

Supplementary Information

**Palladium-catalyzed generation of CO from formic acid for alkoxy carbonylation
of internal alkenes exploits a PTSA-assisted NH-Pd mechanism: a DFT
mechanistic study**

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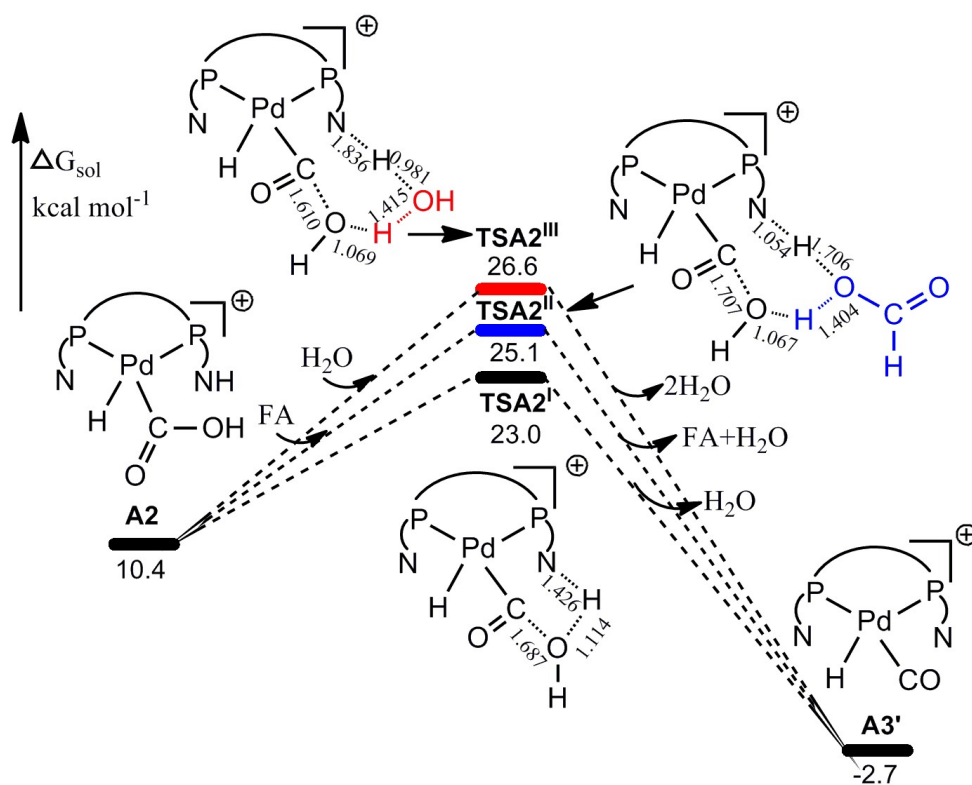


Fig. S1 Calculated free energy profiles with schematic structures for the CO-generation along the NH-Pd pathway.

Table S1. Calculated thermodynamic corrections for Gibbs free energies (ΔG_{cor} in hartree), single-point energies (ΔE in hartree) of each species and the imaginary vibrational frequency (in cm^{-1}) of transition states.

Structure	ΔG_{cor}	ΔE	IF
Computational Level: M06/def2-TVZP/M06/6-31G(d,p)-LANL2DZ/SMD			
HCOOH	0.00967	-189.755106591	-
CO	-0.01409	-113.284950804	-
H₂O	0.00387	-76.4343553864	-
CO₂	-0.00889	-188.576293145	-
PTSA	0.105376	-895.309130408	-
MeOH	0.028675	-115.702430033	-
HCOOMe	0.034791	-229.033030017	-
A1	0.490506	-1931.46652037	-
TSA-A'	0.486987	-1931.43963822	-727.16
A1'	0.490423	-1931.45910735	-
TSA1'	0.516185	-2121.18531357	-1514.77
TSA1	0.522596	-2121.22282454	-455.49
A2	0.524151	-2121.22896479	-
TSA2	0.653527	-3016.55245985	-466.68
A3	0.652378	-3016.56136059	-
TSA3	0.645588	-3016.55105796	-1152.55
A4	0.653276	-3016.58060215	-
TSA2^I	0.520263	-2121.20507102	-490.11
TSA2^{II}	0.551841	-2310.97870787	-444.68
TSA2^{III}	0.543885	-2197.65334373	-377.83
A3'	0.495417	-2044.79076899	-
IV	0.494833	-2044.7747646	-
TSB1'	0.515279	-2121.23024928	-337.23

TSB1	0.517331	-2121.21636449	-1102.25
B2	0.520010	-2121.23686838	-
TSB2	0.522906	-2121.21848165	-134.89
B3-CO₂	0.518735	-2121.23315065	-
B3	0.508079	-1932.64547445	-
TSB3	0.507677	-1932.64195353	-757.56
B4	0.509120	-1932.65277314	-
TSB4	0.509385	-1932.64040778	-112.79
R	0.131810	-235.743633208	
A1-R	0.650825	-2167.23564769	-
TSC1	0.646424	-2167.20821770	-1071.21
C2	0.650657	-2167.23233811	-
TSC2	0.643412	-2167.21316420	-343.74
C3	0.643853	-2167.21474418	-
C3'	0.647205	-2167.22274153	-
TSC3	0.646909	-2167.22237086	-328.85
C4	0.649127	-2167.24015192	-
C4-CO	0.658007	-2280.54690874	-
TSC4	0.659015	-2280.54560152	-276.05
C5	0.659752	-2280.56460235	-
C5-MeOH	0.712732	-2396.28880895	-
TSC5	0.709855	-2396.25215606	-255.83
C5-MeOH-PTSA	0.848277	-3291.60986717	-
TSC6	0.844326	-3291.59464027	-426.59
A1-P	0.711903	-2396.30109887	-
A1-MF	0.550584	-2160.51021744	-
TSD1'	0.54884	-2160.47659925	-97.49
D2'	0.548034	-2160.47660038	-
TSD1	0.549767	-2160.50066922	-469.23

D2	0.551760	-2160.50737481	-
TSD2	0.677956	-3055.82962811	-459.89
D3	0.678531	-3055.83417233	-
TSD3	0.673313	-3055.82717930	-1098.60
D4	0.679278	-3055.85636485	-
D2-R	0.706336	-2396.24217784	-
TSD4	0.709676	-2396.22604346	-367.21
D5	0.711152	-2396.24294911	-
D5'	0.710205	-2396.24195968	-
TSD5	0.709119	-2396.22068597	-703.35
D6	0.707145	-2396.24234622	-
TSD6	0.705020	-2396.22023826	-361.53
D7	0.712469	-2396.25084346	-
TSD7	0.710106	-2396.24412516	-262.41

Computational Level: M06/def2-TVZP/M06/6-31G(d,p)-LANL2DZ

PTSA	0.105222	-895.294123418	
HCOOMe	0.034898	-229.030504756	
CH₃OH	0.028550	-115.694297751	
H₂O	0.004161	-76.4196666513	
HCOOH	0.010135	-189.738864299	
A1^{H₂O}	0.567249	-2160.70908522	
TSD2^{H₂O}	0.750937	-3285.05473000	-361.82
A3^{H₂O}	0.567885	-2274.03690020	
TSC1^{H₂O}	0.716987	-2396.45340128	-691.72
C5	0.659692	-2280.4831612	
PTSA^{H₂O}	0.176215	-1124.61418908	
TSC6^{H₂O}	0.917564	-3520.82114021	-476.10
A1^{HCOOMe}	0.664581	-2618.51046595	

TSD2 ^{HCOOMe}	0.855611	-3742.85940227	-243.92
A3 ^{HOOme}	0.673014	-2731.84097681	
TSC1 ^{HCOOMe}	0.814885	-2854.25271583	-753.52
PTSA ^{HCOOMe}	0.274764	-1582.41816655	
TSC6 ^{HCOOMe}	1.013308	-3978.60656203	-431.58

Cartesian coordinates of all the structures

Computational Level: M06/def2-TVZP/M06/6-31G(d,p)-LANL2DZ/SMD

HCOOH

C	-0.12440900	0.40017600	-0.00001600
H	-0.09207500	1.50063300	-0.00001200
O	-1.13594100	-0.26209900	-0.00016100
O	1.10876000	-0.09240800	0.00016000
H	1.05598100	-1.06562600	0.00011500

CO

C	0.00000000	0.00000000	-0.64983400
O	0.00000000	0.00000000	0.48737600

H₂O

O	0.00000000	0.00000000	0.11940900
H	0.00000000	0.75599800	-0.47763700
H	0.00000000	-0.75599800	-0.47763700

CO₂

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16446400
O	0.00000000	0.00000000	-1.16446400

PTSA

H	3.10459300	-0.45074600	1.60008400
C	-1.94733300	1.20783500	0.01206700
C	-0.55980100	1.23256900	-0.03235600
C	0.12530000	0.02274800	-0.07404900
C	-0.54140700	-1.20203300	-0.07207600
C	-1.92586400	-1.20216800	-0.02498100
C	-2.64717300	-0.00211700	0.01599500
H	-2.50085000	2.14451200	0.04493300

H	-0.01774600	2.17485800	-0.03668400
H	0.01457400	-2.13643100	-0.10657900
H	-2.46421300	-2.14842300	-0.02116100
C	-4.14131600	-0.02260600	0.04155900
H	-4.54383600	-0.19483500	-0.96521200
H	-4.51857000	-0.83044700	0.67833500
H	-4.55117000	0.92651900	0.40151100
S	1.87786500	0.02781700	-0.11215500
O	2.37331800	1.36162200	-0.42442800
O	2.37860500	-1.09606800	-0.89389000
O	2.15519500	-0.28248500	1.44360400

MeOH

C	-0.65898800	-0.01905900	-0.00001200
H	-1.09396100	0.98542000	0.00009100
H	-1.02786100	-0.54795500	-0.89080700
H	-1.02780800	-0.54793600	0.89082000
O	0.74678600	0.12341200	-0.00001800
H	1.12927400	-0.76247400	0.00011000

MF

C	-0.82362000	0.43857200	0.00005100
H	-1.41602100	1.36686200	0.00001100
O	-1.28796000	-0.67883000	-0.00003200
O	0.47073800	0.72976300	0.00000500
C	1.35644000	-0.39955100	0.00002000
H	1.19109300	-1.01265800	-0.89059000
H	2.36663100	0.01047200	-0.00612100
H	1.19914700	-1.00626800	0.89648300

A1

C	-0.57957800	-4.57745600	1.37817400
C	-1.28479900	-3.38223400	1.38793300
C	-0.64811400	-2.13270100	1.37577600
C	0.76477000	-2.10354800	1.38918200
C	1.46071700	-3.32073500	1.40312600
C	0.81083100	-4.54720000	1.38433500
H	-1.11417200	-5.52487400	1.38583300
H	-2.37423700	-3.40697400	1.42037200
H	2.54947000	-3.29410500	1.44990000
H	1.38667400	-5.47000200	1.39584300
C	1.58759600	-0.84321000	1.44973100
C	-1.53061400	-0.91359500	1.42498100
P	2.03999500	-0.12660300	-0.21969000

P	-2.00853600	-0.16095000	-0.23040700
C	3.66231400	-0.91774100	-0.79624200
C	-3.52002400	-1.10857600	-0.87151800
C	2.62190500	1.54459700	0.35139500
C	3.34922800	1.85323300	1.49119200
C	2.55938800	3.86115000	-0.22139600
C	3.68643400	3.17704800	1.76264400
H	3.64901600	1.06150400	2.17139400
C	3.29622000	4.19322700	0.89607900
H	2.19207500	4.58208400	-0.94336700
H	4.25781200	3.41514600	2.65595300
H	3.54577300	5.23123700	1.08637800
C	-2.75357900	1.43857200	0.33097100
C	-3.38137200	1.61388100	1.56603500
C	-3.91279300	2.85964000	1.88362500
H	-3.45867000	0.79395500	2.27566800
C	-3.16736600	3.62512900	-0.24678800
C	-3.80903300	3.88888900	0.95875200
H	-4.40399100	3.01838200	2.84114000
H	-3.06474400	4.41185800	-0.99487900
H	-4.21088600	4.87793300	1.16134800
N	-2.64087700	2.43924400	-0.56081800
N	2.25051900	2.57389100	-0.44717600
C	4.64265400	-1.24498100	0.32006900
H	4.25055700	-1.99468700	1.01779400
H	5.56221500	-1.65863200	-0.11829900
H	4.93066800	-0.35644800	0.89601700
C	3.26888400	-2.19013000	-1.54650800
H	4.17454600	-2.67422000	-1.93827100
H	2.75717600	-2.91458500	-0.90016000
H	2.61050000	-1.96776600	-2.39687400
C	4.30152500	0.06223200	-1.77795900
H	3.58831000	0.40349700	-2.54171400
H	4.71375900	0.94560000	-1.27263500
H	5.12981000	-0.43690300	-2.29938800
C	-4.52572000	-1.46648700	0.21435500
H	-5.40555600	-1.94031000	-0.24500200
H	-4.12173600	-2.17824900	0.94501200
H	-4.87885500	-0.58035900	0.75795000
C	-3.00551200	-2.37050500	-1.56065200
H	-2.46738600	-3.03330400	-0.87211500
H	-3.85316100	-2.93531000	-1.97492300
H	-2.32908900	-2.12365700	-2.39043800
C	-4.19394100	-0.22157700	-1.91645700

H	-4.67068200	0.65954800	-1.46893800
H	-3.48433400	0.12448200	-2.68077000
H	-4.97656300	-0.79910500	-2.42878000
H	1.03849300	-0.02962700	1.94178600
H	2.49215900	-1.02261300	2.04536200
H	-1.02779900	-0.08449800	1.94087700
H	-2.42800400	-1.14892900	2.01218500
Pd	0.03984900	0.04940100	-1.32721700
H	1.66829400	2.33732200	-1.25991200

TSA-A'

C	-1.54858100	4.53813900	-1.37513300
C	-1.98537600	3.22407900	-1.46290400
C	-1.10533700	2.13423800	-1.40722600
C	0.27885800	2.39389800	-1.29024300
C	0.70223000	3.72932200	-1.22306100
C	-0.18751000	4.79380500	-1.24901500
H	-2.26581200	5.35467400	-1.42067500
H	-3.04898300	3.02186600	-1.58901700
H	1.77098100	3.93321600	-1.16581100
H	0.18335400	5.81474400	-1.19315600
C	1.35982700	1.34181400	-1.33359800
C	-1.71043200	0.75798000	-1.49828800
P	1.78100000	0.38804100	0.21247800
P	-2.05745900	-0.02089200	0.16838100
C	2.49782700	1.53203800	1.51015100
C	-3.69155400	0.63869400	0.84721400
C	3.18831700	-0.65782600	-0.39667900
C	4.32356300	-0.25255600	-1.08657800
C	3.84853400	-2.89151700	-0.49601500
C	5.24218100	-1.22161200	-1.48462600
H	4.48708400	0.79602200	-1.32329000
C	5.00719400	-2.55794300	-1.18488800
H	3.60358000	-3.92024000	-0.24116200
H	6.13451000	-0.93166600	-2.03364500
H	5.70248200	-3.33524900	-1.48699600
C	-2.38571200	-1.78130600	-0.32497900
C	-3.34124500	-2.28541700	-1.19883300
C	-3.37647500	-3.65657400	-1.44071600
H	-4.04686600	-1.61901300	-1.68895400
C	-1.50015500	-3.90404300	0.01730500
C	-2.44942000	-4.48091300	-0.81707900
H	-4.11992500	-4.07405900	-2.11548000
H	-0.73533700	-4.50603300	0.50372700

H	-2.44604300	-5.55433600	-0.98214300
N	-1.46751300	-2.58977200	0.26194600
N	2.97763000	-1.95310300	-0.12295900
C	3.56028200	2.47726200	0.96546700
H	3.18447500	3.10530300	0.14957200
H	3.88794200	3.14650400	1.77330200
H	4.44674900	1.93765800	0.61109300
C	1.33273300	2.32259800	2.10626500
H	1.70510300	2.93431600	2.93957600
H	0.87329100	3.00026200	1.37561300
H	0.55174100	1.65774600	2.49918900
C	3.10535600	0.63195200	2.58495600
H	2.36822000	-0.07457900	2.99026700
H	3.96088000	0.05765300	2.20573500
H	3.46643500	1.25426400	3.41529100
C	-4.77368400	0.87715900	-0.19534700
H	-5.68057400	1.24909300	0.30369200
H	-4.47659500	1.62834900	-0.93663800
H	-5.05160700	-0.04092300	-0.72710600
C	-3.36073800	1.94580900	1.56951300
H	-2.95406500	2.70582200	0.89036400
H	-4.27605800	2.35517400	2.02025500
H	-2.63252400	1.78803200	2.37614500
C	-4.16884300	-0.38636500	1.87575100
H	-4.51225300	-1.31592600	1.40480000
H	-3.38020000	-0.63930600	2.59906100
H	-5.01326000	0.03362900	2.44001200
H	1.11357600	0.54589900	-2.05093300
H	2.29153200	1.80453800	-1.68648800
H	-1.02574400	0.04414000	-1.97684700
H	-2.62575600	0.78601500	-2.10382800
Pd	0.15931200	-1.09312800	0.76126100
H	1.63632100	-1.94309000	0.45219500

Al'

C	-1.01622800	4.73049100	-1.22707000
C	-1.64463400	3.50941200	-1.42666300
C	-0.94057100	2.29848700	-1.42277700
C	0.45733200	2.32555600	-1.22637300
C	1.07620300	3.57235600	-1.05768300
C	0.36112300	4.76115000	-1.03892200
H	-1.59642500	5.65036900	-1.23567600
H	-2.72029700	3.48216800	-1.59912900
H	2.16068400	3.60594400	-0.96284000

H	0.88136200	5.70641200	-0.90188000
C	1.36818300	1.12547500	-1.31727600
C	-1.74270900	1.04000000	-1.62715600
P	1.73397600	0.03496000	0.16061300
P	-1.97438200	0.12138100	-0.04285600
C	2.24247300	1.00817400	1.68392800
C	-3.28065700	0.93906400	1.03235200
C	3.28632100	-0.82293400	-0.38964800
C	4.29764400	-0.12872700	-1.05744000
C	4.51363500	-2.76255700	-0.42893600
C	5.45266200	-0.81207400	-1.42321100
H	4.20501900	0.92893300	-1.28998600
C	5.56613900	-2.15759300	-1.10738600
H	4.56691100	-3.81692100	-0.15836700
H	6.25091100	-0.29260100	-1.94764400
H	6.44806600	-2.73211900	-1.37662200
C	-2.67747200	-1.51754700	-0.51437100
C	-3.74230700	-1.85052400	-1.33705100
C	-4.04443500	-3.19970600	-1.51402100
H	-4.32282700	-1.07321200	-1.82811300
C	-2.19641100	-3.75641100	-0.09726400
C	-3.27285900	-4.16275900	-0.87692100
H	-4.87954000	-3.49390600	-2.14477700
H	-1.54122600	-4.47453500	0.39050000
H	-3.48504900	-5.22148400	-0.99257900
N	-1.90614200	-2.46451700	0.07938400
N	3.39851600	-2.11920200	-0.08007200
C	3.37248900	1.99286900	1.40625000
H	3.10016900	2.74025400	0.65340700
H	3.60308100	2.53026000	2.33662100
H	4.29168000	1.48929900	1.08473600
C	1.01121100	1.73687600	2.21520600
H	1.28207000	2.27068500	3.13658900
H	0.61912200	2.47538600	1.50359600
H	0.20978000	1.02613700	2.45676600
C	2.70281800	-0.02310900	2.71445900
H	1.91794700	-0.75773300	2.93729300
H	3.59938200	-0.56417800	2.38664900
H	2.95324800	0.49787000	3.64866000
C	-4.49851800	1.35900000	0.22031500
H	-5.24558400	1.79556300	0.89841200
H	-4.25160700	2.11968200	-0.53035600
H	-4.97453200	0.51023200	-0.28623400
C	-2.65894100	2.15244500	1.72164800

H	-2.30161700	2.90539500	1.00866700
H	-3.42187700	2.62825800	2.35337900
H	-1.82254100	1.86558600	2.37056900
C	-3.67399800	-0.08854200	2.09285200
H	-4.20317100	-0.94896400	1.66407800
H	-2.79967300	-0.45945700	2.64621900
H	-4.34725900	0.38867000	2.81794700
H	1.00073100	0.39859400	-2.05548600
H	2.33547800	1.47453800	-1.69553600
H	-1.22828000	0.31991200	-2.27969500
H	-2.70923700	1.26927200	-2.09351800
Pd	-0.07325200	-1.29794600	0.49478700
H	1.04318500	-2.41109900	0.58157500

TSA1'

C	-1.07100600	4.99447500	-0.47071800
C	-1.68299100	3.75505000	-0.59957600
C	-0.97931000	2.61299700	-1.00519000
C	0.39438100	2.74059000	-1.29376600
C	0.98272400	4.00906300	-1.21534200
C	0.27314700	5.12679100	-0.80025900
H	-1.65152000	5.85634300	-0.14987700
H	-2.75118300	3.66940500	-0.40545100
H	2.02761800	4.11738800	-1.50062100
H	0.76528100	6.09510700	-0.74606100
C	1.27794100	1.58673500	-1.68507900
C	-1.76737400	1.35417200	-1.25362700
P	1.73389700	0.51270500	-0.24742400
P	-1.95574000	0.05280700	0.06574100
C	2.84336300	1.46822200	0.93754200
C	-3.00763800	0.69644500	1.48247300
C	2.86862900	-0.73999700	-1.00014100
C	3.72178100	-0.53770500	-2.07809700
C	3.57530400	-2.95696200	-0.79272900
C	4.51704600	-1.59702200	-2.51119000
H	3.77353200	0.42742900	-2.57531000
C	4.44889900	-2.82349200	-1.86264700
H	3.46528000	-3.88921400	-0.24109700
H	5.19040200	-1.45902800	-3.35311300
H	5.05595900	-3.66622500	-2.17817300
C	-2.99581800	-1.18571500	-0.83618300
C	-4.06504900	-0.78367000	-1.63971600
C	-4.81310500	-1.75669900	-2.29430900
H	-4.32478900	0.26500000	-1.75613600

C	-3.39165500	-3.39570700	-1.30897300
C	-4.47240800	-3.09100100	-2.12943400
H	-5.65183000	-1.46881600	-2.92338500
H	-3.09322100	-4.43267800	-1.15630700
H	-5.02556600	-3.88408100	-2.62461700
N	-2.66456300	-2.47300900	-0.67680900
N	2.81311700	-1.93849700	-0.39548700
C	3.86875400	2.33378400	0.21835100
H	3.40950500	3.17193200	-0.31490400
H	4.55796800	2.75835000	0.96198500
H	4.47299800	1.75503000	-0.49250900
C	1.93306800	2.31403600	1.82768500
H	2.55311700	2.90529400	2.51590200
H	1.31113900	3.01463600	1.25575600
H	1.27105600	1.67949500	2.43274800
C	3.57121200	0.44304400	1.80649400
H	2.88708600	-0.27989300	2.27007400
H	4.33313600	-0.10943700	1.24194900
H	4.08690200	0.97627400	2.61699300
C	-4.26110400	1.41185900	0.98658100
H	-4.79148800	1.82404700	1.85560500
H	-4.04069900	2.24536000	0.31150800
H	-4.95075000	0.72678100	0.47916900
C	-2.13505400	1.64210400	2.30635800
H	-1.83417400	2.53426300	1.74248000
H	-2.70202900	1.97662300	3.18588600
H	-1.22809900	1.13514100	2.66329100
C	-3.42978000	-0.48934900	2.34778600
H	-4.00861300	-1.23113400	1.78234500
H	-2.57207100	-0.99487400	2.80757100
H	-4.07149300	-0.11604900	3.15734900
H	0.79096500	0.90420400	-2.39605000
H	2.18700600	1.96353800	-2.16952300
H	-1.34920400	0.78521200	-2.09585900
H	-2.78160000	1.64309900	-1.55781000
Pd	0.02325900	-0.87419500	0.75868800
H	-1.14394500	-1.79386500	1.32102500
C	1.25688500	-2.51238000	1.77157100
H	1.88498400	-2.03742600	0.63402100
O	0.95661200	-3.78878700	1.44635000
O	1.47323800	-2.19257000	2.93130800
H	0.96232100	-4.32357700	2.26434600

TSA1

C	1. 63578600	-4. 66570400	-1. 36517300
C	2. 24089800	-3. 41931400	-1. 25086200
C	1. 53444500	-2. 23401100	-1. 47896200
C	0. 16782700	-2. 31580900	-1. 81818800
C	-0. 41547000	-3. 57690800	-1. 97109300
C	0. 30028600	-4. 74650500	-1. 74307300
H	2. 21345500	-5. 56895300	-1. 18148800
H	3. 30043800	-3. 35802000	-1. 00331000
H	-1. 45851000	-3. 63550900	-2. 28090800
H	-0. 18257100	-5. 71329100	-1. 86730500
C	-0. 69112500	-1. 09329900	-2. 01144700
C	2. 27852000	-0. 92871600	-1. 43945300
P	-1. 48161900	-0. 57425300	-0. 40754100
P	1. 98552200	0. 10711700	0. 08877500
C	-3. 15670000	-1. 44735400	-0. 23978200
C	3. 67418300	0. 21141600	0. 92389000
C	-1. 98659000	1. 16827900	-0. 77954300
C	-2. 14244400	1. 72448100	-2. 03979200
C	-2. 52798100	3. 27058800	0. 20197000
C	-2. 49094600	3. 06774700	-2. 16996000
H	-1. 99762800	1. 11155500	-2. 92432500
C	-2. 69373400	3. 85074800	-1. 03958400
H	-2. 65366700	3. 80261900	1. 13908300
H	-2. 61026200	3. 49878900	-3. 16043400
H	-2. 96781000	4. 89751500	-1. 11059400
C	1. 72854500	1. 81085100	-0. 58410500
C	2. 19803300	2. 24846200	-1. 82392400
C	1. 89609800	3. 54151200	-2. 23951300
H	2. 79634300	1. 60096000	-2. 46106500
C	0. 74519400	3. 84900600	-0. 17519300
C	1. 14933200	4. 36049100	-1. 40422300
H	2. 24622100	3. 90184700	-3. 20411500
H	0. 17048500	4. 46954600	0. 51419600
H	0. 88575600	5. 37531200	-1. 68971800
N	1. 01555900	2. 60718800	0. 23173400
N	-2. 18017900	1. 97768300	0. 29373700
C	-3. 84592900	-1. 64248800	-1. 58347400
H	-3. 30836700	-2. 33962200	-2. 23651000
H	-4. 84563300	-2. 06545400	-1. 41121200
H	-3. 98010200	-0. 69453800	-2. 12161500
C	-2. 89011900	-2. 79048600	0. 43845800
H	-3. 84249200	-3. 32687900	0. 55224200
H	-2. 21521800	-3. 42889600	-0. 14317800
H	-2. 45791600	-2. 65518500	1. 43834200

C	-4.05272100	-0.60762300	0.66971300
H	-3.56821800	-0.34308000	1.61904600
H	-4.39535600	0.31397800	0.18269400
H	-4.94525700	-1.19858300	0.91559800
C	4.76177300	0.73757900	-0.00519600
H	5.71727400	0.75888400	0.53807400
H	4.90861400	0.10680900	-0.89063300
H	4.55229800	1.76092800	-0.34141700
C	4.01235600	-1.19873200	1.39870700
H	4.15546200	-1.89209800	0.56001400
H	4.94913300	-1.17948200	1.97302500
H	3.22747600	-1.60726300	2.05071400
C	3.54339600	1.14295000	2.12536000
H	3.30438100	2.17112900	1.82474000
H	2.76908500	0.80299300	2.82594400
H	4.49900600	1.16969600	2.66741700
H	-0.09552600	-0.22588900	-2.32736700
H	-1.44947200	-1.26463700	-2.78479900
H	2.00057100	-0.31956500	-2.30752400
H	3.35320400	-1.12253500	-1.53510900
Pd	0.02775700	-0.37874200	1.43751600
H	-2.02737200	1.59454200	1.24005500
C	-1.19938700	-0.36582900	3.06123800
O	-1.78165400	0.87128300	3.17120200
O	-1.62004400	-1.29969300	3.72036500
H	0.37074100	-0.14004700	3.04967600
H	-2.52916600	0.79678200	3.79592000

A2

C	1.74685000	-4.61021600	-1.35941800
C	2.33015600	-3.35548400	-1.22569600
C	1.60738900	-2.18267400	-1.46341900
C	0.24930500	-2.28106200	-1.82628400
C	-0.31011400	-3.54978600	-2.00204300
C	0.42177500	-4.70863300	-1.76827200
H	2.33361900	-5.50573500	-1.16738700
H	3.38271000	-3.27622500	-0.95396900
H	-1.34519900	-3.62786500	-2.33197700
H	-0.04286500	-5.68200000	-1.90929600
C	-0.61580400	-1.06073900	-2.01113200
C	2.32699800	-0.86580900	-1.41428500
P	-1.43285600	-0.58492200	-0.41067900
P	1.98756100	0.17540800	0.09501000
C	-3.07314900	-1.53259900	-0.27907500

C	3.67418100	0.35807100	0.92368700
C	-2.00362400	1.14207200	-0.74208500
C	-2.15532900	1.72765200	-1.98847900
C	-2.68161700	3.17716800	0.28876000
C	-2.57876900	3.05234200	-2.08688600
H	-1.95228300	1.15185600	-2.88660900
C	-2.84885800	3.78700500	-0.93891100
H	-2.85821700	3.67249800	1.23787700
H	-2.69865400	3.50689700	-3.06671800
H	-3.17775900	4.81923600	-0.98499600
C	1.64198400	1.86237800	-0.57460800
C	2.07022300	2.31513800	-1.82328800
C	1.71860100	3.59977100	-2.22617500
H	2.67771400	1.69054300	-2.47422900
C	0.60677700	3.86630500	-0.13392400
C	0.96959600	4.39378600	-1.36953300
H	2.03567600	3.97364100	-3.19691500
H	0.02665000	4.46550200	0.56951100
H	0.67194600	5.40199000	-1.64464800
N	0.92234500	2.63123300	0.26081500
N	-2.26929300	1.90212100	0.35096700
C	-3.70629400	-1.75885900	-1.64610600
H	-3.13153400	-2.44739600	-2.27498700
H	-4.69983900	-2.20534100	-1.50155900
H	-3.84712400	-0.81920400	-2.19694000
C	-2.77064700	-2.85994400	0.41527700
H	-3.70002600	-3.44197600	0.48657700
H	-2.03946100	-3.46413500	-0.13340100
H	-2.38993200	-2.70293200	1.43242400
C	-4.04725000	-0.73146000	0.58362200
H	-3.62775200	-0.44793700	1.55646400
H	-4.40437000	0.17339100	0.07630800
H	-4.92393300	-1.36246600	0.78152700
C	4.71971100	0.90810700	-0.04211000
H	5.68301300	0.97691500	0.48229000
H	4.87559100	0.26809000	-0.91870300
H	4.46321200	1.91616100	-0.39103200
C	4.08077300	-1.02772500	1.41791100
H	4.21839200	-1.73945800	0.59357400
H	5.03794000	-0.95516600	1.95261900
H	3.34058500	-1.44706900	2.11265900
C	3.54376300	1.31341000	2.10595200
H	3.25628200	2.32426700	1.79007200
H	2.81001100	0.96119300	2.84140000

H	4.51700100	1.38853800	2.61043200
H	-0.02436500	-0.18468500	-2.31083700
H	-1.36927600	-1.22322800	-2.79041900
H	2.06695000	-0.26840900	-2.29550300
H	3.40592500	-1.04431400	-1.47644600
Pd	0.09043100	-0.40381100	1.46258600
H	-2.13542000	1.49458600	1.29196100
C	-1.33787100	-0.54101500	2.91369800
O	-1.94930800	0.68163400	3.07258800
O	-1.71064700	-1.47525000	3.59878600
H	0.97699500	-0.21682800	2.78878200
H	-2.65687000	0.58732700	3.74161400

TSA2

C	-4.44221600	3.71549700	-0.91909000
C	-3.45069200	3.52941300	0.03712100
C	-3.13463100	2.25871400	0.52693800
C	-3.88098000	1.15292400	0.07444300
C	-4.87697500	1.35321600	-0.88518800
C	-5.15277200	2.61790000	-1.39281300
H	-4.66602900	4.71602800	-1.28239100
H	-2.90951200	4.38983500	0.43110100
H	-5.46452000	0.49927200	-1.22045200
H	-5.93585900	2.74621300	-2.13660100
C	-3.68900900	-0.22827700	0.64036100
C	-2.02907900	2.11551700	1.53371800
P	-2.23023100	-1.13489700	-0.07075800
P	-0.36549000	1.70748800	0.79518500
C	-2.94332500	-2.63269600	-0.97839200
C	0.54507800	3.33993300	0.49987300
C	-1.45589200	-1.93981000	1.40379700
C	-2.09011100	-2.23439500	2.60027700
C	0.53699200	-2.95174800	2.21766900
C	-1.39006800	-2.88535000	3.61436200
H	-3.13459900	-1.97371800	2.74160500
C	-0.06555800	-3.25736800	3.42195300
H	1.56766100	-3.19312900	1.96630000
H	-1.89011400	-3.11143600	4.55221300
H	0.49884300	-3.77371100	4.19085100
C	0.53413600	0.96541400	2.22483600
C	0.18831300	1.24206100	3.54902900
C	0.94135900	0.66863300	4.56859100
H	-0.64805700	1.89441700	3.78753000
C	2.28067100	-0.36280100	2.88495700

C	2.01419600	-0.14448700	4.23360100
H	0.69268500	0.86380100	5.60907000
H	3.11040800	-1.00810700	2.59239700
H	2.63290300	-0.61064000	4.99540700
N	1.55885300	0.16449000	1.89427200
N	-0.15701800	-2.30169200	1.27118400
C	-3.81239600	-3.49701700	-0.07161600
H	-4.64178000	-2.94280800	0.38477800
H	-4.25641500	-4.29851600	-0.67805400
H	-3.23255700	-3.97612500	0.72687500
C	-3.77857600	-2.08167300	-2.13255600
H	-4.10911900	-2.92087300	-2.75946900
H	-4.67961100	-1.56900200	-1.77497200
H	-3.21485000	-1.38868700	-2.77047800
C	-1.78563600	-3.46882000	-1.51487600
H	-1.12388000	-2.89976100	-2.17740000
H	-1.17652500	-3.90618600	-0.71320900
H	-2.19699300	-4.30363500	-2.09852200
C	0.37003700	4.29245600	1.67884600
H	1.01393000	5.16832700	1.52005900
H	-0.65928200	4.66132000	1.76715800
H	0.66466500	3.83966200	2.63455200
C	0.00402700	3.98507200	-0.77264500
H	-1.07585200	4.16446000	-0.72474400
H	0.49950500	4.95495700	-0.91775100
H	0.20727200	3.36727900	-1.65586000
C	2.02682300	3.02439300	0.30828100
H	2.50692000	2.68324400	1.23383400
H	2.18656500	2.26260600	-0.46691900
H	2.54075100	3.94107800	-0.01465800
H	-3.56235200	-0.18652000	1.72881500
H	-4.58701000	-0.82933000	0.45686300
H	-2.23283500	1.29189400	2.23125100
H	-1.94396800	3.02674000	2.13815500
Pd	-0.56180000	0.29796300	-1.11377900
C	-0.54950800	-0.48693700	-2.99826900
H	0.58558800	1.20413600	-1.74977900
O	-1.20367000	-0.40510500	-3.98839600
O	0.68915400	-1.39978700	-3.19632400
H	0.56310500	-2.08301000	-3.88310400
H	0.36628500	-2.06181800	0.40585200
H	1.06797900	-1.76812700	-2.25825300
C	5.12536900	1.05546100	-0.01738400
C	4.55030000	-0.20558100	0.09133000

C	3.77336300	-0.69066300	-0.95422600
C	3.58466700	0.06107100	-2.11400300
C	4.16793400	1.31676500	-2.20774800
C	4.94100300	1.83470900	-1.16217700
H	5.72640600	1.44526600	0.80305600
H	4.70472400	-0.81093700	0.98087600
H	2.98334100	-0.32310100	-2.93633100
H	4.01669100	1.91333000	-3.10631800
C	5.55963800	3.19285900	-1.26996800
H	4.96763900	3.85211000	-1.91448600
H	5.65784000	3.66534300	-0.28619900
H	6.56700700	3.13442700	-1.70318100
S	3.03175400	-2.29658400	-0.84173800
O	3.31207900	-2.82959900	0.49901200
O	3.52344400	-3.08357200	-1.98131400
O	1.52547000	-2.06472300	-0.99380300

A3

C	-6.02329100	0.79578200	-1.96953600
C	-5.18880200	1.44732300	-1.06845700
C	-4.34251400	0.73860700	-0.21177400
C	-4.38916000	-0.66941000	-0.22110200
C	-5.22784900	-1.31277100	-1.13579300
C	-6.02957100	-0.59409100	-2.01584300
H	-6.67065900	1.37386500	-2.62511400
H	-5.19453600	2.53592100	-1.01772900
H	-5.26923700	-2.40169100	-1.13135300
H	-6.67686000	-1.11981300	-2.71419700
C	-3.64803600	-1.49390000	0.79360500
C	-3.41710400	1.49982100	0.69798800
P	-1.81721200	-1.65087100	0.52085900
P	-1.74811600	1.81785200	-0.04924500
C	-1.52501400	-3.48576500	0.20106000
C	-1.82318500	3.42341800	-1.04391300
C	-1.05254700	-1.34557800	2.16875600
C	-1.74021800	-1.36516600	3.38188400
C	0.92656800	-0.83821200	3.21384900
C	-1.03690700	-1.07359900	4.54733300
H	-2.79728100	-1.61350700	3.43548600
C	0.31994000	-0.79630400	4.46649500
H	1.99589100	-0.64570700	3.11137200
H	-1.54890300	-1.07040500	5.50670900
H	0.90411500	-0.55588900	5.35077300
C	-0.64308100	2.16861100	1.37486100

C	-1.10870700	2.51545800	2.64152800
C	-0.17239400	2.73448400	3.64968200
H	-2.17133700	2.61933400	2.84722900
C	1.54196300	2.26139800	2.05652100
C	1.17742300	2.60584100	3.35623900
H	-0.50038500	3.00409600	4.65083200
H	2.59343400	2.14266200	1.79018200
H	1.93891000	2.76076300	4.11578400
N	0.65953500	2.04415400	1.08334800
N	0.26259500	-1.09508500	2.08765100
C	-2.01661700	-4.32622100	1.37623600
H	-3.08486800	-4.18881600	1.58417700
H	-1.86539200	-5.38855100	1.13993900
H	-1.45584100	-4.10911600	2.29379500
C	-2.28421000	-3.85060100	-1.07199300
H	-2.07409100	-4.89866000	-1.32563200
H	-3.37099500	-3.75299200	-0.95562700
H	-1.97575800	-3.23500600	-1.92828900
C	-0.03143300	-3.73042000	0.00277300
H	0.38220200	-3.14998300	-0.83179300
H	0.55144600	-3.49785300	0.90147900
H	0.12326700	-4.79352200	-0.22809000
C	-2.66870300	4.45357900	-0.29730900
H	-2.57161000	5.42110800	-0.80766900
H	-3.73378100	4.19398400	-0.29254800
H	-2.33637500	4.59597300	0.73974000
C	-2.42227600	3.14475900	-2.41946200
H	-3.40883700	2.67229100	-2.36443900
H	-2.53743000	4.09906500	-2.95132200
H	-1.76921400	2.50127500	-3.02239100
C	-0.40658900	3.96260000	-1.22318800
H	0.03222800	4.31059200	-0.28126800
H	0.26957000	3.22094100	-1.66955700
H	-0.45238500	4.81992200	-1.90840700
H	-3.79649800	-1.06123900	1.78937600
H	-4.07922400	-2.50044400	0.83480800
H	-3.21145000	0.95134900	1.62689900
H	-3.86102300	2.45868700	0.99209500
Pd	-0.92765000	-0.08405300	-1.15545300
C	-0.11721700	-1.29630800	-2.49776600
H	-0.40683500	1.07096400	-2.11942100
O	0.36446300	-1.88956400	-3.34451900
O	2.47570700	1.00767300	-2.68272200
H	1.99607200	0.53952700	-3.37954800

