100	0.80540200	1.82749800
H	-1.57967000	2.53249500	3.14995000	H	6.87456500	-0.56621800	0.79263900
H	-1.35673400	0.08642900	2.78179600	C	2.39889200	-3.61600200	-0.77502100
C	2.16238300	-2.19366200	-2.66266200	H	1.95487100	-2.75039300	-1.29726000
H	1.59795600	-2.91133500	-3.28432800	H	3.45693800	-3.70414000	-1.08082000
H	1.59044100	-1.24959000	-2.61859900	H	1.86585100	-4.52076800	-1.11541900
H	3.12191700	-1.98550000	-3.16873900	C	2.96362300	-4.60804700	1.49728800
H	1.39582400	-2.97551600	-0.81692900	H	4.02659900	-4.68874900	1.20841200
O	-0.06089500	2.12735000	-2.25424400	H	2.91624800	-4.46533700	2.59109600
Cl	0.07038100	3.63678400	-1.69058800	H	2.47733600	-5.57067300	1.26021700
O	1.36314200	3.74409100	-0.94716600	C	-2.81980900	-0.13641700	2.12862300
O	-1.09976600	3.90168000	-0.79952900	H	-2.76299000	-0.13897500	1.02914500
O	0.05068600	4.47790500	-2.91742500	H	-3.65584800	-0.79398200	2.42672800

Int1_CIO4

N	-1.89276000	1.43547400	-2.61898500	H	5.02931800	-0.19145500	-1.25371800
C	-2.45737300	2.40049900	-1.82424900	H	5.49544000	-1.19262000	-1.27073700
C	1.61465900	-0.07073300	0.97721600	H	4.00956700	-0.27776400	-1.66952200
C	2.67957800	0.42120700	2.92509600	H	5.61441600	0.46678900	-1.92022300
C	1.91566400	-0.69550800	3.13975700	H	4.41039300	-0.35482300	0.79530400
H	3.33762300	0.98382900	3.58203900	C	-3.67702300	2.00328900	-1.05548600
H	1.77237600	-1.31188100	4.02301700	C	-4.36564800	0.78757600	-1.23151300
N	1.27097700	-0.97672600	1.94200600	C	-4.13349600	2.89711000	-0.06183400
N	2.48107300	0.78609600	1.60029500	C	-5.45767400	0.45124300	-0.42300400
Au	1.10727000	-0.02014200	-0.98203100	H	-4.06912200	0.07311300	-2.00513000
C	3.09425000	1.91895500	0.94698200	C	-5.21638200	2.57555700	0.75088000
C	4.29766200	1.71169200	0.23935000	H	-3.60490500	3.84670300	0.06219500
C	2.44217100	3.17077200	1.03562200	C	-5.88025700	1.33934100	0.58608100
C	4.84697800	2.82292500	-0.42713700	H	-5.96014400	-0.50533700	-0.58203700
C	3.03490300	4.24560300	0.34948500	H	-5.56582100	3.25903600	1.53076900
C	4.21960400	4.07227300	-0.37816200	O	-6.91215700	1.10269800	1.44476000
H	5.77656300	2.70125000	-0.99245900	C	-7.56542300	-0.16804500	1.35441700
H	2.56222500	5.23132700	0.38269900	H	-6.85676600	-0.99856200	1.52927600
H	4.66037800	4.92338700	-0.90746100	H	-8.32917000	-0.16521300	2.14602100
C	0.35279400	-2.07755800	1.75599700	H	-8.05725500	-0.30359500	0.37362600
C	0.84151000	-3.26952100	1.18091300	O	-1.96633800	3.54484500	-1.73420700
C	-0.98869700	-1.89913500	2.16155000	C	-0.61445400	1.67481800	-3.25455100
C	-0.07731300	-4.32079700	1.01143600	C	0.33870200	0.57701000	-3.01633100
C	-1.85630300	-2.99143700	1.99227700	C	1.09042700	-0.41757800	-3.10091300
C	-1.40868400	-4.18693500	1.41922200	H	1.63104000	-1.26470700	-3.50171400
H	0.25985800	-5.25524500	0.55173300	H	-2.23949200	0.46646800	-2.64265200
H	-2.90550700	-2.89214100	2.28611300	H	-0.71157300	1.77011600	-4.35579200
H	-2.10876500	-5.01539600	1.27277600	H	-0.23516000	2.63903200	-2.87144000
C	1.13674200	3.33613200	1.80657500	O	-2.54013000	-1.34264800	-3.21921600
H	1.10108300	2.54821300	2.58083500	O	-3.16204000	-3.13293800	-1.63118000
C	1.03377100	4.68906900	2.52875900	O	-1.65834100	-1.30748500	-0.92190100

Cl	-2.05087800	-2.21792300	-2.06137400
O	-0.86211400	-3.01834700	-2.52258500

TS1_5exo_CIO4

N	-3.07987300	-0.00675300	-1.07467100
C	-3.66410100	-1.07929300	-1.67346200
C	2.62995400	0.20549000	0.47716400
C	3.70002900	1.65206000	1.86318000
C	4.34205700	0.44583900	1.94917400
H	3.88339500	2.60444900	2.35376700
H	5.20157000	0.12432600	2.53139700
N	3.67340400	-0.42405400	1.09081800
N	2.65480800	1.48286400	0.96011800
Au	1.28896200	-0.54644500	-0.82920000
C	1.71291900	2.49372600	0.53713000
C	1.96374200	3.16655900	-0.67863300
C	0.55909400	2.71137400	1.32708000
C	0.99099000	4.08583400	-1.11509000
C	-0.38102200	3.63722600	0.84122800
C	-0.17050800	4.31051600	-0.36973500
H	1.14809500	4.62272000	-2.05639100
H	-1.30138100	3.82333200	1.40073800
H	-0.93090100	5.00824900	-0.73374900
C	4.01590900	-1.80852300	0.86744500
C	4.99095800	-2.10555200	-0.11251200
C	3.34495900	-2.79578900	1.62203600
C	5.29256900	-3.46255800	-0.32462000
C	3.68741300	-4.13730700	1.36961700
C	4.64949700	-4.46732200	0.40919800
H	6.03516300	-3.73629300	-1.08010800
H	3.18713800	-4.93058000	1.93421100
H	4.89917100	-5.51769200	0.22714300
C	0.31130800	1.93245100	2.61486800
H	1.29229300	1.60955900	3.00895200
C	-0.36936300	2.78001600	3.70292900
H	-0.41356600	2.20867200	4.64667500
H	0.18116100	3.71737800	3.89536200
H	-1.40626200	3.03952700	3.42844000
C	-0.51840100	0.66250200	2.32896100
H	-1.53004800	0.92996200	1.97665500
H	-0.04058800	0.02891300	1.56000800
H	-0.62781700	0.06131700	3.24958900
C	2.28676500	-2.45604800	2.66359400
C	2.72555200	-2.90684600	4.06894700
H	3.68234700	-2.43998600	4.36101100
H	1.96317100	-2.62313300	4.81544700
H	2.85432400	-4.00248800	4.11795400
C	5.64023600	-1.01442100	-0.95574100
H	5.47976300	-0.04766200	-0.44677300
C	3.21927300	2.92950700	-1.50912900
C	4.07478600	4.20765500	-1.58931000
H	3.52642700	5.02633000	-2.08763400
H	4.36732600	4.55928600	-0.58464800
H	4.99590800	4.01757700	-2.16804300
C	4.94945100	-0.93354200	-2.33218100
H	3.86380300	-0.75838600	-2.22413800
H	5.37623700	-0.11079800	-2.93273000
H	5.08596000	-1.87459000	-2.89457200
C	7.15861300	-1.20069900	-1.10987800
H	7.58837200	-0.34178700	-1.65423800
H	7.66046100	-1.26957300	-0.12915400
H	7.40784100	-2.11014900	-1.68385600
C	0.92312100	-3.06326500	2.28444600

H	0.59728200	-2.72294300	1.28512500
H	0.96276100	-4.16695200	2.27084200
H	0.15312700	-2.76242300	3.01606000
H	2.16348800	-1.35978400	2.69091200
C	2.86747700	2.40635700	-2.91333600
H	3.78696400	2.19265300	-3.48637300
H	2.27402200	1.47642300	-2.85254600
H	2.27998500	3.14716400	-3.48366200
H	3.82790500	2.15441700	-1.01127900
C	-4.98361600	-1.54983100	-1.18051400
C	-5.80035700	-0.79872000	-0.31232100
C	-5.44564700	-2.80813500	-1.62823100
C	-7.03950300	-1.28876900	0.11265500
H	-5.49247000	0.18974000	0.04044600
C	-6.67429700	-3.30767900	-1.21021000
H	-4.81476600	-3.38466200	-2.31088500
C	-7.48311200	-2.55096800	-0.33222400
H	-7.65119000	-0.67944200	0.78137200
H	-7.03604400	-4.28347100	-1.54800000
O	-8.66716800	-3.12237600	0.02016200
C	-9.51774600	-2.38875900	0.90974100
H	-9.82793600	-1.42438000	0.46765000
H	-10.40343700	-3.02279900	1.06107400
H	-9.02463700	-2.20883200	1.88251100
O	-3.06106800	-1.64391400	-2.62313900
C	-1.85219700	0.47447200	-1.67645800
C	-0.94589900	-0.64023700	-1.98851900
C	-0.01431900	-1.46588100	-2.19637600
H	0.21910700	-2.39068500	-2.71769200
H	-3.44518000	0.48465300	-0.24135400
H	-2.05129800	1.02793300	-2.61665200
H	-1.37280500	1.18325400	-0.98133000
O	-3.80168700	1.45772500	1.26709100
O	-3.42059400	3.17472900	-0.46919100
O	-3.66638300	3.83587400	1.90368500
Cl	-4.13482400	2.89137300	0.82801400
O	-5.62084400	3.00591000	0.64247300

TS1_6endo_CIO4

N	-3.19730000	0.09680900	-2.20747600
C	-3.83941600	-1.02770300	-1.78929100
C	2.42088500	-0.14661000	0.46044400
C	4.24978600	0.75278000	1.46731400
C	4.34148100	-0.60648600	1.59412700
H	4.90128100	1.55587800	1.80133400
H	5.08671300	-1.24011000	2.06769500
N	3.21731800	-1.13688000	0.96842000
N	3.06974900	1.01271000	0.77455600
Au	0.71846900	-0.47089200	-0.58362000
C	2.56934300	2.33551300	0.48116800
C	2.82908700	2.88829200	-0.79150400
C	1.84626900	3.01050900	1.49094800
C	2.32093500	4.17471400	-1.04719400
C	1.35699800	4.29087400	1.17923900
C	1.58785000	4.86492400	-0.07609800
H	2.49339400	4.63196800	-2.02630200
H	0.76744100	4.83519600	1.92263100
H	1.18527900	5.85747900	-0.30115500
C	2.85723400	-2.53309600	0.91728700
C	3.36686800	-3.32435200	-0.13655200
C	1.97353100	-3.02574300	1.90415300
C	2.96729300	-4.67255900	-0.17598400
C	1.59952700	-4.37893600	1.81118900

C	2.09216400	-5.19363600	0.78510000
H	3.33464300	-5.31865700	-0.97908200
H	0.91294300	-4.79648700	2.55442900
H	1.78916300	-6.24446300	0.73173300
C	1.57210400	2.38139200	2.85270200
H	2.17467600	1.46012100	2.93531500
C	1.99939300	3.30264600	4.00889600
H	1.85776700	2.78577100	4.97456600
H	3.06240800	3.59006500	3.92782200
H	1.39880700	4.22899500	4.04024500
C	0.09220500	1.97383100	2.97926700
H	-0.57299900	2.85031300	2.89088200
H	-0.20363400	1.26743400	2.18683800
H	-0.08945000	1.49810200	3.96031300
C	1.43372400	-2.14981300	3.02873100
C	1.89782100	-2.66318000	4.40430400
H	2.99907100	-2.68413600	4.47919500
H	1.51284300	-2.00791900	5.20522900
H	1.52685800	-3.68538800	4.59852500
C	4.25627400	-2.73673800	-1.22625500
H	4.59476500	-1.74063600	-0.89117900
C	3.60375900	2.13289200	-1.86381400
C	4.78961200	2.95409400	-2.40073100
H	4.44935000	3.86838100	-2.91794200
H	5.47049100	3.25861800	-1.58685400
H	5.36852300	2.35733600	-3.12743600
C	3.44835200	-2.54022200	-2.52464000
H	2.56132400	-1.90429400	-2.35137500
H	4.07269500	-2.06139600	-3.29974900
H	3.09608600	-3.50926800	-2.92110600
C	5.51068000	-3.58948500	-1.48033600
H	6.16503500	-3.09003800	-2.21599400
H	6.09167500	-3.74234000	-0.55423800
H	5.25344100	-4.58269200	-1.88831600
C	-0.09998000	-2.03570800	2.96541900
H	-0.42867100	-1.61953300	1.99686500
H	-0.58833000	-3.01706600	3.10109900
H	-0.46562100	-1.36548200	3.76287300
H	1.84015800	-1.13188600	2.89986000
C	2.66582700	1.69996400	-3.00591200
H	3.21760200	1.11050600	-3.75999000
H	1.83623900	1.07901100	-2.61991700
H	2.22282800	2.57724700	-3.51013600
H	4.01744900	1.21633600	-1.40781500
C	-5.15019000	-0.86914900	-1.09844000
C	-5.57039100	0.32171500	-0.47307900
C	-5.99483700	-2.00040400	-1.03473300
C	-6.80345300	0.39083300	0.18578400
H	-4.93542400	1.21371500	-0.46372900
C	-7.22718600	-1.94087800	-0.39308100
H	-5.66012800	-2.92963300	-1.50453800
C	-7.64271700	-0.74068000	0.22566200
H	-7.09535200	1.32383200	0.67280800
H	-7.88886300	-2.81123500	-0.35018500
O	-8.85893200	-0.78066900	0.83670600
C	-9.30567300	0.40733200	1.50025100
H	-9.41806200	1.24882300	0.79236900
H	-10.28809700	0.15559700	1.92565300
H	-8.61577600	0.69915600	2.31308700
O	-3.34729700	-2.17555700	-1.98573900
C	-1.81894000	0.06146500	-2.66587600
C	-0.99147000	-0.79682600	-1.74240100
C	-1.21355000	-1.92459600	-1.20995800

H	-1.20201500	-2.86097500	-0.67216800
H	-3.53020000	1.02508800	-1.90337000
H	-1.75645000	-0.39242100	-3.67152500
H	-1.44595600	1.09234700	-2.70776600
O	-3.44588300	2.82510900	-1.21283300
O	-2.27486800	4.00506200	0.61886000
O	-0.98368100	2.80905000	-1.11220800
O	-2.30730400	1.53345100	0.55004600
Cl	-2.23575000	2.79543500	-0.27035700

Int2_Sexo_CIO4

N	3.41610900	-0.20866800	0.47046500
C	3.79049700	-1.45730300	0.26767600
C	-2.82965300	0.49455700	0.09556500
C	-3.88785800	2.51079400	0.25363100
C	-4.82776900	1.57955200	-0.09737800
H	-3.96212600	3.58018800	0.43297900
H	-5.89375700	1.66577700	-0.29082300
N	-4.16148400	0.35921600	-0.18683600
N	-2.67902200	1.83025800	0.36420800
Au	-1.32042400	-0.86780700	0.08854100
C	-1.41012000	2.41700600	0.72613000
C	-1.04810100	2.43471300	2.09219000
C	-0.56512300	2.89009700	-0.30308500
C	0.21668600	2.95970700	2.41739900
C	0.68948000	3.40207400	0.07680900
C	1.07786000	3.43616800	1.42121300
H	0.53363200	2.98077600	3.46535000
H	1.38779000	3.75504100	-0.68724700
H	2.06819800	3.82233400	1.68160000
C	-4.76566300	-0.89906400	-0.54825700
C	-5.27006000	-1.72388200	0.48212100
C	-4.78655100	-1.26288600	-1.91300300
C	-5.81950800	-2.96191800	0.10286100
C	-5.34928100	-2.51092400	-2.23727800
C	-5.85938200	-3.35142700	-1.24124200
H	-6.21296500	-3.63317200	0.87276600
H	-5.37696900	-2.83043900	-3.28395600
H	-6.28787700	-4.32135800	-1.51431400
C	-0.94828600	2.82004900	-1.77612200
H	-1.98263900	2.44064200	-1.84775200
C	-0.91541600	4.21174800	-2.43268100
H	-1.23962200	4.14547300	-3.48626800
H	-1.58425000	4.91959100	-1.91239000
H	0.10303900	4.63752300	-2.42228500
C	-0.03849000	1.82825600	-2.52654500
H	1.01959000	2.14160200	-2.48188400
H	-0.11704200	0.81512200	-2.09185300
H	-0.33051500	1.76822900	-3.59022500
C	-4.18893000	-0.37627500	-2.99855700
C	-5.20071000	-0.07868100	-4.11879100
H	-6.11697600	0.39110600	-3.72045900
H	-4.75745300	0.61021700	-4.85925400
H	-5.49658600	-0.99742000	-4.65525700
C	-5.18464300	-1.32727100	1.95077500
H	-4.88659500	-0.26553800	2.00182400
C	-1.94869300	1.86104500	3.17897700
C	-2.24720100	2.89346800	4.27990000
H	-1.32847900	3.19858400	4.81113700
H	-2.71349700	3.80305700	3.86266900
H	-2.93851600	2.46658900	5.02795500

C	-4.09124200	-2.14818900	2.66220300
H	-3.11276000	-2.01883100	2.16542300
H	-3.99102000	-1.82864500	3.71486100
H	-4.33704400	-3.22527800	2.65348800
C	-6.53810000	-1.45874100	2.67006000
H	-6.45272800	-1.09293600	3.70835200
H	-7.32383200	-0.87090700	2.16424400
H	-6.87768200	-2.50832300	2.71725100
C	-2.90048200	-1.00736100	-3.56032900
H	-2.16137100	-1.18029700	-2.75733600
H	-3.11107000	-1.97770500	-4.04481600
H	-2.44277700	-0.34214500	-4.31383100
H	-3.90921800	0.58810900	-2.54040100
C	-1.33040700	0.57704200	3.76429200
H	-2.00677100	0.12744200	4.51305300
H	-1.14869300	-0.16912100	2.96946800
H	-0.36626600	0.78940600	4.26031600
H	-2.91107400	1.58038500	2.71707000
C	5.13913300	-1.96574000	0.15515800
C	6.24931100	-1.09175800	0.20267400
C	5.35453200	-3.35574500	-0.02089600
C	7.54567800	-1.58621200	0.07786000
H	6.10526100	-0.01285600	0.32396000
C	6.64359300	-3.85289800	-0.14318000
H	4.49998200	-4.03607300	-0.06189400
C	7.75221300	-2.97361200	-0.09693800
H	8.38688300	-0.89131900	0.11115600
H	6.82751200	-4.92202500	-0.28003800
O	8.96471400	-3.55745700	-0.23304500
C	10.12752900	-2.71365900	-0.21034000
H	10.23035200	-2.20268800	0.76329900
H	10.98120400	-3.38866000	-0.36329000
H	10.09626000	-1.96770900	-1.02398300
O	2.75546700	-2.29368800	0.15144300
C	1.95999800	-0.08509000	0.46927900
C	1.52840500	-1.51640100	0.22371400
C	0.32127200	-2.07245700	0.06315300
H	0.30544300	-3.15852900	-0.11006300
H	4.04443800	0.62892600	0.52112400
H	1.60518400	0.31763200	1.43476200
H	1.64209100	0.60992300	-0.32613500
O	4.91780500	2.09731700	0.61833600
Cl	4.61294100	2.91748400	-0.65498000
O	3.64581000	2.12864900	-1.50120200
O	4.00448500	4.22538200	-0.23489600
O	5.89545800	3.14427800	-1.39525700

Int2_gendo_CIO4

N	-3.29209600	-0.47409800	-0.23457700
C	-3.63915100	-1.72369500	-0.45699200
C	2.80798400	0.44374900	0.45674500
C	4.25901400	2.08646300	1.08958500
C	4.98045900	1.13453300	0.42026100
H	4.55595900	3.02247500	1.55555500
H	6.03713900	1.06758100	0.17479700
N	4.07659500	0.14220500	0.04606500
N	2.93889400	1.64738800	1.09825300
Au	1.01973000	-0.47295300	0.14129100
C	1.81567300	2.32413000	1.70510800
C	1.06748200	3.23021300	0.91988800
C	1.47491400	1.98870200	3.03479800
C	-0.07449500	3.80155600	1.50994400
C	0.32868500	2.59624000	3.57882600

C	-0.44295600	3.48569800	2.82251600
H	-0.70221400	4.47722900	0.92255500
H	0.02791600	2.35097100	4.60267200
H	-1.34614100	3.92962500	3.25328500
C	4.40935400	-1.04177100	-0.70663200
C	4.27907800	-1.00066300	-2.11226000
C	4.82861600	-2.19115500	0.00069600
C	4.59203700	-2.17509800	-2.82132000
C	5.12780300	-3.33778600	-0.75663500
C	5.01221700	-3.32994800	-2.15223900
H	4.49751000	-2.18214800	-3.91197300
H	5.44826900	-4.25087100	-0.24557400
H	5.24758100	-4.23457300	-2.72257400
C	2.26897500	0.97577200	3.85000200
H	3.14415000	0.66367500	3.25409400
C	2.79742600	1.58699500	5.15979500
H	3.40651800	0.84667600	5.70816000
H	3.42724700	2.47274300	4.96630300
H	1.97205400	1.89773700	5.82453000
C	1.42282800	-0.28229500	4.12159800
H	0.54608400	-0.04431800	4.75028700
H	1.05325900	-0.72040000	3.17721800
H	2.02147400	-1.04579900	4.64967900
C	4.88948000	-2.21632900	1.52300300
C	6.17448000	-2.87069200	2.05606100
H	7.07691500	-2.38573500	1.64492700
H	6.21132700	-2.78649100	3.15626600
H	6.22240300	-3.94547600	1.80800500
C	3.79687500	0.24140500	-2.85090700
H	3.65514900	1.04793800	-2.11111200
C	1.42628400	3.55619700	-0.52503800
C	1.54313300	5.07387600	-0.75382700
H	0.57599900	5.58347200	-0.59899400
H	2.28094300	5.53135600	-0.07149800
H	1.86269700	5.27851300	-1.79078500
C	2.43143100	-0.01712300	-3.51474400
H	1.68440800	-0.33445800	-2.76500900
H	2.06102200	0.90070400	-4.00453800
H	2.50107400	-0.80797600	-4.28304000
C	4.83665200	0.73057100	-3.87490400
H	4.48450700	1.65652800	-4.36249700
H	5.80708900	0.94470300	-3.39397300
H	5.01028800	-0.01910800	-4.66711800
C	3.63484100	-2.91239200	2.08801500
H	2.71165500	-2.41970500	1.73439300
H	3.59808300	-3.97025700	1.77095200
H	3.64166700	-2.88626100	3.19232600
H	4.87890900	-1.17189600	1.88087800
C	0.40505300	2.92477300	-1.49176300
H	0.66501600	3.16431000	-2.53851300
H	0.39334400	1.82534900	-1.38073500
H	-0.61689800	3.29516800	-1.29858200
H	2.41295400	3.11096900	-0.74459400
C	-5.02763600	-2.15725000	-0.57093900
C	-6.07211300	-1.22178200	-0.74585600
C	-5.34334200	-3.53779000	-0.51281400
C	-7.39717600	-1.64273200	-0.84538600
H	-5.86088500	-0.15015700	-0.81875500
C	-6.66077000	-3.96339600	-0.61346700
H	-4.54349100	-4.27025900	-0.37914700
C	-7.70253900	-3.01991800	-0.77648200
H	-8.18319500	-0.89807400	-0.98398800
H	-6.91698000	-5.02537700	-0.56399600

O	-8.95249400	-3.53413200	-0.86015100
C	-10.04641900	-2.61574000	-1.01060300
H	-9.95908500	-2.04049900	-1.94952300
H	-10.95078100	-3.23965900	-1.04550900
H	-10.10810500	-1.92375800	-0.15180300
O	-2.72268500	-2.68024900	-0.58501600
C	-1.90381600	0.02609700	-0.25025400
C	-0.89474900	-1.09609800	-0.17514100
C	-1.34254200	-2.34768200	-0.34543400
H	-0.77495800	-3.27821300	-0.34407500
H	-4.02355100	0.25257900	-0.06540300
H	-1.77078400	0.63202500	-1.16572600
H	-1.80501300	0.72646500	0.59633900
O	-5.20575000	3.98228600	-0.78911700
O	-3.67223700	2.33450500	-1.81261900
Cl	-4.21467700	2.89134300	-0.52164700
O	-3.08865200	3.39267700	0.34286000
O	-4.93317300	1.75230900	0.22837900

TS2_5exo_CIO4

N	-3.55525500	1.14156300	-3.57108500
C	-3.51640200	0.71915900	-2.35273100
C	1.78535000	-0.75785300	0.66040800
C	3.36325500	-1.55852000	2.10235300
C	2.15966900	-2.08906000	2.47597600
H	4.36460200	-1.68517300	2.50476700
H	1.88919700	-2.77367500	3.27493800
N	1.21031900	-1.58712700	1.58819000
N	3.11353000	-0.74957500	0.99640200
Au	0.89317900	0.25256700	-0.84393100
C	4.13207100	-0.07446200	0.22799100
C	4.78105900	-0.80613800	-0.79166100
C	4.42692900	1.27737600	0.52107300
C	5.77968000	-0.14111700	-1.52680500
C	5.43561900	1.89148900	-0.24245400
C	6.10701000	1.19057300	-1.25210600
H	6.29843100	-0.67320800	-2.33071800
H	5.69254000	2.93728300	-0.05171400
H	6.88607200	1.69218500	-1.83569700
C	-0.17975700	-1.97464200	1.59356800
C	-0.58766900	-3.00881000	0.72055900
C	-1.06166900	-1.32820400	2.48917900
C	-1.93547500	-3.40747300	0.77778400
C	-2.39396500	-1.77917700	2.51739600
C	-2.82734200	-2.80903200	1.67339500
H	-2.28552100	-4.20031700	0.10906000
H	-3.10298300	-1.30876800	3.20567500
H	-3.87101700	-3.13767200	1.70491200
C	3.70228900	2.02865600	1.63112800
H	2.70189700	1.57507400	1.73916800
C	4.44578600	1.85896200	2.97184200
H	3.90531300	2.38485100	3.77883500
H	4.53683000	0.79746200	3.25996900
H	5.46467400	2.28232600	2.91027200
C	3.49251000	3.51755200	1.31470900
H	4.44389100	4.07871200	1.32221500
H	3.01052800	3.66042900	0.33318400
H	2.83727100	3.96973500	2.07769000
C	-0.60256400	-0.20217900	3.40652000
C	-0.36756600	-0.72895600	4.83588200
H	0.38531900	-1.53616200	4.85361400
H	-0.01035000	0.08395700	5.49274900
H	-1.30302900	-1.12905400	5.26702600

C	0.36261300	-3.68464100	-0.25981100
H	1.36592100	-3.24217600	-0.13512900
C	4.39425500	-2.23957800	-1.13500700
C	5.61250300	-3.17816900	-1.16125800
H	6.31999300	-2.90671700	-1.96424700
H	6.16053200	-3.15396000	-0.20318400
H	5.28749600	-4.21763200	-1.34389000
C	-0.07678700	-3.42093200	-1.71161700
H	-0.12142300	-2.33609200	-1.91465200
H	0.63792800	-3.87686300	-2.41955500
H	-1.07490100	-3.84889500	-1.91324300
C	0.48407600	-5.19249900	0.02582100
H	1.20779300	-5.65531200	-0.66832100
H	0.83093800	-5.38021900	1.05702500
H	-0.48343500	-5.70928800	-0.10404000
C	-1.58613100	0.98033200	3.41118200
H	-1.79470400	1.33686300	2.38963500
H	-2.54564000	0.71289900	3.88871300
H	-1.15780700	1.82283500	3.98112400
H	0.36269500	0.17298700	3.02466900
C	3.62793800	-2.27973100	-2.47164700
H	3.31087600	-3.31213400	-2.70447200
H	2.72813100	-1.64021000	-2.43320600
H	4.26282100	-1.92375700	-3.30277900
H	3.71051900	-2.61133400	-0.35211000
C	-4.62448400	0.30117100	-1.50138900
C	-5.93520800	0.28388700	-2.01963600
C	-4.41102400	-0.08199800	-0.15735500
C	-7.01611400	-0.10850100	-1.22751900
H	-6.09936000	0.58272800	-3.05913600
C	-5.48361800	-0.46950200	0.64023100
H	-3.40111100	-0.07418400	0.25945500
C	-6.79361300	-0.48971900	0.11374800
H	-8.02182100	-0.11451300	-1.65325900
H	-5.33151200	-0.76292500	1.68285500
O	-7.76835400	-0.89167700	0.97442600
C	-9.10962700	-0.95734000	0.47614000
H	-9.19109800	-1.66572400	-0.36851300
H	-9.71978300	-1.31861200	1.31663200
H	-9.47351700	0.03775000	0.16106900
O	-2.24765900	0.64953900	-1.76219900
C	-2.16617900	1.43078700	-3.93553400
C	-1.34774200	1.11538000	-2.69856700
C	-0.02495300	1.27094000	-2.39221000
H	0.56506100	1.62558100	-3.25344400
H	-0.02614100	2.47605600	-1.50508800
H	-1.85260900	0.81886900	-4.80300500
H	-2.05100200	2.48900500	-4.23718400
O	0.05350800	3.57982800	-1.08783500
O	-0.87284800	5.15524400	0.54963300
O	0.19440300	3.08340000	1.38144100
O	-1.98800100	2.95960400	0.22607900
Cl	-0.69773300	3.69273600	0.35524300

