

Probing Enantioselectivity in Rhodium-Catalyzed Si–C Bond Cleavage to Construct Silicon-Stereocenter: A Theoretical Study

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1. Figure S1, S2 and S3.

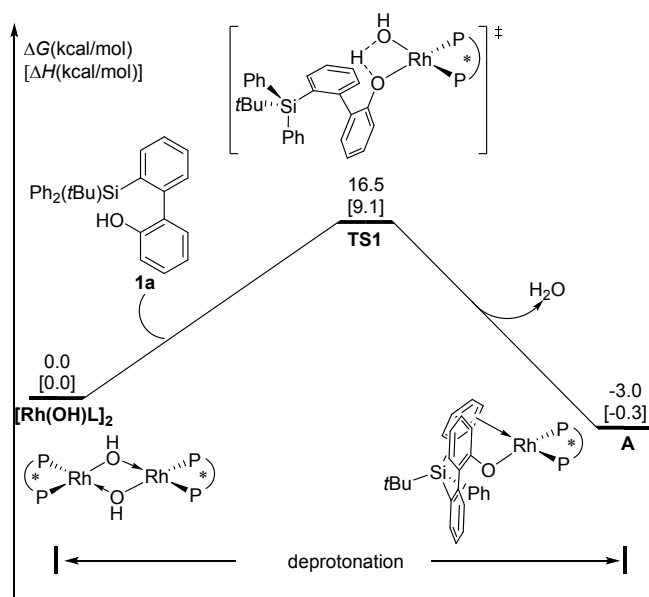


Figure S1. Free-energy profile calculated for deprotonation step.

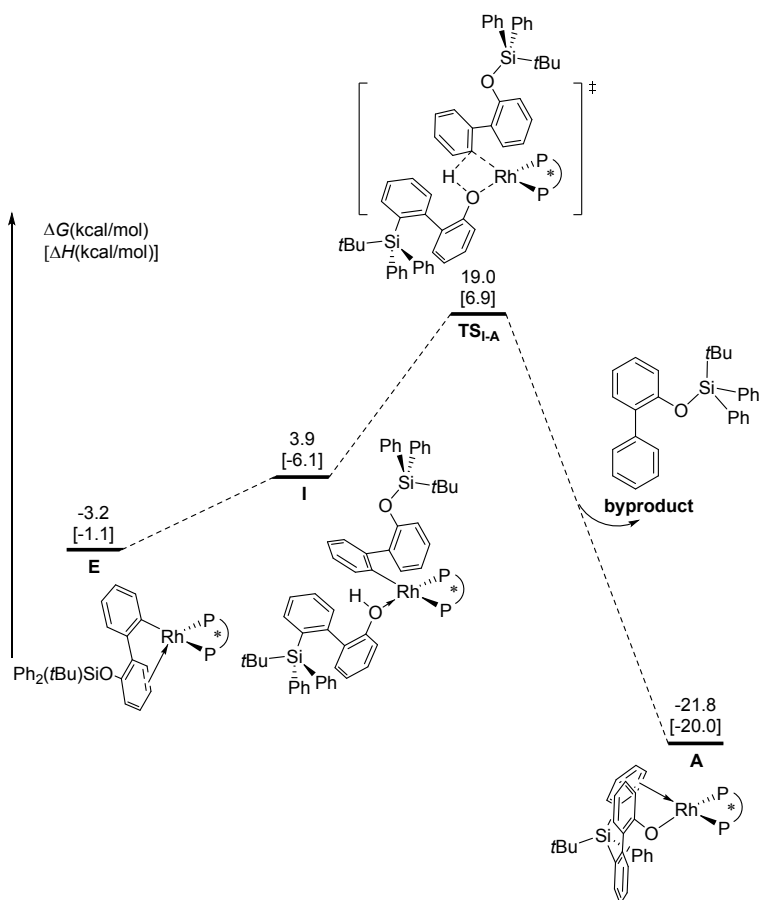


Figure S2. Free-energy profile calculated for the pathway from complex **E** to byproduct and active species **A**.

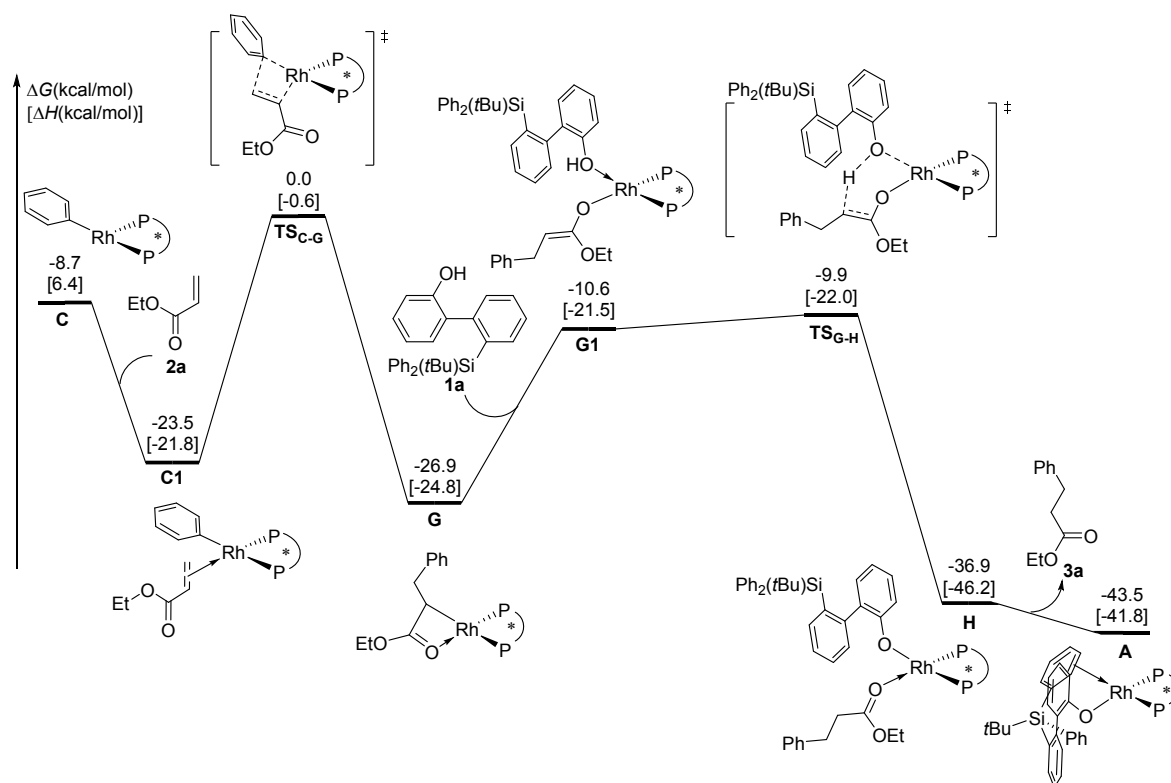


Figure S3. Free-energy profile calculated for the pathway from phenylrhodium complex **C** to active aryloxorhodium species **A**.

2. B3LYP and MN12-L absolute calculation energies, enthalpies, and free energies.

Geometry	E _{B3LYP(elec)} ¹	E _{MN12-L(THF)} ²	Correction of H _(gas phase) ³	Correction of G _(gas phase) ⁴	IF ⁵
[Rh(OH)L] ₂	-3141.820744	-3138.736887	0.930988	0.791979	-
1a	-1448.558975	-1447.766281	0.511803	0.425435	-
2a	-345.780538	-345.536718	0.133218	0.091786	-
3a	-578.060942	-577.648248	0.243252	0.186719	-
TS1	-3019.457616	-3017.117649	0.974789	0.830660	-
H₂O	-76.40702351	-76.38177163	0.024919	0.003474	-
A	-2943.030425	-2940.751311	0.950233	0.811569	-
TS_{A-B(R)}	-2942.977459	-2940.724567	0.949992	0.818626	-87.4
B-R	-2942.984037	-2940.732422	0.951731	0.817079	-
TS_{B-C(R)}	-2942.974639	-2940.721002	0.950277	0.817013	-127.8
C	-1726.678707	-1725.016355	0.545139	0.456206	-
TS_{A-C(R)}	-2942.985100	-2940.721162	0.950103	0.817049	-184.8
TS_{A-D}	-2942.984624	-2940.730031	0.950084	0.816893	-117.3
D	-2943.000719	-2940.752488	0.951897	0.817429	-
TS_{D-E}	-2942.980889	-2940.725198	0.950189	0.816068	-131.3
E	-2943.046832	-2940.753098	0.950237	0.808264	-
TS_{A-E}	-2942.993626	-2940.732902	0.949344	0.815257	-88.2
TS_{E-C(R)}	-2942.967779	-2940.703669	0.948688	0.814432	-199.2
TS_{E-F(R)}	-2942.998691	-2940.738031	0.949633	0.815502	-98.2
F-R	-2943.002652	-2940.755209	0.951515	0.818592	-
TS_{F-C(R)}	-2942.99786	-2940.740039	0.950648	0.818242	-85.9
TS_{E-F(S)}	-2943.000277	-2940.741616	0.949728	0.816793	-91.9
F-S	-2943.006406	-2940.75195	0.951505	0.818588	-
TS_{F-C(S)}	-2942.995563	-2940.737557	0.950863	0.819988	-73.0
C1	-2072.483835	-2070.599644	0.679891	0.570966	-
TS_{C-G}	-2072.469341	-2070.56583	0.679950	0.574739	-314.1
G	-2072.516057	-2070.606109	0.681678	0.572061	-

G1	-3521.069911	-3518.368496	1.194796	1.019601	-
TS_{G-H}	-3521.068049	-3518.365105	1.190665	1.017340	-796.6
H	-3521.108772	-3518.409235	1.196087	1.018381	-
I	-4391.610618	-4388.529532	1.464207	1.25516	-
TS_{I-A}	-4391.590411	-4388.503227	1.458718	1.252858	-1247.3
(R)-product	-1216.369830	-1215.722553	0.402950	0.329034	-
(S)-product	-1216.369830	-1215.722553	0.402950	0.329034	-
byproduct	-1448.609559	-1447.79771	0.511432	0.422140	-

¹The electronic energy calculated by B3LYP in gas phase. ²The electronic energy calculated by MN12-L in tetrahydrofuran. ³The thermal correction to enthalpy calculated by B3LYP in gas phase. ⁴The thermal correction to Gibbs free energy calculated by B3LYP in gas phase. ⁵The B3LYP calculated imaginary frequencies for the transition states in gas phase.

3. B3LYP geometries for all the optimized compounds and transition states.

[Rh(OH)L]₂				C	1.58639700	2.55590500	-2.18093000
C	5.84441800	1.42138400	-0.90025900	H	1.74714500	1.64293400	-2.76414000
C	4.69505100	0.72546400	-0.49663000	H	0.68786000	2.40368400	-1.57492300
C	4.71346700	-0.68443600	-0.46895900	H	1.40695400	3.38075300	-2.88407500
C	5.88669500	-1.36250300	-0.83335700	H	3.69481300	2.92723000	-1.90399400
C	7.02499800	-0.65980100	-1.23015100	C	4.68898800	2.43527500	2.31062900
C	7.00337300	0.73594300	-1.26577900	H	4.50495500	1.47316600	2.80200600
H	5.83934800	2.50762300	-0.92970100	H	5.64452800	2.36331200	1.77973100
H	5.91696300	-2.44856500	-0.81308800	H	4.79875800	3.19495800	3.09538500
H	7.92477200	-1.19967700	-1.51364200	H	2.61229900	2.83455600	1.95497800
H	7.88683800	1.28854100	-1.57488000	C	3.26842900	-2.53912500	2.74329500
C	2.71355700	-2.80893000	-1.27337500	H	3.69908700	-1.60082000	3.10848600
C	3.69436000	-2.83003800	1.30281200	H	2.17937100	-2.45154600	2.81727600
C	3.30810300	-4.14138900	-0.78056900	H	3.59572500	-3.34675500	3.41186700
C	3.15720000	-4.16570000	0.74728500	H	4.79140900	-2.85225800	1.25557700
H	2.80685600	-4.99577800	-1.25449300	C	3.04497800	-2.43303700	-2.71776500
H	4.37118000	-4.20802200	-1.05515600	H	2.68230000	-3.20716700	-3.40629300
H	2.09341900	-4.26164000	1.00500800	H	2.56742200	-1.48775700	-2.99847200
H	3.67805700	-5.01813600	1.20242800	H	4.12405900	-2.32559400	-2.87461000
C	3.54122200	2.80372700	1.36963100	H	1.62209600	-2.87283400	-1.17428000
C	2.78834100	2.86712100	-1.28630400	C	-5.84459800	-1.42228100	-0.89832200
C	3.68758400	4.15638600	0.64685000	C	-4.69512600	-0.72603700	-0.49565800
C	2.65316200	4.18012000	-0.48748800	C	-4.71396500	0.68388400	-0.46797200
H	3.55070200	4.99298900	1.34487200	C	-5.88772200	1.36157100	-0.83139200
H	4.70207200	4.25449100	0.23285600	C	-7.02613400	0.65849700	-1.22723600
H	1.64304700	4.23543300	-0.05903000	C	-7.00407400	-0.73723200	-1.26287300
H	2.77635000	5.05287200	-1.14184100	H	-5.83920400	-2.50850300	-0.92778200
P	3.13185000	-1.51922800	0.04765900	H	-5.91829700	2.44762600	-0.81113200
P	3.10644300	1.53700900	0.02759900	H	-7.92630300	1.19809900	-1.50998500
Rh	1.57344400	-0.00028100	0.49734400	H	-7.88760800	-1.29011300	-1.57124600
O	0.00282200	-1.41350300	0.91804100	C	-2.71542700	2.80912100	-1.27438500
H	-0.01105500	-1.46171900	1.88853800	C	-3.69424100	2.83020200	1.30256600

C	-3.30999700	4.14145800	-0.78128900
C	-3.15801400	4.16600600	0.74645200
H	-2.80935700	4.99597000	-1.25565400
H	-4.37329300	4.20772000	-1.05512800
H	-2.09407000	4.26240300	1.00339400
H	-3.67886700	5.01829400	1.20187900
C	-3.53895200	-2.80389500	1.36954000
C	-2.78837500	-2.86702600	-1.28697800
C	-3.68598100	-4.15651000	0.64681300
C	-2.65255000	-4.18014000	-0.48843400
H	-3.54845400	-4.99315700	1.34464200
H	-4.70083600	-4.25459900	0.23374000
H	-1.64209300	-4.23556300	-0.06084700
H	-2.77634600	-5.05280000	-1.14278600
P	-3.13214600	1.51935200	0.04724700
P	-3.10578600	-1.53707100	0.02719200
Rh	-1.57313100	0.00082800	0.49593800
O	-0.00300300	1.41389000	0.91740300
H	0.01049100	1.46292800	1.88780200
C	-1.58699600	-2.55554600	-2.18228900
H	-1.74823500	-1.64255500	-2.76532200
H	-0.68814800	-2.40320800	-1.57681100
H	-1.40781000	-3.38029600	-2.88560800
H	-3.69518100	-2.92718000	-1.90415600
C	-4.68575100	-2.43558700	2.31177500
H	-4.50126200	-1.47350000	2.80301700
H	-5.64184700	-2.36365200	1.78189300
H	-4.79464800	-3.19531700	3.09659900
H	-2.60941000	-2.83471000	1.95387900
C	-3.26717600	2.53971600	2.74281400
H	-3.69722200	1.60130200	3.10845300
H	-2.17802500	2.45257600	2.81602800
H	-3.59430200	3.34733700	3.41147900
H	-4.79133000	2.85194400	1.25611100
C	-3.04795200	2.43290100	-2.71843800
H	-2.68605500	3.20702100	-3.40739900
H	-2.57039600	1.48768900	-2.99937800
H	-4.12714400	2.32515700	-2.87432200
H	-1.62388000	2.87335200	-1.17621100

1a

C	2.76885700	1.04717300	0.60583200
C	2.63639400	-0.32466900	0.34630100
C	3.54482700	-0.92211900	-0.55332400
C	4.52657100	-0.15778000	-1.19075400
C	4.62758300	1.20582000	-0.92347500
C	3.75079600	1.81366400	-0.02177500
H	2.09130900	1.51294700	1.31370100
H	5.19868500	-0.65227100	-1.88520100
H	5.39570800	1.79269900	-1.42015600
H	3.83060600	2.87474300	0.19491800
C	1.64822000	-1.18150200	1.07794200
C	0.23618100	-1.13048300	0.89946700
C	2.20327200	-2.08111100	2.00920300
C	-0.53577200	-1.97747700	1.72361700

C	1.40815200	-2.91832000	2.79057400
H	3.28331000	-2.09561800	2.13485800
C	0.02556200	-2.85667400	2.65164500
H	-1.61626700	-1.95644300	1.63742000
H	1.86797700	-3.59519700	3.50582500
H	-0.62020100	-3.48721600	3.25723400
O	3.50124200	-2.25578300	-0.85562000
Si	-0.75191600	0.01293600	-0.30202300
C	-0.76074400	1.76453500	0.44551900
C	-0.55839500	1.93447200	1.82964300
C	-1.04879400	2.92047400	-0.30553400
C	-0.62589900	3.19268200	2.43202500
H	-0.34252900	1.06876100	2.45103600
C	-1.11634100	4.18271500	0.28916600
H	-1.22817000	2.84513600	-1.37418500
C	-0.90172700	4.32327800	1.66102400
H	-0.46291100	3.28890200	3.50265700
H	-1.33621300	5.05542200	-0.32075000
H	-0.95240100	5.30464000	2.12565100
C	-2.56515600	-0.58904500	-0.24744900
C	-3.60810700	0.28543400	0.10901400
C	-2.92893100	-1.90154100	-0.61597200
C	-4.94477800	-0.12390900	0.09648500
H	-3.37713800	1.30547600	0.40213200
C	-4.26073000	-2.31764900	-0.63146100
H	-2.16004900	-2.62273100	-0.88329300
C	-5.27594300	-1.42636000	-0.27533900
H	-5.72597800	0.57750900	0.37921800
H	-4.50571600	-3.33691300	-0.91999500
H	-6.31452800	-1.74711200	-0.28588200
C	-0.20060500	-0.04005800	-2.17450400
C	-1.41378700	0.31228000	-3.07196100
H	-1.81881100	1.30953600	-2.86237900
H	-1.09883900	0.30586700	-4.12538200
H	-2.23448600	-0.40285700	-2.96499700
C	0.26374200	-1.46702800	-2.54836400
H	1.16198400	-1.77061600	-2.00252500
H	-0.51482800	-2.21845800	-2.37074800
H	0.50802000	-1.50650000	-3.61986100
C	0.93738100	0.94783100	-2.51265200
H	1.15177600	0.89764700	-3.59033700
H	0.67305200	1.98415000	-2.27982500
H	1.86294000	0.71630200	-1.98425900
H	2.80961100	-2.67043700	-0.31096300

2a

C	-0.00802000	-1.15244100	-0.84246200
H	-0.02111200	-1.06441700	-1.92483900
C	0.09822200	-2.32928900	-0.22149800
H	0.17750600	-3.26147900	-0.77264700
H	0.10724500	-2.37788900	0.86378100
C	-0.11569400	0.10928800	-0.06467400
O	-0.11295800	0.19672200	1.14767400
O	-0.22018900	1.17283300	-0.89445700
C	-0.33281900	2.46176900	-0.25290000

H	-1.20225100	2.44972300	0.41255100
H	0.55397600	2.62483500	0.36855300
C	-0.46404500	3.50663500	-1.34569600
H	-0.55140900	4.50305500	-0.89884300
H	0.41212400	3.49896800	-2.00218900
H	-1.35386000	3.32364200	-1.95673200

3a

C	-0.12148800	-0.94918300	-1.22594800
H	0.60750700	-0.76924200	-2.02659800
C	0.15186300	-2.29129300	-0.52791900
H	1.12739900	-2.23936600	-0.03219200
H	-0.58725600	-2.43256200	0.26851900
C	-0.07686100	0.22855100	-0.26995000
O	0.16678400	0.16397900	0.91649300
O	-0.34604300	1.38438200	-0.91669200
C	-0.32787900	2.58176400	-0.10648100
H	-1.05118500	2.46855900	0.70762800
H	0.66351100	2.68653400	0.34646900
C	-0.66721600	3.75093300	-1.01243500
H	-0.66293800	4.68216500	-0.43533400
H	0.06371100	3.84406100	-1.82226000
H	-1.65960700	3.62584900	-1.45760800
C	0.11381000	-3.45617500	-1.49458500
C	-1.08909900	-4.11946500	-1.77429000
C	1.27469300	-3.87865000	-2.15695800
C	-1.13356700	-5.17094600	-2.69110700
H	-1.99912700	-3.81185900	-1.26285400
C	1.23622000	-4.92969700	-3.07474300
H	2.21982700	-3.38232700	-1.94565900
C	0.03031200	-5.57925900	-3.34577100
H	-2.07609800	-5.67465200	-2.88999500
H	2.14921300	-5.24457200	-3.57370700
H	-0.00120500	-6.40018600	-4.05716600
H	-1.10128100	-0.95559300	-1.72021900