H	2.07200900	1.88573800	-2.65097200
C	6.57648300	0.54642300	0.76198000
C	5.39266000	-0.16849600	0.68751900
C	4.94461800	-0.59625100	-0.56273600
C	5.65103800	-0.31434100	-1.72635600
C	6.83848800	0.40179000	-1.62845200
C	7.31572400	0.84098100	-0.39177800
H	6.94268500	0.88448600	1.73027700
H	4.82374200	-0.39901700	1.58627400
H	5.28383500	-0.65767400	-2.69033400
H	7.40750500	0.62447200	-2.52935400
C	8.59468400	1.60841000	-0.28675600
H	9.32317100	1.07317900	0.33482900
H	9.04616700	1.77665600	-1.26954500
H	8.43241200	2.58413500	0.18745900
S	3.41462200	-1.46296300	-0.65595700
O	3.26916800	-2.32445100	0.51032100
O	3.27196200	-2.04086000	-1.98900200
O	2.32796200	-0.32367400	-0.47059600
H	2.30602500	0.26047400	-1.30442900

TSA3

C	-5.17327600	2.57260800	-1.62366900
C	-4.19506600	2.71889100	-0.64690600
C	-3.72374900	1.62979800	0.09256700
C	-4.31277500	0.36662000	-0.12184200
C	-5.29620900	0.23178500	-1.10631500
C	-5.71913700	1.31671500	-1.86524600
H	-5.51285300	3.44004700	-2.18528900
H	-3.78924300	3.70845800	-0.44020100
H	-5.74786700	-0.74778400	-1.26175000
H	-6.48711800	1.18449600	-2.62412600
C	-3.94475300	-0.84277600	0.69545300
C	-2.63484800	1.84912500	1.10747100
P	-2.30907900	-1.54459600	0.16468100
P	-0.88888500	1.74987800	0.44603700
C	-2.62215500	-3.28393100	-0.48552300
C	-0.38792700	3.48188600	-0.13592500
C	-1.43479300	-1.85379700	1.76457600
C	-2.01791500	-2.04635000	3.00716000
C	0.72240800	-2.00256200	2.76554400
C	-1.21418400	-2.20427600	4.13497100
H	-3.09988000	-2.07879900	3.09853400
C	0.17080900	-2.18560500	4.01785000

H	1.78991500	-1.97644500	2.56659400
H	-1.67708300	-2.34851400	5.10761000
H	0.81872500	-2.30560100	4.87925500
C	0.09474300	1.48985900	1.98893200
C	-0.42412300	1.67098300	3.27196700
C	0.40618300	1.44837700	4.36735100
H	-1.45182200	1.98735900	3.42871100
C	2.15124900	0.91514400	2.83439900
C	1.72224700	1.06800100	4.14987200
H	0.02281800	1.57762100	5.37683700
H	3.17903800	0.61229300	2.62391800
H	2.40552300	0.88689100	4.97494500
N	1.36425900	1.10636900	1.77535100
N	-0.08002800	-1.83640700	1.70337400
C	-3.28820300	-4.19138500	0.54086000
H	-4.25039500	-3.79968400	0.89422600
H	-3.48586300	-5.16731100	0.07566200
H	-2.64423000	-4.36841900	1.41132300
C	-3.51535200	-3.11947200	-1.71354100
H	-3.63317500	-4.09622200	-2.20231000
H	-4.51783200	-2.76083900	-1.44716100
H	-3.08650300	-2.42639900	-2.45088900
C	-1.27044600	-3.86594700	-0.89304700
H	-0.74975200	-3.23856700	-1.62913700
H	-0.60384300	-4.00919900	-0.03203000
H	-1.42978800	-4.85256500	-1.34913800
C	-0.97573000	4.56325900	0.76358500
H	-0.54998700	5.53417900	0.47468500
H	-2.06438400	4.64644600	0.66735500
H	-0.73175400	4.39961300	1.82211200
C	-0.87463800	3.65386700	-1.57384500
H	-1.95731100	3.51583500	-1.67625200
H	-0.63254500	4.67035600	-1.91436000
H	-0.37803100	2.94412800	-2.24871600
C	1.13534200	3.58926600	-0.12294500
H	1.54222200	3.61370700	0.89452400
H	1.62135100	2.77172700	-0.66755700
H	1.41745700	4.52930200	-0.61831500
H	-3.88857200	-0.59254600	1.76174600
H	-4.71730300	-1.61451900	0.59611900
H	-2.66625400	1.07895500	1.88872300
H	-2.77173500	2.81268800	1.61390800
Pd	-0.81824000	-0.03973700	-1.14777700
O	3.91121700	2.78952100	-1.94610700

H	3.60691400	3.45799800	-2.56971900
H	0.38778300	-1.65669100	0.79859300
H	3.29549400	2.05143200	-2.07639000
C	5.78728100	0.40617700	0.41479800
C	4.48626500	0.29053100	-0.04591300
C	4.20155300	-0.65084400	-1.03549800
C	5.19214800	-1.46704200	-1.56516000
C	6.49361500	-1.33613700	-1.08988800
C	6.80807600	-0.40848500	-0.09536000
H	6.02398200	1.14130800	1.18317600
H	3.69511000	0.93539300	0.33498500
H	4.95128800	-2.19109200	-2.33977300
H	7.28069300	-1.96735000	-1.49897800
C	8.20263000	-0.27861500	0.43015000
H	8.25794100	-0.60522100	1.47657400
H	8.90924200	-0.88313900	-0.14731300
H	8.53954200	0.76454200	0.40633200
S	2.52081600	-0.85520100	-1.53598500
O	1.80126200	-1.45053600	-0.38508900
O	2.46905400	-1.66679700	-2.75979000
O	2.04684200	0.57724100	-1.79085600
C	-0.64214700	-0.80816300	-2.95472300
O	-0.60431400	-1.25148100	-4.00978800
H	0.63067900	0.67569500	-1.61531000

A4

C	-5.80905300	0.58113500	-2.12575500
C	-5.03534400	1.28476600	-1.20994100
C	-4.23838900	0.63295800	-0.26207100
C	-4.26793900	-0.77696700	-0.21340700
C	-5.05101800	-1.47195700	-1.14011000
C	-5.80879600	-0.80932100	-2.09852500
H	-6.41697800	1.11899900	-2.85006200
H	-5.04917500	2.37486100	-1.22035600
H	-5.07720200	-2.56022400	-1.09157500
H	-6.41142200	-1.37641400	-2.80453400
C	-3.52616500	-1.56928500	0.83018000
C	-3.38477900	1.45940300	0.66138000
P	-1.70477500	-1.74152100	0.46144100
P	-1.68676100	1.83630800	-0.03977500
C	-1.38485600	-3.58547400	0.18209100
C	-1.80921500	3.51853100	-0.91714100
C	-0.96920400	-1.48616600	2.14240800
C	-1.58640700	-1.66389600	3.37323600

C	1.02712700	-0.81384000	3.26060400
C	-0.88382800	-1.40749800	4.54770500
H	-2.61141000	-2.01959400	3.42170900
C	0.43864400	-0.97926900	4.49709800
H	2.05321200	-0.49176700	3.11041300
H	-1.37231800	-1.55175200	5.50767100
H	1.00835100	-0.77654800	5.39750700
C	-0.71824600	2.22670800	1.48510500
C	-1.28213000	2.58821900	2.71046400
C	-0.44020500	2.81126400	3.79658600
H	-2.35852500	2.69477500	2.82493000
C	1.40454600	2.33591900	2.36297800
C	0.93171200	2.68667000	3.62401400
H	-0.85572500	3.08625900	4.76348700
H	2.47644700	2.22531500	2.18820100
H	1.62440200	2.85106900	4.44488600
N	0.60958500	2.09914600	1.31844000
N	0.31524500	-1.05627000	2.14807500
C	-1.73923900	-4.45313300	1.38200900
H	-2.78367700	-4.33229900	1.69654900
H	-1.60065300	-5.51028200	1.11440500
H	-1.09280100	-4.24681500	2.24426300
C	-2.22546200	-3.98229100	-1.02868600
H	-1.93800500	-4.99327700	-1.34832900
H	-3.29748300	-4.00322000	-0.79717600
H	-2.06681700	-3.30501400	-1.88035100
C	0.09727400	-3.73325300	-0.15301000
H	0.37086800	-3.16343100	-1.05216700
H	0.74749300	-3.41147300	0.67258400
H	0.31949700	-4.79199000	-0.34670400
C	-2.79363000	4.46539000	-0.24287100
H	-2.72184300	5.45647600	-0.71368000
H	-3.83412700	4.13425100	-0.34622900
H	-2.57531600	4.59580600	0.82575400
C	-2.22880200	3.24667200	-2.36016100
H	-3.17494200	2.69580400	-2.42238600
H	-2.35710200	4.20056000	-2.89146100
H	-1.46581200	2.66141000	-2.89178800
C	-0.42411700	4.16128700	-0.92715800
H	-0.11920200	4.50270200	0.06926900
H	0.35129900	3.48475600	-1.31063400
H	-0.44980900	5.04035800	-1.58672200
H	-3.62209000	-1.08871700	1.81083800
H	-3.97302600	-2.56610600	0.92759700

H	-3.17994400	0.92033100	1.59533500
H	-3.90343500	2.38516400	0.93906400
Pd	-0.92188200	-0.16353800	-1.21207600
C	-0.29635500	-0.73146800	-2.95412900
H	2.42945000	-0.07123900	-2.17072800
O	0.05698100	-1.18305200	-3.96027200
O	1.95550900	1.41402600	-2.19368300
H	1.97689400	1.73920300	-3.10513600
H	1.00348000	1.31521000	-1.99026400
C	7.20353600	-0.67174700	-0.79257300
C	5.95708500	-1.27810500	-0.77288900
C	4.83318300	-0.48794300	-0.53753800
C	4.93343900	0.88574800	-0.32954100
C	6.19229500	1.47132600	-0.35722500
C	7.33950200	0.70659400	-0.58814900
H	8.09335100	-1.27464700	-0.96773000
H	5.85634300	-2.34954800	-0.92806300
H	4.04557600	1.48758400	-0.14382000
H	6.28928400	2.54292500	-0.19257700
C	8.69385600	1.33823500	-0.61829600
H	9.17252900	1.19298300	-1.59471800
H	8.64245300	2.41334300	-0.42113900
H	9.35747600	0.88488800	0.12807600
S	3.24154800	-1.23713200	-0.54783800
O	3.36136200	-2.67200300	-0.34309900
O	2.71295000	-1.04571200	-2.02155300
O	2.38012200	-0.46587700	0.35674900
H	0.80196700	-0.90007700	1.25086100

TSA2¹

C	-2.97085200	4.03097100	-1.20371300
C	-3.17335100	2.65872500	-1.11543300
C	-2.14668600	1.74883900	-1.38489300
C	-0.87186400	2.23841000	-1.73064900
C	-0.69645500	3.61927300	-1.85931500
C	-1.72741600	4.51397600	-1.59621700
H	-3.78827200	4.71648800	-0.99193300
H	-4.15910100	2.27340300	-0.85576600
H	0.27322300	3.99744900	-2.18075500
H	-1.55871600	5.58310700	-1.70393100
C	0.30103700	1.32306200	-1.96122500
C	-2.46757300	0.28167100	-1.39532900
P	1.21089400	0.96247000	-0.38197800
P	-1.88044100	-0.69067600	0.07868700

C	2.47576400	2.35382600	-0.11705700
C	-3.45354900	-1.35996400	0.87051800
C	2.25648300	-0.50079000	-0.78639200
C	2.55277900	-0.92191900	-2.07768300
C	3.49527900	-2.25070900	0.11247100
C	3.34903400	-2.05114700	-2.25717900
H	2.17861700	-0.37507200	-2.93906100
C	3.83114700	-2.72903300	-1.14666800
H	3.83983500	-2.74339400	1.02046300
H	3.59076400	-2.39114600	-3.26102400
H	4.45331500	-3.61299400	-1.24515200
C	-1.05039600	-2.18237500	-0.62381000
C	-1.31256100	-2.69012200	-1.89654300
C	-0.61239300	-3.81444700	-2.32370900
H	-2.05303500	-2.23308600	-2.54852900
C	0.49174400	-3.83208600	-0.20932000
C	0.31258800	-4.39623800	-1.46863000
H	-0.79262100	-4.22830600	-3.31298200
H	1.20207300	-4.26901300	0.49341600
H	0.88500200	-5.27180600	-1.76263500
N	-0.16496200	-2.74951900	0.21179700
N	2.72765200	-1.17204800	0.28547500
C	3.02777000	2.85794700	-1.44636500
H	2.27729600	3.38454400	-2.04590400
H	3.83955800	3.56964500	-1.24274000
H	3.45005500	2.04427100	-2.05168900
C	1.77368100	3.47667600	0.64519600
H	2.48057900	4.30477200	0.79445800
H	0.90584200	3.87125100	0.10358000
H	1.43420800	3.14127600	1.63399700
C	3.64208600	1.83495700	0.72266000
H	3.32621300	1.39370800	1.67449700
H	4.24889800	1.09841900	0.18260600
H	4.29285300	2.68694800	0.96194100
C	-4.27552600	-2.16073400	-0.13721400
H	-5.20442100	-2.48615400	0.35091400
H	-4.56434100	-1.58092800	-1.02192000
H	-3.74703400	-3.06218700	-0.47087700
C	-4.25028100	-0.16044900	1.37854400
H	-4.61594300	0.47254100	0.56008100
H	-5.12891600	-0.52028900	1.93094900
H	-3.65843400	0.46581000	2.06011300
C	-3.08762200	-2.27269300	2.03535100
H	-2.49797600	-3.13930300	1.71206900

H	-2.52526300	-1.74614500	2.81596800
H	-4.01407000	-2.65182500	2.48789600
H	-0.01387600	0.34328500	-2.34475400
H	0.98959400	1.74859400	-2.70030800
H	-2.03936800	-0.18775500	-2.28893600
H	-3.55281800	0.15325400	-1.47631200
Pd	-0.23488200	0.29625600	1.46292800
H	2.42349500	-0.85777800	1.64281300
C	1.14827000	0.63258700	2.91130300
O	2.19886600	-0.67314300	2.71783200
O	1.48842200	1.30181300	3.81768100
H	-1.15819800	-0.17303500	2.67532100
H	3.02479900	-0.49090800	3.20158700

TSA2^{II}

C	5.10731400	1.08784600	-0.95944100
C	3.88759800	1.73450700	-1.12504200
C	2.71774500	1.02755600	-1.41450200
C	2.79572700	-0.36706700	-1.59973700
C	4.02775900	-1.00515800	-1.43331400
C	5.17488700	-0.29384800	-1.10050400
H	6.00121400	1.66424600	-0.73183100
H	3.83609000	2.81999700	-1.04354500
H	4.08810800	-2.08057700	-1.59558200
H	6.12180700	-0.81509500	-0.97895400
C	1.61577000	-1.17489300	-2.06381200
C	1.41603800	1.76965100	-1.53341100
P	0.39180600	-1.59251200	-0.72910900
P	0.45844900	1.83948400	0.05934400
C	0.44035700	-3.47356800	-0.58256400
C	0.94607000	3.42815800	0.96697200
C	-1.23862800	-1.28673100	-1.55283600
C	-1.45143100	-1.17671800	-2.91874100
C	-3.54594200	-0.86714100	-1.16944000
C	-2.72742700	-0.89245800	-3.40294500
H	-0.63273300	-1.32338500	-3.61652300
C	-3.78750900	-0.72539000	-2.52217400
H	-4.29689800	-0.77079700	-0.38680400
H	-2.88694600	-0.80496800	-4.47424700
H	-4.78899700	-0.49538900	-2.86974400
C	-1.27871900	2.14963900	-0.47227100
C	-1.62582600	2.61135600	-1.74200900
C	-2.97202800	2.82656700	-2.02652300
H	-0.86995200	2.81302500	-2.49729200

C	-3.47348000	2.11900500	0.19658500
C	-3.91555100	2.58356000	-1.03901900
H	-3.27338600	3.18346600	-3.00862000
H	-4.18786800	1.90172200	0.99065000
H	-4.97582000	2.74104800	-1.21727800
N	-2.18962900	1.89476000	0.48110400
N	-2.30678300	-1.13759000	-0.73365400
C	0.08808900	-4.15255200	-1.90142000
H	0.73828800	-3.84541900	-2.72972000
H	0.20927500	-5.23771500	-1.77976000
H	-0.95373200	-3.96798500	-2.19104800
C	1.86141400	-3.83635100	-0.15499500
H	1.89061100	-4.90422700	0.10027500
H	2.58952000	-3.67285500	-0.95828400
H	2.18796900	-3.27272500	0.72923900
C	-0.55199300	-3.90780000	0.49151400
H	-0.31777700	-3.48064800	1.47333800
H	-1.58807900	-3.64612900	0.23945600
H	-0.50685000	-5.00098400	0.58799300
C	1.04926600	4.59320400	-0.01453700
H	1.18379400	5.52208600	0.55602400
H	1.90944100	4.49888100	-0.68811800
H	0.14192700	4.71100700	-0.62165300
C	2.28089500	3.22112300	1.67608700
H	3.09326600	2.97041200	0.98526000
H	2.55593900	4.15466600	2.18624600
H	2.21879700	2.43053900	2.43466300
C	-0.12249100	3.74093900	2.01120000
H	-1.07725200	4.02982800	1.55742500
H	-0.30445800	2.89673600	2.68871200
H	0.22846500	4.58545300	2.61997100
H	1.08064600	-0.63809200	-2.85398700
H	1.96176600	-2.11306900	-2.51231500
H	0.74441200	1.27041900	-2.24387400
H	1.57745700	2.78669700	-1.90983000
Pd	0.63285600	-0.18839400	1.26505200
C	0.96355600	-1.60301700	2.69546400
H	0.81628600	0.76029400	2.52590000
O	1.79786300	-2.27683200	3.17568200
O	-0.48005000	-1.75053900	3.59532700
H	-0.51668600	-2.62863500	4.01291900
H	-2.20689300	-1.23100300	0.31106100
H	-1.30492900	-1.62863500	2.93000300
C	-3.39278000	-0.85915000	2.50204800

H	-3.37213700	-0.72470700	3.60614200
O	-2.33343600	-1.38972000	2.00520800
O	-4.38888800	-0.51087500	1.86526500

TSA2^{III}

C	4.80586200	-0.43220000	-1.77664300
C	3.86869500	0.59208200	-1.70919900
C	2.49648600	0.34126400	-1.79864600
C	2.05716000	-0.98868400	-1.96912200
C	3.01435500	-2.00201700	-2.07275400
C	4.37480500	-1.74009100	-1.96653300
H	5.86700700	-0.20370100	-1.70628100
H	4.20759600	1.62221200	-1.60720300
H	2.67880200	-3.01937500	-2.26711600
H	5.09345700	-2.55223400	-2.05070500
C	0.60165500	-1.34771000	-2.10025600
C	1.54221500	1.50495200	-1.76037400
P	-0.30707100	-1.53826400	-0.48300900
P	0.76750500	1.77472200	-0.09251400
C	-0.46145500	-3.39821700	-0.16002500
C	1.52939000	3.35088500	0.60966300
C	-2.04635500	-1.09697700	-0.92184400
C	-2.52004800	-1.00989300	-2.23044600
C	-4.14009400	-0.62227300	-0.07570300
C	-3.86144000	-0.70474900	-2.44019500
H	-1.86758800	-1.19327800	-3.08003800
C	-4.69216000	-0.51000400	-1.34577200
H	-4.75124800	-0.46727200	0.81390200
H	-4.25107400	-0.62908800	-3.45250500
H	-5.74492200	-0.27162800	-1.46700900
C	-0.97787900	2.26531100	-0.41156900
C	-1.44613300	2.73342100	-1.63723000
C	-2.79591400	3.05277500	-1.75831300
H	-0.77451100	2.85910800	-2.48332000
C	-3.06590400	2.44797100	0.53341300
C	-3.62496800	2.90571400	-0.65526300
H	-3.18924300	3.41485600	-2.70522800
H	-3.68445900	2.31240000	1.42152600
H	-4.68560400	3.13498800	-0.70790800
N	-1.77585500	2.13147600	0.66178100
N	-2.85194600	-0.90377400	0.13687400
C	-1.14341400	-4.12168000	-1.31670600
H	-0.61615200	-3.99155600	-2.27004000
H	-1.15502000	-5.19898300	-1.09960900

H	-2.18420800	-3.80160400	-1.45014100
C	0.94252400	-3.95996400	0.04560100
H	0.86276400	-4.99460400	0.40730000
H	1.50980800	-3.98617500	-0.89046300
H	1.52089900	-3.39217400	0.78514700
C	-1.28851400	-3.60140100	1.10873700
H	-0.84711300	-3.10854600	1.98355500
H	-2.31757500	-3.24044200	0.99779900
H	-1.33266100	-4.67740500	1.32714900
C	1.28782900	4.52904400	-0.33056400
H	1.77971200	5.41860000	0.08622200
H	1.70674400	4.36874300	-1.33196900
H	0.22105800	4.76169300	-0.43567900
C	3.02633400	3.12147900	0.78854100
H	3.54416500	3.02337400	-0.17283700
H	3.46077800	3.98641000	1.30799800
H	3.23888800	2.22802200	1.39098700
C	0.88598800	3.64712300	1.96093100
H	-0.19100500	3.83475300	1.87534800
H	1.03620700	2.82911000	2.67743500
H	1.34943400	4.55067900	2.38030400
H	0.06136900	-0.56506400	-2.64663400
H	0.49284000	-2.26786500	-2.68747700
H	0.72223000	1.35941100	-2.47397700
H	2.05866900	2.42324100	-2.06475400
Pd	0.76994600	-0.16764300	1.24658400
C	0.92348400	-1.52387600	2.75981600
H	1.56711000	0.71864900	2.30881000
O	1.58522500	-2.42274500	3.15457300
O	-0.22021900	-1.13774400	3.82565800
H	-0.49513900	-1.90486100	4.36158500
H	-2.32525800	-0.47284700	1.84239000
H	-1.04344100	-0.65470000	3.34373300
O	-2.05544700	0.04405000	2.64322200
H	-1.68419900	0.85572300	2.23421000

A3'

C	3.18869800	3.33213300	-1.88004300
C	1.82413300	3.06590400	-1.88761500
C	1.33395500	1.76181500	-1.78224000
C	2.24888300	0.69221100	-1.73878300
C	3.61794300	0.97286900	-1.72346500
C	4.09150300	2.27919000	-1.77768200
H	3.54270500	4.35750400	-1.95925600

H	1.11400600	3.88737600	-1.98006900
H	4.32383800	0.14295900	-1.69400300
H	5.16228100	2.47012300	-1.76735200
C	1.79821200	-0.74011700	-1.80988500
C	-0.15083400	1.53149800	-1.71862100
P	1.06684800	-1.42335000	-0.24429900
P	-0.81508500	1.52923800	0.01495600
C	2.21792000	-2.83424400	0.24945400
C	-1.21108600	3.30782300	0.51575200
C	-0.49331800	-2.27123000	-0.73270400
C	-0.82920100	-2.61590800	-2.04102300
C	-2.44638100	-3.16132200	0.07918200
C	-2.05152300	-3.23999300	-2.27201600
H	-0.15652800	-2.41949800	-2.87205100
C	-2.88157000	-3.51485700	-1.19497500
H	-3.06501800	-3.37960400	0.95014100
H	-2.34290200	-3.51222100	-3.28370100
H	-3.84585300	-3.99729000	-1.32997200
C	-2.44389500	0.68864600	-0.10205600
C	-3.13081600	0.53458100	-1.30505000
C	-4.36836700	-0.10465900	-1.28156800
H	-2.72265000	0.90557800	-2.24222300
C	-4.11326600	-0.33832500	1.08093600
C	-4.87411200	-0.54436600	-0.06750500
H	-4.92641600	-0.24919000	-2.20356600
H	-4.48035300	-0.67851100	2.04934700
H	-5.83597600	-1.04545500	-0.00264900
N	-2.91894400	0.25276000	1.07456800
N	-1.28740600	-2.54487100	0.31508300
C	2.31470600	-3.86976800	-0.86801100
H	2.67556000	-3.44966100	-1.81513000
H	3.02812600	-4.64917000	-0.56656200
H	1.35020700	-4.35862700	-1.05264800
C	3.58880900	-2.22583300	0.53468900
H	4.26269300	-3.01380700	0.89759000
H	4.04745100	-1.79167300	-0.36250400
H	3.54484300	-1.44701500	1.30869400
C	1.67374700	-3.50766900	1.50505200
H	1.57051000	-2.81169200	2.34678600
H	0.69760400	-3.97518000	1.33185700
H	2.37273400	-4.29691000	1.81409600
C	-1.82229700	4.05210000	-0.66869700
H	-2.18121900	5.02929400	-0.31893600
H	-1.09402700	4.23913800	-1.46617300

H	-2.68337900	3.52196800	-1.09678200
C	0.06513500	4.00554600	0.97850300
H	0.85845700	3.98820300	0.22382400
H	-0.16930700	5.05704800	1.19387300
H	0.45944500	3.55556600	1.89811100
C	-2.20921300	3.29108100	1.67063300
H	-3.19817800	2.93311700	1.36320800
H	-1.86374800	2.68028400	2.51459600
H	-2.32406000	4.32134400	2.03374100
H	1.05469500	-0.85267200	-2.60770600
H	2.64612100	-1.37219100	-2.09576700
H	-0.42406000	0.54915200	-2.12617700
H	-0.69244900	2.28150300	-2.30766700
Pd	0.58280900	0.29188000	1.45147000
C	1.67788900	-0.30890400	2.98073500
H	0.12334500	1.44866700	2.44700500
O	2.29204400	-0.55846100	3.90812400

IV

C	0.69571000	4.70949100	1.28351400
C	1.37240200	3.50026600	1.33276400
C	0.70752600	2.26493200	1.35409400
C	-0.70725200	2.26496500	1.35410500
C	-1.37205400	3.50033800	1.33276100
C	-0.69529400	4.70952500	1.28350500
H	1.25147700	5.64422300	1.26629900
H	2.46124200	3.50036100	1.36961200
H	-2.46089100	3.50050200	1.36960900
H	-1.25101400	5.64428600	1.26627600
C	-1.57518800	1.03727000	1.45314800
C	1.57539900	1.03719700	1.45307700
P	-2.10493300	0.20888100	-0.13778200
P	2.10498200	0.20875800	-0.13788000
C	-3.39778600	1.21311700	-1.05647100
C	3.39775900	1.21289200	-1.05676200
C	-3.00311500	-1.28155400	0.47536200
C	-3.75835200	-1.28169300	1.64784300
C	-3.46647300	-3.49445800	0.08905500
C	-4.37951500	-2.46468200	2.03818300
H	-3.86399400	-0.38289900	2.24988000
C	-4.23084800	-3.59541500	1.24783800
H	-3.32756100	-4.36198900	-0.55654200
H	-4.97024100	-2.49663800	2.95053700
H	-4.69367900	-4.54031000	1.51848900

C	3.00312900	-1.28166300	0.47535100
C	3.75840500	-1.28168900	1.64781100
C	4.37937900	-2.46470000	2.03837900
H	3.86421800	-0.38279300	2.24966200
C	3.46614600	-3.49470800	0.08945900
C	4.23050400	-3.59556700	1.24826400
H	4.97010900	-2.49656900	2.95073600
H	3.32709400	-4.36234200	-0.55597000
H	4.69315400	-4.54049300	1.51911600
N	2.86151800	-2.36996800	-0.29396600
N	-2.86167500	-2.36973900	-0.29415900
C	-4.48778600	1.71888600	-0.11873700
H	-4.09940900	2.40732900	0.64103800
H	-5.23758600	2.26548900	-0.70724900
H	-5.00777700	0.89811700	0.39110600
C	-2.70748200	2.37713900	-1.76178500
H	-3.46178000	2.94956900	-2.31904800
H	-2.21792600	3.06409000	-1.06142600
H	-1.95741300	2.02276100	-2.48069000
C	-4.00672100	0.28426400	-2.10636800
H	-3.24169700	-0.16250300	-2.75614800
H	-4.59245800	-0.52538900	-1.65477900
H	-4.68299700	0.87067100	-2.74320900
C	4.48800600	1.71847800	-0.11921600
H	5.23772500	2.26507500	-0.70783500
H	4.09982900	2.40687900	0.64070000
H	5.00803500	0.89761700	0.39043800
C	2.70747000	2.37703900	-1.76188500
H	2.21814000	3.06402600	-1.06140400
H	3.46173600	2.94939100	-2.31926900
H	1.95721600	2.02279300	-2.48066100
C	4.00633900	0.28400000	-2.10683200
H	4.59193900	-0.52584400	-1.65540600
H	3.24110900	-0.16251400	-2.75654500
H	4.68266300	0.87030700	-2.74371400
H	-1.06871900	0.22409300	1.99196700
H	-2.47563300	1.28588700	2.03057600
H	1.06892800	0.22404300	1.99192900
H	2.47589700	1.28576600	2.03044200
Pd	-0.00000400	-0.36443600	-1.01850700
H	0.00004600	1.22046200	-1.03041300
C	-0.00005500	-2.39899100	-1.02821200
O	-0.00009500	-3.53926500	-1.06180500

TSB1'

C	-1.44906400	4.91343300	-0.60263000
C	-1.95311300	3.62804400	-0.73984000
C	-1.13543400	2.53294200	-1.05053800
C	0.24031400	2.76149000	-1.24714800
C	0.72607300	4.07210100	-1.15079800
C	-0.09499800	5.14088400	-0.82198700
H	-2.11698200	5.73569900	-0.35676000
H	-3.02393500	3.46742500	-0.62740400
H	1.78133100	4.25290900	-1.35101400
H	0.31835000	6.14437200	-0.75206100
C	1.22987600	1.68058300	-1.58797200
C	-1.80775900	1.20806200	-1.29534900
P	1.70012200	0.59760300	-0.15888300
P	-1.98698200	-0.04733300	0.06860600
C	2.65167500	1.62362000	1.10918700
C	-3.10834500	0.60238600	1.42994900
C	3.01412600	-0.47387400	-0.90464700
C	3.80507100	-0.14830200	-1.99939600
C	4.08638200	-2.55159500	-0.71917700
C	4.75685400	-1.06130300	-2.44940100
H	3.69039400	0.80585600	-2.50488000
C	4.90468400	-2.28067600	-1.80365900
H	4.13532500	-3.48725900	-0.16643800
H	5.37934500	-0.81354100	-3.30533900
H	5.63456000	-3.01338800	-2.13201800
C	-2.95598900	-1.36184700	-0.80581700
C	-4.01715100	-1.03846600	-1.65500000
C	-4.72044300	-2.06952900	-2.26935100
H	-4.30675400	-0.00756300	-1.84029700
C	-3.27119300	-3.60615500	-1.16636900
C	-4.34403300	-3.38124000	-2.02214300
H	-5.55255400	-1.84264800	-2.93124200
H	-2.94367800	-4.62303100	-0.95171800
H	-4.86302900	-4.21691800	-2.48297200
N	-2.58805100	-2.62736000	-0.57045100
N	3.17573300	-1.67018800	-0.29766400
C	3.68160100	2.54214700	0.46550700
H	3.22062800	3.32337900	-0.14833600
H	4.25343100	3.04541800	1.25798000
H	4.39834100	1.98863500	-0.15532400
C	1.62672200	2.42323000	1.91461100
H	2.15272100	2.99322900	2.69350900
H	1.06570900	3.13816600	1.30019600

H	0.90734700	1.76008200	2.41530700
C	3.35810600	0.64891000	2.05196400
H	2.66412500	-0.07529800	2.49758700
H	4.16427900	0.09591700	1.55370000
H	3.81300500	1.22375400	2.87003600
C	-4.38923600	1.21388500	0.86863900
H	-4.96326500	1.64088700	1.70194300
H	-4.20492300	2.02035900	0.15208900
H	-5.02394200	0.46052100	0.38692400
C	-2.31601200	1.63404500	2.23159600
H	-2.04956700	2.51610200	1.63619000
H	-2.92745800	1.97372800	3.07869500
H	-1.39222200	1.19890800	2.63745100
C	-3.48872700	-0.56175800	2.34276600
H	-4.01250800	-1.36052700	1.80188600
H	-2.61803100	-0.99664600	2.84786200
H	-4.17102400	-0.18417500	3.11646500
H	0.83877800	0.98256700	-2.34170800
H	2.12862300	2.14074400	-2.01485000
H	-1.29554300	0.63801600	-2.08335300
H	-2.81892600	1.40661500	-1.67136600
Pd	-0.01064100	-0.84249800	0.83376900
H	-1.16172500	-1.74932100	1.43244600
C	1.33086000	-3.45088700	1.68686100
H	0.47974600	-3.63913400	2.36868200
O	1.91821900	-4.34896800	1.10989400
O	1.64189500	-2.17873600	1.59036500
H	2.45265400	-1.97926500	0.68449700

TSB1

C	0.77510300	5.04292200	-0.71191400
C	1.43629600	3.86228600	-1.01797700
C	0.75742100	2.64837200	-1.19436600
C	-0.64923200	2.63707300	-1.08445300
C	-1.29993400	3.84594900	-0.79876500
C	-0.61076900	5.03313400	-0.59758700
H	1.33670300	5.96528900	-0.58205300
H	2.51910300	3.87352900	-1.13897700
H	-2.38798800	3.85234100	-0.75470000
H	-1.15641700	5.94773500	-0.37615000
C	-1.51438900	1.43732200	-1.37334700
C	1.58980200	1.44008400	-1.54016500
P	-1.91029200	0.23023700	0.00006500
P	1.92207200	0.32869200	-0.08878800

C	-3.08872900	1.05037400	1.22149300
C	3.26599200	1.10209900	0.99105300
C	-2.97448500	-0.96440700	-0.93851800
C	-3.91388600	-0.55395900	-1.88769300
C	-3.50570900	-3.17205400	-1.29203200
C	-4.66693000	-1.51603300	-2.55180200
H	-4.06356200	0.49905700	-2.11143300
C	-4.46100700	-2.85493500	-2.25132300
H	-3.31498600	-4.21357100	-1.03241400
H	-5.40280800	-1.21802100	-3.29487800
H	-5.02189100	-3.64169500	-2.74822500
C	2.85815200	-1.04017000	-0.92498300
C	3.63312900	-0.92999100	-2.06970900
C	4.26506400	-2.05351300	-2.59761500
H	3.75042600	0.03664600	-2.55042700
C	3.34462800	-3.37215700	-0.84351200
C	4.12349400	-3.29006400	-1.97912000
H	4.87161600	-1.95870300	-3.49412100
H	3.17100700	-4.29266100	-0.29658300
H	4.60317900	-4.18143500	-2.36802400
N	2.74247500	-2.27197900	-0.36376000
N	-2.77383300	-2.25951800	-0.64838200
C	-4.23148300	1.80363000	0.55174800
H	-3.88658100	2.58594500	-0.13396700
H	-4.84002700	2.29318300	1.32508500
H	-4.89517100	1.12976500	-0.00414800
C	-2.25565900	1.99197800	2.09085400
H	-2.90015500	2.44714400	2.85612500
H	-1.79795900	2.80329200	1.51100900
H	-1.45144200	1.44889000	2.60750200
C	-3.67028600	-0.05518300	2.10166700
H	-2.88727400	-0.60736300	2.63726100
H	-4.26740200	-0.77399900	1.52547400
H	-4.33244800	0.39829300	2.85254400
C	4.39900000	1.73179600	0.19483200
H	5.15392400	2.12583500	0.89024200
H	4.05959600	2.56857400	-0.42701500
H	4.89997800	1.00224100	-0.45491100
C	2.56986700	2.13988300	1.87257100
H	2.14937500	2.96948500	1.29170300
H	3.29930500	2.56192700	2.57817700
H	1.75821600	1.68710000	2.45932900
C	3.81216500	-0.01270400	1.88216100
H	4.39662800	-0.75035000	1.31726600

H	3.01196600	-0.53962400	2.42012200
H	4.48211100	0.42840400	2.63290600
H	-1.04672100	0.79023100	-2.12943000
H	-2.45727600	1.79221900	-1.80838500
H	1.07901600	0.78963600	-2.26465700
H	2.52763700	1.76940200	-2.00468000
Pd	-0.04415200	-0.69896800	0.92254500
H	2.15288700	-2.38501000	0.47902000
C	0.10681500	-3.14850500	2.49566800
H	0.39471800	-4.06157900	3.04360400
O	-1.13049400	-2.92330000	2.38623900
O	1.02573700	-2.42005900	2.04158900
H	-1.16200300	-1.72554700	1.62094600

B2

C	1.53851300	4.90126600	0.61202900
C	2.01844600	3.60957900	0.77311800
C	1.17330900	2.52901400	1.05877300
C	-0.20368600	2.77950800	1.21434800
C	-0.66745800	4.09539300	1.08795000
C	0.18027800	5.14878400	0.77732700
H	2.22682100	5.71258600	0.38689900
H	3.08964600	3.43143200	0.70040100
H	-1.72508500	4.29572700	1.25350600
H	-0.21629800	6.15710900	0.68386600
C	-1.20627400	1.71248600	1.56369000
C	1.80859500	1.18923700	1.31508400
P	-1.70764900	0.63085800	0.14434400
P	1.97331400	-0.04884400	-0.06530800
C	-2.83452800	1.63582600	-0.99246200
C	3.18538300	0.57732100	-1.36265500
C	-2.87897900	-0.52819700	0.99233000
C	-3.50850400	-0.32004600	2.20959900
C	-3.90123600	-2.66771000	0.83342200
C	-4.34492000	-1.30525400	2.73274300
H	-3.35579100	0.60633600	2.75417400
C	-4.54753200	-2.49281400	2.04159000
H	-3.98599900	-3.56122500	0.22264300
H	-4.83880600	-1.13850000	3.68642800
H	-5.19193800	-3.27482100	2.42790800
C	2.83847400	-1.42815500	0.81624900
C	3.88017300	-1.17384000	1.71108600
C	4.51342000	-2.24903800	2.32504900
H	4.20654300	-0.16089900	1.93033100

C	3.03581600	-3.69170300	1.13500600
C	4.08702100	-3.53595700	2.03230500
H	5.32920200	-2.07659900	3.02270500
H	2.66944700	-4.68740200	0.88628700
H	4.55186400	-4.40506500	2.48926400
N	2.41975200	-2.66965300	0.53795600
N	-3.10130500	-1.70491000	0.35722200
C	-3.80890000	2.51004600	-0.21440000
H	-3.30862300	3.29167700	0.36581300
H	-4.47871400	3.01049000	-0.92741600
H	-4.43808400	1.91986700	0.46503100
C	-1.91127100	2.47828700	-1.87209000
H	-2.52306900	3.09484000	-2.54509900
H	-1.27259100	3.15381100	-1.28986600
H	-1.26443500	1.84218300	-2.49179500
C	-3.62295600	0.67730100	-1.88199700
H	-2.97554900	-0.02090400	-2.42478200
H	-4.36780600	0.10122900	-1.31821700
H	-4.17028800	1.27225200	-2.62590800
C	4.45217500	1.15872800	-0.73902600
H	5.08686900	1.54908500	-1.54588500
H	4.25522300	1.98610400	-0.05046200
H	5.03425800	0.39586700	-0.20816500
C	2.45715200	1.62978300	-2.19742500
H	2.17578700	2.51155300	-1.60802300
H	3.11815600	1.96640500	-3.00795400
H	1.54699200	1.21752100	-2.65489100
C	3.58670000	-0.59254400	-2.25903500
H	4.07756500	-1.39695300	-1.69597800
H	2.73275700	-1.01734100	-2.79992300
H	4.30460500	-0.22502500	-3.00488300
H	-0.81014200	1.01413100	2.31409600
H	-2.09804100	2.17906600	1.99886300
H	1.26001900	0.62587000	2.08331700
H	2.81510800	1.35599200	1.71807100
Pd	-0.00007500	-0.74567700	-0.94504300
H	1.13751500	-1.64244400	-1.57685200
C	-1.32170700	-3.18479300	-2.06497200
H	-0.40518600	-3.38771800	-2.66237500
O	-1.99827200	-4.11661100	-1.63450300
O	-1.59885000	-1.93330600	-1.89743400
H	-2.61062400	-1.87905700	-0.56125600