TS2_6endo_CIO4

N	2.80060700	-2.23170300	0.56795400
C	3.33486400	-1.92193900	-0.56865600
C	-1.27309600	1.29627600	0.57991800
C	-1.12850100	3.47362900	1.24373900
C	-2.44310100	3.10365500	1.32652800
H	-0.62717700	4.41309600	1.46166900
H	-3.32954500	3.65283000	1.63296600
N	-2.51172200	1.77279900	0.91798700

N	-0.43291600	2.35872200	0.79026600
Au	-0.58960500	-0.49476200	-0.06187000
C	0.97852600	2.29053100	0.48845900
C	1.87361900	1.87773200	1.50098800
C	1.38533500	2.55868200	-0.83816400
C	3.22569400	1.72627700	1.14220000
C	2.74931200	2.39685900	-1.14037600
C	3.65983100	1.97863200	-0.16404100
H	3.94538000	1.38359300	1.89210800
H	3.09717000	2.58555000	-2.16132900
H	4.71338400	1.83704200	-0.42525100
C	-3.72597800	0.99919400	0.82965000
C	-4.12892800	0.25282800	1.95879200
C	-4.43409700	1.00786400	-0.39144100
C	-5.29598700	-0.52048800	1.83110100
C	-5.59812300	0.22247500	-0.46187900
C	-6.02299500	-0.53583500	0.63469200
H	-5.63289600	-1.12624800	2.67787000
H	-6.16886700	0.19435100	-1.39555300
H	-6.92546300	-1.15059300	0.55451800
C	0.40374000	2.97415500	-1.92707700
H	-0.59646100	3.07866000	-1.47176300
C	0.77941000	4.33916000	-2.53143700
H	0.03003800	4.64358600	-3.28336700
H	0.82490900	5.12368000	-1.75598300
H	1.76217500	4.30267900	-3.03369200
C	0.30003700	1.88931500	-3.01541000
H	-0.02574600	0.92784800	-2.57989600
H	-0.43185200	2.18636600	-3.78724800
H	1.27267800	1.72695700	-3.51341700
C	-3.96001200	1.80145100	-1.60347000
C	-5.03344600	2.79238800	-2.08800200
H	-5.33324600	3.48838400	-1.28502200
H	-4.64823800	3.39013700	-2.93297800
H	-5.94019000	2.26797700	-2.43743800
C	-3.32031400	0.24122500	3.25092100
H	-2.58427600	1.06263800	3.19907100
C	1.41021200	1.55533200	2.91586000
C	2.23964800	2.29932200	3.97756800
H	2.23528900	3.38986000	3.80547800
H	1.82537500	2.10952800	4.98337800
H	3.29067800	1.96134000	3.98411700
C	-2.53254400	-1.07646400	3.38589100
H	-1.86922500	-1.23159400	2.51771100
H	-1.91439600	-1.06295400	4.30175200
H	-3.21549400	-1.94193600	3.44558900
C	-4.19912300	0.49303000	4.48824800
H	-3.56997300	0.55911900	5.39340500
H	-4.76622000	1.43583700	4.39585400
H	-4.92362900	-0.32436000	4.64994700
C	-3.51909000	0.85957100	-2.73952400
H	-2.71213900	0.18616900	-2.40588400
H	-4.35868400	0.23270500	-3.08776600
H	-3.15187600	1.44592300	-3.60099400
H	-3.07575100	2.39168100	-1.30557300
C	1.43451900	0.03336500	3.15773300
H	1.09427100	-0.20019000	4.18241300
H	0.77354400	-0.48805400	2.44346200
H	2.45220800	-0.37518000	3.02868200
H	0.36403600	1.89262700	3.01956500
C	4.67939400	-1.33827800	-0.71761200
C	5.51629800	-1.22960300	0.41139600
C	5.13998800	-0.82765300	-1.95236900

C	6.77263300	-0.62409000	0.32764400
H	5.16008300	-1.62241900	1.36794300
C	6.39246100	-0.22429200	-2.04921200
H	4.50206200	-0.89630100	-2.83659300
C	7.21972900	-0.11483400	-0.91064300
H	7.39743100	-0.55730000	1.22115000
H	6.75537200	0.17387100	-3.00144400
O	8.42319800	0.49187400	-1.10959000
C	9.29530900	0.61905200	0.01871700
H	9.57775600	-0.36962700	0.42443800
H	10.19366800	1.12975600	-0.35738800
H	8.83539800	1.22827400	0.81856300
O	2.66587500	-2.04222900	-1.80899900
C	1.44939600	-2.80885900	0.51102200
C	0.59356900	-2.14700200	-0.57016400
C	1.29811500	-1.87947500	-1.71245100
H	0.89228100	-1.48535600	-2.65038100
H	-0.61911600	-2.98621000	-0.88840200
H	1.53961300	-3.89535000	0.29818000
H	0.99075400	-2.72219500	1.50882300
O	-1.25956000	-3.88189700	-1.16420600
O	-3.28722200	-2.44978600	-1.52166200
O	-2.86573200	-3.43141300	0.71108100
O	-3.49907200	-4.89502400	-1.18637200
Cl	-2.82654800	-3.64044800	-0.76072200

TsOH

H	-2.03385400	2.26011200	0.30432200
O	-1.46202600	2.26385200	-0.50229400
S	0.08016900	1.88107300	-0.01859800
O	0.26250600	2.36894600	1.36424600
O	0.92406100	2.35704100	-1.12636600
C	0.06755200	0.09759600	-0.01060400
C	-0.01186500	-0.58556700	1.21075100
C	0.11963900	-0.58996400	-1.23384500
C	-0.04119000	-1.98510400	1.19901400
H	-0.04256000	-0.02956800	2.15166000
C	0.08370800	-1.98659000	-1.22164700
H	0.19271500	-0.04014600	-2.17621700
C	0.00440900	-2.70633600	-0.01025200
H	-0.10163500	-2.52870100	2.14779600
H	0.12268600	-2.53269800	-2.17023100
C	-0.00242500	-4.21318500	-0.01412200
H	-0.56283300	-4.61149200	-0.87671100
H	1.02798400	-4.60867900	-0.08715300
H	-0.44628600	-4.61894600	0.90972300

IPrAuOTs

C	1.78788200	-0.03144900	0.13923700
C	3.90734000	0.60900100	0.64132900
C	3.88647600	-0.75068800	0.62647500
H	4.70882100	1.31712500	0.83363400
H	4.66478100	-1.48768400	0.80462400
N	2.58437300	-1.12440400	0.31859300
N	2.61804400	1.03179400	0.33755100
Au	-0.13955700	-0.02673900	-0.22999500
C	2.19790300	2.41066900	0.27583300
C	2.40633900	3.13441100	-0.92663600
C	1.60432300	2.96659400	1.42404600
C	1.99593200	4.47975300	-0.94032300
C	1.21462800	4.31585200	1.35464200
C	1.40974600	5.06439700	0.18755500

H	2.13268700	5.07505100	-1.84800500
H	0.75008700	4.78331100	2.22818500
H	1.09726800	6.11333900	0.15497700
C	2.10802000	-2.48355900	0.23686100
C	2.14318100	-3.13759100	-1.01608400
C	1.60575300	-3.08275500	1.41248400
C	1.66256900	-4.45864500	-1.06318000
C	1.13866000	-4.40538900	1.30798500
C	1.16810800	-5.08665600	0.08566700
H	1.66714000	-4.99717100	-2.01596900
H	0.73771300	-4.90213800	2.19732700
H	0.79531100	-6.11443800	0.02621900
C	1.41100600	2.16480500	2.70385100
H	1.62054700	1.10410200	2.47960600
C	2.41501700	2.61879600	3.78069800
H	2.30085200	2.00914800	4.69443600
H	3.45763300	2.52022500	3.43030000
H	2.24986900	3.67595100	4.05593100
C	-0.03600300	2.24048500	3.22076800
H	-0.30266600	3.26334400	3.54105200
H	-0.76162100	1.92641800	2.45086600
H	-0.15707600	1.57690200	4.09527000
C	1.55462300	-2.34922000	2.74634600
C	2.46941500	-3.02660700	3.78395200
H	3.51275300	-3.08376700	3.42696900
H	2.46195500	-2.45751900	4.73042000
H	2.13214700	-4.05457200	4.00670700
C	2.62342000	-2.44394900	-2.28420800
H	3.05366400	-1.46808900	-2.00082200
C	2.98110400	2.47357400	-2.17530000
C	3.92376300	3.39413300	-2.96654800
H	3.38938600	4.25724300	-3.40067100
H	4.74108000	3.78211900	-2.33398800
H	4.37560800	2.83611400	-3.80495000
C	1.43314300	-2.16794500	-3.22346700
H	0.65086100	-1.58032300	-2.71049600
H	1.76501800	-1.60246800	-4.11210100
H	0.97426800	-3.11074200	-3.57101300
C	3.72634500	-3.24257500	-3.00087600
H	4.08969200	-2.68199500	-3.88008300
H	4.58649300	-3.43161900	-2.33516000
H	3.35529700	-4.21847800	-3.36067300
C	0.11010500	-2.23312400	3.26599700
H	-0.55189600	-1.74251600	2.53194800
H	-0.31538900	-3.22646400	3.49454200
H	0.08774500	-1.63770100	4.19611800
H	1.93401300	-1.32412600	2.59151200
C	1.83604400	1.95897300	-3.07217100
H	2.24161200	1.42032800	-3.94728300
H	1.16847200	1.27432500	-2.51983300
H	1.22298100	2.80083800	-3.44089000
H	3.57288300	1.59820500	-1.85603300
O	-2.17140600	-0.08426600	-0.64726500
S	-3.08675800	0.28043900	0.58743000
O	-2.94098200	1.72768800	0.96454500
O	-2.94500500	-0.73018400	1.69019800
C	-4.71316500	0.06472100	-0.14483100
C	-5.33596800	1.14655800	-0.78363400
C	-5.34350800	-1.18612300	-0.06876100
C	-6.60104000	0.96480900	-1.35719700
H	-4.83983300	2.12077200	-0.81318300
C	-6.60744100	-1.35036500	-0.64842400
H	-4.85162400	-2.01203900	0.45271000

C	-7.25428000	-0.28277800	-1.30406400
H	-7.09503900	1.80939700	-1.85034200
H	-7.10662300	-2.32377600	-0.58504000
C	-8.60416700	-0.47877200	-1.94832800
H	-9.22220600	-1.19713400	-1.38334000
H	-9.15894500	0.47127100	-2.02520600
H	-8.49801600	-0.87942400	-2.97427200

Int1_TsO

N	2.08042200	0.89139600	-2.43356400
C	3.26641000	0.20494300	-2.40263900
C	-0.95661700	-1.58153600	0.83269600
C	-0.54721300	-3.34422100	2.20662800
C	-1.67352800	-2.71856200	2.66535500
H	-0.00732700	-4.21575300	2.56704200
H	-2.32598100	-2.93098200	3.50774600
N	-1.90498800	-1.64088800	1.81404000
N	-0.12503900	-2.63425700	1.08680900
Au	-0.90337000	-0.36870700	-0.78528000
C	1.07597400	-2.91130400	0.33403700
C	0.97005500	-3.64826000	-0.86702600
C	2.29897300	-2.41139800	0.83624500
C	2.15930900	-3.88604800	-1.57862200
C	3.45686000	-2.68764500	0.08781800
C	3.38820700	-3.41009300	-1.10825000
H	2.11790400	-4.44718400	-2.51747200
H	4.42036700	-2.30676900	0.43879600
H	4.29955900	-3.59755200	-1.68406200
C	-2.96530700	-0.67681700	1.98543400
C	-4.15341900	-0.83646500	1.23843900
C	-2.76385300	0.36806500	2.91715600
C	-5.16799700	0.11867800	1.43466900
C	-3.81511700	1.28943700	3.07870700
C	-5.00207200	1.16865500	2.34539700
H	-6.10243600	0.02924200	0.87093800
H	-3.70142500	2.11197300	3.79130300
H	-5.80515800	1.89930300	2.48780100
C	2.39615900	-1.61103200	2.12973500
H	1.38023200	-1.49519300	2.54551900
C	3.24177800	-2.36324400	3.17486100
H	3.27362800	-1.79472600	4.12112700
H	2.82981400	-3.36522800	3.39003500
H	4.28198800	-2.49454500	2.82721100
C	2.95179200	-0.19725100	1.87970400
H	3.96861300	-0.23337200	1.45263900
H	2.30776300	0.38087000	1.19693200
H	3.00782100	0.35625700	2.83444600
C	-1.49786700	0.47991400	3.75980200
C	-1.79577000	0.04384200	5.20859000
H	-2.20406100	-0.98127800	5.25135000
H	-0.87244000	0.06988400	5.81366800
H	-2.53124600	0.71942700	5.68093800
C	-4.36871000	-1.99862100	0.27663900
H	-3.46855200	-2.63739900	0.30063000
C	-0.35725400	-4.19128100	-1.38202700
C	-0.37334100	-5.73100500	-1.34816100
H	0.40047100	-6.15499500	-2.01234700
H	-0.18878700	-6.11284100	-0.32881200
H	-1.35358700	-6.11293200	-1.68452800

C	-4.54648400	-1.50631800	-1.17100400
H	-3.65661100	-0.94478000	-1.50815100
H	-4.68793700	-2.36370800	-1.85277400
H	-5.42692900	-0.84650200	-1.26886600
C	-5.56232600	-2.86415000	0.72180800
H	-5.67766300	-3.73173000	0.04859900
H	-5.42380400	-3.24317000	1.74935500
H	-6.50655000	-2.29166500	0.69771500
C	-0.87406400	1.88481900	3.71931800
H	-0.55848500	2.15481500	2.69762500
H	-1.56592500	2.65752100	4.09852500
H	0.02628200	1.90684100	4.35942000
H	-0.74722000	-0.21723300	3.34890000
C	-0.67229800	-3.66222300	-2.79259300
H	-1.66439600	-4.01694800	-3.12466700
H	-0.68084400	-2.55783800	-2.80558900
H	0.07334100	-4.00564400	-3.53118700
H	-1.15887100	-3.83771900	-0.71026700
C	4.31738300	0.70796700	-1.46362800
C	4.22115600	1.90295800	-0.72503500
C	5.46613600	-0.09602300	-1.29770500
C	5.23054100	2.28138600	0.16937500
H	3.35452100	2.56440400	-0.83011500
C	6.47492500	0.26425400	-0.40887600
H	5.53923700	-1.01640500	-1.88368200
C	6.36075700	1.45711400	0.33971500
H	5.12250200	3.21244800	0.73068300
H	7.36448900	-0.35848400	-0.27210700
O	7.39345300	1.71995100	1.19054400
C	7.30576800	2.90385000	1.99017200
H	6.42134500	2.87987100	2.65337400
H	8.22017300	2.91724300	2.60164600
H	7.27190200	3.81535600	1.36535900
O	3.45456300	-0.80596900	-3.11223800
C	1.03114400	0.44141400	-3.32286100
C	-0.30722400	0.59533200	-2.73568800
C	-1.48623800	0.88729200	-2.44686200
H	-2.46512000	1.35085100	-2.44662000
H	1.90490900	1.77429800	-1.91616500
H	1.01870400	1.00897300	-4.27810100
H	1.24402700	-0.61295800	-3.57721900
O	1.33021800	3.40113900	-1.38131600
S	0.47283000	3.42729700	-0.12512100
O	0.69338800	4.64571400	0.71391900
O	0.52476700	2.12767600	0.63341100
C	-1.21997400	3.54455400	-0.75456500
C	-2.28543000	3.01154500	-0.01267800
C	-1.46666200	4.16654200	-1.98733500
C	-3.58932200	3.08114200	-0.52027100
H	-2.09292800	2.51659400	0.94321300
C	-2.77488800	4.23287200	-2.48474300
H	-0.62718700	4.56089900	-2.56703000
C	-3.85812600	3.68810400	-1.76456900
H	-4.41122300	2.64369600	0.05681700
H	-2.95943500	4.70616000	-3.45620000
C	-5.26784500	3.77120500	-2.29768400
H	-5.28339400	3.81045300	-3.40011900
H	-5.87490700	2.90811600	-1.97413200
H	-5.77872600	4.68214300	-1.93255300

TS1_5exo_TsO

N	-2.26106100	-0.34177400	-0.74716700
C	-2.84730900	-1.45710500	-1.26028700

C	3.35532900	0.39360200	0.42124900
C	4.19867700	2.04872000	1.72914600
C	5.04682200	0.97731500	1.81918700
H	4.22506000	3.03314100	2.18882300
H	5.97003800	0.82955900	2.37319400
N	4.51197400	-0.02390000	1.01181400
N	3.17318700	1.67081800	0.86931500
Au	2.07853200	-0.60405200	-0.77519800
C	2.02915700	2.46805100	0.49273800
C	2.11413100	3.24748600	-0.68263000
C	0.85824100	2.37140200	1.27834700
C	0.95677900	3.94580700	-1.07359800
C	-0.27162700	3.08391800	0.83619300
C	-0.22574800	3.85794900	-0.32988300
H	0.98028200	4.54915000	-1.98690200
H	-1.21061000	3.00280000	1.39058700
H	-1.13457900	4.36258400	-0.66935600
C	5.07468800	-1.33994300	0.83092900
C	6.01830300	-1.52804100	-0.20351500
C	4.63888500	-2.37756400	1.68563700
C	6.54811100	-2.82151900	-0.36046900
C	5.20112000	-3.65138600	1.48364000
C	6.14724800	-3.87049900	0.47551300
H	7.27851700	-3.00855500	-1.15401300
H	4.88659300	-4.48221400	2.12331900
H	6.57174900	-4.87002700	0.33595600
C	0.77752900	1.51200700	2.53432000
H	1.77868600	1.09047500	2.73514200
C	0.37587400	2.35498800	3.75826800
H	0.37483900	1.73034900	4.66898000
H	1.07621400	3.19358100	3.91755100
H	-0.63735100	2.77609200	3.63934900
C	-0.19660100	0.33546100	2.32994100
H	-1.21893000	0.69621600	2.12230300
H	0.12055000	-0.30161100	1.48451900
H	-0.23166500	-0.29522000	3.23649300
C	3.58583800	-2.15796200	2.76442600
C	4.11331700	-2.53555100	4.16009500
H	5.02436100	-1.96648800	4.41473200
H	3.34911700	-2.31919900	4.92699700
H	4.35625600	-3.61082800	4.22420900
C	6.41360100	-0.40490600	-1.15423300
H	5.98686400	0.53796400	-0.77049200
C	3.37705500	3.30754900	-1.53331000
C	3.86235900	4.75500600	-1.72863100
H	3.12477300	5.35730300	-2.28738700
H	4.04101600	5.25383900	-0.76025800
H	4.80653100	4.76851400	-2.30129700
C	5.80823800	-0.65202200	-2.54975700
H	4.70922200	-0.75107500	-2.49615200
H	6.04621800	0.18703800	-3.22725600
H	6.21052600	-1.57776700	-2.99838500
C	7.93853200	-0.21897000	-1.23475500
H	8.18126300	0.63645400	-1.88921900
H	8.37461500	-0.02330100	-0.23979400
H	8.43755500	-1.10978300	-1.65473000
C	2.29499800	-2.92790200	2.42708000
H	1.90194200	-2.62814400	1.43901600
H	2.47267800	-4.01779300	2.40699000
H	1.51611300	-2.72400200	3.18259800
H	3.33203700	-1.08393500	2.78582200
C	3.15186500	2.60785700	-2.88766100
H	4.08367000	2.59949900	-3.48078100

H	2.82490900	1.56190400	-2.74477400	H	0.50317600	4.91853900	1.73052200
H	2.37649600	3.12651000	-3.47924200	H	1.17163100	5.91926600	-0.44164200
H	4.17701400	2.75878500	-1.00609500	C	3.24482400	-2.31766700	0.99470500
C	-4.13257200	-1.91763700	-0.67604800	C	4.01456500	-2.96798600	0.00473500
C	-4.63994100	-1.43030400	0.54433100	C	2.25141500	-2.96994500	1.75899100
C	-4.89617100	-2.85495300	-1.40542900	C	3.75451200	-4.33226800	-0.21814500
C	-5.88520000	-1.84942300	1.02176800	C	2.03251700	-4.33445700	1.49510500
H	-4.08034200	-0.69545600	1.13018100	C	2.77295200	-5.00833200	0.51654800
C	-6.14552300	-3.26513500	-0.95006700	H	4.32344700	-4.86730300	-0.98521900
H	-4.49469000	-3.23873000	-2.34783900	H	1.26553900	-4.87137700	2.06246800
C	-6.65545600	-2.75291400	0.26350500	H	2.58224900	-6.06906100	0.32336300
H	-6.25679400	-1.44463400	1.96500800	C	1.30023300	2.54975300	2.83625600
H	-6.75453100	-3.97362700	-1.51947000	H	1.87709000	1.62323200	3.00326300
O	-7.90370500	-3.18267000	0.60888000	C	1.58256900	3.48647900	4.02495200
C	-8.46195800	-2.67360700	1.82631800	H	1.29040400	2.99986800	4.97227600
H	-8.53237900	-1.57118900	1.80998000	H	2.65318200	3.74970700	4.09056100
H	-9.47181900	-3.10434600	1.89201100	H	1.00851900	4.42617200	3.94261800
H	-7.86928800	-2.99193600	2.70361900	C	-0.18790400	2.15693100	2.77437300
O	-2.28944300	-2.05458800	-2.21914700	H	-0.83141500	3.03619000	2.59951400
C	-1.12034200	0.15464900	-1.49202400	H	-0.37935200	1.45142700	1.95119100
C	-0.18910700	-0.93752300	-1.79791900	H	-0.49797000	1.68420900	3.72387200
C	0.77614700	-1.73020300	-1.98722600	C	1.41619600	-2.24211600	2.80537300
H	1.02940600	-2.68228300	-2.44604300	C	1.52658700	-2.91303900	4.18590500
H	-2.71394000	0.31729400	-0.07029800	H	2.57557800	-2.96326000	4.52632200
H	-1.42752200	0.63069000	-2.44590100	H	0.95032400	-2.34044800	4.93365900
H	-0.61751600	0.93196900	-0.89154400	H	1.12564700	-3.94181000	4.17144500
O	-3.26992200	1.48562900	1.07090200	C	5.05316100	-2.22917400	-0.82990500
S	-3.99884200	2.59852200	0.31173900	H	5.18283300	-1.22030200	-0.40129800
O	-3.34537700	2.89269400	-1.00743500	C	4.06390700	2.36703000	-1.51059300
O	-4.26954400	3.78149500	1.18359600	C	5.34128300	3.20873600	-1.68751200
C	-5.60268600	1.86881700	-0.08904100	H	5.12010300	4.17912100	-2.16610000
C	-5.76696400	1.17304300	-1.29715900	H	5.82573000	3.41384500	-0.71687900
C	-6.65093700	1.92447900	0.83926400	H	6.06657600	2.67534400	-2.32734200
C	-6.97538000	0.52078800	-1.56402300	C	4.55532000	-2.05503000	-2.27761900
H	-4.94633200	1.15008000	-2.01992700	H	3.58946800	-1.51876800	-2.30173300
C	-7.85813600	1.26904700	0.55968700	H	5.28629100	-1.47683100	-2.87049900
H	-6.52033200	2.48779500	1.76814700	H	4.41329800	-3.03329000	-2.77063400
C	-8.03803300	0.54878500	-0.63789000	C	6.42428400	-2.92597600	-0.78927900
H	-7.09544000	-0.03041200	-2.50351500	H	7.16700400	-2.33594500	-1.35434300
H	-8.68041000	1.32070100	1.28311600	H	6.79058800	-3.03618300	0.24627700
C	-9.31997500	-0.19796700	-0.91601400	H	6.38410400	-3.93153400	-1.24340700
H	-9.16185400	-1.29063500	-0.85108400	C	-0.05191500	-2.13296400	2.35093600
H	-10.11013100	0.07019800	-0.19484000	H	-0.12297100	-1.62690900	1.37239100
H	-9.69962600	0.01195300	-1.93164300	H	-0.51635300	-3.13117700	2.25623300

TS1_6endo_TsO

N	-2.37142600	0.11522900	-2.91944500	H	1.80621300	-1.21423200	2.90480200
C	-2.90524100	-1.12595400	-2.74585000	C	3.42719000	2.03022700	-2.87136800
C	2.71269700	0.05233700	0.55614300	H	4.14221600	1.47367900	-3.50322900
C	4.20484500	1.02640000	1.96790000	H	2.52418400	1.40588600	-2.73924000
C	4.36654400	-0.32868800	2.07347500	H	3.13006700	2.94316500	-3.41690200
H	4.70734600	1.85488100	2.46001900	H	4.35887300	1.41223300	-1.04125000
H	5.03714900	-0.93322200	2.67837700	C	-4.24867000	-1.23032300	-2.11060600
N	3.44673300	-0.90429600	1.20155600	C	-5.05773500	-0.12152500	-1.79210500
N	3.18790300	1.23747100	1.04049500	C	-4.67262800	-2.51469600	-1.70333500
Au	1.30030300	-0.28820500	-0.85305600	C	-6.23633000	-0.27848900	-1.05650000
C	2.66852700	2.52756400	0.65183400	H	-4.76414200	0.89257000	-2.07787100
C	3.06959700	3.06631300	-0.59117900	C	-5.84138100	-2.68476500	-0.96865700
C	1.75567200	3.16817600	1.51950800	H	-4.04424200	-3.37375400	-1.95477000
C	2.51473500	4.30452500	-0.96078200	C	-6.62148700	-1.56108300	-0.61913600
C	1.23528000	4.40509700	1.10036000	H	-6.82711200	0.60420400	-0.80389800
C	1.60481400	4.96435300	-0.12748900	H	-6.16317900	-3.67478300	-0.63135000
H	2.79684300	4.75029400	-1.92004600	O	-7.71709700	-1.81846600	0.15242500
				C	-8.50281000	-0.69714900	0.57505200

H	-8.95416600	-0.17309800	-0.28717000	H	-2.02960300	5.48729000	-1.33597700
H	-9.30133100	-1.11609800	1.20457200	H	-0.43507100	5.07471000	-2.02811500
H	-7.90157300	0.01583900	1.16778100	C	-0.83421600	2.32822800	-2.28450200
O	-2.25512500	-2.16895500	-3.04930400	H	0.24741100	2.55061400	-2.25110400
C	-0.96541700	0.28402600	-3.24311400	H	-0.98687900	1.29380200	-1.92842700
C	-0.13161600	-0.60107700	-2.34742800	H	-1.16705700	2.38364100	-3.33688600
C	-0.26863300	-1.81260700	-2.00017300	C	-4.35677100	-0.31041900	-3.01097100
H	-0.18627200	-2.82075700	-1.62104400	C	-5.36623900	0.01635500	-4.12525000
H	-2.79372300	0.94760400	-2.44829100	H	-6.30310100	0.42802400	-3.71078300
H	-0.76025700	-0.02707600	-4.28355100	H	-4.94079400	0.76336300	-4.81839600
H	-0.71674600	1.34459800	-3.11947100	H	-5.62318500	-0.87944200	-4.71762900
O	-3.13796900	2.50791700	-1.68262500	C	-5.46561300	-1.59280200	1.83675700
S	-2.30496900	2.54991400	-0.40436400	H	-5.26799200	-0.51269200	1.95253400
O	-2.34865600	3.88508700	0.26882700	C	-2.32303800	1.48768400	3.33451700
O	-0.93414000	1.97292000	-0.62177600	C	-2.83819400	2.35972700	4.49415100
C	-3.14589400	1.39805300	0.70757000	H	-2.00412800	2.80234300	5.06699500
C	-4.21966800	1.84412600	1.49151600	H	-3.47016300	3.18664400	4.12549300
C	-2.78907300	0.04109100	0.71395300	H	-3.44138400	1.75284400	5.19249100
C	-4.94415400	0.92568200	2.26274700	C	-4.32123700	-2.34912700	2.53988200
H	-4.47513100	2.90808500	1.49943700	H	-3.34451500	-2.10073200	2.08668500
C	-3.52026300	-0.86798900	1.48819500	H	-4.28543300	-2.08524300	3.61201700
H	-1.94008500	-0.29517700	0.11193300	H	-4.46458600	-3.44186200	2.46173400
C	-4.61890500	-0.44589500	2.26292600	C	-6.82043300	-1.88471400	2.50375500
H	-5.78119100	1.27830700	2.87703100	H	-6.79652800	-1.56984400	3.56175800
H	-3.24310400	-1.92827000	1.47918500	H	-7.64163200	-1.34262500	2.00328300
C	-5.45154600	-1.44246300	3.03179100	H	-7.06423300	-2.96151800	2.48476600
H	-5.97828000	-0.96758100	3.87696200	C	-3.03414300	-0.84763500	-3.59092900
H	-6.21947300	-1.89732100	2.37744300	H	-2.30880400	-1.06354200	-2.78529800
H	-4.83557000	-2.26759800	3.42889900	H	-3.19836300	-1.78043300	-4.15991900