A

C	-1.19905700	-3.76325200	2.70633900
C	-0.82224200	-3.00024800	1.59404500
C	0.33994100	-2.17346200	1.66522200
C	1.04736200	-2.14268000	2.89122900
C	0.64031100	-2.89784900	3.98800400
C	-0.48903100	-3.71732200	3.90862200
H	-2.07901900	-4.39844000	2.62326400
H	1.91329200	-1.48782900	2.95721200
H	1.21107000	-2.84528000	4.91343500
H	-0.80783600	-4.31273200	4.75971100
C	-1.56699000	-3.13501600	0.30691300
C	-2.30563300	-2.08658300	-0.30147100
C	-1.51940400	-4.39321100	-0.31948300
C	-2.93538100	-2.36283800	-1.53375900
C	-2.16357700	-4.64136900	-1.53058300
H	-0.94865200	-5.18434800	0.15986200
C	-2.87146400	-3.61386900	-2.14927700
H	-3.49081200	-1.57618500	-2.03755700

H	-2.10455800	-5.62651700	-1.98734000
H	-3.37275800	-3.77871800	-3.09988200
O	0.71206300	-1.49367900	0.59599800
Si	-2.70322400	-0.36712100	0.43082100
C	-2.53873500	0.88872100	-1.00123400
C	-1.67854500	0.63656300	-2.08784500
C	-3.19373600	2.13598200	-0.98392600
C	-1.49400600	1.57168200	-3.11008400
H	-1.14653300	-0.30865800	-2.13884700
C	-3.01642700	3.07588000	-2.00155500
H	-3.85416800	2.39002400	-0.15985000
C	-2.16572300	2.79470200	-3.07221700
H	-0.82939300	1.34023500	-3.93915800
H	-3.54385800	4.02579600	-1.95821000
H	-2.02838300	3.52162100	-3.86899800
C	-1.55677100	0.30388900	1.80248000
C	-1.66873900	-0.07585400	3.14656700
C	-0.57700100	1.27823300	1.49141400
C	-0.85311900	0.47168400	4.14592200
H	-2.39038000	-0.83104100	3.43940000
C	0.24689100	1.82535200	2.48485800
H	-0.50016700	1.65417300	0.47557400
C	0.11061300	1.41714600	3.82055800
H	-0.97308800	0.14274800	5.17448400
H	0.92962200	2.63182600	2.23861200
H	0.73993900	1.85320500	4.59234100
C	-4.54092400	-0.44967600	1.10232200
C	-4.88248700	0.72864900	2.04270400
H	-4.81846600	1.70063900	1.54043200
H	-5.91550400	0.62417700	2.40641800
H	-4.22696200	0.76994200	2.91794800
C	-4.75356000	-1.76959700	1.88263200
H	-4.57904200	-2.64657100	1.25112400
H	-4.09869900	-1.85862400	2.75681000
H	-5.78994800	-1.82133700	2.24824900
C	-5.54451800	-0.43943500	-0.07317800
H	-6.57178600	-0.50279700	0.31519800
H	-5.47415800	0.47316800	-0.67477800
H	-5.39784000	-1.29527300	-0.74066300
C	5.48615400	2.54753000	-1.35158600
C	4.50192200	1.65251700	-0.90250700
C	4.47400300	0.34790000	-1.43082100
C	5.41993200	-0.03381200	-2.39446700
C	6.38872800	0.86660100	-2.83552100
C	6.42316200	2.15964500	-2.30933300
H	5.52993100	3.55787100	-0.95620800
H	5.39971300	-1.03848800	-2.80764800
H	7.11292600	0.56170300	-3.58605900
H	7.17840600	2.86569800	-2.64403900
C	2.21431800	-1.53956400	-2.22039700
C	4.08141200	-2.38177400	-0.36587300
C	2.85404500	-2.92175100	-2.46123400
C	3.27481400	-3.47747900	-1.09292000
H	2.14752800	-3.58827800	-2.97151600
H	3.73223000	-2.82599400	-3.11744200

H	2.38008800	-3.71806000	-0.50613200
H	3.86782600	-4.39631100	-1.18469200
C	4.14717600	2.68544600	1.89706200
C	2.67849400	3.83067600	-0.14249100
C	4.27478400	4.21297000	1.74147500
C	2.98506700	4.72182600	1.08050400
H	4.45316200	4.69354100	2.71218800
H	5.14139600	4.45322200	1.10975000
H	2.15533000	4.65975600	1.79931700
H	3.06196900	5.77578800	0.78464600
P	3.16239700	-0.77995500	-0.78055400
P	3.20609800	2.07081700	0.36851700
Rh	1.84069800	0.28411400	0.63327000
C	1.24684100	3.96176000	-0.66745900
H	1.06220500	3.30542300	-1.52353600
H	0.50832400	3.71584200	0.10217900
H	1.05579300	4.99416600	-0.98790800
H	3.36424900	4.11433800	-0.95030000
C	5.44997100	1.95176400	2.22209200
H	5.27901200	0.87619600	2.34170300
H	6.20043000	2.08950100	1.43613000
H	5.87439800	2.32918500	3.16094300
H	3.43603300	2.48572000	2.71063300
C	4.31408500	-2.64646100	1.12121300
H	4.89532100	-1.84329600	1.58833800
H	3.36563700	-2.73411700	1.65721400
H	4.87143800	-3.58301600	1.25305900
H	5.05608300	-2.28489000	-0.86471300
C	2.05460600	-0.66435100	-3.46338800
H	1.42658500	-1.17577600	-4.20384300
H	1.57340500	0.28906000	-3.21933300
H	3.01730400	-0.44492800	-3.93905400
H	1.23257500	-1.69940700	-1.75741800

B-R

C	-5.14094800	-0.05086100	-0.95992300
C	-3.77886000	-0.38670100	-0.83961900
C	-2.86253900	0.14936500	-1.78668200
C	-3.39069300	0.88952800	-2.87225700
C	-4.74410400	1.19148700	-2.97351700
C	-5.63107100	0.74668900	-1.99130600
H	-5.83165000	-0.43690300	-0.21403500
H	-2.70065100	1.20670500	-3.64889200
H	-5.10352900	1.77827700	-3.81599900
H	-6.68826700	0.99204800	-2.03987100
C	-3.41701400	-1.42603800	0.17136400
C	-2.39730800	-1.35175400	1.16427500
C	-4.24293200	-2.57167000	0.13070800
C	-2.34282400	-2.40964500	2.10020100
C	-4.14456600	-3.60587400	1.05621200
H	-4.98369100	-2.63821400	-0.66038400
C	-3.19496300	-3.51273400	2.06780500
H	-1.61227700	-2.37721900	2.89851300
H	-4.80673100	-4.46547300	0.98566400
H	-3.10213500	-4.29112300	2.82127200

O	-1.55994600	-0.11144200	-1.75468400
Si	-1.16115200	0.10143300	1.49300200
C	-0.40190800	2.50157000	-0.57638800
C	-1.01203700	2.96932700	-1.75724800
C	0.00583800	3.48570000	0.34223700
C	-1.21332100	4.33261200	-1.99908800
H	-1.33300800	2.25795000	-2.50502700
C	-0.19984900	4.85137100	0.11526300
H	0.49225200	3.19181400	1.26473000
C	-0.81406400	5.28479200	-1.06035400
H	-1.69146400	4.64587400	-2.92486300
H	0.12441600	5.57508600	0.86087500
H	-0.97648200	6.34421000	-1.24168000
C	-2.25437200	1.46902700	2.41905100
C	4.73304500	-0.49203200	-0.15620400
C	3.34791500	-0.53018800	-0.39973700
C	2.80307200	-1.65227200	-1.06684800
C	3.66950200	-2.68739200	-1.46355000
C	5.03638300	-2.64028800	-1.20040600
C	5.57155600	-1.53621900	-0.53792900
H	5.17194900	0.36962600	0.33544100
H	3.27603800	-3.54666400	-1.99588400
H	5.67879900	-3.45707600	-1.51809500
H	6.63575400	-1.48238500	-0.32532200
C	0.53022400	-3.55263600	-1.39879500
C	0.80427900	-1.57854900	-3.30301000
C	0.08130300	-3.88589200	-2.84062900
C	0.86878000	-3.02135400	-3.82538300
H	-0.98894400	-3.66117500	-2.93832200
H	0.20213200	-4.95924400	-3.03458100
H	0.45684000	-3.08263300	-4.84127500
H	1.91391400	-3.35662300	-3.88785400
C	3.23045900	2.31885000	-0.90395800
C	2.88151800	1.60567500	1.74551800
C	3.44829200	3.44421700	0.12109300
C	3.82957400	2.79282600	1.45217200
H	2.53296500	4.03502300	0.22317400
H	4.23318600	4.12540300	-0.23295000
H	3.80300100	3.50829300	2.28375600
H	4.86280100	2.42115800	1.39651100
P	0.97655600	-1.68795600	-1.41889200
P	2.29064800	0.94438200	0.04944300
Rh	0.04363200	0.49724200	-0.57358300
C	0.07391800	-0.67459500	2.76962100
C	0.14186800	-0.33662400	4.13577700
C	0.86754000	-1.76915100	2.36646300
C	0.92851500	-1.05672000	5.04212500
H	-0.44189200	0.48751600	4.52542100
C	1.64447600	-2.50525700	3.26175300
H	0.86050900	-2.06666200	1.32491700
C	1.67600400	-2.15236300	4.61298500
H	0.94415100	-0.76182600	6.08864200
H	2.22678800	-3.35070100	2.90310600
H	2.27694500	-2.72072900	5.31818000
C	-3.11467400	0.70849400	3.46989300

H	-2.52383600	0.17118000	4.21817300
H	-3.78667300	-0.01471800	3.00127600
H	-3.73628300	1.43922500	4.00753500
C	-3.24775900	2.17029800	1.46695300
H	-2.74079000	2.70847000	0.66276500
H	-3.83941300	2.90153100	2.03857000
H	-3.94825100	1.46783200	1.01015800
C	-1.45958700	2.58124300	3.15239300
H	-1.22684400	3.40321900	2.47550200
H	-0.51923200	2.24978900	3.60360800
H	-2.07737800	2.99821900	3.96057200
C	1.73035700	-0.60439900	-4.02761100
H	2.78791300	-0.84368100	-3.86660400
H	1.53977800	-0.64313000	-5.10762000
H	1.55616500	0.42540200	-3.70382500
C	2.66258200	2.80177100	-2.23760700
H	2.63902800	1.99981100	-2.98026600
H	1.65405200	3.20606800	-2.13356300
H	3.30881900	3.59426500	-2.63722600
C	3.48089800	0.62819800	2.75994400
H	4.42561100	0.20048800	2.41183900
H	3.69117700	1.17148400	3.69005400
H	2.80573100	-0.19086000	2.99796400
C	-0.50374500	-4.00498700	-0.36711100
H	-0.16075100	-3.87005900	0.66085100
H	-1.44702200	-3.46578000	-0.47946900
H	-0.70725700	-5.07475400	-0.50835500
H	4.20781900	1.86076100	-1.10133100
H	1.95340600	1.99803300	2.17674000
H	1.47255700	-4.07295200	-1.19282800
H	-0.22836700	-1.21604300	-3.39314300

C

C	-3.61852800	1.18087400	-0.08158500
C	-2.27530200	0.77348700	-0.04253300
C	-1.26035500	1.75144200	0.00212800
C	-1.61908800	3.10942300	0.01330400
C	-2.95704000	3.50046800	-0.02526700
C	-3.96155100	2.53225700	-0.07310500
H	-4.40939800	0.43708700	-0.11612900
H	-0.84975500	3.87507000	0.04849800
H	-3.21393600	4.55645200	-0.01982600
H	-5.00695600	2.82801600	-0.10158200
C	1.42073900	2.13247100	-1.32909400
C	1.28286600	2.21693500	1.42856700
C	2.05222000	3.36082800	-0.64430400
C	2.47923300	2.92951100	0.76595200
H	2.90029000	3.73711800	-1.23082900
H	1.32274400	4.18154800	-0.58376300
H	3.32402100	2.23136000	0.69600400
H	2.81181300	3.77947700	1.37542000
C	-2.69835600	-1.84504400	1.38188400
C	-2.81470900	-1.81091000	-1.37693000
C	-3.95245800	-2.46996600	0.74060800
C	-3.55760800	-2.95794600	-0.65982600

H	-4.34918600	-3.28394000	1.36148800
H	-4.74921400	-1.71622100	0.66417200
H	-2.88761000	-3.82514100	-0.56775300
H	-4.42528500	-3.28986600	-1.24400600
P	0.51585900	1.17677000	0.03652000
P	-1.73957900	-1.00619400	-0.03087000
Rh	0.59810300	-1.00922300	-0.01872000
C	-2.01889800	-2.25877100	-2.60580400
H	-1.52256600	-1.41355800	-3.09371600
H	-1.24183900	-2.98232100	-2.33226700
H	-2.67942700	-2.73522900	-3.34207300
H	-3.55332700	-1.06070600	-1.68761400
C	-2.95898000	-0.99871300	2.62961600
H	-2.02536700	-0.60787600	3.04906700
H	-3.61218900	-0.14646100	2.41421000
H	-3.44398600	-1.60536800	3.40504600
H	-2.02410000	-2.66548000	1.66678100
C	1.63976900	1.44075900	2.69622100
H	0.76162600	0.94774300	3.12661000
H	2.38603800	0.66994700	2.48450200
H	2.05100500	2.12101800	3.45386500
H	0.52741900	2.97374800	1.67936300
C	0.62748200	2.42701600	-2.60295400
H	1.27355800	2.91554900	-3.34350700
H	0.24378000	1.50533500	-3.05422900
H	-0.22424400	3.08943000	-2.41527000
H	2.23511300	1.44490100	-1.58423400
C	2.63581100	-1.11442400	-0.00474400
C	3.28233000	-1.62016900	1.14601500
C	3.41895400	-1.01493800	-1.17484300
C	4.61897700	-2.03344700	1.12119700
H	2.72972100	-1.70174500	2.08129600
C	4.75618000	-1.42435700	-1.20751600
H	2.97190700	-0.62705500	-2.08947700
C	5.36286900	-1.93348800	-0.05674100
H	5.08253600	-2.42587900	2.02469400
H	5.32606800	-1.34500800	-2.13174800
H	6.40454100	-2.24534500	-0.07680700

C1

C	-3.85297300	0.85425500	-0.38467200
C	-2.50516300	0.48732300	-0.22786400
C	-1.51423600	1.49160400	-0.23437100
C	-1.90441700	2.83377300	-0.38333800
C	-3.24456500	3.18353200	-0.53616400
C	-4.22422700	2.18853500	-0.53826000
H	-4.62592700	0.09126600	-0.38689000
H	-1.15386200	3.61861200	-0.37985400
H	-3.52314400	4.22725500	-0.65434700
H	-5.27218700	2.45072800	-0.65639700
C	1.29797600	1.93508900	-1.29339000
C	0.82523800	2.08848600	1.42244200
C	1.85031800	3.17591700	-0.56110800
C	2.10233300	2.77862400	0.90141000
H	2.76406200	3.53801100	-1.04943300

H	1.12135700	3.99850600	-0.60456800
H	2.94986300	2.08474800	0.95270400
H	2.35167200	3.64593800	1.52624700
C	-3.03344200	-2.01415400	1.37709800
C	-2.89848100	-2.19720600	-1.37433200
C	-4.21086700	-2.72148000	0.67685800
C	-3.68152400	-3.30618500	-0.64004400
H	-4.64493100	-3.49503000	1.32359300
H	-5.01269700	-1.99922400	0.46880400
H	-3.01080800	-4.15063100	-0.42547600
H	-4.48828400	-3.69790200	-1.27246300
P	0.26537900	0.98654200	-0.01806800
P	-1.95864500	-1.27528900	-0.00471700
Rh	0.42482600	-1.33972000	0.07080300
C	-2.00805000	-2.70208500	-2.51329200
H	-1.51242600	-1.87385400	-3.03169600
H	-1.22709500	-3.37316400	-2.14068700
H	-2.60526500	-3.24996400	-3.25369900
H	-3.62276500	-1.48427900	-1.78866100
C	-3.41883000	-1.07241200	2.52011700
H	-2.53348200	-0.62682900	2.98742600
H	-4.06176200	-0.25619200	2.17510700
H	-3.96284400	-1.62343000	3.29752900
H	-2.38264500	-2.79633300	1.79300100
C	0.95488900	1.38036300	2.77216800
H	-0.02201200	1.03859400	3.13182300
H	1.60192000	0.50088900	2.72672300
H	1.35983600	2.07160600	3.52292200
H	0.04590400	2.85764600	1.50881800
C	0.64641200	2.20902800	-2.65043900
H	1.37172400	2.68090300	-3.32514900
H	0.30897700	1.28141000	-3.12703400
H	-0.21720900	2.87727400	-2.56918500
H	2.13449700	1.24378000	-1.45343200
C	2.45972600	-1.23941500	-0.27983600
C	3.49800900	-0.68405400	0.48986600
C	2.81961900	-1.74700500	-1.54565500
C	4.81961500	-0.63621700	0.02679700
H	3.28564100	-0.29477100	1.48271300
C	4.13592100	-1.70249200	-2.01856700
H	2.05777000	-2.19781300	-2.18358000
C	5.14702400	-1.14449400	-1.23191400
H	5.59472200	-0.19815300	0.65382200
H	4.37164000	-2.10853300	-3.00088000
H	6.17138700	-1.10654000	-1.59479200
C	0.50512500	-3.54572800	0.46281800
H	-0.45147800	-3.99407100	0.20979300
H	1.37326800	-3.96838300	-0.03256400
C	0.65998700	-2.85564700	1.66804400
H	-0.19244400	-2.67339600	2.31667500
C	1.94176200	-2.73719200	2.41721400
O	2.08897800	-2.03244500	3.40223700
O	2.91040800	-3.54028900	1.93064400
C	4.19289500	-3.46322700	2.58510100
H	4.50374400	-2.41642600	2.63441600

H	4.08539200	-3.83178000	3.61165800
C	5.16580000	-4.30006700	1.77490400
H	5.26412900	-3.89651300	0.76236800
H	6.15285200	-4.28920900	2.25135700
H	4.82806500	-5.33970500	1.70662700
D			
C	-4.54206700	1.94925100	-1.65977200
C	-3.18952100	1.65075600	-1.36790000
C	-2.64446900	0.48071900	-1.96843000
C	-3.43549500	-0.27461900	-2.87138000
C	-4.73911200	0.07902700	-3.16562600
C	-5.30856900	1.19651200	-2.53772300
H	-5.02022400	2.78100500	-1.15370800
H	-2.97608300	-1.15421800	-3.31324200
H	-5.32381500	-0.52182700	-3.85822100
H	-6.34409100	1.46850200	-2.72342100
C	-2.41202200	2.51258200	-0.44790600
C	-1.23707800	2.11216000	0.26572400
C	-2.89332500	3.83527700	-0.24641900
C	-0.75871100	3.00718400	1.25190900
C	-2.35832400	4.70294000	0.69120600
H	-3.70803600	4.19486800	-0.86488900
C	-1.29304300	4.26959700	1.48436700
H	0.07574300	2.69795200	1.86737300
H	-2.76876700	5.70324300	0.80395000
H	-0.87140200	4.91183700	2.25459200
O	-1.41142700	0.05913800	-1.77003400
Si	-0.92000700	-0.80483800	1.56299900
C	0.31497900	-2.23724200	1.97603100
C	1.69087600	-2.14866300	1.70411200
C	-0.11365600	-3.42864600	2.60387300
C	2.59146800	-3.16822400	2.02706500
H	2.07420800	-1.26768600	1.20757600
C	0.77348700	-4.45851600	2.92627100
H	-1.16126500	-3.56834200	2.84519500
C	2.13405800	-4.33414500	2.63970200
H	3.64652300	-3.04816600	1.79250100
H	0.39693000	-5.36041800	3.40304700
H	2.82533100	-5.13494100	2.88986900
C	-2.53832800	-1.60439100	0.92291500
C	-3.70087800	-0.81997400	0.77644700
C	-2.66374800	-2.97634100	0.62427300
C	-4.92373300	-1.37514300	0.39428300
H	-3.65452900	0.24850700	0.94558100
C	-3.88285900	-3.53922600	0.23962900
H	-1.80169800	-3.62864100	0.69953500
C	-5.02211700	-2.74092300	0.13051600
H	-5.79190000	-0.73122400	0.28402600
H	-3.93951500	-4.60447700	0.02688800
H	-5.97253300	-3.17666700	-0.16767500
C	-1.39122200	-0.07745800	3.35928800
C	-1.85587600	-1.26454300	4.24318800
H	-1.04196400	-1.95394200	4.48239300
H	-2.23461200	-0.86597300	5.19585800