TSB2

C	-1.51966700	4.84086600	-0.97423100
C	-2.00066400	3.54296800	-1.09485500
C	-1.14406900	2.46218600	-1.32316400
C	0.23460800	2.70693000	-1.47891100
C	0.70313400	4.01915400	-1.36469200
C	-0.15577700	5.07978000	-1.10273900
H	-2.21001500	5.66206300	-0.79552000
H	-3.07225500	3.35722100	-1.02574800
H	1.76552500	4.21169400	-1.50951800
H	0.23823100	6.09022200	-1.02160900
C	1.20433300	1.61595500	-1.84628700
C	-1.72978700	1.08420100	-1.44448300
P	1.71422200	0.54737500	-0.41060300
P	-1.86698300	0.12450500	0.13853400
C	3.53951700	0.94698900	-0.11259400
C	-3.51034300	0.53765200	0.96230300
C	1.75918100	-1.15353200	-1.14747500
C	1.80748900	-1.46489300	-2.49705800
C	1.54114700	-3.46493400	-0.63114400
C	1.69530100	-2.79163100	-2.90864400
H	1.92890400	-0.67665900	-3.23413200
C	1.55122700	-3.80511500	-1.96967500
H	1.45066700	-4.18673500	0.17431000
H	1.72202100	-3.02820400	-3.96883900
H	1.44939100	-4.84467100	-2.26168000
C	-1.98834600	-1.62756200	-0.42531900
C	-2.46511900	-1.96832700	-1.69085600
C	-2.50977300	-3.31529900	-2.04135500
H	-2.80228800	-1.21115300	-2.39395600
C	-1.63175900	-3.82475600	0.11845800
C	-2.08763000	-4.26406000	-1.12238600
H	-2.87478800	-3.61220200	-3.02156500
H	-1.29340900	-4.54411300	0.86453800
H	-2.10315100	-5.32521900	-1.35499800
N	-1.57238900	-2.53929700	0.46634400
N	1.64527500	-2.17894900	-0.26592100
C	4.38161400	0.64006100	-1.34454400
H	4.03179700	1.16064000	-2.24459500
H	5.41190700	0.97343300	-1.15760500
H	4.41836100	-0.43582200	-1.55742300
C	3.60805900	2.43234300	0.23410600
H	4.62564900	2.66714500	0.57409300
H	3.39696500	3.07193700	-0.63023200
H	2.91598000	2.69925700	1.04572000

C	4.04639000	0.13412900	1.07328500
H	3.55925300	0.43266400	2.00827700
H	3.92395600	-0.94833500	0.93827900
H	5.12180000	0.32599000	1.18972300
C	-4.60871500	0.68531900	-0.08781700
H	-5.56977800	0.79647000	0.43127000
H	-4.47490600	1.57351900	-0.71510200
H	-4.68870100	-0.19711000	-0.73651600
C	-3.34734800	1.83554600	1.74920900
H	-3.00983200	2.66740500	1.11999000
H	-4.31899000	2.11341400	2.17973600
H	-2.63330600	1.72041000	2.57432600
C	-3.88326800	-0.59360400	1.91608000
H	-4.12494800	-1.52235800	1.38542400
H	-3.09445700	-0.80449600	2.64979300
H	-4.77703700	-0.28681900	2.47575500
H	0.76693300	0.96123500	-2.60899800
H	2.10270400	2.05391900	-2.29628000
H	-1.12705100	0.44321200	-2.10017300
H	-2.72820800	1.13639400	-1.89610100
Pd	0.04050300	0.22407400	1.35667900
C	1.81805200	-0.72148400	3.32046700
H	1.37006800	0.31682700	3.13312500
O	1.48159000	-1.62255500	2.49555700
O	2.55942200	-0.81938900	4.29940100
H	-1.14724400	-0.08247000	2.34933000
H	1.59349200	-1.96431300	0.75396900

B3-CO₂

C	5.11670600	0.99035500	-0.63261500
C	4.23263800	-0.04636800	-0.90694400
C	2.88978900	0.19742500	-1.20887700
C	2.42744800	1.52801500	-1.26671700
C	3.33312800	2.55930600	-1.00020800
C	4.66014100	2.30315300	-0.67487300
H	6.15680500	0.77289900	-0.40021400
H	4.58637300	-1.07752400	-0.90374400
H	2.98919200	3.59014900	-1.06757600
H	5.33786800	3.12967500	-0.47293200
C	1.01648400	1.87297600	-1.66552700
C	1.98507100	-0.97477300	-1.46326400
P	-0.23333200	1.76669800	-0.28172400
P	1.06928200	-1.48626400	0.07248500
C	-0.74027400	3.56476000	0.03059000

C	1.99257600	-2.94594400	0.84648000
C	-1.75120300	1.04299300	-1.04892000
C	-1.90193000	0.73716200	-2.40163900
C	-3.86949200	0.27443200	-0.57973200
C	-3.09097100	0.15242600	-2.82813100
H	-1.12055800	0.95245600	-3.12566300
C	-4.10120300	-0.07998900	-1.90504400
H	-4.63971200	0.11150400	0.17677800
H	-3.22573600	-0.10632600	-3.87597100
H	-5.04565100	-0.53044500	-2.19789200
C	-0.40883000	-2.31304700	-0.67144700
C	-0.47855700	-2.94008800	-1.90500900
C	-1.68279700	-3.49947600	-2.32965900
H	0.40444100	-2.99092000	-2.53561500
C	-2.71197700	-2.80262600	-0.29803200
C	-2.81116700	-3.43730700	-1.52006800
H	-1.73538200	-3.98910400	-3.29823600
H	-3.52976200	-2.70118400	0.40925600
H	-3.75857800	-3.86515500	-1.82888500
N	-1.53898700	-2.26772500	0.07314700
N	-2.72344300	0.80544200	-0.14990400
C	-1.40082300	4.16555400	-1.20754800
H	-0.76354500	4.11481000	-2.10004000
H	-1.61144700	5.22781100	-1.01966000
H	-2.35480600	3.67600000	-1.44082700
C	0.51734700	4.34991800	0.39439600
H	0.22552400	5.35499300	0.72907400
H	1.19115900	4.47708600	-0.46049000
H	1.07638900	3.87736700	1.21411300
C	-1.71408400	3.62477800	1.20374800
H	-1.26159100	3.24034900	2.12650400
H	-2.63462100	3.06373900	1.00882900
H	-1.98740900	4.67511600	1.37775300
C	2.56569000	-3.89850100	-0.19440900
H	2.98363800	-4.77239200	0.32402200
H	3.38237400	-3.44270700	-0.76714200
H	1.80558500	-4.26762600	-0.89495500
C	3.12039200	-2.36111800	1.69419800
H	3.82184500	-1.76690100	1.09535400
H	3.68427600	-3.18480800	2.15315700
H	2.73441100	-1.72455700	2.49985000
C	1.00829700	-3.68990400	1.74544700
H	0.25846900	-4.24632200	1.16895300
H	0.48907800	-3.01503200	2.43974700

H	1.56467000	-4.41902900	2.34970300
H	0.68037500	1.20256200	-2.46318500
H	0.98723300	2.88346100	-2.08938000
H	1.20994800	-0.73536800	-2.20248400
H	2.55231200	-1.82356400	-1.86230500
Pd	0.38129300	0.29888100	1.52876400
H	-1.50157600	-1.77705600	0.97430400
C	-2.85386100	0.06692100	2.78172600
H	0.01157500	1.34946200	2.68599800
O	-3.01630700	1.16710700	3.11967600
O	-2.72425000	-1.05409200	2.48129200
H	0.62835100	-0.53279400	2.89126600

B3

C	4.73498800	-0.98099900	-1.32237900
C	3.47439000	-1.55582700	-1.43212200
C	2.31501700	-0.77578000	-1.46927900
C	2.42896800	0.62872600	-1.42540500
C	3.70524700	1.19063100	-1.32713200
C	4.84940900	0.40347800	-1.26440900
H	5.62114300	-1.61105300	-1.29530200
H	3.37609500	-2.63941900	-1.50343000
H	3.80110700	2.27516300	-1.31929500
H	5.82713700	0.87401400	-1.18857700
C	1.23385800	1.53625800	-1.55021600
C	0.98514800	-1.46944300	-1.55784800
P	0.28636000	1.80822000	0.03597600
P	0.21760300	-1.71153600	0.11889800
C	0.60168200	3.62535900	0.46281200
C	0.60642800	-3.47273200	0.69126200
C	-1.49618300	1.80283900	-0.44907000
C	-1.97492200	1.68021100	-1.75344000
C	-3.63635500	1.89728300	0.39027500
C	-3.35064000	1.64130900	-1.96149600
H	-1.30223300	1.62513600	-2.60499300
C	-4.20340800	1.75791100	-0.87271500
H	-4.27298500	1.99540900	1.27037900
H	-3.74709300	1.53157800	-2.96835600
H	-5.28318700	1.73671300	-0.99180200
C	-1.57070900	-1.83056000	-0.33903400
C	-2.08738600	-2.30589000	-1.53383900
C	-3.46626300	-2.31486400	-1.73788200
H	-1.41538400	-2.66730700	-2.30719400
C	-3.78111300	-1.38221600	0.43193300

C	-4.32477200	-1.85755700	-0.74496000
H	-3.86800100	-2.68491400	-2.67737900
H	-4.36573100	-0.99777900	1.26113800
H	-5.40071200	-1.85544000	-0.87811200
N	-2.44845600	-1.37867400	0.58936800
N	-2.32028100	1.90162000	0.61026500
C	0.04735600	4.54025800	-0.62594900
H	0.44888200	4.31170700	-1.62188100
H	0.32214100	5.57931500	-0.39542800
H	-1.04757100	4.49337400	-0.67994700
C	2.10966000	3.81822900	0.60271300
H	2.30504400	4.82314100	1.00196900
H	2.63101900	3.74574900	-0.35874700
H	2.55567200	3.09332800	1.29799300
C	-0.06266400	3.96137200	1.79399100
H	0.34328800	3.35475800	2.61331700
H	-1.14820500	3.81695200	1.76450300
H	0.13359600	5.01725700	2.02779200
C	0.58236600	-4.48354300	-0.44762600
H	0.71541600	-5.48912700	-0.02536400
H	1.39686700	-4.32439900	-1.16480600
H	-0.37048400	-4.48323200	-0.99252900
C	1.99385300	-3.43609900	1.32951200
H	2.76589400	-3.10034100	0.62581200
H	2.25946200	-4.44970000	1.66023500
H	2.02030400	-2.77602900	2.20535100
C	-0.43140400	-3.85532800	1.74361200
H	-1.42157300	-4.03179000	1.30398500
H	-0.52577100	-3.09467000	2.53054000
H	-0.11590600	-4.79019800	2.22620900
H	0.53189700	1.12644700	-2.28405000
H	1.54723200	2.50990400	-1.94482600
H	0.25725300	-0.88321600	-2.13360600
H	1.08592200	-2.43637200	-2.06425900
Pd	0.54496200	0.07600500	1.69052100
H	-2.06405400	-0.98037800	1.45394500
H	0.80163900	1.09399800	2.90745500
H	0.66005000	-0.89380700	2.97687400

TSB3

C	-2.16899700	4.27792000	-1.32813200
C	-0.95802600	3.60887600	-1.46202600
C	-0.89040100	2.21270600	-1.48019300
C	-2.08386100	1.46658100	-1.40324600

C	-3.29438100	2.15460100	-1.27087100
C	-3.34472400	3.54323300	-1.22066300
H	-2.19268800	5.36526200	-1.31584200
H	-0.03318200	4.17757000	-1.56311500
H	-4.22019600	1.58188500	-1.22485900
H	-4.30303800	4.04766600	-1.11716800
C	-2.10732900	-0.03306400	-1.52992000
C	0.46137700	1.55964200	-1.56212400
P	-1.62188700	-0.96505200	0.01825500
P	1.14460900	1.22703100	0.13848500
C	-3.17832600	-1.95725500	0.43597900
C	2.20779600	2.70468900	0.66516100
C	-0.42874500	-2.26060100	-0.54596400
C	0.06631800	-2.40031900	-1.84292000
C	0.89608700	-3.98888800	0.20275700
C	1.03118000	-3.37208000	-2.09327400
H	-0.28195600	-1.77326300	-2.65893500
C	1.45349800	-4.19129600	-1.05581700
H	1.20104900	-4.61107300	1.04505800
H	1.43916400	-3.48948100	-3.09487600
H	2.20266400	-4.96345900	-1.20840400
C	2.43886800	-0.03695000	-0.26474800
C	3.23378400	-0.08222600	-1.39957600
C	4.19377500	-1.08285700	-1.53422900
H	3.10729100	0.66742400	-2.17556600
C	3.53254900	-1.98389000	0.57004600
C	4.35296200	-2.03963900	-0.53822100
H	4.82103100	-1.11039700	-2.42112800
H	3.57449400	-2.69059700	1.39210100
H	5.09392400	-2.82758600	-0.61769100
N	2.61790100	-1.00509700	0.66586400
N	-0.00423900	-3.04057100	0.46576300
C	-3.50470700	-2.95460900	-0.67077600
H	-3.60376000	-2.47820500	-1.65522200
H	-4.46200100	-3.44827800	-0.44986200
H	-2.73976600	-3.73753600	-0.75069700
C	-4.32078300	-0.95995900	0.61605700
H	-5.19471100	-1.48649600	1.02389600
H	-4.63400300	-0.50010800	-0.32873500
H	-4.05781200	-0.15801800	1.32077000
C	-2.96708900	-2.69614300	1.75417200
H	-2.74261900	-2.00072600	2.57406100
H	-2.15347200	-3.42652800	1.69360000
H	-3.89008300	-3.23406600	2.01335800

C	2.93444100	3.36847700	-0.49557400
H	3.58281900	4.16306700	-0.10076400
H	2.24194900	3.83563300	-1.20606900
H	3.57710600	2.66867900	-1.04457800
C	1.27454200	3.70644700	1.34296600
H	0.48937100	4.06820000	0.66763500
H	1.86136400	4.57658700	1.66864500
H	0.79042600	3.27342000	2.22765800
C	3.21814600	2.19147600	1.68852100
H	3.99637100	1.56895100	1.22821300
H	2.73826400	1.61545100	2.49226400
H	3.71739500	3.05086800	2.15607500
H	-1.45254600	-0.34730300	-2.34953900
H	-3.11456900	-0.35284900	-1.82004300
H	0.40884500	0.57563100	-2.04742700
H	1.15863900	2.17276800	-2.14537300
Pd	-0.45792100	0.32901400	1.70180400
H	2.00173600	-0.98950500	1.48718700
H	-1.20966300	0.06287600	3.10763300
H	-0.07766700	0.87966200	3.17797200

B4

C	-0.31642200	-4.79715600	-1.29314600
C	-1.03423600	-3.61618500	-1.43706400
C	-0.40422700	-2.36754200	-1.45060900
C	1.00311500	-2.31086300	-1.36380500
C	1.71049800	-3.50927200	-1.21669600
C	1.06724000	-4.74129000	-1.16782100
H	-0.83548600	-5.75322000	-1.28702700
H	-2.11722400	-3.65480800	-1.55525800
H	2.79786100	-3.47017800	-1.15723900
H	1.64859900	-5.65392400	-1.05585800
C	1.77467800	-1.02495500	-1.50126500
C	-1.26420200	-1.13788300	-1.53936200
P	1.92633000	-0.02582300	0.07847700
P	-1.68644000	-0.47908200	0.16168400
C	3.79777200	0.01367900	0.39868700
C	-3.40045100	-1.14379800	0.63817400
C	1.58881500	1.71951800	-0.45006500
C	1.31520100	2.13814500	-1.75386100
C	1.32915200	3.86853000	0.34132300
C	1.00928700	3.47592800	-1.98506000
H	1.34350400	1.44748000	-2.59225400
C	1.02043000	4.36674100	-0.92045000

H	1.35477400	4.53718900	1.20296100
H	0.77745700	3.81565700	-2.99223000
H	0.79177700	5.42033800	-1.05664700
C	-2.09331400	1.27413900	-0.29079500
C	-2.71264600	1.72846000	-1.44553800
C	-2.94956300	3.09049500	-1.61671700
H	-3.01435100	1.01862600	-2.21026500
C	-1.93196900	3.52200200	0.49397000
C	-2.56716800	3.99827500	-0.63468800
H	-3.44099700	3.44225500	-2.51994800
H	-1.58263400	4.15173700	1.30557000
H	-2.74182800	5.06311100	-0.74349600
N	-1.71820400	2.20236100	0.62202300
N	1.58506200	2.58214500	0.58492300
C	4.55945600	0.73428500	-0.70780000
H	4.37170000	0.30416000	-1.70078200
H	5.64044200	0.65669300	-0.52013200
H	4.30938500	1.80208800	-0.74642900
C	4.27623300	-1.43125100	0.51787500
H	5.31090000	-1.43847900	0.88864300
H	4.27671200	-1.95524100	-0.44532600
H	3.66616600	-2.00858600	1.22778500
C	4.03763000	0.71430400	1.73321800
H	3.52149100	0.19993500	2.55555300
H	3.69914100	1.75628800	1.71884700
H	5.11395700	0.70845000	1.95696200
C	-4.37489900	-1.26090700	-0.52538700
H	-5.34955000	-1.59621400	-0.14301400
H	-4.04987700	-1.99889800	-1.26847700
H	-4.53946500	-0.30286200	-1.03482800
C	-3.16939900	-2.51497200	1.27065600
H	-2.72851500	-3.23065600	0.56593100
H	-4.13242700	-2.92540200	1.60551300
H	-2.50759400	-2.44927400	2.14449900
C	-3.96138600	-0.19760000	1.69717100
H	-4.25617800	0.77234400	1.27552200
H	-3.24330300	-0.01974500	2.51061700
H	-4.85802400	-0.64894500	2.14378200
H	1.30274400	-0.39334500	-2.25976900
H	2.77886800	-1.24710700	-1.88055600
H	-0.74068100	-0.31426400	-2.04224900
H	-2.17293100	-1.34233900	-2.11780300
Pd	0.17060000	-0.52835000	1.63524500
H	-1.21852600	1.85833300	1.45231600

H	0.64281300	-0.81643500	3.37102700
H	-0.19041100	-0.89361600	3.38608000

TSB4

C	-0.49937900	-4.79795400	-1.11785000
C	-1.18442100	-3.59751000	-1.25816400
C	-0.51754100	-2.36918200	-1.33383900
C	0.89428700	-2.35577900	-1.29809000
C	1.56746800	-3.57556900	-1.16144200
C	0.89005500	-4.78485200	-1.06087500
H	-1.04749700	-5.73611200	-1.06426300
H	-2.27305000	-3.60294000	-1.32329200
H	2.65690400	-3.57063500	-1.15146100
H	1.44746400	-5.71361300	-0.95886300
C	1.71065600	-1.10183800	-1.47067400
C	-1.35258600	-1.12425500	-1.44774300
P	2.02848000	-0.14394100	0.11411400
P	-1.80341200	-0.41226500	0.22821200
C	3.91190800	-0.22236700	0.34063500
C	-3.52185900	-1.06318000	0.69629700
C	1.77310600	1.62936700	-0.37882000
C	1.49561300	2.07772900	-1.67273900
C	1.58778000	3.77400200	0.44733500
C	1.22183500	3.42613000	-1.87929400
H	1.50255100	1.40062300	-2.52256900
C	1.26620600	4.29890500	-0.80047300
H	1.64679800	4.42866800	1.31780000
H	0.98667900	3.78808000	-2.87796200
H	1.05820200	5.35933600	-0.91551500
C	-2.17314200	1.33018900	-0.31206400
C	-2.81841400	1.74309200	-1.46823000
C	-2.98264700	3.10269500	-1.72474000
H	-3.18871900	1.00405400	-2.17278900
C	-1.85231700	3.61237700	0.30982500
C	-2.50452900	4.04940900	-0.82500500
H	-3.49007700	3.42206300	-2.63117600
H	-1.43458900	4.27367700	1.06153300
H	-2.62113700	5.11320600	-1.00123900
N	-1.70971500	2.29388700	0.51984700
N	1.81643600	2.47801800	0.66743000
C	4.66406400	0.48675300	-0.77893900
H	4.39964500	0.10134600	-1.77291600
H	5.74607800	0.33725200	-0.64862700
H	4.47892000	1.56836300	-0.77374600

C	4.31779800	-1.69206100	0.40300300
H	5.36125700	-1.76502400	0.74132000
H	4.26150900	-2.18390900	-0.57567600
H	3.70026000	-2.26208500	1.11206000
C	4.23215200	0.43296500	1.68179700
H	3.73041400	-0.08469100	2.51136600
H	3.92846500	1.48606600	1.70684800
H	5.31567700	0.38779600	1.86318300
C	-4.44604800	-1.34016600	-0.47992100
H	-5.42317600	-1.66706100	-0.09607200
H	-4.07022900	-2.14184900	-1.12708000
H	-4.62190600	-0.44938100	-1.09600300
C	-3.27264000	-2.35199500	1.48081200
H	-2.75152800	-3.10948800	0.88057900
H	-4.23510500	-2.77816100	1.79700000
H	-2.67360700	-2.16380500	2.38163200
C	-4.15047000	-0.02558500	1.62268500
H	-4.45738100	0.87959000	1.08238400
H	-3.46697100	0.27001200	2.43145300
H	-5.04857000	-0.45265100	2.08987600
H	1.20018500	-0.42703000	-2.16382400
H	2.66840200	-1.35404800	-1.94198600
H	-0.80756300	-0.31562900	-1.95160800
H	-2.25405700	-1.32050100	-2.04166500
Pd	0.12853100	-0.39365600	1.48590400
H	-1.17500700	1.97320300	1.33904800
H	0.70817600	0.22730100	3.53970500
H	0.66547100	0.75798200	4.07423000

R

C	0.67353300	0.00000100	0.00000000
C	-0.67354100	0.00000000	0.00000000
C	1.51833500	1.24108600	-0.01402800
H	2.25797100	1.18771900	-0.82632700
H	0.95876200	2.17122000	-0.14104800
C	-1.51833600	1.24109100	0.01402400
H	-2.10217000	1.32588000	-0.91470900
H	-2.25764000	1.18796300	0.82664100
H	-0.95869900	2.17125300	0.14056200
C	-1.51833300	-1.24109200	-0.01402400
H	-2.10215500	-1.32589200	0.91471500
H	-2.25764600	-1.18796100	-0.82663400
H	-0.95869300	-2.17124900	-0.14057600
C	1.51833400	-1.24108600	0.01402900

H	0.95876000	-2.17121900	0.14104500
H	2.10179600	-1.32613000	-0.91491600
H	2.25797000	-1.18771800	0.82632700
H	2.10179500	1.32613100	0.91491700

A1-R

C	-0.21698200	5.14782900	-0.89599900
C	-1.03451600	4.04751600	-1.12590500
C	-0.50691600	2.78997700	-1.44150300
C	0.89130200	2.65356900	-1.55177100
C	1.70145000	3.77478100	-1.34214100
C	1.16338200	5.01124600	-1.00631800
H	-0.65857100	6.11146300	-0.65119500
H	-2.11787100	4.16174800	-1.07865900
H	2.77979900	3.66904400	-1.46412000
H	1.81786800	5.86542400	-0.84769100
C	1.53685500	1.34982500	-1.91985500
C	-1.44492300	1.65236500	-1.71823100
P	1.86155500	0.24915500	-0.44413400
P	-1.80659600	0.51610800	-0.26870500
C	3.66209400	0.61223400	0.05423100
C	-3.39659500	1.24003100	0.48947800
C	2.00678700	-1.36695700	-1.35567100
C	2.58557400	-1.61265700	-2.59243700
C	1.36898000	-3.66255400	-1.20701600
C	2.56142600	-2.89988100	-3.12385200
H	3.04719000	-0.79898600	-3.14405100
C	1.95416300	-3.93921700	-2.42545800
H	0.85661800	-4.39875800	-0.59600200
H	3.01873100	-3.09027700	-4.09132300
H	1.92173900	-4.94842100	-2.82084600
C	-2.43159100	-0.96410500	-1.19875500
C	-3.08527400	-0.88241400	-2.43147400
C	-3.50509400	-2.05266500	-3.05440400
H	-3.26440400	0.07972700	-2.90549900
C	-2.60619200	-3.25877900	-1.20630900
C	-3.26316700	-3.26986300	-2.43206800
H	-4.01622900	-2.00998700	-4.01355800
H	-2.39876600	-4.19549200	-0.68696800
H	-3.57247400	-4.20942100	-2.88178200
N	-2.19409100	-2.14330600	-0.59896800
N	1.41710500	-2.41049200	-0.72654600
C	4.59268200	0.97431800	-1.09477000
H	4.30664900	1.90831800	-1.59292400

H	5.60421900	1.12218100	-0.69034800
H	4.65973800	0.18124200	-1.84982600
C	3.58242200	1.77912400	1.03949700
H	4.59153100	2.01794500	1.40403500
H	3.17322300	2.68498900	0.57412300
H	2.95732700	1.53506400	1.90783400
C	4.20232900	-0.62042200	0.77169700
H	3.56255600	-0.91625300	1.61160500
H	4.31314400	-1.48073000	0.09759800
H	5.19602300	-0.39182800	1.18166800
C	-4.36860800	1.83763800	-0.51982400
H	-5.28494500	2.14025800	0.00771800
H	-3.97023600	2.73401800	-1.01117700
H	-4.66375200	1.11829900	-1.29484800
C	-2.95210300	2.32220800	1.47270900
H	-2.39475000	3.12480200	0.97165000
H	-3.83327100	2.77610600	1.94932000
H	-2.31297100	1.91345200	2.26576800
C	-4.09850900	0.11491900	1.24290100
H	-4.54129600	-0.61874900	0.55679500
H	-3.41604800	-0.41849900	1.91571300
H	-4.91097600	0.53390000	1.85369100
H	0.89098500	0.75860800	-2.58076100
H	2.46870200	1.52794500	-2.46856400
H	-1.03217500	0.98916400	-2.48858200
H	-2.38498200	2.04361800	-2.12331300
Pd	0.08125100	-0.14755900	1.16618500
C	0.82090800	-1.11762100	3.06914300
C	-0.57921900	-1.00584000	3.15445400
C	1.46376700	-2.46915900	2.86053200
H	0.88523200	-3.14358100	2.21962100
H	2.47029100	-2.38633300	2.43129400
H	1.58191100	-2.98090300	3.83200700
C	-1.44848100	-2.23514000	3.02882700
H	-1.42235200	-2.81592800	3.96765200
H	-2.49918700	-1.97114300	2.85915100
H	-1.14893700	-2.91237400	2.22223200
C	-1.20637500	0.05279900	4.03035000
H	-2.26256300	0.21192100	3.77716400
H	-1.18380000	-0.26643900	5.08769000
H	-0.70221900	1.02357900	3.97767200
C	1.71013100	-0.18122000	3.85309000
H	1.38307300	0.86370400	3.82746600
H	1.73951500	-0.48558100	4.91446700

H	2.74661000	-0.21490300	3.49329100
H	0.93880300	-2.18786500	0.16258400

TSC1

C	-0.80877100	5.37629100	-0.41766800
C	-1.46672100	4.17012100	-0.61826000
C	-0.79020400	2.99646000	-0.97729800
C	0.60745500	3.06445400	-1.15012500
C	1.25207600	4.29772200	-0.99017400
C	0.56555900	5.44491100	-0.61755400
H	-1.37380900	6.26237000	-0.13674200
H	-2.55033500	4.13867000	-0.51890500
H	2.32465200	4.35299200	-1.17345000
H	1.09785000	6.38596600	-0.49830400
C	1.45914300	1.88180900	-1.51599400
C	-1.60215900	1.76739600	-1.28747800
P	1.73414200	0.67039500	-0.13718600
P	-1.91705800	0.42893700	-0.00413900
C	2.60491400	1.52645000	1.30231900
C	-3.15458000	1.15250600	1.22189800
C	3.04640100	-0.41864400	-0.85413300
C	4.12230300	0.00469700	-1.62736800
C	3.77551600	-2.61901100	-0.95636200
C	5.04265100	-0.93635300	-2.07753100
H	4.24626400	1.05509400	-1.87859600
C	4.87199500	-2.27001400	-1.73173400
H	3.60758700	-3.65311700	-0.66252100
H	5.88717500	-0.62749400	-2.68834800
H	5.56912000	-3.03524600	-2.05910100
C	-2.79348600	-0.71969400	-1.17234800
C	-4.13580500	-1.09647100	-1.15341800
C	-4.58478700	-2.03662900	-2.07736800
H	-4.83605400	-0.68073200	-0.43594700
C	-2.37597700	-2.11282300	-2.96045600
C	-3.69195800	-2.56360500	-2.99832500
H	-5.62671400	-2.34826400	-2.07209400
H	-1.64426800	-2.49193100	-3.67476600
H	-4.00108900	-3.30170900	-3.73298500
N	-1.93104300	-1.22069700	-2.07542400
N	2.88107300	-1.71414100	-0.54460500
C	3.79733100	2.37593000	0.88441400
H	3.51405600	3.19978200	0.21976400
H	4.24841200	2.82131200	1.78282700
H	4.57655700	1.78190800	0.39114400

C	1. 57228200	2. 38028900	2. 03986100
H	2. 03010600	2. 77860400	2. 95642900
H	1. 22726600	3. 23368500	1. 44319100
H	0. 69582200	1. 78713300	2. 33518500
C	3. 07357000	0. 41019600	2. 23650100
H	2. 23420300	-0. 21580100	2. 56931200
H	3. 82488200	-0. 23994300	1. 76945700
H	3. 53327700	0. 85824700	3. 12835100
C	-4. 28321300	1. 95213200	0. 57774000
H	-4. 97741500	2. 28580200	1. 36206100
H	-3. 91834500	2. 84843900	0. 06563300
H	-4. 86444300	1. 37046800	-0. 14683800
C	-2. 33802200	2. 06027900	2. 14682800
H	-1. 84158700	2. 87968600	1. 61187500
H	-3. 00883600	2. 50759300	2. 89395600
H	-1. 57142100	1. 48790000	2. 68833300
C	-3. 73043600	0. 02935500	2. 08365800
H	-4. 35850800	-0. 67524000	1. 52866200
H	-2. 93399900	-0. 53714700	2. 58021800
H	-4. 35444900	0. 47543000	2. 87081200
H	1. 00734100	1. 27541100	-2. 31484400
H	2. 42759600	2. 23407600	-1. 89112400
H	-1. 13521800	1. 19909200	-2. 10260800
H	-2. 59135000	2. 07316000	-1. 65446100
Pd	0. 07448200	-0. 86557100	0. 56235000
C	0. 58023400	-3. 06570400	0. 98464100
C	-0. 69669200	-2. 67015800	1. 50233500
C	0. 58017300	-3. 96292400	-0. 23836200
H	-0. 01309100	-3. 55982500	-1. 06649600
H	1. 59157700	-4. 14064600	-0. 61492400
H	0. 16196500	-4. 94701500	0. 02380800
C	-1. 96218100	-3. 22198000	0. 89998900
H	-2. 13370700	-4. 24627900	1. 27413100
H	-2. 83276500	-2. 62510300	1. 19647000
H	-1. 94496500	-3. 27314100	-0. 19310300
C	-0. 82062300	-2. 38266600	2. 98088500
H	-1. 81545600	-1. 99578500	3. 22591400
H	-0. 68683500	-3. 30828900	3. 56571000
H	-0. 08399300	-1. 65886000	3. 35173400
C	1. 69058300	-3. 39495800	1. 96102400
H	1. 74102400	-2. 70857400	2. 81114800
H	1. 52688500	-4. 40743700	2. 36369100
H	2. 67589700	-3. 39994100	1. 48147400
H	1. 57707300	-1. 86132100	0. 21601300

C2

C	0.61185600	5.36961100	0.29187000
C	1.27549400	4.19204500	0.60673900
C	0.59747200	3.01429000	0.95008600
C	-0.80991300	3.05517600	1.00851300
C	-1.46525100	4.26160100	0.72762200
C	-0.77618000	5.40743600	0.35713200
H	1.18022900	6.25783500	0.02482500
H	2.36289400	4.19119200	0.61094100
H	-2.55078100	4.29718600	0.81125500
H	-1.31907400	6.32470200	0.13997400
C	-1.66156700	1.88237100	1.40156300
C	1.40527000	1.81190100	1.36422000
P	-1.83591900	0.54565100	0.12571500
P	1.90781700	0.48504400	0.13305300
C	-2.76880500	1.26261600	-1.35007500
C	3.19606900	1.25378900	-1.01095600
C	-3.07791300	-0.57186900	0.93028500
C	-4.00682400	-0.14000700	1.87961500
C	-3.89668200	-2.71929400	1.02611000
C	-4.90408300	-1.06148500	2.41042100
H	-4.04327400	0.89542200	2.20737100
C	-4.85312000	-2.37858700	1.97721600
H	-3.82675300	-3.74468300	0.66014600
H	-5.63560600	-0.74609600	3.15093900
H	-5.53470300	-3.13061000	2.36503000
C	2.70234200	-0.65416000	1.36064300
C	4.05964200	-0.93418100	1.50516200
C	4.45059700	-1.88440000	2.44616300
H	4.81479600	-0.43658500	0.90537000
C	2.15576200	-2.14460000	3.02806200
C	3.48519500	-2.51103300	3.21904300
H	5.50403900	-2.12659300	2.56697100
H	1.36694000	-2.60154900	3.62644500
H	3.74694200	-3.26344900	3.95755700
N	1.76699300	-1.24509800	2.12474300
N	-3.02392100	-1.84849800	0.51618300
C	-4.00600700	2.04982700	-0.94025600
H	-3.76206200	2.91684600	-0.31575700
H	-4.51341300	2.42540200	-1.84044900
H	-4.72451800	1.42547700	-0.39358600
C	-1.79703100	2.14391700	-2.13760300
H	-2.28466500	2.47491400	-3.06556100

H	-1.49202900	3.04024500	-1.58441500
H	-0.88722100	1.58984500	-2.41311200
C	-3.18205000	0.08877700	-2.23721400
H	-2.31439800	-0.51251700	-2.54417600
H	-3.90519100	-0.57448900	-1.74723100
H	-3.65393000	0.48035600	-3.14924700
C	4.20742300	2.13814900	-0.28666800
H	4.93712200	2.50630000	-1.02133100
H	3.75487800	3.01510000	0.18118500
H	4.76648800	1.59898700	0.48682400
C	2.39880200	2.07729600	-2.02660100
H	1.80758700	2.87198800	-1.55479900
H	3.09802000	2.55271500	-2.72850600
H	1.71879700	1.44136700	-2.61153300
C	3.95492500	0.16993600	-1.77381000
H	4.58037500	-0.45830600	-1.13038800
H	3.28158400	-0.47929800	-2.33965000
H	4.62016600	0.66012300	-2.49825000
H	-1.25658100	1.36220900	2.28230800
H	-2.65582900	2.25005600	1.67961200
H	0.87163300	1.22843600	2.12621300
H	2.34060800	2.14594300	1.83548800
Pd	0.05793400	-0.74180600	-0.67162100
C	-0.32830700	-3.05041500	-1.25619000
C	0.97160800	-2.40497400	-1.64935100
C	-0.27069800	-3.94378100	-0.02490900
H	0.16871800	-3.43983000	0.84316300
H	-1.27997900	-4.26748100	0.25419500
H	0.31722700	-4.84770700	-0.23380300
C	2.23440500	-2.99826500	-1.09577800
H	2.36280100	-4.01804200	-1.50076800
H	3.11196200	-2.41975600	-1.40149400
H	2.23775700	-3.07853300	-0.00294000
C	1.07335400	-1.98704400	-3.09398500
H	1.97634500	-1.40075800	-3.28488400
H	1.12936600	-2.87465700	-3.74680000
H	0.20746000	-1.39791800	-3.42688300
C	-1.08321900	-3.75409800	-2.38674100
H	-1.27770000	-3.10859500	-3.24739800
H	-0.50335900	-4.62215300	-2.72944000
H	-2.04973200	-4.11766700	-2.01504400
H	-1.09428400	-2.21082100	-0.98379400

TSC2

C	1. 22537600	5. 22761500	-1. 10694000
C	0. 20817400	4. 30355700	-1. 29922900
C	0. 44415900	2. 92195800	-1. 29149500
C	1. 76919400	2. 46747700	-1. 15175500
C	2. 78703900	3. 41343900	-0. 97401400
C	2. 52836800	4. 77638300	-0. 92590000
H	1. 00234600	6. 29219600	-1. 11171100
H	-0. 80869600	4. 65711500	-1. 46414800
H	3. 81623600	3. 06496900	-0. 89768700
H	3. 34445100	5. 48092800	-0. 78268100
C	2. 17308300	1. 02952300	-1. 33183300
C	-0. 72937300	2. 01053200	-1. 49131900
P	2. 06251700	-0. 17578100	0. 07640600
P	-1. 45109500	1. 10838300	-0. 01315200
C	3. 37007700	0. 27625700	1. 35688500
C	-1. 92224800	2. 41025800	1. 26846300
C	2. 73439900	-1. 71315900	-0. 72447200
C	3. 45471900	-1. 71182600	-1. 91988500
C	2. 92964400	-3. 99912900	-0. 54487300
C	3. 90870900	-2. 92471800	-2. 43084700
H	3. 66939100	-0. 79267000	-2. 45668300
C	3. 64427200	-4. 09427100	-1. 73496600
H	2. 70069000	-4. 89385400	0. 03471600
H	4. 46670400	-2. 94637900	-3. 36386700
H	3. 97792500	-5. 06125200	-2. 10072500
C	-2. 96830800	0. 49130300	-0. 87930600
C	-4. 28797700	0. 60584800	-0. 44093200
C	-5. 29777900	0. 00875900	-1. 19081900
H	-4. 54228500	1. 14986800	0. 46323400
C	-3. 62531800	-0. 73690200	-2. 71223200
C	-4. 96718300	-0. 67809900	-2. 35024400
H	-6. 33295200	0. 08544300	-0. 86648700
H	-3. 32272200	-1. 26724100	-3. 61611000
H	-5. 72487700	-1. 15869900	-2. 96265100
N	-2. 64738100	-0. 17548700	-2. 00089500
N	2. 47773500	-2. 84550900	-0. 05391100
C	4. 71793000	0. 53718400	0. 69216300
H	4. 70335500	1. 41557200	0. 03783500
H	5. 46794000	0. 72650600	1. 47250200
H	5. 06254300	-0. 32470200	0. 10635200
C	2. 89273500	1. 51482500	2. 11284700
H	3. 66277900	1. 80440800	2. 84142600
H	2. 71906000	2. 37366600	1. 45275900
H	1. 96927500	1. 31104700	2. 67123500

C	3.51248900	-0.87737000	2.34693000
H	2.55843300	-1.12420600	2.83115400
H	3.90635400	-1.78637500	1.87828600
H	4.21698400	-0.57322200	3.13325300
C	-2.77841500	3.53514600	0.69343200
H	-3.03258100	4.23773700	1.49978700
H	-2.25154000	4.10527200	-0.07911400
H	-3.72084500	3.17553500	0.26342400
C	-0.62126500	2.97985500	1.84500100
H	-0.03131100	3.54766700	1.11827400
H	-0.87559600	3.66080200	2.66946200
H	0.00907000	2.18204500	2.25924600
C	-2.64367300	1.73364200	2.43421400
H	-3.60326800	1.28104800	2.16561100
H	-2.01464900	0.95879500	2.89019000
H	-2.84511000	2.49168000	3.20380700
H	1.56609100	0.55460800	-2.11687400
H	3.21104200	1.01392600	-1.68701000
H	-0.49585700	1.19262500	-2.18507600
H	-1.55599400	2.57384900	-1.94350900
Pd	-0.08949400	-0.73706600	0.84259900
C	-2.38568400	-2.87300400	0.05382700
C	-1.86402500	-2.30219600	1.36022300
C	-3.19116900	-4.14341800	0.34615300
H	-4.03540700	-3.96150900	1.02039100
H	-3.59622800	-4.55700400	-0.58566300
H	-2.54767500	-4.90859800	0.80214900
C	-2.89624800	-1.69045700	2.26101600
H	-3.55272800	-2.48196100	2.65181900
H	-2.44478900	-1.19092100	3.12440900
H	-3.54224400	-0.98101300	1.73009400
C	-0.65944800	-2.72709100	1.89605600
H	-0.45212700	-2.55490300	2.95251600
H	-0.09579900	-3.53529300	1.43181400
H	0.93056800	-1.84035800	1.33738100
C	-1.32266200	-3.17590400	-0.99254400
H	-0.71493200	-2.29224700	-1.23367000
H	-0.64373500	-3.97675100	-0.66906000
H	-1.80206100	-3.51322000	-1.92028200
H	-3.07987300	-2.12806300	-0.36645700
C3			
C	1.33761200	5.19140400	-1.10884600
C	0.29931500	4.29611300	-1.32334800