Int2_5exo_TsO

N	2.91891700	-0.69817500	-1.77220300	H	-2.09235600	-0.32855600	4.53116700
C	3.38928800	-1.66959500	-1.01091400	H	-1.14036900	-0.32816900	3.01406700
C	-3.16280900	0.48498400	0.15625300	H	-0.60149100	0.64611100	4.41201400
C	-4.38964900	2.38214200	0.48165100	H	-3.20364000	1.07099700	2.81575500
C	-5.24469000	1.41302600	0.03228100	C	4.77378800	-2.01010200	-0.77210900
H	-4.55561300	3.42030600	0.75744800	C	5.81610100	-1.31304100	-1.42315200
H	-6.31265900	1.42780200	-0.16867800	C	5.09360500	-3.00755000	0.18256600
N	-4.47709800	0.26677300	-0.15830400	C	7.14888100	-1.60311200	-1.13596600
N	-3.12734900	1.79821800	0.54649400	H	5.58850600	-0.51443600	-2.13557600
Au	-1.58478700	-0.80111700	0.08619100	C	6.41844400	-3.29679100	0.47555600
C	-1.92430700	2.46577500	0.98576700	H	4.29041500	-3.54122400	0.69703000
C	-1.52631800	2.31325000	2.33241600	C	7.45948100	-2.59645900	-0.18047900
C	-1.18742500	3.21665400	0.04058000	H	7.93855300	-1.04802800	-1.64611500
C	-0.33540900	2.94987000	2.72763100	H	6.68219700	-4.06011500	1.21276800
C	0.00361300	3.81923200	0.48410000	O	8.71555300	-2.94882800	0.18023200
C	0.42404700	3.68842100	1.81370100	C	9.81289600	-2.27113900	-0.45167800
H	0.00487900	2.85178700	3.76363200	H	9.78943200	-1.18758300	-0.23855000
H	0.63114500	4.36232100	-0.22713700	H	10.72010600	-2.71161000	-0.01453300
H	1.36161800	4.15449900	2.13291800	H	9.81026000	-2.43889100	-1.54329700
C	-4.98182900	-1.00434300	-0.61570100	O	2.42917900	-2.36314200	-0.39194900
C	-5.47295400	-1.91401300	0.34753100	C	1.46089900	-0.61885900	-1.65488600
C	-4.93081800	-1.29145200	-1.99742100	C	1.16971600	-1.66820400	-0.60364700
C	-5.92785900	-3.16049800	-0.11852400	C	0.07771500	-1.97399500	0.10518100
C	-5.40143000	-2.55153400	-2.41021700	H	0.18967500	-2.82111900	0.79930700
C	-5.89368800	-3.47614600	-1.48212800	H	3.49410300	0.13318600	-2.13032300
H	-6.30493700	-3.89580000	0.59909300	H	1.15931400	0.39477700	-1.34628700
H	-5.37136800	-2.81204200	-3.47324200	H	0.98403300	-0.83756600	-2.62857500
H	-6.24977800	-4.45369200	-1.82361000	O	4.30287400	1.47531900	-2.44184200
C	-1.62402300	3.32739500	-1.41548400	S	4.03388400	2.57675600	-1.40234300
H	-2.69169100	3.04973100	-1.47288900	O	2.64472200	3.12811000	-1.51745600
C	-1.49041000	4.75757200	-1.96505100	O	5.13799300	3.58010600	-1.37027900
H	-1.90985200	4.80855300	-2.98523200				

C	4.09263200	1.68825800	0.17057100
C	2.90607700	1.33058100	0.82374700
C	5.33169300	1.26231800	0.67873400
C	2.95780700	0.52058300	1.96781400
H	1.94765500	1.68800000	0.43882000
C	5.37145000	0.45480000	1.81978800
H	6.25648500	1.56001300	0.17541700
C	4.18614200	0.05583600	2.47397100
H	2.02432900	0.24154900	2.46999400
H	6.33893000	0.11025200	2.20294700
C	4.24173000	-0.86194500	3.67012700
H	4.93341000	-0.48266700	4.44339600
H	3.24762300	-0.98664000	4.13043500
H	4.60624800	-1.86504600	3.37971000

H	-2.83924500	-5.14359300	-2.81692400
H	-3.95502800	-5.19545800	-1.42581300
H	-4.50353100	-4.53242200	-2.99360900
C	-5.38918800	0.87622500	-2.75047400
H	-4.31416800	0.94424700	-2.50645500
H	-5.51525800	0.12697400	-3.55242600
H	-5.71100800	1.85636700	-3.14576100
C	-7.70811400	0.33901700	-1.85556000
H	-7.84656800	-0.44080100	-2.62491900
H	-8.30172600	0.05402800	-0.96945700
H	-8.12825800	1.27815400	-2.25645600
C	-2.67629800	2.52754700	2.84371100
H	-2.16776200	2.31367800	1.88616400
H	-2.84912400	3.61720100	2.90265800
H	-1.99555100	2.24560600	3.66623800
H	-3.75577300	0.67403100	2.89121800
C	-2.81069900	-2.33563400	-3.10834500
H	-3.66715000	-2.24514800	-3.80027600
H	-2.50050200	-1.32006800	-2.80272500
H	-1.97220100	-2.79429100	-3.66226500
H	-4.05233400	-2.69249500	-1.39288000
C	3.93596000	2.30921100	-1.25297800
C	4.99618300	1.38456500	-1.38601600
C	4.22892700	3.63605600	-0.85067700
C	6.30925800	1.75656300	-1.10289000
H	4.80156300	0.35307600	-1.69483600
C	5.53642600	4.01754700	-0.58172100
H	3.41678000	4.35835700	-0.73864600
C	6.58828700	3.07838600	-0.69297200
H	7.10188900	1.01084200	-1.18986600
H	5.77424200	5.03660100	-0.26415900
O	7.82393700	3.54287200	-0.38408800
C	8.91313400	2.60852500	-0.41720700
H	9.07470400	2.21631300	-1.43745700
H	9.79868600	3.17632600	-0.09777400
H	8.73474300	1.77096800	0.27937100
O	1.64722900	2.89651800	-1.46875000
C	0.77043800	0.28035500	-1.88717400
C	-0.18828900	1.29171800	-1.28708400
C	0.28967800	2.53665700	-1.15122800
H	-0.21303000	3.42438600	-0.76569000
H	2.84084800	-0.14628400	-1.49294000
H	0.61192500	0.18338600	-2.97987100
H	0.64316300	-0.72260200	-1.45128200
O	3.63481100	-1.58782000	-1.36126200
S	3.75173800	-1.95160800	0.12290300
O	3.58733500	-3.42134200	0.35181400
O	2.91651300	-1.05720200	0.98726300
C	5.47311500	-1.57385400	0.52886600
C	6.50644700	-2.11270200	-0.25648500
C	5.77278600	-0.74722700	1.61812300
C	7.83776000	-1.82515500	0.06181300
H	6.26675300	-2.74660700	-1.11586000
C	7.11199300	-0.46924300	1.92989800
H	4.95410900	-0.32109700	2.20479500
C	8.16462800	-1.00697200	1.16555200
H	8.64292700	-2.24619500	-0.55153400
H	7.34501400	0.17805100	2.78317400
C	9.60713900	-0.73823500	1.52138800
H	9.70279600	0.11527900	2.21307900
H	10.06268400	-1.61603300	2.01732400
H	10.21682600	-0.52823900	0.62491300

Int2_gendo_TsO

N	2.16897400	0.66274000	-1.63690000
C	2.55060600	1.90931000	-1.47381800
C	-3.41182200	-0.50944000	0.37525000
C	-4.42099300	-2.30682100	1.35288500
C	-5.28170300	-1.24642700	1.45171000
H	-4.50499500	-3.33861500	1.68392500
H	-6.27416000	-1.15894800	1.88608600
N	-4.64584700	-0.16161400	0.84989200
N	-3.28918000	-1.83634100	0.69626300
Au	-1.91338900	0.53763800	-0.51384400
C	-2.10178400	-2.59429600	0.37195300
C	-2.04035900	-3.23248900	-0.88730900
C	-1.02038500	-2.57625300	1.28229200
C	-0.83454600	-3.87254800	-1.22822400
C	0.16819300	-3.21307600	0.88180200
C	0.26355500	-3.85101300	-0.36028000
H	-0.74924800	-4.36735800	-2.20139300
H	1.04861300	-3.17890700	1.52856800
H	1.21472400	-4.30725200	-0.65052400
C	-5.19554900	1.16700200	0.74660700
C	-5.97926000	1.48363700	-0.38538600
C	-4.90683400	2.09354300	1.77284500
C	-6.49832400	2.78871400	-0.46351300
C	-5.45363700	3.38382800	1.64676300
C	-6.24321700	3.72729900	0.54336300
H	-7.10440300	3.07387900	-1.32929300
H	-5.24711700	4.13090600	2.42002200
H	-6.65674900	4.73798500	0.46302800
C	-1.09162700	-1.86880900	2.62983200
H	-2.12489100	-1.50653100	2.77627400
C	-0.77218700	-2.83546500	3.78513000
H	-0.88323800	-2.32003400	4.75566600
H	-1.44735900	-3.70932700	3.78175700
H	0.26505300	-3.20842300	3.72210900
C	-0.15692600	-0.64431100	2.65593100
H	0.89439200	-0.93321200	2.48440400
H	-0.43518400	0.07455100	1.86434400
H	-0.22463800	-0.13118500	3.63240400
C	-4.00148500	1.74839000	2.94841200
C	-4.69238900	1.99311200	4.30111200
H	-5.63086600	1.41758500	4.38421400
H	-4.02790400	1.68665500	5.12806300
H	-4.93555200	3.06027900	4.44807400
C	-6.21599900	0.48376700	-1.51027500
H	-5.85743100	-0.50433600	-1.17297400
C	-3.19391100	-3.18575100	-1.88163200
C	-3.64653200	-4.59562800	-2.29976900

TS2_5exo_TsO

N	3.41240200	-0.10615100	-3.16054200
C	3.27391400	0.13912700	-1.90164900
C	-2.29959500	0.84779000	0.69267100
C	-4.02272200	1.46005500	2.05554600
C	-2.96662400	2.28255600	2.33596800
H	-5.03057900	1.41533000	2.45932200
H	-2.85692300	3.10093700	3.04246200
N	-1.92620400	1.89318300	1.49552900
N	-3.59540600	0.59215100	1.05281100
Au	-1.19662800	-0.10965800	-0.69288300
C	-4.42941000	-0.38803700	0.39841000
C	-5.25892500	0.05321600	-0.65640900
C	-4.36530400	-1.73531100	0.82621400
C	-6.07376000	-0.90844700	-1.28176900
C	-5.20249900	-2.65278400	0.16673800
C	-6.05032800	-2.24484400	-0.87078500
H	-6.72323300	-0.60593700	-2.10944300
H	-5.18070700	-3.70562400	0.46099300
H	-6.68920600	-2.98030700	-1.37086100
C	-0.62944400	2.52297500	1.45428000
C	-0.38473900	3.49586400	0.45844100
C	0.33395000	2.13943700	2.41364600
C	0.88623000	4.09929900	0.44649500
C	1.58089000	2.78858400	2.36713000
C	1.85776700	3.75401800	1.39229000
H	1.11351800	4.84926400	-0.31817300
H	2.34956300	2.52163200	3.09936500
H	2.84192700	4.23268300	1.36425300
C	-3.44550700	-2.17105300	1.96111300
H	-2.55018200	-1.52515500	1.93109800
C	-4.13451500	-1.96087400	3.32513200
H	-3.45564800	-2.25424500	4.14544400
H	-4.42256300	-0.90740400	3.48430200
H	-5.04830300	-2.57793400	3.40007600
C	-2.95726200	-3.62029300	1.81966000
H	-3.76939900	-4.34828200	1.99735100
H	-2.53118600	-3.80719200	0.82056100
H	-2.16536100	-3.81842600	2.56017800
C	0.06176600	1.06707100	3.45978400
C	-0.00236600	1.67872800	4.87170600
H	-0.77938800	2.46032100	4.94106400
H	-0.23473400	0.89919500	5.61851800
H	0.96281500	2.13808700	5.15165100
C	-1.42956200	3.89202200	-0.57756100
H	-2.35372200	3.32555400	-0.37112300
C	-5.24252800	1.49333700	-1.15538400
C	-6.65353800	2.10086100	-1.23294400
H	-7.28353100	1.58225400	-1.97688400
H	-7.16934500	2.04838900	-0.25830300
H	-6.59407000	3.16206800	-1.53269400
C	-0.96888400	3.51112900	-1.99637900
H	-0.77693000	2.42516400	-2.06392600
H	-1.74598400	3.77269800	-2.73644400
H	-0.04166100	4.04288100	-2.27496300
C	-1.77562800	5.38918000	-0.48261100
H	-2.57031000	5.64330800	-1.20633300
H	-2.13383700	5.65657000	0.52693300
H	-0.90029800	6.02357700	-0.70934700
C	1.10254700	-0.06400700	3.38626600
H	1.12493400	-0.51855800	2.38268800
H	2.11553000	0.29856100	3.63841400
H	0.84614600	-0.86185000	4.10532500

H	-0.92193100	0.61706200	3.24287500
C	-4.52025300	1.57538600	-2.51447500
H	-4.46159400	2.62389600	-2.85784600
H	-3.49389900	1.17404500	-2.44275700
H	-5.05822900	0.99482200	-3.28530500
H	-4.66339100	2.10081600	-0.43880300
C	4.24842200	0.70254800	-0.97527700
C	5.52711600	1.06497600	-1.44356400
C	3.94283100	0.87599900	0.39399400
C	6.49245700	1.57897200	-0.57472800
H	5.75904500	0.94021300	-2.50524300
C	4.89892500	1.38614600	1.26714200
H	2.95384500	0.60452200	0.77008200
C	6.18189700	1.73932600	0.79333700
H	7.47539500	1.85295700	-0.96419100
H	4.67796200	1.52091500	2.32998600
O	7.04151600	2.22607300	1.72896500
C	8.35306000	2.60470900	1.29405400
H	8.31067500	3.41512800	0.54359400
H	8.87060900	2.96641700	2.19419300
H	8.90373000	1.74222400	0.87619400
O	2.02017100	-0.16311100	-1.34846200
C	2.12795900	-0.65180700	-3.60269000
C	1.24262900	-0.65876000	-2.37250400
C	-0.05028400	-1.05867300	-2.16040900
H	-0.53615200	-1.39286800	-3.09195300
H	-0.11719700	-2.18315100	-1.34619200
H	1.69741100	-0.03532800	-4.41430900
H	2.25432100	-1.67209100	-4.01267100
O	-0.25124600	-3.37009300	-0.91018500
S	0.61745300	-3.66340600	0.36749200
O	0.48304900	-5.10668200	0.69934100
O	0.35656700	-2.68753500	1.46320500
C	2.29189800	-3.34815000	-0.20569800
C	3.22462500	-2.78469500	0.67364900
C	2.65601600	-3.67787800	-1.52185900
C	4.52811800	-2.53517500	0.22428000
H	2.92075200	-2.51723000	1.68966400
C	3.95927300	-3.41740800	-1.95600900
H	1.91583500	-4.10946500	-2.20142000
C	4.91379600	-2.83615400	-1.09501800
H	5.25288500	-2.07120400	0.90166800
H	4.24202000	-3.65505500	-2.98788400
C	6.29530500	-2.50902800	-1.60089000
H	6.80885800	-3.40832100	-1.98656500
H	6.24144400	-1.78538900	-2.43445500
H	6.92229700	-2.06791200	-0.80908700

TS2_6endo_TsO

N	-2.84730700	0.68380200	-2.32065600
C	-3.44442600	-0.36163500	-1.88535500
C	1.47624300	1.27306500	1.21846700
C	2.19066400	3.06470800	2.43489800
C	2.41493400	1.94223000	3.18395400
H	2.38400600	4.11578500	2.63251900
H	2.84051900	1.80991500	4.17500000
N	1.97152600	0.85962900	2.42540500
N	1.61756300	2.63500800	1.24204800
Au	0.54202600	0.27345300	-0.25713700
C	1.17267900	3.48608500	0.16394000
C	2.07453900	3.77074100	-0.88551500
C	-0.16281300	3.94907500	0.18522100
C	1.59587700	4.55933200	-1.94783300

C	-0.58821800	4.73463400	-0.90128800
C	0.28007000	5.03595400	-1.95715900
H	2.26288100	4.78983900	-2.78460000
H	-1.61928900	5.10161500	-0.92424500
H	-0.07397100	5.64251900	-2.79718000
C	2.00818500	-0.51468900	2.86175900
C	3.23742500	-1.20974600	2.78504300
C	0.82030000	-1.09567100	3.36196700
C	3.25296400	-2.54126900	3.23950700
C	0.89458700	-2.42928800	3.80492800
C	2.09629600	-3.14468200	3.74684900
H	4.18692600	-3.10960500	3.19755900
H	-0.00478600	-2.91025600	4.20321600
H	2.13183100	-4.18144100	4.09746400
C	-1.13623000	3.59249000	1.30210100
H	-0.57962300	3.04337000	2.08146500
C	-1.72997300	4.85035100	1.96043700
H	-2.39024800	4.56585100	2.79861200
H	-0.93885100	5.51084900	2.35658300
H	-2.33350200	5.43695200	1.24552600
C	-2.24319200	2.65743100	0.77864800
H	-2.83616100	3.14092000	-0.01764900
H	-1.80970100	1.73286300	0.35855600
H	-2.93210100	2.37918200	1.59651400
C	-0.49520600	-0.33263000	3.46168100
C	-0.89182600	-0.12036400	4.93451700
H	-0.10684100	0.42500800	5.48728800
H	-1.82672500	0.46387900	4.99974000
H	-1.05871000	-1.08410000	5.44786600
C	4.51514700	-0.55520300	2.27513900
H	4.24648400	0.41087300	1.81383500
C	3.49424700	3.22045400	-0.91455900
C	4.53619600	4.34440800	-1.05836500
H	4.42933200	4.87669300	-2.02003700
H	4.44465300	5.08879900	-0.24782200
H	5.55667700	3.92429000	-1.02308200
C	5.21822400	-1.39655200	1.19547000
H	4.56152600	-1.57775500	0.32820100
H	6.11442500	-0.86123700	0.83479300
H	5.55532700	-2.37202900	1.58900800
C	5.46642100	-0.26237300	3.45241600
H	6.37339100	0.25504100	3.09305700
H	4.98813200	0.37478500	4.21691900
H	5.78278200	-1.19841900	3.94674300
C	-1.61504500	-1.03587400	2.67452000
H	-1.33367200	-1.15585100	1.61392000
H	-1.83748200	-2.03594300	3.08779200
H	-2.54432100	-0.44056600	2.71526400
H	-0.35447800	0.66307300	3.00855300
C	3.64329300	2.17010600	-2.03194900
H	4.65506800	1.72844600	-2.01287300
H	2.91573600	1.34953300	-1.91222600
H	3.48751400	2.62407800	-3.02704600
H	3.68614400	2.71209700	0.04602400
C	-4.87117300	-0.40343000	-1.52574000
C	-5.67585800	0.73224600	-1.74898700
C	-5.46296400	-1.54931400	-0.94739200
C	-7.03005400	0.73946400	-1.40732700
H	-5.21785800	1.61900000	-2.19644400
C	-6.81329700	-1.55475800	-0.60545000
H	-4.85477900	-2.43819800	-0.76323800
C	-7.60956600	-0.41151800	-0.83138400
H	-7.62637400	1.63581300	-1.59214300

H	-7.27857100	-2.43794000	-0.15779600
O	-8.91647600	-0.51838200	-0.46226400
C	-9.76469800	0.61148700	-0.69503300
H	-9.81869200	0.86050200	-1.77062800
H	-10.76135800	0.31180400	-0.33958700
H	-9.42396600	1.49674700	-0.12722700
O	-2.80922500	-1.60146400	-1.64759300
C	-1.42830000	0.54835300	-2.67724500
C	-0.68647500	-0.45828700	-1.79810600
C	-1.45937100	-1.51036800	-1.39652400
H	-1.11936200	-2.37644200	-0.82144500
H	0.51641300	-0.87543300	-2.43890300
H	-1.36782500	0.23022900	-3.73985000
H	-0.96360000	1.54684200	-2.62797100
O	1.35527300	-1.22251600	-3.27423000
S	2.44349500	-2.16787100	-2.63395900
O	3.29993200	-1.42977300	-1.66439100
O	3.11812000	-2.91379400	-3.72618900
C	1.44454300	-3.32854100	-1.69296600
C	1.46582800	-3.30424600	-0.29316400
C	0.59355800	-4.20672400	-2.38474500
C	0.61891500	-4.16740400	0.41814500
H	2.13278800	-2.61630200	0.23249600
C	-0.24204500	-5.06231600	-1.66088500
H	0.58544900	-4.21493100	-3.47872200
C	-0.24602300	-5.05519800	-0.24873400
H	0.63179800	-4.14299300	1.51253300
H	-0.90967700	-5.74558900	-2.19766300
C	-1.14757700	-5.98839900	0.52063300
H	-2.18363100	-5.95376300	0.14023800
H	-0.80711400	-7.03633600	0.42742000
H	-1.16620100	-5.73790900	1.59414200

HTFA

C	0.60616000	-0.00073200	0.00001100
C	-0.93744000	0.16141800	0.00005000
O	-1.49859600	1.23862300	-0.00000100
O	-1.51991900	-1.05027800	-0.00001600
H	-2.49805300	-0.91032300	-0.00004900
F	1.00687700	-0.68291100	1.09735000
F	1.19318500	1.20611600	-0.00004000
F	1.00682600	-0.68298200	-1.09730300

IPrAuTFA

C	1.13930600	0.03376600	0.26106700
C	3.09745500	0.78624200	1.14312300
C	3.14711700	-0.58112500	1.13898400
H	3.81296900	1.53374400	1.47508400
H	3.91361000	-1.27844400	1.46633900
N	1.94320200	-1.02145600	0.59604600
N	1.86428400	1.14218900	0.60358000
Au	-0.68521400	-0.04321600	-0.46394900
C	1.38437300	2.49364800	0.44395900
C	1.68359500	3.17332300	-0.75744600
C	0.61690100	3.05898100	1.48649800
C	1.19048700	4.48337600	-0.89356700
C	0.15271500	4.37373700	1.29962400
C	0.43584300	5.07852200	0.12416700
H	1.39403700	5.03970700	-1.81429200
H	-0.44681100	4.84511300	2.08495000
H	0.05974200	6.09900300	-0.00258600
C	1.55810400	-2.40302200	0.43711400

C	4.32412200	1.27907900	-0.86570200	H	-0.17131800	3.44282800	4.05863900
C	5.38854600	-0.89765300	-0.88183300	H	-1.74212300	2.85285600	3.43857200
C	5.33057200	1.76997400	-0.02452300	C	-0.86007100	0.54902500	2.20473900
H	3.52289400	1.96522800	-1.16258100	H	-1.82366800	0.88391100	1.78003000
C	6.39160800	-0.42585700	-0.03972400	H	-0.33941300	-0.04748000	1.43379000
H	5.39566300	-1.93349600	-1.23318300	H	-1.07303600	-0.11256000	3.06380300
C	6.36852400	0.91659400	0.39999400	C	2.26729000	-2.61757400	2.78915100
H	5.28935800	2.81185800	0.30121700	C	2.66796700	-3.11899000	4.18856000
H	7.20910400	-1.07332200	0.29233100	H	3.59529200	-2.63333500	4.53930200
O	7.39003000	1.28637400	1.22485500	H	1.86793400	-2.89777400	4.91661200
C	7.38769400	2.63179800	1.71265200	H	2.83470700	-4.21065100	4.19327400
H	6.48193700	2.84321200	2.31058200	C	5.64162500	-0.87235500	-0.67607300
H	8.27736200	2.71705600	2.35378000	H	5.29220000	0.07646800	-0.23299700
H	7.46149900	3.36284400	0.88649200	C	3.12868800	2.86610600	-1.27192800
O	3.36523900	-1.85036100	-2.57525700	C	4.00633400	4.13057000	-1.31613100
C	1.17535500	-0.40973600	-3.35599000	H	3.48815100	4.96185500	-1.82562200
C	-0.14590500	0.12693700	-3.00020100	H	4.27416800	4.47041300	-0.30052200
C	-1.26445900	0.67781300	-2.92814200	H	4.94167100	3.92885600	-1.86751900
H	-2.13966300	1.27225500	-3.15514100	C	5.15628700	-0.90459300	-2.13856500
H	2.12861600	1.13343200	-2.24126900	H	4.05367000	-0.86092800	-2.19313400
H	1.33102500	-0.17444600	-4.43088800	H	5.56498800	-0.04594200	-2.70031400
H	1.20114500	-1.51093700	-3.26026700	H	5.48476300	-1.82983800	-2.64499500
O	1.52271000	2.77146000	-2.09810000	C	7.17814200	-0.87624200	-0.59848200
C	0.77874800	2.88785100	-1.07716400	H	7.58672900	-0.00232100	-1.13541300
O	0.85693200	2.35245300	0.05573400	H	7.52949700	-0.83024300	0.44692700
C	-0.43766000	3.85680500	-1.25321100	H	7.60913000	-1.78138600	-1.06122400
F	-0.57490300	4.34058200	-2.51603800	C	0.94518000	-3.25579300	2.32434100
F	-1.62411100	3.23654100	-0.94448500	H	0.64379900	-2.87293200	1.33277400
F	-0.33646900	4.93276700	-0.41772100	H	1.03180700	-4.35455300	2.25241300

TS1_5exo_TFA

N	-2.91769000	-0.31341300	-1.39839200	C	2.80594500	2.36109400	-2.68992000
C	-3.42400200	-1.48862400	-1.84350500	H	3.73660500	2.15460500	-3.24757700
C	2.53655600	0.12727600	0.65151800	H	2.21276300	1.42951300	-2.65161100
C	3.44813900	1.59424300	2.12770100	H	2.22844300	3.10841500	-3.26180400
C	4.14398500	0.42029300	2.23199500	H	3.71133200	2.07565700	-0.76721700
H	3.55380900	2.54575000	2.64216600	C	-4.74115800	-1.95149700	-1.33239500
H	4.98312500	0.12899600	2.85822300	C	-5.54964400	-1.18630700	-0.46850700
N	3.57128100	-0.46177400	1.32000900	C	-5.20131000	-3.22107000	-1.74720900
N	2.46795300	1.39350000	1.15881500	C	-6.78308700	-1.67377200	-0.02215500
Au	1.35860400	-0.71736000	-0.74685800	H	-5.22853500	-0.19513500	-0.12878000
C	1.53567400	2.39689600	0.70070400	C	-6.42627200	-3.71533200	-1.31109900
C	1.85120800	3.10954700	-0.47702600	H	-4.57186400	-3.80940400	-2.42112100
C	0.35317900	2.61279700	1.44713000	C	-7.22935600	-2.94367500	-0.44184400
C	0.92247000	4.07380100	-0.91324700	H	-7.38858200	-1.05878200	0.64743800
C	-0.52532000	3.60168200	0.97551900	H	-6.78857200	-4.69809400	-1.62769500
C	-0.25221700	4.31771200	-0.19621800	O	-8.41037200	-3.51136500	-0.06875300
H	1.12689000	4.63572700	-1.83049800	C	-9.25710300	-2.76093900	0.80913300
H	-1.44771500	3.80177700	1.52318500	H	-9.57096800	-1.80608300	0.34885100
H	-0.97985400	5.04976300	-0.55662900	H	-10.14148600	-3.39258300	0.97805900
C	4.00807700	-1.81429700	1.07291800	H	-8.76025800	-2.55988800	1.77602800
C	5.02252400	-2.02119100	0.11079200	O	-2.75897700	-2.16478400	-2.67800300
C	3.37670400	-2.86428700	1.77552600	C	-1.68630700	0.11086100	-2.03200700
C	5.41088700	-3.35032700	-0.13525500	C	-0.74533100	-1.01050600	-2.13350300
C	3.80495800	-4.17399500	1.49126400	C	0.23991700	-1.80225100	-2.15202200
C	4.80993900	-4.41491700	0.54744200	H	0.53693900	-2.77985600	-2.52300100
H	6.18648700	-3.55195800	-0.88084000	H	-3.35536800	0.34183500	-0.69495100
H	3.33583300	-5.01383500	2.01372800	H	-1.86482500	0.50226800	-3.05455000
H	5.12479300	-5.44240600	0.33794300	H	-1.25523800	0.94033100	-1.44718700
C	-0.00637800	1.75511500	2.65491600	O	-3.87374200	1.49429300	0.43484900
H	0.93137200	1.36084800	3.08719800	C	-3.62057700	2.61290200	-0.12742700
C	-0.73317800	2.54107400	3.75847600	O	-3.06669300	2.86346300	-1.21801400
H	-0.85806700	1.90352500	4.65093800	C	-4.12553500	3.83626400	0.70267500