H	-2.67056700	-1.83376600	3.78174300
C	-2.55112000	0.94150400	3.36878000
H	-2.38525300	1.78925000	2.70234200
H	-3.50035000	0.47082300	3.09802100
H	-2.67038600	1.33814900	4.38860900
C	-0.17663200	0.55790300	4.06236100
H	-0.41136900	0.73928600	5.12183000
H	0.70906300	-0.08721200	4.03143800
H	0.07914400	1.52714700	3.62629900
C	4.76151400	0.70059900	-0.21385000
C	3.41134000	0.37711700	-0.44115000
C	3.11103300	-0.68073300	-1.32850400
C	4.16495000	-1.39426900	-1.92529100
C	5.49634000	-1.07774000	-1.66605000
C	5.79552400	-0.01776200	-0.81039700
H	5.01823200	1.52779100	0.43754400
H	3.94646300	-2.20458700	-2.61337300
H	6.29275800	-1.64572400	-2.13919400
H	6.82841500	0.25139000	-0.60689500
C	1.17738000	-0.42993000	-3.54949200
C	1.20211200	-2.83163500	-2.18469100
C	1.43920100	-1.68577000	-4.39753100
C	0.79260300	-2.86645900	-3.67468300
H	1.03852900	-1.55727100	-5.41157200
H	2.52150800	-1.84688400	-4.50416100
H	-0.29993000	-2.77884700	-3.74177200
H	1.06458000	-3.83131500	-4.12107500
C	2.70701000	1.78672400	2.13016600
C	2.47399700	3.12878000	-0.27902200
C	3.41698600	3.15457700	2.03229800
C	2.70400700	3.99869100	0.97238200
H	3.41569600	3.64735800	3.01317100
H	4.47196200	3.01808200	1.75931900
H	1.73755900	4.34751800	1.35339400
H	3.28259200	4.89313500	0.70804400
P	1.33247500	-0.98143100	-1.73758600
P	2.05070500	1.37372400	0.38018500
Rh	-0.07777100	0.53340300	-0.32389500
C	1.50765300	3.76787000	-1.27837000
H	1.36700000	3.15216300	-2.17018400
H	0.52570400	3.94150000	-0.83508100
H	1.91349600	4.73403300	-1.60593700
H	3.44173900	2.98671600	-0.77616400
C	3.51140700	0.72977000	2.89393500
H	4.45118700	0.47770500	2.39394800
H	3.76068100	1.12086100	3.88854200
H	1.77918800	1.94389200	2.68678400
C	0.25370200	-3.65619300	-1.31608800
H	0.59074500	-3.71352100	-0.27982900
H	-0.75353600	-3.23040100	-1.32651600
H	0.19253800	-4.67928200	-1.71059100
H	2.21490500	-3.23896900	-2.08202800
C	2.00839900	0.77653600	-3.98440400
H	1.80372000	1.00546900	-5.03784300
H	1.76705400	1.67108100	-3.40513500

H	3.08336300	0.58774400	-3.88617200
H	0.11179300	-0.17563000	-3.61240500
H	2.94828300	-0.19519200	3.03599100
E			
C	-1.68178000	-3.69353500	-1.37568900
C	-0.34916900	-3.22945900	-1.29436200
C	0.56001200	-3.96736900	-0.48799400
C	0.12360300	-5.10769000	0.18886200
C	-1.19453700	-5.56550300	0.06614500
C	-2.10151800	-4.85903200	-0.71273400
H	-2.35650500	-3.19160000	-2.06723600
H	0.82373500	-5.63199600	0.83006800
H	-1.49661500	-6.47223800	0.58391200
H	-3.12072400	-5.21301300	-0.83512400
C	0.01283500	-2.01844500	-2.08994200
C	-0.78615600	-0.87791800	-1.83928500
C	0.99769700	-2.04188400	-3.08509400
C	-0.55662000	0.23453100	-2.66867500
C	1.20249000	-0.91399500	-3.88072800
H	1.57930100	-2.94319500	-3.25819600
C	0.41501600	0.22088100	-3.67555300
H	-1.14944500	1.13800300	-2.54954700
H	1.95821600	-0.92782700	-4.66194000
H	0.55568500	1.09861600	-4.30409800
O	1.83193800	-3.51357700	-0.30968000
Si	3.41851300	-3.91410200	-0.72091800
C	4.25882300	-2.22921700	-0.85907100
C	3.53537300	-1.05970000	-0.55829800
C	5.60612600	-2.07765400	-1.24669300
C	4.13168800	0.20091800	-0.63234700
H	2.49049700	-1.13768000	-0.27689600
C	6.20442500	-0.81886700	-1.32727100
H	6.20576700	-2.94982000	-1.49489000
C	5.46734700	0.32534800	-1.01633900
H	3.54644000	1.08599100	-0.39654700
H	7.24436300	-0.73296100	-1.63259100
H	5.93098900	1.30683500	-1.07732200
C	3.43758300	-4.84674900	-2.36711500
C	4.19193400	-4.38880000	-3.46467800
C	2.67554800	-6.01963100	-2.55069700
C	4.20197000	-5.07660700	-4.68032700
H	4.76860500	-3.47262700	-3.37739300
C	2.67574100	-6.70581600	-3.76594900
H	2.05918600	-6.40181200	-1.74183100
C	3.44490700	-6.23858100	-4.83351600
H	4.79508600	-4.69887500	-5.50941300
H	2.07319800	-7.60343200	-3.87952500
H	3.44768500	-6.77278500	-5.78019200
C	4.21295500	-4.94626800	0.70469200
C	5.75109400	-4.95779900	0.54883500
H	6.18199000	-3.95628900	0.64052800
H	6.19867000	-5.58176900	1.33577500
H	6.06455800	-5.37957900	-0.41510700
C	3.73970200	-6.41585800	0.71312000

H	2.65608500	-6.51317300	0.84048200
H	4.01542300	-6.93924600	-0.20882700
H	4.20959700	-6.95227800	1.55025800
C	3.85365800	-4.28647700	2.05460200
H	4.33358200	-4.82991100	2.88157700
H	4.19473300	-3.24536700	2.10134900
H	2.77300900	-4.28904200	2.23577800
C	-3.68939800	1.94703700	2.68981000
C	-3.35345600	0.76233000	2.01223300
C	-3.74678900	-0.47317400	2.56123700
C	-4.46936500	-0.49119400	3.76587500
C	-4.79517600	0.69055500	4.42870200
C	-4.40285200	1.91584000	3.88706800
H	-3.39434500	2.90971300	2.28497400
H	-4.78031400	-1.43811300	4.19696900
H	-5.34990400	0.65552800	5.36264600
H	-4.65243700	2.84446800	4.39357600
C	-2.45443800	-3.16570400	2.89609900
C	-4.89057600	-2.99414100	1.61195200
C	-3.57666500	-4.07504400	3.43468100
C	-4.55090300	-4.34381100	2.27847300
H	-3.16378000	-5.00654800	3.84428000
H	-4.10333500	-3.57748200	4.26152600
H	-4.07053300	-5.00407000	1.54437500
H	-5.46294000	-4.85268300	2.61660800
C	-3.38633300	1.87709700	-0.75920500
C	-1.05354000	2.04107000	0.71712500
C	-2.81473700	3.29492500	-0.55857700
C	-1.30255200	3.16422100	-0.31492500
H	-3.02941600	3.92881300	-1.42906600
H	-3.29900700	3.77670400	0.30200000
H	-0.80055000	2.90548800	-1.25522400
H	-0.86193400	4.10917600	0.02829800
P	-3.26204800	-2.00519100	1.62985800
P	-2.40835900	0.74021600	0.40079600
Rh	-2.01152100	-1.34397100	-0.24747900
C	0.37807000	1.49969900	0.71298800
H	0.51606900	0.72913100	1.47854700
H	0.62870900	1.05499100	-0.25446700
H	1.08723000	2.31308800	0.91882200
H	-1.26777500	2.43614300	1.71764900
C	-4.90947600	1.76585000	-0.67052900
H	-5.23664500	0.73228600	-0.83087200
H	-5.28713700	2.09288500	0.30418700
H	-5.38221200	2.38922000	-1.44005000
H	-3.08211900	1.52458400	-1.75208600
C	-5.53588000	-3.11485000	0.22955300
H	-5.79858600	-2.13218600	-0.17669000
H	-4.85852100	-3.59265100	-0.48556400
H	-6.45463800	-3.71395300	0.28219700
H	-5.58242000	-2.45341300	2.27013800
C	-1.58148000	-2.50102000	3.96275600
H	-1.09325400	-3.26348500	4.58341200
H	-0.79422000	-1.89113500	3.50588700
H	-2.16541000	-1.85403800	4.62628700

H	-1.80288400	-3.78148800	2.26260400
F-R			
C	4.42632100	-1.41182900	-0.56560500
C	3.54546700	-0.33534200	-0.31453600
C	3.49947700	0.14386300	1.01136700
C	4.38922300	-0.35719500	1.97680200
C	5.26330800	-1.39911100	1.68786100
C	5.26244300	-1.95286200	0.40678900
H	4.45370400	-1.82632500	-1.56883600
H	4.38823700	0.11072200	2.95644900
H	5.93505800	-1.77312300	2.45599800
H	5.92036000	-2.78112700	0.15846600
C	2.84447000	0.28224600	-1.48318800
C	1.48901600	0.69009100	-1.55985700
C	3.65936200	0.41600100	-2.63773000
C	1.01983500	1.10532800	-2.82780500
C	3.17267000	0.85483900	-3.86137200
H	4.71484400	0.17496300	-2.55167300
C	1.82018500	1.17763100	-3.96592000
H	-0.01797600	1.41903800	-2.92899400
H	3.83949400	0.94811000	-4.71457600
H	1.39716700	1.51737900	-4.90856700
O	2.68478100	1.16289800	1.39188300
Si	1.00484400	1.27082300	1.65457700
C	0.49399700	-0.04722500	2.96526700
C	-0.86495700	-0.26078800	3.26090900
C	1.42636000	-0.70706400	3.79020600
C	-1.27995900	-1.06019900	4.32932000
H	-1.61736400	0.21257800	2.64135600
C	1.02398800	-1.51631100	4.85576000
H	2.48689500	-0.58387400	3.61135400
C	-0.33215000	-1.69064200	5.13688700
H	-2.34128100	-1.19109400	4.52786600
H	1.77461400	-2.00712600	5.47091700
H	-0.64594500	-2.31330800	5.97084500
C	-0.17507800	2.85827000	-0.56955000
C	0.91000900	3.58385700	-1.11031400
C	-1.36390900	3.60046100	-0.39933000
C	0.79495800	4.91671400	-1.51578400
H	1.87687400	3.10689200	-1.21730000
C	-1.49187900	4.93713100	-0.79584100
H	-2.22803900	3.13700800	0.06174700
C	-0.41149200	5.60347500	-1.37126100
H	1.66248100	5.42198900	-1.93529800
H	-2.43858500	5.45354400	-0.64744500
H	-0.50233500	6.64023100	-1.68567500
C	1.05194300	2.93636800	2.70852600
C	-0.34577200	3.46872800	3.06243600
H	-0.94697300	2.72031100	3.59179300
H	-0.25532600	4.34057900	3.72741200
H	-0.88993700	3.78943400	2.17046900
C	1.86398900	4.05544100	2.02546900
H	2.86117500	3.71049800	1.73308700
H	1.36559600	4.44876600	1.13957300

H	1.99320700	4.88944500	2.73174300
C	1.78146800	2.60592100	4.03726800
H	1.89667600	3.53379600	4.61614100
H	1.22881400	1.89730400	4.65993800
H	2.78433000	2.20176900	3.86266700
C	-2.38579500	-3.65541100	0.02707600
C	-2.06214200	-2.28684100	-0.00953200
C	-3.08599200	-1.33473000	0.19996500
C	-4.39483000	-1.80184000	0.42942900
C	-4.69456400	-3.16132800	0.47364200
C	-3.68161400	-4.09765300	0.27550900
H	-1.61095600	-4.39480400	-0.14442200
H	-5.21002800	-1.10220200	0.57008700
H	-5.71630600	-3.48322500	0.65600200
H	-3.89726900	-5.16211500	0.30740900
C	-3.54614800	1.03701300	-1.51205400
C	-4.07996400	1.27136400	1.18875600
C	-5.01435800	1.30968500	-1.14676200
C	-5.02387000	2.01432400	0.21136400
H	-5.49591900	1.91966600	-1.92225100
H	-5.57149100	0.36468300	-1.10069600
H	-4.66709500	3.04545800	0.08517900
H	-6.03277600	2.08271500	0.63783200
C	0.89020000	-2.81239200	0.59479200
C	-0.00757700	-2.75413600	-2.00316500
C	1.54586900	-3.80046900	-0.40224500
C	1.43761000	-3.24226500	-1.82493500
H	2.58627300	-3.98836600	-0.11330500
H	1.02009400	-4.76510800	-0.35463400
H	2.13244700	-2.40821800	-1.97080900
H	1.67981100	-4.00272800	-2.57913000
P	-2.69040200	0.49301700	0.10304700
P	-0.33083500	-1.74294800	-0.41814400
Rh	-0.16921900	0.77406100	-0.33437000
C	-0.29870000	-2.11261300	-3.35794500
H	-1.35813700	-1.86101300	-3.46619200
H	0.29174700	-1.20815600	-3.51744500
H	-0.05066200	-2.82382600	-4.15691900
H	-0.66155200	-3.63000400	-1.90220800
C	0.36907600	-3.50444600	1.85746700
H	-0.14409000	-2.81563600	2.52938800
H	-0.31601100	-4.32487600	1.62283200
H	1.21731100	-3.93307500	2.40515200
H	1.64121100	-2.07858900	0.89835900
C	-3.65589800	2.16604200	2.35755400
H	-3.09205500	1.62124600	3.11846000
H	-3.04756300	3.01253700	2.03176900
H	-4.55406400	2.56994000	2.84293800
H	-4.61600700	0.42019800	1.61784200
C	-3.36455100	0.12697100	-2.72567900
H	-3.91485200	0.53739900	-3.58182800
H	-2.31363600	0.05298000	-3.01894300
H	-3.74294700	-0.88428800	-2.53941300
H	-3.06676200	1.99908800	-1.73107300

F-S			
C	4.53830200	-1.42468900	1.39935300
C	3.51402500	-0.50564000	1.05586800
C	3.39521200	-0.21152400	-0.32483200
C	4.32193000	-0.73969600	-1.24727400
C	5.34037800	-1.59703600	-0.85754300
C	5.43828400	-1.96187700	0.48651200
H	4.60940300	-1.73978300	2.43475900
H	4.20479600	-0.44527600	-2.28586300
H	6.03619300	-1.98680500	-1.59585700
H	6.19988900	-2.65993900	0.82241500
C	2.69412100	0.03122200	2.19306000
C	1.29339800	0.28004700	2.20717900
C	3.40887300	0.18063200	3.41201400
C	0.68898100	0.40310600	3.48046700
C	2.79030700	0.38649400	4.63655000
H	4.49278900	0.12964900	3.38299800
C	1.39717900	0.43484700	4.67998200
H	-0.39360800	0.50720100	3.53520300
H	3.38531200	0.49091000	5.54005500
H	0.86786600	0.54067200	5.62428400
O	2.43818400	0.54821900	-0.88883800
Si	1.15486800	1.59960600	-0.52434500
C	2.14008900	3.27226300	-0.19958900
C	-0.85006400	2.34228400	1.26925800
C	-0.47137900	3.04546300	2.43275700
C	-1.80150900	3.00209000	0.46172200
C	-1.03460600	4.27636200	2.78674200
H	0.27610000	2.63192200	3.09670900
C	-2.36056500	4.24152300	0.79283100
H	-2.12807400	2.54155400	-0.46189300
C	-1.98747800	4.88733400	1.97073000
H	-0.71098800	4.76406200	3.70412400
H	-3.09191400	4.69613600	0.12688700
H	-2.42018400	5.84713500	2.24116600
Rh	-0.27577600	0.33952700	0.86266900
C	0.38970300	1.76020200	-2.28355600
C	-0.52931300	2.76483400	-2.65041000
C	0.79672400	0.87826000	-3.30502700
C	-1.02374100	2.87395700	-3.95354100
H	-0.85998600	3.49054900	-1.91705600
C	0.30501600	0.97819100	-4.60858500
H	1.53030500	0.11415000	-3.07977200
C	-0.61342500	1.97579600	-4.93942100
H	-1.72352300	3.67001900	-4.19792200
H	0.64941400	0.28070700	-5.36891000
H	-0.99391300	2.06027800	-5.95437800
C	2.88711800	3.27193200	1.14890500
H	3.47815400	4.19595400	1.23771100
H	3.58090100	2.43110400	1.23784100
H	2.20440800	3.23491200	2.00164100
C	3.20419400	3.35445100	-1.32765300
H	3.75533100	4.30107600	-1.22993200
H	2.75179900	3.33884000	-2.32564700
H	3.93199700	2.53973500	-1.27448100

C	1.29220400	4.55792200	-0.28655500
H	1.94966500	5.42736900	-0.13618600
H	0.51057300	4.60459500	0.47310000
H	0.82959000	4.67891500	-1.27110000
C	-1.95371800	-4.26390900	0.60102800
C	-1.74681300	-2.87691600	0.46433700
C	-2.84349300	-2.05560800	0.13813100
C	-4.10083800	-2.65632200	-0.07368100
C	-4.28704300	-4.02841300	0.05827500
C	-3.20632700	-4.83796000	0.41139600
H	-1.12020400	-4.91021500	0.85190700
H	-4.95437900	-2.04557300	-0.34772500
H	-5.26877400	-4.46191300	-0.11211200
H	-3.33608300	-5.91028200	0.53000500
C	-3.30545600	0.28156700	-1.67927800
C	-4.18141300	0.38296500	0.94636500
C	-4.78712900	0.65598900	-1.45620500
C	-4.92594100	1.28424700	-0.06142400
H	-5.13357400	1.33525300	-2.24587100
H	-5.41273700	-0.24476300	-1.52530500
H	-4.48675700	2.28836300	-0.05349800
H	-5.97815000	1.39523700	0.23105200
C	0.85023100	-3.05973200	1.99244700
C	0.81476900	-3.21730400	-0.75923800
C	1.57597900	-4.26751000	1.36272700
C	2.01888400	-3.86614100	-0.05060400
H	2.43025700	-4.56200700	1.98548000
H	0.90902200	-5.13961900	1.31700700
H	2.84884400	-3.15441300	0.00762700
H	2.37495500	-4.72946300	-0.62771600
P	-2.61955300	-0.21093000	0.02366000
P	-0.03510700	-2.14960600	0.58216000
C	1.14299200	-2.53058600	-2.08106000
H	0.24915800	-2.10387000	-2.54838400
H	1.87039600	-1.73007900	-1.94282300
H	1.56949000	-3.26063400	-2.78151900
H	0.08082800	-4.00635900	-0.96287700
C	0.02654300	-3.36601300	3.24620700
H	-0.38310600	-2.44929900	3.68275000
H	-0.80429600	-4.05087000	3.04818000
H	0.66869300	-3.83089800	4.00479800
H	1.61557100	-2.33084600	2.27652000
C	-3.96992100	1.00078600	2.33126400
H	-3.45882400	0.30305500	3.00487000
H	-3.38275700	1.91917600	2.28528600
H	-4.94338800	1.23696500	2.78073600
H	-4.78046500	-0.52360400	1.08492200
C	-3.05637300	-0.71193800	-2.81684200
H	-3.44432600	-0.30191100	-3.75729000
H	-1.98615000	-0.89403200	-2.95909100
H	-3.54997400	-1.67288900	-2.63802000
H	-2.75313700	1.19641100	-1.92254300