C	0.49672800	2.90867500	-1.30839800
C	1.80512500	2.41662000	-1.14192300
C	2.84453400	3.33424000	-0.94249700
C	2.62281400	4.70382200	-0.89823500
H	1.14494800	6.26181800	-1.11941100
H	-0.70287200	4.67774500	-1.51401700
H	3.86159500	2.95789700	-0.84474500
H	3.45503900	5.38484000	-0.73586300
C	2.17076800	0.96832500	-1.32592600
C	-0.69945400	2.03091000	-1.51698200
P	2.08710900	-0.23860400	0.08541000
P	-1.42305500	1.13337100	-0.03853800
C	3.44221100	0.18875600	1.32353800
C	-1.85698200	2.43753100	1.25324700
C	2.68322400	-1.79478100	-0.73463500
C	3.37458300	-1.80920300	-1.94701600
C	2.81100700	-4.08506800	-0.56802000
C	3.77887100	-3.03331300	-2.47275900
H	3.60583300	-0.89496600	-2.48517000
C	3.49402300	-4.19681500	-1.77514900
H	2.56873700	-4.97505200	0.01324500
H	4.31430800	-3.06817000	-3.41843300
H	3.78942800	-5.17209700	-2.15155100
C	-2.95046400	0.54636300	-0.90641700
C	-4.27330200	0.75181100	-0.51441800
C	-5.29249000	0.17610800	-1.26867400
H	-4.52352700	1.34814400	0.35733400
C	-3.62101300	-0.71847200	-2.70901200
C	-4.96716600	-0.57599200	-2.38824600
H	-6.33075000	0.32174100	-0.97964300
H	-3.32302700	-1.29864000	-3.58328900
H	-5.73217600	-1.04220700	-3.00267000
N	-2.63423700	-0.18086000	-1.99146700
N	2.40700500	-2.92044700	-0.06154800
C	4.76699700	0.43186500	0.60437300
H	4.74500100	1.30706700	-0.05316900
H	5.54712600	0.61129000	1.35655700
H	5.07747800	-0.43772600	0.01078600
C	3.00656300	1.42740700	2.10426300
H	3.80368000	1.69978100	2.80974000
H	2.82115800	2.29455300	1.45904900
H	2.09940000	1.22778000	2.68989500
C	3.62297800	-0.96708300	2.30482400
H	2.70002100	-1.19465700	2.85330800

H	3.97305900	-1.88395600	1.81717200
H	4.38107700	-0.67063700	3.04257100
C	-2.65391200	3.61081700	0.69182500
H	-2.92736600	4.28427600	1.51659900
H	-2.07162100	4.19870000	-0.02496600
H	-3.58356900	3.30091000	0.20052800
C	-0.53709200	2.93917100	1.85056100
H	0.08434000	3.48878200	1.13516300
H	-0.76682200	3.62073600	2.68187700
H	0.05165200	2.10597900	2.25709100
C	-2.62269600	1.77129700	2.39649200
H	-3.60197600	1.37711300	2.10579000
H	-2.04142600	0.95188100	2.83861700
H	-2.79236100	2.51902400	3.18371200
H	1.53245800	0.50272600	-2.09058300
H	3.19726400	0.92868300	-1.71167500
H	-0.49172100	1.21551200	-2.22202300
H	-1.51536100	2.62107400	-1.95404400
Pd	-0.04806700	-0.67079400	0.88551500
C	-2.49541800	-2.87807600	0.09745900
C	-2.06823500	-2.26677900	1.41616100
C	-3.34488300	-4.12386400	0.37336800
H	-4.23753400	-3.90302500	0.96884400
H	-3.68063600	-4.56824200	-0.57146200
H	-2.75414400	-4.87916000	0.90993900
C	-3.15112100	-1.59104800	2.19859500
H	-3.86462900	-2.35012200	2.55047400
H	-2.76167200	-1.08148200	3.08543000
H	-3.72863600	-0.88108100	1.59356700
C	-0.87973900	-2.57823300	2.01524300
H	-0.70842900	-2.30921100	3.05803900
H	-0.22143800	-3.33827600	1.59926800
H	1.09588800	-1.62214400	1.42255700
C	-1.35950900	-3.23659000	-0.84815900
H	-0.69443800	-2.38122100	-1.03618400
H	-0.74681100	-4.05979200	-0.45595500
H	-1.76692700	-3.56692200	-1.81219000
H	-3.14195500	-2.14061800	-0.40350800
C3'			
C	-1.39153100	5.33777200	0.35360800
C	-0.32101000	4.47796400	0.55608400
C	-0.50132600	3.13186800	0.90096700
C	-1.81405700	2.64737400	1.05394100

C	-2.88199800	3.54056800	0.89755900
C	-2.68686900	4.86743500	0.54083300
H	-1.21091200	6.37585900	0.08399900
H	0.69334100	4.86446700	0.46561700
H	-3.89442400	3.17683300	1.06768300
H	-3.54013300	5.53147600	0.42339800
C	-2.12845500	1.22913900	1.42827200
C	0.72484200	2.32627100	1.24062000
P	-1.97366100	-0.07223300	0.09564900
P	1.51281800	1.18177900	0.00628700
C	-3.24476900	0.33134600	-1.23340500
C	2.24014900	2.20933200	-1.39239600
C	-2.56876100	-1.51814500	1.08535100
C	-1.78827700	-1.90697700	2.18091400
C	-3.97874800	-3.30032400	1.38318700
C	-2.14796100	-3.04470900	2.88943300
H	-0.90034600	-1.33998000	2.46100000
C	-3.26670400	-3.76367400	2.48109500
H	-4.86200800	-3.83727900	1.03642500
H	-1.55832200	-3.36959300	3.74366400
H	-3.58181200	-4.66477100	2.99977700
C	2.98596000	0.58572300	0.96703800
C	3.40666200	1.16495400	2.16480400
C	4.51252900	0.62615600	2.81704200
H	2.89472400	2.01766300	2.59916400
C	4.68904900	-0.95745700	1.04723300
C	5.16867100	-0.45748300	2.25423800
H	4.85198500	1.05563300	3.75653500
H	5.18023400	-1.80467000	0.56700300
H	6.03023700	-0.91286800	2.73442800
N	3.62447700	-0.45771900	0.42086900
N	-3.64771600	-2.20254100	0.69343200
C	-4.62166000	0.62153600	-0.64497200
H	-4.61648700	1.49552000	0.01545000
H	-5.32107200	0.83841300	-1.46491300
H	-5.01159700	-0.23543500	-0.08548100
C	-2.73171000	1.54620100	-2.01132500
H	-3.42883300	1.74941000	-2.83657900
H	-2.66658700	2.45484100	-1.40295300
H	-1.74488300	1.35291900	-2.45382100
C	-3.33238600	-0.83556700	-2.21806700
H	-2.38161100	-0.98384000	-2.74651200
H	-3.62557200	-1.77200700	-1.73304500
H	-4.08992400	-0.59207300	-2.97623300

C	3.09965900	3.33878900	-0.82961400
H	3.54581300	3.89531900	-1.66501300
H	2.52415500	4.05338700	-0.23127000
H	3.92225500	2.95728900	-0.21051500
C	1.08829300	2.75939100	-2.23300100
H	0.40816500	3.39991900	-1.65939900
H	1.50564000	3.36373200	-3.05030200
H	0.50296800	1.94743200	-2.68626700
C	3.10436500	1.31923500	-2.28285200
H	3.96468600	0.89641100	-1.75184600
H	2.52605100	0.49366800	-2.71839200
H	3.48748100	1.93164400	-3.11064300
H	-1.46200700	0.87927800	2.22864200
H	-3.15114800	1.16205200	1.82204600
H	0.52627300	1.66743300	2.09878900
H	1.50399000	3.02924900	1.56048100
Pd	0.26243900	-0.65666500	-0.64910100
C	1.86674400	-3.56167200	-0.74995800
C	0.80614900	-2.87679600	-1.58927800
C	1.95061600	-5.02745400	-1.18547400
H	2.21424300	-5.13371700	-2.24388800
H	2.71440600	-5.55214700	-0.59923400
H	0.98989800	-5.53514100	-1.02096300
C	1.13465600	-2.68161000	-3.04226600
H	1.02592600	-3.63803300	-3.57268700
H	0.45782600	-1.96140200	-3.51560100
H	2.16778800	-2.34430100	-3.18564400
C	-0.49835900	-2.75692300	-1.16361500
H	-1.28650200	-2.58200000	-1.89326300
H	-0.80861200	-3.15786400	-0.19871900
H	1.77178600	-0.93363600	-1.06546000
C	1.64603100	-3.47262600	0.75133600
H	1.53242100	-2.43078600	1.08302900
H	0.75159100	-4.02786800	1.06645400
H	2.50278800	-3.90674100	1.28127200
H	2.83045000	-3.08632600	-0.99069500

TSC3

C	3.79281800	4.04521700	-0.57487000
C	3.65279700	2.70761300	-0.91589900
C	2.39765500	2.10804100	-1.08278100
C	1.24521500	2.90824400	-0.95813600
C	1.40519700	4.26112100	-0.62869100
C	2.65416600	4.82774700	-0.41578900

H	4.78382500	4.47509500	-0.44745100
H	4.54362800	2.09862900	-1.06278600
H	0.51906200	4.89062100	-0.55927100
H	2.73580300	5.88110900	-0.15756400
C	-0.14358500	2.42782500	-1.29201900
C	2.35889600	0.64991900	-1.42919400
P	-1.15113300	1.49599100	-0.03820100
P	1.93259900	-0.55476400	-0.07159700
C	-1.58474700	2.67214900	1.36846900
C	3.26173200	-0.44230500	1.25455800
C	-2.74947100	1.26046900	-0.95483400
C	-3.06520700	1.93070100	-2.13749000
C	-4.76055400	0.14607300	-0.98270400
C	-4.28514800	1.66527900	-2.75371000
H	-2.38525000	2.64929400	-2.58494600
C	-5.15286600	0.75410000	-2.17151500
H	-5.41708300	-0.57221100	-0.49024800
H	-4.54791200	2.17153600	-3.67953400
H	-6.11135400	0.51332900	-2.62262100
C	2.11439000	-2.10385300	-1.06770600
C	2.97732300	-3.17284700	-0.83510600
C	2.87246500	-4.30366700	-1.64175800
H	3.72181600	-3.14493000	-0.04566100
C	1.12327600	-3.20699900	-2.82844200
C	1.92616100	-4.33041300	-2.65508900
H	3.52966200	-5.15340400	-1.47268000
H	0.37314400	-3.18293900	-3.61946800
H	1.80972500	-5.19511700	-3.30212200
N	1.20314900	-2.12354300	-2.05674100
N	-3.59140000	0.38359000	-0.38981900
C	-2.11582400	3.99632900	0.82894700
H	-1.36927000	4.54748600	0.24690400
H	-2.40729300	4.63530500	1.67396100
H	-3.00535100	3.85311500	0.20168200
C	-0.32614000	2.87981800	2.20935700
H	-0.55023200	3.58389600	3.02302200
H	0.51447800	3.28806700	1.63529600
H	-0.00125900	1.93641900	2.66863600
C	-2.65173600	2.02579000	2.24906800
H	-2.32517900	1.05439100	2.64387000
H	-3.60030000	1.88115500	1.72013900
H	-2.84088700	2.68843300	3.10491000
C	4.67418200	-0.49214000	0.67889500
H	4.87133800	-1.40995400	0.11304700

H	5.39962100	-0.45240100	1.50353100
H	4.88190300	0.35786800	0.01997500
C	3.04905800	0.87421300	2.00907600
H	3.21645500	1.76051200	1.38797600
H	3.76129000	0.91619800	2.84509900
H	2.03823100	0.93488600	2.43427900
C	3.05127300	-1.56871600	2.26894800
H	3.10600000	-2.57463400	1.83886100
H	2.08504600	-1.46372400	2.77862700
H	3.83495000	-1.49699700	3.03570400
H	-0.11755000	1.74693100	-2.15581800
H	-0.73453500	3.29963500	-1.59943000
H	1.60052100	0.43193400	-2.19260700
H	3.32584000	0.33690000	-1.84495000
Pd	-0.36066600	-0.59539200	0.65467100
H	-1.13501300	-1.58326100	3.54797300
C	-1.55236000	-2.46718800	1.61860000
C	-1.92087300	-2.15842000	3.04564100
C	-0.21468000	-2.71546900	1.31054000
H	-1.90578800	-0.68552600	1.05872600
H	0.05246700	-3.27646500	0.41405200
H	0.51610700	-2.72469700	2.11821800
C	-2.67781000	-2.98533500	0.73753700
H	-3.54562700	-2.32749600	0.90140300
H	-2.04980900	-3.09771400	3.60031600
H	-2.86415500	-1.60337000	3.11242700
C	-3.05948300	-4.38929800	1.21269500
H	-3.41800200	-4.39912000	2.24810000
H	-3.85952000	-4.79481800	0.58180600
H	-2.19843400	-5.06851100	1.14222900
C	-2.36058800	-3.00705700	-0.74901300
H	-3.26395100	-3.25256500	-1.32089900
H	-1.98679700	-2.03531400	-1.10121800
H	-1.60717900	-3.76994800	-0.98896700

C4

C	4.24710200	3.14728200	0.20316100
C	3.90935400	1.92514300	-0.36694100
C	2.62901500	1.68211400	-0.87417100
C	1.67901500	2.72211200	-0.84944400
C	2.03712100	3.95240700	-0.28871700
C	3.30065900	4.16638600	0.24916600
H	5.24961800	3.30587600	0.59447800
H	4.65990600	1.13872800	-0.44496200

H	1.30556800	4.76113800	-0.29567300
H	3.55092700	5.13297900	0.68109900
C	0.31584000	2.57092500	-1.45934900
C	2.32732200	0.34683600	-1.49138700
P	-0.88447900	1.61350100	-0.41377300
P	1.65241200	-0.95847500	-0.34973700
C	-1.86840700	2.90075900	0.56265500
C	3.13012500	-1.90378500	0.34985300
C	-2.08787800	0.95791600	-1.64509600
C	-2.35314300	1.55976700	-2.87544100
C	-3.58409100	-0.73252600	-2.07022900
C	-3.27741800	0.95899400	-3.72523100
H	-1.84961000	2.47781700	-3.17106700
C	-3.90474300	-0.21114600	-3.32004900
H	-4.05972700	-1.64770100	-1.71380700
H	-3.50157700	1.40314600	-4.69225900
H	-4.62837400	-0.71450400	-3.95510400
C	0.84115400	-2.12521600	-1.52602200
C	1.23819400	-2.26276400	-2.85666900
C	0.51435400	-3.11945100	-3.68135900
H	2.08858000	-1.71160900	-3.25157500
C	-0.87592700	-3.62012800	-1.80715300
C	-0.56988600	-3.80585200	-3.15299400
H	0.79569500	-3.24134700	-4.72498200
H	-1.71619400	-4.14923600	-1.35477000
H	-1.17067800	-4.47275400	-3.76501800
N	-0.19189900	-2.80442800	-1.00408000
N	-2.69791100	-0.17011900	-1.24780600
C	-2.24909600	4.11044400	-0.28425200
H	-1.37926300	4.71597500	-0.56656000
H	-2.91499100	4.75888500	0.30200900
H	-2.78931200	3.82656200	-1.19737800
C	-0.99329800	3.33361000	1.73734600
H	-1.52191200	4.09664000	2.32651000
H	-0.04092100	3.76911100	1.40681000
H	-0.76666800	2.48906200	2.40338200
C	-3.14148300	2.24176700	1.08896100
H	-2.93840400	1.32027200	1.65284300
H	-3.84547600	2.00194300	0.28257900
H	-3.64325300	2.94136100	1.77124100
C	4.21859800	-2.08724100	-0.70382600
H	5.00139600	-2.73543300	-0.28639500
H	4.69790400	-1.14248200	-0.98640900
H	3.84134200	-2.57446200	-1.61298700

C	3.67987600	-1.11949600	1.53866900
H	3.98486000	-0.10396400	1.25958300
H	4.56497800	-1.63724200	1.93415700
H	2.94744600	-1.03841200	2.35076300
C	2.65333600	-3.27983200	0.80864800
H	2.32288800	-3.90158700	-0.03249700
H	1.83835500	-3.22189800	1.53820500
H	3.49314600	-3.79668600	1.29322500
H	0.36891500	2.02935500	-2.41276900
H	-0.10295700	3.55663000	-1.69109300
H	1.55886800	0.43792500	-2.26851400
H	3.22286800	-0.04957500	-1.98419400
Pd	-0.05953700	-0.16955100	1.01476700
H	0.14113800	0.59933600	4.19424800
C	-1.08969100	-0.81166800	3.10560700
C	-0.76918000	0.00513200	4.35073900
C	0.07237300	-1.55726600	2.56896800
H	-1.38236600	0.02362000	2.32769800
H	-0.11270300	-2.56558300	2.18915100
H	1.00609700	-1.46956200	3.12977900
C	-2.42350400	-1.58923100	3.17773600
H	-3.20252100	-0.83529700	3.38439000
H	-0.59631400	-0.65181600	5.21327200
H	-1.59250800	0.68868600	4.60058100
C	-2.42232700	-2.59622900	4.32382800
H	-2.32614300	-2.11728800	5.30610800
H	-3.36169200	-3.16453800	4.33010400
H	-1.59930700	-3.31899900	4.21659100
C	-2.77295400	-2.26957300	1.86122300
H	-3.81408800	-2.61663000	1.87766400
H	-2.65371700	-1.58966800	1.00418800
H	-2.14390300	-3.15214500	1.68454600

C4-CO

C	-0.02168600	0.02111000	0.02203700
C	-0.00549200	0.00985100	1.41219800
C	1.19189500	0.01536900	2.13326400
C	2.40446600	0.11339300	1.42217700
C	2.37717400	0.12394500	0.02541400
C	1.17944400	0.06197600	-0.67781000
H	-0.97055300	0.00860400	-0.50966100
H	-0.94831000	0.00266700	1.95805100
H	3.31984500	0.20047300	-0.51626100
H	1.18509600	0.07137500	-1.76549500

C	3.72332400	0.23616000	2.13051400
C	1.15665200	-0.05974000	3.63700500
P	4.25972300	-1.37465100	2.87999400
P	1.06215200	-1.78257900	4.34864300
C	5.82012700	-1.87616600	1.94868400
C	-0.77731700	-2.25647700	4.41062300
C	4.85098500	-0.96266600	4.57524700
C	5.17989400	0.32122000	5.00726200
C	5.29995300	-1.85195200	6.64399200
C	5.55605000	0.50068000	6.33523300
H	5.15879600	1.16835300	4.32573600
C	5.61224000	-0.60327200	7.17501600
H	5.35447800	-2.74552700	7.26864100
H	5.80805700	1.49254400	6.70301300
H	5.89652600	-0.50822800	8.21954900
C	1.55884500	-1.54482200	6.10710700
C	1.62398800	-0.29842800	6.72885200
C	2.04921700	-0.23816800	8.05379900
H	1.34736200	0.61122600	6.20209500
C	2.26910500	-2.61316600	8.00813300
C	2.37901700	-1.41492800	8.70956900
H	2.11930400	0.72103600	8.56156800
H	2.52000900	-3.55796500	8.49285100
H	2.71681600	-1.41325800	9.74218800
N	1.87923300	-2.68630400	6.73621500
N	4.91606700	-2.03569600	5.38063300
C	6.94197000	-0.86914800	2.17994600
H	6.66200100	0.15177000	1.88963800
H	7.81144300	-1.15442300	1.57095500
H	7.26385200	-0.85137500	3.22853000
C	5.48126100	-1.96342900	0.46288400
H	6.35175500	-2.36388200	-0.07494200
H	5.24999200	-0.98504200	0.02488900
H	4.63678900	-2.63883000	0.26749000
C	6.25103500	-3.25264400	2.44923000
H	5.48173000	-4.01346000	2.25731400
H	6.47620700	-3.25378700	3.52314600
H	7.16243000	-3.55713600	1.91597700
C	-1.62568100	-1.03260900	4.75107100
H	-2.65773500	-1.36439200	4.92935400
H	-1.65980700	-0.29556700	3.94125500
H	-1.28098500	-0.53167900	5.66568900
C	-1.18825700	-2.82948400	3.05435100
H	-0.98686300	-2.14593800	2.22190700

H	-2.26971200	-3.02488100	3.06776000
H	-0.68295200	-3.77844300	2.84026900
C	-1.01080100	-3.31348100	5.49046200
H	-0.79806700	-2.93594900	6.49727600
H	-0.42497200	-4.22397100	5.32910800
H	-2.07212400	-3.59646200	5.46022700
H	3.65477000	0.98175300	2.93133800
H	4.49184300	0.60000400	1.43938400
H	2.06499700	0.36845000	4.07818400
H	0.31626700	0.52388100	4.03099900
Pd	2.56452100	-3.13387400	3.13517300
H	2.25036100	-6.19080100	1.47275700
C	2.87421600	-5.80137900	3.51976000
C	2.55763300	-6.74693100	2.36917900
C	1.69831100	-4.91417900	3.84476200
H	3.72123700	-5.15315600	3.17198000
H	1.53809000	-4.73290300	4.90981400
H	0.76488900	-5.17248400	3.33696000
C	3.45644300	-6.52781400	4.75541900
H	4.26340200	-7.17075200	4.36575300
H	1.73375800	-7.42374400	2.62817100
H	3.42883400	-7.35760800	2.10157000
C	2.43714300	-7.42485400	5.44596100
H	1.99644000	-8.15976100	4.76133500
H	2.90860800	-7.98185600	6.26544300
H	1.61764200	-6.83596700	5.88068300
C	4.08028900	-5.55098200	5.74151700
H	4.55871400	-6.08659400	6.57141500
H	4.84622700	-4.92913700	5.25757000
H	3.33252600	-4.87097800	6.17582100
C	2.20581200	-3.58835300	1.11651300
O	1.61482800	-3.25730200	0.18959500

TSC4

C	-2.14922800	-3.75845100	2.96334400
C	-1.46209500	-2.57042000	3.18664100
C	-1.68539700	-1.43699800	2.39951200
C	-2.68147800	-1.48972200	1.40495700
C	-3.36417200	-2.68962300	1.18699800
C	-3.09476500	-3.82368900	1.94524700
H	-1.95134400	-4.62575000	3.58924300
H	-0.73845200	-2.50948700	3.99913300
H	-4.14055600	-2.72048000	0.42282500
H	-3.64162600	-4.74529600	1.75842900

C	-3.09239500	-0.26446200	0.63905900
C	-0.87388000	-0.19528700	2.64059500
P	-1.92686200	0.24508600	-0.71227500
P	0.68023700	-0.10370700	1.61382300
C	-2.92208500	0.05219200	-2.30133400
C	2.05279200	-0.94002400	2.62978900
C	-1.71809800	2.06603000	-0.54009900
C	-2.57207000	2.88952100	0.19242100
C	-0.38677000	3.84106100	-1.12410100
C	-2.27889500	4.24796400	0.27090600
H	-3.45686600	2.49575100	0.68625500
C	-1.16101600	4.73556700	-0.39026400
H	0.49022400	4.19075300	-1.67012000
H	-2.92160100	4.91281600	0.84302700
H	-0.89009100	5.78700200	-0.34746900
C	1.11810200	1.68370100	1.65745000
C	0.58684600	2.60088800	2.56252200
C	0.99609200	3.92976100	2.47782200
H	-0.12604700	2.29374900	3.32398700
C	2.40249600	3.30026800	0.65583300
C	1.92378400	4.28978700	1.51088800
H	0.59447200	4.66972400	3.16633800
H	3.13103600	3.54396300	-0.11914600
H	2.27032800	5.31493800	1.41234700
N	2.00711900	2.02936300	0.71297700
N	-0.64805700	2.53582600	-1.19980600
C	-4.14913200	0.96117900	-2.27762000
H	-4.79694300	0.78232500	-1.41043900
H	-4.74851300	0.76474200	-3.17712900
H	-3.87211900	2.02244200	-2.28824300
C	-3.35076300	-1.40898900	-2.41137800
H	-3.81643600	-1.56965000	-3.39333900
H	-4.09069900	-1.68304800	-1.64954300
H	-2.50196100	-2.10118600	-2.33055400
C	-2.04518400	0.42843000	-3.49192900
H	-1.19400300	-0.25163300	-3.61210400
H	-1.66015900	1.45268400	-3.41843100
H	-2.64830100	0.36289100	-4.40799000
C	1.90382500	-0.62599200	4.11573200
H	2.78918800	-1.00871900	4.64227400
H	1.02786800	-1.10901000	4.56437600
H	1.84900700	0.45343000	4.31141200
C	1.97070000	-2.44871000	2.40355000
H	0.98751700	-2.85935200	2.65871600

H	2.71435900	-2.94479600	3.04306700
H	2.19164500	-2.71966500	1.36487400
C	3.41753300	-0.43656800	2.16245100
H	3.57193200	0.62469500	2.38828500
H	3.58901000	-0.58542700	1.08930900
H	4.19134400	-1.00500000	2.69721400
H	-3.19624300	0.58293600	1.32579100
H	-4.08336400	-0.41936800	0.19747800
H	-1.43641800	0.70827100	2.37259400
H	-0.61786100	-0.09750300	3.70163900
Pd	0.21653100	-0.84256000	-0.69020900
H	4.03416200	-3.74626200	-2.16259400
C	3.03930000	-1.82980000	-2.46336800
C	4.28634500	-2.68002900	-2.20374200
C	2.13412500	-2.01605700	-1.25139500
H	2.55163300	-2.25171500	-3.35609800
H	2.57390000	-1.54571000	-0.36971300
H	1.94516200	-3.07244600	-1.03245800
C	3.41739700	-0.37939200	-2.81861600
H	4.09706900	-0.47577100	-3.68249600
H	4.76934100	-2.42026700	-1.25235900
H	5.02457000	-2.54132000	-3.00507100
C	4.17990600	0.35560400	-1.72339800
H	5.06877400	-0.19242400	-1.38732100
H	4.52307300	1.33117100	-2.09303700
H	3.54600500	0.55467900	-0.84866300
C	2.22664500	0.45204100	-3.27717600
H	2.56238000	1.41314800	-3.68824000
H	1.64674200	-0.05835200	-4.05835400
H	1.54520800	0.68216700	-2.44289700
C	0.25558600	-1.90191600	-2.26526000
O	0.11560900	-2.57888900	-3.18960400

C5

C	5.57983700	-1.94806000	-0.98986200
C	4.88042300	-0.78555300	-1.28106800
C	3.48067900	-0.74536800	-1.30715400
C	2.75944500	-1.93186700	-1.05630100
C	3.48634200	-3.10070500	-0.78698800
C	4.87275900	-3.11754700	-0.73273500
H	6.66729200	-1.94173300	-0.97579500
H	5.42936800	0.13052900	-1.49800800
H	2.94098300	-4.03047900	-0.62865800
H	5.39621000	-4.04573100	-0.51468800

C	1.26460300	-2.07514900	-1.21115000
C	2.83373500	0.58385800	-1.58282200
P	0.01335300	-1.71649000	0.13793400
P	2.11110300	1.31669500	-0.04798500
C	0.42836800	-2.70059100	1.68520000
C	3.46446300	1.98874100	1.07206000
C	-1.49067700	-2.50527200	-0.59369400
C	-1.58022300	-2.91260600	-1.92623600
C	-3.68811200	-3.05896600	-0.21218100
C	-2.79583200	-3.40512200	-2.39282400
H	-0.73462200	-2.84803900	-2.60347200
C	-3.87316900	-3.48895500	-1.52249700
H	-4.50893600	-3.10832300	0.50408300
H	-2.89090100	-3.72251200	-3.42852600
H	-4.83741500	-3.87060800	-1.84611300
C	1.18903300	2.79766300	-0.64223600
C	1.58322900	3.80994200	-1.50476300
C	0.67845000	4.83012000	-1.79054900
H	2.57729400	3.79973900	-1.94502600
C	-0.92195600	3.73523300	-0.38768800
C	-0.58466800	4.80074200	-1.21410700
H	0.96098300	5.64220200	-2.45568800
H	-1.91079400	3.65697000	0.06094700
H	-1.31219100	5.58300700	-1.40857400
N	-0.05858800	2.75416400	-0.11074800
N	-2.53671800	-2.56415200	0.24312000
C	0.51513300	-4.18792100	1.36315700
H	1.29616100	-4.41000000	0.62694800
H	0.76066200	-4.74133200	2.28030200
H	-0.43667900	-4.58075000	0.98415800
C	1.75657000	-2.17457800	2.22651700
H	2.00807500	-2.73061400	3.14019600
H	2.58917600	-2.29473300	1.52462400
H	1.67585200	-1.11262900	2.49474900
C	-0.64062100	-2.45212700	2.75003100
H	-0.74956800	-1.38264100	2.97347400
H	-1.61966500	-2.84124500	2.45706200
H	-0.32574700	-2.95657400	3.67436700
C	4.52264000	2.76513000	0.30147700
H	5.26235900	3.16266200	1.01115100
H	5.06047800	2.13274000	-0.41495300
H	4.09701500	3.61997300	-0.23823300
C	4.09825400	0.81327000	1.81446700
H	4.58476400	0.09905700	1.13882600

H	4.86519900	1.19844500	2.50098400
H	3.35844700	0.27014900	2.41575300
C	2.77134000	2.89903700	2.08485400
H	2.35656000	3.80173400	1.61887200
H	1.96029300	2.38045600	2.61577000
H	3.50646000	3.22171600	2.83477600
H	0.90739900	-1.45045200	-2.04241300
H	1.06761700	-3.11648700	-1.49849100
H	1.97820600	0.50019200	-2.26936900
H	3.55120600	1.27665700	-2.04105300
Pd	-0.19422100	0.57622100	0.44473000
C	-2.19723700	0.43252000	0.71042900
O	-2.60069300	0.36769400	1.84790400
C	-3.04313300	0.58533000	-0.52438900
H	-2.78864900	1.57170600	-0.94666600
H	-2.63959200	-0.13046300	-1.25659300
C	-4.56293500	0.39712000	-0.40440900
H	-4.73074900	-0.55145300	0.13139000
C	-5.35377700	1.50593100	0.34134500
H	-6.32598700	1.56654100	-0.17516600
C	-5.10639900	0.23792600	-1.82147600
H	-6.17787900	0.00397900	-1.81000800
H	-4.97500000	1.16710100	-2.39512800
H	-4.59350100	-0.56474100	-2.36808500
C	-4.71814600	2.88606000	0.24696400
H	-3.80598800	2.94152200	0.85963000
H	-4.45891300	3.16063800	-0.78454700
H	-5.40594200	3.65143700	0.62770800
C	-5.66438900	1.16661300	1.79435600
H	-4.75687300	1.14064800	2.40906800
H	-6.34218800	1.91376000	2.22813300
H	-6.15445600	0.18800400	1.88127200

C5-MeOH

C	2.32224300	3.17106400	2.73037700
C	0.97660900	3.11320700	2.38634600
C	0.28951100	1.89737100	2.31024100
C	0.97910600	0.70919000	2.62397000
C	2.33263900	0.78006900	2.96860500
C	3.00765500	1.99463600	3.01718500
H	2.82920200	4.13210900	2.78370000
H	0.43090800	4.03344800	2.17630500
H	2.85707600	-0.14232200	3.22042800
H	4.05980000	2.02165700	3.29360200

C	0.29681400	-0.62891100	2.64590100
C	-1.15421200	1.90265900	1.89140100
P	0.18801700	-1.47865000	0.99306600
P	-1.35634100	1.53830500	0.07608800
C	1.15201400	-3.08812600	1.20303900
C	-1.27690700	3.19137400	-0.84715300
C	-1.55375000	-2.07485300	0.83757300
C	-2.51606900	-2.01614600	1.84431300
C	-3.03193600	-3.05887800	-0.61887800
C	-3.79309600	-2.50147800	1.57133600
H	-2.29296400	-1.61637500	2.82989200
C	-4.06115300	-3.03407000	0.31821700
H	-3.20270400	-3.46895600	-1.61598200
H	-4.56507000	-2.46468800	2.33665800
H	-5.04593400	-3.41629400	0.06338300
C	-3.12280600	1.04094200	-0.07859700
C	-4.11828100	1.43255500	0.81578500
C	-5.42852900	1.02720400	0.57911500
H	-3.88130800	2.04961600	1.67930400
C	-4.64516400	-0.10769800	-1.36736800
C	-5.70179800	0.24620800	-0.53499900
H	-6.22460000	1.32465700	1.25752300
H	-4.81787500	-0.72950700	-2.24633600
H	-6.71027600	-0.08968200	-0.75889500
N	-3.38369500	0.27128200	-1.15075400
N	-1.80884100	-2.59184500	-0.37375500
C	0.42366200	-4.00399800	2.18608400
H	0.21585200	-3.51559500	3.14735300
H	1.06314600	-4.87354100	2.39337900
H	-0.52374500	-4.37759700	1.77909600
C	2.54028800	-2.75885100	1.74549100
H	3.17414200	-3.65270100	1.67159600
H	2.51484400	-2.46582000	2.80171500
H	3.03293400	-1.95461000	1.18527900
C	1.26504900	-3.78103800	-0.15217800
H	1.79782600	-3.16940200	-0.89072200
H	0.28092400	-4.02873600	-0.56556300
H	1.82472600	-4.71810000	-0.02621100
C	-1.95119000	4.31990700	-0.07798400
H	-1.96572300	5.22132700	-0.70722000
H	-1.41749600	4.57934900	0.84446200
H	-2.99276900	4.08314200	0.17708300
C	0.19735800	3.51343100	-1.08890000
H	0.76135700	3.62435200	-0.15475600

H	0.27334700	4.46171200	-1.63994100
H	0.67941800	2.73279400	-1.69432300
C	-1.96840100	3.01418100	-2.19858600
H	-3.05268000	2.88231400	-2.09564900
H	-1.56893100	2.16211600	-2.76405000
H	-1.79919300	3.92025900	-2.79683900
H	-0.72117600	-0.53340000	3.03699300
H	0.82456700	-1.30046100	3.33209400
H	-1.72953100	1.12379800	2.40928800
H	-1.62244800	2.86100400	2.14410200
Pd	0.39314700	0.01711400	-0.78523700
H	5.59249800	-1.66745400	-3.23065800
C	4.58850500	-0.22924400	-1.94917400
C	5.76155000	-1.14100500	-2.28366600
C	3.35282800	-1.10637200	-1.66803200
H	4.36178200	0.37631600	-2.84035300
H	3.42138200	-1.61007100	-0.69951800
H	3.28834200	-1.90076100	-2.43055900
C	4.93103100	0.75600000	-0.81393200
H	5.80369900	1.31861000	-1.18639100
H	5.92056500	-1.90456500	-1.51094000
H	6.69125400	-0.56561900	-2.37862400
C	5.34676900	0.08077000	0.48755100
H	6.14996900	-0.65269600	0.34894100
H	5.71055400	0.82956600	1.20265300
H	4.49952100	-0.43144400	0.96641600
C	3.82448600	1.76671100	-0.53981300
H	4.16184300	2.51978500	0.18438800
H	3.51021500	2.29349700	-1.45015800
H	2.93638700	1.28441900	-0.09615600
C	2.05822700	-0.37619000	-1.79500200
O	1.79232200	0.42595500	-2.66588800
C	-1.06549500	-1.57983400	-3.51364200
H	-0.26209700	-1.55380800	-4.25888200
H	-1.98426400	-1.91312000	-4.01901800
H	-0.80156600	-2.31918800	-2.74261600
O	-1.20087200	-0.27842300	-2.97706300
H	-1.97483800	-0.24243100	-2.37426700

TSC5

C	-0.58926300	4.97264800	1.72854300
C	-1.54033200	4.09333400	1.22139400
C	-1.49101300	2.72328100	1.49215200
C	-0.48377100	2.23467900	2.35131100

C	0.47087900	3.12823200	2.84549900
C	0.43663600	4.48246500	2.52933000
H	-0.65194500	6.03414100	1.49905900
H	-2.34583000	4.47117500	0.59102300
H	1.24092100	2.75036600	3.51808000
H	1.19101900	5.15477400	2.93227700
C	-0.47961200	0.81820500	2.85281500
C	-2.45698200	1.80742100	0.78798000
P	0.27707300	-0.50868400	1.76504400
P	-1.61154700	1.18046300	-0.75232000
C	1.68041400	-1.19155800	2.82946400
C	-2.07587100	2.33112100	-2.19015100
C	-1.00235400	-1.85261800	1.84618600
C	-1.99887900	-1.93173000	2.82303200
C	-1.78055000	-3.76317600	0.82955600
C	-2.92690800	-2.96562100	2.75778900
H	-2.05535900	-1.21643800	3.63902600
C	-2.82679100	-3.89935200	1.73585100
H	-1.65176600	-4.49369600	0.02846900
H	-3.71349900	-3.04018100	3.50524600
H	-3.53294000	-4.71991100	1.64346100
C	-2.51605700	-0.37616400	-1.19201000
C	-3.86217400	-0.56608500	-0.88899700
C	-4.50873200	-1.72185000	-1.31748800
H	-4.40593000	0.19149800	-0.32971900
C	-2.45858100	-2.40030000	-2.31924400
C	-3.80083400	-2.64894600	-2.06748900
H	-5.55778400	-1.88273400	-1.08128000
H	-1.86013300	-3.11046300	-2.89022600
H	-4.26620500	-3.55483700	-2.44389500
N	-1.81540600	-1.31246300	-1.87726100
N	-0.89275200	-2.76888900	0.87319400
C	1.19918700	-1.74383900	4.16642700
H	0.65313300	-1.00125000	4.76242700
H	2.07025500	-2.05769000	4.75957600
H	0.55432800	-2.62197200	4.03856600
C	2.66514700	-0.04549000	3.05868600
H	3.60238100	-0.44492600	3.47207500
H	2.28010700	0.68766800	3.77847300
H	2.91097100	0.48779500	2.12912700
C	2.35008400	-2.30761400	2.03285000
H	2.68289900	-1.96055000	1.04512700
H	1.67468700	-3.15998600	1.88239700
H	3.23168300	-2.67022400	2.58019400

C	-3.48129500	2.90030600	-2.06290900
H	-3.71840200	3.48121300	-2.96585600
H	-3.58165500	3.57721200	-1.20570300
H	-4.23865600	2.10974400	-1.97323700
C	-1.03927700	3.45404800	-2.22153100
H	-1.03318000	4.04671100	-1.29875500
H	-1.26612900	4.13359900	-3.05533100
H	-0.02646800	3.05537800	-2.37346000
C	-1.96354100	1.53258600	-3.48785100
H	-2.76582400	0.79153000	-3.59326300
H	-0.99915600	1.01566900	-3.57669400
H	-2.04554900	2.22857700	-4.33441400
H	-1.51352000	0.51940900	3.05059400
H	0.03250000	0.78614400	3.82141300
H	-2.69660700	0.91638300	1.38465400
H	-3.40060900	2.31810400	0.56434400
Pd	0.60518800	0.30492700	-0.42560900
H	5.19532600	-1.47645800	-3.72366800
C	4.23933700	-0.23888400	-2.20843100
C	5.44504800	-0.98731000	-2.77425700
C	3.15661100	-1.28941800	-1.90142900
H	3.84859100	0.41134400	-3.00646300
H	3.38495100	-1.84526900	-0.98290800
H	3.19192200	-2.03065200	-2.71638300
C	4.67263600	0.68881600	-1.05494100
H	5.53483100	1.24416600	-1.46189400
H	5.79726200	-1.77007800	-2.08911800
H	6.28432800	-0.30578200	-2.95990000
C	5.16613900	-0.06107500	0.17614200
H	5.97787200	-0.75981100	-0.06095400
H	5.55119000	0.64197300	0.92643600
H	4.35989200	-0.63258900	0.65553500
C	3.63576200	1.73776900	-0.66999000
H	4.06844900	2.46663600	0.02873800
H	3.26775200	2.28959900	-1.54544200
H	2.76023100	1.29156300	-0.16731500
C	1.74341700	-0.77079700	-1.90235000
O	1.36150500	0.25982600	-2.49308200
C	0.99266900	-3.22143200	-1.62636900
H	1.82590200	-3.67251900	-2.16709700
H	0.09219700	-3.81534800	-1.78925900
H	1.19567200	-3.13562400	-0.55640600
O	0.74327800	-1.91301900	-2.19613800
H	-0.26368400	-1.56162200	-2.03572200