F	-5.47231700	4.00199100	0.56239400
F	-3.53908500	5.00919000	0.32976700
F	-3.88381100	3.69054100	2.04430200

C	4.46625700	-1.53063200	-2.64402000
H	3.37557700	-1.47905900	-2.47818000
H	4.72178000	-0.85864900	-3.48255300
H	4.71350600	-2.56331800	-2.94839800
C	6.76095800	-1.17046700	-1.60863100
H	7.03888800	-0.48576700	-2.42907200
H	7.31639200	-0.86512800	-0.70472800
H	7.10273900	-2.18199800	-1.88999600
C	1.31662400	-2.30042900	2.99566100
H	0.85157400	-2.05200400	2.02468400
H	1.31017000	-3.39936000	3.10820300
H	0.68599400	-1.87230400	3.79418500
H	2.68439400	-0.64672800	2.96020200
C	1.88846200	1.50785000	-3.46569700
H	2.67337300	1.16832800	-4.16447500
H	1.40734500	0.61421200	-3.02805800
H	1.12806800	2.05269300	-4.05232100
H	3.23958600	1.78121600	-1.82353400
C	-4.67556200	-1.90874800	-0.97566600
C	-5.40126100	-0.72217200	-0.74968200
C	-5.19752600	-3.12162100	-0.47228000
C	-6.60298300	-0.73556900	-0.03339000
H	-5.03325900	0.24296200	-1.11043000
C	-6.39912500	-3.15152000	0.22804700
H	-4.63017400	-4.04109200	-0.64188000
C	-7.11173200	-1.95390100	0.45950200
H	-7.12464100	0.20765000	0.14381700
H	-6.80602600	-4.08871700	0.61964000
O	-8.27057500	-2.08113700	1.16527200
C	-9.00208800	-0.88461400	1.45429500
H	-9.33135600	-0.37704500	0.52891600
H	-9.88461500	-1.20787700	2.02561100
H	-8.40486700	-0.18418100	2.06644500
O	-2.75038700	-3.06317200	-1.81359300
C	-1.49052600	-0.75527500	-2.67547500
C	-0.55125100	-1.43724700	-1.70720100
C	-0.62591700	-2.53248600	-1.07947100
H	-0.49169100	-3.41576600	-0.47296900
H	-3.16122200	0.13537800	-1.79103100
H	-1.40780800	-1.29807300	-3.63472900
H	-1.22272300	0.29730600	-2.83830700
O	-3.38059700	1.72136800	-1.23356000
O	-2.32385100	0.85898500	0.61098400
C	-3.05310200	1.66712200	-0.00146100
C	-3.76689800	2.76262500	0.85091400
F	-3.25847100	2.88907400	2.11117200
F	-5.09558900	2.46506700	0.99114000
F	-3.69910500	4.00097700	0.27522500

TS1_gendo_TFA

N	-2.84641200	-0.79962100	-2.16866200
C	-3.36319300	-1.96323700	-1.68309000
C	2.51144900	0.35565400	0.32369700
C	3.76127600	2.09459900	1.08691300
C	4.46253700	0.94466500	1.33230600
H	3.99545200	3.13780400	1.28235600
H	5.43080300	0.77370400	1.79542700
N	3.68259100	-0.10553600	0.85419200
N	2.57072300	1.71350000	0.47603500
Au	1.02629400	-0.67355600	-0.58308100
C	1.52374200	2.59618500	0.01561100
C	1.44522600	2.86842700	-1.36906000
C	0.60072800	3.09762700	0.96303400
C	0.35482900	3.64138100	-1.80982000
C	-0.46042600	3.87210200	0.46531200
C	-0.59584900	4.12375000	-0.90547700
H	0.25223100	3.86314800	-2.87706500
H	-1.20751600	4.26467300	1.15704300
H	-1.45718300	4.69383600	-1.26607900
C	4.05343300	-1.49985800	0.87624800
C	4.82094100	-2.00174900	-0.19879100
C	3.60840200	-2.29827100	1.95294100
C	5.15072800	-3.36881800	-0.16914900
C	3.96396000	-3.65945100	1.93035400
C	4.72769800	-4.18885100	0.88375300
H	5.73776800	-3.79671700	-0.98809600
H	3.63219900	-4.31149600	2.74445400
H	4.99168000	-5.25144300	0.88610200
C	0.71499700	2.76813600	2.44916200
H	1.79045700	2.70194100	2.69924100
C	0.09706600	3.84779900	3.35220200
H	0.34590500	3.63594200	4.40645600
H	0.47018500	4.85791500	3.10847100
H	-1.00372300	3.85645800	3.27308300
C	0.07549900	1.39694300	2.75660700
H	-0.99153500	1.39754900	2.47959200
H	0.55432300	0.58631100	2.18257900
H	0.17378000	1.16589100	3.83292000
C	2.74969700	-1.74183900	3.08178200
C	3.37199900	-2.01607500	4.46250300
H	4.39391100	-1.60424900	4.53373400
H	2.75858800	-1.54944000	5.25301900
H	3.42582100	-3.09774700	4.67866000
C	5.24087400	-1.12811700	-1.37414900
H	4.97331100	-0.08317300	-1.14001500
C	2.49757400	2.39380900	-2.36499700
C	3.24596300	3.59599500	-2.97202200
H	2.56264700	4.24442900	-3.54858100
H	3.71622800	4.21450500	-2.18780900
H	4.03871000	3.24762500	-3.65767300

Int2_Sexo_TFA

N	3.34775300	-0.52283800	0.43704500
C	3.67577200	-1.76660800	0.16867000
C	-2.85857700	0.40379600	0.19532500
C	-3.84589000	2.44250200	0.48601600
C	-4.81425200	1.57417900	0.06082800
H	-3.88286600	3.49923500	0.73739300
H	-5.87359000	1.71355300	-0.13834200
N	-4.19178900	0.33912900	-0.10932500
N	-2.66402400	1.71127600	0.56074700
Au	-1.40340700	-1.01297700	0.09722900
C	-1.37488000	2.24022800	0.94033600
C	-0.99111500	2.16974200	2.29873700
C	-0.53598500	2.75915000	-0.07191500

C	0.29226600	2.64188800	2.63202100
C	0.73547600	3.22011800	0.31593000
C	1.14835400	3.15852100	1.65181700
H	0.62601700	2.59201300	3.67354400
H	1.42711500	3.59730500	-0.44136200
H	2.15042000	3.50686400	1.92024000
C	-4.83935300	-0.85453700	-0.59527800
C	-5.42475500	-1.73554200	0.34045800
C	-4.83728000	-1.09468100	-1.98796500
C	-6.03087100	-2.90068600	-0.16371000
C	-5.45586900	-2.27462700	-2.43864100
C	-6.04767200	-3.16766700	-1.53767000
H	-6.48665900	-3.61137100	0.53299300
H	-5.46432500	-2.49783200	-3.51038900
H	-6.52086000	-4.08252100	-1.90933100
C	-0.94347100	2.78891300	-1.53946700
H	-1.99460000	2.45938900	-1.61391200
C	-0.86236200	4.21184700	-2.12097000
H	-1.21953800	4.21672400	-3.16600200
H	-1.48201300	4.92020400	-1.54345000
H	0.17499300	4.58986000	-2.12112300
C	-0.08662100	1.80273400	-2.35692600
H	0.98488600	2.06517400	-2.30773900
H	-0.20562200	0.77250300	-1.97526700
H	-0.39567700	1.81241500	-3.41766400
C	-4.16407600	-0.14925600	-2.97525500
C	-5.12533900	0.29786500	-4.09041500
H	-6.02915300	0.77850300	-3.67693500
H	-4.62440100	1.02482200	-4.75357000
H	-5.44961100	-0.55303300	-4.71533600
C	-5.36673300	-1.47710800	1.84042000
H	-4.97094600	-0.45876600	1.99693800
C	-1.89374000	1.56712100	3.36823000
C	-2.13914000	2.54747100	4.52881100
H	-1.20331400	2.78537400	5.06450400
H	-2.57355200	3.49671400	4.16955700
H	-2.83867500	2.10605400	5.26064000
C	-4.38905300	-2.45959000	2.51321500
H	-3.38458000	-2.39099200	2.05876300
H	-4.29741100	-2.23537600	3.59106500
H	-4.73991200	-3.50213500	2.41032600
C	-6.75768200	-1.53681600	2.49446500
H	-6.68251800	-1.29119700	3.56842300
H	-7.45560900	-0.82006500	2.02747700
H	-7.20387000	-2.54390000	2.41542200
C	-2.89229700	-0.79417500	-3.55877000
H	-2.19074000	-1.08372100	-2.75575500
H	-3.13642000	-1.70052400	-4.14139200
H	-2.37478700	-0.08620800	-4.23015300
H	-3.85276700	0.75601400	-2.42613400
C	-1.31383400	0.23321200	3.87617700
H	-1.99709300	-0.23108000	4.60970800
H	-1.16844000	-0.47678000	3.04210100
H	-0.33719300	0.38501800	4.37004600
H	-2.87229900	1.34699800	2.90742000
C	5.01226000	-2.30627700	0.01633000
C	6.13995100	-1.45633900	0.06750900
C	5.19613900	-3.69283200	-0.20588600
C	7.42438500	-1.97261000	-0.09759800
H	6.01497700	-0.37896200	0.22170700
C	6.47320200	-4.21212300	-0.36842600
H	4.32716800	-4.35449900	-0.25095100
C	7.59971500	-3.35749600	-0.31729700

H	8.28061100	-1.29624200	-0.05906800
H	6.63230400	-5.28006000	-0.54175600
O	8.79923600	-3.96146700	-0.49413000
C	9.97610600	-3.13953600	-0.47146400
H	10.10427100	-2.65134000	0.51102200
H	10.81600500	-3.82498300	-0.65280700
H	9.94577300	-2.37504000	-1.26821300
O	2.61773300	-2.57685100	0.01386500
C	1.89522000	-0.36245400	0.42154000
C	1.41677700	-1.77065800	0.13646800
C	0.18754700	-2.28179900	-0.01449900
H	0.12700900	-3.35940300	-0.22654100
H	4.00369200	0.35293900	0.47318600
H	1.53707000	0.02882300	1.39045300
H	1.62063600	0.36551800	-0.36129900
O	4.75774700	1.68661400	0.49747800
O	3.40885100	2.07205100	-1.31540100
C	4.24141000	2.38931000	-0.44163300
C	4.68532600	3.88269300	-0.43164400
F	3.72987700	4.64428800	0.20143700
F	4.81651800	4.38418400	-1.68713600
F	5.85648600	4.10076400	0.21878700

Int2_6endo_TFA

N	-3.05665600	-0.64510500	-0.64039300
C	-3.43112600	-1.89588100	-0.77006000
C	2.81487600	0.38481200	0.34848000
C	3.97415500	2.05388400	1.38653500
C	4.88786000	1.21320200	0.80944100
H	4.09763400	2.96230000	1.97042600
H	5.97416600	1.23560500	0.78309900
N	4.15932200	0.20335000	0.18254900
N	2.71897000	1.53216700	1.09350600
Au	1.16469200	-0.60628300	-0.30572700
C	1.44225800	2.04954200	1.53096700
C	0.73669000	2.92859000	0.67858700
C	0.91489800	1.57287800	2.75233000
C	-0.55695300	3.31311600	1.07595600
C	-0.38033000	1.99403700	3.10424400
C	-1.11605900	2.84258200	2.26937700
H	-1.14599100	3.96740900	0.42763100
H	-0.82580300	1.62844000	4.03516400
H	-2.14084800	3.12168800	2.52948100
C	4.73503000	-0.90388000	-0.54035600
C	5.00399100	-0.74075900	-1.91755600
C	4.98942100	-2.10275500	0.16207200
C	5.56569800	-1.83686500	-2.59734600
C	5.55132900	-3.16756200	-0.56538200
C	5.83999400	-3.03574400	-1.92866000
H	5.78369700	-1.74977500	-3.66659300
H	5.75723700	-4.11390400	-0.05502700
H	6.27642800	-3.87736500	-2.47649100
C	1.67531500	0.60311400	3.64808400
H	2.67194000	0.43205200	3.20525100
C	1.88945600	1.18907900	5.05523400
H	2.48124400	0.49210200	5.67474100
H	2.42805800	2.15191300	5.01289300
H	0.92838500	1.36176400	5.57129500
C	0.95833800	-0.75823200	3.71293900
H	-0.04518200	-0.65932900	4.16362300
H	0.83468600	-1.18879800	2.70348700
H	1.53738800	-1.47038300	4.32775300
C	4.63221900	-2.27405100	1.63313300

C	5.83498900	-2.74325300	2.46972700	C	1.75830400	-0.46881300	0.86335500
H	6.68472100	-2.04414700	2.38121300	C	3.30829300	-0.91504600	2.47635600
H	5.55425200	-2.80704000	3.53571000	C	2.12634000	-1.47299300	2.87756200
H	6.18461700	-3.74291800	2.15725400	H	4.29292300	-0.90112900	2.93567000
C	4.66146700	0.54359300	-2.66158500	H	1.86358800	-2.04749100	3.76147400
H	4.35682400	1.29976100	-1.91762700	N	1.19206100	-1.18862800	1.88363100
C	1.30563500	3.42434500	-0.64451900	N	3.06297300	-0.30663200	1.24767300
C	1.41403300	4.95999600	-0.66022900	Au	0.87206100	0.24422300	-0.79494100
H	0.42043500	5.43408500	-0.57310500	C	4.07786100	0.29884800	0.41839600
H	2.03819600	5.32865300	0.17256400	C	4.78196700	-0.53722400	-0.47743800
H	1.86748900	5.30314400	-1.60688600	C	4.32153400	1.68622600	0.53693900
C	3.46109300	0.31293300	-3.60005300	C	5.78108500	0.05930600	-1.26783700
H	2.58829400	-0.06924500	-3.04109100	C	5.33685300	2.22852200	-0.27115300
H	3.16813600	1.25794900	-4.09142900	C	6.06006100	1.42598700	-1.16199400
H	3.70742800	-0.41994300	-4.38915200	H	6.34009800	-0.55795300	-1.97835100
C	5.86975800	1.11089000	-3.42664400	H	5.55887500	3.29777900	-0.20741300
H	5.60046900	2.06843500	-3.90596000	H	6.84219800	1.87315900	-1.78436800
H	6.72477400	1.29416400	-2.75274000	C	-0.17068400	-1.66715300	1.89116400
H	6.20805300	0.42502000	-4.22321800	C	-0.47384100	-2.83283600	1.15055200
C	3.43702500	-3.23539000	1.78219800	C	-1.13350600	-0.96667500	2.65516100
H	2.56339000	-2.87231100	1.21169400	C	-1.79944700	-3.30158100	1.19891600
H	3.69098700	-4.24484600	1.41211300	C	-2.43872800	-1.49024400	2.68010900
H	3.14379700	-3.32549100	2.84316800	C	-2.77033200	-2.64412000	1.96033200
H	4.31745600	-1.29189600	2.02668100	H	-2.06948700	-4.19690000	0.63002400
C	0.46956900	2.91048900	-1.83204300	H	-3.20838600	-0.97826500	3.26526300
H	0.89999100	3.26283000	-2.78666600	H	-3.79596600	-3.02568400	1.98326100
H	0.45582600	1.80603800	-1.84871300	C	3.54697600	2.55575600	1.51838900
H	-0.57511100	3.26478800	-1.77787400	H	2.59744000	2.04284800	1.74814100
H	2.32550300	3.01616700	-0.75559400	C	4.33345700	2.70040000	2.83666800
C	-4.80598300	-2.33071200	-0.56807300	H	3.75837400	3.30177400	3.56295400
C	-5.86609700	-1.40261000	-0.68247600	H	4.54165600	1.71841700	3.29644900
C	-5.09185000	-3.68262300	-0.25872200	H	5.30123100	3.20546800	2.66519800
C	-7.18405100	-1.80801300	-0.46731700	C	3.18605200	3.93317200	0.94062600
H	-5.66435400	-0.36128800	-0.97207800	H	4.08343400	4.54321600	0.73601400
C	-6.40209600	-4.08922600	-0.04577700	H	2.60710600	3.83865500	0.00669700
H	-4.27390300	-4.40303300	-0.17359500	H	2.56713000	4.48831200	1.66361100
C	-7.45988200	-3.15376700	-0.14043000	C	-0.78511400	0.28591900	3.44939300
H	-7.98916700	-1.07712200	-0.56860300	C	-0.54585000	-0.06675400	4.93130500
H	-6.64076400	-5.12669000	0.20450200	H	0.25733800	-0.81414900	5.05265300
O	-8.69946600	-3.65160300	0.09358700	H	-0.26089200	0.83572500	5.50079000
C	-9.80947200	-2.74400100	0.03948800	H	-1.46311400	-0.48118000	5.38755100
H	-9.92721900	-2.31303200	-0.97087500	C	0.56204400	-3.57934100	0.31851200
H	-10.69456300	-3.34853700	0.28418500	H	1.53734400	-3.07869200	0.44556400
H	-9.70060700	-1.93223900	0.78079900	C	4.46598500	-2.02011900	-0.62680300
O	-2.54273700	-2.84553000	-1.09029100	C	5.70858700	-2.89785400	-0.39625800
C	-1.72031200	-0.18496400	-1.03991000	H	6.48940900	-2.70805300	-1.15379200
C	-0.68440100	-1.27587200	-0.83161900	H	6.15133500	-2.71501600	0.59860100
C	-1.15172100	-2.53198300	-0.89368900	H	5.43685200	-3.96648200	-0.45798300
H	-0.60479200	-3.47060500	-0.79686300	C	0.20358300	-3.52094900	-1.17781800
H	-3.66511000	0.10166000	-0.15645300	H	0.15084000	-2.47334600	-1.52417000
H	-1.75331900	0.13751900	-2.10016700	H	0.96622900	-4.04653800	-1.77930500
H	-1.51380300	0.71280900	-0.43858200	H	-0.77335700	-3.99689400	-1.37601900
O	-5.13566700	1.82195700	-1.44029700	C	0.72491600	-5.03372900	0.79724400
O	-4.00006900	1.51112400	0.52369600	H	1.51629500	-5.54029700	0.21677400
C	-4.50281000	2.19556400	-0.42782300	H	1.00233600	-5.07864300	1.86494600
C	-4.21660000	3.72653900	-0.34051200	H	-0.20800800	-5.60958000	0.66455300
F	-5.25688800	4.47748700	-0.78560100	C	-1.85383400	1.38443400	3.31977500
F	-3.91950700	4.15878300	0.91781400	H	-2.06301300	1.62746000	2.26526000
F	-3.13404000	4.04238800	-1.12921500	H	-2.80190400	1.09084400	3.80473300
				H	-1.50317400	2.30522900	3.81552300
				H	0.15540600	0.69525500	3.04117000
				C	3.82445000	-2.29830600	-1.99911000
				H	3.55446600	-3.36570400	-2.08829700
TS2_5exo_TFA							
N	-3.28989500	-0.15941800	-3.95649000				
C	-3.36400700	-0.23444000	-2.67092200				

H	2.90904000	-1.69516100	-2.13298700
H	4.51848600	-2.05358500	-2.82296800
H	3.72341900	-2.29488800	0.14199300
C	-4.48897200	-0.63993800	-1.83773200
C	-5.64427200	-1.18551900	-2.43249900
C	-4.44550900	-0.47658500	-0.43358100
C	-6.73843900	-1.56845900	-1.65404800
H	-5.67602200	-1.30933000	-3.51903600
C	-5.53471600	-0.85022300	0.34790100
H	-3.56131200	-0.03731700	0.03471400
C	-6.68791500	-1.40129900	-0.25269700
H	-7.62099800	-1.99322500	-2.13713300
H	-5.52002700	-0.71797300	1.43354900
O	-7.69341200	-1.73744400	0.60099200
C	-8.89609000	-2.27018400	0.03412100
H	-8.70696500	-3.22297700	-0.49377700
H	-9.56833400	-2.45278300	0.88502100
H	-9.36823100	-1.55023300	-0.65898900
O	-2.20574700	0.12879100	-1.96534300
C	-1.93802000	0.32397300	-4.24621600
C	-1.27702600	0.51560800	-2.89647800
C	-0.05351200	1.00595800	-2.51557900
H	0.57749900	1.26911000	-3.37991600
H	-0.22712200	2.14293400	-1.78299000
H	-1.38421700	-0.40180700	-4.87207600
H	-1.97247400	1.27055300	-4.81830400
O	-0.19055400	3.25599300	-1.11372500
O	-2.07109500	2.51032600	-0.03100300
C	-1.04602500	3.19334000	-0.13905100
C	-0.61576900	4.06724700	1.07309700
F	-1.67504100	4.44285400	1.82980000
F	0.21707600	3.33225000	1.88095000
F	0.05795900	5.19086600	0.71910600

TS2_gendo_TFA

N	2.39462500	-2.60942800	0.54980700
C	3.07682500	-2.32371300	-0.49683900
C	-0.94838200	1.50732300	0.30436800
C	-0.65627600	3.61967100	1.10574000
C	-2.00216700	3.41677400	0.95430100
H	-0.09125200	4.47978500	1.45532000
H	-2.85420200	4.06589400	1.13702400
N	-2.15839700	2.12050800	0.46869100
N	-0.03182000	2.44241900	0.70577100
Au	-0.46775600	-0.33395500	-0.34017200
C	1.38975200	2.18583000	0.68959400
C	1.97515700	1.57822300	1.82331900
C	2.11019000	2.48050000	-0.48932400
C	3.34271100	1.25820300	1.74543400
C	3.47499600	2.14067700	-0.51182900
C	4.08475000	1.53297500	0.59132300
H	3.82745000	0.76473400	2.59359400
H	4.06190300	2.33625100	-1.41518800
H	5.14175000	1.25247000	0.54420300
C	-3.41975900	1.49351500	0.15487100
C	-4.10749100	0.81397300	1.18689000
C	-3.89290500	1.57216700	-1.17319600
C	-5.34091900	0.22692000	0.85413000
C	-5.12772000	0.95864800	-1.45255400
C	-5.84642000	0.30004500	-0.44957200
H	-5.90256300	-0.31395900	1.62053600
H	-5.52124900	0.98689900	-2.47376100
H	-6.80133300	-0.17886600	-0.68895300

C	1.44660900	3.08898100	-1.71865400
H	0.41105300	3.36291300	-1.45120600
C	2.15920600	4.37292700	-2.17916000
H	1.62876400	4.81547400	-3.04073200
H	2.19230100	5.12777600	-1.37426000
H	3.19736500	4.16992300	-2.49582900
C	1.37022400	2.05405200	-2.85745600
H	2.37958100	1.72883600	-3.16736700
H	0.80915700	1.15837700	-2.53647600
H	0.86383100	2.48551900	-3.73936200
C	-3.08942500	2.23666700	-2.28352100
C	-3.90715100	3.29710300	-3.04095600
H	-4.29489400	4.07316400	-2.35795900
H	-3.27475700	3.79247200	-3.79862300
H	-4.76751400	2.84933700	-3.56885600
C	-3.54688100	0.72817600	2.60157900
H	-2.45500600	0.88489200	2.53788600
C	1.16659100	1.22308200	3.06449500
C	1.81705800	1.76337800	4.34990700
H	2.79253600	1.28522500	4.54722900
H	1.97993000	2.85401800	4.29340600
H	1.16729200	1.55780000	5.21864000
C	-3.77140600	-0.64826200	3.24985100
H	-3.41696600	-1.46697200	2.60173900
H	-3.22049400	-0.70026700	4.20555500
H	-4.83750100	-0.82511700	3.47891800
C	-4.13047700	1.85034400	3.48324800
H	-3.69982300	1.80627700	4.49955300
H	-3.91911500	2.85044000	3.06670400
H	-5.22690800	1.74619200	3.57277500
C	-2.52987600	1.17041000	-3.24507900
H	-1.91226500	0.43441300	-2.69810100
H	-3.34600300	0.62156200	-3.74808000
H	-1.90366600	1.64214100	-4.02339100
H	-2.22773900	2.75150700	-1.82366000
C	0.94550700	-0.30022700	3.14386300
H	0.34511100	-0.55759800	4.03490000
H	0.41040600	-0.66393700	2.24822900
H	1.90541600	-0.84278500	3.20120900
H	0.17302200	1.69746100	2.97510300
C	4.48034700	-1.88226500	-0.46474700
C	5.20214900	-1.95950400	0.74294100
C	5.11189200	-1.31847600	-1.59577500
C	6.51439500	-1.48805800	0.83561600
H	4.71147300	-2.39129800	1.61984100
C	6.41950200	-0.84330700	-1.51600300
H	4.56442300	-1.24294600	-2.53845000
C	7.13267000	-0.92132700	-0.30006800
H	7.04805800	-1.56627000	1.78561700
H	6.91348600	-0.40029700	-2.38587600
O	8.40259000	-0.42787600	-0.32658300
C	9.15961500	-0.47586700	0.88764900
H	9.31572200	-1.51645600	1.22683300
H	10.13205600	-0.02108300	0.64877500
H	8.67183600	0.10512500	1.69222600
O	2.54690700	-2.32548900	-1.80585500
C	1.00452200	-3.02949600	0.31361000
C	0.35244300	-2.22483400	-0.80816500
C	1.20225000	-2.00256000	-1.85281800
H	0.96050700	-1.52009700	-2.80602600
H	-1.03500700	-2.66533600	-1.06871700
H	1.00524100	-4.10640500	0.03889700
H	0.43985400	-2.94682700	1.25439800

O	-2.12296400	-3.08238700	-1.25365800
O	-2.33481200	-2.97280000	1.02638600
C	-2.77424200	-3.08378400	-0.12051100
C	-4.29790900	-3.28901700	-0.34254400
F	-5.00651600	-2.95280100	0.76160800
F	-4.55908300	-4.59858500	-0.61711100
F	-4.76714200	-2.55213000	-1.38170400

HSbF₆

H	-0.03508800	0.92825300	-0.67430500
Sb	-1.39833200	2.35396400	-2.61526500
F	-1.25338700	4.11545100	-1.94917900
F	0.27959600	2.55628200	-3.46300600
F	-2.46561700	2.70932300	-4.12180100
F	-2.81614000	2.04222700	-1.40158200
F	-1.24232200	0.47542600	-2.83031000
F	-0.09497100	1.88735500	-0.79017000