G			
C	4.57912600	4.98426500	-1.98040500

C	4.36810400	3.74217800	-1.36098000
C	5.43762800	2.82833500	-1.26437000
C	6.69209600	3.18447800	-1.78423400
C	6.88766900	4.41843000	-2.40420400
C	5.82762400	5.32180400	-2.50234000
H	3.76503200	5.69945500	-2.05871200
H	7.52726900	2.49362500	-1.71104400
H	7.86333000	4.67370200	-2.80924700
H	5.97339400	6.28659500	-2.98094600
C	5.82069800	-0.17013500	-1.51837300
C	6.50924200	1.08619100	0.84052100
C	7.23060200	-0.46070000	-0.96640400
C	7.17642800	-0.27461700	0.55716600
H	7.55886000	-1.47058400	-1.24454700
H	7.95989500	0.23793300	-1.40169200
H	6.57661800	-1.07936100	1.00528700
H	8.17205700	-0.32528600	1.01611900
C	2.31505800	4.50221400	0.69867500
C	1.43228800	3.82649600	-1.83155400
C	1.40683300	5.52817700	-0.00523100
C	0.52500100	4.75387400	-0.99399900
H	0.80885000	6.09111700	0.72330700
H	2.02208900	6.26312400	-0.54378600
H	-0.19891500	4.14390900	-0.43560800
H	-0.05539100	5.42175500	-1.64311200
P	5.09434500	1.20004600	-0.42375800
P	2.75216400	3.20561100	-0.61852700
Rh	2.93671100	1.02166200	0.04295000
C	0.67574000	2.69919800	-2.53893900
H	1.34563200	2.10508700	-3.17009800
H	0.21677400	2.02056700	-1.81221100
H	-0.11521600	3.11194500	-3.17905200
H	1.95378400	4.43336100	-2.58293500
C	3.48954500	5.09840500	1.47635600
H	4.07721400	4.31726300	1.97169900
H	4.16356700	5.66382500	0.82350700
H	3.12384700	5.78136700	2.25368400
H	1.69626500	3.92631400	1.40046000
C	6.08396900	1.29562500	2.29385300
H	5.65402300	2.29146400	2.44572800
H	5.32847100	0.56367000	2.59422600
H	6.94669000	1.19580400	2.96557000
H	7.22246100	1.87549700	0.56803800
C	5.73793200	0.04504600	-3.03049100
H	6.10923300	-0.84220900	-3.55898500
H	4.70342000	0.21366400	-3.34913500
H	6.33506000	0.90259700	-3.35808100
H	5.17861800	-1.02227700	-1.26297200
C	2.08722800	-2.25196600	2.91608100
C	2.89835600	-3.31516500	3.33442600
C	0.69640400	-2.39223700	3.03353100
C	2.34117800	-4.48713000	3.85024500
H	3.98025400	-3.22147500	3.25799200
C	0.13444800	-3.56037800	3.54981500
H	0.05290600	-1.57466000	2.71587500

C	0.95527900	-4.61393200	3.95997800
H	2.98995500	-5.29882800	4.17081700
H	-0.94604500	-3.64682700	3.63652500
H	0.51862000	-5.52344000	4.36454800
C	2.69263100	-0.98951700	2.32125100
H	2.09354200	-0.12222800	2.61776900
H	3.69314400	-0.84222900	2.74203600
C	2.79292500	-1.04242000	0.79140900
H	3.41225800	-1.86000000	0.42181000
C	1.57818900	-0.84834700	0.03711200
O	0.84736700	0.16956000	0.24972600
O	1.31248900	-1.71475400	-0.96550900
C	0.24277000	-1.36816000	-1.86595100
H	-0.67574400	-1.21042100	-1.29144200
H	0.48885000	-0.42827600	-2.37124700
C	0.09559400	-2.51243700	-2.85360000
H	-0.13836200	-3.44709100	-2.33357900
H	-0.71502100	-2.29633100	-3.55873200
H	1.01933700	-2.65858500	-3.42330100

G1

C	8.58451600	3.26521900	2.36044400
C	7.27806500	2.88420000	2.70403600
C	7.02465400	1.54206000	3.04713500
C	8.07695700	0.61438300	3.05698500
C	9.37249400	1.00830600	2.72395300
C	9.62523600	2.33617900	2.37222800
H	8.79917200	4.29267400	2.08192100
H	7.88686700	-0.42224200	3.32150100
H	10.18071700	0.28206900	2.73371900
H	10.63210700	2.64836900	2.10828400
C	4.73021100	-0.27949500	2.28252200
C	5.30888900	0.03387900	4.97391000
C	4.91136200	-1.57047200	3.10475600
C	4.54442900	-1.24216200	4.55950700
H	4.29042000	-2.37895600	2.69891100
H	5.95546600	-1.91229200	3.04648200
H	3.46678800	-1.04648100	4.62834400
H	4.77316400	-2.07093800	5.24136500
C	6.35805500	5.56965200	3.71716800
C	5.92853100	4.93336300	1.06080500
C	6.92020600	6.56228600	2.68126500
C	6.07020700	6.43062000	1.40942200
H	6.90574200	7.58679400	3.07498900
H	7.97089200	6.32522600	2.46267700
H	5.07400500	6.85033800	1.59619500
H	6.49863400	6.98834500	0.56720900
P	5.26772700	1.12100700	3.42860000
P	5.82111000	4.04272300	2.73466000
Rh	3.99040500	2.91024500	3.37217300
C	4.76291500	4.62019100	0.11869200
H	4.71634200	3.55305100	-0.12246900
H	3.80477700	4.89849300	0.56991900
H	4.87200200	5.17587000	-0.82176000
H	6.86265900	4.59119400	0.59676900

C	7.25170500	5.31406400	4.93256500
H	6.78404700	4.61142500	5.63131300
H	8.22422800	4.90100400	4.64420600
H	7.43238900	6.25157200	5.47303700
H	5.39895300	5.96787000	4.07628700
C	4.75713500	0.71392800	6.22976000
H	5.36506600	1.57830200	6.51821400
H	3.73485900	1.06195200	6.05653900
H	4.75471300	0.00867500	7.07137000
H	6.36414300	-0.22719400	5.13482500
C	5.35796200	-0.29167300	0.88845800
H	4.91901700	-1.09627600	0.28624900
H	5.17411700	0.65184700	0.36268400
H	6.44113300	-0.45202500	0.92731200
H	3.65419800	-0.09207300	2.17790500
C	1.16020700	2.16949600	2.02925800
H	2.10246900	2.34277200	1.51007600
C	1.28625600	1.69030700	3.31942500
O	2.35516800	1.68591800	4.04634800
O	0.13807600	1.21847800	3.92112300
C	0.20856400	0.87408100	5.30988700
H	0.93196500	0.06358000	5.45624500
H	0.55811600	1.73464100	5.89147500
C	-1.18602700	0.44676500	5.73882000
H	-1.18351900	0.16076600	6.79686100
H	-1.90358700	1.26310400	5.60409400
H	-1.52958900	-0.41034600	5.14984100
C	0.02615500	0.75808400	0.25137600
C	-0.06400000	-0.54173600	0.77573700
C	0.22490500	0.90085400	-1.12730000
C	0.03925700	-1.65870400	-0.05226900
H	-0.21947400	-0.66609200	1.84476300
C	0.33520900	-0.21567400	-1.96161300
H	0.29114800	1.90039700	-1.55314900
C	0.24178100	-1.50078500	-1.42726400
H	-0.04269600	-2.65631900	0.37362400
H	0.48953600	-0.07903000	-3.02955300
H	0.32157400	-2.37136600	-2.07352700
C	-0.06921100	1.97079500	1.16797300
H	-0.25197900	2.86069300	0.55047400
H	-0.94531800	1.85764700	1.81542900
C	0.44481000	6.53064500	5.82933000
C	0.70269100	5.90326700	4.59723800
C	1.91399400	5.18811200	4.47527600
C	2.82305700	5.14553200	5.53744500
C	2.55152900	5.80116700	6.73623900
C	1.35173600	6.49675100	6.88649500
H	-0.49728200	7.05368700	5.95142100
H	3.73072500	4.56044400	5.40219300
H	3.26926500	5.75310100	7.55097100
H	1.11541000	7.00060200	7.81928100
C	-0.36219200	5.92447400	3.54244700
C	-0.80243500	7.10245200	2.87147600
C	-1.01849000	4.70345600	3.31255600
C	-1.91765500	6.96533600	2.01624300

C	-2.11189500	4.60777400	2.45284000	H	10.34137400	2.85464100	1.08228700
H	-0.68524300	3.81421600	3.83891400	C	5.05823800	-0.61955400	2.87745100
C	-2.56960300	5.74986200	1.80599700	C	5.84367600	0.54729800	5.25375000
H	-2.29630900	7.83767800	1.49593300	C	5.59251900	-1.57358900	3.96254400
H	-2.60223600	3.64983700	2.30642600	C	5.33477000	-0.90880400	5.32225600
H	-3.42810000	5.70434000	1.14077200	H	5.11258900	-2.55839400	3.89103200
O	2.30833800	4.56502500	3.29892200	H	6.67014800	-1.73885800	3.82157300
Si	-0.12042100	8.89585800	3.03422000	H	4.25504400	-0.90577800	5.52786600
C	-0.80960800	9.65260300	4.64299700	H	5.81436900	-1.45217400	6.14607900
C	-2.01177700	9.15488500	5.18424800	C	5.95333900	5.58440900	2.75261800
C	-0.22431900	10.75586200	5.29295000	C	5.28363300	4.43042200	0.33021000
C	-2.59351400	9.71917200	6.32138300	C	6.34679800	6.39336400	1.50160100
H	-2.50243400	8.30868300	4.70938100	C	5.40642300	5.97261000	0.36130200
C	-0.79909200	11.32551200	6.43193400	H	6.27838000	7.47080600	1.69908800
H	0.69505800	11.18859500	4.90965900	H	7.39376500	6.19173600	1.23541500
C	-1.98545300	10.80630600	6.95194400	H	4.41357000	6.39886600	0.54225800
H	-3.52090300	9.30952500	6.71415200	H	5.74593100	6.35327900	-0.61016000
H	-0.31863000	12.17457900	6.91199600	P	5.42437200	1.13557800	3.49799100
H	-2.43404400	11.24697500	7.83865900	P	5.51051700	3.86573600	2.12338700
C	-0.89499200	9.91099700	1.60853600	Rh	3.90892700	2.74716400	3.16016600
C	-1.56260200	11.12242700	1.86558000	C	3.97131700	3.94302800	-0.29368700
C	-0.76001500	9.52938200	0.25694300	H	3.94308700	2.85064900	-0.36308700
C	-2.06540000	11.91692000	0.83114600	H	3.11750300	4.26383100	0.31159500
H	-1.69534500	11.45459400	2.89125400	H	3.85922800	4.35100400	-1.30699100
C	-1.25881900	10.31707000	-0.78138800	H	6.13095500	4.01121500	-0.22776600
H	-0.27336900	8.59005200	0.00530400	C	6.94833100	5.64314600	3.91276100
C	-1.91316000	11.51805900	-0.49640700	H	6.59592400	5.05607700	4.76816000
H	-2.57833700	12.84658900	1.06563500	H	7.93426400	5.26234500	3.62379100
H	-1.13960500	9.99189900	-1.81208800	H	7.07477400	6.67918800	4.25031100
H	-2.30388700	12.13343300	-1.30292100	H	4.98271500	5.95546500	3.10666000
C	1.80922500	9.10340700	2.83962000	C	5.29099100	1.45311000	6.35715600
C	2.12931000	10.53357600	2.33628700	H	5.70847300	2.46330000	6.29275300
H	1.79642600	11.31237800	3.03258600	H	4.20208900	1.54205400	6.28372300
H	3.21816800	10.64406600	2.22538600	H	5.53891800	1.04633100	7.34639400
H	1.67233800	10.74602500	1.36553200	H	6.93992700	0.53401300	5.31718300
C	2.31237500	8.10557400	1.77236900	C	5.49388300	-0.94132300	1.44691200
H	2.17836600	7.06357600	2.08049800	H	5.16773700	-1.95136500	1.16826700
H	1.81061000	8.24214900	0.80741600	H	5.05513000	-0.24040900	0.72813800
H	3.38577900	8.26878400	1.59683100	H	6.58235200	-0.89875400	1.33482100
C	2.60359800	8.87296700	4.14252500	H	3.96076800	-0.65489200	2.91809600
H	3.67196300	9.06035800	3.95494500	C	1.15808200	1.05278500	2.05501800
H	2.29194900	9.54615000	4.94741800	H	2.03255700	0.42434800	1.85271500
H	2.50922200	7.85128000	4.51309400	C	1.18071900	1.37589100	3.53146800
H	1.59609900	3.98560800	2.88394000	O	2.20710700	1.64225800	4.15868300
H				O	-0.01345800	1.36419800	4.11092100
C	8.27516300	3.29805800	1.49638500	C	-0.08948200	1.78959900	5.50647200
C	7.08370000	2.87601500	2.10693700	H	0.38400900	1.01451300	6.11790300
C	7.05437600	1.63452000	2.77147300	H	0.47805200	2.71589600	5.61421600
C	8.21954700	0.85516300	2.83373300	C	-1.55705400	1.96794900	5.84049500
C	9.40019300	1.28969700	2.23192600	H	-1.65539600	2.26988600	6.88870400
C	9.42597200	2.51204400	1.55723200	H	-2.00229400	2.74973700	5.21787600
H	8.31255200	4.24627600	0.96922100	H	-2.11629100	1.03799300	5.69378600
H	8.21016100	-0.09935200	3.35238800	C	-0.00379700	0.01921000	0.05518800
H	10.29502700	0.67540900	2.28538100	C	0.05158700	-1.32502800	-0.33408400
				C	0.07055600	1.00508600	-0.94090300

C	0.17467700	-1.68007400	-1.67948500
H	-0.00930600	-2.10283600	0.42440700
C	0.19436800	0.65478300	-2.28563300
H	0.02791600	2.05578700	-0.66282800
C	0.24671000	-0.69027000	-2.66020000
H	0.21126700	-2.72982900	-1.95948700
H	0.24634400	1.43366900	-3.04195600
H	0.34032200	-0.96324900	-3.70793700
C	-0.12871800	0.39937000	1.51794900
H	-0.96826700	1.08955800	1.66023600
H	-0.36256200	-0.49307100	2.10963600
C	-0.01362000	6.09200700	4.85839400
C	0.61778300	5.57689300	3.71623100
C	1.84758100	4.84671400	3.85707100
C	2.39738100	4.76924600	5.16612600
C	1.75461700	5.30743800	6.27804900
C	0.52969000	5.96501000	6.13823700
H	-0.96492300	6.60109600	4.73460300
H	3.34390700	4.24213900	5.27385200
H	2.21558900	5.21056500	7.25964200
H	0.01347300	6.38131800	6.99855600
C	-0.07752900	5.69237300	2.39692000
C	-0.36723800	6.92287700	1.74246800
C	-0.55085100	4.49172800	1.83761200
C	-1.14762700	6.85826900	0.56415500
C	-1.31280700	4.46245400	0.67343300
H	-0.34518100	3.56853500	2.36842900
C	-1.61705700	5.66009000	0.02975600
H	-1.40086500	7.77631200	0.04533000
H	-1.68487900	3.51648800	0.28628300
H	-2.21962100	5.66754800	-0.87517700
O	2.43440000	4.28006600	2.81729000
Si	0.09667600	8.70134100	2.31122000
C	-1.17980200	9.27038800	3.60911100
C	-2.44667800	8.65555900	3.65930900
C	-0.95542800	10.34357000	4.49302100
C	-3.43439600	9.08174500	4.54978200
H	-2.66490400	7.82531000	2.99224600
C	-1.93756800	10.77463700	5.38831000
H	-0.00044600	10.86112800	4.48991200
C	-3.18134900	10.14266500	5.42099400
H	-4.40080100	8.58340600	4.56367100
H	-1.72897600	11.60365200	6.06034300
H	-3.94689800	10.47499600	6.11773000
C	-0.16879500	9.83273600	0.78772100
C	-0.93490800	11.00938500	0.87511900
C	0.45403900	9.56727300	-0.44994700
C	-1.06940600	11.88083500	-0.20980300
H	-1.43920900	11.25376000	1.80593900
C	0.32603000	10.43229800	-1.53753600
H	1.03567200	8.65720000	-0.57733500
C	-0.43669500	11.59685200	-1.41973300
H	-1.67176800	12.78047700	-0.10756800
H	0.81826300	10.19568400	-2.47799200
H	-0.53968200	12.27229800	-2.26545200

C	1.94551400	9.00499400	2.85855000
C	2.33128300	10.48398000	2.60171700
H	1.71639800	11.18701700	3.17628200
H	3.37545600	10.64373500	2.90901400
H	2.24773200	10.76256000	1.54712100
C	2.86481000	8.12037800	1.98904700
H	2.67521600	7.05305100	2.14142600
H	2.75299100	8.33858700	0.91985700
H	3.91605500	8.31830600	2.24881500
C	2.23103800	8.69434300	4.34290900
H	3.27017000	8.97265600	4.57610400
H	1.58246700	9.25819500	5.02121600
H	2.11221300	7.63596400	4.57573800
H	1.35936800	2.00336300	1.54512500

H₂O

O	0.00000000	0.00000000	0.11942600
H	0.00000000	0.76261700	-0.47770500
H	0.00000000	-0.76261700	-0.47770500

I

C	-1.21234500	-0.85425000	-1.94951800
C	-2.07457200	-1.21145400	-0.90042800
C	-3.35075900	-1.71424400	-1.25966500
C	-3.70719800	-1.84658000	-2.60908000
C	-2.81731200	-1.49206100	-3.62258100
C	-1.56093000	-0.98860800	-3.29258400
H	-0.23458800	-0.46970600	-1.68961000
H	-4.69830700	-2.20539800	-2.86340000
H	-3.11567900	-1.60672100	-4.66146700
H	-0.85028500	-0.71122000	-4.06616900
C	-1.59246300	-1.10124000	0.51223200
C	-0.94122300	0.06211800	1.01459700
C	-1.72612100	-2.24245600	1.32986000
C	-0.47897000	-0.01132800	2.35220900
C	-1.25568100	-2.27319900	2.64170100
H	-2.20284700	-3.12718100	0.92136500
C	-0.62261200	-1.14285100	3.15965800
H	0.00004900	0.86746100	2.78401800
H	-1.38250700	-3.16892400	3.24583800
H	-0.24676000	-1.13875700	4.18114000
O	-4.24524900	-2.01483500	-0.26332000
Si	-5.72002900	-2.82318200	-0.13498500
C	-6.99896700	-2.03866500	-1.29248100
C	-6.85799500	-0.68260600	-1.64796600
C	-8.13796700	-2.71454900	-1.76994600
C	-7.80477300	-0.03409800	-2.44180300
H	-5.99000500	-0.12671000	-1.30640800
C	-9.09184700	-2.07028900	-2.56187700
H	-8.29412600	-3.76191200	-1.52767200
C	-8.92685800	-0.72695800	-2.90084000
H	-7.66529300	1.01189600	-2.70362100
H	-9.96071700	-2.61972400	-2.91563100
H	-9.66605400	-0.22395900	-3.51906600
C	-6.21930800	-2.45843500	1.64673300