A1-P

C	-4.36563800	3.74646300	-0.19240100
C	-4.14517300	2.41702200	0.13328900
C	-2.91878300	1.94782100	0.63068900
C	-1.87060300	2.87970700	0.81264500
C	-2.13207600	4.22809200	0.51964300
C	-3.34523300	4.66813000	0.01375000
H	-5.33429900	4.06241700	-0.57324000
H	-4.96296900	1.70571900	0.02341900
H	-1.34578400	4.95794400	0.70770600
H	-3.49624000	5.72403600	-0.19979200
C	-0.50378400	2.57267700	1.37212000
C	-2.88684200	0.49695800	1.04559700
P	0.80874400	1.92272700	0.18932300
P	-2.19186800	-0.75346200	-0.16419800
C	1.30153900	3.34903000	-0.95624500
C	-3.42258800	-0.99167400	-1.58007200
C	2.26569100	1.80297700	1.32979100
C	2.31610300	2.32170500	2.62572700
C	4.35553600	0.85986700	1.57571200
C	3.43600500	2.06651900	3.41180300
H	1.49750400	2.91293900	3.02734700
C	4.47940000	1.31850700	2.88328500
H	5.15327700	0.26932900	1.11803700
H	3.48907800	2.45210200	4.42754800
H	5.36849000	1.09178500	3.46524600
C	-2.52550200	-2.29138400	0.83704900
C	-3.56749900	-2.51913500	1.72719700
C	-3.65613100	-3.73248800	2.40422700
H	-4.31806800	-1.75277600	1.89323200
C	-1.66951500	-4.46222500	1.32206500
C	-2.69926200	-4.72156800	2.20190000
H	-4.47755100	-3.90303400	3.09501900
H	-0.86146400	-5.15523900	1.10791200
H	-2.74121800	-5.67214700	2.72201700
N	-1.62066200	-3.28479700	0.68079600
N	3.28019300	1.08039200	0.81915900
C	1.57544400	4.64219200	-0.19901900
H	0.68010500	5.03944900	0.29243800
H	1.93113300	5.41077000	-0.90062400
H	2.35209700	4.51050600	0.56650000
C	0.18250300	3.54027200	-1.98017800
H	0.47043100	4.33196400	-2.68682600

H	-0.76842200	3.83327400	-1.52134500
H	0.01199100	2.62161500	-2.55949900
C	2.56056300	2.92929900	-1.71390500
H	2.41550300	1.97828000	-2.24507200
H	3.43256900	2.82517200	-1.05825200
H	2.79285000	3.69795400	-2.46495200
C	-4.87511200	-1.12231300	-1.14285700
H	-5.51247900	-1.21731100	-2.03362000
H	-5.22644900	-0.24881100	-0.58111700
H	-5.04426700	-2.01613800	-0.52871500
C	-3.24639700	0.20602000	-2.51470700
H	-3.54118000	1.15105900	-2.04212300
H	-3.87443600	0.06448100	-3.40542700
H	-2.20318900	0.30187300	-2.84763400
C	-2.99373800	-2.25860700	-2.32063700
H	-3.15782500	-3.16615900	-1.72508300
H	-1.93428900	-2.22391500	-2.61430800
H	-3.59107800	-2.35710800	-3.23775700
H	-0.55690700	1.78172400	2.13523400
H	-0.12865800	3.47594800	1.87162700
H	-2.25335900	0.35329700	1.93250500
H	-3.90674100	0.20965400	1.33084500
Pd	-0.03777700	-0.08839000	-0.61152000
H	5.17527200	-4.04581600	-0.48447400
C	3.62327200	-2.80340400	-1.36402300
C	5.08478800	-3.19176400	-1.16701500
C	3.05364400	-2.29951800	-0.03056000
H	3.06740300	-3.71256900	-1.63846100
H	3.07442600	-1.19920600	0.04089000
H	3.68426800	-2.64383000	0.80273000
C	3.46377100	-1.81963300	-2.54082800
H	3.85423200	-2.35882400	-3.42090400
H	5.66674000	-2.36725300	-0.73340100
H	5.55652400	-3.47157500	-2.11773600
C	4.29276400	-0.54865700	-2.38535500
H	5.36731900	-0.75734100	-2.31955900
H	4.14564900	0.10811300	-3.25264700
H	4.00419100	0.02500100	-1.49137800
C	2.01111800	-1.47046200	-2.83957900
H	1.94093100	-0.85527600	-3.74647200
H	1.39265200	-2.36434200	-2.98815200
H	1.56016100	-0.87898400	-2.01762600
C	1.65584600	-2.73450000	0.27495900
O	0.92877000	-3.33758600	-0.50691800

C	1.85293800	-1.71990000	2.46968200
H	2.85892100	-2.10919800	2.65372300
H	1.89435300	-0.66951400	2.16076100
H	1.26464000	-1.80417500	3.38487600
O	1.15517200	-2.49835700	1.49128300
H	-0.79178800	-3.13667700	0.07253000

C5-MeOH-PTSA

C	3.99136700	-0.44452500	4.24742400
C	3.21607200	-1.45482100	3.69076100
C	3.11459500	-1.62176600	2.30596300
C	3.86794100	-0.78159800	1.46439700
C	4.64408700	0.23170500	2.03574000
C	4.69756900	0.41604400	3.41273900
H	4.04860900	-0.33560500	5.32817600
H	2.67090900	-2.13888000	4.34124800
H	5.23633400	0.87236000	1.38281800
H	5.31157300	1.21041900	3.83137100
C	3.92347200	-0.99718500	-0.02094300
C	2.18600200	-2.66520300	1.75622800
P	2.62789300	-0.10981800	-1.02103900
P	0.53535700	-1.93232100	1.28573800
C	3.66422200	1.00776700	-2.15669100
C	-0.54912200	-2.05518400	2.83842000
C	1.90792100	-1.33906600	-2.19574600
C	2.40401900	-2.62271900	-2.41375200
C	0.21347800	-1.65402700	-3.71131000
C	1.74192400	-3.44394000	-3.32326100
H	3.29279200	-2.98746700	-1.90557000
C	0.62613400	-2.95521100	-3.98687500
H	-0.65921900	-1.23598700	-4.21383500
H	2.10201000	-4.45333900	-3.50868100
H	0.07819700	-3.56510800	-4.70000000
C	-0.18386200	-3.20408700	0.16435800
C	0.14728200	-4.55895300	0.20470300
C	-0.49166400	-5.42753600	-0.67548900
H	0.88484700	-4.93406900	0.91071300
C	-1.68889000	-3.55044400	-1.53560900
C	-1.43120300	-4.91845300	-1.56180400
H	-0.25694300	-6.48942200	-0.66447600
H	-2.40926100	-3.10785800	-2.22683600
H	-1.95142700	-5.56101100	-2.26684200
N	-1.08403800	-2.70616400	-0.69863700
N	0.82780200	-0.86009600	-2.83464600

C	4.52012600	0.12413300	-3.06507900
H	5.10040900	-0.63169100	-2.52108100
H	5.23842000	0.76644600	-3.59322100
H	3.91610000	-0.38758300	-3.82387100
C	4.55969600	1.89740100	-1.29651100
H	5.03212400	2.64714400	-1.94612400
H	5.36709400	1.34192400	-0.80514900
H	3.99258300	2.43915200	-0.52835300
C	2.77991500	1.89366900	-3.02883600
H	2.30157600	2.69373900	-2.45386500
H	2.00258000	1.32889700	-3.55660400
H	3.41863500	2.37183400	-3.78422400
C	-0.28806400	-3.31968000	3.64697900
H	-1.02482300	-3.38009800	4.46077500
H	0.70479800	-3.32379200	4.11082700
H	-0.39465000	-4.22928300	3.04090500
C	-0.25751600	-0.81794400	3.68598800
H	0.76617200	-0.82470300	4.07826300
H	-0.94349600	-0.78587300	4.54479300
H	-0.38447800	0.10960000	3.11248200
C	-2.01189000	-2.05572500	2.39855600
H	-2.28795000	-2.98993500	1.89281400
H	-2.25613000	-1.23046500	1.72098800
H	-2.65267000	-1.95126300	3.28557300
H	3.84858700	-2.06427800	-0.25334200
H	4.90159900	-0.67669000	-0.39476500
H	2.57815000	-3.11359600	0.83372400
H	2.04876500	-3.48205400	2.47343200
Pd	0.71100100	0.38381600	0.25004900
H	-1.91821800	0.20668000	0.53945800
O	-1.54080000	1.08260900	0.71477000
H	3.45310000	4.92399400	-0.20289600
C	1.29543700	4.72731000	-0.04084200
C	2.61507700	5.39375600	0.32813500
C	1.30787800	3.27066400	0.45855500
H	1.22971200	4.69482100	-1.14011700
H	0.79706700	3.15227300	1.42971300
H	2.33144700	2.92028000	0.65571700
C	0.08703800	5.54975500	0.44587600
H	0.19642800	6.53721200	-0.03409500
H	2.82358800	5.31623600	1.40347400
H	2.60740500	6.45960800	0.06552000
C	0.07755800	5.77846100	1.95244700
H	0.97500700	6.30257200	2.30193100

H	-0.78857700	6.38766300	2.24024300
H	0.00260400	4.83383300	2.50973900
C	-1.24278600	4.96466500	-0.00974600
H	-2.07088200	5.63927700	0.24146600
H	-1.26514300	4.79043100	-1.09240600
H	-1.44970100	4.00610000	0.48848500
C	0.69424300	2.25687900	-0.46655200
O	0.06815800	2.47916200	-1.47061500
C	-2.19567400	1.66604200	1.84984500
H	-3.12227200	2.16217800	1.53074900
H	-2.43338200	0.90909200	2.60582500
H	-1.51401700	2.40345600	2.28477000
C	-5.24175200	-1.04316000	0.96119900
C	-4.38957200	-0.71765300	-0.08977700
C	-4.54806100	0.51222500	-0.71846000
C	-5.54400300	1.41120200	-0.33040800
C	-6.37767900	1.06779100	0.71955700
C	-6.23832900	-0.16074200	1.38149700
H	-5.13329300	-2.00426700	1.46170100
H	-3.60830300	-1.40708900	-0.40878700
H	-5.65603200	2.36885700	-0.83564800
H	-7.15497100	1.75999000	1.03960400
C	-7.14975600	-0.50795000	2.51403500
H	-6.91243300	-1.48926800	2.93606000
H	-7.08057300	0.23714600	3.31601400
H	-8.19634100	-0.52078500	2.18581500
S	-3.46003000	0.99081100	-2.01803600
O	-2.80354800	2.33291200	-1.45173500
O	-4.22406000	1.42018400	-3.17821300
O	-2.41508700	-0.01667500	-2.16758700
H	-2.13139300	2.09872000	-0.76282400

TSC6

C	3.29704000	-1.13669400	4.78096600
C	2.58487700	-1.98595000	3.94248400
C	2.72943500	-1.93816800	2.55215200
C	3.66939800	-1.04671900	1.99564300
C	4.37604500	-0.19582600	2.85235300
C	4.18704800	-0.22159700	4.22922800
H	3.16101100	-1.19580600	5.85850700
H	1.89501500	-2.71351400	4.37006500
H	5.11278400	0.48352400	2.42441400
H	4.75570100	0.45022100	4.86850600
C	4.00729800	-1.03965300	0.53150900

C	1.86129900	-2.82849100	1.70472900
P	2.94086900	0.05191700	-0.55425900
P	0.36282500	-1.90625700	1.08415000
C	4.18316400	1.26291700	-1.31865500
C	-1.04631400	-2.19641600	2.32642400
C	2.49099400	-1.04667100	-1.98167400
C	3.18080500	-2.20281600	-2.34901200
C	0.91297500	-1.40065100	-3.61793600
C	2.67349200	-2.98963600	-3.37927000
H	4.10249100	-2.49412300	-1.85073800
C	1.51124000	-2.58997300	-4.02369800
H	0.00702900	-1.04187600	-4.11018400
H	3.18741600	-3.90195800	-3.67363400
H	1.07353700	-3.17927500	-4.82517400
C	-0.17521700	-2.98698900	-0.32094400
C	0.20591800	-4.30260700	-0.54595300
C	-0.31063700	-4.99985600	-1.63578900
H	0.89001100	-4.79440100	0.13897800
C	-1.55492700	-3.07177400	-2.26421200
C	-1.20897800	-4.38614400	-2.50242700
H	-0.01501400	-6.03248700	-1.80084500
H	-2.23123300	-2.49377900	-2.88945200
H	-1.62900100	-4.90908400	-3.35445000
N	-1.03362100	-2.42641900	-1.20896200
N	1.37721600	-0.64698600	-2.62042300
C	5.28377900	0.54209700	-2.08943200
H	5.84542800	-0.17143100	-1.47310400
H	6.00437400	1.28528900	-2.46062600
H	4.88751300	0.00732000	-2.96142500
C	4.79023800	2.08790600	-0.18634200
H	5.37791400	2.91155400	-0.61569200
H	5.46912200	1.49646400	0.43972000
H	4.02333100	2.53159200	0.46462000
C	3.42650500	2.18274400	-2.27277200
H	2.66099200	2.77349100	-1.75697700
H	2.93579800	1.62694700	-3.08225700
H	4.13814000	2.88318800	-2.73244100
C	-1.09981900	-3.62275800	2.85310000
H	-1.98820800	-3.73209800	3.49123000
H	-0.22714500	-3.87492800	3.46750500
H	-1.18336600	-4.36357700	2.04675400
C	-0.82145100	-1.21323600	3.47387300
H	0.12075900	-1.39419800	4.00236000
H	-1.63778800	-1.31923100	4.20204100

H	-0.81743200	-0.17282700	3.12377900
C	-2.36386900	-1.85037200	1.63140000
H	-2.68296900	-2.62915400	0.92636600
H	-2.31080800	-0.89422800	1.09204700
H	-3.15271200	-1.76025200	2.39176200
H	3.95202100	-2.05689800	0.13015300
H	5.04882000	-0.72132800	0.40896300
H	2.38969200	-3.16829600	0.80443100
H	1.56169100	-3.72496400	2.26051800
Pd	0.77924000	0.41478500	0.33796200
H	-1.64398300	1.04697200	-0.44956200
O	-1.09280200	1.81800700	0.29737400
H	2.93085000	5.32606100	-0.00518200
C	0.81561000	4.88698500	-0.23965500
C	1.96013200	5.73345600	0.30783200
C	0.91753700	3.48879700	0.40421400
H	0.98606100	4.74974100	-1.31951500
H	0.55331400	3.48108400	1.43813100
H	1.98381400	3.23217200	0.47042400
C	-0.53764600	5.60874200	-0.09276400
H	-0.38705100	6.58806700	-0.57926000
H	1.95804500	5.76060900	1.40587700
H	1.89925800	6.76860600	-0.05168600
C	-0.92122500	5.88690600	1.35570300
H	-0.16506400	6.48498700	1.87856800
H	-1.86578500	6.44358200	1.40276500
H	-1.06460000	4.95991300	1.92782000
C	-1.68122800	4.92386700	-0.83331900
H	-2.57832400	5.55640000	-0.81869300
H	-1.43147100	4.72966300	-1.88433500
H	-1.95779600	3.96544200	-0.37661900
C	0.30340400	2.37592400	-0.40951800
O	0.16416600	2.36766400	-1.62065900
C	-1.63250000	2.08845500	1.59165900
H	-2.21628600	3.01681600	1.57256700
H	-2.28987200	1.25483600	1.86774300
H	-0.83244300	2.17221600	2.33467700
C	-5.98174500	-1.31621900	0.47506300
C	-5.12089500	-1.01337900	-0.57300700
C	-4.59065400	0.27015700	-0.65738500
C	-4.89144500	1.24459100	0.29262900
C	-5.74827800	0.92115200	1.33496300
C	-6.30664200	-0.35867100	1.44032900
H	-6.40960800	-2.31466200	0.54910100

H	-4.86655200	-1.76486400	-1.31805500
H	-4.46438200	2.24273700	0.21016200
H	-5.99616900	1.67386600	2.08188100
C	-7.24919200	-0.67882800	2.55642500
H	-7.41939800	-1.75654000	2.64492400
H	-6.87176000	-0.30702900	3.51606500
H	-8.22366800	-0.20080500	2.39218500
S	-3.38206800	0.62360600	-1.89274000
O	-2.04896000	0.22586800	-1.19937000
O	-3.37601900	2.06531600	-2.14575100
O	-3.58247400	-0.27947500	-3.02629000
H	-1.30924300	-1.43527400	-1.09667000

A1-MF

C	1.23569500	-4.00431900	-2.66728900
C	1.43802000	-2.62985000	-2.68846300
C	0.45634900	-1.72546000	-2.26808400
C	-0.80153800	-2.23585400	-1.87437400
C	-0.99074900	-3.62215000	-1.86095100
C	0.01321700	-4.50666700	-2.23484800
H	2.02509700	-4.67610500	-2.99741700
H	2.38591400	-2.23436300	-3.05323700
H	-1.96567500	-4.01144900	-1.56898100
H	-0.16960800	-5.57882800	-2.21349100
C	-1.97795600	-1.36010800	-1.53439200
C	0.78769700	-0.25847500	-2.27238000
P	-2.00054700	-0.74918000	0.23696600
P	1.50150400	0.36440300	-0.64940300
C	-3.57689800	-1.47337800	0.99375200
C	3.39146300	0.28117600	-0.80134400
C	-2.49196700	1.02767300	-0.03542500
C	-3.29283100	1.53655100	-1.04744000
C	-2.17217800	3.24195200	0.79993400
C	-3.52126700	2.90782200	-1.13364100
H	-3.73901700	0.86265700	-1.77317800
C	-2.96434200	3.77237500	-0.19745100
H	-1.69806800	3.83159300	1.57716700
H	-4.14441100	3.29954400	-1.93308700
H	-3.13118200	4.84320400	-0.23905100
C	1.14963900	2.17843400	-0.77920500
C	0.81875800	2.82911400	-1.97066200
C	0.51978900	4.18782500	-1.93756100
H	0.79546900	2.29082100	-2.91508200
C	0.94420900	4.13994600	0.40652000

C	0.58756800	4.86365500	-0.72726200
H	0.24845900	4.71153100	-2.85160700
H	1.01345100	4.63850900	1.37420900
H	0.36741200	5.92523600	-0.65547100
N	1.20007500	2.83028400	0.39770100
N	-1.96092400	1.91640400	0.83917900
C	-4.85142000	-1.16934200	0.21879600
H	-4.80074900	-1.50244100	-0.82566000
H	-5.69133300	-1.70177100	0.68774600
H	-5.09762000	-0.10030400	0.23033800
C	-3.34372800	-2.98112400	1.05486700
H	-4.14138600	-3.44765700	1.64925500
H	-3.36623900	-3.43971600	0.05856400
H	-2.38330100	-3.23029700	1.52847600
C	-3.68111400	-0.91374600	2.40921800
H	-2.77918200	-1.12759200	2.99924500
H	-3.84739200	0.17222200	2.41453800
H	-4.53524700	-1.37793200	2.92208300
C	3.90735400	0.70528800	-2.16882100
H	5.00722700	0.71094600	-2.15874100
H	3.59587800	0.01722400	-2.96450600
H	3.57820200	1.71786500	-2.43892600
C	3.80841100	-1.15596100	-0.49510300
H	3.44780000	-1.86855400	-1.24534300
H	4.90586100	-1.22271100	-0.47524500
H	3.43108700	-1.48393300	0.48335700
C	3.98039300	1.19290300	0.27401100
H	3.79866900	2.25384100	0.06542700
H	3.58003600	0.96807900	1.27269100
H	5.06873400	1.03998100	0.31049100
H	-1.99763100	-0.47715400	-2.18364600
H	-2.90864600	-1.90773900	-1.72957200
H	-0.11854400	0.34584300	-2.41012400
H	1.45978800	-0.02223200	-3.10772500
Pd	0.18059600	-0.58609000	1.05441300
C	1.64025200	-0.68343700	3.18380700
H	0.56412000	-0.99376500	3.06185900
O	2.00496500	0.42342200	3.52267000
O	2.43410400	-1.74389500	3.04812000
H	-1.31173100	1.54122600	1.54355600
C	3.82537300	-1.52103800	3.32739800
H	3.95124300	-1.14500600	4.34714000
H	4.31292600	-2.49002200	3.21556500
H	4.25201800	-0.80481400	2.61580900

TSD1'

C	1. 14576200	-4. 66500300	-1. 69956000
C	1. 57812200	-3. 35121100	-1. 83855300
C	0. 68284600	-2. 27764300	-1. 80838300
C	-0. 69360500	-2. 54569700	-1. 67434800
C	-1. 11586500	-3. 87205300	-1. 54239200
C	-0. 21078200	-4. 92713300	-1. 54258200
H	1. 86646100	-5. 47930600	-1. 72604300
H	2. 63863700	-3. 14665300	-1. 98545100
H	-2. 18259500	-4. 07864400	-1. 46165400
H	-0. 56808700	-5. 94951900	-1. 44165700
C	-1. 72738000	-1. 45542900	-1. 74322600
C	1. 20965900	-0. 87662100	-1. 94068700
P	-1. 84940300	-0. 42827400	-0. 19097400
P	1. 70100100	-0. 10418200	-0. 31768100
C	-3. 56215900	-0. 81938300	0. 50511600
C	3. 53327900	-0. 50964900	-0. 04342800
C	-2. 05507600	1. 28156500	-0. 87265900
C	-2. 60076300	1. 63381100	-2. 09732600
C	-1. 64020400	3. 58564700	-0. 40941300
C	-2. 65048300	2. 97336900	-2. 47763900
H	-2. 99590300	0. 86419900	-2. 75472300
C	-2. 17057500	3. 96198100	-1. 62639200
H	-1. 25030300	4. 28434900	0. 32334800
H	-3. 07478400	3. 24320200	-3. 44086200
H	-2. 20161800	5. 01189400	-1. 89589400
C	1. 69820700	1. 69999000	-0. 71105400
C	1. 79127200	2. 19861200	-2. 01001400
C	1. 77972700	3. 57780700	-2. 20102200
H	1. 87485500	1. 53150800	-2. 86419300
C	1. 60895800	3. 81999200	0. 16619700
C	1. 69535900	4. 40843500	-1. 09299100
H	1. 84635100	3. 99226900	-3. 20417600
H	1. 53772500	4. 44264900	1. 05831900
H	1. 69004600	5. 49017600	-1. 19347100
N	1. 59472700	2. 50050300	0. 36445100
N	-1. 59085200	2. 28326300	-0. 08427400
C	-4. 68966500	-0. 55037800	-0. 48189500
H	-4. 57598600	-1. 09465500	-1. 42741900
H	-5. 63655500	-0. 88019200	-0. 03178800
H	-4. 78976400	0. 51892000	-0. 70698800
C	-3. 52079000	-2. 29854000	0. 88487600
H	-4. 44482100	-2. 55440200	1. 42127800

H	-3.46249300	-2.95155300	0.00597500
H	-2.67522900	-2.53059100	1.54813200
C	-3.76545300	0.01982500	1.76233900
H	-3.00087900	-0.19435300	2.51923000
H	-3.76533300	1.09716100	1.54838100
H	-4.74690500	-0.22235900	2.19322700
C	4.29883400	-0.59044500	-1.35950400
H	5.37170200	-0.66913300	-1.13486400
H	4.02807700	-1.47035400	-1.95451200
H	4.16007800	0.30665900	-1.97734600
C	3.61782200	-1.84110700	0.70125800
H	3.06231800	-2.64306900	0.19966000
H	4.67020200	-2.15160100	0.76403100
H	3.23778000	-1.75453200	1.72648000
C	4.15673600	0.58573900	0.82008900
H	4.24313000	1.53619200	0.27987400
H	3.59806100	0.75957100	1.74628600
H	5.17205300	0.26926200	1.09769500
H	-1.51373000	-0.77807700	-2.57864700
H	-2.71107400	-1.89482800	-1.94483000
H	0.45058200	-0.20097700	-2.35602600
H	2.05750500	-0.85186200	-2.63511500
Pd	0.10050700	-0.41584800	1.36777400
C	1.31942700	-0.54882700	2.96110000
O	1.97042100	0.32979400	3.47681500
H	-1.14843600	2.02729800	0.80579900
H	1.31448200	-1.60416400	3.31668300
O	-0.73615900	-0.35672600	3.37708800
C	-0.94089600	0.96524500	3.76992800
H	-0.00811600	1.56344700	3.76338500
H	-1.66700100	1.50269200	3.12917700
H	-1.33285100	1.00692300	4.80144300

D2'

C	0.03122400	0.06097000	-0.03964300
C	0.00936400	0.07398600	1.35013600
C	1.18714300	0.03514900	2.10130500
C	2.42030400	-0.06400800	1.42793900
C	2.42829500	-0.08095600	0.03018300
C	1.25060800	-0.00766600	-0.70499000
H	-0.90164100	0.09261600	-0.59818200
H	-0.94666300	0.10475100	1.87245300
H	3.38107000	-0.18059100	-0.48884100
H	1.28668300	-0.02552100	-1.79190400

C	3.71809400	-0.23077900	2.17041100
C	1.10681300	0.08357400	3.60040400
P	4.35661900	1.34106500	2.93957100
P	1.11588400	1.81084800	4.29721300
C	5.95752200	1.71796200	2.00734700
C	-0.69851000	2.34127700	4.47494700
C	4.97954500	0.76984500	4.58450200
C	5.42327400	-0.49796700	4.92572600
C	5.41579200	1.50937700	6.81061500
C	5.85502900	-0.75686000	6.22508300
H	5.44435000	-1.28577700	4.17825200
C	5.86075000	0.25582200	7.17755000
H	5.38872300	2.36197400	7.48073400
H	6.19784400	-1.75383600	6.48808000
H	6.19999300	0.08301100	8.19300000
C	1.66237200	1.55050500	6.04107800
C	1.61231600	0.31647300	6.68881000
C	2.03637400	0.23803000	8.01300800
H	1.24052500	-0.57044000	6.18173100
C	2.49702100	2.57693400	7.91781800
C	2.48155400	1.38990800	8.64562300
H	2.00976200	-0.71232000	8.54094300
H	2.84698700	3.49946800	8.38181200
H	2.81692400	1.37663000	9.67888400
N	2.11339000	2.66539800	6.64295500
N	4.98693000	1.71765600	5.55486600
C	6.95467000	0.56812200	2.04059700
H	6.55061100	-0.36530900	1.62954000
H	7.82501200	0.83967700	1.42665100
H	7.31959400	0.37010200	3.05638600
C	5.53882600	2.02511100	0.57046900
H	6.41608300	2.38595000	0.01629800
H	5.16350800	1.13671600	0.04795400
H	4.76961100	2.80881900	0.52328900
C	6.57752600	2.96348500	2.63185300
H	5.89135100	3.81752100	2.57906400
H	6.87264600	2.80314000	3.67778500
H	7.48871800	3.22310000	2.07523200
C	-1.59738300	1.15793100	4.81735600
H	-2.59780600	1.53957700	5.06400200
H	-1.71599900	0.45846200	3.98209100
H	-1.23553600	0.60094800	5.69188400
C	-1.13948700	2.97651800	3.15772600
H	-0.95504100	2.32658500	2.29413800

H	-2.21877900	3.17983300	3.19930100
H	-0.63316800	3.93332000	2.97917700
C	-0.80816000	3.37936600	5.59205100
H	-0.65317600	2.93569400	6.58300700
H	-0.10298500	4.20830100	5.46753300
H	-1.82473000	3.79678100	5.57161600
H	3.60769600	-0.97415700	2.96953500
H	4.48491700	-0.61979500	1.49102600
H	1.96786200	-0.41550900	4.06094600
H	0.21770900	-0.45009400	3.95511000
Pd	2.73362700	3.20388500	3.32528500
C	1.70587100	4.92035100	3.36088900
O	1.43626100	5.60813300	4.31571800
H	4.61055300	2.64395700	5.32280600
H	1.43931900	5.19745400	2.31384000
O	3.86210700	5.00652700	2.86614200
C	4.47232900	5.50017900	4.01614200
H	3.75376200	5.70715800	4.83543000
H	5.23758700	4.81576500	4.43592900
H	4.98639900	6.45537700	3.80542200

TSD1

C	-3.10782500	4.09493900	-0.91757600
C	-3.33892900	2.72791700	-0.81531700
C	-2.38036500	1.78770600	-1.20751800
C	-1.14359000	2.24807800	-1.70357000
C	-0.94073900	3.62489400	-1.83690800
C	-1.90403000	4.54743700	-1.44617200
H	-3.87440500	4.80075300	-0.60546400
H	-4.29914600	2.37046600	-0.44354700
H	-0.00107000	3.97636800	-2.26249500
H	-1.71498800	5.61250200	-1.56068500
C	-0.02824200	1.31063300	-2.08654300
C	-2.73899700	0.32842000	-1.16774700
P	1.08700000	0.98649000	-0.63268200
P	-1.96315600	-0.64202900	0.23013400
C	2.43942900	2.31509500	-0.58330200
C	-3.43162700	-1.25680200	1.24331700
C	2.03073300	-0.50421800	-1.19623600
C	2.18408100	-0.93183600	-2.50570100
C	3.28207400	-2.38867500	-0.44838900
C	2.88874900	-2.10349600	-2.77811800
H	1.75538100	-0.35300100	-3.31798200
C	3.45071600	-2.83973000	-1.74196700

H	3.67334800	-2.89917200	0.42561700
H	3.00102300	-2.43561600	-3.80668700
H	4.00522900	-3.75342000	-1.92572300
C	-1.32679000	-2.16850500	-0.59939600
C	-1.81094300	-2.67113900	-1.80818300
C	-1.20581200	-3.79560400	-2.36093100
H	-2.64834200	-2.19932200	-2.31675400
C	0.24779600	-3.83901500	-0.47217700
C	-0.14925100	-4.39096000	-1.68606500
H	-1.56112400	-4.19946400	-3.30617500
H	1.06434000	-4.29047100	0.09364800
H	0.35745100	-5.26644700	-2.08299300
N	-0.31327900	-2.75330300	0.06360500
N	2.58753100	-1.26402200	-0.21844200
C	2.83227200	2.79456200	-1.97376000
H	2.02203800	3.33524100	-2.47607200
H	3.67894500	3.48936400	-1.88393100
H	3.15163800	1.96723000	-2.62179800
C	1.90248400	3.46771600	0.26417000
H	2.66005200	4.26262800	0.30477200
H	0.98410000	3.90258800	-0.14701600
H	1.69656400	3.14597800	1.29341800
C	3.66424300	1.72363900	0.11069600
H	3.42131000	1.27556300	1.08367900
H	4.16949400	0.97101100	-0.50755500
H	4.38226000	2.53327000	0.29818300
C	-4.44997600	-2.01864000	0.40318500
H	-5.29216700	-2.32038700	1.04217200
H	-4.86707800	-1.41514300	-0.41229500
H	-4.02250300	-2.93220400	-0.02880900
C	-4.07147700	-0.02179800	1.87156500
H	-4.49593000	0.65534200	1.11858500
H	-4.89019400	-0.33024300	2.53667500
H	-3.34797400	0.54654700	2.47269000
C	-2.89508000	-2.17132700	2.34039600
H	-2.43532100	-3.08029400	1.93144200
H	-2.14975500	-1.66374800	2.96690600
H	-3.72557500	-2.48114600	2.99013700
H	-0.41338600	0.32295800	-2.37484300
H	0.53664300	1.70476100	-2.94011200
H	-2.44287600	-0.15124000	-2.10849900
H	-3.82875200	0.22739600	-1.10375900
Pd	-0.02792900	0.29490100	1.36272200
H	2.44788800	-0.99139300	0.76865400

C	1.38687900	0.49890500	2.82109600
O	2.24625300	-0.56823800	2.73373500
O	1.65890800	1.46353200	3.51236300
H	-0.06668800	-0.10281600	2.97934600
C	3.45539800	-0.47120900	3.50171600
H	3.22678500	-0.41034500	4.57040500
H	4.01767500	-1.38354900	3.29492900
H	4.04402700	0.40408800	3.20660300

D2

C	-2.89418800	4.18930900	-1.03637500
C	-3.19454200	2.83910100	-0.89889700
C	-2.28265600	1.84510300	-1.26637000
C	-1.02328900	2.22743400	-1.76857300
C	-0.75169400	3.58778900	-1.94117500
C	-1.66986300	4.56641900	-1.57711000
H	-3.62372000	4.94112600	-0.74369700
H	-4.17110000	2.53790600	-0.51993600
H	0.20346400	3.88268400	-2.37428000
H	-1.42922500	5.61730100	-1.72118600
C	0.03676700	1.21264500	-2.11104500
C	-2.71047600	0.40739300	-1.19460500
P	1.13168700	0.87516000	-0.64527500
P	-1.98935000	-0.55903500	0.22871800
C	2.55874500	2.12815300	-0.66779400
C	-3.48896000	-1.09563200	1.24138800
C	1.98232300	-0.69334700	-1.13179600
C	2.10900900	-1.18787500	-2.41977100
C	3.15306100	-2.58913800	-0.29709700
C	2.76925200	-2.39581600	-2.63887500
H	1.70200000	-0.63038200	-3.25789400
C	3.30103900	-3.10555200	-1.56923500
H	3.52608600	-3.07506200	0.59857100
H	2.86771900	-2.77898900	-3.65094200
H	3.81812900	-4.04834100	-1.70994200
C	-1.38607000	-2.12886100	-0.53688300
C	-1.84125500	-2.63840000	-1.75338300
C	-1.27587600	-3.81257400	-2.24190600
H	-2.62864600	-2.13873300	-2.31261500
C	0.08186500	-3.87797900	-0.28273400
C	-0.29027900	-4.44541600	-1.49772800
H	-1.60893200	-4.22608700	-3.19097300
H	0.84356200	-4.35575000	0.33520400
H	0.18345500	-5.35998200	-1.84403700

N	-0.44194600	-2.74687200	0.19353400
N	2.50752900	-1.42717300	-0.11832200
C	2.94482500	2.51915500	-2.08855300
H	2.16611200	3.10010200	-2.59446000
H	3.84374900	3.14936200	-2.04548800
H	3.18835600	1.64599000	-2.70862900
C	2.09845300	3.34978300	0.12790700
H	2.88410700	4.11680200	0.08427300
H	1.17838900	3.79098700	-0.27292700
H	1.92648500	3.10203300	1.18283200
C	3.77580600	1.51243400	0.02058200
H	3.54815100	1.11491000	1.01755100
H	4.23233200	0.71564800	-0.57989100
H	4.53125800	2.29916100	0.14900500
C	-4.51000500	-1.83560300	0.38213400
H	-5.37595800	-2.09913100	1.00546500
H	-4.88752500	-1.23333700	-0.45270600
H	-4.10178900	-2.76978800	-0.02378000
C	-4.10106900	0.17229600	1.83044900
H	-4.48811600	0.84664400	1.05564600
H	-4.94430100	-0.09820100	2.48093500
H	-3.37503300	0.73016400	2.43720900
C	-3.02413700	-2.01872300	2.36260500
H	-2.59027400	-2.94932300	1.97595500
H	-2.28133400	-1.53815200	3.01129500
H	-3.88980000	-2.28855200	2.98336000
H	-0.40496000	0.24118400	-2.37186900
H	0.63252600	1.53919200	-2.97173300
H	-2.43722300	-0.10883400	-2.12256500
H	-3.80357500	0.36097800	-1.13245100
Pd	-0.08240300	0.36879100	1.38488500
H	2.39446100	-1.09161300	0.85429600
C	1.47081200	0.73327400	2.65992200
O	2.29686100	-0.36890100	2.66135200
O	1.74570300	1.69117300	3.35756400
H	-0.75068300	0.01575800	2.80489600
C	3.45231900	-0.31218100	3.51456500
H	3.15245700	-0.25401600	4.56517500
H	4.00351900	-1.23831700	3.33928700
H	4.08227000	0.54939100	3.26899300

TSD2

C	-6.29989500	0.48744300	-1.01439200
C	-5.32957500	1.32820000	-0.48059700

C	-4.28901200	0.83405000	0.31016500
C	-4.27269300	-0.53863100	0.62631900
C	-5.24604800	-1.37625100	0.07519100
C	-6.24585900	-0.87726000	-0.75209700
H	-7.09620900	0.89980100	-1.62994600
H	-5.37477200	2.39897300	-0.67863000
H	-5.22714800	-2.43698400	0.32430200
H	-6.99355600	-1.54958600	-1.16683500
C	-3.29934400	-1.11202800	1.61852200
C	-3.21401000	1.77212300	0.78546200
P	-1.58434200	-1.39902900	0.96011000
P	-1.76616500	1.83576600	-0.38556800
C	-1.27949900	-3.24883700	1.16915300
C	-2.13510700	3.13943600	-1.70703200
C	-0.50627800	-0.64521300	2.26690900
C	-0.85286000	-0.39306700	3.58544800
C	1.65529400	0.26444700	2.67464500
C	0.06529600	0.21089300	4.44241100
H	-1.83336600	-0.67330400	3.95858000
C	1.33316200	0.54869700	3.98662700
H	2.62582100	0.46867900	2.23084700
H	-0.21440300	0.41021400	5.47331400
H	2.06655700	1.01965100	4.63203600
C	-0.40583400	2.57139300	0.61565900
C	-0.61558200	3.25541400	1.81238500
C	0.48836600	3.77299000	2.48591600
H	-1.61654700	3.39328000	2.21416500
C	1.86167500	2.89878100	0.74118800
C	1.75166500	3.60238400	1.93778800
H	0.35567400	4.30754200	3.42363300
H	2.84111200	2.74416800	0.28560700
H	2.63944500	3.99481300	2.42599700
N	0.81792600	2.37996100	0.09336900
N	0.74260100	-0.30134000	1.87071500
C	-1.42616300	-3.68829700	2.62160900
H	-2.40222200	-3.42832600	3.04915900
H	-1.33209800	-4.78186600	2.66945900
H	-0.64274800	-3.26337800	3.26130000
C	-2.31769100	-3.94586400	0.29125600
H	-2.10653600	-5.02364200	0.28289600
H	-3.33828700	-3.81554700	0.67235700
H	-2.28817100	-3.59194200	-0.74758600
C	0.12846100	-3.57858800	0.67928400
H	0.27845000	-3.32576200	-0.37815700

H	0.90504500	-3.07704000	1.27172100
H	0.28905400	-4.66021300	0.78405100
C	-2.83279900	4.34891100	-1.09266000
H	-2.90076200	5.14018300	-1.85178600
H	-3.85568800	4.12465100	-0.76871600
H	-2.27772800	4.76123200	-0.23945900
C	-3.00796700	2.51682800	-2.79580200
H	-3.95152700	2.11452700	-2.40995100
H	-3.25216900	3.29165800	-3.53575400
H	-2.48187400	1.70741400	-3.31781400
C	-0.81820600	3.58639300	-2.33747900
H	-0.20084400	4.17128800	-1.64601300
H	-0.22302100	2.74065300	-2.70448800
H	-1.05085300	4.22612400	-3.19994300
H	-3.22923700	-0.45189300	2.48994200
H	-3.67920400	-2.06919300	1.99297600
H	-2.79159100	1.44593300	1.74617800
H	-3.61369800	2.78182500	0.93943400
Pd	-1.11725100	-0.31029300	-1.16045600
C	-0.52688800	-1.89319200	-2.30440200
H	-0.79567000	0.42301300	-2.54138600
O	-1.07110500	-2.75312000	-2.92815400
O	0.97879500	-1.86745600	-2.51885600
H	1.04080200	-0.48153200	0.89274100
H	1.50846600	-1.49996300	-1.65379700
C	6.43032900	0.84418100	0.48232400
C	5.43600100	-0.09787900	0.73064900
C	4.66896000	-0.56322500	-0.32970300
C	4.88300100	-0.10533500	-1.63072900
C	5.87484600	0.83394500	-1.85916500
C	6.66179800	1.32385700	-0.80728000
H	7.03709200	1.21490400	1.30685300
H	5.25707000	-0.46726300	1.73759400
H	4.27414700	-0.47412900	-2.45545000
H	6.04767400	1.20248500	-2.86950300
C	7.72274300	2.34337400	-1.07645400
H	8.45285800	1.97083500	-1.80553100
H	7.29196300	3.25845100	-1.50175900
H	8.26253900	2.61572000	-0.16381300
S	3.37075300	-1.73165200	-0.04910300
O	3.30452500	-1.98843000	1.39614400
O	3.59438000	-2.90658800	-0.90377300
O	2.11443100	-0.98768900	-0.51746000
C	1.59148300	-2.95796800	-3.24343500