IPrAuSbF₆

C	-0.81852800	-1.44107800	1.20612200
C	-0.61841300	-3.47192300	2.19206300
C	-1.86169400	-2.98529100	2.49581600
H	-0.11911300	-4.40008400	2.45715900
H	-2.67610500	-3.39826200	3.08491800
N	-1.96599300	-1.74073700	1.88200600
N	0.00504400	-2.51179700	1.40039400
Au	-0.46297300	0.15797900	0.15906400
C	1.31166200	-2.63450400	0.79857400
C	1.40261200	-3.24979900	-0.47040500
C	2.42293900	-2.10123200	1.48763300
C	2.68185100	-3.33342600	-1.04932800
C	3.67763100	-2.21123000	0.86142600
C	3.80631700	-2.82114100	-0.39193200
H	2.79260400	-3.79670400	-2.03479800
H	4.56290400	-1.80479300	1.36080800
H	4.79149200	-2.89170000	-0.86424600
C	-3.12338800	-0.87738500	1.92098000
C	-4.10640600	-1.02958300	0.91757600
C	-3.20370100	0.08678100	2.95049200
C	-5.21590400	-0.16687000	0.97521600
C	-4.33440600	0.92321100	2.95843900
C	-5.33101100	0.79612900	1.98379500
H	-5.99618800	-0.24918900	0.21193200
H	-4.42712700	1.69064600	3.73359100
H	-6.20061500	1.46094600	2.00424000
C	2.28610700	-1.39697500	2.83144500
H	1.24121800	-1.50499400	3.17127600
C	3.18686800	-2.03140200	3.90562900
H	3.03082400	-1.53025900	4.87705000
H	2.96612200	-3.10530700	4.03512300
H	4.25624200	-1.93389100	3.64858100
C	2.57079100	0.10966000	2.68202000
H	3.61076800	0.28959600	2.35667000
H	1.89789500	0.56859100	1.93492500
H	2.42068900	0.62805200	3.64570100
C	-2.09676600	0.27033200	3.98002900
C	-2.62590100	0.17891000	5.42201100
H	-3.14073900	-0.78075800	5.60287900
H	-1.79088100	0.25947400	6.13996800
H	-3.33782100	0.99238400	5.64673400
C	-4.00129500	-2.07004700	-0.19095700

H	-3.03562300	-2.59430900	-0.08593800
C	0.18284800	-3.77773200	-1.21515100
C	0.32496000	-5.27700500	-1.53494000
H	1.17293800	-5.46693100	-2.21643300
H	0.48673500	-5.87227500	-0.61943700
H	-0.58940800	-5.64905700	-2.02958000
C	-4.02132600	-1.42043800	-1.58692400
H	-3.19621300	-0.70188200	-1.71898700
H	-3.92435600	-2.19816300	-2.36523600
H	-4.96863300	-0.88298600	-1.76853400
C	-5.11733000	-3.12286300	-0.05202500
H	-5.01724900	-3.89564500	-0.83453400
H	-5.08134300	-3.62371100	0.93129800
H	-6.11514400	-2.66198000	-0.15993900
C	-1.36106600	1.60164300	3.73442000
H	-0.97041600	1.65147800	2.70183000
H	-2.03672800	2.46275800	3.88111900
H	-0.51186400	1.71056900	4.43235900
H	-1.36198300	-0.54282700	3.84582800
C	-0.08137900	-2.95922100	-2.49325500
H	-0.98556700	-3.33447600	-3.00447000
H	-0.23856100	-1.89005000	-2.26951100
H	0.76344800	-3.03642100	-3.20052500
H	-0.69931800	-3.66327100	-0.56166800
Sb	-1.29879400	2.32318100	-2.55816400
F	-1.25565200	4.13056200	-1.96937500
F	0.26745700	2.61035000	-3.59713200
F	-2.45281800	2.71075300	-4.01621200
F	-2.76038600	1.97587700	-1.37783400
F	-1.24034400	0.46119400	-2.99752800
F	-0.06372300	1.90646200	-1.01142400

Int1_SbF₆

N	1.60127800	1.12129200	-2.50222500
C	2.57133000	0.20775000	-2.84106800
C	-0.96528000	-1.46934500	1.08928800
C	-0.46192200	-3.25292600	2.39899900
C	-1.71064500	-2.82260500	2.75566500
H	0.15096900	-4.07308600	2.76319800
H	-2.41792600	-3.18740000	3.49535200
N	-1.99926200	-1.73336000	1.94107300
N	-0.01917100	-2.40861600	1.38270600
Au	-1.02868400	-0.01905100	-0.31867900
C	1.27008800	-2.51419500	0.73947800
C	1.33659600	-3.09497900	-0.54762000
C	2.40635000	-2.05269000	1.44448500
C	2.60628800	-3.17769000	-1.14790700
C	3.65163700	-2.18914700	0.80672600
C	3.75116200	-2.73535900	-0.47766600
H	2.69506700	-3.59547800	-2.15507100
H	4.55494200	-1.84330500	1.31738600
H	4.72850800	-2.80290500	-0.96449200
C	-3.21744300	-0.95968000	1.96606300
C	-4.28995500	-1.37540000	1.14653600
C	-3.25837900	0.19239400	2.78622000
C	-5.45909300	-0.59264600	1.17651900
C	-4.45340600	0.93399600	2.77947000
C	-5.54109400	0.54507500	1.98698500
H	-6.31090800	-0.87738100	0.55051200
H	-4.53036800	1.83335100	3.39724700
H	-6.45949900	1.14108000	1.99641100
C	2.31986900	-1.47156500	2.85131500
H	1.25855600	-1.26621900	3.07660900

C	2.82628500	-2.49906300	3.88278500
H	2.73686500	-2.09420300	4.90643600
H	2.25286100	-3.44130100	3.83620600
H	3.88892100	-2.74327400	3.70499900
C	3.07542400	-0.13836600	2.98695900
H	4.15897900	-0.25812700	2.81083800
H	2.68578400	0.61004500	2.28017700
H	2.94842000	0.25971600	4.00930400
C	-2.07717900	0.59700000	3.66045400
C	-2.23898800	0.00617900	5.07569900
H	-2.31455600	-1.09505900	5.05275700
H	-1.37198100	0.27550900	5.70449000
H	-3.14977000	0.39917200	5.56223300
C	-4.19180800	-2.58685300	0.22691700
H	-3.22935500	-3.09121000	0.42163500
C	0.11284100	-3.64206700	-1.27322100
C	0.28455400	-5.13737200	-1.59989700
H	1.12057100	-5.30532500	-2.30120100
H	0.48264300	-5.72906300	-0.68930700
H	-0.63219800	-5.53182900	-2.07272700
C	-4.18946600	-2.14853100	-1.25042100
H	-3.35763700	-1.45065400	-1.45582100
H	-4.07375600	-3.02526100	-1.91222700
H	-5.13312600	-1.64148200	-1.51959300
C	-5.30987600	-3.60779100	0.50278500
H	-5.17689500	-4.49876700	-0.13556100
H	-5.30404200	-3.93798900	1.55609100
H	-6.30718700	-3.18657600	0.28534000
C	-1.86438400	2.11776400	3.72026000
H	-1.80226600	2.56208500	2.71412000
H	-2.67108600	2.62603100	4.27807800
H	-0.91496600	2.34125500	4.23495400
H	-1.16353200	0.16078500	3.21938800
C	-0.19524500	-2.82848800	-2.54250800
H	-1.08483900	-3.23668800	-3.05469000
H	-0.40034800	-1.77366900	-2.28464300
H	0.65093900	-2.83815700	-3.25018100
H	-0.75855800	-3.55260600	-0.60101400
C	3.86314100	0.34207100	-2.10586900
C	3.96514100	0.96408700	-0.84915600
C	5.02282500	-0.22307400	-2.67840600
C	5.19020100	1.04938700	-0.17857400
H	3.07383100	1.33429900	-0.33944800
C	6.24939400	-0.14781100	-2.02370000
H	4.93910100	-0.72548500	-3.64671500
C	6.34357900	0.49383200	-0.76694400
H	5.22538700	1.54354300	0.79461800
H	7.15579700	-0.57593500	-2.46262800
O	7.58461800	0.51232900	-0.20388400
C	7.71365900	1.12900800	1.08177600
H	7.09077200	0.61761400	1.83926700
H	8.77461100	1.02976200	1.35384700
H	7.44248200	2.19991600	1.04730100
O	2.38287800	-0.66426800	-3.711107400
C	0.29238900	1.08460200	-3.11762100
C	-0.78372200	1.28641900	-2.13263400
C	-1.73047200	1.69580800	-1.42960200
H	-2.54284600	2.28018100	-1.01830900
H	1.80420800	1.92294400	-1.89907700
H	0.17402900	1.87553800	-3.88668000
H	0.19956700	0.11072700	-3.62918600
Sb	1.16547600	3.62947000	0.92134000
F	1.07758100	3.62314100	2.83064400

F	3.07820100	3.64461400	0.98617900
F	1.11378200	5.53549100	0.88074100
F	-0.75248700	3.56026100	0.81302100
F	1.24870500	3.58800000	-1.01060400
F	1.21561300	1.69906200	0.91625100

TS1_5exo_SbF6

N	2.99269100	-0.95743800	0.60186200
C	3.44308700	-2.23128400	0.41642100
C	-3.05056900	0.51555700	0.07783500
C	-4.29554400	2.41458700	0.07219200
C	-5.08213600	1.40526300	-0.41349700
H	-4.49652000	3.46932600	0.24119500
H	-6.11086700	1.39357800	-0.76336000
N	-4.30131100	0.25256800	-0.40125700
N	-3.05647400	1.85048700	0.36456700
Au	-1.54749200	-0.81123100	0.30231800
C	-1.91923700	2.54677000	0.91899000
C	-1.67525800	2.42614300	2.30470600
C	-1.08901000	3.28055700	0.03838900
C	-0.52808100	3.06710200	2.80982200
C	0.04406500	3.89383000	0.59793200
C	0.32504800	3.78379800	1.96595400
H	-0.30242700	2.99563000	3.87878600
H	0.73423700	4.44345300	-0.04506000
H	1.22830400	4.25170100	2.36662200
C	-4.73924500	-1.06382200	-0.79892300
C	-5.39531700	-1.86496100	0.16300800
C	-4.46249700	-1.49617000	-2.11485800
C	-5.78221400	-3.15714800	-0.23578300
C	-4.87280400	-2.79731200	-2.45971000
C	-5.52483500	-3.61805800	-1.53244500
H	-6.28327000	-3.81271800	0.48335000
H	-4.67223700	-3.17059200	-3.46892700
H	-5.83181600	-4.62847300	-1.82151500
C	-1.37500300	3.34560900	-1.45901000
H	-2.47034900	3.28354100	-1.59646800
C	-0.89650800	4.65393300	-2.10846200
H	-1.25615700	4.70377500	-3.15083400
H	-1.27275700	5.54337100	-1.57377200
H	0.20490800	4.70643800	-2.14030300
C	-0.74387700	2.13766200	-2.18420500
H	0.35396100	2.17756300	-2.10578300
H	-1.07417700	1.17947300	-1.74666900
H	-1.01903900	2.14641700	-3.25410500
C	-3.72816400	-0.62438900	-3.12484300
C	-4.56266300	-0.40894700	-4.40034800
H	-5.54862300	0.03009600	-4.16853200
H	-4.03525400	0.27565800	-5.08736800
H	-4.73191600	-1.35799900	-4.93926800
C	-5.63104100	-1.38903800	1.59132700
H	-5.39303200	-0.31199700	1.64070400
C	-2.59448600	1.65204100	3.24309500
C	-3.25159000	2.59409500	4.26881800
H	-2.49567300	3.07366000	4.91549300
H	-3.82467200	3.39421300	3.76877000
H	-3.94393900	2.03131100	4.91980500
C	-4.68103300	-2.11650200	2.56301400
H	-3.62523700	-1.97636400	2.27002700

H	-4.80977200	-1.72998700	3.58960900	C	-0.14183000	-4.51061500	-0.12313200
H	-4.88611100	-3.20173600	2.57938900	H	-1.03271700	-4.71783700	-2.08310900
C	-7.09906700	-1.55240400	2.02164600	H	0.54107600	-4.13642100	1.88496100
H	-7.24502300	-1.14133200	3.03588900	H	0.74203600	-5.10360400	-0.37238700
H	-7.78163500	-1.02172000	1.33541300	C	-4.78567100	1.28253500	0.68650500
H	-7.40243700	-2.61360700	2.04747700	C	-5.50439800	1.65317900	-0.47236500
C	-2.34762800	-1.22138900	-3.45772900	C	-4.33282300	2.21004100	1.65092700
H	-1.73779300	-1.34781400	-2.54453600	C	-5.77623900	3.02203000	-0.64734000
H	-2.44574800	-2.21026600	-3.93990300	C	-4.63444500	3.56611000	1.42686400
H	-1.79652300	-0.55897600	-4.14787700	C	-5.34802500	3.96795200	0.29180600
H	-3.56103400	0.36621300	-2.66764800	H	-6.32381200	3.34945200	-1.53674600
C	-1.84248700	0.50455500	3.94123300	H	-4.30077800	4.31419300	2.15329600
H	-2.52941600	-0.07235700	4.58508200	H	-5.56957000	5.02871300	0.13518700
H	-1.40395300	-0.18792300	3.20007600	C	-1.46750400	-2.53755500	2.89665300
H	-1.02409200	0.88509600	4.57765600	H	-2.51558200	-2.22051700	3.04515900
H	-3.40357100	1.19807300	2.64499200	C	-1.12956600	-3.53766000	4.01532000
C	4.76106400	-2.42802100	-0.24096000	H	-1.31854200	-3.07833200	5.00138300
C	5.42079400	-1.42309500	-0.97604700	H	-1.74021700	-4.45418500	3.94053200
C	5.36027200	-3.70413600	-0.14445500	H	-0.06675400	-3.83403300	3.98970600
C	6.65526600	-1.67259300	-1.58533800	C	-0.57844500	-1.28168300	2.99927600
H	4.97149700	-0.43657800	-1.11701800	H	0.48289300	-1.53822100	2.84732900
C	6.59046600	-3.96168100	-0.73933500	H	-0.84931700	-0.53449400	2.23199300
H	4.83807600	-4.48794400	0.41183100	H	-0.68634100	-0.81308700	3.99421800
C	7.25207300	-2.94404200	-1.46342800	C	-3.54724100	1.78701300	2.88533500
H	7.13611700	-0.87612200	-2.15736200	C	-4.32517700	2.10903200	4.17452800
H	7.06527100	-4.94433500	-0.66175600	H	-5.30928000	1.60897400	4.18533500
O	8.44930600	-3.29212000	-2.00867100	H	-3.75815500	1.76781800	5.05836800
C	9.15697900	-2.29151500	-2.75097000	H	-4.49596500	3.19482000	4.28246500
H	9.40494300	-1.41952300	-2.11892700	C	-5.92964800	0.63708300	-1.52515100
H	10.08576700	-2.77546900	-3.08631700	H	-5.74060100	-0.37415100	-1.12485400
H	8.57924900	-1.95795000	-3.63234000	C	-3.28565200	-3.18376300	-1.87103200
O	2.72421200	-3.19154700	0.78645500	C	-4.02045500	-4.47221600	-2.28485900
C	1.73746900	-0.79410400	1.31439400	H	-3.32349900	-5.20780700	-2.72399200
C	0.73620000	-1.75281100	0.83110000	H	-4.51479100	-4.94930200	-1.42071200
C	-0.23471900	-2.44699100	0.43306000	H	-4.79377500	-4.24799200	-3.04071000
H	-0.55142900	-3.45492700	0.18041200	C	-5.07839000	0.79363600	-2.79995700
H	3.58932900	-0.12963600	0.49356500	H	-4.00281800	0.67481200	-2.57873600
H	1.86014100	-0.94040000	2.40721000	H	-5.36287900	0.03229300	-3.54768800
H	1.38679000	0.23763400	1.14615700	H	-5.22262200	1.78941100	-3.25614600
Sb	3.61881900	2.73352100	-0.75942400	C	-7.43266400	0.73082600	-1.84037600
F	4.54847100	1.48057400	0.39416300	H	-7.71824400	-0.05158100	-2.56504400
F	3.19400900	3.79468000	0.77466300	H	-8.04346200	0.59464700	-0.93102000
F	2.64219400	3.93403100	-1.88851500	H	-7.69801200	1.70647300	-2.28388800
F	5.22299900	3.73838900	-0.99630100	C	-2.14671000	2.42717000	2.90265600
F	4.07993400	1.63185000	-2.25666500	H	-1.57539900	2.16382600	1.99453100
F	2.03120700	1.67516400	-0.50162700	H	-2.20559300	3.52862600	2.96039100

TS1_gendo_SbF6

N	2.38710600	0.84042100	-1.88584400	H	-3.40793000	0.69321200	2.84662100
C	2.53271800	2.19825200	-1.94102200	C	-2.65271600	-2.48960500	-3.09104800
C	-3.28392200	-0.66499300	0.46181400	H	-3.42836300	-2.23404600	-3.83451500
C	-4.60600100	-2.26017800	1.39152600	H	-2.13776800	-1.55796400	-2.79415000
C	-5.28887500	-1.07407900	1.44649900	H	-1.91114600	-3.14145200	-3.58550300
H	-4.87080600	-3.26214000	1.71866600	H	-4.03839400	-2.49369700	-1.45086900
H	-6.27189600	-0.82350400	1.83643300	C	3.86639100	2.75776700	-1.58407200
N	-4.46333100	-0.11221800	0.86880300	C	5.04473100	1.98791200	-1.52105000
N	-3.38255300	-1.98594800	0.78908100	C	3.95166200	4.14599400	-1.33461200
Au	-1.70541100	0.21133000	-0.44989200	C	6.27418100	2.57589700	-1.20557200
C	-2.31991700	-2.92172500	0.50390400	H	5.02597700	0.91483400	-1.72891100
C	-2.24251300	-3.46702400	-0.79693300	C	5.16639400	4.74280000	-1.01603500
C	-1.35759700	-3.16259400	1.51064500	H	3.03844700	4.74436300	-1.39764600
C	-1.13151400	-4.28123800	-1.08404900	C	6.34162500	3.96069200	-0.94917500
C	-0.25749900	-3.96288900	1.16040700	H	7.17018400	1.95286300	-1.16708300
				H	5.23756400	5.81590800	-0.81507400

O	7.48235500	4.63397000	-0.63743200	H	-5.15368600	0.72071300	-4.85678100
C	8.70089600	3.88201800	-0.58395800	H	-5.89094600	-0.89696500	-4.74404200
H	8.93206100	3.42096800	-1.56166600	C	-5.58363900	-1.61227900	1.81495400
H	9.48582700	4.60814800	-0.32762900	H	-5.31670800	-0.54628600	1.92240900
H	8.65816300	3.09800300	0.19381700	C	-2.31110700	1.53809500	3.21953600
O	1.58574900	2.95563700	-2.28495000	C	-2.60346300	2.51002700	4.37620600
C	1.12618000	0.17612500	-2.16113200	H	-1.68005000	2.79779900	4.90891800
C	-0.00202000	0.87457800	-1.45135900	H	-3.08641200	3.43397300	4.01330300
C	-0.30023700	2.08308300	-1.23488900	H	-3.27859100	2.03692500	5.11100500
H	-0.69037900	3.05000800	-0.95336600	C	-4.47012800	-2.43696400	2.48987200
H	3.06912900	0.28918800	-1.34934800	H	-3.49473500	-2.26188300	2.00150200
H	0.89399800	0.21735100	-3.24196500	H	-4.37866500	-2.16350200	3.55629000
H	1.22348300	-0.87804100	-1.87138800	H	-4.68952200	-3.51826700	2.43231800
Sb	3.49882500	-2.56900300	0.23499200	C	-6.93600900	-1.81965300	2.51793700
F	2.09674000	-1.58398300	1.09721200	H	-6.86565900	-1.50635200	3.57437800
F	4.17586900	-0.88957600	-0.46943100	H	-7.73532500	-1.22841400	2.03814500
F	4.60997100	-2.34222200	1.77009000	H	-7.24594400	-2.87947200	2.50738200
F	4.89835400	-3.48349100	-0.68728900	C	-3.28168900	-0.96594400	-3.67446900
F	2.85253800	-4.23386400	0.92909700	H	-2.54127600	-1.19770000	-2.88762200
F	2.37884200	-2.74430600	-1.31666700	H	-3.49289100	-1.89785300	-4.22900400

Int2_5exo_SbF6

N	3.02971200	-0.30535300	0.30700400	H	-4.28966100	0.55709700	-2.54751900
C	3.42413400	-1.51130900	-0.06535400	C	-1.67126200	0.23394700	3.73248100
C	-3.22664000	0.33104700	0.06732100	H	-2.33322200	-0.25920300	4.46648100
C	-4.31074800	2.31889100	0.35705000	H	-1.49187800	-0.47092400	2.90090800
C	-5.24058200	1.39784400	-0.04390900	H	-0.70352900	0.43253800	4.22750400
H	-4.39805000	3.37428700	0.60150500	H	-3.27821300	1.27067500	2.75979700
H	-6.30902400	1.48075300	-0.22504700	C	4.77499800	-1.96640400	-0.29615000
N	-4.55863800	0.19489500	-0.21375000	C	5.86460300	-1.06710400	-0.23548500
N	-3.09202300	1.64946700	0.41725000	C	5.01176000	-3.32699200	-0.61871600
Au	-1.69722800	-1.00293900	-0.06046200	C	7.16103700	-1.50760500	-0.48862000
C	-1.82563000	2.23412900	0.79096300	H	5.70349900	-0.01116100	-0.00489200
C	-1.43611100	2.17810900	2.14859600	C	6.30156800	-3.77086500	-0.86689500
C	-1.01179800	2.78731900	-0.22328600	H	4.17330200	-4.02629600	-0.67173800
C	-0.17256400	2.70262100	2.47981500	C	7.38912000	-2.86565600	-0.80809200
C	0.24135400	3.29725000	0.16242800	H	7.98398700	-0.79151900	-0.44799800
C	0.65954000	3.25316900	1.49753300	H	6.50229500	-4.81623000	-1.11660500
H	0.16368800	2.66838200	3.52128400	O	8.60283900	-3.39625400	-1.07628600
H	0.91339900	3.71568800	-0.59032700	C	9.74377500	-2.52247500	-1.05412300
H	1.64738000	3.64413400	1.75979600	H	9.89087900	-2.08436200	-0.05121100
C	-5.14795000	-1.04640100	-0.65131400	H	10.60348300	-3.15884400	-1.30680900
C	-5.65123500	-1.93250000	0.32716900	H	9.64491600	-1.71845200	-1.80455900
C	-5.15642000	-1.33243200	-2.03444500	O	2.40106800	-2.34696800	-0.24572900
C	-6.18142800	-3.15450600	-0.12447700	C	1.57198400	-0.20729300	0.35113200
C	-5.70042700	-2.56734100	-2.43231600	C	1.16145900	-1.61128000	-0.04349400
C	-6.20616700	-3.46890500	-1.48863800	C	-0.03883700	-2.17301100	-0.22883800
H	-6.57163600	-3.87176200	0.60444100	H	-0.04075900	-3.23257100	-0.52358800
H	-5.71669700	-2.82701900	-3.49590600	H	3.64615800	0.51447500	0.43231800
H	-6.61926700	-4.42770100	-1.81885500	H	1.23086800	0.07540700	1.36242400
C	-1.42415500	2.80083600	-1.68981200	H	1.22832700	0.56565500	-0.35625300
H	-2.46883800	2.45010300	-1.75893600	Sb	4.42742800	3.07347800	-1.10183200
C	-1.37043500	4.22027500	-2.28234800	F	4.57346700	1.99196800	0.52454900
H	-1.73320600	4.21085700	-3.32527900	F	3.27124900	4.27716100	-0.15971500
H	-1.99855900	4.92251400	-1.70676300	F	4.27181200	4.11335900	-2.69052400
H	-0.33977500	4.61586400	-2.29188900	F	5.94566600	4.07267800	-0.52667000
C	-0.55058700	1.82510300	-2.50231400	F	5.56450200	1.80497100	-1.96922100
H	0.51537100	2.10912800	-2.45697700	F	2.90072600	2.01499300	-1.59374500
H	-0.64876500	0.79487100	-2.11412500				
H	-0.85871600	1.82296700	-3.56317800				
C	-4.56817700	-0.37717400	-3.06465100				
C	-5.59014700	-0.01219300	-4.15557900				
H	-6.50323800	0.43103300	-3.72113100				

Int2_6endo_SbF6

N	2.49808400	0.80865100	-0.80384700
C	2.69364600	2.02337600	-1.27808700
C	-3.40647800	-0.57448600	0.47826000
C	-4.66856300	-2.35261300	1.14646700

C	-5.45553700	-1.23501900	1.22703800	H	-3.95137500	-2.42350800	-1.57902700
H	-4.87261800	-3.39688000	1.36838900	C	4.01547300	2.59798700	-1.49688100
H	-6.48925300	-1.10059800	1.53453700	C	5.17970900	1.79639000	-1.49465600
N	-4.66630600	-0.16337500	0.81381300	C	4.14247900	3.99244500	-1.72039600
N	-3.42501800	-1.92809400	0.69072600	C	6.43693700	2.36279600	-1.69696300
Au	-1.75598700	0.42840300	-0.15543400	H	5.11988500	0.71574800	-1.33963000
C	-2.27645000	-2.76477900	0.42513600	C	5.39080000	4.56218500	-1.92528600
C	-2.10089100	-3.25669500	-0.88784000	H	3.24996400	4.62267000	-1.72156600
C	-1.34185300	-2.97898900	1.46346500	C	6.55231300	3.75417200	-1.91307300
C	-0.92964200	-3.99106900	-1.14847400	H	7.31841500	1.71881100	-1.69095500
C	-0.18440900	-3.71100000	1.14474200	H	5.50097400	5.63719800	-2.09255100
C	0.02361700	-4.20728300	-0.14719400	O	7.72074600	4.40446100	-2.12008400
H	-0.75397400	-4.37767600	-2.15777600	C	8.93113200	3.63060600	-2.10684600
H	0.58359000	-3.87010500	1.90600700	H	8.92578000	2.86837400	-2.90610800
H	0.94646700	-4.74985200	-0.36801700	H	9.74143100	4.35005200	-2.29026300
C	-5.09662200	1.21124900	0.74702100	H	9.08240200	3.14491600	-1.12662400
C	-5.65832100	1.68194900	-0.46115800	O	1.66459500	2.80982000	-1.57675300
C	-4.90284900	2.02963000	1.88191800	C	1.17672000	0.15571100	-0.68900100
C	-6.04408600	3.03380300	-0.50672400	C	0.05089800	1.16185700	-0.74594800
C	-5.31058600	3.37254700	1.78345100	C	0.34293300	2.39528700	-1.17972800
C	-5.87559600	3.86968200	0.60359400	H	-0.32345700	3.24780400	-1.30986300
H	-6.47387100	3.43772600	-1.42874600	H	3.31073200	0.25807900	-0.48107500
H	-5.17171500	4.03774100	2.64161500	H	1.08430200	-0.60050400	-1.49042200
H	-6.18142200	4.91947300	0.54603900	H	1.18695300	-0.40091100	0.26028900
C	-1.53356100	-2.40607400	2.86266900	Sb	3.82133200	-2.70041800	0.59404700
H	-2.56355500	-2.01411000	2.93644800	F	2.48165500	-1.83399600	1.66428000
C	-1.36812000	-3.48356900	3.94930200	F	4.52097800	-0.93217600	0.15059400
H	-1.57350400	-3.05399400	4.94568100	F	4.97452500	-2.75834100	2.11241500
H	-2.05996500	-4.32933700	3.79111900	F	5.17884000	-3.49648100	-0.48473800
H	-0.33987200	-3.88490200	3.96673200	F	3.08882000	-4.41489400	1.02879700
C	-0.56872400	-1.22805100	3.10177000	F	2.68933100	-2.55651900	-0.94516400
H	0.48272100	-1.55338500	3.02515200				
H	-0.73039400	-0.42992800	2.35414300	TS2_5exo_SbF6			
H	-0.72572800	-0.79826500	4.10755400	N	2.04254100	0.77403200	-2.97855200
C	-4.23938600	1.51571000	3.15332600	C	2.56075300	0.34234800	-1.87810100
C	-5.12754500	1.73468300	4.39068100	C	-2.01864000	0.68901700	0.67621000
H	-6.11108500	1.24780800	4.27022000	C	-3.70408600	1.56277100	1.92442800
H	-4.64268000	1.31070800	5.28752100	C	-2.56862600	2.26976000	2.21107900
H	-5.30294500	2.80802000	4.58262500	H	-4.72385200	1.65827000	2.28684400
C	-5.79600900	0.79278600	-1.69090700	H	-2.39179800	3.10525500	2.88220200
H	-5.59671900	-0.24916300	-1.38522500	N	-1.54544300	1.71870200	1.44151300
C	-3.09635700	-2.97601400	-2.00645600	N	-3.34680900	0.60194300	0.98233300
C	-3.64595800	-4.27820300	-2.61527200	Au	-0.98834000	-0.50336900	-0.57000800
H	-2.84344200	-4.87703100	-3.08081100	C	-4.27526600	-0.26183900	0.29039700
H	-4.13500100	-4.90566900	-1.84985600	C	-4.91755700	0.25758200	-0.85652500
H	-4.38988400	-4.04978700	-3.39884800	C	-4.48212700	-1.57403600	0.77212100
C	-4.73696000	1.17480800	-2.74334700	C	-5.82877200	-0.58429800	-1.51960600
H	-3.71760400	1.10317000	-2.32333600	C	-5.41003100	-2.36895300	0.07486500
H	-4.79994200	0.50249200	-3.61722300	C	-6.07890800	-1.87980200	-1.05380900
H	-4.88720200	2.21041300	-3.09788500	H	-6.34040700	-0.22000900	-2.41622800
C	-7.21401800	0.83203800	-2.28581100	H	-5.60309800	-3.38994800	0.41659400
H	-7.28915900	0.12486700	-3.13053000	H	-6.79338500	-2.51981500	-1.58184500
H	-7.97465300	0.55170100	-1.53648400	C	-0.19010200	2.22258900	1.38890900
H	-7.47113800	1.83446300	-2.67101500	C	0.17556500	3.04308400	0.29214600
C	-2.85327300	2.16464700	3.33168700	C	0.69832600	1.88158300	2.43342400
H	-2.21064200	1.97177500	2.45396500	C	1.48755600	3.54834100	0.28297200
H	-2.93902600	3.25891700	3.45747900	C	1.99320400	2.43031100	2.37724400
H	-2.34810500	1.75778600	4.22537900	C	2.38272300	3.25463900	1.31803500
H	-4.08404400	0.42822800	3.04646100	H	1.81640700	4.17346300	-0.55158500
C	-2.46173700	-2.07935300	-3.08604100	H	2.71291200	2.18561900	3.16357200
H	-3.20174800	-1.83445600	-3.86883000	H	3.40182700	3.65188500	1.28385300
H	-2.09293100	-1.13507700	-2.64644800	C	-3.75017900	-2.10202700	1.99879700
H	-1.60770800	-2.58305300	-3.57306900	H	-2.81995200	-1.52129400	2.11490400