C	-5.26687900	-2.09872900	2.61864000	H	-4.63923100	2.04316100	-2.28078400
C	-7.56563000	-2.54815100	2.04823500	H	-4.26016000	3.68527900	-0.42639200
C	-5.64550100	-1.84828700	3.94000800	C	-2.66673300	3.36934200	3.46267200
H	-4.22246000	-2.00178300	2.33835900	H	-1.58376000	3.36071600	3.63062100
C	-7.94714000	-2.30275300	3.36827800	H	-2.97687900	4.41157000	3.33444000
H	-8.33325800	-2.79967900	1.31928700	H	-3.14619000	2.98849400	4.37362000
C	-6.98527200	-1.95278500	4.31856100	H	-2.68216200	1.48227500	2.46561100
H	-4.89083200	-1.57138800	4.67212900	C	2.54028500	3.75080400	1.68489500
H	-8.99381900	-2.37697500	3.65305200	H	1.76019100	3.67508500	2.44980400
H	-7.28005700	-1.75799400	5.34682800	H	2.77740300	2.73594500	1.35244000
C	-5.48305500	-4.71914700	-0.41874100	H	3.43686900	4.17520400	2.15608800
C	-6.64890200	-5.51057400	0.21980400	H	1.81610800	5.61495600	0.90350900
H	-7.61927400	-5.28100700	-0.23566500	C	0.17221800	5.13764300	-3.05707900
H	-6.47938800	-6.58873800	0.08623900	H	0.63949600	5.33992000	-4.02955400
H	-6.73435100	-5.31887000	1.29464200	H	-0.66611400	4.45251900	-3.22748300
C	-4.17433300	-5.15869100	0.27594500	H	-0.23892000	6.08030100	-2.68169600
H	-3.29496200	-4.70677400	-0.19475100	H	1.55267200	3.59454900	-2.52886800
H	-4.16390900	-4.89690500	1.34090200	C	3.74877500	-1.56051500	-2.39300000
H	-4.06170900	-6.25026600	0.20445400	C	3.19581200	-1.07973700	-1.19517200
C	-5.38614000	-5.08115000	-1.91801100	C	2.34901800	0.04515000	-1.27666700
H	-5.24728500	-6.16621600	-2.03245200	C	2.09428800	0.66875900	-2.49929700
H	-6.28929800	-4.80548200	-2.47367100	C	2.67738700	0.18136000	-3.66786500
H	-4.53407700	-4.59050700	-2.40116700	C	3.50651900	-0.93983100	-3.61762300
C	-2.99504500	5.64354000	0.89820700	H	4.37623500	-2.44382900	-2.35396800
C	-1.98465300	4.73614700	0.53774800	H	1.40534400	1.50648400	-2.51479100
C	-0.74705500	5.23039800	0.08598900	H	2.46800600	0.67055400	-4.61529200
C	-0.54669700	6.61951200	0.01906600	H	3.95335300	-1.33789600	-4.52373900
C	-1.55385200	7.51021700	0.38656100	C	3.39623900	-1.81465900	0.09382500
C	-2.78459300	7.01953800	0.82739600	C	4.65475300	-1.98300100	0.74186600
H	-3.95793200	5.27564300	1.23991800	C	2.24094800	-2.40362100	0.64081700
H	0.40493800	7.01505600	-0.32336900	C	4.66142100	-2.78445500	1.90335200
H	-1.38001300	8.58146700	0.32748100	C	2.28641500	-3.17000400	1.80514200
H	-3.57639500	7.70561900	1.11654600	H	1.29021100	-2.28844700	0.12541200
C	1.19583900	4.53593800	-2.09215700	C	3.50959200	-3.36879000	2.43403300
C	2.08596100	4.62471900	0.51422900	H	5.59836800	-2.95745900	2.42040100
C	2.43942000	5.40486200	-1.82063500	H	1.37141000	-3.60134600	2.19824500
C	3.14560200	4.81980400	-0.58910700	H	3.57770900	-3.97324800	3.33484000
H	3.09974000	5.43112200	-2.69765400	O	1.74432500	0.59632300	-0.15968700
H	2.14039100	6.44378800	-1.62229700	Si	6.37525600	-1.29833400	0.20178900
H	3.59220500	3.84954200	-0.84799100	C	7.01772700	-2.37562100	-1.23228300
H	3.96311400	5.46226000	-0.23706900	C	6.53562400	-3.69031400	-1.39165900
C	-3.05001900	2.49421700	2.26761400	C	8.03081300	-1.95423300	-2.11477000
C	-3.82778900	2.67695700	-0.37123300	C	7.02769500	-4.53604800	-2.38811000
C	-4.56188100	2.39164000	1.97969300	H	5.75850400	-4.06134700	-0.72774300
C	-4.72672200	1.83744800	0.55635300	C	8.52732900	-2.79352600	-3.11508800
H	-5.05394000	1.75157900	2.72279300	H	8.44895900	-0.95603700	-2.02454900
H	-5.03476500	3.38248800	2.05050700	C	8.02427700	-4.08759800	-3.25693300
H	-4.41621000	0.78503600	0.53139200	H	6.63215400	-5.54403300	-2.48542500
H	-5.77233600	1.87425100	0.22423500	H	9.30668500	-2.43501400	-3.78301400
P	0.54118100	3.97851000	-0.38900600	H	8.40787200	-4.74200400	-4.03548500
P	-2.21549000	2.88784200	0.60823300	C	7.56461800	-1.60812200	1.66659900
Rh	-0.31813100	1.85241600	0.12229500	C	8.76258600	-2.32395700	1.48882300
C	-3.66040900	2.14306100	-1.79239400	C	7.32004100	-1.07974200	2.95196000
H	-3.05458500	2.82312000	-2.40206500	C	9.67342600	-2.50120700	2.53448400
H	-3.16984500	1.16758500	-1.79840600	H	8.99316900	-2.75325200	0.51805800

C	8.22440100	-1.25177400	4.00050000
H	6.39847800	-0.53697300	3.14877200
C	9.40860100	-1.96365800	3.79353100
H	10.58897500	-3.06194300	2.36255400
H	8.00377000	-0.83250900	4.97913500
H	10.11483000	-2.10004000	4.60858100
C	6.45714600	0.61769900	-0.16715200
C	7.89571600	1.13159600	0.09382900
H	8.64040700	0.65150700	-0.55241400
H	7.93843300	2.21114100	-0.11202100
H	8.21290700	0.97687700	1.12894400
C	5.50570700	1.36187100	0.79664600
H	4.45973200	1.07906800	0.64177400
H	5.75204000	1.18113800	1.84940600
H	5.58192000	2.44645700	0.63107500
C	6.07553200	0.99848300	-1.61380100
H	6.21541600	2.08099700	-1.75130200
H	6.69652500	0.49199700	-2.35962200
H	5.03320700	0.77108900	-1.84248600
H	1.72503200	-0.05132800	0.57039300

(R)-product

C	3.70505300	-1.00147700	-0.23197300
C	2.37121100	-0.54774500	-0.17239200
C	1.41395000	-1.46886900	0.32053000
C	1.77858500	-2.77668300	0.66194800
C	3.09995000	-3.19528000	0.55917700
C	4.07405900	-2.29471200	0.12106000
H	4.48245200	-0.31297800	-0.54484500
H	0.99778200	-3.44284000	1.01574800
H	3.36924100	-4.21138000	0.83431300
H	5.11611100	-2.59479400	0.05984500
C	2.00553800	0.82592500	-0.61861200
C	0.76457000	1.42621400	-0.27072300
C	2.89505300	1.56544000	-1.42450300
C	0.48864600	2.73322500	-0.70633200
C	2.60390600	2.86256900	-1.83446000
H	3.82260400	1.11573200	-1.76116600
C	1.39770000	3.46204700	-1.46893900
H	-0.46652000	3.18951900	-0.45662900
H	3.31719500	3.40051400	-2.45364100
H	1.16236100	4.47296400	-1.79028400
O	0.09293300	-1.15581300	0.47887600
Si	-0.49385000	0.41718300	0.67818600
C	-2.19296900	0.39222800	-0.13383800
C	-2.67138200	-0.80457400	-0.70032400
C	-3.02017500	1.52941900	-0.21565700
C	-3.92224600	-0.86395500	-1.31791200
H	-2.05383700	-1.69702900	-0.65761300
C	-4.26922400	1.47566600	-0.83618500
H	-2.69353900	2.47745000	0.20496100
C	-4.72408800	0.27631600	-1.38777100
H	-4.26908700	-1.80076600	-1.74674600
H	-4.88647200	2.36897500	-0.88863500
H	-5.69713200	0.23219300	-1.87028600

C	-0.56652700	0.82381300	2.54936800
C	-1.53304600	-0.15640900	3.24890300
H	-1.21293400	-1.19760200	3.12463300
H	-1.56936600	0.05261800	4.32790300
H	-2.55435800	-0.07049800	2.86020500
C	-1.05208500	2.27189000	2.77612100
H	-0.40628200	3.00565300	2.27765800
H	-2.07907700	2.42189700	2.42315700
H	-1.04309800	2.50748700	3.85011500
C	0.84473700	0.66868000	3.15862100
H	0.81582300	0.90001600	4.23320500
H	1.22697900	-0.35276700	3.05282500
H	1.56903100	1.34868500	2.69477800

(S)-product

C	3.70505300	-1.00147700	0.23197300
C	2.37121100	-0.54774500	0.17239200
C	1.41395000	-1.46886900	-0.32053000
C	1.77858500	-2.77668300	-0.66194800
C	3.09995000	-3.19528000	-0.55917700
C	4.07405900	-2.29471200	-0.12106000
H	4.48245200	-0.31297800	0.54484500
H	0.99778200	-3.44284000	-1.01574800
H	3.36924100	-4.21138000	-0.83431300
H	5.11611100	-2.59479400	-0.05984500
C	2.00553800	0.82592500	0.61861200
C	0.76457000	1.42621400	0.27072300
C	2.89505300	1.56544000	1.42450300
C	0.48864600	2.73322500	0.70633200
C	2.60390600	2.86256900	1.83446000
H	3.82260400	1.11573200	1.76116600
C	1.39770000	3.46204700	1.46893900
H	-0.46652000	3.18951900	0.45662900
H	3.31719500	3.40051400	2.45364100
H	1.16236100	4.47296400	1.79028400
O	0.09293300	-1.15581300	-0.47887600
Si	-0.49385000	0.41718300	-0.67818600
C	-2.19296900	0.39222800	0.13383800
C	-2.67138200	-0.80457400	0.70032400
C	-3.02017500	1.52941900	0.21565700
C	-3.92224600	-0.86395500	1.31791200
H	-2.05383700	-1.69702900	0.65761300
C	-4.26922400	1.47566600	0.83618500
H	-2.69353900	2.47745000	-0.20496100
C	-4.72408800	0.27631600	1.38777100
H	-4.26908700	-1.80076600	1.74674600
H	-4.88647200	2.36897500	0.88863500
H	-5.69713200	0.23219300	1.87028600
C	-0.56652700	0.82381300	-2.54936800
C	-1.53304600	-0.15640900	-3.24890300
H	-1.21293400	-1.19760200	-3.12463300
H	-1.56936600	0.05261800	-4.32790300
H	-2.55435800	-0.07049800	-2.86020500
C	-1.05208500	2.27189000	-2.77612100
H	-0.40628200	3.00565300	-2.27765800

H	-2.07907700	2.42189700	-2.42315700
H	-1.04309800	2.50748700	-3.85011500
C	0.84473700	0.66868000	-3.15862100
H	0.81582300	0.90001600	-4.23320500
H	1.22697900	-0.35276700	-3.05282500
H	1.56903100	1.34868500	-2.69477800

TS1

C	-2.79458900	-1.63133100	-1.85609400
C	-1.98173100	-0.71788000	-1.16595000
C	-0.90582700	-1.22760000	-0.40473700
C	-0.70247000	-2.61414800	-0.33328900
C	-1.52979100	-3.49771200	-1.01984700
C	-2.58463600	-3.00779300	-1.79181700
H	-3.60849900	-1.24120700	-2.45942300
H	0.10628100	-2.97635900	0.29387400
H	-1.35182600	-4.56796900	-0.94689000
H	-3.23398100	-3.68454300	-2.33983600
C	-2.22023400	0.75187100	-1.33722700
C	-3.32766000	1.44226200	-0.77161300
C	-1.32128800	1.43809200	-2.16886600
C	-3.47900300	2.80062700	-1.11883400
C	-1.49571700	2.78321300	-2.48310100
H	-0.47420700	0.89531800	-2.57882100
C	-2.58958700	3.46792300	-1.96118500
H	-4.31690400	3.36339000	-0.72406600
H	-0.78405900	3.28676800	-3.13213100
H	-2.75183900	4.51610500	-2.19991000
O	-0.06638100	-0.44291700	0.32046300
Si	-4.61051700	0.63509400	0.39782400
C	-3.75085500	-0.58878300	1.57238900
C	-4.07598300	-1.95657900	1.62843800
C	-2.76724200	-0.12554200	2.46949400
C	-3.47058800	-2.81405400	2.54930300
H	-4.79748200	-2.36919000	0.93057700
C	-2.15933500	-0.97637700	3.39393600
H	-2.45232000	0.91435300	2.44044200
C	-2.51569500	-2.32525300	3.44171700
H	-3.74261000	-3.86677300	2.56456000
H	-1.40448700	-0.58629900	4.07232300
H	-2.04651900	-2.99065000	4.16234100
C	-5.93707200	-0.22308700	-0.66878100
C	-6.89344300	-1.11122800	-0.13562600
C	-6.05184800	0.09035000	-2.03738400
C	-7.90083100	-1.66658500	-0.92809300
H	-6.85646800	-1.38412700	0.91540200
C	-7.05826000	-0.45823000	-2.83555600
H	-5.34219400	0.77845800	-2.48964600
C	-7.98599300	-1.34237900	-2.28296300
H	-8.61916900	-2.35238400	-0.48533700
H	-7.11643900	-0.19439500	-3.88882600
H	-8.76938100	-1.77328000	-2.90137400
C	-5.55693000	1.94963100	1.50330400
C	-6.29809500	1.19048000	2.63083400
H	-5.61026500	0.63676000	3.27796700

H	-6.84477400	1.90800400	3.26025300
H	-7.03612700	0.48333600	2.23578900
C	-6.62887600	2.71397600	0.69092200
H	-6.20960400	3.31975300	-0.11961100
H	-7.35889600	2.03155900	0.24345700
H	-7.17666400	3.39939800	1.35436600
C	-4.60650200	2.96596600	2.17549800
H	-5.18978500	3.67670500	2.77981800
H	-3.90226700	2.47338100	2.85408000
H	-4.02260300	3.54769900	1.45564400
O	0.69452300	1.82251800	0.31920700
H	0.68580300	2.13716400	1.23847600
H	-0.11177500	0.63705000	0.26515700
C	6.70217100	1.05328200	-0.39116800
C	5.42054400	0.51321700	-0.20576200
C	5.24317700	-0.88418600	-0.23143900
C	6.36012800	-1.71220300	-0.42216900
C	7.63136600	-1.16609600	-0.60126000
C	7.80276600	0.21984600	-0.58995500
H	6.84791600	2.12992200	-0.37932700
H	6.24388800	-2.79209400	-0.43612400
H	8.48561500	-1.82049400	-0.75302500
H	8.79076400	0.64958500	-0.73170100
C	3.16283400	-2.67501600	-1.47166400
C	3.65282000	-2.90335500	1.23820400
C	3.54698200	-4.08022500	-0.96996600
C	3.14316500	-4.16692100	0.50946100
H	3.05749700	-4.85775800	-1.57061200
H	4.62981400	-4.23638600	-1.07716800
H	2.04814200	-4.20987500	0.58333300
H	3.52728000	-5.07542900	0.99020800
C	4.26379700	2.64992900	1.58204200
C	3.95433600	2.93607600	-1.15289400
C	4.72458300	3.99044300	0.97686500
C	3.90368600	4.22207200	-0.30025300
H	4.59929000	4.80836300	1.69820100
H	5.79661200	3.94584400	0.73551900
H	2.85954800	4.43135800	-0.03160200
H	4.26757800	5.08374900	-0.87378600
P	3.49809700	-1.49691100	-0.02969800
P	3.89843800	1.52327200	0.10450300
Rh	2.11125000	0.25337900	0.21292500
C	2.85290500	2.85636400	-2.21398400
H	2.95285000	1.95352800	-2.82603500
H	1.86783500	2.83162100	-1.73779000
H	2.90816100	3.72641400	-2.88208600
H	4.93730900	2.87640200	-1.63983200
C	5.17015600	2.07174700	2.66975200
H	4.77199800	1.12802000	3.05923700
H	6.18231200	1.88143200	2.29719400
H	5.24907800	2.77289500	3.51006600
H	3.26455000	2.80241800	2.01123900
C	2.93769900	-2.61959100	2.56230700
H	3.36611000	-1.74960300	3.07111700
H	1.87415100	-2.41265600	2.40084500

H	3.02196300	-3.48215100	3.23649900
H	4.72659100	-3.02169400	1.43248000
C	3.75795600	-2.27339000	-2.82265400
H	3.43728300	-2.97583300	-3.60215000
H	3.42587400	-1.27256200	-3.11999700
H	4.85335200	-2.27277900	-2.80182700
H	2.06758800	-2.63674700	-1.55408900

TS_{A-B(R)}

C	4.85217300	1.78606100	-0.69986300
C	3.50504800	1.54308300	-0.36821900
C	2.53035700	1.64148800	-1.39688100
C	2.96614700	1.98275000	-2.70402300
C	4.30438400	2.21044300	-2.99874300
C	5.26621800	2.10640100	-1.98997900
H	5.59757400	1.69662700	0.08677300
H	2.20152800	2.08088800	-3.47082400
H	4.59728900	2.46680500	-4.01466400
H	6.31878900	2.27093300	-2.20241900
C	3.18637900	1.27762000	1.06598200
C	2.45625200	0.16347900	1.58209800
C	3.77581300	2.18465600	1.97335800
C	2.47431700	-0.00633200	2.98521400
C	3.73822000	2.00434300	3.35258900
H	4.28878000	3.05089200	1.56564500
C	3.10204700	0.87824400	3.86312700
H	1.99217700	-0.87168900	3.42193700
H	4.21230000	2.72786400	4.01131600
H	3.08077900	0.68423500	4.93269200
O	1.23037300	1.53255300	-1.18839400
Si	1.54502700	-1.24634000	0.59056900
C	0.50298000	-1.51278400	-1.61823000
C	1.22004200	-1.18150800	-2.79101000
C	-0.08480300	-2.79549900	-1.58725000
C	1.28645100	-2.05170200	-3.88275200
H	1.71233100	-0.22054800	-2.86456800
C	-0.02003800	-3.67110700	-2.67504300
H	-0.60114100	-3.12471100	-0.69118300
C	0.65685700	-3.29856100	-3.83686100
H	1.83246900	-1.74995300	-4.77378500
H	-0.49636400	-4.64738200	-2.61058800
H	0.70731900	-3.97440800	-4.68672100
C	3.08354700	-2.43208800	0.10987600
C	-4.97905800	0.56835000	0.15164800
C	-3.58356300	0.74112000	0.09596300
C	-3.04989700	2.01250300	0.37429200
C	-3.91304000	3.06578900	0.72486800
C	-5.28943900	2.87267000	0.79927000
C	-5.82468200	1.61686800	0.50533800
H	-5.41887400	-0.39443100	-0.08617800
H	-3.50814300	4.05249800	0.92946000
H	-5.94162700	3.69810000	1.07132300
H	-6.89827500	1.45450000	0.54847400
C	-0.72281500	3.33997000	1.61293800
C	-0.97323700	3.59644200	-1.12213800

C	0.10972200	4.45260800	0.94658300
C	-0.63660500	4.87481100	-0.32641100
H	1.10401000	4.06646100	0.69003900
H	0.25230500	5.29128500	1.63997300
H	-0.04395800	5.56478600	-0.94014300
H	-1.56174100	5.40504300	-0.05435700
C	-3.27012800	-1.17259900	-2.03761700
C	-3.09949500	-2.18445100	0.53504100
C	-3.54646300	-2.68130400	-1.89566600
C	-4.01218200	-2.94604000	-0.45728400
H	-2.63500900	-3.24517100	-2.11423100
H	-4.30148900	-2.99984600	-2.62635700
H	-4.02096300	-4.01809300	-0.22248200
H	-5.04736200	-2.59620000	-0.33763200
P	-1.23365600	2.23518900	0.16434700
P	-2.44280500	-0.65685200	-0.39610400
Rh	-0.21724100	0.17561700	-0.54908400
C	0.45876800	-2.20191700	1.86453500
C	0.38438400	-3.60703800	1.92967200
C	-0.26826600	-1.49310500	2.84444800
C	-0.34112100	-4.26797200	2.92716500
H	0.91178800	-4.21265100	1.20271700
C	-0.96418800	-2.14222700	3.86472300
H	-0.26665600	-0.40795200	2.82217000
C	-1.00487400	-3.53801000	3.91164600
H	-0.36725600	-5.35500200	2.94118900
H	-1.48206500	-1.55689900	4.62113500
H	-1.54811300	-4.04691200	4.70389400
C	3.70754200	-2.90395800	1.45123800
H	3.04737400	-3.56763800	2.01845800
H	3.98344400	-2.06773200	2.09996800
H	4.62810700	-3.46490200	1.23415200
C	4.17572300	-1.64116100	-0.64094200
H	3.81151400	-1.20668300	-1.57691600
H	5.00191200	-2.32231600	-0.89389300
H	4.59200200	-0.83540800	-0.03570700
C	2.80429400	-3.68500400	-0.74501700
H	2.55461800	-3.42605800	-1.77455800
H	2.00737700	-4.32679800	-0.36124900
H	3.71864200	-4.29625100	-0.77601800
C	-2.06485800	3.76535400	-2.17945500
H	-3.01847100	4.08489200	-1.74443900
H	-1.75946200	4.52518000	-2.90975100
H	-2.24138200	2.83395800	-2.72958600
C	-2.55225700	-0.76742600	-3.32588100
H	-2.40885600	0.31754500	-3.38067000
H	-1.57187100	-1.23857000	-3.41301400
H	-3.15535600	-1.06575300	-4.19358100
C	-3.76476400	-1.93835100	1.89483500
H	-4.73644200	-1.44751900	1.79352800
H	-3.92538600	-2.89792500	2.40064400
H	-3.14096000	-1.32655700	2.54924400
C	-0.05058900	2.64176500	2.79081600
H	-0.71847900	1.90474800	3.25158700
H	0.86311900	2.13110500	2.48539600

H	0.21113900	3.37694700	3.56233100
H	-4.23824100	-0.65693200	-2.01665000
H	-2.19511500	-2.77532800	0.71538900
H	-1.65964800	3.79180400	1.96627900
H	-0.05838700	3.23758600	-1.60722300