H	2.64843600	-2.71120100	-3.34443600
H	1.46393000	-3.89749700	-2.69865500
H	1.12038300	-3.01559100	-4.22510000

D3

C	-5.90970400	1.00565100	-2.10567300
C	-5.19855100	1.47127600	-1.00562400
C	-4.39440500	0.62096400	-0.24209600
C	-4.35873200	-0.75110000	-0.55976800
C	-5.07687600	-1.20634800	-1.66899100
C	-5.83491300	-0.34002000	-2.44922700
H	-6.52554200	1.68974900	-2.68512200
H	-5.26713900	2.52089900	-0.72047300
H	-5.05794300	-2.26981200	-1.90575000
H	-6.38603500	-0.72137800	-3.30599500
C	-3.64432800	-1.74820600	0.30926000
C	-3.59023900	1.19480300	0.89211300
P	-1.79405400	-1.75955000	0.13096400
P	-1.89877000	1.75449100	0.36917900
C	-1.37267900	-3.45599500	-0.57659800
C	-2.00261800	3.55850400	-0.17906200
C	-1.13121500	-1.82892400	1.84676800
C	-1.86970000	-2.18689900	2.97409400
C	0.77801900	-1.55396500	3.09002400
C	-1.22521300	-2.20870200	4.20816700
H	-2.91904400	-2.46322000	2.90429700
C	0.12227200	-1.88390600	4.27310800
H	1.83866600	-1.29530500	3.09692000
H	-1.77523700	-2.48240600	5.10557100
H	0.66063800	-1.88438100	5.21702800
C	-0.88350200	1.76695100	1.90129900
C	-1.42382800	1.78570700	3.18556700
C	-0.54737100	1.76868000	4.26859100
H	-2.49905400	1.82007900	3.34591800
C	1.26019400	1.71822600	2.70788000
C	0.81882600	1.73390300	4.02895900
H	-0.93346600	1.78063600	5.28502300
H	2.32694000	1.67974300	2.48165500
H	1.53536300	1.71082600	4.84560100
N	0.43612600	1.73553800	1.66195900
N	0.17225800	-1.51958100	1.90444100
C	-1.87058200	-4.56741800	0.34344600
H	-2.95243700	-4.52294100	0.52021100
H	-1.65934600	-5.53767800	-0.12722900

H	-1.36072000	-4.55268800	1.31453500
C	-2.03929200	-3.56643200	-1.94523800
H	-1.73438000	-4.51125400	-2.41538700
H	-3.13396400	-3.57303400	-1.87334100
H	-1.74583500	-2.75202700	-2.62201000
C	0.14271000	-3.56896500	-0.72342100
H	0.55699700	-2.80690200	-1.39575600
H	0.66098900	-3.48784200	0.23934700
H	0.38239900	-4.55071600	-1.15498800
C	-2.96324500	4.31779300	0.73393800
H	-2.87234100	5.39118300	0.52053000
H	-4.00998300	4.03997300	0.56323200
H	-2.73013100	4.17444400	1.79754300
C	-2.47146100	3.63571500	-1.62894400
H	-3.41955300	3.11474700	-1.80093200
H	-2.61625200	4.69216200	-1.89307600
H	-1.72434600	3.21839800	-2.31660900
C	-0.61290000	4.18266100	-0.07990700
H	-0.27268800	4.28331400	0.95712200
H	0.13912900	3.61301300	-0.64039200
H	-0.66075600	5.18967500	-0.51600600
H	-3.87302000	-1.54957200	1.36309100
H	-4.02089700	-2.75637300	0.10096400
H	-3.41264600	0.45252700	1.68018700
H	-4.11694300	2.03318300	1.36303200
Pd	-0.92067500	0.19482100	-1.09508100
C	-0.00840000	-0.65255600	-2.63422400
H	-0.45304900	1.56079100	-1.76415500
O	0.51279600	-1.03244300	-3.57511500
O	2.67470700	1.30132500	-2.43771000
H	2.49384700	0.90147500	-3.29863300
C	6.56892800	0.49342500	0.91777500
C	5.35994600	-0.17471000	0.81663500
C	4.89746700	-0.53518000	-0.44920100
C	5.61289300	-0.23187000	-1.60203500
C	6.82572300	0.43538100	-1.47726900
C	7.31869800	0.80625400	-0.22386200
H	6.94511700	0.78183300	1.89807800
H	4.78122700	-0.41768200	1.70611400
H	5.22874100	-0.51729500	-2.57856300
H	7.40095800	0.67645600	-2.36946200
C	8.63047100	1.51101400	-0.08814400
H	9.39505900	0.83403200	0.31442900
H	8.99079500	1.88496800	-1.05168400

H	8.55728200	2.35461100	0.60789900
S	3.33184200	-1.33072100	-0.57193400
O	3.15940100	-2.23941100	0.55336200
O	3.15217000	-1.84078300	-1.92874000
O	2.29659000	-0.15149100	-0.32681100
H	2.32637500	0.47407100	-1.12359700
C	2.28554900	2.66799500	-2.45364900
H	2.40794400	3.04908200	-1.43524500
H	2.92531000	3.25203700	-3.12623900
H	1.23727500	2.79270700	-2.75800800

TSD3

C	-5.08310300	3.17880400	-0.33951600
C	-4.09222700	2.86836100	0.58398200
C	-3.68747400	1.55040700	0.81639600
C	-4.34971000	0.51097600	0.13055800
C	-5.34762200	0.83586100	-0.79335200
C	-5.70942500	2.15472900	-1.04173100
H	-5.37103000	4.21543500	-0.49953500
H	-3.62002000	3.66797100	1.15379800
H	-5.86396800	0.02920600	-1.31279700
H	-6.49187800	2.37699400	-1.76379400
C	-4.04108500	-0.94157800	0.37780400
C	-2.59682600	1.29130000	1.81950000
P	-2.45811200	-1.44780400	-0.45358600
P	-0.84842700	1.36332200	1.15569800
C	-2.90149200	-2.71667500	-1.77224200
C	-0.23836300	3.15033100	1.30389600
C	-1.59835500	-2.47508100	0.82151800
C	-2.18644500	-3.16458800	1.87135100
C	0.54818100	-3.18760700	1.56947500
C	-1.38866600	-3.85707000	2.78001700
H	-3.26698700	-3.16966200	1.98028100
C	-0.00647800	-3.87161900	2.63220800
H	1.61359300	-3.14298300	1.36314900
H	-1.85478500	-4.39126900	3.60347300
H	0.63732200	-4.39942500	3.32725100
C	0.08543800	0.46942600	2.47839600
C	-0.41195400	0.31874900	3.77417900
C	0.35873700	-0.36149600	4.71276100
H	-1.37946000	0.72445600	4.05735700
C	2.01409600	-0.64941500	3.02133200
C	1.59789200	-0.85610900	4.33336600
H	-0.00789300	-0.49421500	5.72788200

H	2.98453800	-1.02492900	2.68964500
H	2.23351500	-1.39304800	5.03193300
N	1.28324900	-0.00962000	2.10599800
N	-0.24758200	-2.52273400	0.71803800
C	-3.66654400	-3.90794700	-1.21092800
H	-4.59206800	-3.61222800	-0.70109300
H	-3.94944700	-4.57157300	-2.04010400
H	-3.05846500	-4.49728300	-0.51352700
C	-3.75158000	-1.97449200	-2.80111600
H	-3.94199300	-2.64119400	-3.65294600
H	-4.72487200	-1.67785500	-2.39110000
H	-3.24914300	-1.07579500	-3.18526400
C	-1.59893300	-3.18509400	-2.41513100
H	-0.99919300	-2.34756300	-2.79734300
H	-0.97762400	-3.76868300	-1.72297000
H	-1.83756500	-3.83860900	-3.26542300
C	-0.75861000	3.82350900	2.56878900
H	-0.27296700	4.80398400	2.67183000
H	-1.83981200	4.00204500	2.54008200
H	-0.52173900	3.24803600	3.47361700
C	-0.70161700	3.91137700	0.06403600
H	-1.79274100	3.91917300	-0.04234200
H	-0.36420800	4.95522800	0.13518600
H	-0.27811700	3.47911400	-0.85284900
C	1.28914400	3.13583500	1.33593900
H	1.67957500	2.70985600	2.26810400
H	1.72687200	2.58590600	0.49436700
H	1.64614100	4.17374300	1.27034700
H	-3.94941300	-1.14830300	1.45073200
H	-4.85904500	-1.56985900	0.00535100
H	-2.68583800	0.28164900	2.24200500
H	-2.68901500	1.98924700	2.66087700
Pd	-0.84815900	0.37503900	-1.02717000
O	3.74049400	3.25770600	-0.96532700
H	0.22802300	-1.99597200	-0.03455600
H	3.37772800	2.36024300	-1.03636000
C	5.62579700	-0.18706800	0.78399200
C	4.35364300	-0.09442900	0.24321100
C	4.15362300	-0.49116700	-1.08042200
C	5.19711100	-0.97711600	-1.85649600
C	6.46735800	-1.06312000	-1.29509500
C	6.70011200	-0.67216200	0.02440600
H	5.79853600	0.12407200	1.81384300
H	3.51956300	0.29155400	0.83134100

H	5.02025900	-1.27738000	-2.88649200
H	7.29545400	-1.43767200	-1.89442700
C	8.06665300	-0.75703500	0.62692000
H	8.06680700	-1.39150000	1.52193200
H	8.79470700	-1.16625600	-0.08073800
H	8.41992500	0.23246000	0.94302600
S	2.51879400	-0.41336400	-1.74466000
O	1.69994600	-1.41784500	-1.02780400
O	2.58360200	-0.61886700	-3.19749400
O	2.06836200	1.00391900	-1.39131300
C	-0.68821400	0.46875100	-2.99130000
O	-0.62955200	0.55657000	-4.13131200
H	0.65470100	1.09678000	-1.15500500
C	2.97737000	4.05438200	-1.84384300
H	1.91018300	4.09002300	-1.56690100
H	3.36569200	5.07790300	-1.80116800
H	3.04374700	3.71044600	-2.88739700

D4

C	-5.81839400	0.90781800	-1.94653300
C	-5.05717600	1.43243500	-0.90860900
C	-4.25723600	0.62312700	-0.09579500
C	-4.28154300	-0.77292800	-0.30396800
C	-5.05210400	-1.28772200	-1.35117200
C	-5.80441900	-0.46310500	-2.17958200
H	-6.42707000	1.56678800	-2.56192300
H	-5.08356300	2.50402700	-0.71204600
H	-5.07588600	-2.36671700	-1.50171600
H	-6.39587700	-0.89385700	-2.98449300
C	-3.55423900	-1.73888300	0.59348100
C	-3.40129900	1.27409400	0.95685800
P	-1.72604600	-1.84140900	0.23423500
P	-1.71334700	1.77642300	0.31045900
C	-1.39661200	-3.60713900	-0.35243500
C	-1.84606200	3.57534500	-0.28771100
C	-1.01503600	-1.86657800	1.94490300
C	-1.65781200	-2.23416100	3.11864600
C	0.94671800	-1.35357700	3.20041200
C	-0.98846600	-2.14457400	4.33634000
H	-2.67857500	-2.60396500	3.08539700
C	0.32924500	-1.70204300	4.38386100
H	1.97482800	-1.01160500	3.12643000
H	-1.49945200	-2.43290600	5.25114500
H	0.87329500	-1.62730700	5.31902700

C	-0.72740500	1.92365100	1.86591400
C	-1.27879300	2.09633200	3.13660300
C	-0.42690400	2.15172400	4.23627600
H	-2.35417900	2.18285800	3.27335000
C	1.40300200	1.88594900	2.73019800
C	0.94258300	2.04812400	4.03368800
H	-0.83302300	2.27917800	5.23729200
H	2.47250900	1.79323000	2.53236800
H	1.64359500	2.08373900	4.86322000
N	0.59870800	1.81636200	1.66824700
N	0.26523300	-1.43456900	2.04610100
C	-1.79597600	-4.67106700	0.66062500
H	-2.85121800	-4.60253300	0.95375400
H	-1.64779300	-5.66485300	0.21449200
H	-1.18217400	-4.62601400	1.56898400
C	-2.18816000	-3.77852700	-1.64674800
H	-1.90909400	-4.73279300	-2.11416200
H	-3.27018900	-3.80278900	-1.46679700
H	-1.97320100	-2.97714900	-2.36831700
C	0.09828900	-3.69974500	-0.65036600
H	0.40490900	-2.96707500	-1.40986400
H	0.71460300	-3.54656000	0.24663300
H	0.32984900	-4.70209100	-1.03675100
C	-2.81742300	4.40397800	0.54233700
H	-2.77074500	5.45219900	0.21351400
H	-3.85701800	4.07496400	0.42636200
H	-2.56582300	4.38573100	1.61152100
C	-2.28058300	3.54168000	-1.75134900
H	-3.24932500	3.04751100	-1.89371600
H	-2.37017500	4.56982400	-2.13027200
H	-1.54231300	3.01468900	-2.37243500
C	-0.45693100	4.20754300	-0.21173700
H	-0.14040800	4.38924900	0.82261900
H	0.31172900	3.59296900	-0.69850000
H	-0.48370000	5.17727300	-0.72885400
H	-3.67442900	-1.44177300	1.64168000
H	-3.99498200	-2.73870500	0.49961900
H	-3.18088200	0.57536100	1.77522700
H	-3.92007100	2.13182100	1.40235800
Pd	-0.95138600	-0.01744000	-1.15896400
C	-0.38329900	-0.31838000	-2.98614100
H	2.37428300	0.36697900	-2.00009400
O	-0.09791200	-0.61661500	-4.06815500
O	1.78921800	1.79533600	-1.78811900

H	0.87684200	1.54656600	-1.52448000
C	7.17350100	-0.71026900	-0.68620700
C	5.91163400	-1.26692900	-0.82875200
C	4.79864500	-0.48690100	-0.52410200
C	4.92346000	0.83105500	-0.08953900
C	6.19681400	1.36793600	0.04164200
C	7.33490200	0.61064400	-0.25269200
H	8.05413400	-1.30877900	-0.91415600
H	5.78662800	-2.29391800	-1.16304500
H	4.04604100	1.43094200	0.14683700
H	6.31282300	2.39459800	0.38403800
C	8.70479800	1.19367100	-0.11681800
H	9.19013100	1.28295600	-1.09693900
H	8.67621800	2.18956800	0.33614100
H	9.34860400	0.55336200	0.49795700
S	3.19171900	-1.17563200	-0.73059200
O	3.28821100	-2.61718300	-0.89466900
O	2.68028900	-0.60449500	-2.11023300
O	2.33263000	-0.63927900	0.33213200
H	0.77255100	-1.15083600	1.19302400
C	1.71297600	2.43570600	-3.06207300
H	2.69112200	2.87793300	-3.26594400
H	1.47299500	1.71877600	-3.85903600
H	0.95938500	3.23193600	-3.05283900

D2-R

C	-0.91532200	5.14941600	-0.99619800
C	-1.56865500	3.94063200	-1.18630200
C	-0.88286500	2.73998300	-1.42035100
C	0.52708200	2.78032600	-1.49279800
C	1.16717600	4.01741000	-1.33426800
C	0.47202000	5.18902500	-1.07361700
H	-1.48835400	6.05566400	-0.81334600
H	-2.65736700	3.92096700	-1.17167500
H	2.24961400	4.05822800	-1.43946200
H	1.00954000	6.12708800	-0.95477300
C	1.40617900	1.59483100	-1.80290700
C	-1.71722100	1.51072800	-1.66508800
P	2.03200900	0.62078000	-0.33728300
P	-2.17090200	0.44302500	-0.19500100
C	3.51281500	1.49964200	0.44414200
C	-3.60863100	1.25678500	0.72763800
C	2.88533500	-0.77681800	-1.21619400
C	3.37885000	-0.77061500	-2.51172500

C	3.56232700	-3.05447400	-0.98582900
C	3.96710700	-1.91950300	-3.03753800
H	3.30707400	0.12638000	-3.11798000
C	4.06731300	-3.07386900	-2.26939900
H	3.57654600	-3.90512400	-0.31270600
H	4.34832200	-1.90797200	-4.05488500
H	4.51787400	-3.98083400	-2.65676900
C	-2.99022900	-0.99587500	-1.02466900
C	-3.45603900	-0.97104000	-2.33971300
C	-3.98629100	-2.13739200	-2.88406800
H	-3.40615600	-0.06733000	-2.94012500
C	-3.57640700	-3.20437000	-0.79270600
C	-4.04787300	-3.28022000	-2.10040700
H	-4.34605600	-2.14631500	-3.91030000
H	-3.61248900	-4.08045100	-0.14444600
H	-4.44804700	-4.21364500	-2.48652500
N	-3.05499200	-2.09786900	-0.26195000
N	3.00030600	-1.93005700	-0.51351600
C	4.41406500	2.15127300	-0.59708800
H	3.92500000	2.97796000	-1.12275100
H	5.29585000	2.56305200	-0.08669500
H	4.77545400	1.43260800	-1.34376500
C	2.96981400	2.53974800	1.42062100
H	3.81581400	3.08969300	1.85501800
H	2.30868800	3.26804200	0.93464900
H	2.41744400	2.06771700	2.24375300
C	4.31353600	0.45240800	1.21724900
H	3.67408700	-0.18723400	1.84076200
H	4.90849800	-0.18916200	0.55535600
H	5.01341900	0.97010300	1.88686900
C	-4.64226800	1.81968400	-0.24321200
H	-5.51762600	2.15409700	0.33139500
H	-4.27280700	2.68599400	-0.80295700
H	-4.99123400	1.06501100	-0.96008900
C	-3.06795600	2.36188800	1.62993800
H	-2.52302900	3.13351500	1.07346500
H	-3.91141400	2.84962800	2.13865700
H	-2.39740800	1.96112800	2.40021700
C	-4.28175500	0.19237100	1.59610000
H	-4.83391200	-0.54195200	0.99861600
H	-3.56770500	-0.35306900	2.22630400
H	-5.00077600	0.69125000	2.26060800
H	0.87694200	0.83912300	-2.39865500
H	2.26638900	1.93428000	-2.39454900

H	-1.20014100	0.80714100	-2.33042200
H	-2.64348100	1.80979500	-2.17292200
Pd	-0.01231100	-0.01462400	0.63047100
C	0.98946300	-1.20311000	3.69425200
C	-0.36189500	-1.19368100	3.66710000
C	1.83346200	-2.37073300	3.26764100
H	1.31018500	-3.11054800	2.65645800
H	2.71478600	-2.02719600	2.70496400
H	2.23650400	-2.89417100	4.14838500
C	-1.20622500	-2.35253100	3.21948100
H	-1.79824200	-2.72988200	4.06752900
H	-1.93202300	-2.03669700	2.45633400
H	-0.64120000	-3.19327900	2.80985200
C	-1.19020100	-0.07900700	4.24412100
H	-2.11141100	0.05786900	3.66373700
H	-1.50944600	-0.32890800	5.26769400
H	-0.68014000	0.88782000	4.28870000
C	1.81211900	-0.10172500	4.29880700
H	1.24789000	0.80511500	4.53267600
H	2.27789000	-0.44842500	5.23429200
H	2.64500900	0.18122700	3.63910200
H	2.59909500	-1.96757800	0.42707400
H	-0.05085700	1.45272500	1.39141500
C	0.02087600	-1.85732900	-0.34291100
O	0.14169500	-2.95750000	0.18253900
O	-0.05480800	-1.77554300	-1.70590100
C	-0.02829300	-3.00937500	-2.43163600
H	-0.16678200	-2.75005900	-3.48317900
H	0.93125900	-3.52469300	-2.30106400
H	-0.83210300	-3.68016800	-2.10688500

TSD4

C	-0.11350300	5.32224200	-0.81577400
C	-0.89683300	4.20270100	-1.05462000
C	-0.34529900	2.93331400	-1.28256000
C	1.05941200	2.81239800	-1.31285600
C	1.83597100	3.96122600	-1.10462200
C	1.27193900	5.20050300	-0.84136500
H	-0.58356700	6.28750700	-0.64085400
H	-1.97992800	4.31154600	-1.09084500
H	2.91935500	3.87211900	-1.17636600
H	1.90892900	6.06767300	-0.68291000
C	1.78400900	1.53556000	-1.63991000
C	-1.28927700	1.81323800	-1.62618500

P	2.25013300	0.48896100	-0.15961000
P	-1.97261800	0.71983700	-0.27516200
C	3.93124800	1.13609000	0.46781200
C	-3.33083400	1.69783300	0.61247100
C	2.83665500	-1.00351800	-1.10284000
C	3.32893100	-1.04880500	-2.40093900
C	3.07936000	-3.37906200	-0.95920200
C	3.70461900	-2.26454800	-2.96565600
H	3.42091500	-0.13295900	-2.97580400
C	3.58259100	-3.44651000	-2.24024700
H	2.93279400	-4.24051400	-0.31558300
H	4.09435800	-2.28744300	-3.97979900
H	3.86433100	-4.40603600	-2.65931600
C	-2.94879000	-0.49643300	-1.28519900
C	-3.21708200	-0.34034000	-2.64622200
C	-3.89478800	-1.35296500	-3.31898500
H	-2.90674700	0.54760300	-3.18938300
C	-3.99885300	-2.54190200	-1.25873700
C	-4.29258900	-2.48184300	-2.61749300
H	-4.10569600	-1.25496000	-4.38149400
H	-4.30038100	-3.40902000	-0.67014900
H	-4.81655600	-3.29962500	-3.10446900
N	-3.34316200	-1.58310600	-0.60331200
N	2.73620600	-2.18464400	-0.44658500
C	4.88339800	1.60961400	-0.62117400
H	4.50127700	2.48228900	-1.16496800
H	5.83629100	1.90736700	-0.15984600
H	5.10868200	0.82067200	-1.35105100
C	3.61248900	2.27826000	1.43254300
H	4.54875500	2.66851100	1.85649000
H	3.09785600	3.11188500	0.94082100
H	2.98301800	1.93961300	2.26599300
C	4.58163900	-0.00105900	1.25599700
H	3.89802900	-0.43803900	1.99915300
H	4.94790400	-0.80594000	0.60579500
H	5.44825200	0.39445800	1.80395400
C	-4.26013500	2.38644700	-0.38303800
H	-5.09373800	2.84861400	0.16393000
H	-3.76036800	3.18452900	-0.94456400
H	-4.69148600	1.67938000	-1.10374000
C	-2.69571500	2.72839500	1.54344200
H	-2.03300700	3.42749000	1.02198400
H	-3.49500000	3.31479300	2.01822700
C	-4.14256600	0.72489400	1.46579600

H	-4.76018800	0.05264100	0.86086200
H	-3.49920100	0.11298500	2.11293600
H	-4.81446700	1.30551900	2.11353100
H	1.16574300	0.86662100	-2.25284100
H	2.67937200	1.77467100	-2.22686000
H	-0.81966300	1.09838800	-2.31451000
H	-2.14752200	2.24147100	-2.16001200
Pd	-0.53692600	-0.50639900	1.16285000
H	-0.60788600	0.69032200	2.25871900
C	-0.00320200	-1.85777800	2.86578100
C	-0.09377400	-0.58627900	3.48432600
C	-1.14718200	-2.83520300	2.97920700
H	-2.13362200	-2.36715900	2.89621200
H	-1.07682400	-3.59673800	2.19492500
H	-1.10487600	-3.35744400	3.94967400
C	-1.28012600	-0.24663900	4.35310500
H	-1.14286700	-0.72738500	5.33467300
H	-1.34926500	0.83375800	4.52426400
H	-2.23626200	-0.58954600	3.94963000
C	1.15697400	0.14544900	3.89921600
H	0.94726800	1.20475000	4.08730100
H	1.53378400	-0.28991000	4.83782000
H	1.96022200	0.08551400	3.15900200
C	1.32603900	-2.55371900	2.72189300
H	2.17239000	-1.87944100	2.54711900
H	1.55647700	-3.10737700	3.64739300
H	1.28531800	-3.30374800	1.92048600
H	2.34085800	-2.17482100	0.49636800
C	-0.38877500	-2.05449400	-0.28660200
O	-0.47123900	-3.27648700	-0.22597300
O	-0.17287700	-1.49552800	-1.53129700
C	-0.16205100	-2.37126300	-2.65747200
H	0.01178200	-1.74012500	-3.53421700
H	0.63296600	-3.12382000	-2.58438500
H	-1.12520100	-2.88750400	-2.76695100
H	-2.11853400	2.24481600	2.34223500

D5

C	0.15094800	5.44514300	-0.48334300
C	-0.70981900	4.39301400	-0.76036800
C	-0.24771600	3.11415500	-1.10599100
C	1.14456000	2.91421400	-1.20682200
C	1.99941300	3.99689600	-0.95657500
C	1.52406100	5.24597100	-0.58499600

H	-0.25018600	6.41986500	-0.21462800
H	-1.78494400	4.56497900	-0.72807400
H	3.07123100	3.84919300	-1.08322100
H	2.21968600	6.06109500	-0.39880600
C	1.77139000	1.61635500	-1.63396700
C	-1.27628300	2.07838500	-1.47535500
P	2.23909300	0.48668600	-0.21562800
P	-1.89310300	0.87452700	-0.18186300
C	4.01462000	0.95673100	0.30679000
C	-3.05684900	1.83243600	0.96578900
C	2.62311000	-1.02616100	-1.22926100
C	3.07646900	-1.07365800	-2.54128100
C	2.63270200	-3.41566300	-1.16823900
C	3.31271000	-2.30007900	-3.15622900
H	3.24527400	-0.15156100	-3.08886900
C	3.09624800	-3.48833400	-2.46428200
H	2.41355500	-4.28047900	-0.54955800
H	3.66970800	-2.32598200	-4.18227400
H	3.26957400	-4.45617500	-2.92180000
C	-3.06427900	-0.13551500	-1.20853900
C	-3.41641200	0.16094500	-2.52655700
C	-4.21669600	-0.73637400	-3.22855200
H	-3.07854500	1.07055900	-3.01345400
C	-4.26778700	-2.09575500	-1.27433600
C	-4.64829300	-1.89371600	-2.59796000
H	-4.49391600	-0.52728800	-4.25967200
H	-4.59589800	-2.98752700	-0.73925500
H	-5.26539400	-2.62605100	-3.11108100
N	-3.49541300	-1.24890800	-0.59210900
N	2.41911700	-2.21241000	-0.60892900
C	4.91533600	1.43304300	-0.82283500
H	4.55889300	2.36274200	-1.28329500
H	5.91793600	1.63502500	-0.41858700
H	5.03046200	0.67880700	-1.61199300
C	3.86165900	2.05028700	1.36409000
H	4.85573300	2.36086200	1.71584200
H	3.35244700	2.94065700	0.97609900
H	3.29616100	1.69276300	2.23465600
C	4.62826800	-0.28030700	0.96158100
H	3.97024400	-0.71784200	1.72691400
H	4.87193900	-1.06034700	0.22851400
H	5.56415500	0.00493300	1.46211800
C	-4.04243100	2.70321900	0.19536600
H	-4.75484900	3.15441200	0.90080200

H	-3.55255600	3.52446100	-0.33990300
H	-4.62426400	2.11979900	-0.53067300
C	-2.20826800	2.68508400	1.90794900
H	-1.57011400	3.40102100	1.37786900
H	-2.87222300	3.25924200	2.56991400
C	-3.83328100	0.82324500	1.80971400
H	-4.54099600	0.23635400	1.21445300
H	-3.16299600	0.12314000	2.32800700
H	-4.40442300	1.36830700	2.57486800
H	1.08347700	1.02081700	-2.24859300
H	2.65348100	1.82496200	-2.25181400
H	-0.89916400	1.41409800	-2.26553700
H	-2.14844300	2.59610000	-1.89526300
Pd	-0.48660500	-0.72834900	1.03196800
H	-0.33994600	0.13860000	2.75685300
C	0.05838600	-2.00386900	2.61209500
C	0.06784200	-0.72117000	3.42479700
C	-1.10715300	-2.94264900	2.83417600
H	-2.08330000	-2.44503800	2.78731000
H	-1.10242100	-3.72879900	2.07064500
H	-1.03328600	-3.44093900	3.81718600
C	-0.88693000	-0.69149200	4.61586900
H	-0.56551300	-1.42538600	5.36820900
H	-0.87402800	0.29858300	5.08773200
H	-1.92162300	-0.91926900	4.34208700
C	1.44453900	-0.22434000	3.84830600
H	1.36233500	0.76715500	4.31077000
H	1.88985200	-0.90259300	4.58884800
H	2.13658000	-0.13896200	3.00288200
C	1.34702700	-2.78556200	2.53103500
H	2.23309500	-2.17308700	2.31992100
H	1.54915900	-3.30339400	3.48593400
H	1.26769300	-3.57561000	1.76958100
H	2.03516200	-2.19704300	0.34163700
C	-0.56324600	-2.14346800	-0.44707500
O	-0.81110400	-3.34078700	-0.40596700
O	-0.34646800	-1.55727400	-1.66596900
C	-0.51770000	-2.38062000	-2.82258200
H	-0.30996400	-1.73963000	-3.68339100
H	0.17445600	-3.23181400	-2.82101900
H	-1.54600400	-2.75794000	-2.88408500
H	-1.56557200	2.06145400	2.54531300

D5'

C	0.00903800	0.14287600	0.00524400
C	0.01168000	0.09900900	1.39171400
C	1.19838500	0.08057500	2.13834900
C	2.42630700	0.05454900	1.44535700
C	2.40478300	0.07813800	0.04412900
C	1.22134700	0.13796400	-0.67765900
H	-0.93338500	0.15859300	-0.53770800
H	-0.93750300	0.06453800	1.92658200
H	3.35094600	0.01421700	-0.49119800
H	1.24640600	0.15272800	-1.76493300
C	3.75429300	-0.12049800	2.13115600
C	1.08044000	-0.02545000	3.63278200
P	4.79497900	1.42247600	2.32787100
P	1.20974700	1.52881100	4.66163200
C	5.93668400	1.53388800	0.79699800
C	-0.44585800	2.44135300	4.48713600
C	6.01651200	0.71322200	3.53911800
C	6.30508400	-0.62763700	3.76323900
C	7.58309600	1.30012100	5.24943600
C	7.23786500	-0.99387000	4.72917400
H	5.80266800	-1.39433000	3.18244700
C	7.88879600	-0.02267800	5.48460600
H	8.02867000	2.13259200	5.78504800
H	7.45832700	-2.04586100	4.89042100
H	8.61519600	-0.28132300	6.24677600
C	1.09878000	0.79286300	6.36173800
C	0.92949100	-0.57012200	6.61646300
C	0.93401300	-1.01501400	7.93503800
H	0.79259700	-1.28852700	5.81388400
C	1.24799800	1.24489700	8.61346200
C	1.09732800	-0.09433400	8.95953800
H	0.80727500	-2.07317800	8.15289900
H	1.37493600	2.00127900	9.38895400
H	1.10993300	-0.39820200	10.00252400
N	1.25507600	1.68444000	7.35404400
N	6.68038200	1.61236500	4.30413200
C	6.28239100	0.19111600	0.17242100
H	5.41440600	-0.30426500	-0.27801500
H	7.01554500	0.34867900	-0.63203700
H	6.73578600	-0.49929200	0.89623800
C	5.19704400	2.42500700	-0.20064200
H	5.78357300	2.50741400	-1.12677700
H	4.21006100	2.02688600	-0.46655000
H	5.05532600	3.43857100	0.19937200

C	7.22751900	2.23828400	1.21464800
H	7.04326700	3.17069800	1.76877300
H	7.87544000	1.59512900	1.82382300
H	7.79159400	2.50721500	0.31069700
C	-1.63540800	1.52603800	4.75458100
H	-2.56275900	2.11590200	4.72134900
H	-1.73244600	0.73142600	4.00405800
H	-1.57977100	1.05760500	5.74592200
C	-0.54225900	3.03216900	3.08151900
H	-0.56485800	2.27009700	2.29727800
H	-1.47222300	3.61367800	3.00608500
C	-0.45841800	3.60329600	5.48056400
H	-0.46502700	3.26649100	6.52202500
H	0.41123400	4.26274600	5.34129300
H	-1.36480600	4.20101700	5.30827000
H	3.61639500	-0.46517300	3.16365000
H	4.32815700	-0.89614600	1.60736300
H	1.87227200	-0.66885800	4.03913200
H	0.12796400	-0.51188500	3.88023100
Pd	3.05660400	3.13001500	4.50662900
H	5.63218000	4.27661100	3.14633600
C	4.00330400	5.01110000	4.29217000
C	5.47610000	5.06824800	3.90178100
C	3.05994000	5.10445800	3.12803300
H	2.34701700	5.93610000	3.19973000
H	3.56413300	5.11703300	2.15511500
C	5.83639000	6.39357200	3.22228600
H	5.69346400	7.24200200	3.90477900
H	6.89189900	6.39246600	2.91974100
H	5.23530300	6.57780000	2.32378900
C	6.42692900	4.84642900	5.07260800
H	7.45308600	4.68248600	4.71389900
H	6.45859600	5.72932100	5.72532200
H	6.13222200	3.99991700	5.70612200
C	3.62552300	5.86409400	5.48028000
H	4.11416700	5.52444500	6.40136800
H	3.91106800	6.91945700	5.32908100
H	2.54175800	5.84599300	5.65390600
H	6.46962600	2.60348600	4.17631800
C	4.03411000	2.40078100	6.14394500
O	4.33132300	2.95560200	7.19331100
O	4.25146700	1.05184000	6.02619300
C	4.69788200	0.37974200	7.20881400
H	4.74233400	-0.68404800	6.96207200

H	5.68832400	0.73248200	7.52221000
H	3.99108200	0.53482400	8.03409600
H	0.28959100	3.71593600	2.86762300
H	2.35740600	4.20070600	3.02975300

TSD5

C	-1.87672800	5.16595000	-0.02271200
C	-2.35040900	3.91765200	-0.40020700
C	-1.50075600	2.89234800	-0.83902700
C	-0.12139300	3.16688400	-0.94576100
C	0.33736200	4.44082500	-0.58090600
C	-0.51386300	5.42874200	-0.10726000
H	-2.57047800	5.93139400	0.31788600
H	-3.42180300	3.72274500	-0.36665500
H	1.39618800	4.66593800	-0.69793500
H	-0.11761600	6.40369200	0.16759400
C	0.87909000	2.20906900	-1.53923200
C	-2.13597200	1.59074800	-1.24500900
P	1.72065800	1.04304000	-0.34679600
P	-2.17249700	0.22534200	0.03242300
C	3.16283100	2.00201900	0.44518900
C	-3.56178000	0.64583100	1.25948100
C	2.64753400	0.00374100	-1.57756700
C	2.87205900	0.27607400	-2.92032400
C	3.74197900	-2.10533300	-1.84789500
C	3.53094200	-0.65404700	-3.72009500
H	2.53030200	1.21240600	-3.34946100
C	3.97217500	-1.86068300	-3.18451500
H	4.04042400	-3.01208500	-1.33073300
H	3.70119300	-0.43215100	-4.77033200
H	4.48065600	-2.60289200	-3.78956400
C	-2.92896100	-1.14706200	-0.95852700
C	-3.50286400	-0.97788100	-2.22011800
C	-3.97137800	-2.09663900	-2.90344900
H	-3.59173300	0.00522000	-2.67380300
C	-3.29091100	-3.41649300	-1.04107800
C	-3.86151000	-3.34533400	-2.30843800
H	-4.41748300	-1.98667100	-3.88949100
H	-3.19411100	-4.37904200	-0.53728600
H	-4.20745000	-4.24625400	-2.80767100
N	-2.83096100	-2.35443400	-0.37851100
N	3.10672900	-1.18111200	-1.10804800
C	3.84064400	2.98023000	-0.50573700
H	3.19491100	3.81887400	-0.78630700

H	4.72223100	3.40621000	-0.00577600
H	4.19097000	2.49161200	-1.42437800
C	2.57461500	2.73528000	1.64980500
H	3.35747700	3.34728600	2.11912800
H	1.74958100	3.40361500	1.37175900
H	2.20342600	2.02931500	2.40495700
C	4.20328400	0.99620500	0.93563200
H	3.75732300	0.16495900	1.49968000
H	4.79957800	0.57898800	0.11501000
H	4.89903200	1.51107200	1.61198000
C	-4.84102300	1.07499600	0.55030700
H	-5.63827600	1.21085900	1.29540200
H	-4.72915100	2.02903500	0.02213300
H	-5.18903400	0.32156100	-0.16850800
C	-3.08429300	1.75348200	2.19665700
H	-2.85262400	2.68623900	1.67120400
H	-3.87995300	1.97090400	2.92358600
C	-3.85043400	-0.59675000	2.10161600
H	-4.30567700	-1.40389200	1.51772700
H	-2.94573600	-0.99113300	2.58317800
H	-4.55607100	-0.32223900	2.89874100
H	0.39850800	1.54694400	-2.27174900
H	1.64010500	2.78229800	-2.08403100
H	-1.59686300	1.13293500	-2.08603600
H	-3.15627600	1.78855000	-1.59849600
Pd	0.05136100	-0.35958000	0.87614800
H	2.60172900	-0.88836500	2.75423200
C	0.61936100	-1.63525400	2.83602200
C	2.11525900	-1.84715800	2.99274500
C	0.09007600	-0.41124600	3.24953800
H	-0.14587900	0.76828300	2.03814900
H	-0.94942100	-0.35868600	3.57383100
H	0.75810700	0.31529200	3.71509100
C	2.43994800	-2.16811800	4.45529700
H	1.92679300	-3.08283000	4.78160100
H	3.51753700	-2.33326800	4.58436400
H	2.14096800	-1.35349000	5.12585700
C	2.69110400	-2.93621400	2.09591300
H	3.78686200	-2.87751300	2.06849000
H	2.43093700	-3.93518700	2.47242200
H	2.30543600	-2.88479100	1.07031500
C	-0.24464600	-2.86084800	2.77073100
H	-0.03643200	-3.46333500	1.87863800
H	-0.06257200	-3.50216200	3.64744400

H	-1.30874000	-2.59907700	2.75900600
H	2.93095700	-1.40937100	-0.12629200
C	0.21707400	-1.93176700	-0.53936000
O	0.37946000	-3.14284800	-0.44162700
O	0.07728200	-1.41086900	-1.80818900
C	0.07342400	-2.33312600	-2.89782400
H	-0.07125300	-1.73865500	-3.80349400
H	1.02139500	-2.88204700	-2.96480900
H	-0.74621100	-3.05691300	-2.80345900
H	-2.19214600	1.45258700	2.76073200

D6

C	-1.25157300	4.64816600	-2.28523700
C	-1.90778500	3.45852500	-2.00580000
C	-1.24748300	2.22156400	-1.97899900
C	0.13097300	2.19263900	-2.28331600
C	0.77040500	3.40152400	-2.59359700
C	0.10637500	4.61933400	-2.58320600
H	-1.80314700	5.58560700	-2.29317800
H	-2.98034000	3.47442100	-1.81554700
H	1.82295900	3.37538800	-2.87139600
H	0.64186100	5.53345600	-2.82962500
C	0.95904700	0.93621400	-2.38814900
C	-2.09440000	1.00395100	-1.72318600
P	1.81981000	0.37601700	-0.82723500
P	-2.23094300	0.37862500	0.03285600
C	3.38258800	1.40625000	-0.54925500
C	-3.43110700	1.48837600	0.98470800
C	2.55183700	-1.22511200	-1.42076700
C	2.80415300	-1.59762300	-2.73151800
C	3.24360600	-3.39014400	-0.68803700
C	3.27290500	-2.88006500	-3.01221800
H	2.62800100	-0.89290000	-3.53805400
C	3.49911100	-3.78822200	-1.98398800
H	3.37818000	-4.02360400	0.18228600
H	3.46208200	-3.16696600	-4.04311300
H	3.85843400	-4.79283400	-2.17727500
C	-3.20346400	-1.17661300	-0.21100400
C	-3.85106300	-1.50758100	-1.40211700
C	-4.47363500	-2.74798700	-1.50453600
H	-3.87243900	-0.82108700	-2.24426300
C	-3.78890800	-3.18546500	0.73661600
C	-4.44175200	-3.60962000	-0.41734000
H	-4.97873400	-3.03187400	-2.42498000