C	-4.59864400	-1.88230100	3.26686900
H	-4.05276700	-2.23666900	4.15896700
H	-4.83593700	-0.81406800	3.41548400
H	-5.55277900	-2.43653100	3.20629500
C	-3.33401600	-3.57414400	1.85436100
H	-4.20487400	-4.25348800	1.83790500
H	-2.75100900	-3.73789400	0.93228200
H	-2.69811200	-3.86870000	2.70414000
C	0.29323600	0.96382500	3.58061300
C	-0.13559000	1.78373000	4.81392500
H	-0.98001600	2.45801700	4.59166600
H	-0.44378100	1.11108200	5.63369800
H	0.70321500	2.40320600	5.17947100
C	-0.81055700	3.39749100	-0.81672200
H	-1.50133800	2.54440600	-0.93628300
C	-4.60513000	1.64439300	-1.40636100
C	-5.87259800	2.49531300	-1.59759100
H	-6.54979900	2.05927200	-2.35291500
H	-6.43710700	2.59513700	-0.65433300
H	-5.59983300	3.50881900	-1.94074900
C	-0.13608900	3.62102400	-2.17931800
H	0.55523500	2.79944700	-2.43593000
H	-0.90515600	3.68465400	-2.96903400
H	0.43552500	4.56589400	-2.20728500
C	-1.65373600	4.62702700	-0.42034900
H	-2.39252200	4.85893400	-1.20866700
H	-2.20372900	4.46238800	0.52180700
H	-1.00844100	5.51380200	-0.28613400
C	1.40996200	-0.02399800	3.95877900
H	1.81355600	-0.53634600	3.07287000
H	2.24415100	0.48291700	4.47621000
H	1.01671700	-0.79206900	4.64604500
H	-0.57235900	0.36582400	3.24596300
C	-3.80644900	1.52792200	-2.71910700
H	-3.54016500	2.52996400	-3.10045700
H	-2.87450500	0.95469700	-2.56438100
H	-4.39540500	1.01323900	-3.49906000
H	-3.96547100	2.17098600	-0.67717500
C	3.68533300	0.87960600	-1.12620800
C	4.36645600	2.01369000	-1.61300100
C	4.09334700	0.29959300	0.09743800
C	5.43395700	2.56835800	-0.90481900
H	4.04575400	2.46021000	-2.55863000
C	5.15677000	0.84619100	0.80876300
H	3.56712100	-0.57319400	0.49183600
C	5.83571500	1.98296900	0.31688300
H	5.94677000	3.44641200	-1.30341000
H	5.48135400	0.41005200	1.75787900
O	6.85759800	2.43781300	1.09075600
C	7.58694800	3.58112600	0.62947600
H	6.93408000	4.46905800	0.54301100
H	8.35721200	3.76810200	1.39148700
H	8.07411800	3.38403000	-0.34287200
O	1.95187400	-0.79515400	-1.31720300
C	0.94173500	-0.13874400	-3.29239300
C	0.83639400	-1.05735000	-2.08436800
C	-0.03968500	-2.07457200	-1.74842200
H	-0.76520200	-2.33417700	-2.53362700
H	0.20344600	-2.86912400	-0.86826300
H	0.00778200	0.40925000	-3.49777100
H	1.17954100	-0.72942700	-4.19984100
Sb	0.96135600	-3.59766000	1.92593500
F	-0.44158700	-2.33436200	2.26648800

F	-0.23844500	-5.03599900	2.29376700
F	0.36709000	-3.67485900	0.02841900
F	2.34913000	-4.82889900	1.48621900
F	2.10639600	-2.14260300	1.42774300
F	1.52835700	-3.51863100	3.74336500

TS2_6endo_SbF6

N	-2.15090000	-0.20676600	-2.70901500
C	-2.80344700	-0.78915000	-1.77262100
C	1.08567400	0.98026800	1.08517000
C	1.64572100	2.86211200	2.23258800
C	1.96053000	1.79064500	3.02338600
H	1.73354500	3.93195200	2.40048800
H	2.37682900	1.73002600	4.02522800
N	1.61868800	0.65021000	2.30159600
N	1.11771600	2.34646100	1.05175500
Au	0.39522800	-0.30621900	-0.30360400
C	0.55913500	3.13468000	-0.02261700
C	1.37831800	3.45737000	-1.12980100
C	-0.79391100	3.52600100	0.08608400
C	0.78355000	4.20007000	-2.16528300
C	-1.33802100	4.26022200	-0.98347400
C	-0.55925700	4.59167000	-2.09669300
H	1.37832600	4.46676000	-3.04317400
H	-2.38806100	4.56617800	-0.94402200
H	-1.00227900	5.15887700	-2.92183700
C	1.71464500	-0.70499400	2.79199100
C	2.91766900	-1.41805400	2.57739800
C	0.58867000	-1.25859500	3.44268500
C	2.98003100	-2.72988200	3.07956100
C	0.70711300	-2.57697300	3.92190100
C	1.89025800	-3.30195900	3.74776500
H	3.89115300	-3.31701600	2.93412200
H	-0.14452200	-3.03806100	4.43273500
H	1.96228700	-4.32680200	4.12642900
C	-1.65766000	3.14786700	1.28331200
H	-0.99505500	2.75979500	2.07690600
C	-2.40249000	4.36053300	1.86778600
H	-2.95580200	4.06219200	2.77556400
H	-1.70533900	5.17141900	2.14186700
H	-3.13766300	4.77269100	1.15450700
C	-2.63719800	2.02121700	0.90622200
H	-3.33349300	2.34522900	0.11350700
H	-2.09426000	1.13671800	0.53254900
H	-3.23735800	1.71822500	1.78259300
C	-0.71640300	-0.49211700	3.62421200
C	-1.01991400	-0.25658400	5.11504100
H	-0.20174700	0.29441300	5.61093400
H	-1.94796100	0.33114300	5.22860700
H	-1.15752300	-1.21154500	5.65263200
C	4.09809700	-0.79156700	1.84518200
H	3.69493200	-0.03528800	1.14891800
C	2.84951900	3.06076200	-1.18198700
C	3.71730800	4.12752100	-0.48214400
H	3.61973700	5.10410900	-0.98967100
H	3.43176100	4.26477200	0.57486000
H	4.78120300	3.83229600	-0.51023800
C	4.88842200	-1.80533500	1.00405600
H	4.23174700	-2.39323900	0.34368400

H	5.61511700	-1.27374000	0.36747500	H	4.72475100	1.29415000	0.84922500
H	5.45879900	-2.50709400	1.63832400	H	4.64534300	-1.51868000	0.82865200
C	5.03565500	-0.07073200	2.83545500	N	2.56991400	-1.13212900	0.33090700
H	5.87423900	0.40017400	2.29274500	N	2.63093200	1.03234900	0.34554200
H	4.51238900	0.71960100	3.40002300	Au	-0.13539500	0.03673900	-0.24730100
H	5.45856100	-0.78524600	3.56459400	C	2.21352800	2.41278400	0.29188500
C	-1.88520300	-1.21275700	2.92644800	C	2.28920500	3.09121000	-0.94454100
H	-2.06785300	-2.20756300	3.37043400	C	1.72657600	3.00744600	1.47706200
H	-2.81378000	-0.62392800	3.02600400	C	1.86454900	4.43185700	-0.96719600
H	-1.68371900	-1.35158800	1.85036000	C	1.31811900	4.35126200	1.39812400
H	-0.60615600	0.49729800	3.14741400	C	1.38698500	5.05606900	0.19116900
C	3.35938800	2.81060000	-2.60927500	H	1.89889000	4.98881600	-1.90868900
H	4.37179300	2.37492400	-2.57114700	H	0.93118100	4.84560300	2.29491900
H	2.71293400	2.10717500	-3.15699600	H	1.05844500	6.09975800	0.15088400
H	3.42746200	3.74647900	-3.19219000	C	2.08074400	-2.48758900	0.25903000
H	2.96605200	2.11443400	-0.62625200	C	2.14077400	-3.15874100	-0.98222400
C	-4.11446000	-0.32590700	-1.28590300	C	1.55210300	-3.06824700	1.43311500
C	-4.76911800	0.72790600	-1.95407000	C	1.66148600	-4.48035300	-1.02011400
C	-4.71747400	-0.87384200	-0.13092100	C	1.09124900	-4.39403500	1.33955700
C	-5.98549200	1.23527400	-1.49052800	C	1.14710400	-5.09316500	0.12864500
H	-4.29943200	1.15423800	-2.84500900	H	1.68263600	-5.03136200	-1.96531400
C	-5.93065700	-0.37666700	0.34050100	H	0.67438200	-4.87894600	2.22792000
H	-4.22392600	-1.68909200	0.40373600	H	0.77831300	-6.12282600	0.07732200
C	-6.57496800	0.68349000	-0.33249900	C	1.63162600	2.24860100	2.79474400
H	-6.46817000	2.05223300	-2.03186300	H	1.94680600	1.20573200	2.61646600
H	-6.40149700	-0.79365400	1.23570200	C	2.58712900	2.84653300	3.84457700
O	-7.75353300	1.09903400	0.20925400	H	2.53152400	2.27095000	4.78541400
C	-8.43567800	2.17944200	-0.43661100	H	3.63440900	2.83152900	3.49483200
H	-8.71153000	1.92144000	-1.47545500	H	2.32319700	3.89414200	4.07473400
H	-9.35016700	2.34499100	0.15160700	C	0.18407800	2.20934800	3.31669600
H	-7.82617600	3.10195300	-0.43338900	H	-0.17888000	3.22090800	3.57149500
O	-2.35238400	-1.91211200	-1.05062800	H	-0.50914900	1.78011200	2.57307200
C	-0.86405900	-0.78391800	-3.12287200	H	0.12866200	1.59410700	4.23244800
C	-0.14342900	-1.54996800	-2.02703600	C	1.47042800	-2.31222800	2.75304600
C	-0.97736600	-2.09451800	-1.07598300	C	2.41735700	-2.92911300	3.79961600
H	-0.69505100	-2.83846700	-0.32221700	H	3.46414400	-2.93099400	3.44804800
H	1.14100400	-2.03555500	-2.22111100	H	2.37354200	-2.35510700	4.74211500
H	-1.04944500	-1.47269600	-3.97507400	H	2.13596100	-3.97284300	4.02716000
H	-0.23069900	0.02455700	-3.52149300	C	2.64139000	-2.47632500	-2.24847900
Sb	3.63724200	-1.25860600	-3.12546900	H	3.10507000	-1.51612600	-1.96157500
F	2.09699400	-2.40228100	-2.35459800	C	2.75464200	2.40268900	-2.22104400
F	3.55831900	-2.37363200	-4.66379000	C	3.87845800	3.18169800	-2.92650800
F	2.26050800	-0.16505100	-3.87116500	H	3.53169600	4.16804700	-3.28184900
F	5.04588000	-0.19340600	-3.81996700	H	4.73909400	3.34704200	-2.25520000
F	3.55178300	-0.24330500	-1.50777400	H	4.23385900	2.61904800	-3.80759900
F	4.80659200	-2.49982300	-2.28024900	C	1.45605700	-2.15538000	-3.17990600
MsOH				H	0.70307400	-1.53379900	-2.66276700
O	-1.46013000	2.32672700	0.11741300	H	1.80461100	-1.60671600	-4.07311400
S	-0.04830000	1.89287300	0.08413700	H	0.95623000	-3.08015900	-3.51912500
O	0.88028500	2.37887700	1.12487500	C	3.71365900	-3.30554100	-2.97637200
O	0.58465700	2.21759400	-1.41712000	H	4.09023700	-2.75034500	-3.85333000
C	0.05772600	0.11062900	-0.04839700	H	4.57089500	-3.52680100	-2.31673100
H	-0.32384700	-0.29943700	0.89917300	H	3.31071900	-4.26636600	-3.34215700
H	-0.56167700	-0.22741800	-0.89152800	C	0.02475000	-2.24607800	3.27675900
H	1.11089800	-0.17344400	-0.18836100	H	-0.66046400	-1.80257000	2.53413400
H	0.52743000	3.19825900	-1.54482100	H	-0.35845500	-3.24957300	3.53398300
IPrAuOMs				H	-0.01687900	-1.62932900	4.19225200
C	1.78672200	-0.02617800	0.14488700	H	1.80185400	-1.27440000	2.57569100
C	3.91549000	0.59542200	0.65507800	C	1.55854100	2.16886100	-3.16431100
C	3.87700900	-0.77231800	0.64597600	H	1.87883900	1.61620800	-4.06559300
				H	0.76719900	1.58379100	-2.66205500
				H	1.11644700	3.12733400	-3.48958900
				H	3.15956700	1.41201300	-1.94973600

O	-2.15989100	0.11336900	-0.69671800
S	-3.08446900	0.09358500	0.58314400
O	-2.94864100	1.34938000	1.37534000
O	-2.95657200	-1.18932800	1.33262100
C	-4.70309200	0.11074100	-0.21011400
H	-4.79671000	1.02232100	-0.81861200
H	-4.80417700	-0.78507400	-0.84041600
H	-5.46683400	0.10455800	0.58256500

H	-4.36975600	-3.04526800	-1.66131500
H	-5.31902800	-1.57172100	-1.32117100
C	-5.44383500	-3.34002200	0.88196200
H	-5.42071300	-4.28549900	0.31210800
H	-5.36411100	-3.58417600	1.95559800
H	-6.43037700	-2.87351700	0.71401800
C	-1.63508700	2.41515700	3.62167600
H	-1.80114500	2.95953100	2.67873700
H	-2.34993900	2.79234800	4.37544200
H	-0.61909900	2.66206200	3.97177600
H	-0.89823200	0.59049700	2.79875100
C	-0.75906500	-3.36139000	-2.72934800
H	-1.76693800	-3.67114800	-3.05837000
H	-0.72551200	-2.25766900	-2.71964100
H	-0.03503900	-3.71644900	-3.48350700
H	-1.23330100	-3.56017200	-0.64885200
C	4.26330600	0.66592800	-1.53788700
C	4.31983800	1.79993500	-0.70483000
C	5.36559600	-0.21642200	-1.54688500
C	5.43059500	2.04083900	0.11280600
H	3.49909100	2.52501100	-0.67479700
C	6.47499700	0.00750000	-0.73551800
H	5.32347900	-1.08669700	-2.20786500
C	6.51301600	1.13917500	0.10999800
H	5.43492800	2.92711400	0.75092600
H	7.32877700	-0.67740100	-0.73642500
O	7.63478300	1.27223700	0.87463700
C	7.70247300	2.40542000	1.74740000
H	6.87606700	2.40075700	2.48184300
H	8.66224700	2.31444800	2.27706900
H	7.68544500	3.35443500	1.18039800
O	3.15227000	-0.62576600	-3.23027800
C	0.84004300	0.83482500	-3.13929200
C	-0.44401700	1.01266200	-2.44663800
C	-1.58591100	1.31346400	-2.04062300
H	-2.55578000	1.77988500	-1.92708800
H	1.90111200	1.91522700	-1.64837500
H	0.81928300	1.51138000	-4.02067400
H	0.94413600	-0.19629800	-3.52501300
O	1.49945700	3.45412400	-0.92748600
S	0.88145700	3.45626900	0.46558200
O	1.71320900	4.17769900	1.47840600
O	0.41999400	2.08671800	0.89913600
C	-0.62394900	4.44017900	0.24166600
H	-1.27272800	3.94093200	-0.49516800
H	-1.14793300	4.53043500	1.20534700
H	-0.34386300	5.44044800	-0.12336100

Int1_MsO

N	1.97591000	1.09102600	-2.28090100
C	3.10073200	0.32096700	-2.41645100
C	-0.97136300	-1.46488400	0.94826500
C	-0.55857700	-3.26113300	2.27380100
C	-1.71224900	-2.67782300	2.72040400
H	-0.00980500	-4.13360700	2.61808400
H	-2.39064500	-2.94216600	3.52678100
N	-1.94360300	-1.57553000	1.90078800
N	-0.11966000	-2.50203300	1.19168800
Au	-0.93913700	-0.13553800	-0.57189500
C	1.06051000	-2.78210900	0.40933300
C	0.90352400	-3.46150300	-0.82103600
C	2.31099000	-2.35260100	0.90640800
C	2.06933800	-3.71917800	-1.56339700
C	3.44271600	-2.63835500	0.12162400
C	3.32459600	-3.31168000	-1.09867700
H	1.98822800	-4.24141900	-2.52183900
H	4.42658400	-2.30612100	0.46512700
H	4.21787200	-3.51337800	-1.69790400
C	-3.10763500	-0.72264200	1.95812400
C	-4.25666800	-1.13266400	1.24661800
C	-3.02909400	0.48826800	2.68809300
C	-5.37948100	-0.28498100	1.29353200
C	-4.18291000	1.29221000	2.70294700
C	-5.34352000	0.91140000	2.01603000
H	-6.28721900	-0.56667900	0.75010800
H	-4.17004800	2.23892800	3.24958500
H	-6.22574200	1.55955800	2.04102900
C	2.46482700	-1.61300500	2.22960800
H	1.46939800	-1.52235000	2.69739100
C	3.36220600	-2.40278900	3.20124400
H	3.42745500	-1.87787200	4.17052100
H	2.96962600	-3.41843800	3.38629800
H	4.38893700	-2.50498100	2.80711800
C	3.00343400	-0.18755400	2.01050800
H	3.99342100	-0.20345500	1.52345700
H	2.31979900	0.41610500	1.39051000
H	3.11387600	0.32658700	2.98227900
C	-1.75611900	0.89799300	3.42289700
C	-1.64424600	0.18027900	4.78462300
H	-1.62324600	-0.91708000	4.68051100
H	-0.71510600	0.48676200	5.29638800
H	-2.49630100	0.44429700	5.43684900
C	-4.29661600	-2.41897800	0.43061200
H	-3.35262000	-2.96600600	0.59778300
C	-0.45231500	-3.93314900	-1.33412900
C	-0.53464700	-5.47132200	-1.33202100
H	0.21567900	-5.91381100	-2.01093200
H	-0.36022100	-5.88237000	-0.32229900
H	-1.53276500	-5.80369700	-1.66868300
C	-4.38555500	-2.10893500	-1.07568200
H	-3.53529800	-1.48321100	-1.40162600

TS1_5exo_MsO

N	-2.30473000	-0.38624300	-0.83948300
C	-2.84410300	-1.54734800	-1.29478500
C	3.28636200	0.41063700	0.47461800
C	4.17022300	2.02751400	1.80232900
C	4.99062700	0.93406800	1.88166000
H	4.22048800	3.00570200	2.27314000
H	5.90877500	0.75670300	2.43543200
N	4.43158600	-0.04343100	1.06196900
N	3.13611400	1.68630500	0.93692500
Au	2.02439300	-0.55695100	-0.76051600
C	2.03535800	2.53682900	0.54743700
C	2.15839500	3.28031700	-0.64839400
C	0.87063900	2.53730600	1.34817700
C	1.04801200	4.05017400	-1.04144000

C	-0.20932200	3.32215100	0.90621500
C	-0.12414200	4.06595100	-0.27659500
H	1.10232400	4.63171900	-1.96764100
H	-1.14722700	3.33908300	1.46784100
H	-0.99605600	4.64003200	-0.60216200
C	4.98003000	-1.35829900	0.83365700
C	5.90900800	-1.51975300	-0.21881300
C	4.54520600	-2.42092300	1.65715200
C	6.41651800	-2.81399200	-0.43307500
C	5.08506300	-3.69408300	1.39834500
C	6.01180500	-3.88862000	0.36748300
H	7.13297300	-2.98071100	-1.24369800
H	4.76792000	-4.54423400	2.01064400
H	6.41775000	-4.88846200	0.18222800
C	0.73806600	1.68667800	2.60579000
H	1.73321600	1.27758100	2.85621900
C	0.26662700	2.51965600	3.81057400
H	0.24577600	1.89384700	4.72018500
H	0.93923500	3.37496400	3.99795600
H	-0.75207300	2.91458100	3.65529500
C	-0.21168700	0.49825400	2.35138000
H	-1.22028500	0.84714800	2.06736900
H	0.16694800	-0.14790300	1.53871300
H	-0.30385300	-0.12124000	3.26188200
C	3.50792000	-2.22878300	2.75589400
C	4.02356100	-2.71358400	4.12215700
H	4.95714400	-2.19854300	4.40774100
H	3.26975800	-2.51508700	4.90397800
H	4.22278500	-3.79955700	4.11956000
C	6.31844100	-0.36722600	-1.12775200
H	5.90313600	0.56680700	-0.71121600
C	3.41212800	3.23458200	-1.51375600
C	4.01505700	4.63685100	-1.71303300
H	3.32058100	5.30061300	-2.25737100
H	4.25160500	5.11510200	-0.74665200
H	4.94786000	4.57349400	-2.30065000
C	5.71707800	-0.55500000	-2.53400500
H	4.61616400	-0.63414300	-2.49020100
H	5.97643300	0.30116000	-3.18158500
H	6.10401300	-1.47261800	-3.01191800
C	7.84627600	-0.19773700	-1.19361100
H	8.10406200	0.67844000	-1.81399000
H	8.27865500	-0.04509700	-0.18956100
H	8.33739500	-1.07856400	-1.64297100
C	2.18752400	-2.92817000	2.37902500
H	1.80942100	-2.56560500	1.40615300
H	2.32238800	-4.02204400	2.30510200
H	1.41479300	-2.73059000	3.14259900
H	3.29572500	-1.14945900	2.84575200
C	3.11841300	2.55914800	-2.86678600
H	4.04140800	2.47923500	-3.46835200
H	2.71086500	1.54193600	-2.72273400
H	2.38150700	3.13873100	-3.45073100
H	4.16821000	2.61987300	-0.99459700
C	-4.10466400	-2.05109200	-0.68670500
C	-4.80456100	-1.37298900	0.33116000
C	-4.62442500	-3.27251300	-1.17047200
C	-5.99280400	-1.89544300	0.85499600
H	-4.43526300	-0.42074000	0.72936600
C	-5.80402100	-3.80141500	-0.65716000
H	-4.07866800	-3.79473500	-1.96159700
C	-6.50029500	-3.11532200	0.36293600
H	-6.51321400	-1.34757100	1.64395200

H	-6.21229200	-4.74648900	-1.02781300
O	-7.64387200	-3.71146300	0.80127100
C	-8.38837000	-3.04406800	1.82641300
H	-8.73729300	-2.05013900	1.49105000
H	-9.25780300	-3.68751800	2.02594600
H	-7.79414800	-2.93401700	2.75198600
O	-2.25348600	-2.17518900	-2.21435700
C	-1.18248600	0.11968300	-1.60491800
C	-0.20252300	-0.94364100	-1.85677300
C	0.79376500	-1.69981100	-2.02923100
H	1.09310600	-2.64743800	-2.46866100
H	-2.76365100	0.28170000	-0.17757700
H	-1.50585900	0.53371300	-2.58157700
H	-0.72032200	0.94996600	-1.04618400
O	-3.35605500	1.49015800	0.91356900
S	-3.72598800	2.72273100	0.08278900
O	-3.18779900	2.64579500	-1.31627500
O	-3.43867300	4.00161200	0.80980500
C	-5.52980300	2.63112500	-0.06893300
H	-5.80397500	1.69537800	-0.58081300
H	-5.97831300	2.65477300	0.93627900
H	-5.88167600	3.49461700	-0.65467800

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N	-2.43926800	0.25937000	-2.62293300
C	-3.03563700	-0.96363200	-2.59265000
C	2.89944100	-0.02756300	0.55249200
C	4.52498100	1.01802500	1.74913500
C	4.74809300	-0.32905100	1.84431300
H	5.05833400	1.86854100	2.16510000
H	5.51319800	-0.90146300	2.36200400
N	3.74531000	-0.94910500	1.10403000
N	3.39123700	1.18061600	0.95811800
Au	1.32576800	-0.38581900	-0.66314300
C	2.73663300	2.43769400	0.67986900
C	3.00708900	3.08724000	-0.54440900
C	1.82375600	2.93239500	1.63885900
C	2.31139600	4.28261100	-0.80122500
C	1.16110500	4.13330800	1.33250500
C	1.39676200	4.79753600	0.12413100
H	2.48221400	4.81009000	-1.74542600
H	0.42324100	4.53349100	2.03270900
H	0.84936200	5.71757200	-0.10355700
C	3.54247000	-2.37300900	0.99336400
C	4.20482400	-3.07352200	-0.03844900
C	2.65933100	-2.98850200	1.90952800
C	3.95424500	-4.45411100	-0.13964800
C	2.44328400	-4.37077900	1.76141600
C	3.08296600	-5.09556900	0.74896400
H	4.44318200	-5.03044600	-0.93122900
H	1.76036100	-4.88199800	2.44788600
H	2.89888200	-6.17035600	0.64989600
C	1.54825400	2.21313000	2.95409800
H	2.08212200	1.24669000	2.93704400
C	2.09927000	3.02444400	4.14222500
H	1.92719300	2.48454100	5.09047000
H	3.18420800	3.20660200	4.04467800
H	1.59843000	4.00610000	4.21710800
C	0.05083200	1.90447800	3.13860100
H	-0.54118800	2.83060800	3.24428700
H	-0.35260400	1.35399700	2.27322600
H	-0.09738800	1.30412600	4.05445400
C	1.93991100	-2.20687500	3.00200700