TS_{A-C(R)}

C	2.98732300	-3.57468000	-0.20249200
C	2.36524500	-2.35829100	0.13573300
C	1.91511600	-1.53997600	-0.92160700
C	2.08274300	-1.93549800	-2.25364400
C	2.68935100	-3.15131700	-2.55873200
C	3.14541300	-3.97599600	-1.52625000
H	3.38585700	-4.20239900	0.58910500
H	1.75655500	-1.25916600	-3.03725900
H	2.82628800	-3.44228200	-3.59686900
H	3.64220000	-4.91553800	-1.75167700
C	2.16596300	-1.93132900	1.54112400
C	2.06084400	-0.55356900	1.89454700
C	2.04943400	-2.92075600	2.53733800
C	1.82355200	-0.26394200	3.25144000
C	1.82646900	-2.59235500	3.87023800
H	2.10505800	-3.96841500	2.25630700
C	1.70506400	-1.25118800	4.22974300
H	1.72248800	0.76551300	3.56718200
H	1.73668500	-3.37789100	4.61642300
H	1.51824900	-0.97140100	5.26354900
O	1.35012000	-0.32167900	-0.66673400
Si	2.24480400	0.81251400	0.53681700
C	3.90232400	0.58636700	-0.43439500
C	4.14045200	1.20637800	-1.67594400
C	4.94588800	-0.20245900	0.08747300
C	5.35048300	1.05280500	-2.35737600
H	3.37266000	1.83068500	-2.12415000
C	6.15815500	-0.36447700	-0.58785000
H	4.81486700	-0.70577300	1.04193500
C	6.36616200	0.26377300	-1.81611900
H	5.49829000	1.55203300	-3.31252700
H	6.93848000	-0.98493500	-0.15292300
H	7.30823800	0.14038900	-2.34483300
C	2.76789400	2.46369700	1.57770400
C	3.20162500	3.61549800	0.64356500
H	2.39086500	3.97716500	0.00874200
H	3.54506700	4.46657100	1.25119200
H	4.03508000	3.32183800	-0.00165600
C	4.04084600	2.09651000	2.39333900
H	3.88402900	1.27517100	3.09760200
H	4.87921400	1.82804300	1.74590400
H	4.34968900	2.97608400	2.97760300
C	1.68729000	2.98635800	2.57201700
H	0.75758900	2.41135600	2.54834300
H	2.05425700	2.95574300	3.60594000
H	1.42756300	4.03070800	2.36567600
C	0.41874200	2.12627000	-0.57277700
C	-0.04077400	3.36366100	-0.05560100

C	0.75956500	2.14864500	-1.95095000
C	-0.15102400	4.51921200	-0.83064700
H	-0.32911900	3.43037600	0.98561700
C	0.66777900	3.30180800	-2.74051800
H	1.10322000	1.23185400	-2.41735700
C	0.20966300	4.49496400	-2.18210700
H	-0.51714800	5.44109500	-0.38245500
H	0.94879200	3.26422300	-3.79099700
H	0.13361700	5.39462000	-2.78817300
C	-4.61132800	-2.52212500	-0.00407900
C	-3.65985300	-1.48867800	-0.03858300
C	-4.07738000	-0.15900500	0.12572200
C	-5.44435900	0.11345800	0.30647700
C	-6.38128400	-0.91752000	0.33603900
C	-5.96247500	-2.24192700	0.18708100
H	-4.29962900	-3.55495200	-0.12832700
H	-5.78754000	1.13654300	0.42434700
H	-7.43455100	-0.68894500	0.47516900
H	-6.68650600	-3.05178500	0.21657800
C	-3.33350800	2.46081900	-1.12845900
C	-3.27262200	2.18945300	1.62193900
C	-4.14426600	3.49378700	-0.31846000
C	-3.50979400	3.61314900	1.07630800
H	-4.16419800	4.46096300	-0.83710900
H	-5.18986300	3.16681800	-0.22902100
H	-2.55419300	4.14431700	0.99809000
H	-4.14154600	4.18937900	1.76466200
C	-1.29247900	-3.16944500	0.77739300
C	-1.90528400	-2.86097800	-1.89386300
C	-1.40774600	-4.46006200	-0.05926600
C	-1.07649100	-4.10562100	-1.51715400
H	-0.73712400	-5.23526300	0.33299100
H	-2.42846100	-4.86418500	0.00636700
H	-0.00653500	-3.88644200	-1.61233800
H	-1.29637100	-4.93634700	-2.20033300
P	-2.75460200	1.15035600	0.11055200
P	-1.85323000	-1.75545500	-0.34636900
Rh	-0.72064900	0.24973400	-0.25619700
C	-1.50496400	-2.17891100	-3.20215200
H	-2.14945800	-1.31974300	-3.41835600
H	-0.47301900	-1.82247800	-3.16606800
H	-1.59198100	-2.88354100	-4.03973500
H	-2.95464800	-3.17161600	-1.97850700
C	-1.93267000	-3.22317800	2.16575700
H	-1.78037000	-2.28350900	2.70739100
H	-3.00951100	-3.41785100	2.11721500
H	-1.47232200	-4.02287100	2.75908200
H	-0.22794800	-2.95198200	0.91232100
C	-2.35480900	2.10579000	2.84119600
H	-2.25463900	1.07536400	3.19754200
H	-1.35054000	2.47425600	2.61966900
H	-2.76157400	2.70893000	3.66351900
H	-4.24637700	1.77643600	1.91114400
C	-4.03004800	1.93606500	-2.38566400
H	-4.25225800	2.76712900	-3.06694100

H	-3.39325700	1.22656600	-2.92569800
H	-4.97499200	1.43338900	-2.15276900
H	-2.39211500	2.93133700	-1.43147700

TS_{A-D}

C	3.91824900	1.06476300	-2.76149200
C	2.68430900	0.80088500	-2.11941300
C	2.07946200	1.86521900	-1.38785300
C	2.72324600	3.13305600	-1.37604800
C	3.91120000	3.35749300	-2.04534900
C	4.53094700	2.30696600	-2.73935800
H	4.43198300	0.24833200	-3.26000800
H	2.23534800	3.92684200	-0.81681700
H	4.37011600	4.34354200	-2.01767400
H	5.48455900	2.45544000	-3.23796600
C	2.06768800	-0.53573600	-2.25418800
C	1.17845300	-1.16063900	-1.30768500
C	2.35928800	-1.24410700	-3.44922400
C	0.71563200	-2.46310000	-1.62712400
C	1.86851500	-2.51155100	-3.72287600
H	2.95620200	-0.75190800	-4.20867100
C	1.03639200	-3.14260100	-2.79519200
H	0.07440900	-2.96002800	-0.91334900
H	2.12142300	-2.99692400	-4.66238700
H	0.63828100	-4.13661500	-2.98360100
O	0.93178100	1.77800400	-0.75363800
Si	1.59358800	-1.06518900	0.94482100
C	0.70889900	-0.57879800	2.61768500
C	-0.68076700	-0.65638300	2.82036000
C	1.47758100	-0.24010100	3.75240600
C	-1.27551800	-0.41995000	4.06264800
H	-1.31698600	-0.87686700	1.97398400
C	0.89449800	0.01247800	4.99775900
H	2.55661300	-0.16895800	3.67452100
C	-0.48757400	-0.07905500	5.16258800
H	-2.35601500	-0.49420500	4.16461700
H	1.52846300	0.27786500	5.84063600
H	-0.94250800	0.11350100	6.13101000
C	3.22845900	-0.07325100	0.96352400
C	4.40096100	-0.56567400	0.35941900
C	3.33699300	1.15849000	1.63663600
C	5.62271200	0.10044600	0.46553100
H	4.36395400	-1.47672800	-0.22700100
C	4.55262600	1.83646100	1.74264500
H	2.45850700	1.60065600	2.09253800
C	5.70579200	1.30279600	1.16754300
H	6.50655400	-0.31642500	-0.01111500
H	4.59516500	2.78547000	2.27177600
H	6.65507200	1.82601300	1.25144100
C	2.06731900	-2.96999800	1.37775700
C	2.89042800	-2.95618200	2.69386800
H	2.30603800	-2.61869300	3.55273700
H	3.22537100	-3.98109300	2.91041200
H	3.78439100	-2.32851000	2.61725800
C	2.93480900	-3.72853400	0.34737000

H	2.52298700	-3.72432000	-0.66283000
H	3.95213600	-3.33038200	0.30110000
H	3.02539300	-4.77916700	0.66181800
C	0.80551800	-3.81777100	1.65786700
H	1.09822900	-4.77378000	2.11661700
H	0.11509500	-3.32285900	2.34896700
H	0.25874500	-4.06856700	0.74336400
C	-5.02105200	-0.61446200	0.02746500
C	-3.70966500	-0.11185000	-0.02602500
C	-3.48206700	1.22625700	0.35731800
C	-4.55116700	2.00273100	0.83326000
C	-5.83877500	1.47605600	0.91710300
C	-6.07598700	0.16601400	0.49861100
H	-5.23050600	-1.62720700	-0.29956800
H	-4.38262000	3.03280000	1.13277300
H	-6.65416300	2.08906100	1.29144000
H	-7.07894600	-0.25010800	0.54128800
C	-1.99833000	3.14920100	-1.34149900
C	-1.45499600	3.20963100	1.36977000
C	-2.21761000	4.50091900	-0.63984200
C	-1.30102800	4.53348800	0.58495500
H	-2.01200400	5.33281700	-1.32593500
H	-3.26992700	4.59583700	-0.33501300
H	-0.25867300	4.62489500	0.25450900
H	-1.51003800	5.39008500	1.23818300
C	-2.60130500	-2.90136100	0.07726300
C	-2.83716600	-1.63316200	-2.37177000
C	-3.36333000	-3.66536200	-1.02675400
C	-2.85993300	-3.17448800	-2.38770000
H	-3.22251900	-4.74738900	-0.90520500
H	-4.44278700	-3.48285000	-0.93784500
H	-1.84702300	-3.55291400	-2.57171500
H	-3.48819100	-3.53871600	-3.21066800
P	-1.78725200	1.88385300	0.05030800
P	-2.26328200	-1.14601800	-0.61292500
Rh	-0.31425300	0.14592200	-0.49232400
C	-2.04536600	-1.02475900	-3.53150000
H	-2.09821300	0.06714500	-3.53507900
H	-0.99033200	-1.30421000	-3.48961400
H	-2.45756000	-1.38010700	-4.48541100
H	-3.87462400	-1.27892500	-2.43046700
C	-3.22417900	-3.04609500	1.47067700
H	-4.21767200	-2.59383100	1.53417700
H	-3.32939700	-4.11241700	1.70850600
H	-1.59636200	-3.33163100	0.13277500
C	-0.26079300	2.93417900	2.28433100
H	-0.42682100	2.06989600	2.92978300
H	0.63466200	2.75111000	1.68467300
H	-0.08074100	3.80807200	2.92459400
H	-2.36819100	3.25878800	1.97715800
C	-3.04332800	2.83268500	-2.41090200
H	-3.02900600	3.60886200	-3.18623100
H	-2.84932800	1.87531100	-2.90237600
H	-4.05485000	2.79835500	-1.99106200
H	-0.99923100	3.14876600	-1.79579000

H	-2.59982000	-2.59998200	2.24879300
TS _{A-E}			
C	-1.20463100	0.70219100	4.35672600
C	-1.22069900	0.33078000	2.99906200
C	-1.30678500	1.37551200	2.04805300
C	-1.39254000	2.71219100	2.46216300
C	-1.37836500	3.04397200	3.81504900
C	-1.27980300	2.03093300	4.76902200
H	-1.12144900	-0.05965300	5.12352000
H	-1.47584700	3.48202700	1.70143700
H	-1.44379300	4.08552500	4.11889100
H	-1.26255800	2.26886800	5.82875300
C	-1.15346300	-1.08408200	2.54631500
C	-1.11752000	-1.42245500	1.14738000
C	-1.15655500	-2.11432900	3.50981400
C	-0.98665300	-2.79750700	0.84209400
C	-1.06830300	-3.45525200	3.15001800
H	-1.23704000	-1.87944000	4.56520200
C	-0.95947900	-3.80558500	1.80449700
H	-0.93739700	-3.08900800	-0.20016200
H	-1.08062400	-4.22086400	3.92219000
H	-0.87205100	-4.84852000	1.50880500
O	-1.30804500	1.12996100	0.70432100
Si	-2.36139100	-0.21525200	-0.23375600
C	-2.18707100	-1.61854100	-1.60140400
C	-3.08422000	-2.68373700	-1.80043500
C	-1.08697600	-1.56462300	-2.48039500
C	-2.90609000	-3.63064200	-2.81553600
H	-3.94693800	-2.79817900	-1.15387500
C	-0.89703000	-2.50174500	-3.49941600
H	-0.36031900	-0.76234800	-2.36141400
C	-1.81087700	-3.54403100	-3.67380400
H	-3.62875800	-4.43540300	-2.93213800
H	-0.04014500	-2.41301400	-4.16367300
H	-1.67155800	-4.27386100	-4.46768300
C	-2.70504500	1.24411300	-1.52782700
C	-2.77592800	2.60235200	-1.14594200
C	-3.07173600	0.97453800	-2.86362600
C	-3.16847800	3.61507900	-2.02494500
H	-2.51595100	2.87900300	-0.13274800
C	-3.45694000	1.97932800	-3.75703200
H	-3.06554300	-0.04539400	-3.22864700
C	-3.50510300	3.30984300	-3.34427100
H	-3.21111200	4.64481700	-1.67526100
H	-3.72339500	1.71459400	-4.77807800
H	-3.80556900	4.09426500	-4.03501400
C	-4.14592200	-0.36655100	0.62990400
C	-5.23963600	-0.31162200	-0.47056300
H	-5.12789100	-1.07859400	-1.24183000
H	-6.22421100	-0.45828300	-0.00218000
H	-5.25603700	0.65723100	-0.97652000
C	-4.43993600	0.82216300	1.57375200
H	-3.82109000	0.81014400	2.47386200
H	-4.30160300	1.78757500	1.07573000

H	-5.48972900	0.77376000	1.90061500
C	-4.34409200	-1.66468500	1.44295500
H	-5.37892600	-1.71050700	1.81413300
H	-4.16961400	-2.57179700	0.85614200
H	-3.68476000	-1.71119900	2.31359100
C	5.11174400	-0.77803900	-0.69356800
C	3.82357400	-0.26209000	-0.47593100
C	3.60804200	1.12084700	-0.59504100
C	4.68139500	1.96356900	-0.92710000
C	5.95626200	1.44153700	-1.13724900
C	6.17117300	0.06571000	-1.02263800
H	5.29523700	-1.84503100	-0.60848600
H	4.52578000	3.03463100	-1.02114600
H	6.77974500	2.10426400	-1.38916500
H	7.16184400	-0.34825000	-1.19010000
C	1.93445000	3.14695100	0.91033400
C	1.56395600	2.83391100	-1.80778600
C	1.90831800	4.43202800	0.05783500
C	1.05416100	4.14961300	-1.18716500
H	1.51948100	5.27606200	0.64180500
H	2.92998100	4.70286500	-0.24664600
H	-0.00168800	4.03822200	-0.90827600
H	1.10815900	4.96656700	-1.91776500
C	2.28397000	-2.72476900	-1.26990100
C	3.06271700	-2.39837300	1.36424700
C	3.00584500	-3.91610100	-0.60370400
C	2.75883000	-3.83979500	0.91057900
H	2.65585800	-4.86565600	-1.02816000
H	4.08491600	-3.85978700	-0.80816100
H	1.71192100	-4.07981500	1.13133400
H	3.37898000	-4.55721500	1.46316600
P	1.87654700	1.70729500	-0.31537100
P	2.35609500	-1.30719800	-0.01614200
Rh	0.52868900	-0.01816100	0.29595100
C	2.60021700	-2.04809900	2.77855000
H	2.87561600	-1.02141500	3.04441800
H	1.51675800	-2.14017100	2.88240400
H	3.07297400	-2.72057600	3.50651000
H	4.14929900	-2.25191600	1.31077500
C	2.76106400	-2.39663000	-2.68662300
H	2.22256000	-1.53827900	-3.10229800
H	3.83104600	-2.16602700	-2.71559700
H	2.58361800	-3.25268200	-3.34918000
H	1.21272900	-2.95296100	-1.32028000
C	0.67962400	2.24514900	-2.90575900
H	1.12666800	1.33982200	-3.33256700
H	-0.31300700	1.98818300	-2.52936100
H	0.55677000	2.97038500	-3.72015500
H	2.56126700	3.02625600	-2.22665600
C	3.02905200	3.08770200	1.97796100
H	2.91624900	3.92551900	2.67734900
H	2.96720600	2.16154200	2.56003700
H	4.03287400	3.14733500	1.54390400
H	0.96717500	3.06165000	1.41966500

TS_{B-C(R)}

C	-5.42486800	-0.37756300	-0.70873500
C	-4.06414900	-0.65039500	-0.49537900
C	-3.09525700	0.13757500	-1.17512800
C	-3.53275800	1.11245200	-2.09180200
C	-4.89060300	1.34754200	-2.29604400
C	-5.84805400	0.61371000	-1.59346600
H	-6.16740600	-0.94137000	-0.15037800
H	-2.79431900	1.69941400	-2.62031500
H	-5.19884600	2.11984600	-2.99720900
H	-6.90809000	0.80904300	-1.72935900
C	-3.64337500	-1.76311700	0.39406900
C	-2.48185700	-1.72781700	1.22504400
C	-4.46186900	-2.90897100	0.40870600
C	-2.26778800	-2.83870000	2.06574800
C	-4.21038300	-3.99408000	1.24402800
H	-5.30931200	-2.95136700	-0.26876400
C	-3.10836300	-3.95418000	2.09095200
H	-1.40955900	-2.84968500	2.72581700
H	-4.86815800	-4.85972800	1.22378200
H	-2.88677800	-4.78452800	2.75691000
O	-1.80836200	-0.14291500	-0.96283600
Si	-1.26944700	-0.22497000	1.38957700
C	-0.28176500	2.64371400	-0.76882800
C	-0.62007700	2.90850900	-2.11515000
C	-0.11316200	3.77462300	0.04982500
C	-0.79503200	4.20635300	-2.60764000
H	-0.74378700	2.08091200	-2.81006100
C	-0.29795100	5.07868100	-0.42621400
H	0.15917000	3.65973000	1.09323200
C	-0.64140400	5.30401000	-1.75948200
H	-1.05886900	4.35522100	-3.65285800
H	-0.16963400	5.91970700	0.25249000
H	-0.78660300	6.31517300	-2.13097200
C	-2.25985400	1.22724600	2.29855200
C	4.69013900	-0.47061600	0.24799600
C	3.35477700	-0.43361800	-0.18330700
C	2.81729500	-1.56144000	-0.84497900
C	3.61869400	-2.70166900	-1.01270400
C	4.93263000	-2.73528400	-0.54631400
C	5.47329900	-1.61222500	0.07936200
H	5.12964800	0.39866000	0.72691200
H	3.21700400	-3.57907000	-1.50974000
H	5.53208000	-3.63184200	-0.67913700
H	6.49877400	-1.62331400	0.43839500
C	0.45881500	-3.21716100	-1.75620300
C	1.08142900	-1.06900800	-3.28572000
C	-0.60452200	-2.92526100	-2.83186800
C	0.07364500	-2.07732800	-3.92350600
H	-1.43833100	-2.37782400	-2.37700600
H	-1.00705700	-3.85969900	-3.24226100
H	-0.66678000	-1.54946100	-4.53348300
H	0.62836000	-2.74063800	-4.60015400
C	3.35555700	2.34097400	-0.98902000
C	2.72767900	1.94324500	1.67012700