H	-3.75195800	-3.83150200	1.61423700
H	-4.90927500	-4.58960500	-0.45498000
N	-3.17745100	-2.00517600	0.84554200
N	2.79010800	-2.14752400	-0.45675500
C	4.12192300	1.68625300	-1.85307400
H	3.55025700	2.32975500	-2.53028400
H	5.06072700	2.20801300	-1.62021000
H	4.38367700	0.76536700	-2.39084900
C	2.97343700	2.70855000	0.13417900
H	3.86766800	3.33471400	0.25710400
H	2.24080200	3.28074100	-0.44731700
H	2.55211600	2.52476300	1.13160700
C	4.29401900	0.62283900	0.39319600
H	3.77180500	0.30526600	1.30622700
H	4.73688300	-0.25963200	-0.08504600
H	5.12202700	1.27540500	0.70155700
C	-4.67486500	1.78527700	0.15257500
H	-5.39684300	2.33714100	0.77069800
H	-4.45170200	2.40647300	-0.72304400
H	-5.16945600	0.86809100	-0.19342400
C	-2.73009300	2.78774800	1.37133100
H	-2.35101500	3.34135400	0.50452400
H	-3.45026400	3.43418300	1.89237800
C	-3.83755500	0.75895900	2.26471300
H	-4.44651800	-0.12908100	2.06362300
H	-2.96675600	0.44962200	2.85855500
H	-4.43480600	1.44439900	2.88245000
H	0.34140800	0.06829500	-2.65789000
H	1.70182700	1.06762900	-3.18568400
H	-1.70346000	0.13286600	-2.26630300
H	-3.10492700	1.19112400	-2.10996000
Pd	0.01880300	0.02404400	0.63640500
H	2.73719200	1.12026500	3.00540800
C	1.27447600	-0.34631100	3.42407100
C	2.00397900	0.92265800	3.80941500
C	-0.06428900	-0.42618900	3.30007600
H	0.07361000	1.64352700	0.90276200
H	-0.55128800	-1.37985400	3.09489700
H	-0.71542400	0.42090700	3.50479300
C	1.11828500	2.14939700	3.94973900
H	0.41190600	2.03928700	4.78433500
H	1.73295200	3.03404700	4.15667900
H	0.53961300	2.35059700	3.03909800
C	2.79985600	0.71179300	5.10026000

H	3.31241100	1.63819200	5.38691500
H	2.12980800	0.43209400	5.92528300
H	3.56284300	-0.06880200	5.00551600
C	2.12882600	-1.57058400	3.27099100
H	3.05373500	-1.35492700	2.71569500
H	2.44719200	-1.95313100	4.25060400
H	1.58461500	-2.37466400	2.76373900
H	2.57533600	-1.89947400	0.51268800
C	-0.13043100	-2.01622600	0.15514600
O	-0.00274700	-2.99132400	0.88595100
O	-0.39872800	-2.22721300	-1.17381900
C	-0.53963800	-3.58693600	-1.59561200
H	-0.79396500	-3.55296700	-2.65744200
H	0.39746400	-4.14144500	-1.46061300
H	-1.33840800	-4.09485800	-1.04070500
H	-1.88999000	2.60573400	2.05362300

TSD6

C	-0.04032800	0.19192400	-0.02166500
C	-0.03084300	0.09732300	1.36189500
C	1.15641400	0.05731000	2.10860800
C	2.38039600	0.07875100	1.40659100
C	2.35267200	0.13700500	0.00554100
C	1.16778300	0.21273500	-0.71108800
H	-0.98597300	0.22080200	-0.55863800
H	-0.97892100	0.02534700	1.89331900
H	3.29676900	0.09107400	-0.53545000
H	1.18891300	0.25739300	-1.79749700
C	3.72451600	-0.10607600	2.06297500
C	1.03374100	-0.09470100	3.60000700
P	4.74457400	1.40816700	2.42016300
P	0.79451900	1.51191800	4.54885900
C	5.64238700	1.95666500	0.84609400
C	-1.10193200	1.78019000	4.63401700
C	6.14201700	0.61357600	3.35977100
C	6.52257800	-0.71785300	3.30195500
C	7.87536200	1.02305900	4.94925100
C	7.58870000	-1.17126600	4.07703300
H	5.99116200	-1.40856900	2.65536100
C	8.27821600	-0.29552900	4.90737000
H	8.33948400	1.78141800	5.57041600
H	7.87896300	-2.21713400	4.02798000
H	9.11012500	-0.62342200	5.52061800
C	1.08847200	0.90753200	6.27771500

C	0.91010600	-0.41250500	6.70267900
C	1.12456800	-0.72901200	8.03987900
H	0.60095800	-1.18660600	6.00402500
C	1.68881200	1.55785200	8.40203400
C	1.52072400	0.27536800	8.91374800
H	0.98285000	-1.74841300	8.39273000
H	2.00867400	2.37009600	9.05613600
H	1.70263800	0.07475800	9.96616100
N	1.48100300	1.87796000	7.12232800
N	6.84455200	1.42382000	4.18742900
C	6.18362800	0.77021200	0.05379000
H	5.38768900	0.13967800	-0.35843800
H	6.76790200	1.15368000	-0.79351200
H	6.85187000	0.13723700	0.65141100
C	4.68088400	2.77476600	-0.01502300
H	5.17969000	3.00989300	-0.96495500
H	3.75182600	2.24281400	-0.24712700
H	4.41445900	3.72390400	0.46716400
C	6.80215500	2.86023600	1.26555900
H	6.47828500	3.66912600	1.93591400
H	7.61691100	2.30650100	1.74795900
H	7.21950500	3.32903800	0.36418700
C	-1.91665800	0.49778400	4.72607500
H	-2.97739700	0.75142000	4.87210800
H	-1.85564200	-0.10995900	3.81491300
H	-1.61419100	-0.12770700	5.57677100
C	-1.51439000	2.58233200	3.39887100
H	-1.21262800	2.10880300	2.45731100
H	-2.60879700	2.69160100	3.37966200
C	-1.39077400	2.63933800	5.86555900
H	-1.26404400	2.08271100	6.80230800
H	-0.75000400	3.53132400	5.91062700
H	-2.43398800	2.98507700	5.82388300
H	3.63202100	-0.59240000	3.04193600
H	4.33359800	-0.76509900	1.43107500
H	1.94110400	-0.52939000	4.03670800
H	0.21545200	-0.79232300	3.82024100
Pd	3.86378000	3.11183100	3.75147800
H	2.63024100	6.09215600	1.77461700
C	3.47076300	5.46461200	3.62058500
C	2.28926700	5.98957600	2.81753200
C	3.30515900	4.89270600	4.88907900
H	3.62840600	4.01373400	2.41210700
H	4.11540500	4.96970500	5.61450900

H	2.30834400	4.73440800	5.30276200
C	1.05905700	5.10110400	2.83129300
H	0.63969900	5.00588700	3.84252800
H	0.27713500	5.53500100	2.19573400
H	1.28137400	4.09180700	2.45825900
C	1.92761800	7.38223100	3.34047200
H	1.59275600	7.32513000	4.38521600
H	2.76734300	8.08470500	3.29137800
H	1.10793400	7.80627400	2.74831100
C	4.79966700	6.09174200	3.28702400
H	4.99908600	6.07654300	2.20902700
H	4.80037600	7.14303900	3.60670600
H	5.62390600	5.59040800	3.80627900
H	6.54874300	2.40255200	4.26566700
C	4.27207900	2.04849000	5.52693000
O	4.76559200	2.44447400	6.57626300
O	4.04029400	0.70245500	5.38475200
C	4.44613000	-0.14952800	6.45791700
H	4.19835800	-1.16912400	6.14890600
H	5.52688600	-0.06996400	6.63150000
H	3.91729000	0.09294400	7.38752100
H	-1.08271200	3.59111000	3.41905600

D7

C	0.39831800	5.62331600	-0.78136900
C	1.01517400	4.60090800	-0.07432100
C	0.30843500	3.48891500	0.40252100
C	-1.08169600	3.44318500	0.19075500
C	-1.69874600	4.50157300	-0.48982100
C	-0.97550200	5.57459500	-0.99065400
H	0.98489600	6.46576000	-1.14087300
H	2.08185700	4.66927500	0.13206200
H	-2.78084500	4.48772700	-0.61328900
H	-1.48599700	6.37706900	-1.51819000
C	-1.96619800	2.35843900	0.73894700
C	1.04386500	2.47434800	1.23291200
P	-1.88797800	0.67844400	-0.05809100
P	1.77920400	0.93799000	0.45018700
C	-2.46507100	0.91605300	-1.85181600
C	3.25966200	1.53482000	-0.58451700
C	-3.39201800	-0.05255800	0.76639300
C	-4.13857300	0.54897300	1.77306000
C	-4.80981700	-1.97260900	0.92179600
C	-5.22099500	-0.11773300	2.34114100

H	-3.88508200	1.53984500	2.13075000
C	-5.57339700	-1.39095600	1.90996700
H	-4.98391900	-2.96699200	0.52290400
H	-5.79146700	0.36905900	3.12750600
H	-6.41293200	-1.92911200	2.33531500
C	2.58061700	0.20395100	1.96135300
C	2.48545600	0.75480200	3.24246900
C	3.08400600	0.09114500	4.30910900
H	1.96089000	1.68569900	3.42899400
C	3.82016300	-1.56145800	2.76525700
C	3.76713400	-1.09237600	4.07355400
H	3.01515000	0.50427000	5.31292900
H	4.35358700	-2.48461500	2.53489500
H	4.25046200	-1.64144800	4.87685400
N	3.23945200	-0.94445500	1.73628300
N	-3.76981300	-1.30267600	0.39708500
C	-3.71403100	1.78375200	-1.93898900
H	-3.54089000	2.80842700	-1.59446700
H	-4.03405700	1.84084400	-2.98881700
H	-4.54933000	1.36211800	-1.36410000
C	-1.29792500	1.55776600	-2.60695800
H	-1.60577400	1.71536800	-3.65006400
H	-1.00334700	2.53202000	-2.19837500
H	-0.41751400	0.90081600	-2.61578700
C	-2.75091600	-0.44322700	-2.48974400
H	-1.94353700	-1.16740400	-2.31887000
H	-3.69842500	-0.87687600	-2.14701000
H	-2.84835300	-0.30103000	-3.57469700
C	4.13692400	2.49586200	0.21016000
H	5.00438800	2.78027600	-0.40240800
H	3.62144800	3.42030800	0.48966000
H	4.51961100	2.02997300	1.12814900
C	2.70554300	2.19911300	-1.84432200
H	2.10472300	3.08961000	-1.63439500
H	3.54495100	2.50796100	-2.48354700
C	4.11635400	0.34911600	-1.02540500
H	4.53969100	-0.20779700	-0.18356200
H	3.55024800	-0.34802600	-1.65269900
H	4.94662000	0.73530000	-1.63362500
H	-1.73779000	2.17129100	1.79862500
H	-3.00552800	2.70228800	0.68905400
H	0.37174400	2.06170000	1.99800600
H	1.84990300	2.99025300	1.77059100
Pd	0.07549800	-0.80341000	-0.08410800

H	1.46350700	-3.65223400	-3.87924600
C	1.02641600	-3.19762200	-1.85043800
C	1.85588200	-2.94739700	-3.12492200
C	1.45586200	-2.34172400	-0.65006800
H	-0.00642400	-2.94559400	-2.14194600
H	1.64079900	-2.95960400	0.23797300
H	2.37090100	-1.78054600	-0.84964700
C	1.62221400	-1.54099300	-3.65994300
H	1.96787600	-0.77743000	-2.94905400
H	2.15837800	-1.37450600	-4.60345400
H	0.55407000	-1.36080500	-3.84842600
C	3.34337100	-3.23878200	-2.96865400
H	3.81360400	-2.58206800	-2.22359000
H	3.52962100	-4.27541100	-2.66080100
H	3.87086500	-3.08289800	-3.91885300
C	1.01164900	-4.67438600	-1.46795400
H	0.71845500	-5.30976000	-2.31537500
H	1.99683700	-5.01251700	-1.11845400
H	0.29765900	-4.85734400	-0.65291100
H	-3.20293100	-1.82408700	-0.28369500
C	-1.01321800	-2.50217400	0.24152800
O	-1.80382100	-3.10348700	-0.48283400
O	-0.82797900	-2.92494200	1.51484100
C	-1.59834600	-4.06322900	1.93541700
H	-1.32424100	-4.24327400	2.97602900
H	-2.67188200	-3.85615800	1.86583000
H	-1.35844700	-4.94335800	1.33003000
H	2.08803600	1.50091300	-2.42668700

TSD7

C	1.25910000	5.43467400	-0.99288300
C	1.73398200	4.38696900	-0.21680400
C	0.88385000	3.41518800	0.32861800
C	-0.50056800	3.53171200	0.09930100
C	-0.96813200	4.61788800	-0.65406000
C	-0.10909600	5.55399000	-1.21130200
H	1.95240300	6.16699200	-1.40063100
H	2.80014500	4.32496500	-0.00281200
H	-2.04214200	4.73636500	-0.79081400
H	-0.50883000	6.38168800	-1.79268300
C	-1.52996700	2.61515700	0.70551000
C	1.48173600	2.37222900	1.22949400
P	-1.77294900	0.93511300	-0.07291900
P	1.92956400	0.70801800	0.50347300

C	-2.49244100	1.23792300	-1.80296600
C	3.59634100	0.95311600	-0.37433500
C	-3.27596500	0.40268000	0.88971000
C	-3.95971900	1.16091100	1.83225100
C	-4.77019700	-1.41158400	1.32577700
C	-5.04807400	0.62320900	2.51443400
H	-3.65397600	2.17852900	2.04587900
C	-5.46789600	-0.67699000	2.25980900
H	-5.00763400	-2.43685400	1.05887900
H	-5.57022000	1.23133200	3.24809300
H	-6.31273900	-1.11948100	2.77548800
C	2.43137300	-0.16776200	2.06798500
C	2.66850100	0.47530500	3.28568500
C	3.00536200	-0.28695900	4.40014700
H	2.59771600	1.55464100	3.38080800
C	2.86592000	-2.21982200	3.01913700
C	3.10586400	-1.66440500	4.27149700
H	3.18780100	0.19780400	5.35672200
H	2.94056000	-3.29820800	2.87378200
H	3.36401000	-2.29771900	5.11574000
N	2.53054900	-1.50279800	1.94603600
N	-3.71991900	-0.86533300	0.69056700
C	-3.62391200	2.25648700	-1.79575200
H	-3.29779200	3.25314300	-1.48260100
H	-4.02257300	2.35170700	-2.81565700
H	-4.45402500	1.94555100	-1.14747400
C	-1.32650700	1.70955900	-2.67488600
H	-1.67661900	1.80739400	-3.71189000
H	-0.92832500	2.68145700	-2.36364500
H	-0.50407300	0.98061600	-2.66268600
C	-3.01451800	-0.07847600	-2.37490300
H	-2.26440500	-0.87771400	-2.33611700
H	-3.92850200	-0.42291400	-1.87519600
H	-3.27334900	0.08476600	-3.43000300
C	4.58697100	1.76260400	0.45293500
H	5.55118900	1.79721700	-0.07453000
H	4.26678800	2.79967300	0.60552100
H	4.76615700	1.31030700	1.43728500
C	3.32569000	1.64165900	-1.71128100
H	2.87918400	2.63491500	-1.59196700
H	4.27470500	1.76687000	-2.25232000
C	4.19251100	-0.42545300	-0.65304200
H	4.44662700	-0.96782700	0.26497100
H	3.51639100	-1.05283900	-1.24854800

H	5.11791800	-0.29818600	-1.23283800
H	-1.29213400	2.39284000	1.75627300
H	-2.49258800	3.14029300	0.69740700
H	0.77870300	2.11940000	2.03553400
H	2.37101900	2.79730900	1.71097300
Pd	-0.03277100	-0.72403700	-0.18418300
H	0.81403500	-3.28968900	-4.28732200
C	0.36130100	-3.24944300	-2.21154900
C	1.27388000	-2.84720500	-3.38628900
C	0.81843900	-2.71203100	-0.85478800
H	-0.62747000	-2.82339700	-2.45034500
H	0.92854900	-3.50464600	-0.10652700
H	1.78940200	-2.20858000	-0.90448500
C	1.29022300	-1.33777500	-3.58152300
H	1.71890000	-0.82738700	-2.70733300
H	1.89084200	-1.05166100	-4.45520500
H	0.27494700	-0.94414700	-3.73164000
C	2.68982200	-3.40109100	-3.28545400
H	3.20192800	-3.05143700	-2.37811300
H	2.70540100	-4.49786700	-3.27242600
H	3.29383600	-3.07867300	-4.14349500
C	0.17481400	-4.76218400	-2.13829600
H	-0.14301600	-5.17703900	-3.10470600
H	1.10281800	-5.27065100	-1.84303800
H	-0.58936500	-5.02365600	-1.39440200
H	-3.21629500	-1.49109100	0.04545700
C	-1.07852800	-2.41718800	0.12183800
O	-2.03195300	-2.88621000	-0.49848200
O	-0.86316600	-2.79005400	1.41193300
C	-1.73278900	-3.80111800	1.93697800
H	-1.38053400	-4.00126500	2.95025300
H	-2.77277500	-3.45766900	1.97033000
H	-1.67159100	-4.71486100	1.33535900
H	2.65952900	1.04476500	-2.34893600

Computational Level: M06/def2-TVZP/M06/6-31G(d,p)-LANL2DZ

PTSA

H	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	5.46930170
C	0.68949539	0.00000000	4.26317102
C	0.19907328	0.76530244	3.21281961
C	-0.95638536	1.53127686	3.34641410
C	-1.62931606	1.51804729	4.55754679

C	-1.16519111	0.75116908	5.63242446
H	0.37446495	-0.59018627	6.30388567
H	1.60344685	-0.57300187	4.13210908
H	-1.30430936	2.13881991	2.51455486
H	-2.52986596	2.11774375	4.68161189
C	-1.91819770	0.73662191	6.92714672
H	-2.19571199	1.74989518	7.23873899
H	-2.85000744	0.16514125	6.83235201
H	-1.33159700	0.28160045	7.73111814
S	1.05495509	0.76564302	1.67119597
O	2.39482240	0.26124740	1.87759629
O	0.81349662	2.01364138	0.96648970
O	0.20395263	-0.36923503	0.87302536

HCOOMe

C	-0.82187200	0.43512500	0.00007900
H	-1.40170000	1.37405200	0.00000400
O	-1.28816000	-0.67220600	-0.00004100
O	0.47993500	0.73134400	0.00005400
C	1.34746500	-0.40244100	-0.00009000
H	2.36344300	-0.00732200	-0.01427200
H	1.18510700	-1.01041500	0.89505400
H	1.16539200	-1.02552200	-0.88082900

CH₃OH

C	-0.65358800	-0.01976100	0.00000200
H	-1.08203700	0.98673000	0.00001100
H	-1.03474600	-0.54276800	-0.89126800
H	-1.03473100	-0.54277500	0.89127500
O	0.74267800	0.12182500	-0.00000900
H	1.13161500	-0.75721900	0.00003800

H₂O

O	0.00000000	0.00000000	0.11765300
H	0.00000000	0.75844700	-0.47061100
H	0.00000000	-0.75844700	-0.47061100

HCOOH

C	-0.13056400	0.39895200	-0.00001400
H	-0.08553300	1.50076600	0.00000200
O	-1.13309800	-0.26069500	-0.00015800
O	1.11335300	-0.09353800	0.00015200
H	1.02688100	-1.06060900	0.00013100

A1^{H₂O}

C	-0.02396300	5.23524400	0.06260500
C	0.82985200	4.20936400	0.44236600
C	0.35391300	2.97052200	0.88386200
C	-1.04095100	2.77883400	0.97810800
C	-1.88684200	3.82647100	0.60293800
C	-1.39723800	5.03946000	0.13907500
H	0.38159700	6.18517600	-0.27541500
H	1.90699300	4.37435000	0.41375500
H	-2.96318100	3.69001300	0.69385200
H	-2.08542900	5.83256200	-0.14086800
C	-1.67151300	1.51307500	1.50494600
C	1.36558600	1.92179400	1.25616200
P	-2.10626100	0.27107900	0.15719500
P	1.78355900	0.72113800	-0.13367000
C	-3.99841600	0.07309100	0.31104100
C	3.33370900	1.37146300	-1.00260100
C	-1.54329900	-1.34070600	0.91836000
C	-1.17385300	-1.58597700	2.23926200
C	-0.95666500	-3.58965500	0.37090200
C	-0.69581800	-2.83699100	2.61381200
H	-1.28819900	-0.80609000	2.98620600
C	-0.57976600	-3.85655400	1.67223400
H	-0.88117700	-4.29569600	-0.45759100
H	-0.42147200	-3.01950900	3.65007800
H	-0.20537800	-4.83891000	1.93936800
C	2.43754700	-0.70311100	0.86448600
C	3.06234700	-0.55443700	2.10548600
C	3.53683700	-1.67996300	2.77137700
H	3.19025800	0.43007200	2.54840000
C	2.74756500	-2.98894400	0.94632900
C	3.38232800	-2.92715300	2.18110700
H	4.03154100	-1.57859700	3.73440700
H	2.60883000	-3.94652600	0.44242700
H	3.75019400	-3.83113000	2.65756300
N	2.27489600	-1.91635500	0.30869800
N	-1.42445100	-2.37315200	0.04813900
C	-4.43383100	-0.40482700	1.69128400
H	-4.07829800	0.24768000	2.49940300
H	-5.53098900	-0.41211900	1.74521500
H	-4.09212400	-1.42651100	1.89909000
C	-4.61112100	1.43824600	0.00325200
H	-5.69898600	1.32877400	-0.09603300
H	-4.43466400	2.16538500	0.80454300

H	-4.23351500	1.85797800	-0.93887800
C	-4.45122100	-0.92077100	-0.75531700
H	-4.18642700	-0.58293100	-1.76424600
H	-4.02855900	-1.92321900	-0.61736400
H	-5.54380800	-1.02152100	-0.71144000
C	4.36492900	1.97967900	-0.06110200
H	5.26508900	2.24162300	-0.63345500
H	4.01041000	2.90415100	0.41049600
H	4.67568200	1.28069900	0.72601600
C	2.85576200	2.41348400	-2.01404200
H	2.32374600	3.24592200	-1.53748200
H	3.72058700	2.82803700	-2.54930800
H	2.18052800	1.96726900	-2.75505600
C	3.95176100	0.18963100	-1.75068200
H	4.42895400	-0.52466300	-1.06888300
H	3.21353100	-0.35707300	-2.35241900
H	4.72651700	0.56259400	-2.43357000
H	-0.99456400	1.01419100	2.20546200
H	-2.57849500	1.75891200	2.07203200
H	0.99450200	1.27916900	2.06624100
H	2.27700100	2.40336600	1.63401300
Pd	-0.24978700	0.42086200	-1.24546400
H	-1.67178300	-2.22395600	-0.96653200
H	0.75780900	-1.46668600	-2.46598300
H	0.35467300	-3.75887400	-2.55062900
H	-1.60699500	-3.19985300	-2.84718100
H	1.61053700	-2.16592300	-1.41442000
H	-0.12691000	-5.09865900	-3.21359300
H	-1.93909400	-1.70010600	-3.18127300
O	-0.37031300	-4.42664000	-2.57159400
O	1.23842900	-2.29533300	-2.31566000
O	-2.11651100	-2.41094500	-2.55872800

TSD2_{H₂O}

C	-5.94209300	1.02583800	-2.07733100
C	-5.21365700	1.57298100	-1.02887400
C	-4.41058400	0.78494600	-0.20223800
C	-4.34718300	-0.60097100	-0.44456900
C	-5.11672600	-1.14284100	-1.47597200
C	-5.90141300	-0.34503100	-2.29753700
H	-6.55825200	1.66637400	-2.70254800
H	-5.28549700	2.64145300	-0.83157200
H	-5.11696400	-2.22301700	-1.61994600

H	-6.48828300	-0.79503600	-3.09350000
C	-3.50826000	-1.52422400	0.39480400
C	-3.69946700	1.42998400	0.95829100
P	-1.72241500	-1.62620900	-0.15777400
P	-1.89111900	1.79257500	0.65956700
C	-1.54018900	-3.20270800	-1.19272700
C	-1.77898900	3.67539800	0.55800100
C	-0.92236300	-2.13099200	1.44003300
C	-1.54395300	-2.86301000	2.44139200
C	1.09747100	-2.14488000	2.69613600
C	-0.82881900	-3.23537300	3.57966400
H	-2.58152500	-3.16224100	2.32998100
C	0.50326400	-2.87563500	3.71105800
H	2.13453400	-1.81986700	2.67891400
H	-1.31893800	-3.81642300	4.35682700
H	1.08759700	-3.16149900	4.57866300
C	-1.04083200	1.41341200	2.25353200
C	-1.67601600	1.17976900	3.47306900
C	-0.88988600	0.92378100	4.59424600
H	-2.75865100	1.22526200	3.56651300
C	1.03941100	1.17957100	3.20787400
C	0.49201800	0.92310700	4.46368200
H	-1.35653300	0.74251200	5.55981100
H	2.11953600	1.17775800	3.05484000
H	1.14002200	0.73716900	5.31559200
N	0.29504000	1.40552600	2.12452100
N	0.37218200	-1.78460700	1.62735600
C	-2.18187200	-4.42627100	-0.54806300
H	-3.26814300	-4.32742300	-0.43025300
H	-2.01463700	-5.28996100	-1.20458700
H	-1.73856200	-4.67529800	0.42335400
C	-2.19504400	-2.92539900	-2.54634300
H	-2.03378600	-3.79694600	-3.19407600
H	-3.27644800	-2.77668200	-2.46135000
H	-1.76948600	-2.05378400	-3.05376900
C	-0.04264600	-3.44581800	-1.37158600
H	0.49132200	-2.56957300	-1.76194900
H	0.44569500	-3.76188200	-0.44049700
H	0.10618800	-4.25175000	-2.10152200
C	-2.23220300	4.31699900	1.86796800
H	-2.22514700	5.40852500	1.75115700
H	-3.25334800	4.03531100	2.15498000
H	-1.56074500	4.07085300	2.69894200
C	-2.66488500	4.13655500	-0.59694800

H	-3.73098400	4.00876500	-0.37693000
H	-2.49784000	5.20748700	-0.77000700
H	-2.43605900	3.60716600	-1.53102400
C	-0.33119200	4.06981100	0.27642600
H	0.35248400	3.71131000	1.05572600
H	0.01181100	3.67833200	-0.68939900
H	-0.26581400	5.16573100	0.24144700
H	-3.47680900	-1.19268100	1.44139300
H	-3.94304900	-2.53134500	0.39538200
H	-3.75621900	0.78546600	1.84368800
H	-4.20708500	2.36321100	1.23072500
Pd	-0.92695100	0.49722600	-1.07848100
C	0.03483900	-0.11084400	-2.78430000
H	-0.48971000	1.86499000	-1.74654000
O	-0.26562100	-0.43011800	-3.88332300
O	1.56180400	-0.06875800	-2.55365200
H	0.89243100	-1.26499000	0.88753100
H	1.82456300	-0.30940600	-1.51919900
C	5.36351700	2.84089500	-1.20369900
C	5.09313200	1.53518400	-0.81514100
C	3.85316600	1.24491000	-0.25581300
C	2.88533700	2.23102100	-0.07954100
C	3.17597200	3.52778000	-0.47769300
C	4.41572400	3.85418400	-1.03838700
H	6.32818800	3.08078400	-1.64761100
H	5.82594200	0.74324800	-0.94621200
H	1.91791000	1.97504600	0.35605600
H	2.42552300	4.30827400	-0.35363500
C	4.73054500	5.26379400	-1.43327100
H	5.38543000	5.29961400	-2.30981300
H	3.82309100	5.83184100	-1.66108300
H	5.24937600	5.78876600	-0.62132700
S	3.49795600	-0.39275000	0.29945800
O	3.41879800	-0.40801300	1.76127100
O	4.50205200	-1.27904000	-0.32305900
O	2.10045900	-0.68336300	-0.27777600
C	2.42280700	-0.70825200	-3.52029300
H	3.43283500	-0.33629900	-3.32957400
H	2.38486400	-1.79677000	-3.40420000
H	2.08792600	-0.41061000	-4.51377500
O	2.50538900	-3.60300400	0.94125300
H	2.50928000	-3.46352200	-0.02279800
H	3.36915900	-4.02162400	1.06979600
O	5.13458200	-4.01008600	0.12011800

H	6.01959900	-4.32476200	0.32134100
H	5.16657100	-3.04076100	0.17728400
O	3.17108600	-3.33473400	-1.80479300
H	3.83720800	-4.00745100	-1.59750600
H	3.62237200	-2.52304400	-1.52037300

A3^{H₂O}

C	5.04339100	-1.38052300	-0.83400000
C	3.78530900	-1.81177200	-1.23446500
C	2.73538500	-0.91422500	-1.44257100
C	2.98111100	0.46355700	-1.29520800
C	4.25080200	0.88461100	-0.89411600
C	5.27344200	-0.02264300	-0.64833900
H	5.84168300	-2.10156300	-0.68052300
H	3.61073100	-2.87396200	-1.40607200
H	4.44981300	1.95114000	-0.79698900
H	6.25256200	0.33351400	-0.33991000
C	1.94366600	1.49989500	-1.63547800
C	1.38063900	-1.44696900	-1.81347300
P	0.70274100	1.85190200	-0.29227900
P	0.25663500	-1.66844600	-0.33801800
C	1.01220700	3.63032400	0.24158700
C	0.45806700	-3.45143800	0.27235600
C	-0.95259800	1.89135700	-1.09642600
C	-1.17585200	1.96717000	-2.46862800
C	-3.21017900	1.79850200	-0.65680200
C	-2.49044100	1.94066400	-2.92949200
H	-0.35337900	2.06415800	-3.17351300
C	-3.52661700	1.84872600	-2.01232500
H	-3.98652600	1.70469200	0.10535100
H	-2.69676900	1.99809900	-3.99537600
H	-4.56388600	1.81825400	-2.33311500
C	-1.42217700	-1.67620800	-1.10362100
C	-1.66245100	-2.00719400	-2.43700200
C	-2.97849100	-2.03727900	-2.89111200
H	-0.84617200	-2.25351200	-3.11172800
C	-3.67406900	-1.40251700	-0.69695800
C	-4.00472100	-1.73597100	-2.00756300
H	-3.19479900	-2.30238000	-3.92319100
H	-4.43520400	-1.12304800	0.03430200
H	-5.04427900	-1.75430000	-2.32172100
N	-2.41517300	-1.37166500	-0.25531100
N	-1.95547500	1.81865600	-0.20879400

C	0.80399800	4.56624500	-0.94987400
H	1.45017800	4.33103700	-1.80494700
H	1.04775600	5.58995800	-0.63905500
H	-0.23743000	4.56715300	-1.29215300
C	2.44618400	3.72674200	0.75715600
H	2.59823400	4.71983000	1.19809300
H	3.18641900	3.61343600	-0.04347800
H	2.65717000	2.98208300	1.53574200
C	0.03654700	4.00335800	1.35433600
H	0.15408600	3.37307800	2.24307100
H	-1.00895600	3.94274400	1.03270000
H	0.23221200	5.04055100	1.65482500
C	0.53402400	-4.43290400	-0.89382400
H	0.51205400	-5.45512600	-0.49461000
H	1.46301200	-4.33619900	-1.46825400
H	-0.31728000	-4.33610700	-1.57953800
C	1.73041300	-3.54144600	1.11366100
H	2.62072200	-3.18617400	0.58362200
H	1.90047600	-4.59015300	1.39003700
H	1.64527900	-2.97304200	2.04559700
C	-0.75335200	-3.78934500	1.14357300
H	-1.67100000	-3.87944600	0.55099800
H	-0.93580900	-3.05115600	1.93472000
H	-0.57349800	-4.75847600	1.62688900
H	1.38078000	1.20193400	-2.52788700
H	2.43846200	2.44420500	-1.89043500
H	0.84021100	-0.75767500	-2.47643800
H	1.47553200	-2.39432600	-2.35787700
Pd	0.63140300	0.14533700	1.31840000
H	-1.99357900	0.03762700	2.76526200
H	-5.38319600	0.09170200	2.51763600
H	-2.06103000	1.90725900	1.74352100
O	-2.29827300	1.81757200	2.68371000
O	-4.57312200	0.21925500	2.01529900
O	-2.10643100	-0.92198200	2.58794500
H	-3.25471900	1.65426300	2.66064800
H	-3.92067600	-0.40364900	2.39340300
H	-2.12981700	-0.99167800	1.61242000
H	0.93935300	1.38310800	2.25268400
C	0.65744000	-0.86933100	3.05106600
O	0.69539700	-1.36515200	4.07271600

TSC1^{H₂O}

C	1. 16792100	5. 34520300	0. 54205700
C	1. 72231800	4. 09509400	0. 77493400
C	0. 94534500	2. 94429600	0. 95927300
C	-0. 45670400	3. 09099300	0. 94613400
C	-1. 00300400	4. 36598600	0. 75477800
C	-0. 21404700	5. 48502800	0. 53511600
H	1. 81322300	6. 20808300	0. 39996300
H	2. 80447300	4. 01171400	0. 84829400
H	-2. 08513400	4. 48296400	0. 80211600
H	-0. 67433300	6. 45809900	0. 38682800
C	-1. 41433500	1. 95557800	1. 18097300
C	1. 65098700	1. 65232100	1. 28453700
P	-1. 64150400	0. 79382500	-0. 24926200
P	2. 05027000	0. 40501800	-0. 07406700
C	-2. 23518000	1. 74129700	-1. 77071200
C	3. 42179000	1. 17650600	-1. 12305500
C	-3. 14302600	-0. 16811800	0. 25894200
C	-4. 31870800	0. 32814700	0. 81200300
C	-3. 96119600	-2. 34053700	0. 32842500
C	-5. 34256300	-0. 56023100	1. 11809800
H	-4. 42926600	1. 38855400	1. 02140000
C	-5. 16260100	-1. 91851000	0. 88056500
H	-3. 76727100	-3. 39154200	0. 12120200
H	-6. 27226100	-0. 19612700	1. 54774800
H	-5. 93636200	-2. 64245100	1. 11747700
C	2. 81978600	-0. 86174500	1. 04361500
C	4. 17027800	-1. 17831800	1. 18969800
C	4. 53149800	-2. 21934100	2. 04027400
H	4. 93893400	-0. 63741000	0. 64816800
C	2. 22364700	-2. 50645200	2. 54986100
C	3. 54444300	-2. 90259600	2. 73518300
H	5. 57854800	-2. 48850800	2. 15581400
H	1. 40397400	-3. 00180800	3. 07252700
H	3. 78546300	-3. 72307300	3. 40460400
N	1. 86776400	-1. 52256900	1. 72220100
N	-2. 98966700	-1. 47570600	0. 02682900
C	-3. 37867800	2. 70696500	-1. 47809300
H	-3. 10192000	3. 48034800	-0. 75364500
H	-3. 65438000	3. 22221500	-2. 40795900
H	-4. 27709200	2. 18944500	-1. 12159700
C	-1. 04228200	2. 49325300	-2. 36389900
H	-1. 35594500	2. 97574400	-3. 29935700
H	-0. 65842900	3. 27409800	-1. 69701200
H	-0. 21984900	1. 80574300	-2. 59951800

C	-2.70278400	0.69135700	-2.78119200
H	-1.90094700	-0.01769700	-3.02530300
H	-3.56857700	0.11772700	-2.42623800
H	-3.00052000	1.19729000	-3.70897400
C	4.49152800	1.93214100	-0.33533800
H	5.29907700	2.22566800	-1.01964900
H	4.10253300	2.85300000	0.10622500
H	4.94446000	1.34677700	0.47173700
C	2.72153900	2.14265000	-2.08382500
H	2.17114600	2.93380100	-1.55953800
H	3.47131400	2.62633200	-2.72458000
H	2.02205500	1.60593300	-2.73888300
C	4.07692000	0.08380200	-1.96997100
H	4.63167700	-0.65457700	-1.38205500
H	3.33364000	-0.45066700	-2.57189700
H	4.78565900	0.55046200	-2.66693000
H	-1.08979600	1.31667700	2.01558500
H	-2.39458000	2.35718400	1.46894400
H	1.06719900	1.06040700	2.00587900
H	2.60498400	1.88205400	1.77872200
Pd	-0.02435100	-0.81805700	-0.80268300
C	-0.39206200	-3.01197900	-1.57307300
C	0.88038400	-2.58324700	-1.96445700
C	-0.55904700	-3.96465100	-0.41562900
H	0.10491400	-3.75573600	0.42687700
H	-1.58257300	-3.94249500	-0.02738700
H	-0.36415900	-4.99360200	-0.75469800
C	2.12266100	-3.15836400	-1.33519600
H	2.37003200	-4.10943100	-1.83308700
H	2.98613700	-2.49772200	-1.47020000
H	2.01982900	-3.36697900	-0.26686400
C	1.09355600	-2.05714000	-3.36628300
H	2.09165400	-1.62367700	-3.47781300
H	1.02075700	-2.87606600	-4.09874100
H	0.36743300	-1.29065900	-3.66224700
C	-1.52109900	-3.08825900	-2.57110000
H	-1.47484300	-2.32317500	-3.34961600
H	-1.48218200	-4.06771900	-3.07280600
H	-2.50282500	-3.01650900	-2.08935000
H	-1.58038500	-1.53404900	-0.55930200
H	-0.13166700	-0.75172400	3.52681200
H	-1.68184400	-1.65207100	2.50341300
H	-2.04216800	0.02466500	3.76626400
O	-0.19435400	0.16776700	3.86099600

O	-0.81810000	-2.10353100	2.48393200
O	-2.82758800	-0.31687500	3.29614800
H	-3.39862200	-0.68536700	3.97583400
H	-0.31298200	-1.74133600	1.73554100
H	0.36037000	0.22746000	4.64293800

C5

C	1.92725000	4.56775900	-1.95262900
C	0.68747200	4.18314000	-1.45913300
C	0.56507700	3.29408800	-0.38773600
C	1.73637300	2.83760500	0.24618500
C	2.97734700	3.22832600	-0.26241800
C	3.08259700	4.07034300	-1.36179900
H	1.98897500	5.26179100	-2.78667300
H	-0.21791600	4.59123000	-1.90844800
H	3.88306700	2.88633500	0.23666900
H	4.06161400	4.36129100	-1.73253900
C	1.70078400	2.03125200	1.51541600
C	-0.80695000	2.86206900	0.04903800
P	1.52687200	0.18339800	1.32853100
P	-1.30513200	1.19540000	-0.63649400
C	3.08296300	-0.54629900	2.09385500
C	-2.10150600	1.50413800	-2.32776300
C	0.16469000	-0.30762300	2.46988000
C	-0.28595100	0.44884300	3.55091000
C	-1.39555900	-1.93989800	2.85773900
C	-1.36608000	-0.02917600	4.28870900
H	0.19691400	1.38236500	3.83216500
C	-1.93933800	-1.24167500	3.93413300
H	-1.80539700	-2.90477100	2.55658700
H	-1.74604400	0.53911400	5.13422300
H	-2.78621800	-1.64718200	4.48061400
C	-2.71972300	0.70623400	0.43974700
C	-3.40612100	1.57783400	1.28685600
C	-4.46881800	1.07930700	2.03562200
H	-3.13535900	2.62902900	1.35391100
C	-4.07244000	-1.04791600	1.03087200
C	-4.81397000	-0.25830400	1.90655700
H	-5.02509900	1.73495400	2.70116200
H	-4.31288500	-2.10393200	0.89895600
H	-5.64204200	-0.68507500	2.46532700
N	-3.04389900	-0.58921200	0.32081600
N	-0.37579000	-1.48718600	2.13474300
C	3.21461900	-0.09979400	3.54876500