C	2.23345200	-2.78473900	4.39790500	C	3.50749700	-1.49724400	-0.19027400
H	3.31694200	-2.79816900	4.60925400	C	-3.20360300	0.36836300	0.10097000
H	1.74040100	-2.17314100	5.17379400	C	-4.35939800	2.31762200	0.38439700
H	1.85641400	-3.81784700	4.49787000	C	-5.25028100	1.36937300	-0.04035000
C	5.11089800	-2.37070800	-1.04120100	H	-4.48697200	3.36751300	0.63472200
H	5.29545400	-1.34555600	-0.67599600	H	-6.31745700	1.41793900	-0.24037900
C	3.98786800	2.52785100	-1.56701200	N	-4.52579800	0.19095700	-0.20553500
C	5.09561200	3.54308100	-1.90148100	N	-3.12052500	1.68836100	0.46178700
H	4.68405100	4.44875400	-2.38050100	Au	-1.63304900	-0.92236600	0.00769200
H	5.63939200	3.85850700	-0.99386000	C	-1.88093900	2.30538800	0.87048100
H	5.82502900	3.09819500	-2.60135600	C	-1.52435900	2.24593400	2.23648600
C	4.40705400	-2.25409300	-2.40763400	C	-1.05639800	2.88377600	-0.12030700
H	3.44252400	-1.72357700	-2.31278900	C	-0.28191500	2.79511500	2.60241800
H	5.03874800	-1.69620900	-3.12172600	C	0.18287700	3.40525500	0.29567600
H	4.20587600	-3.25204400	-2.83668200	C	0.56507000	3.36078200	1.64171500
C	6.47667400	-3.06566300	-1.17350200	H	0.03015300	2.76052500	3.65138300
H	7.13356400	-2.48805700	-1.84714400	H	0.87446700	3.80740200	-0.44958200
H	6.98087100	-3.15283300	-0.19532800	H	1.53756200	3.76439100	1.94420400
H	6.37965800	-4.08100900	-1.59655700	C	-5.07200400	-1.06460100	-0.65731800
C	0.42552900	-2.14956700	2.72600600	C	-5.57472500	-1.96446500	0.30872300
H	0.21866800	-1.69436600	1.74093900	C	-5.04624600	-1.34765400	-2.04076100
H	-0.02140500	-3.15992500	2.73714800	C	-6.06819600	-3.19688600	-0.15596600
H	-0.08338000	-1.54360900	3.49610100	C	-5.55387900	-2.59359800	-2.45216700
H	2.31597000	-1.16936200	2.98972600	C	-6.05845800	-3.50857600	-1.52091000
C	3.25193200	2.06703000	-2.83928900	H	-6.45638500	-3.92434500	0.56384100
H	3.96056400	1.61019200	-3.55311200	H	-5.54270300	-2.85082700	-3.51639700
H	2.47639500	1.31752500	-2.59489000	H	-6.44336600	-4.47554100	-1.86125900
H	2.75644700	2.91490000	-3.34481600	C	-1.45257200	2.92295500	-1.59101200
H	4.47619400	1.64125000	-1.12589200	H	-2.48680500	2.54615600	-1.67778700
C	-4.46574900	-1.03627900	-2.16815600	C	-1.43855000	4.36194700	-2.13827100
C	-5.24707700	0.08482500	-1.82210900	H	-1.79600300	4.37520800	-3.18308100
C	-5.06111900	-2.31633500	-2.10783200	H	-2.09010300	5.02649200	-1.54386900
C	-6.57963200	-0.06271000	-1.41860500	H	-0.41976600	4.78741900	-2.12942500
H	-4.82479300	1.09490000	-1.83926600	C	-0.54874100	1.99966100	-2.43043400
C	-6.38516400	-2.47596400	-1.71220600	H	0.50879000	2.31265500	-2.37750800
H	-4.45275300	-3.18403600	-2.37800600	H	-0.61873200	0.95588300	-2.07411600
C	-7.15821200	-1.34673000	-1.36179100	H	-0.86019400	2.02036500	-3.49034400
H	-7.15597400	0.82619200	-1.15260600	C	-4.46108900	-0.37594900	-3.05695900
H	-6.84875800	-3.46590200	-1.66274200	C	-5.47417400	-0.02417000	-4.16036500
O	-8.44185300	-1.60214100	-0.98335700	H	-6.40022000	0.40195600	-3.73622600
C	-9.25503200	-0.48498500	-0.60756500	H	-5.04090300	0.71874800	-4.85301400
H	-9.38638900	0.22019400	-1.44873900	H	-5.75220700	-0.91164900	-4.75589800
H	-10.23153600	-0.90903200	-0.33166300	C	-5.54397200	-1.64763500	1.79831500
H	-8.83013000	0.05069000	0.26106400	H	-5.29992200	-0.57705900	1.91437500
O	-2.40956100	-2.01662700	-2.90691000	C	-2.40849600	1.57448800	3.27991600
C	-1.01536600	0.40095800	-2.85663000	C	-2.75279400	2.52640900	4.43869700
C	-0.24836500	-0.58796700	-2.01731400	H	-1.84931200	2.83500100	4.99359300
C	-0.41862000	-1.81268600	-1.75267000	H	-3.25480700	3.43977600	4.07467100
H	-0.38897700	-2.83828900	-1.41632000	H	-3.42908600	2.02677700	5.15455800
H	-2.85763800	1.07355000	-2.11489800	C	-4.42871700	-2.45297200	2.49333400
H	-0.76717800	0.18623400	-3.91267100	H	-3.44689800	-2.25559900	2.02708100
H	-0.73800900	1.43570500	-2.62246800	H	-4.36578300	-2.18310400	3.56272900
O	-3.19912000	2.55938900	-1.26020500	H	-4.62516700	-3.53813100	2.42609900
S	-2.45920500	2.49896800	0.07449400	C	-6.90632600	-1.88406400	2.47227100
O	-2.17095300	3.85473400	0.63776300	H	-6.86318100	-1.57580800	3.53167100
O	-1.28432500	1.56002300	0.01495900	H	-7.70658700	-1.30496700	1.97933800
C	-3.62693600	1.71461100	1.21772100	H	-7.19608800	-2.94941900	2.44920000
H	-4.54407900	2.32117400	1.27941600	C	-3.15514900	-0.93748800	-3.65061000
H	-3.87114600	0.70560300	0.85100100	H	-2.42344900	-1.16183800	-2.85365900
H	-3.15713800	1.64510100	2.21152600	H	-3.34136400	-1.86888700	-4.21504800
				H	-2.69950200	-0.20648100	-4.34177400
				H	-4.20841400	0.56017900	-2.53025400
				C	-1.74709000	0.28175400	3.79437800

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N 3.16858500 -0.23688800 -0.01582800

H	-2.41968200	-0.24514000	4.49459300	H	-5.14443700	4.07662800	2.56028600
H	-1.51347500	-0.40103500	2.95784700	H	-6.45851400	4.84430600	0.59302100
H	-0.80471800	0.50131500	4.32783200	C	-1.32818600	-2.09606000	2.66852200
H	-3.35764200	1.28851700	2.79478500	H	-2.34581500	-1.67776200	2.76730000
C	4.83962900	-2.03777500	-0.36507200	C	-1.15287000	-3.15791800	3.77053000
C	5.96768700	-1.18663300	-0.40278100	H	-1.29416700	-2.70395500	4.76746600
C	5.01656700	-3.43603000	-0.51352600	H	-1.88312900	-3.97900500	3.66048300
C	7.24540400	-1.71517000	-0.57911100	H	-0.14087700	-3.59842000	3.74247900
H	5.84799000	-0.10081600	-0.30968800	C	-0.32710200	-0.93920900	2.84802800
C	6.28695800	-3.96539700	-0.69075800	H	0.71571500	-1.27689600	2.71967500
H	4.14723000	-4.09826400	-0.49021200	H	-0.51102900	-0.14236300	2.10490300
C	7.41433900	-3.11052600	-0.72431800	H	-0.42803100	-0.50004300	3.85717800
H	8.10187100	-1.03873900	-0.60927300	C	-4.04528900	1.61123600	3.01775100
H	6.44077600	-5.04178000	-0.80737600	C	-4.77653100	1.84016700	4.35191800
O	8.60780700	-3.72523400	-0.90293800	H	-5.74852600	1.31721900	4.37483100
C	9.78790500	-2.90735000	-0.92700300	H	-4.16423600	1.46121100	5.18903600
H	9.92660000	-2.37997400	0.03348800	H	-4.96416000	2.91281400	4.53603100
H	10.62343700	-3.60294800	-1.08858900	C	-6.12422800	0.67889700	-1.58312800
H	9.75211400	-2.17575600	-1.75357000	H	-5.90117400	-0.35226200	-1.25799400
O	2.45636900	-2.32586900	-0.20674000	C	-3.26445500	-3.18881300	-1.97643500
C	1.71543200	-0.09450000	0.06543200	C	-3.72331800	-4.58387100	-2.43743400
C	1.24931200	-1.52951100	-0.07370500	H	-2.90672300	-5.13262800	-2.93891000
C	0.03169700	-2.08683100	-0.10501700	H	-4.06826600	-5.19695500	-1.58649900
H	0.00893100	-3.18023100	-0.22653500	H	-4.55636100	-4.49510000	-3.15729300
H	3.82824200	0.60592400	-0.04074600	C	-5.13343000	1.03456400	-2.71024000
H	1.42349500	0.36471400	1.02667400	H	-4.08955900	0.99460400	-2.35084800
H	1.36472200	0.56726700	-0.74354800	H	-5.23762400	0.32943900	-3.55414200
O	4.78872500	1.88819100	-0.06166900	H	-5.32184700	2.05472800	-3.09077100
S	4.23829300	2.88558000	-1.09272700	C	-7.57467000	0.69686200	-2.09203500
O	2.82041600	2.55643800	-1.46857700	H	-7.69805300	-0.03829300	-2.90646300
O	5.16928400	3.11061000	-2.23826600	H	-8.28898300	0.44136600	-1.29013600
C	4.16753200	4.43964400	-0.16828700	H	-7.85706200	1.68489200	-2.49590500
H	3.52086300	4.30455400	0.71239300	C	-2.67294300	2.31153500	3.00350600
H	5.18311700	4.71792600	0.15260400	H	-2.13518300	2.10414700	2.06038900
H	3.75417300	5.22367300	-0.82176700	H	-2.78239900	3.40655800	3.10191600

Int2_gendo_MsO

N	2.39933800	0.62523600	-1.14739100	H	-2.04947900	1.95421200	3.84201000
C	2.68009400	1.89847300	-1.29696300	H	-3.86082000	0.52734400	2.92260600
C	-3.45501600	-0.54856000	0.37723800	C	-2.83268600	-2.32084500	-3.17387200
C	-4.60788600	-2.33882800	1.19785500	H	-3.66295900	-2.21563000	-3.89493400
C	-5.41909300	-1.24074100	1.30506200	H	-2.52889500	-1.31180200	-2.84333600
H	-4.76306300	-3.38039700	1.46730600	H	-1.97766800	-2.77476500	-3.70584800
H	-6.42922500	-1.12346500	1.68859800	H	-4.13117800	-2.69305800	-1.50521200
N	-4.69623200	-0.16087900	0.79951100	C	4.04033000	2.43500400	-1.32561900
N	-3.41848300	-1.89544600	0.63104500	C	5.17283700	1.59293300	-1.25369500
Au	-1.83524900	0.44666500	-0.34583100	C	4.23309900	3.83598200	-1.41826900
C	-2.24548700	-2.68550400	0.33259000	C	6.46074000	2.12892400	-1.27112300
C	-2.14555600	-3.27874900	-0.94582100	H	5.06045500	0.50567100	-1.17376600
C	-1.20389800	-2.72847600	1.28769100	C	5.51264200	4.37452900	-1.43983700
C	-0.93583400	-3.92278700	-1.26511300	H	3.36542200	4.49761400	-1.46978800
C	-0.00941100	-3.36738300	0.90860700	C	6.64126300	3.52605500	-1.36622300
C	0.12853300	-3.94937900	-0.35676300	H	7.31838900	1.45563200	-1.21092300
H	-0.81936800	-4.38091400	-2.25299200	H	5.67043000	5.45437300	-1.51078600
H	0.84363400	-3.37746000	1.59241600	O	7.84586400	4.14727800	-1.39229200
H	1.08750200	-4.39929400	-0.63069400	C	9.02416800	3.33000000	-1.33219700
C	-5.17508500	1.19802900	0.74441900	H	9.07876300	2.64022100	-2.19358200
C	-5.90485300	1.60632600	-0.39456900	H	9.86925100	4.03202700	-1.36982400
C	-4.87998700	2.05863100	1.82499000	H	9.06540200	2.75478700	-0.38979700
C	-6.36168300	2.93608900	-0.42317300	O	1.71122700	2.80968500	-1.42178200
C	-5.35845700	3.37937000	1.74400000	C	1.03341500	0.07009500	-1.13370600
C	-6.09541000	3.81219800	0.63600100	C	-0.01991800	1.14067800	-0.95577700
H	-6.92568700	3.29094900	-1.29141000	C	0.36300700	2.41398200	-1.12269400
				H	-0.23992600	3.31925900	-1.04706600
				H	3.15942300	-0.09850000	-0.98768600

H	0.87372100	-0.49611700	-2.07224200
H	1.01375100	-0.66572600	-0.31268600
O	4.11094700	-1.44843000	-0.80368600
S	3.80580800	-2.10918500	0.54613400
O	3.42588400	-3.55055900	0.40488600
O	2.87308200	-1.27371700	1.37459000
C	5.39504400	-2.08635300	1.41348300
H	5.26459400	-2.54688800	2.40511800
H	6.13561900	-2.65623700	0.83135200
H	5.72655200	-1.04235000	1.52642000

TS2_5exo_MsO

N	3.37292300	-0.17136000	-3.36141200
C	3.27518600	0.19334900	-2.12775600
C	-2.25252800	0.76001400	0.70094200
C	-4.01708700	1.42533700	1.98326900
C	-2.94418100	2.20022900	2.32748800
H	-5.04524300	1.41855300	2.33472800
H	-2.84244900	3.01082700	3.04337900
N	-1.87539600	1.77524900	1.54088300
N	-3.57373900	0.55147500	0.99270000
Au	-1.12835900	-0.21444100	-0.65265400
C	-4.41606700	-0.37594000	0.27555100
C	-5.16457300	0.12313300	-0.81325600
C	-4.44434000	-1.73149800	0.68102700
C	-5.99420100	-0.78436000	-1.49773000
C	-5.29172700	-2.59331900	-0.03783300
C	-6.06206900	-2.12619000	-1.11045700
H	-6.58209400	-0.43348900	-2.35203500
H	-5.34038600	-3.65004800	0.23929800
H	-6.71159500	-2.81920400	-1.65553400
C	-0.56696400	2.38711900	1.53372300
C	-0.30738600	3.38762000	0.56979400
C	0.39179500	1.95853700	2.48183300
C	0.96883300	3.98046700	0.58102000
C	1.64567500	2.59467600	2.45493300
C	1.93372900	3.59200600	1.51514900
H	1.20675600	4.75145600	-0.15910200
H	2.41395900	2.29298300	3.17261800
H	2.92421900	4.05813400	1.50369300
C	-3.60787600	-2.23086800	1.85344800
H	-2.68036700	-1.63348600	1.88166100
C	-4.35450800	-2.00945500	3.18470900
H	-3.72913300	-2.34215000	4.03211200
H	-4.60232000	-0.94624100	3.34560700
H	-5.29743100	-2.58575300	3.20761300
C	-3.18039400	-3.69893000	1.71202800
H	-4.03550300	-4.39253700	1.80588500
H	-2.68316200	-3.88208700	0.74473000
H	-2.45715800	-3.94565000	2.50611000
C	0.08015800	0.87755400	3.50932700
C	-0.43495600	1.51047000	4.81843700
H	-1.33020400	2.13387700	4.65401500
H	-0.69772500	0.72333100	5.54741100
H	0.34248300	2.15106000	5.27335200
C	-1.33892200	3.81944300	-0.46517100
H	-2.27133700	3.25921500	-0.28031500
C	-5.04723700	1.56644400	-1.28811900
C	-6.41800300	2.25556900	-1.39582600
H	-7.05721000	1.77861500	-2.15963600
H	-6.95995600	2.22482400	-0.43441600
H	-6.29073700	3.31412600	-1.68370500
C	-0.86778200	3.46477600	-1.88733300
H	-0.68035100	2.37963700	-1.97530900

H	-1.63656700	3.74592500	-2.62882300
H	0.06521600	3.99631500	-2.14634000
C	-1.67155800	5.31737900	-0.34183700
H	-2.45656900	5.59443500	-1.06779300
H	-2.03738400	5.56725200	0.66949900
H	-0.78840100	5.94819800	-0.54698500
C	1.27880300	-0.04055100	3.79588000
H	1.68453800	-0.47878900	2.86996900
H	2.08777200	0.49391500	4.32625700
H	0.95667900	-0.87282600	4.44498700
H	-0.72260200	0.24270700	3.09497000
C	-4.28158900	1.62192000	-2.62464000
H	-4.14350200	2.66881200	-2.94927100
H	-3.28623600	1.15341600	-2.52816600
H	-4.83252600	1.08899800	-3.42031300
H	-4.45472700	2.12858700	-0.54579600
C	4.26772600	0.84647500	-1.28299700
C	5.45258800	1.35398900	-1.85198500
C	4.06520700	0.96193900	0.11206500
C	6.42155300	1.97138000	-1.05803900
H	5.60725400	1.26324600	-2.93129700
C	5.02899400	1.57170700	0.90984600
H	3.15970700	0.54926700	0.56370400
C	6.21276400	2.08311800	0.33405300
H	7.32885100	2.36190300	-1.52381900
H	4.89160800	1.65707800	1.99172500
O	7.08829500	2.66067200	1.20213500
C	8.31909700	3.16393500	0.66993400
H	8.14314100	3.97729000	-0.05777000
H	8.87333000	3.56151300	1.53251000
H	8.91097100	2.36136700	0.19292700
O	2.04946700	-0.07432000	-1.50106800
C	2.08758900	-0.79205900	-3.69232000
C	1.26521000	-0.72468700	-2.42138200
C	0.03031900	-1.20788100	-2.07719300
H	-0.47412100	-1.71126800	-2.91752900
H	0.23086800	-2.17018400	-1.09408500
H	1.59333800	-0.25744300	-4.52613200
H	2.22955500	-1.83666600	-4.02837000
O	0.39517400	-3.23109600	-0.40548400
S	0.99276400	-2.92190600	1.01728100
O	-0.06758700	-2.58982200	2.01314800
O	2.14385100	-1.97692100	0.92877200
C	1.63990000	-4.54857000	1.45608100
H	2.07531800	-4.47537000	2.46482400
H	0.81484900	-5.27681500	1.45322200
H	2.41213400	-4.83874900	0.72852000

TS2_6endo_MsO

N	-1.86379000	0.13406700	-2.93325200
C	-2.98095800	-0.11666800	-2.36008800
C	1.04748800	0.81691800	1.50369200
C	1.31436100	2.80001400	2.59862400
C	2.10292000	1.87415700	3.22540900
H	1.14531100	3.85616300	2.79146800
H	2.76627400	1.95061200	4.08283300
N	1.92635400	0.67249400	2.54202200
N	0.67981600	2.13583000	1.55434500
Au	0.26046900	-0.48040700	0.17358300
C	-0.22483300	2.74377100	0.60677900
C	0.31616200	3.26541700	-0.58991600
C	-1.60498400	2.76497100	0.90673900
C	-0.58496500	3.83683300	-1.50621100

C	-2.46105200	3.35159200	-0.04261900
C	-1.95689400	3.88313200	-1.23464700
H	-0.20531100	4.23860100	-2.45094100
H	-3.53914400	3.37365800	0.14711800
H	-2.64352900	4.32201600	-1.96496500
C	2.62670100	-0.54684100	2.85987500
C	3.92976600	-0.71769500	2.34074000
C	1.98793700	-1.50220400	3.68185600
C	4.61450400	-1.89336600	2.69765300
C	2.70948600	-2.67085700	3.98793400
C	4.01230800	-2.86003600	3.51159500
H	5.62856900	-2.05668400	2.31860000
H	2.24369900	-3.43975300	4.61246000
H	4.55948200	-3.77289600	3.76876600
C	-2.17262600	2.16203300	2.18465300
H	-1.33636900	1.73596400	2.76596900
C	-2.84327400	3.23796600	3.05774100
H	-3.21631700	2.79454900	3.99794000
H	-2.13442800	4.04393300	3.31678300
H	-3.70249700	3.69897700	2.53897000
C	-3.14507700	1.01139000	1.86520400
H	-4.02465400	1.37017400	1.30215400
H	-2.64963200	0.23443000	1.25711400
H	-3.50567600	0.54359800	2.79885400
C	0.56854100	-1.30979700	4.20052800
C	0.48767800	-1.45619200	5.73001700
H	1.17158800	-0.75492700	6.23896400
H	-0.53948200	-1.24508400	6.07600200
H	0.74443300	-2.47890900	6.05779400
C	4.58253700	0.30138500	1.41509500
H	3.85758400	1.11232700	1.22889200
C	1.80106200	3.17452500	-0.91831400
C	2.39601200	4.54351000	-1.29098300
H	1.94803100	4.94606100	-2.21654700
H	2.23810700	5.28472000	-0.48793800
H	3.48294200	4.45164400	-1.46306200
C	4.92561300	-0.32597700	0.05129000
H	4.03431900	-0.74968900	-0.44197000
H	5.35342800	0.44016700	-0.61962900
H	5.67429200	-1.13221500	0.15324500
C	5.82492500	0.93147400	2.07110800
H	6.26435600	1.69459400	1.40480800
H	5.57366600	1.41829300	3.02984700
H	6.60217100	0.17265800	2.27170400
C	-0.39993000	-2.27736900	3.49395500
H	-0.36897100	-2.13097000	2.39827200
H	-0.14222300	-3.33005400	3.70780000
H	-1.43603300	-2.10217600	3.83507500
H	0.24912900	-0.28317900	3.95015700
C	2.03729900	2.13619500	-2.03215500
H	3.11598900	2.03625800	-2.24773700
H	1.65413400	1.14411300	-1.73261600
H	1.52541100	2.43000200	-2.96576400
H	2.33201700	2.81895000	-0.01777000
C	-4.15332500	0.77043400	-2.42023000
C	-4.13933200	1.87832100	-3.29100600
C	-5.27662500	0.58138200	-1.58357800
C	-5.20222100	2.78450300	-3.32921900
H	-3.26872100	2.02573100	-3.93596700
C	-6.34178400	1.47961800	-1.61052100
H	-5.30488100	-0.27117100	-0.90072700
C	-6.31314600	2.59130400	-2.47994400
H	-5.16151400	3.63186500	-4.01782200

H	-7.21233100	1.34268800	-0.96208800
O	-7.39866700	3.41339600	-2.42686600
C	-7.39667400	4.56236600	-3.28056300
H	-7.35066800	4.27458600	-4.34698000
H	-8.34665000	5.08083700	-3.08541500
H	-6.55504900	5.23948100	-3.04455300
O	-3.20926700	-1.24088800	-1.53193400
C	-0.79556000	-0.85949400	-2.74812400
C	-0.81145700	-1.46498800	-1.34472600
C	-2.07876400	-1.68302100	-0.87978100
H	-2.35068200	-2.19523800	0.04958700
H	0.02415300	-2.65186400	-1.26647500
H	-0.93111800	-1.66900500	-3.49637900
H	0.16987200	-0.38226800	-2.97722100
O	0.54882100	-3.70830200	-1.39771700
S	2.12985800	-3.58193700	-1.40327700
O	2.55285300	-2.29801100	-2.02980400
O	2.70223900	-4.84094100	-1.93971900
C	2.52856000	-3.49175900	0.34664900
H	2.15171300	-4.39571400	0.84816900
H	3.62091900	-3.42596300	0.45282600
H	2.04830000	-2.59231200	0.76594600

TfOH

O	-1.47255400	2.33957900	0.12667500
S	-0.05156800	1.95766400	0.09479000
O	0.87921800	2.39498700	1.14697400
O	0.58562800	2.23183600	-1.40014500
C	0.06099600	0.09050500	-0.05067300
H	0.53443500	3.20580100	-1.58586100
F	-0.40423100	-0.41915000	1.09921000
F	1.33591200	-0.27625200	-0.23049500
F	-0.68870000	-0.33484000	-1.07451400

IPrAuOTf

C	1.80077700	-0.01835400	0.16485100
C	3.93658500	0.59072900	0.64819300
C	3.88958300	-0.77703500	0.63909100
H	4.75241900	1.28448600	0.83242100
H	4.65537600	-1.52835100	0.81185500
N	2.57677500	-1.12944500	0.34038200
N	2.65139000	1.03580800	0.35470400
Au	-0.12217500	0.06768300	-0.20795800
C	2.23801700	2.41795300	0.30261900
C	2.30569000	3.09402600	-0.93556800
C	1.75999600	3.01457600	1.49047000
C	1.88062200	4.43461000	-0.95734900
C	1.35004300	4.35792800	1.41176700
C	1.41033200	5.06051200	0.20302400
H	1.90870400	4.99005900	-1.89987300
H	0.96927000	4.85386400	2.31032200
H	1.08095000	6.10389100	0.16307300
C	2.07970400	-2.48227600	0.26601900
C	2.12716000	-3.14703300	-0.97922300
C	1.55733500	-3.06589600	1.44129700
C	1.64116800	-4.46612800	-1.01965800
C	1.08959800	-4.38904000	1.34482200
C	1.13298200	-5.08224500	0.13004600
H	1.65207000	-5.01251100	-1.96762900
H	0.67709500	-4.87637300	2.23386800
H	0.75881000	-6.10977900	0.07640300
C	1.67230400	2.25779900	2.80982800
H	2.00254300	1.21880700	2.63552700

C	2.61534700	2.87070300	3.86206200	C	3.26159700	-3.39917900	-1.19914100
H	2.56553200	2.29475900	4.80293700	H	1.85834200	-4.32572500	-2.55840800
H	3.66352000	2.87046900	3.51492600	H	4.43818600	-2.39710200	0.31249500
H	2.33593200	3.91439300	4.09117500	H	4.12832700	-3.62543300	-1.82778200
C	0.22310400	2.20114100	3.32588700	C	-3.05923700	-0.69963300	1.98395700
H	-0.15721000	3.20926200	3.56790800	C	-4.17612100	-1.02971300	1.18384300
H	-0.45854400	1.75421400	2.58172900	C	-3.01490200	0.42877800	2.83586800
H	0.17105300	1.59331800	4.24663000	C	-5.27931200	-0.15728900	1.23209400
C	1.48506300	-2.31474100	2.76440400	C	-4.14729300	1.26224400	2.84727700
C	2.42930700	-2.94122400	3.80747600	C	-5.26385400	0.97665400	2.05125900
H	3.47554100	-2.94730400	3.45452800	H	-6.16098700	-0.37568400	0.62090700
H	2.38978200	-2.37078500	4.75229600	H	-4.15187200	2.15125100	3.48441600
H	2.14232400	-3.98422300	4.03092900	H	-6.13073900	1.64523800	2.07206900
C	2.62109100	-2.46108900	-2.24620700	C	2.55369600	-1.63663500	2.13093000
H	3.09023900	-1.50346500	-1.95939300	H	1.57348400	-1.49497200	2.61784400
C	2.76312200	2.40434200	-2.21439800	C	3.43933200	-2.44594200	3.09730300
C	3.88680700	3.18036800	-2.92347700	H	3.54529500	-1.90898900	4.05634700
H	3.54141600	4.16793200	-3.27665100	H	3.01145400	-3.44229300	3.30702400
H	4.75038000	3.34255600	-2.25526900	H	4.45227300	-2.59486800	2.68288200
H	4.23703300	2.61727300	-3.80630200	C	3.14650500	-0.23995000	1.87125400
C	1.43040400	-2.13365600	-3.16848200	H	4.12850600	-0.30689600	1.37228100
H	0.68238500	-1.51111800	-2.64534600	H	2.47837600	0.37328800	1.24543600
H	1.77452600	-1.58382300	-4.06259500	H	3.28886400	0.29333200	2.82821300
H	0.92514100	-3.05571700	-3.50682600	C	-1.81657200	0.70394500	3.73540100
C	3.68556600	-3.29124700	-2.98441100	C	-2.03607900	0.05784900	5.11941200
H	4.05751200	-2.73435700	-3.86221800	H	-2.20931400	-1.02957500	5.04837900
H	4.54667900	-3.51717300	-2.33146700	H	-1.15306100	0.22188500	5.76168900
H	3.27691400	-4.24958200	-3.35024200	H	-2.91179200	0.50615600	5.62249700
C	0.04012000	-2.24296800	3.28976200	C	-4.22324900	-2.28060200	0.31440900
H	-0.64362700	-1.80654000	2.54171500	H	-3.27453500	-2.82955700	0.44314100
H	-0.34479900	-3.24394500	3.55326900	C	-0.53009100	-3.96528600	-1.28562800
H	-0.00205500	-1.61896700	4.20010700	C	-0.62928400	-5.50222100	-1.25794400
H	1.82284400	-1.27821100	2.59076600	H	0.08799900	-5.96218900	-1.96053300
C	1.56277800	2.17653000	-3.15368400	H	-0.41817000	-5.90104600	-0.25043400
H	1.87759900	1.62432200	-4.05704500	H	-1.64382800	-5.82750600	-1.54910900
H	0.77035000	1.59362600	-2.65061500	C	-4.35016800	-1.92770800	-1.17808500
H	1.12301200	3.13702500	-3.47589600	H	-3.49985500	-1.30455300	-1.50797000
H	3.16581700	1.41196400	-1.94586800	H	-4.36237300	-2.84657100	-1.79057800
O	-2.16084400	0.20209500	-0.63528300	H	-5.28228400	-1.37264300	-1.38512800
S	-3.09003300	-0.00952100	0.59993000	C	-5.35814100	-3.21842000	0.76619900
O	-3.06771100	1.12847400	1.55148200	H	-5.34982300	-4.14600800	0.16704000
O	-3.02624100	-1.38592600	1.15111900	H	-5.25009200	-3.49554500	1.82928900
C	-4.72577300	0.10511700	-0.30080800	H	-6.34785600	-2.74546500	0.63926100
F	-4.85300400	1.30663000	-0.89424700	C	-1.50322200	2.19935200	3.89018000
F	-4.81567600	-0.85981900	-1.23502700	H	-1.40603200	2.69915600	2.91595500
F	-5.72526800	-0.05202800	0.58996700	H	-2.27893400	2.72275900	4.47725500
Int1_TfO				H	-0.54697100	2.32212300	4.42675600
N	2.00327700	0.94619600	-2.36387200	H	-0.93312700	0.22842400	3.27439400
C	3.17063000	0.23938600	-2.48911400	C	-0.88435200	-3.41081300	-2.67661500
C	-0.94010200	-1.45988600	0.95428800	H	-1.90384800	-3.72172500	-2.96598700
C	-0.50888500	-3.23832700	2.29734500	H	-0.84893400	-2.30703200	-2.68117000
C	-1.65720500	-2.64950800	2.75083700	H	-0.18860900	-3.77785800	-3.45129300
H	0.04318300	-4.10732900	2.64517900	H	-1.28021300	-3.57261300	-0.57746700
H	-2.32184200	-2.90132700	3.57213400	C	4.30143500	0.65720500	-1.60300300
N	-1.90204500	-1.56100300	1.91833200	C	4.31872700	1.84467800	-0.84722900
N	-0.08549600	-2.49490700	1.19900200	C	5.41266700	-0.20932200	-1.51650500
Au	-0.92986400	-0.18982500	-0.61726800	C	5.39236900	2.15104200	-0.00297400
C	1.06330300	-2.80599100	0.38145100	H	3.49729000	2.56555900	-0.90478500
C	0.84976800	-3.50284300	-0.83098400	C	6.48663200	0.07875800	-0.67842700
C	2.33872300	-2.39354400	0.82681300	H	5.40617800	-1.11986000	-2.12228200
C	1.98297000	-3.79013700	-1.61205400	C	6.48006400	1.26079700	0.09624900
C	3.43645200	-2.71315900	0.00712600	H	5.36585900	3.07881200	0.57276500
				H	7.34588100	-0.59483500	-0.60184500