C	3.50593200	3.56392700	-0.06842200
C	3.76737200	3.03948400	1.34679600
H	2.58610100	4.15994000	-0.09135100
H	4.32126900	4.20846300	-0.42171300
H	3.71680500	3.83736200	2.09833900
H	4.78100200	2.61739400	1.40610100
P	1.06101400	-1.46640100	-1.41788000
P	2.30913000	1.09814100	0.01579400
Rh	0.11629700	0.61899700	-0.54891800
C	0.03441300	-0.96350700	2.64263300
C	-0.07000700	-0.83099400	4.04381500
C	1.05415600	-1.82001500	2.18884300
C	0.79874500	-1.48574400	4.92239100
H	-0.85441400	-0.22771900	4.48146300
C	1.92562700	-2.48604200	3.05268000
H	1.16986000	-1.97922600	1.12644500
C	1.80679200	-2.31579000	4.43209700
H	0.67695900	-1.34908300	5.99437500
H	2.69787500	-3.13300700	2.64327400
H	2.48199300	-2.82665800	5.11381500
C	-3.27107400	0.59119100	3.28790700
H	-2.81617100	-0.09814300	4.00602800
H	-4.05328300	0.03864800	2.75961700
H	-3.75879000	1.39198600	3.86349400
C	-3.07965500	2.12806300	1.35069500
H	-2.46505000	2.58168000	0.57234100
H	-3.53149600	2.94140400	1.93861900
H	-3.89330000	1.58322700	0.86937900
C	-1.28969500	2.13890700	3.08444300
H	-0.49398300	2.52098700	2.44344900
H	-0.81233700	1.64312000	3.93158300
H	-1.83840100	3.00554100	3.48047700
C	2.45606000	-1.12075600	-3.96405800
H	2.90913800	-2.11561000	-3.88243000
H	2.34921500	-0.89320700	-5.03243800
H	3.16253300	-0.40161300	-3.53759700
C	2.90150200	2.67311300	-2.40965100
H	2.82096800	1.77599500	-3.03280600
H	1.93462700	3.17966100	-2.41844600
H	3.63916000	3.33410300	-2.88323000
C	3.10746400	1.07686100	2.87340300
H	4.01673000	0.49474600	2.69700900
H	3.29646300	1.73078200	3.73456000
H	2.31096100	0.38516200	3.14731600
C	-0.03653500	-4.04284900	-0.57209900
H	0.75417400	-4.21667000	0.16626000
H	-0.87220800	-3.55631700	-0.06469500
H	-0.38149000	-5.02379000	-0.92306400
H	4.33687300	1.85194200	-1.05082900
H	1.78028800	2.44079300	1.90617700
H	1.28784600	-3.75048100	-2.24570300
H	0.68815700	-0.05085600	-3.37130800

TS_{C-G}

C	7.48811300	1.47745100	-0.16224000
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C	6.17239400	1.06914600	0.11421500
C	5.84126700	-0.29498200	0.02413200
C	6.83689200	-1.21954200	-0.33446400
C	8.13833900	-0.80326600	-0.60851900
C	8.46575200	0.55175300	-0.52189000
H	7.75759100	2.52733400	-0.09452400
H	6.59739800	-2.27667000	-0.40197100
H	8.89403000	-1.53236000	-0.88863900
H	9.47887500	0.88506400	-0.73065600
C	3.54218000	-1.94888500	-0.98514500
C	4.32994500	-2.19946400	1.64422600
C	3.78758800	-3.38159100	-0.47032600
C	3.53537900	-3.37691900	1.04460200
H	3.13718000	-4.09671900	-0.99066300
H	4.82279700	-3.69002700	-0.67720300
H	2.46404700	-3.23864300	1.24046800
H	3.83098700	-4.32408900	1.51431000
C	5.51664500	3.26898000	2.05473500
C	5.01283800	3.65976900	-0.62919300
C	6.06406300	4.56681400	1.42646900
C	5.15339100	4.92355500	0.24292200
H	6.10158200	5.37356200	2.17035500
H	7.09476400	4.41519400	1.07406100
H	4.16854600	5.22829300	0.62145400
H	5.54861200	5.76161100	-0.34568100
P	4.08614800	-0.77864600	0.40334400
P	4.82176000	2.23855300	0.61962100
Rh	2.84164900	1.12350400	0.87047500
C	3.93366400	3.73404400	-1.71013300
H	3.90409600	2.81715700	-2.30842300
H	2.93840800	3.87596300	-1.27885400
H	4.13260400	4.57409200	-2.38851200
H	5.97705900	3.48549200	-1.12437500
C	6.46946500	2.54938000	3.01066200
H	6.00539900	1.65162700	3.43460400
H	7.39710100	2.24479700	2.51483500
H	6.73768000	3.20927400	3.84572000
H	4.60784500	3.53282100	2.60593500
C	3.98652200	-1.86556000	3.09654800
H	4.58638100	-1.02795500	3.46890100
H	2.93356400	-1.59353600	3.20240700
H	4.18415500	-2.73225500	3.74131100
H	5.39743200	-2.45131000	1.59053100
C	4.07989100	-1.65100200	-2.38609100
H	3.62393900	-2.33158600	-3.11662500
H	3.84299500	-0.62632600	-2.69474300
H	5.16599400	-1.77486600	-2.44824700
H	2.45797500	-1.79093000	-0.99970700
C	0.64803400	1.96575000	0.91016000
H	0.27751600	2.04308400	-0.10787800
H	-0.12723500	1.77740500	1.64380200
C	1.65825000	2.90717400	1.30308400
H	1.94907900	3.68946900	0.61043800
C	1.72073400	3.25708500	2.72899700
O	1.23529600	2.62136100	3.65188300

O	2.39189600	4.43432800	2.93548100
C	2.45741700	4.87979400	4.30428600
H	1.44508500	4.90525700	4.71961800
H	3.03252600	4.15533800	4.89188400
C	3.10473700	6.25356500	4.31225200
H	3.16401600	6.63290300	5.33861500
H	4.12002500	6.21546000	3.90251500
H	2.52125100	6.96282000	3.71598100
C	0.95729800	-0.03253100	0.93542900
C	0.64561400	-0.61262400	2.18336900
C	0.40812100	-0.63212000	-0.21350000
C	-0.11719000	-1.77846900	2.26885200
H	0.98157400	-0.11989100	3.09196800
C	-0.36960500	-1.79120300	-0.12999700
H	0.58646100	-0.18249700	-1.18880900
C	-0.62662600	-2.37826400	1.11132900
H	-0.33127800	-2.21135200	3.24384100
H	-0.77823200	-2.23300900	-1.03664600
H	-1.23501100	-3.27649100	1.17946800

TS_{D-E}

C	-2.86930400	1.55128100	-3.45489100
C	-2.25106700	1.23797600	-2.22732600
C	-2.09154600	-0.13660900	-1.91945800
C	-2.63695600	-1.11636500	-2.77036100
C	-3.27123400	-0.76745200	-3.95739500
C	-3.37185300	0.57903000	-4.31480900
H	-2.93590300	2.59250800	-3.75430300
H	-2.53209300	-2.15585400	-2.47534300
H	-3.66868200	-1.54367100	-4.60689800
H	-3.83282500	0.87107500	-5.25434700
C	-1.81334700	2.32254200	-1.30640400
C	-0.74729900	2.18941900	-0.36352900
C	-2.49937500	3.55693800	-1.38938400
C	-0.40512900	3.34139900	0.37471300
C	-2.12065200	4.67432700	-0.65328200
H	-3.36614500	3.63632800	-2.03804200
C	-1.04380600	4.57300400	0.22623300
H	0.39144600	3.27683800	1.10778300
H	-2.67053500	5.60631300	-0.75727800
H	-0.72376000	5.43069900	0.81420700
O	-1.40576100	-0.58885000	-0.84731300
Si	-1.70852200	-0.23520700	1.34253400
C	-0.92559100	-1.78324300	2.17190300
C	0.46421700	-1.85341200	2.38608300
C	-1.70277500	-2.79922800	2.76511500
C	1.05421400	-2.88104900	3.12595500
H	1.09551100	-1.08708200	1.94901800
C	-1.12201200	-3.83863900	3.49761300
H	-2.78345500	-2.77876500	2.67795700
C	0.26074200	-3.88753600	3.67889100
H	2.13268900	-2.89540100	3.26653800
H	-1.75636200	-4.60673900	3.93360900
H	0.71234400	-4.69439600	4.25067300
C	-3.49936200	-0.63465300	0.78044900

C	-4.45460800	0.36823200	0.52498000
C	-3.88833200	-1.95870000	0.48733300
C	-5.74007600	0.06477500	0.06723100
H	-4.19467400	1.41211200	0.65077800
C	-5.17322200	-2.27125800	0.04171100
H	-3.17202400	-2.76726500	0.58954100
C	-6.11271500	-1.25880300	-0.15962200
H	-6.44622500	0.87043500	-0.11880900
H	-5.43577800	-3.30743800	-0.15958900
H	-7.11388700	-1.49782700	-0.50946000
C	-1.93027400	0.97251600	2.91697400
C	-2.68458200	0.14211200	3.98988600
H	-2.09314500	-0.69559500	4.36830600
H	-2.91418400	0.79721300	4.84363000
H	-3.63720900	-0.25083700	3.61679900
C	-2.76559500	2.24959300	2.68147900
H	-2.43144000	2.83275500	1.82179700
H	-3.82687900	2.01951400	2.55623500
H	-2.68677300	2.89658600	3.56842800
C	-0.57338100	1.38446600	3.50824400
H	-0.72547000	1.90628700	4.46524200
H	0.07759900	0.52568000	3.70205700
H	-0.05230800	2.07098000	2.83873500
C	5.06081800	0.20138700	0.22243300
C	3.70385700	-0.04168500	-0.05551100
C	3.33913100	-1.28552800	-0.62121200
C	4.33837700	-2.24798800	-0.84975000
C	5.67465400	-1.99854300	-0.54397700
C	6.03946700	-0.76253400	-0.01196900
H	5.36664300	1.15572500	0.63730500
H	4.07567700	-3.21049800	-1.27522500
H	6.42545700	-2.76225800	-0.72819800
H	7.07822800	-0.54904100	0.22514800
C	1.54121300	-1.40750000	-2.95887600
C	1.32629700	-3.43242600	-1.12679800
C	2.05649100	-2.76155600	-3.46444900
C	1.35711100	-3.83857300	-2.62827600
H	1.84780900	-2.88590400	-4.53525500
H	3.14710600	-2.81276000	-3.34761000
H	0.32078900	-3.93315800	-2.97839800
H	1.81995600	-4.82598500	-2.74896300
C	2.82502800	1.89023000	2.06311600
C	3.17365600	2.80068300	-0.52460900
C	3.74024700	3.11989100	1.88469100
C	3.32018500	3.84485200	0.60187100
H	3.67276300	3.77440000	2.76340000
H	4.79023200	2.80522400	1.81405100
H	2.36060100	4.35360500	0.75538700
H	4.04464300	4.61658000	0.31198000
P	1.55564000	-1.53582800	-1.06965600
P	2.40507600	1.25999400	0.31365600
Rh	0.28793900	0.42147500	-0.27886600
C	2.46752300	3.34661900	-1.76759800
H	2.47212900	2.62459600	-2.58865900
H	1.43007900	3.61662600	-1.55754700

H	2.99181300	4.24531500	-2.11857300
H	4.18029900	2.47768800	-0.81705700
C	3.33358500	0.86568900	3.08056000
H	4.29059300	0.42718900	2.78176700
H	3.47903600	1.35506400	4.05185500
H	1.85630900	2.25139200	2.42049800
C	0.05629000	-3.95092700	-0.44046000
H	0.09845900	-3.83505900	0.64230400
H	-0.83358800	-3.42570100	-0.80149200
H	-0.06461200	-5.01949700	-0.66332800
H	2.19231400	-3.85889900	-0.60866500
C	2.23424300	-0.18820600	-3.56281300
H	2.15722500	-0.21418500	-4.65699700
H	1.76338900	0.73829700	-3.22103000
H	3.29861900	-0.15426500	-3.30269600
H	0.46727600	-1.34236800	-3.18639000
H	2.61878100	0.05096200	3.22890700

TS_{E-C(R)}

C	-2.14060400	4.22086000	-0.23188900
C	-2.23743100	2.81422000	-0.19120600
C	-2.89215800	2.17520200	-1.26598900
C	-3.42432300	2.93381500	-2.32433300
C	-3.31526500	4.31852800	-2.33246200
C	-2.66725500	4.97120700	-1.27793000
H	-1.61912400	4.73879100	0.56745200
H	-3.92628600	2.40118600	-3.12621300
H	-3.73154100	4.88862200	-3.15908100
H	-2.56739500	6.05292500	-1.27484400
C	-1.69925900	2.01542800	0.92818100
C	-1.41680000	0.60925000	0.78995000
C	-1.51678800	2.64298500	2.17183000
C	-0.86844800	-0.03123400	1.93747800
C	-0.97683000	1.96817000	3.27031000
H	-1.82101700	3.67711200	2.29891600
C	-0.62727800	0.63107100	3.15217600
H	-0.78213900	-1.11120300	1.95335700
H	-0.85597400	2.49063800	4.21636400
H	-0.23535000	0.08060800	4.00345300
O	-3.06499100	0.84748000	-1.32719700
Si	-2.55819500	-0.55401600	-0.41767200
C	-3.74026700	-0.95418600	1.06226800
C	-4.58956700	0.07418100	1.51797200
C	-3.82173300	-2.18654400	1.73626900
C	-5.47416100	-0.11623600	2.58045000
H	-4.56744900	1.04610400	1.03047200
C	-4.69640900	-2.38271800	2.80989600
H	-3.19936400	-3.01991400	1.42468400
C	-5.52855200	-1.34805000	3.23641800
H	-6.12038100	0.69925600	2.89752200
H	-4.72893500	-3.34915600	3.30842900
H	-6.21212700	-1.49882300	4.06834200
C	-0.64557400	-1.98052000	-0.56228300
C	-0.70045600	-3.13877800	0.25149300
C	-0.23314700	-2.20610200	-1.90150900

C	-0.41854500	-4.42220000	-0.23133000
H	-0.97786600	-3.04923700	1.29944100
C	0.05550500	-3.47855500	-2.40192600
H	-0.13226700	-1.35507000	-2.57026200
C	-0.04325900	-4.59595800	-1.56537900
H	-0.49308700	-5.28251500	0.43045800
H	0.36054200	-3.60074700	-3.43907100
H	0.17207000	-5.58986500	-1.95009100
C	-3.52114500	-1.63954900	-1.86034100
C	-5.00484500	-1.18006800	-1.81043200
H	-5.11733000	-0.11706700	-2.03547100
H	-5.57387700	-1.74484400	-2.56481400
H	-5.47058000	-1.37611500	-0.84046900
C	-3.53445500	-3.15953700	-1.62789100
H	-2.54491800	-3.61204200	-1.68848200
H	-3.97570300	-3.42112000	-0.66064000
H	-4.15650300	-3.63961500	-2.39931900
C	-3.02318400	-1.35824800	-3.29183600
H	-3.70967600	-1.82040600	-4.01828200
H	-2.98878900	-0.28582000	-3.50508400
H	-2.03555100	-1.78280700	-3.48686700
C	4.83360400	2.14864000	-0.07148200
C	3.78512200	1.21600700	0.00572400
C	4.08529000	-0.14771700	0.14549500
C	5.42906600	-0.54735500	0.24752700
C	6.46130900	0.38643900	0.18554200
C	6.16267200	1.73998000	0.01539600
H	4.61608700	3.20365400	-0.20013900
H	5.67882900	-1.59568400	0.37262300
H	7.49453300	0.05856500	0.26234900
H	6.96142000	2.47440400	-0.04396200
C	3.18935500	-2.71547500	-1.05393200
C	3.02918600	-2.39969000	1.67868000
C	3.90477900	-3.78413500	-0.20457600
C	3.19403400	-3.84088100	1.15431300
H	3.88041300	-4.75670800	-0.71350900
H	4.96504600	-3.53053800	-0.06993000
H	2.20310000	-4.29452200	1.02615300
H	3.74020100	-4.45639700	1.88072000
C	1.83353500	3.16402600	1.12120600
C	1.88516100	2.75229100	-1.61255700
C	2.06138500	4.41911100	0.25384000
C	1.45019600	4.15331400	-1.13006500
H	1.61031800	5.30048800	0.72896700
H	3.13503700	4.63376200	0.16461600
H	0.35703500	4.18353200	-1.05937700
H	1.74355900	4.91875800	-1.85976500
P	2.65821100	-1.33740100	0.13446500
P	1.99044500	1.68351900	-0.04154100
Rh	0.65616400	-0.19168000	0.04261900
C	0.99887000	2.18085000	-2.72269900
H	1.34682900	1.19507600	-3.04878400
H	-0.03922600	2.08071800	-2.39047400
H	1.00865200	2.84789900	-3.59450800
H	2.91717400	2.81119200	-1.98198200

C	2.63850900	3.10842400	2.42165900
H	2.39229300	2.21260700	3.00198600
H	3.71889300	3.11137200	2.24348600
H	2.40033200	3.98048000	3.04394500
H	0.77313800	3.13493400	1.39022800
C	2.04021500	-2.27063600	2.83662200
H	1.94276200	-1.23368500	3.17210200
H	1.04590000	-2.62311700	2.54750200
H	2.37792000	-2.87465900	3.68899600
H	4.00912500	-2.04443700	2.02306000
C	3.92652500	-2.27561300	-2.32031300
H	4.09872300	-3.14056400	-2.97341500
H	3.34110500	-1.54386300	-2.88884500
H	4.89950000	-1.82518000	-2.09885300
H	2.22992100	-3.14082600	-1.35984100

TS_{E-F(R)}

C	-4.48490500	1.93332200	0.13039300
C	-3.48380500	0.94445300	-0.01053500
C	-3.10771800	0.26155200	1.16932700
C	-3.74356900	0.55438000	2.39317500
C	-4.73540000	1.52225900	2.48490800
C	-5.10826900	2.22773500	1.33889600
H	-4.76125200	2.50459300	-0.75043800
H	-3.43057100	-0.01257900	3.26482200
H	-5.20813200	1.72507300	3.44251000
H	-5.86907600	3.00198400	1.38373000
C	-2.92971700	0.70382200	-1.37703000
C	-1.56272700	0.47352800	-1.68326300
C	-3.86448200	0.81456500	-2.43870000
C	-1.21052500	0.52734900	-3.05376700
C	-3.48659100	0.81052600	-3.77424100
H	-4.91982400	0.89889900	-2.19493100
C	-2.12985700	0.70035000	-4.08593100
H	-0.16191900	0.41586300	-3.32578700
H	-4.23643700	0.89814600	-4.55640800
H	-1.79245200	0.72855600	-5.12002400
O	-2.14976400	-0.67521300	1.24629000
Si	-1.12859200	-1.79832400	0.47359400
C	-0.20312000	-2.36864500	2.05814800
C	0.38767700	-3.63655500	2.22798100
C	-0.20111100	-1.52046100	3.18277500
C	0.94997100	-4.03449700	3.44454700
H	0.41758600	-4.33833400	1.40105900
C	0.36590900	-1.90452000	4.39944800
H	-0.67065500	-0.54649500	3.10464300
C	0.94559800	-3.16707300	4.53707500
H	1.38822800	-5.02567400	3.53572100
H	0.34591600	-1.21920500	5.24384900
H	1.38126700	-3.47343600	5.48484100
C	0.22156900	-2.12310000	-1.16313600
C	-0.26845600	-2.37630000	-2.46475300
C	1.31945700	-2.91741400	-0.75934200
C	0.31768100	-3.31781900	-3.31383800
H	-1.11730000	-1.81802400	-2.83447500

C	1.89364700	-3.88483300	-1.58728800
H	1.73394900	-2.77704500	0.22977800
C	1.40173900	-4.08215400	-2.87839800
H	-0.08569900	-3.46230800	-4.31333800
H	2.73398900	-4.47367500	-1.22646300
H	1.85083100	-4.82583100	-3.53189600
C	-2.46580500	-3.18880300	0.05508700
C	-1.87469200	-4.54103100	-0.39589600
H	-1.24866300	-4.99834000	0.37679600
H	-2.69615600	-5.24552800	-0.59391800
H	-1.28564900	-4.46379200	-1.31346300
C	-3.47130000	-2.72169300	-1.01955500
H	-3.99102800	-1.80497600	-0.72836500
H	-3.00163700	-2.54412900	-1.99153900
H	-4.23522500	-3.50008400	-1.16683700
C	-3.26603100	-3.44588500	1.35794300
H	-4.03134900	-4.21273200	1.16760300
H	-2.62804100	-3.81215000	2.16944200
H	-3.77886700	-2.54704400	1.71163400
C	2.37648500	4.20342300	0.59515400
C	2.03026500	2.87480300	0.28241400
C	3.06146700	1.94173500	0.06472300
C	4.39862400	2.37937300	0.10513100
C	4.72371600	3.70335900	0.38525400
C	3.70445300	4.61797400	0.65047300
H	1.60426000	4.93461200	0.80636500
H	5.20546500	1.67968100	-0.08546600
H	5.76439900	4.01564900	0.40410700
H	3.93978200	5.65018900	0.89555200
C	3.46034900	-0.33149900	-1.83867400
C	3.93895200	-0.70752000	0.85508400
C	4.84566900	-0.89424100	-1.46044600
C	4.70926100	-1.62477900	-0.11684600
H	5.22079600	-1.56004200	-2.24862700
H	5.57370800	-0.07596300	-1.37190900
H	4.15700100	-2.56064300	-0.26325400
H	5.68664700	-1.89486700	0.30412000
C	-0.46590600	2.64178000	1.87546000
C	-0.55981500	3.86642300	-0.60682200
C	-1.04699800	4.06977800	1.83287700
C	-1.61524500	4.30845100	0.42820300
H	-1.81652000	4.18977900	2.60577300
H	-0.25836800	4.80226400	2.05571500
H	-2.52794700	3.71685700	0.29840900
H	-1.88626800	5.36051600	0.26940900
P	2.60509700	0.15883700	-0.21332800
P	0.25142400	2.31048800	0.14938900
Rh	0.18099100	0.09818100	-0.60778300
C	-1.08782400	3.79366300	-2.04069000
H	-0.31910400	3.45249400	-2.74123700
H	-1.94374400	3.12394600	-2.13327400
H	-1.40354000	4.79721000	-2.35638300
H	0.24228800	4.61097000	-0.60457200
C	0.47918600	2.37535000	3.04885200
H	0.84831000	1.34453400	3.04110300