H	3.25630700	0.99037700	3.66605100
H	4.15296900	-0.49984200	3.95530300
H	2.39701700	-0.48444200	4.16990700
C	4.27619000	-0.06838700	1.26832900
H	5.18042500	-0.58222400	1.61915200
H	4.45662400	1.00782800	1.37978500
H	4.15617300	-0.30100500	0.20362000
C	2.98676100	-2.07057600	2.03892800
H	2.97083500	-2.44131400	1.00964200
H	2.10222200	-2.45058700	2.56327000
H	3.87360500	-2.49256300	2.52946200
C	-3.08017500	2.67306700	-2.29923300
H	-3.57476200	2.75453500	-3.27622700
H	-2.58498900	3.63348900	-2.11339300
H	-3.86668300	2.53487000	-1.54640500
C	-0.97757600	1.77050900	-3.33025200
H	-0.40202900	2.67174200	-3.09711600
H	-1.40941000	1.89807900	-4.33195600
H	-0.26930900	0.93151000	-3.37901400
C	-2.84108900	0.23341800	-2.74719800
H	-3.70005800	0.01491500	-2.10521700
H	-2.18976700	-0.65080100	-2.73975700
H	-3.20839200	0.36727800	-3.77328300
H	0.87538400	2.36687000	2.15366000
H	2.61876900	2.21857700	2.08447400
H	-0.86457900	2.74077300	1.13984200
H	-1.55407900	3.61902000	-0.22133900
Pd	0.61651900	-0.40517000	-0.74503100
H	0.68488800	-3.52591300	-4.88348600
C	0.71225800	-3.53201800	-2.70439300
C	0.03875100	-3.80635800	-4.04425800
C	1.00481600	-2.01922200	-2.62614200
H	1.69421700	-4.03240900	-2.69626800
H	0.03561300	-1.47105400	-2.60205500
H	1.50864000	-1.66558900	-3.53576900
C	-0.09854700	-4.09935900	-1.52194900
H	-0.30626800	-5.14231600	-1.81155100
H	-0.90070600	-3.24767700	-4.14803300
H	-0.19574600	-4.87154300	-4.14683200
C	-1.43987300	-3.40795900	-1.29915800
H	-2.06085200	-3.37317600	-2.20263900
H	-2.01505800	-3.94460500	-0.53461900
H	-1.32487500	-2.38010300	-0.92096600
C	0.69031100	-4.14045600	-0.21935000

H	0.14246900	-4.71211500	0.53985300
H	1.67477800	-4.60816900	-0.34671900
H	0.83237900	-3.13549100	0.20335900
C	1.96175500	-1.65541300	-1.48817400
O	3.07858900	-2.00955800	-1.31430800

PTSA^{H₂O}

H	-2.30654800	-0.49813200	-1.19110500
C	2.62251900	1.29260300	0.14510700
C	1.28268200	0.95277100	0.24880000
C	0.92719200	-0.38846600	0.12448400
C	1.87245300	-1.38198000	-0.09145300
C	3.21023800	-1.01896400	-0.18499500
C	3.60243200	0.31578100	-0.06640200
H	2.92214500	2.33575300	0.23340500
H	0.51615700	1.70880700	0.41375200
H	1.55266700	-2.41713600	-0.18026200
H	3.96646600	-1.78394200	-0.35297800
C	5.04921800	0.69798900	-0.13698400
H	5.48021200	0.78434700	0.86853100
H	5.63738600	-0.04782800	-0.68107800
H	5.18519300	1.66708100	-0.62898800
S	-0.77048400	-0.83164200	0.26148100
O	-1.35949100	-0.08776500	1.37132700
O	-0.92898200	-2.27456700	0.22101000
O	-1.31812300	-0.21357700	-1.11163600
O	-1.79149100	2.54429500	-0.51929300
H	-1.88142800	3.17931900	-1.23432300
H	-1.53488300	1.70656900	-0.93750200
O	-3.83329800	1.17298900	0.82627300
H	-3.17453600	0.76579000	1.40884200
H	-3.30189900	1.85996700	0.38118300
O	-3.79390600	-0.77484400	-0.99206300
H	-4.00564300	-0.07770400	-0.31442700
H	-3.92563500	-1.62726100	-0.56503100

TSC6^{H₂O}

C	3.06555700	2.16811900	4.77045900
C	2.74930800	0.86773300	4.39840500
C	3.00834200	0.38714300	3.11225200
C	3.67732700	1.22441500	2.19813400
C	3.98580700	2.53096700	2.58404300

C	3.66892300	3.01356700	3.84735800
H	2.85258600	2.51298100	5.77885200
H	2.29957000	0.19663200	5.13024100
H	4.51318500	3.17440300	1.88049700
H	3.92562400	4.03391400	4.11990200
C	4.17074700	0.72572100	0.87038500
C	2.55178200	-1.00095900	2.74701500
P	2.92987500	0.70577800	-0.53666700
P	0.82565500	-0.96744300	2.01269600
C	3.72232300	1.85997600	-1.81867700
C	-0.38236000	-1.21127600	3.47044800
C	3.22837400	-0.97287400	-1.28131500
C	4.42125400	-1.68943800	-1.15774200
C	2.27830900	-2.69161000	-2.49691600
C	4.51382600	-2.95994800	-1.72036200
H	5.28188000	-1.26308800	-0.64833900
C	3.41901700	-3.48042500	-2.39476900
H	1.39978300	-3.07852200	-3.01727500
H	5.43644800	-3.52887600	-1.63176300
H	3.42349600	-4.47293300	-2.83617400
C	0.77609800	-2.63100700	1.18620700
C	1.56597000	-3.72658000	1.50297500
C	1.50713900	-4.88436400	0.72445300
H	2.24154900	-3.67455900	2.35187500
C	-0.13094700	-3.84223700	-0.65432800
C	0.65921400	-4.94445400	-0.37124400
H	2.13723200	-5.73379000	0.97660600
H	-0.80387000	-3.78727400	-1.51294400
H	0.62004700	-5.78653500	-1.05559100
N	-0.05442100	-2.74941600	0.11764000
N	2.18111500	-1.47476400	-1.95302200
C	5.09490800	1.38085800	-2.28268800
H	5.81069000	1.26142100	-1.45895000
H	5.51930000	2.12913600	-2.96589200
H	5.03650300	0.43406600	-2.83117900
C	3.85707400	3.24517600	-1.18443400
H	4.05788900	3.98681000	-1.96926400
H	4.69364700	3.29632700	-0.47670800
H	2.95238800	3.56133600	-0.64825300
C	2.78235100	1.91528700	-3.02181100
H	1.80008100	2.32623800	-2.76982700
H	2.61653700	0.92271600	-3.46007100
H	3.22653700	2.55197000	-3.79876300
C	0.16459700	-2.14424200	4.54472700

H	-0.60656500	-2.29534000	5.31185400
H	1.04478900	-1.73784600	5.05606400
H	0.41836300	-3.13541200	4.14606000
C	-0.65694300	0.17632700	4.05276700
H	0.24201600	0.66113500	4.44719400
H	-1.37901600	0.08558700	4.87526600
H	-1.08929700	0.84468200	3.29830100
C	-1.69432600	-1.78172700	2.93109400
H	-1.57917700	-2.79586200	2.52682600
H	-2.13815200	-1.15390400	2.15007800
H	-2.41244200	-1.84206700	3.75970200
H	4.55193700	-0.29505500	0.98282300
H	5.03069400	1.33000800	0.55824800
H	3.18538000	-1.44750100	1.96900100
H	2.59525000	-1.66475900	3.61893200
Pd	0.66794000	0.78739100	0.24066100
H	-1.88946200	0.25836700	-0.18305400
O	-1.50687400	1.48784800	-0.07411200
H	1.34821600	5.42702500	-2.42494000
C	-0.55473400	4.39539600	-2.20784600
C	0.29762100	5.66092700	-2.20857100
C	-0.07485800	3.50757400	-1.04089400
H	-0.34435600	3.84152900	-3.13611700
H	-0.46296800	3.85129700	-0.07528300
H	1.01570400	3.60531000	-0.96635200
C	-2.06026000	4.72144600	-2.21943400
H	-2.19427500	5.38953000	-3.08659800
H	0.26969500	6.17094000	-1.23681900
H	-0.04942100	6.37234700	-2.96662700
C	-2.52958200	5.49193900	-0.99023000
H	-1.97928100	6.42773800	-0.84131500
H	-3.58972300	5.75231600	-1.08811400
H	-2.43280500	4.89865600	-0.06989100
C	-2.93971900	3.49932600	-2.46105400
H	-3.98764500	3.80224000	-2.57533800
H	-2.64805300	2.95429600	-3.36557300
H	-2.89199700	2.78458600	-1.62882800
C	-0.31359300	2.03421000	-1.23611600
O	-0.46591300	1.43593100	-2.26557900
C	-2.09565400	2.16376700	1.02128700
H	-2.90909500	2.81918400	0.67911100
H	-2.52044600	1.40820100	1.69959000
H	-1.36023100	2.75775500	1.58005600
C	-6.37535000	-1.15194100	1.53818600

C	-5.31430600	-1.58929000	0.75742600
C	-4.74303600	-0.70462900	-0.15122500
C	-5.20180400	0.60289100	-0.28276700
C	-6.26119200	1.02188000	0.51072100
C	-6.86524500	0.15325200	1.42516900
H	-6.84087300	-1.83509500	2.24661800
H	-4.93456700	-2.60568300	0.83333400
H	-4.73736700	1.27009600	-1.00750400
H	-6.63906000	2.03843100	0.41385200
C	-8.03512300	0.60100800	2.24573900
H	-8.07196000	0.08589800	3.21103400
H	-8.00891600	1.67935600	2.43217900
H	-8.97787800	0.38475000	1.72786800
S	-3.33277900	-1.20500000	-1.08601900
O	-2.15357700	-0.81577000	-0.10903000
O	-3.24633700	-0.38477400	-2.28533800
O	-3.31160900	-2.66195000	-1.19213900
H	-0.65356500	-1.94865900	-0.16204100
H	-0.35817100	-4.83772200	-3.45631600
H	-1.29358600	-2.75633400	-3.33614800
H	0.36915400	-1.06005900	-2.38767200
O	-0.55503900	-1.34968900	-2.50764000
O	-1.69337800	-3.64400800	-3.42918700
O	0.50413200	-5.28177200	-3.32314900
H	-1.05322000	-0.53984900	-2.69045600
H	-2.51804500	-3.57097500	-2.92926600
H	0.62646600	-5.82521400	-4.10517800

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C	4.19332200	4.13834400	-0.61653600
C	4.21642000	2.84190400	-0.12311200
C	3.11868500	2.26832100	0.52837700
C	1.95558000	3.05187000	0.69964600
C	1.96373500	4.36912400	0.22682900
C	3.05509800	4.91418000	-0.43428200
H	5.06764500	4.54701300	-1.11617300
H	5.12772500	2.25226100	-0.22437000
H	1.08711500	4.99263500	0.40377200
H	3.02237500	5.94196700	-0.78559000
C	0.71079700	2.57294700	1.40161700
C	3.28498900	0.87232100	1.06713300
P	-0.59721500	1.83129800	0.25169700
P	2.63436400	-0.52143900	-0.01622900
C	-1.74996600	3.22997700	-0.28587300

C	4.02485200	-1.09317300	-1.15797600
C	-1.53124600	0.85982500	1.54252200
C	-2.60647200	1.22599700	2.33794900
C	-1.63654500	-1.34273400	2.45908200
C	-3.21049400	0.29173300	3.17382900
H	-3.00894900	2.23117900	2.27880000
C	-2.72180000	-1.01065100	3.24277100
H	-1.17881600	-2.32710300	2.42587100
H	-4.07627700	0.58468400	3.76076400
H	-3.17581900	-1.75612000	3.88673800
C	2.51680800	-1.85972200	1.26565900
C	3.54352700	-2.15685500	2.16659700
C	3.39089500	-3.22280300	3.04544600
H	4.45346800	-1.56186200	2.18288200
C	1.23738900	-3.58435400	2.09369200
C	2.21996800	-3.96854100	2.99851200
H	4.17979800	-3.47232700	3.75076100
H	0.30174400	-4.14432400	2.02558300
H	2.06586900	-4.82355800	3.65032600
N	1.36232000	-2.54797700	1.25999800
N	-1.08658700	-0.41716500	1.66264500
C	-1.92968300	4.36553100	0.71659900
H	-0.99865300	4.91764300	0.89025600
H	-2.65863500	5.08442400	0.31913000
H	-2.30397400	4.03494800	1.69299000
C	-1.09670800	3.77374700	-1.56346800
H	-1.70044600	4.60544000	-1.95037300
H	-0.07897100	4.14580800	-1.39379000
H	-1.04401200	3.00066000	-2.34087500
C	-3.09992900	2.61831000	-0.66841100
H	-2.96899500	1.72250900	-1.29048300
H	-3.71715200	2.32487800	0.18886200
H	-3.66915900	3.35869700	-1.24755300
C	5.40729800	-1.17207900	-0.52284800
H	6.13563400	-1.47918100	-1.28561400
H	5.75080800	-0.20790800	-0.12647500
H	5.45516400	-1.91764400	0.27958200
C	4.03975500	-0.10529600	-2.32652900
H	4.27051700	0.91823700	-2.00594800
H	4.80306000	-0.41144600	-3.05459100
H	3.07035900	-0.08603100	-2.84091000
C	3.60663900	-2.47161300	-1.67153600
H	3.61813700	-3.22880900	-0.87675900
H	2.60416500	-2.45454900	-2.12053700

H	4.31073500	-2.79704500	-2.44894700
H	0.93958700	1.76174500	2.10547000
H	0.26622000	3.38595100	1.99136400
H	2.73564600	0.74513300	2.01034300
H	4.34305700	0.69896800	1.30496800
Pd	0.62595800	0.24539500	-0.91121500
H	-0.31258000	-0.69832200	1.02357100
C	-3.25833700	-1.65440700	-1.15811600
H	-3.80808000	-2.55583300	-0.83886300
O	-3.09538400	-0.67219300	-0.47082400
O	-2.81848500	-1.82281100	-2.39429200
C	-2.11858800	-0.72301000	-2.99153100
H	-1.29647300	-0.37764800	-2.34260900
H	-1.71971000	-1.10017500	-3.93218500
H	-2.81173700	0.10761400	-3.16522300
C	-0.29639700	-3.02920500	-1.52892400
H	0.05188200	-2.24669200	-0.82480200
O	0.01580500	-3.10486200	-2.68873900
O	-1.10516400	-3.87973100	-0.88368600
C	-1.63945700	-4.92971400	-1.70095100
H	-2.23411200	-5.55903000	-1.03806900
H	-2.26355800	-4.50550800	-2.49431800
H	-0.83308200	-5.50959000	-2.15778800
C	-5.64627400	-0.33695600	0.85488900
H	-5.57978600	-1.27649200	1.43306400
O	-5.38652500	0.75754400	1.28893800
O	-6.06984300	-0.61766400	-0.37048200
C	-6.15876300	0.49689300	-1.26326500
H	-6.70275400	0.14306400	-2.13876300
H	-6.68552900	1.33004900	-0.79097200
H	-5.14869100	0.81989200	-1.54119800

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C	-5.76468900	-2.79299300	-2.19246400
C	-5.50170200	-2.06027400	-1.04229700
C	-4.31851600	-2.22666800	-0.31976200
C	-3.40323600	-3.21199100	-0.73895800
C	-3.67880100	-3.94140600	-1.89709700
C	-4.83704600	-3.72841000	-2.63346900
H	-6.69440400	-2.63978000	-2.73388000
H	-6.23900600	-1.34396100	-0.67991700
H	-2.97744900	-4.71117800	-2.21602500
H	-5.02617400	-4.31160500	-3.53054700

C	-2.19569400	-3.57821100	0.08223700
C	-4.06801900	-1.35119000	0.87753500
P	-0.71453000	-2.44850300	-0.11354300
P	-3.03122700	0.15271500	0.47303000
C	0.63171300	-3.51930100	-0.89505600
C	-4.20889300	1.55957100	0.01046900
C	-0.17068400	-2.30066700	1.66109700
C	-0.43795500	-3.21695300	2.67083700
C	0.96977700	-0.93139600	3.23325000
C	-0.01536400	-2.96504900	3.97401800
H	-0.96170500	-4.14018400	2.44270500
C	0.68699700	-1.80490200	4.26677500
H	1.57578500	-0.03021800	3.32027700
H	-0.22682100	-3.68924300	4.75667400
H	1.03885500	-1.58850300	5.26949000
C	-2.37055100	0.67236200	2.11495300
C	-2.92268400	0.30330400	3.34333600
C	-2.32031300	0.76990300	4.50935400
H	-3.80918700	-0.32549400	3.39608100
C	-0.73694500	1.91845300	3.13784700
C	-1.20912600	1.59598600	4.40935000
H	-2.72623700	0.50048500	5.48168800
H	0.13229600	2.56768000	3.00922500
H	-0.71797300	1.99148100	5.29423200
N	-1.28894700	1.45859000	2.01619100
N	0.52105900	-1.19170400	1.99796500
C	1.08219000	-4.65794700	0.01472400
H	0.25258900	-5.28283900	0.37205600
H	1.75086000	-5.31520300	-0.55797300
H	1.65138700	-4.28341400	0.87566000
C	0.04475400	-4.05743200	-2.20088400
H	0.85524700	-4.51169700	-2.78524200
H	-0.70996400	-4.83590500	-2.03704100
H	-0.39578800	-3.26161700	-2.81657800
C	1.82353300	-2.62164500	-1.21348100
H	1.58738100	-1.89757900	-1.99881400
H	2.21288300	-2.07812100	-0.34515400
H	2.64709700	-3.23961300	-1.59474700
C	-5.39879100	1.62377400	0.96456400
H	-5.99238300	2.51831700	0.73569500
H	-6.07044900	0.76285400	0.86026500
H	-5.08636600	1.70014500	2.01436500
C	-4.68361400	1.34879800	-1.42649700
H	-5.22974600	0.40945200	-1.55994400

H	-5.35867500	2.17015400	-1.70153900
H	-3.84198000	1.34777300	-2.12980800
C	-3.42801800	2.87233900	0.08060800
H	-3.14474200	3.14522700	1.10309100
H	-2.51284900	2.83158000	-0.52339800
H	-4.06457300	3.67330400	-0.31852100
H	-2.46813700	-3.58183600	1.14350400
H	-1.88347000	-4.60224000	-0.15675000
H	-3.50130900	-1.88447300	1.65470200
H	-5.01587600	-1.04382100	1.33707300
Pd	-1.28243400	-0.27804400	-1.07031700
C	0.03149900	-0.12912000	-2.63457100
H	-1.62959800	1.12218800	-1.72701400
O	0.06838100	-0.43856200	-3.77553900
O	1.26500200	0.63842500	-2.15051600
H	0.82371700	-0.50996100	1.26038800
H	1.45793600	0.57938600	-1.09046900
C	1.50416900	5.19328800	2.00118700
C	2.13746400	3.95808000	1.94087400
C	1.79924500	3.07039300	0.92324600
C	0.85382500	3.40772800	-0.04233600
C	0.23347500	4.64824400	0.03520700
C	0.54221900	5.55474900	1.05455900
H	1.76232500	5.89440000	2.79302300
H	2.88282800	3.67172000	2.67922400
H	0.59462900	2.71459800	-0.84292500
H	-0.50294900	4.93020000	-0.71845300
C	-0.15563400	6.87780000	1.13285300
H	0.40584000	7.59391300	1.74067900
H	-0.30018200	7.31339700	0.13826200
H	-1.15014200	6.77286700	1.58458800
S	2.65717600	1.52282200	0.84088600
O	2.94401300	1.12308400	2.22691600
O	3.79236400	1.65764800	-0.06851600
O	1.62721800	0.54487800	0.24656200
C	2.40290600	0.86037300	-3.00279700
H	2.69423200	1.90786800	-2.89114000
H	3.21030400	0.18734000	-2.69774600
H	2.07632500	0.65713100	-4.02401300
C	-0.58741200	3.95734000	-3.39743400
H	-1.68669700	4.03921700	-3.45092600
O	0.02673400	2.92277200	-3.33573100
O	-0.05461600	5.17614500	-3.40557600
C	1.37625000	5.21644900	-3.36322900

H	1.80004000	4.62738700	-4.18172100
H	1.65055900	6.26604500	-3.46611800
H	1.74003400	4.82032200	-2.40828500
C	5.49076700	-0.72602700	-1.13588000
H	5.44021000	0.20438200	-0.54938200
O	4.52760400	-1.37855200	-1.47296700
O	6.75073200	-1.02215600	-1.43140100
C	6.94238900	-2.19834800	-2.21597100
H	6.37023100	-2.14095400	-3.14649900
H	8.01024300	-2.25242600	-2.42655200
H	6.62150800	-3.08699900	-1.66229200
C	4.18322000	-1.78453000	1.74931000
H	4.38652500	-0.72646600	1.99083200
O	3.11600800	-2.33403300	1.91529100
O	5.26809100	-2.36642000	1.25384600
C	5.09337400	-3.71446400	0.81283700
H	4.44599600	-3.72812600	-0.07243800
H	6.08953600	-4.08235000	0.56373100
H	4.64748600	-4.32740600	1.60134900

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C	-6.02764600	-0.33197600	-1.49657900
C	-5.11693400	-1.19232600	-0.89832200
C	-4.17278600	-0.73751500	0.02519000
C	-4.17057100	0.62632800	0.37838800
C	-5.10507200	1.47625700	-0.21727800
C	-6.01914500	1.01429500	-1.15510600
H	-6.75274000	-0.71688700	-2.20862200
H	-5.15517200	-2.25591900	-1.13076200
H	-5.13325900	2.52259800	0.07922300
H	-6.73644900	1.70067400	-1.59687200
C	-3.23570400	1.18019400	1.42425400
C	-3.22679700	-1.72810000	0.64453400
P	-1.56137700	1.68137800	0.78454400
P	-1.51354400	-1.73013600	-0.09526100
C	-1.52106600	3.56760900	0.78129700
C	-1.42265400	-3.22083000	-1.25700100
C	-0.31237700	1.21393900	2.03951800
C	-0.58198300	0.78230100	3.33479200
C	1.95286900	1.07443400	2.35302000
C	0.50094500	0.45514000	4.15025100
H	-1.59929500	0.70917200	3.71429000
C	1.78828800	0.60097200	3.65435500

H	2.94526200	1.21120800	1.92821600
H	0.33323300	0.09358800	5.16202600
H	2.66211400	0.34708600	4.24821000
C	-0.43212600	-2.24561400	1.29952800
C	-0.87481200	-2.94403400	2.42352300
C	0.07039000	-3.32465700	3.37276900
H	-1.92207300	-3.20948700	2.55221800
C	1.75255400	-2.31573100	2.00231500
C	1.40449600	-3.00495400	3.16285900
H	-0.23521400	-3.87504700	4.25945900
H	2.78918800	-2.04490900	1.79107900
H	2.17059600	-3.28819100	3.87909400
N	0.85226200	-1.93730900	1.09398400
N	0.92696600	1.35294600	1.55215800
C	-1.59790700	4.05991400	2.22805400
H	-2.46798600	3.66793600	2.77088400
H	-1.69023900	5.15335200	2.22310600
H	-0.69554500	3.80651900	2.79524000
C	-2.70925900	4.09103200	-0.02082800
H	-2.59749900	5.17528000	-0.14803500
H	-3.66259800	3.92609000	0.49332400
H	-2.76741300	3.64526000	-1.02260100
C	-0.22512100	4.06347500	0.14410200
H	-0.19660000	3.83354200	-0.92888700
H	0.67011500	3.64182000	0.61510200
H	-0.18757900	5.15581000	0.24586100
C	-1.79537300	-4.51584400	-0.53960900
H	-1.72324800	-5.34702700	-1.25307200
H	-2.82465900	-4.51428100	-0.16012300
H	-1.11691500	-4.73775800	0.29172500
C	-2.37460800	-2.98231800	-2.42589400
H	-3.42372200	-2.98655300	-2.11142200
H	-2.24939100	-3.78510300	-3.16415100
H	-2.18532800	-2.03024700	-2.93777400
C	0.01625200	-3.32655600	-1.76248600
H	0.73959200	-3.46859800	-0.95197500
H	0.32484500	-2.43696800	-2.32521500
H	0.08998800	-4.18480700	-2.44290600
H	-3.05098600	0.43991700	2.21260000
H	-3.69211800	2.04755800	1.91740200
H	-3.08213300	-1.51980200	1.71323900
H	-3.64818700	-2.73938900	0.58591300
Pd	-0.97100500	0.46592600	-1.13426500
C	5.18756700	0.05631600	0.85988400

H	5.10215300	1.14412100	0.69628800
O	4.64918400	-0.54977100	1.75609500
O	5.95176500	-0.47780800	-0.08799100
C	6.16156800	-1.89445900	0.01551600
H	5.20593600	-2.41785700	-0.07617800
H	6.82772200	-2.15727400	-0.80631500
H	6.62735300	-2.13471800	0.97528500
C	2.66433200	-0.71752200	-0.99397000
H	2.07585500	-0.19109500	-0.22141300
O	3.17494700	-1.80155600	-0.87570300
O	2.71682700	0.02620800	-2.10705200
C	3.51805500	-0.51054900	-3.16466100
H	3.55299100	0.25961500	-3.93618800
H	4.52376800	-0.73582400	-2.79329400
H	3.07319300	-1.42946000	-3.55896600
C	2.95601500	2.65039200	-1.22843400
H	1.87705300	2.74239400	-1.44574700
O	3.41926100	2.46154700	-0.12988700
O	3.65460100	2.78088900	-2.34874800
C	5.06720700	2.60630000	-2.20301000
H	5.49269900	2.73451900	-3.19831100
H	5.48001100	3.34837900	-1.51363700
H	5.28617000	1.60237200	-1.81908500
H	-0.74555000	1.95382100	-1.64017500
C	-0.31119400	-0.03313100	-2.94730000
O	0.08130100	-0.21736200	-3.99998400

TSC1^{HCOOMe}

C	6.94845000	-1.12922400	-0.43102300
C	5.79269700	-1.64688600	0.13503600
C	4.73761400	-0.83544300	0.57085300
C	4.88647400	0.56021400	0.44679600
C	6.07898700	1.07133600	-0.07964700
C	7.09861900	0.24814100	-0.53273700
H	7.73934300	-1.79841200	-0.75933000
H	5.71422600	-2.72377300	0.27027800
H	6.21594800	2.15142800	-0.11543200
H	8.00997600	0.67917900	-0.93846900
C	3.84416400	1.54676300	0.89547200
C	3.57216900	-1.48724700	1.26387200
P	2.35827600	1.70667800	-0.21317900
P	1.99090200	-1.93126700	0.33943100
C	2.91425300	2.24351600	-1.93450000

C	2.43539600	-3.39925300	-0.76348700
C	1.55065000	3.23074300	0.47317800
C	2.17310200	4.38277700	0.94098400
C	-0.55729700	4.13877800	0.86160000
C	1.38081200	5.43793100	1.38692800
H	3.25712100	4.46427000	0.96215500
C	-0.00233100	5.32013700	1.34142700
H	-1.63797700	3.99694400	0.80528500
H	1.84302500	6.34683000	1.76375700
H	-0.64935500	6.12440600	1.67763400
C	1.10250800	-2.54370500	1.84877800
C	0.71464400	-3.84937200	2.14686200
C	-0.00992100	-4.08538900	3.31173200
H	0.96005000	-4.67730400	1.48931500
C	0.13408700	-1.75530500	3.78108900
C	-0.31422300	-3.02149700	4.14760400
H	-0.32877600	-5.09487300	3.55976200
H	-0.07196400	-0.89212600	4.41436900
H	-0.87939700	-3.16285200	5.06409300
N	0.81739600	-1.51482500	2.66404200
N	0.21610800	3.12832300	0.45535300
C	3.95417400	3.35748800	-1.91676000
H	4.88877000	3.04660100	-1.43980100
H	4.19724500	3.63703500	-2.95074600
H	3.58268200	4.26174700	-1.41877300
C	3.45637600	1.00590100	-2.65333800
H	3.71817000	1.27744600	-3.68492400
H	4.35578200	0.59600600	-2.17659400
H	2.69639100	0.21411500	-2.69518900
C	1.66363800	2.73141000	-2.66919600
H	0.87728600	1.96545600	-2.68684700
H	1.24501700	3.64322500	-2.22454500
H	1.93007600	2.96373600	-3.70869500
C	3.32219000	-4.44993700	-0.09763600
H	3.47978700	-5.28279600	-0.79624100
H	4.31100200	-4.05923500	0.16099200
H	2.88633200	-4.86688700	0.81711500
C	3.15562200	-2.79879300	-1.97605900
H	4.07037200	-2.25813900	-1.70532700
H	3.43525300	-3.60437800	-2.66842600
H	2.49609600	-2.10769900	-2.51869200
C	1.15162800	-4.05244400	-1.27784300
H	0.56112800	-4.53877000	-0.49438900
H	0.51159700	-3.32155900	-1.78482400

H	1.41471000	-4.82312600	-2.01477700
H	3.41511300	1.27779000	1.87170500
H	4.30836200	2.53382200	1.01723900
H	3.18204300	-0.84728400	2.06636100
H	3.91351800	-2.41010400	1.75137000
Pd	0.65979800	0.09460400	-0.25937400
C	-1.63999200	0.49954800	-0.35985000
C	-1.39692400	-0.83549200	-0.71387400
C	-2.13106100	0.83309800	1.03364800
H	-1.51825900	0.36640000	1.81181800
H	-2.12988900	1.91269100	1.20544100
H	-3.16450900	0.48574200	1.18347200
C	-1.75369200	-1.96064200	0.22163500
H	-2.81762800	-2.21573800	0.08738500
H	-1.18501900	-2.86545900	-0.01674900
H	-1.59277200	-1.72348300	1.27696100
C	-1.36107000	-1.22841200	-2.17448700
H	-1.10820200	-2.28683100	-2.28758800
H	-2.35328900	-1.10694000	-2.63473600
H	-0.64396700	-0.64355700	-2.76483900
C	-1.99818700	1.50519600	-1.43119600
H	-1.44466900	1.35286100	-2.36166600
H	-3.06748800	1.41719600	-1.68736400
H	-1.83243100	2.53644700	-1.10475300
H	0.00961000	1.68861900	-0.02124300
C	-5.46955900	-2.85232100	-2.19859600
H	-5.84237300	-2.59772000	-3.20414600
O	-4.31852000	-2.76634100	-1.84521600
O	-6.48457400	-3.25880900	-1.44480100
C	-6.14894600	-3.66870500	-0.11033600
H	-7.05859400	-4.10527000	0.30187900
H	-5.34462100	-4.40908600	-0.13198600
H	-5.83674200	-2.80536800	0.48643000
C	-5.06048700	-0.28144800	-0.47744100
H	-4.03966000	-0.35588500	-0.88955400
O	-5.35450800	-0.47580300	0.67600700
O	-5.90646200	0.05483600	-1.44882900
C	-7.28568800	0.12977500	-1.05770200
H	-7.83348300	0.43015700	-1.95056100
H	-7.63005100	-0.85083000	-0.71240100
H	-7.41251000	0.86674900	-0.25976200
C	-4.84660900	3.07351700	0.23428300
H	-4.83697200	2.52555600	-0.72616800
O	-3.90149900	3.64853900	0.71598700

O	-6.05813700	2.99163300	0.76525500
C	-6.22243100	3.64058000	2.03255100
H	-7.25399500	3.45899100	2.33133600
H	-5.52981800	3.21887300	2.76596900
H	-6.03392500	4.71327400	1.93615500

PTSA^{HCOOMe}

H	-0.77190900	-0.31387900	1.07462800
C	4.51429600	-1.73018000	0.20075900
C	3.14515700	-1.84146600	-0.00662700
C	2.40307900	-0.68193500	-0.19454100
C	2.99322900	0.58002000	-0.18694900
C	4.36139300	0.66550000	0.02156900
C	5.13816400	-0.48182400	0.21847100
H	5.11242300	-2.62775500	0.34782300
H	2.65221800	-2.80960900	-0.03208400
H	2.39354900	1.47434800	-0.35269500
H	4.84325600	1.64210300	0.02604900
C	6.61545300	-0.35828700	0.43508800
H	7.10225900	0.11179400	-0.42796000
H	6.83646000	0.26999100	1.30620000
H	7.08474400	-1.33381600	0.59503300
S	0.66430800	-0.81452900	-0.43107300
O	0.33602500	-2.15629000	-0.88761100
O	0.17733600	0.32768000	-1.20014700
O	0.17204800	-0.63727100	1.08012200
C	-2.85690300	-2.66733900	0.13317200
H	-1.81888300	-2.72426000	-0.23938600
O	-3.27535900	-3.14719000	1.15180000
O	-3.60136400	-1.96444100	-0.74025300
C	-4.96460800	-1.80325500	-0.35621200
H	-5.42537000	-1.17691700	-1.12177700
H	-5.46788700	-2.77315400	-0.29873500
H	-5.03135300	-1.32200600	0.62603000
C	-0.08630400	3.15613800	-0.85944100
H	-0.66201700	3.20575800	-1.79872800
O	1.09842000	3.33349800	-0.75634600
O	-0.91980800	2.89027300	0.15038700
C	-0.28373400	2.70829500	1.41875200
H	-1.07690400	2.43109300	2.11464800
H	0.45480000	1.90137200	1.35998500
H	0.21146500	3.63146200	1.73364600
C	-2.65680500	0.68000300	-0.23781600
H	-2.18001900	0.30901700	-1.15516900

O	-2.30028200	0.39889200	0.89281900
O	-3.67179600	1.47405100	-0.51799000
C	-4.27638000	2.12460600	0.60387800
H	-5.10180500	2.71109000	0.20113500
H	-4.64070300	1.39318800	1.33052100
H	-3.54123600	2.77736800	1.08512500

TSC6^{HCOOMe}

C	6.09720700	0.96995700	3.65495500
C	5.39759000	-0.17770200	3.30447800
C	5.07834000	-0.46739600	1.97556000
C	5.53969700	0.39472200	0.96195100
C	6.23591700	1.54886200	1.33010800
C	6.50132700	1.85115800	2.65954200
H	6.33278900	1.16752600	4.69741700
H	5.09777300	-0.87846400	4.08366400
H	6.60403200	2.21151700	0.54749100
H	7.05075100	2.75410400	2.91272400
C	5.41090500	0.06422800	-0.49803700
C	4.24006700	-1.68280900	1.67517700
P	3.75391400	0.42944800	-1.30679400
P	2.41803900	-1.24924300	1.64715200
C	4.23644500	1.56025700	-2.75445100
C	1.78216900	-1.44870400	3.43626200
C	3.37643000	-1.17480400	-2.16884300
C	4.34497600	-2.05886400	-2.65430700
C	1.68452600	-2.52507100	-2.93992800
C	3.93567000	-3.22343500	-3.29593100
H	5.40641200	-1.84315100	-2.55344400
C	2.57719100	-3.46527600	-3.44750300
H	0.60831900	-2.67135300	-3.04601600
H	4.67173900	-3.92393100	-3.68350800
H	2.21243700	-4.35557900	-3.95242200
C	1.70726400	-2.76702600	0.84759500
C	2.30461600	-4.01352900	0.71646200
C	1.63050200	-5.05171200	0.07160300
H	3.29517200	-4.18245000	1.12857700
C	-0.21283600	-3.59438900	-0.30049000
C	0.35443500	-4.84846300	-0.43835400
H	2.10618300	-6.02531700	-0.01844900
H	-1.20905200	-3.34439100	-0.66058700
H	-0.22446100	-5.62181100	-0.93267700
N	0.46887100	-2.61674700	0.31265300

N	2.06429300	-1.41658400	-2.30478300
C	5.27961400	0.95385600	-3.68879400
H	6.20742300	0.67015300	-3.17572300
H	5.55185500	1.70063600	-4.44726100
H	4.89546000	0.07675700	-4.22178600
C	4.78357000	2.85626100	-2.15501400
H	4.84939800	3.62408000	-2.93786000
H	5.79396500	2.72853100	-1.74702400
H	4.15049700	3.24979100	-1.34865800
C	2.96284500	1.83670400	-3.55218300
H	2.19940500	2.35312900	-2.96219500
H	2.50839500	0.91164300	-3.92810300
H	3.20740500	2.46843800	-4.41710500
C	2.48448500	-2.56153100	4.20379600
H	2.00752300	-2.67559400	5.18666600
H	3.54356400	-2.35016500	4.38812900
H	2.40648200	-3.53150400	3.69466200
C	1.99534400	-0.09685600	4.12008900
H	3.04453900	0.21793200	4.12656700
H	1.65491400	-0.16104900	5.16234200
H	1.41461500	0.69067600	3.62305000
C	0.28199700	-1.73958800	3.39444500
H	0.06294300	-2.75534000	3.04185100
H	-0.27365700	-1.02956500	2.76864400
H	-0.11642900	-1.66117500	4.41472700
H	5.62841900	-0.99915800	-0.65540300
H	6.18348100	0.61087700	-1.05135600
H	4.45436200	-2.07868400	0.67321100
H	4.44819800	-2.48403200	2.39565100
Pd	1.94896000	0.69384500	0.23005900
H	-0.74063900	0.66788200	0.62574600
O	-0.10134000	1.74257600	0.67642400
H	2.20870700	5.25125500	-2.68903000
C	0.37779500	4.45681300	-1.82700200
C	1.30517600	5.61437000	-2.18167400
C	1.10964300	3.55631200	-0.81056700
H	0.22659400	3.85301500	-2.73529000
H	1.07004800	3.96568100	0.20521600
H	2.17415500	3.53314800	-1.07401600
C	-1.01632900	4.94610000	-1.39118200
H	-1.37889900	5.54848900	-2.24092700
H	1.63029900	6.16505100	-1.28924400
H	0.80957700	6.32852200	-2.84949400
C	-0.98897300	5.86241800	-0.17305700

H	-0.37003500	6.75278800	-0.32986600
H	-2.00177100	6.20642100	0.06601900
H	-0.60975900	5.34508700	0.72031500
C	-2.00940300	3.80623800	-1.18757700
H	-3.02804900	4.19278200	-1.05676400
H	-2.01194800	3.10619100	-2.03116800
H	-1.76422200	3.21876700	-0.29233200
C	0.65531300	2.12200500	-0.83773400
O	0.12368700	1.50262700	-1.70779300
C	-0.12517200	2.47805200	1.88570400
H	-0.84331100	3.30762600	1.82455100
H	-0.43889900	1.80189200	2.69382800
H	0.86872100	2.87419300	2.13025600
C	-4.61324700	-0.15934400	3.60894600
C	-3.89640900	-0.70048800	2.55012200
C	-3.58428800	0.11245200	1.46564700
C	-3.97271300	1.44651800	1.42294200
C	-4.69686400	1.96745100	2.48823600
C	-5.02607400	1.17753000	3.59412400
H	-4.86882300	-0.78416000	4.46330200
H	-3.59395500	-1.74517400	2.55043900
H	-3.74132900	2.05867100	0.55374000
H	-5.01796000	3.00802500	2.45600500
C	-5.83248300	1.73979800	4.72443900
H	-5.60810300	1.23541000	5.66979800
H	-5.65026100	2.81119300	4.85638100
H	-6.90674800	1.61467400	4.53954700
S	-2.63744200	-0.54522500	0.12616100
O	-1.16120600	-0.38795200	0.66962300
O	-2.81198200	0.29248700	-1.04665700
O	-2.85570000	-1.98796200	0.03186200
H	-0.01344100	-1.69541600	0.37400900
C	-3.56467100	-4.65213900	-0.83481100
H	-3.57062600	-4.50625000	0.25755100
O	-2.58780200	-4.95752500	-1.48353600
O	-4.77486500	-4.43546500	-1.31004500
C	-4.93860400	-4.56144600	-2.73056800
H	-5.90291000	-4.10598000	-2.95494000
H	-4.13357900	-4.03547600	-3.25167400
H	-4.91854400	-5.61750300	-3.01433200
C	-5.68368200	-1.37003600	-1.67881800
H	-4.70428700	-1.34368600	-2.18771000
O	-6.66183400	-1.95477100	-2.05970500
O	-5.60480400	-0.64043600	-0.56004400

C	-6.83284700	-0.49790400	0.15438900
H	-6.60011500	0.13175900	1.01805600
H	-7.57821700	-0.01682300	-0.48769300
H	-7.20846700	-1.47263700	0.47949100
C	-5.59623100	2.03079000	-1.72592500
H	-4.56924200	1.69447400	-1.94659700
O	-6.60438400	1.58579800	-2.20678000
O	-5.55532600	3.01334900	-0.81207800
C	-6.83525600	3.49749800	-0.40249600
H	-6.64488400	4.32911800	0.27706000
H	-7.41717500	3.83506400	-1.26461400
H	-7.39667600	2.70703900	0.10871000