O	7.56672400	1.45220200	0.89628300	H	5.00424300	-2.18435600	4.40339000
C	7.57550500	2.62032000	1.72490000	H	3.32199600	-2.50875700	4.91164000
H	6.71856700	2.62599700	2.42330300	H	4.27674700	-3.79000800	4.12401200
H	8.51351800	2.56974600	2.29713900	C	6.32796000	-0.35860700	-1.13932900
H	7.56580500	3.54655600	1.12143800	H	5.91624900	0.57530100	-0.71895500
O	3.27613300	-0.71169900	-3.29029300	C	3.38710000	3.22840000	-1.51965700
C	0.87817500	0.62372200	-3.21605300	C	3.98297700	4.63017100	-1.74224100
C	-0.40937800	0.84568700	-2.54334900	H	3.27943900	5.28736900	-2.28279900
C	-1.55266900	1.17841300	-2.16815900	H	4.23379200	5.11867300	-0.78464000
H	-2.50873100	1.67726200	-2.08259100	H	4.90670800	4.56213500	-2.34336000
H	1.88798300	1.75695000	-1.73294300	C	5.71088700	-0.54838300	-2.53855300
H	0.86136500	1.23956900	-4.14080400	H	4.61080300	-0.63139100	-2.48213200
H	0.98842600	-0.42917800	-3.53451400	H	5.95994400	0.30857100	-3.18909100
O	1.26038900	3.29951900	-1.03376600	H	6.09544000	-1.46484400	-3.02055200
S	0.96132700	3.47763600	0.43563800	C	7.85457500	-0.18695100	-1.22312300
O	1.78788800	4.51603700	1.11063400	H	8.10349400	0.68802100	-1.84877300
O	0.75611800	2.20360800	1.19063000	H	8.29825800	-0.03099300	-0.22454100
C	-0.75214400	4.23360800	0.36774600	H	8.34216600	-1.06793800	-1.67595200
F	-0.80441800	5.24364000	-0.52677200	C	2.22553100	-2.93408200	2.39427800
F	-1.68110200	3.30754300	0.00913700	H	1.83909800	-2.57469900	1.42342400
F	-1.11103100	4.72530900	1.57866000	H	2.36586600	-4.02726400	2.32088600

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N	-2.30188400	-0.41852600	-0.82828600
C	-2.84259700	-1.58318900	-1.27837300
C	3.30142100	0.40836200	0.47996500
C	4.18944000	2.03348300	1.79490900
C	5.01461400	0.94356800	1.87159300
H	4.23965400	3.01365200	2.26159800
H	5.93801500	0.77195900	2.41839900
N	4.45291100	-0.03890300	1.05991000
N	3.14961400	1.68509700	0.93887900
Au	2.03608300	-0.57872400	-0.73570100
C	2.04165500	2.53151000	0.56194700
C	2.14785300	3.27749300	-0.63402900
C	0.88925100	2.53265400	1.37999300
C	1.03400900	4.05198000	-1.00738100
C	-0.19357900	3.32562700	0.95897300
C	-0.12453200	4.07428200	-0.22191500
H	1.07500800	4.63561500	-1.93274900
H	-1.11568500	3.34600000	1.54568600
H	-0.99401700	4.66170700	-0.53031100
C	5.00461200	-1.35234100	0.83076400
C	5.92935600	-1.51136200	-0.22580900
C	4.57644600	-2.41588000	1.65660600
C	6.44030500	-2.80397200	-0.44141100
C	5.11912800	-3.68747500	1.39584900
C	6.04224500	-3.87950400	0.36129700
H	7.15364200	-2.96891700	-1.25509800
H	4.80728600	-4.53833400	2.00986700
H	6.45062500	-4.87812000	0.17485000
C	0.77232500	1.67743300	2.63612000
H	1.76783200	1.25741100	2.86546700
C	0.33226300	2.50831800	3.85417000
H	0.32518100	1.87835700	4.76100600
H	1.01568600	3.35710500	4.03129200
H	-0.68612600	2.91267700	3.72253900
C	-0.19176800	0.49817400	2.39319800
H	-1.20203800	0.85671800	2.12878400
H	0.16620000	-0.14815100	1.57141700
H	-0.27431000	-0.12427400	3.30240400
C	3.54448000	-2.22668500	2.76104000
C	4.07160400	-2.70513800	4.12525800

H	5.00424300	-2.18435600	4.40339000
H	3.32199600	-2.50875700	4.91164000
H	4.27674700	-3.79000800	4.12401200
C	6.32796000	-0.35860700	-1.13932900
H	5.91624900	0.57530100	-0.71895500
C	3.38710000	3.22840000	-1.51965700
C	3.98297700	4.63017100	-1.74224100
H	3.27943900	5.28736900	-2.28279900
H	4.23379200	5.11867300	-0.78464000
H	4.90670800	4.56213500	-2.34336000
C	5.71088700	-0.54838300	-2.53855300
H	4.61080300	-0.63139100	-2.48213200
H	5.95994400	0.30857100	-3.18909100
H	6.09544000	-1.46484400	-3.02055200
C	7.85457500	-0.18695100	-1.22312300
H	8.10349400	0.68802100	-1.84877300
H	8.29825800	-0.03099300	-0.22454100
H	8.34216600	-1.06793800	-1.67595200
C	2.22553100	-2.93408200	2.39427800
H	1.83909800	-2.57469900	1.42342400
H	2.36586600	-4.02726400	2.32088600
H	1.45691600	-2.73983900	3.16288200
H	3.32682400	-1.14827000	2.84958600
C	3.07215500	2.53952200	-2.86108400
H	3.98435400	2.46122600	-3.47901700
H	2.67516200	1.52052200	-2.70089700
H	2.31997400	3.10888500	-3.43549000
H	4.15351900	2.62059300	-1.00752900
C	-4.11613100	-2.07008200	-0.68896900
C	-4.84174700	-1.36378800	0.29052800
C	-4.62721700	-3.30210000	-1.15571000
C	-6.04541000	-1.86744000	0.79491900
H	-4.48466800	-0.40382700	0.67514600
C	-5.82195100	-3.81362800	-0.66122700
H	-4.06304800	-3.84580800	-1.91886200
C	-6.54350200	-3.09827300	0.32089800
H	-6.58681200	-1.29416600	1.55076400
H	-6.22377100	-4.76650500	-1.01848900
O	-7.70086700	-3.67797900	0.74253100
C	-8.46620100	-2.98460300	1.73521400
H	-8.80084000	-1.99608400	1.37105600
H	-9.34388000	-3.61900300	1.92707500
H	-7.89275800	-2.85888000	2.67179800
O	-2.23458400	-2.22269100	-2.17727800
C	-1.16835500	0.07685900	-1.58439300
C	-0.19363400	-0.99578300	-1.81897000
C	0.80514100	-1.75162600	-1.97684700
H	1.10763500	-2.70626700	-2.39863700
H	-2.76728000	0.24944400	-0.18509300
H	-1.47902000	0.48696800	-2.56686600
H	-0.70394100	0.90436000	-1.02351400
O	-3.32962100	1.55658700	0.90862100
S	-3.67950600	2.76338900	0.05931200
O	-3.21208300	2.66174600	-1.35463300
O	-3.46076400	4.06887700	0.74412000
C	-5.54118100	2.63088600	-0.06572400
F	-5.89695600	1.48901600	-0.70135600
F	-6.10262800	2.62086700	1.16485600
F	-6.04797100	3.67566500	-0.75707500

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N	2.32811300	0.80788600	-1.61748800
C	2.66526000	2.09406300	-1.75760600

C	-3.37579200	-0.54337700	0.37580100	H	-2.58307600	-1.48378000	-2.90589800
C	-4.49146200	-2.29373600	1.30681500	H	-2.08004100	-2.99863500	-3.70349200
C	-5.29119400	-1.18846000	1.42105000	H	-4.14099200	-2.76264700	-1.42459700
H	-4.63729800	-3.32408600	1.61986500	C	4.06501600	2.52444400	-1.52435700
H	-6.27914900	-1.05436300	1.85330400	C	5.08180000	1.63423200	-1.12224900
N	-4.59326000	-0.12776700	0.84703400	C	4.38450000	3.89357900	-1.68681200
N	-3.32883600	-1.88154200	0.66787500	C	6.37901900	2.09277200	-0.87771500
Au	-1.84176800	0.45499800	-0.50471100	H	4.88409300	0.56698500	-0.98216200
C	-2.17837400	-2.70831800	0.35127600	C	5.67592700	4.35507300	-1.45982600
C	-2.14129700	-3.35330400	-0.90755500	H	3.59664900	4.58686200	-1.99270600
C	-1.10920400	-2.75250200	1.27882700	C	6.68650800	3.45722400	-1.04917300
C	-0.95759000	-4.03668100	-1.24100300	H	7.13235500	1.37568400	-0.54409700
C	0.05775700	-3.42670000	0.87541000	H	5.93403700	5.41056500	-1.58521300
C	0.13974300	-4.05298700	-0.37308900	O	7.91611700	4.00905800	-0.84382400
H	-0.88679300	-4.53866900	-2.21196300	C	8.96928000	3.13914200	-0.42615700
H	0.93822400	-3.43113900	1.52322900	H	9.16306100	2.34945700	-1.17572900
H	1.08276600	-4.52501000	-0.66295000	H	9.85901300	3.77746000	-0.32774500
C	-5.08646000	1.23023300	0.77418600	H	8.74362800	2.66879400	0.54889800
C	-5.84538200	1.61178000	-0.35728100	O	1.80943900	3.00604100	-2.09447000
C	-4.79187500	2.11128000	1.84124300	C	0.99047800	0.26010700	-1.78869600
C	-6.31747500	2.93647900	-0.39697100	C	-0.11343400	1.20380200	-1.33837700
C	-5.29414700	3.42214000	1.74766500	C	0.00741700	2.48792200	-1.43037200
C	-6.04801000	3.83214200	0.64325700	H	-0.37346500	3.48954800	-1.28690100
H	-6.90251600	3.27013600	-1.26030300	H	3.02882800	0.08321100	-1.32614300
H	-5.08498000	4.13258500	2.55411400	H	0.80863800	0.01271300	-2.85363800
H	-6.42604000	4.85843200	0.59120800	H	0.96554000	-0.68158200	-1.22070700
C	-1.17486300	-2.09863200	2.65717100	O	3.87349400	-1.41660600	-1.14095100
H	-2.19917700	-1.70936400	2.80851800	S	3.61854800	-2.09873900	0.19291600
C	-0.91478700	-3.13570900	3.77004200	O	3.33946000	-3.55696600	0.09572100
H	-1.02690600	-2.66475000	4.76238100	O	2.73692600	-1.30116100	1.09677900
H	-1.61870500	-3.98402600	3.70831800	C	5.30919000	-2.10851900	0.99900800
H	0.10925300	-3.54156400	3.70748800	F	5.26188500	-2.51332600	2.25385900
C	-0.19806700	-0.90969300	2.77126200	F	6.21407600	-2.72634900	0.29131800
H	0.84200600	-1.21099900	2.56188800	F	5.74618100	-0.73121000	1.07201700
H	-0.45765700	-0.11566700	2.04851100				
H	-0.24367800	-0.47800600	3.78770300				
C	-3.96432900	1.69413700	3.05310100	Int2_5exo_TfO			
C	-4.78815600	1.78770400	4.35386400	N	3.18895500	-0.23941300	-0.78063300
H	-5.70058200	1.16885800	4.30107600	C	3.54648400	-1.48062400	-0.51225200
H	-4.18756200	1.44084300	5.21253900	C	-3.17331300	0.43275800	0.10830400
H	-5.09938300	2.82675900	4.56132300	C	-4.39007300	2.34639800	0.37346200
C	-6.13389800	0.66003800	-1.51467900	C	-5.24937000	1.36819700	-0.04803600
H	-5.75543900	-0.34026100	-1.23957000	H	-4.55203300	3.39261500	0.61963800
C	-3.29947600	-3.29842000	-1.90069400	H	-6.31675800	1.38271700	-0.25210100
C	-3.80522900	-4.70960700	-2.26248900	N	-4.48794700	0.21191300	-0.20207500
H	-3.02218800	-5.30247500	-2.76636900	N	-3.13152300	1.75788400	0.45728300
H	-4.12041500	-5.26797500	-1.36431200	Au	-1.57404800	-0.82723400	0.06793700
H	-4.66758800	-4.64419800	-2.94916300	C	-1.92489200	2.40690400	0.91348400
C	-5.37963700	1.10043000	-2.78638000	C	-1.56605300	2.26125900	2.27194600
H	-4.29242800	1.15464200	-2.60383500	C	-1.13738400	3.11329400	-0.02523200
H	-5.55730600	0.38230000	-3.60619100	C	-0.35756000	2.85075900	2.68515100
H	-5.71779900	2.09482200	-3.12819400	C	0.07286600	3.66229500	0.43597900
C	-7.64621600	0.51980700	-1.77980800	C	0.45787800	3.53361300	1.77681900
H	-7.82537200	-0.21539400	-2.58343600	H	-0.04940900	2.75952300	3.73175200
H	-8.18550700	0.18151900	-0.87828600	H	0.73471000	4.17517400	-0.26640900
H	-8.09475100	1.47648000	-2.10024700	H	1.40693700	3.96271600	2.10904900
C	-2.66422000	2.51784400	3.15287200	C	-5.00049200	-1.06911700	-0.62077300
H	-2.05873800	2.41584600	2.23598200	C	-5.47952700	-1.95437800	0.37090600
H	-2.87583800	3.59078300	3.30714400	C	-4.96880000	-1.38993900	-1.99562600
H	-2.05538200	2.16858000	4.00474800	C	-5.94218400	-3.21109900	-0.05868500
H	-3.66940900	0.63833300	2.92386500	C	-5.44489200	-2.65954800	-2.37130100
C	-2.90898400	-2.50635800	-3.16552000	C	-5.92543400	-3.56060600	-1.41432200
H	-3.76636900	-2.43384700	-3.85839100	H	-6.31128700	-3.92764900	0.68183300
				H	-5.42740800	-2.94661300	-3.42774600

H	-6.28595700	-4.54616200	-1.72688600
C	-1.54778300	3.23278900	-1.48866200
H	-2.63442600	3.04376000	-1.55193500
C	-1.28767200	4.63630600	-2.06186400
H	-1.69742800	4.70559300	-3.08484000
H	-1.76156300	5.42281300	-1.44887300
H	-0.20780000	4.85551800	-2.12687700
C	-0.83678400	2.16111900	-2.33986900
H	0.25383300	2.33151700	-2.34130700
H	-1.03191600	1.14674600	-1.94685700
H	-1.19358000	2.20156500	-3.38495100
C	-4.41094800	-0.43263700	-3.04060500
C	-5.44041600	-0.12974200	-4.14332300
H	-6.36886400	0.29326200	-3.72123800
H	-5.02696100	0.60012900	-4.86155500
H	-5.71007700	-1.03866500	-4.70951400
C	-5.45393500	-1.59898000	1.85198600
H	-5.23818100	-0.51986600	1.94202500
C	-2.42715500	1.49945400	3.27197700
C	-2.98203300	2.44515500	4.35346200
H	-2.16679900	2.91083800	4.93531700
H	-3.58374200	3.25658900	3.90788700
H	-3.62518200	1.88917700	5.05851500
C	-4.31581300	-2.35836600	2.56168100
H	-3.34004700	-2.13890100	2.09200900
H	-4.26225400	-2.06878900	3.62637100
H	-4.47981600	-3.44990000	2.51259800
C	-6.80763200	-1.85375200	2.53658000
H	-6.76867300	-1.51807000	3.58777200
H	-7.62386100	-1.30736300	2.03262300
H	-7.07033400	-2.92630000	2.54101800
C	-3.09917100	-0.98367900	-3.63083100
H	-2.35738000	-1.17377300	-2.83424100
H	-3.27119400	-1.93266200	-4.16987600
H	-2.66370000	-0.26187600	-4.34429000
H	-4.17230300	0.52129100	-2.54059700
C	-1.64770400	0.32912200	3.89815800
H	-2.30160600	-0.25273100	4.57161400
H	-1.26312200	-0.34962100	3.11646100
H	-0.78783200	0.68807300	4.49105800
H	-3.28765700	1.07013900	2.73063300
C	4.87961800	-2.04184000	-0.53514500
C	5.99936900	-1.25011500	-0.87861100
C	5.06938400	-3.40560400	-0.19705900
C	7.27925900	-1.80083800	-0.88668700
H	5.87793600	-0.19460000	-1.14215300
C	6.34177400	-3.95770300	-0.20342000
H	4.20755300	-4.02205700	0.07094000
C	7.45999600	-3.16118000	-0.54809500
H	8.12948400	-1.17054300	-1.15434900
H	6.50492200	-5.00738300	0.05547300
O	8.65588100	-3.79300100	-0.52302200
C	9.82818600	-3.03482800	-0.86236100
H	9.97880000	-2.19569100	-0.16044700
H	10.66626500	-3.74069400	-0.77673700
H	9.77117500	-2.65345500	-1.89712600
O	2.51293300	-2.25650600	-0.17800800
C	1.74398300	-0.06096400	-0.62900700
C	1.30148400	-1.45248000	-0.22077000
C	0.10315700	-1.97862700	0.05926200
H	0.10283300	-3.04978700	0.31207900
H	3.83242900	0.53491500	-1.09328800
H	1.53120600	0.70966800	0.13183600

H	1.29825700	0.27160600	-1.58102000
O	4.81042900	1.79961200	-1.60932200
S	4.04110300	3.10794300	-1.58523500
O	2.59915200	2.95589800	-1.93969700
O	4.77157600	4.25497700	-2.17988400
C	3.99930900	3.47924100	0.24522800
F	3.41661600	2.45652400	0.92281300
F	5.24371200	3.65248100	0.73613600
F	3.28782400	4.60727100	0.49044600

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N	2.28745200	0.64003300	-1.43083800
C	2.60996400	1.91512500	-1.42090300
C	-3.43167200	-0.53563700	0.38800400
C	-4.53188500	-2.31711500	1.29453200
C	-5.35378600	-1.22691000	1.40032900
H	-4.66289700	-3.35273500	1.59744200
H	-6.35216100	-1.11216300	1.81435000
N	-4.66279000	-0.15253400	0.84239800
N	-3.36829300	-1.87434400	0.67588300
Au	-1.86823400	0.47043500	-0.43340100
C	-2.19838400	-2.66372000	0.36571900
C	-2.12583200	-3.28444300	-0.90171100
C	-1.13889700	-2.69033100	1.30083700
C	-0.93001700	-3.95122900	-1.22571200
C	0.04048800	-3.35518500	0.91821000
C	0.14756400	-3.97467600	-0.33243800
H	-0.83518900	-4.43350500	-2.20418000
H	0.90114400	-3.36319400	1.59243600
H	1.08923000	-4.45825800	-0.60957400
C	-5.16237700	1.19721500	0.75607600
C	-5.91661500	1.56107200	-0.38152700
C	-4.85755300	2.09381500	1.80413100
C	-6.38464800	2.88610000	-0.44575100
C	-5.35038600	3.40659500	1.68987900
C	-6.10825100	3.79783200	0.58002900
H	-6.96640800	3.20842200	-1.31530300
H	-5.12919100	4.13227200	2.47919600
H	-6.48026600	4.82530400	0.51006100
C	-1.22689900	-2.01211200	2.66223300
H	-2.23770600	-1.57994500	2.76967400
C	-1.03727700	-3.03409400	3.79832700
H	-1.14636000	-2.53967500	4.77983700
H	-1.78313500	-3.84624500	3.73838400
H	-0.03310500	-3.49165300	3.76285700
C	-0.21220000	-0.85868900	2.77377200
H	0.82492200	-1.21340300	2.64692400
H	-0.39880300	-0.09661300	1.99583000
H	-0.29427700	-0.37175900	3.76230800
C	-3.99531500	1.69032600	2.99289200
C	-4.69921600	1.95732800	4.33447200
H	-5.66697800	1.42937600	4.39407900
H	-4.06667800	1.60868100	5.16968900
H	-4.89011300	3.03394600	4.48925300
C	-6.16955500	0.58941800	-1.52722000
H	-5.84858100	-0.41544200	-1.20225700
C	-3.25814300	-3.19645300	-1.91760100
C	-3.73140600	-4.58974400	-2.36837800
H	-2.92627400	-5.14489400	-2.88120400
H	-4.06777000	-5.19873800	-1.51117600
H	-4.57437900	-4.49690900	-3.07597700
C	-5.31056700	0.97576000	-2.74735100
H	-4.23847200	1.00921000	-2.48391000

H	5.14549700	1.47151000	2.00030400	C	-1.58785800	-0.29597100	4.84707600
O	7.35859600	2.41195500	1.19255000	H	-0.80909100	0.15027800	5.48950800
C	8.59339400	2.87695100	0.65181200	H	-2.49090900	0.33588300	4.91193300
H	8.43735200	3.69453400	-0.07748900	H	-1.84214500	-1.28514800	5.26663000
H	9.16850600	3.25805300	1.50794300	C	3.83782400	-0.90085200	2.01751100
H	9.15808100	2.05908700	0.16571100	H	3.56121700	-0.08263800	1.32970800
O	2.18207500	-0.12128400	-1.49367300	C	3.16197800	3.33982000	-0.71978100
C	2.19636400	-0.78443500	-3.70139200	C	4.10179700	4.15988900	0.19225700
C	1.37252900	-0.70477200	-2.42787500	H	4.17305900	5.20561300	-0.15762000
C	0.10858800	-1.13944500	-2.11168600	H	3.75586600	4.17667500	1.24054000
H	-0.39901000	-1.61521000	-2.96502500	H	5.11667900	3.72588800	0.17812400
H	0.27056400	-2.09451600	-1.10448600	C	4.63157300	-1.92308600	1.18572000
H	1.72531900	-0.21705600	-4.52782200	H	5.43434600	-1.40603800	0.63540000
H	2.29533600	-1.82873400	-4.05567900	H	5.10455300	-2.69411800	1.82093000
O	0.39876000	-3.12341000	-0.33404200	H	3.99276500	-2.42186400	0.44190600
S	0.96476000	-2.78220300	1.07694100	C	4.72851500	-0.31545400	3.13648100
O	-0.06664100	-2.27638900	2.02049700	H	5.65192900	0.10841100	2.70466100
O	2.26710500	-2.07230600	1.02783500	H	4.22109600	0.48643300	3.69983300
C	1.33845300	-4.52917200	1.65579700	H	5.01846000	-1.10204600	3.85619200
F	1.88234200	-4.47336800	2.88879200	C	-2.22842000	-0.98036300	2.47853700
F	0.20434900	-5.25805700	1.71500000	H	-1.90344800	-1.01988600	1.42484500
F	2.20522100	-5.13242000	0.82266300	H	-2.51064900	-2.00273800	2.78666900

TS2_gendo_TfO

N	-2.36301800	0.48328100	-2.61086200	H	-0.90670000	0.61654700	3.02718900
C	-2.69191800	-0.59855200	-2.00732400	C	3.74932700	3.23323500	-2.13866700
C	1.02315800	1.18305200	1.13365200	H	4.67663700	2.63868300	-2.11245200
C	1.55849900	2.89111100	2.53662900	H	3.05521700	2.72326100	-2.82675900
C	1.72231000	1.72361200	3.22844600	H	3.99707400	4.22386900	-2.56173900
H	1.69666100	3.92802700	2.82986800	H	3.11162400	2.30902400	-0.32709300
H	2.02927900	1.53028300	4.25229800	C	-4.02159200	-0.80920500	-1.40184600
N	1.39735800	0.68820800	2.35519700	C	-5.02379100	0.16304000	-1.58775400
N	1.13439300	2.54385500	1.25662500	C	-4.32667300	-1.95715800	-0.63614900
Au	0.47013200	0.19919900	-0.53949600	C	-6.29413100	0.01088700	-1.02592200
C	0.76929600	3.50943200	0.23630600	H	-4.78358800	1.04565400	-2.18722600
C	1.74896100	3.91895700	-0.70320400	C	-5.59061000	-2.11960300	-0.07189300
C	-0.55188500	4.01735900	0.25007800	H	-3.56276800	-2.72386700	-0.48624900
C	1.36495300	4.90592600	-1.62971300	C	-6.58568900	-1.13802400	-0.26128400
C	-0.87266400	5.00341400	-0.70041300	H	-7.04937700	0.78275300	-1.19225500
C	0.07548400	5.44941600	-1.62502400	H	-5.83765900	-3.00492300	0.52118800
H	2.09131100	5.24376900	-2.37384000	O	-7.79056400	-1.39530000	0.33029700
H	-1.88560300	5.41816200	-0.71799600	C	-8.83297900	-0.43981800	0.14785600
H	-0.19478600	6.21661900	-2.35809200	H	-9.09171600	-0.31885800	-0.92114200
C	1.36939400	-0.70952100	2.73935300	H	-9.70193700	-0.83983900	0.69002300
C	2.54985000	-1.48005600	2.59688200	H	-8.56108400	0.54677600	0.56914800
C	0.16278400	-1.22935500	3.26548300	O	-1.85278900	-1.71239700	-1.81498300
C	2.49286200	-2.81676200	3.03196600	C	-1.03513500	0.55846200	-3.23722600
C	0.16806400	-2.57476900	3.67766600	C	0.01393700	-0.34748500	-2.61430700
C	1.32006600	-3.35845400	3.56951100	C	-0.49855600	-1.45201600	-1.96759500
H	3.38237300	-3.44546300	2.93555600	H	0.08399400	-2.32051800	-1.64169800
H	-0.74944200	-3.01208700	4.08515500	H	1.24880700	-0.31008900	-3.05332100
H	1.30278200	-4.40310500	3.89745900	H	-1.14230800	0.28697600	-4.30985900
C	-1.61536600	3.53725000	1.23385300	H	-0.70966300	1.61331400	-3.22818500
H	-1.20010100	2.68465300	1.79934400	O	2.33896900	-0.25255900	-3.59729200
C	-1.96975300	4.64094100	2.25183700	S	3.62373600	-0.48799900	-2.77628400
H	-2.38274700	5.53108600	1.74514500	O	3.48440500	-0.04788600	-1.35770800
H	-2.72816300	4.27797600	2.96780600	O	4.85426100	-0.12090700	-3.50478400
H	-1.08391200	4.96462900	2.82574000	C	3.63992700	-2.36057100	-2.66061700
C	-2.87419700	3.02463700	0.50462100	F	3.54877400	-2.92757600	-3.87614000
H	-3.40368800	3.84345600	-0.01398500	F	4.77318200	-2.78579500	-2.06514100
H	-2.62331000	2.25618200	-0.24574900	F	2.58529600	-2.78923700	-1.90860000
H	-3.57929200	2.58260300	1.23054600				
C	-1.11774900	-0.40718200	3.38261800				