H	1.34438400	3.04716900	3.03613600
H	-0.05157700	2.53151600	3.99675700
H	-1.30199400	1.93964900	1.93970000
C	3.46038700	-1.38586600	2.13860500
H	2.92762800	-0.68627700	2.78969400
H	2.78946600	-2.22698500	1.95078800
H	4.32352100	-1.76970000	2.69830100
H	4.61598100	0.10000500	1.15375400
C	3.47786700	0.74031500	-2.93099900
H	3.92271300	0.33617200	-3.84922700
H	2.46398000	1.07807100	-3.17365100
H	4.06231900	1.61780300	-2.63372200
H	2.84313700	-1.16619600	-2.19003000

TS_{E-F(S)}

C	4.85117700	0.76421600	0.17168100
C	3.62240300	0.07742300	0.02712900
C	3.08289100	-0.48889100	1.20693500
C	3.79620200	-0.41364000	2.42045000
C	5.01664400	0.24243300	2.51104100
C	5.54612800	0.85419800	1.37334900
H	5.25937800	1.26242300	-0.70193100
H	3.34859900	-0.88700600	3.28921200
H	5.53982000	0.28594900	3.46279300
H	6.48509100	1.39884100	1.41867000
C	3.02920600	0.00560100	-1.34330700
C	1.64895800	0.11875300	-1.65680500
C	3.96673100	-0.09795700	-2.40436600
C	1.32765600	0.29085200	-3.02606300
C	3.60693400	0.02334200	-3.73918400
H	5.00815000	-0.28827200	-2.16137700
C	2.26758200	0.26220900	-4.05417500
H	0.28178000	0.42636400	-3.29992200
H	4.35965000	-0.06136300	-4.51896600
H	1.95341400	0.39432100	-5.08756300
O	1.88592800	-1.09372100	1.29987000
Si	0.64291500	-1.96938000	0.53957100
C	-0.48010600	-2.21706500	2.07913600
C	-0.31957600	-1.35274800	3.18026700
C	-1.39858500	-3.27460800	2.24249600
C	-1.04030600	-1.51952000	4.36451700
H	0.39563700	-0.54276200	3.11068900
C	-2.12408000	-3.45038300	3.42473200
H	-1.55728900	-3.98797400	1.44074400
C	-1.95134100	-2.56940700	4.49239800
H	-0.88304500	-0.83118100	5.19189700
H	-2.81801500	-4.28342100	3.51027300
H	-2.51092100	-2.70524600	5.41457900
C	-0.62827200	-2.02264900	-1.18061500
C	-1.88193400	-2.58410800	-0.84549900
C	-0.10321300	-2.41465600	-2.43540800
C	-2.56315500	-3.46721100	-1.68702800
H	-2.33587400	-2.33342800	0.10370900
C	-0.79134700	-3.26695600	-3.30077800
H	0.85735700	-2.03529600	-2.75348300

C	-2.02503200	-3.80540200	-2.92862600
H	-3.52178100	-3.87699500	-1.37700200
H	-0.35227500	-3.52194300	-4.26232900
H	-2.55460300	-4.48340200	-3.59311700
C	1.61556400	-3.66425200	0.25198000
C	0.73461000	-4.85463800	-0.17997200
H	0.22275600	-4.68429600	-1.13022100
H	1.36844000	-5.74502100	-0.30609500
H	-0.01653400	-5.10889900	0.57491100
C	2.26733700	-4.04163600	1.60739000
H	2.98414800	-3.28818200	1.94553100
H	1.52403000	-4.18084400	2.40005600
H	2.81214000	-4.99062800	1.49539000
C	2.75214400	-3.50398900	-0.78098900
H	3.31826700	-4.44514500	-0.85078400
H	2.37969900	-3.27787000	-1.78452900
H	3.45946400	-2.71858200	-0.50033300
C	-1.40730400	4.71847200	0.12599200
C	-1.35460400	3.31521300	0.02801800
C	-2.55501600	2.58305400	0.05010600
C	-3.77343100	3.27588300	0.17963500
C	-3.81211000	4.66411200	0.27329900
C	-2.62052400	5.39115000	0.23975600
H	-0.48947200	5.29695000	0.11690900
H	-4.70883100	2.72655700	0.20886100
H	-4.76584500	5.17550100	0.37250800
H	-2.63608100	6.47574100	0.30584000
C	-3.56762500	0.04517600	1.27893600
C	-3.82190600	0.46221600	-1.44416200
C	-4.97569300	-0.15895900	0.67670400
C	-4.82732200	-0.52073300	-0.80914600
H	-5.52559700	-0.93113800	1.23055400
H	-5.55807200	0.76738600	0.77735600
H	-4.45736400	-1.54681600	-0.91122200
H	-5.79009800	-0.47810900	-1.33511300
C	1.41972400	3.38521600	-1.17060500
C	1.07169900	3.08154600	1.54185400
C	2.22209200	4.33743900	-0.26001600
C	2.43660700	3.62731200	1.08447500
H	3.17417500	4.60531000	-0.73578100
H	1.67524800	5.27833600	-0.10473700
H	3.15033300	2.80416600	0.96520100
H	2.84903700	4.30458200	1.84373100
P	-2.47639200	0.73186900	-0.12043300
P	0.26075100	2.39181700	-0.04422800
Rh	-0.16145600	0.15024400	-0.62035400
C	1.11069400	2.16288000	2.75864600
H	0.10519300	1.83160800	3.03954600
H	1.72528200	1.28021200	2.57622600
H	1.53677600	2.70015700	3.61623400
H	0.44056900	3.94341800	1.79303900
C	0.79294900	4.02762900	-2.41008500
H	0.30323400	3.27608600	-3.03830900
H	0.05173300	4.79225300	-2.15635600
H	1.57331100	4.50522100	-3.01584700

H	2.10682600	2.60690700	-1.51687500
C	-3.31473900	0.06961600	-2.83378000
H	-2.65465600	0.84180700	-3.24483800
H	-2.75997500	-0.87057100	-2.81626100
H	-4.16101400	-0.04496200	-3.52409900
H	-4.32367600	1.43248800	-1.53730200
C	-3.54489300	0.82257100	2.59788500
H	-4.13473900	0.28997000	3.35408100
H	-2.52584300	0.91544500	2.98638600
H	-3.96381500	1.82821100	2.48940500
H	-3.12731300	-0.93889200	1.47786300

TS_{F-C(R)}

C	-4.42775000	1.98970200	-0.16776800
C	-3.58262000	0.86307900	-0.06642200
C	-3.38137900	0.33500400	1.22688700
C	-4.02804000	0.89790300	2.34160500
C	-4.85864000	2.00240300	2.20211400
C	-5.05401400	2.56185500	0.93517600
H	-4.58377500	2.44169300	-1.14192300
H	-3.85221700	0.43740200	3.30887400
H	-5.34663300	2.42739300	3.07535400
H	-5.69083000	3.43236100	0.80587800
C	-3.02619000	0.20652700	-1.28008100
C	-1.81604500	-0.56585800	-1.34079900
C	-3.84283700	0.29335300	-2.43055300
C	-1.59026100	-1.25121900	-2.55645300
C	-3.51938800	-0.31476500	-3.63654500
H	-4.78643200	0.82328600	-2.36092800
C	-2.38053400	-1.11151500	-3.69570000
H	-0.76028700	-1.93443300	-2.62059300
H	-4.17749800	-0.20702800	-4.49507400
H	-2.12105900	-1.65205500	-4.60275400
O	-2.59501300	-0.72204600	1.47293400
Si	-1.42068400	-1.63245100	0.62473900
C	-0.38690400	-2.00928500	2.22402800
C	0.15617400	-3.26084300	2.56887300
C	-0.27368300	-0.98976600	3.19137400
C	0.76066100	-3.49178600	3.80870800
H	0.08609500	-4.09473200	1.87762400
C	0.32958900	-1.20762100	4.43121100
H	-0.69511600	-0.01190200	2.98137000
C	0.84835500	-2.46553600	4.74875100
H	1.15256000	-4.47956700	4.04019000
H	0.38446400	-0.39710500	5.15474100
H	1.30972900	-2.64332900	5.71695500
C	1.13868200	-1.96956400	-1.33805300
C	1.49193600	-1.86893200	-2.70647500
C	1.54189900	-3.15441300	-0.70034700
C	2.18060900	-2.87823000	-3.38579800
H	1.21615500	-0.97704500	-3.26725400
C	2.23285100	-4.17556300	-1.36885000
H	1.31632300	-3.29998900	0.34790300
C	2.55805300	-4.04601000	-2.71763400
H	2.42004600	-2.74962900	-4.43978800

H	2.51316300	-5.07592100	-0.82512900
H	3.09112500	-4.83632300	-3.24008800
C	-2.43965300	-3.28086500	0.22264500
C	-1.65548500	-4.36067100	-0.54938500
H	-0.77395300	-4.71717900	-0.00754500
H	-2.30303800	-5.23295000	-0.72512800
H	-1.31339800	-4.00317700	-1.52549600
C	-3.72633400	-2.96911700	-0.57876700
H	-4.33824200	-2.20162200	-0.09299000
H	-3.52310300	-2.64899000	-1.60218300
H	-4.33758800	-3.88162200	-0.63790000
C	-2.92621000	-3.87452800	1.57152600
H	-3.59989500	-4.71948400	1.36761600
H	-2.11607800	-4.24805900	2.20014800
H	-3.48694500	-3.13746900	2.15640300
C	1.81878100	4.23018600	0.83670900
C	1.64163900	2.86628600	0.53640900
C	2.74004600	1.99757400	0.66240800
C	3.96825800	2.51260400	1.11931200
C	4.11735000	3.85741200	1.44554100
C	3.03647800	4.72572800	1.29309000
H	0.99394600	4.92166100	0.71528700
H	4.83463200	1.86719700	1.20805100
H	5.07610500	4.22607600	1.80010500
H	3.13946200	5.78183100	1.52738600
C	3.71192900	0.28778300	-1.49420800
C	3.82638400	-0.71177800	1.07647700
C	5.08770500	-0.20111000	-1.00346000
C	4.83987500	-1.27575600	0.06005300
H	5.67735300	-0.58614700	-1.84535800
H	5.65924600	0.63404000	-0.57432600
H	4.42616000	-2.17715400	-0.40919500
H	5.76440100	-1.57109900	0.57302000
C	-1.24818700	3.11460700	1.09502600
C	-0.35811600	3.33717000	-1.51587900
C	-1.65533900	4.40415100	0.34913600
C	-1.64662400	4.10714000	-1.15636500
H	-2.64746000	4.72979700	0.68570100
H	-0.96481600	5.22582400	0.57968700
H	-2.51368000	3.48681200	-1.40826800
H	-1.72479900	5.02376700	-1.75527600
P	2.56368800	0.25874200	0.02817900
P	-0.00777200	2.20151100	-0.02191200
Rh	0.26002600	-0.24237300	-0.51313300
C	-0.43360000	2.63018700	-2.87180100
H	0.50452700	2.12193200	-3.11919700
H	-1.23042200	1.88150600	-2.88923600
H	-0.63409200	3.36218100	-3.66546400
H	0.47745400	4.04771600	-1.53723200
C	-0.86187300	3.30231500	2.56455500
H	-0.60842600	2.34729900	3.03757400
H	-0.00957800	3.97532500	2.69619700
H	-1.71325900	3.72364500	3.11301700
H	-2.11192400	2.45200200	1.07445100
C	3.30177100	-1.73862900	2.07422300

H	2.57781400	-1.30656200	2.76794200
H	2.82767500	-2.58129800	1.57321600
H	4.14161800	-2.12815400	2.66497500
H	4.33393700	0.06600300	1.65619800
C	3.74869900	1.58831500	-2.29810500
H	4.38512100	1.45742800	-3.18245200
H	2.75197900	1.87628500	-2.65048300
H	4.15311600	2.42213600	-1.71495700
H	3.29424500	-0.49691600	-2.13038800

TS_{F-C(S)}

C	0.79889900	-3.80402400	2.67174500
C	-0.01231400	-3.03571900	1.80779000
C	-0.98478300	-2.21245100	2.41698400
C	-1.16066900	-2.22372700	3.81190600
C	-0.36348700	-3.01694200	4.62705900
C	0.63862000	-3.80467100	4.05330200
H	1.58709800	-4.41527400	2.24431300
H	-1.94392000	-1.59656300	4.22672400
H	-0.51456200	-3.01138600	5.70326700
H	1.28944700	-4.41329100	4.67435400
C	0.07596700	-3.19306400	0.33176200
C	-0.35312100	-2.21240900	-0.62773800
C	0.53502800	-4.44460000	-0.13167000
C	-0.29540600	-2.59974400	-1.98820300
C	0.64203800	-4.75255800	-1.48365700
H	0.78193200	-5.21619700	0.58905700
C	0.22133100	-3.81940300	-2.42521600
H	-0.66858700	-1.92631600	-2.74470500
H	1.01140700	-5.72848000	-1.78888900
H	0.25862100	-4.04173500	-3.48855200
O	-1.80960700	-1.41216300	1.72234500
Si	-1.96650500	-0.97992300	0.07470100
C	-2.85217800	0.71731200	0.40758200
C	-3.37188200	1.53848200	-0.61109000
C	-3.09821000	1.12753800	1.73382700
C	-4.10405400	2.69494600	-0.32891200
H	-3.20192900	1.28408200	-1.65069400
C	-3.82379600	2.28662400	2.02523600
H	-2.72659600	0.52088400	2.55184300
C	-4.33415300	3.07731400	0.99478700
H	-4.49821400	3.29482000	-1.14627200
H	-3.99526500	2.56661300	3.06247700
H	-4.90640800	3.97434000	1.21798400
C	-0.31281700	0.34606800	-2.71012700
C	0.86461700	0.60112100	-3.44726400
C	-1.49607100	0.23074200	-3.45945400
C	0.86434400	0.71538000	-4.84100500
H	1.81200600	0.72343600	-2.92569100
C	-1.50879000	0.35080200	-4.85522300
H	-2.43760200	0.02355000	-2.96792300
C	-0.32913800	0.59421700	-5.55766700
H	1.79913800	0.90811100	-5.36398000
H	-2.45111200	0.25101900	-5.39049500
H	-0.33723800	0.68905000	-6.64047700

C	-3.48112400	-2.11949500	-0.50524200
C	-3.91844200	-1.91793100	-1.96861900
H	-4.23893500	-0.88785600	-2.16436300
H	-4.77925200	-2.56606300	-2.19185200
H	-3.12718500	-2.17475200	-2.68082200
C	-3.17349200	-3.61924100	-0.29902400
H	-2.87718900	-3.84255700	0.73216200
H	-2.38731000	-3.98376100	-0.96542300
H	-4.07946600	-4.20716700	-0.50851000
C	-4.68786000	-1.77702100	0.40437700
H	-5.51782900	-2.46322900	0.18013400
H	-5.05121200	-0.75703700	0.25096000
H	-4.44355100	-1.88961400	1.46630500
Rh	0.13550400	0.03991000	-0.72106500
C	2.97018600	3.80308200	-0.62802700
C	2.31444900	2.59978800	-0.30873400
C	3.07803800	1.53343600	0.22112800
C	4.46253500	1.71054500	0.39237500
C	5.09909100	2.90086000	0.04831400
C	4.34523600	3.95633300	-0.45956700
H	2.41087200	4.64585900	-1.01601000
H	5.06244300	0.90328000	0.79728600
H	6.17330700	3.00059300	0.17872300
H	4.82024000	4.89722700	-0.72422500
C	3.29234100	-1.45378300	-0.05056600
C	3.02321500	-0.31999500	2.45850100
C	4.36434700	-1.83678900	0.98908300
C	3.75315200	-1.67663200	2.38445400
H	4.71392800	-2.86310000	0.81460100
H	5.24578100	-1.18995900	0.88086200
H	3.03354900	-2.48132500	2.56974500
H	4.51233700	-1.74101600	3.17521800
C	-0.25983600	3.21307500	0.97559700
C	0.00213600	3.80544500	-1.69339800
C	-0.09421300	4.71066600	0.68670400
C	-0.53406500	4.93500600	-0.76464600
H	-0.69963200	5.30610800	1.38242200
H	0.95063500	5.01053000	0.83976800
H	-1.63037100	4.90782000	-0.80006300
H	-0.22924700	5.91848100	-1.14390800
P	2.24082300	-0.06379400	0.71827500
P	0.47199400	2.35224100	-0.53465200
C	-0.98533800	3.53696000	-2.83452500
H	-0.56919000	2.88593500	-3.60252000
H	-1.91312400	3.09055400	-2.46930700
H	-1.23945500	4.49779400	-3.30309900
H	0.94140400	4.11894200	-2.15636700
C	0.25680100	2.76694300	2.33906600
H	0.04159400	1.71000200	2.51480300
H	1.33734700	2.92521000	2.43597900
H	-0.23718800	3.34449300	3.13071900
H	-1.32538200	2.96676100	0.91221800
C	2.07180700	-0.21071000	3.65065400
H	1.68399000	0.80487500	3.76777200
H	1.22316600	-0.89184500	3.55784000

H	2.60597300	-0.46723200	4.57516500
H	3.77535400	0.47213100	2.54662500
C	3.84305100	-1.21144200	-1.45773600
H	4.40135300	-2.09519500	-1.79230800
H	3.04050600	-1.03703800	-2.18012400
H	4.52517500	-0.35479200	-1.48893300
H	2.57096100	-2.27707600	-0.11097600

TS_{G-H}

C	8.53106000	3.71845200	2.20831700
C	7.27056300	3.18858600	2.52527200
C	7.17651200	1.84709600	2.94192000
C	8.33828200	1.06788300	3.04945100
C	9.58608600	1.60974700	2.74299100
C	9.68142800	2.93709300	2.31904500
H	8.62361300	4.74737900	1.87430300
H	8.27339300	0.03196800	3.37092500
H	10.48004400	0.99817300	2.83004700
H	10.65077500	3.36389000	2.07604100
C	5.17893800	-0.30487200	2.21642200
C	5.58915500	0.24417300	4.89835200
C	5.50876300	-1.50744000	3.12187400
C	5.04033100	-1.15436500	4.54099100
H	5.02774600	-2.42006800	2.74776900
H	6.59233100	-1.69615200	3.11740000
H	3.94311400	-1.12356700	4.56506600
H	5.36202000	-1.89877300	5.28013600
C	5.96009000	5.79738300	3.28649400
C	5.71907500	4.89224400	0.68334800
C	6.45439100	6.76156000	2.19031100
C	5.69963500	6.42211000	0.89609300
H	6.29185600	7.80504100	2.48961800
H	7.53722900	6.64487800	2.04372000
H	4.65879300	6.75454400	0.98731300
H	6.12390900	6.93982400	0.02669400
P	5.47068100	1.22530100	3.28474600
P	5.67581800	4.14119000	2.42603300
Rh	3.98362700	2.84480200	3.09372800
C	4.60421100	4.39015900	-0.23854800
H	4.66568500	3.30840600	-0.39478700
H	3.61788400	4.60888300	0.18394700
H	4.67299900	4.87900500	-1.21913000
H	6.68997800	4.60438500	0.25989800
C	6.80549600	5.76000700	4.56105700
H	6.38047400	5.07028900	5.29855900
H	7.83512000	5.44527700	4.35928500
H	6.84220000	6.75585800	5.01960900
H	4.93940000	6.09500700	3.56170300
C	4.88275200	0.90591100	6.08442900
H	5.33085800	1.87525800	6.32741200
H	3.82503200	1.07086000	5.85931800
H	4.95750700	0.26701000	6.97420500
H	6.66104800	0.15352800	5.12163500
C	5.85300400	-0.31122600	0.84407300
H	5.56160400	-1.20870600	0.28484200

H	5.55415800	0.55965700	0.25041600
H	6.94541600	-0.30599700	0.92636300
H	4.09133000	-0.27737900	2.07134200
C	1.23492000	2.17902300	1.77917000
H	2.18783300	2.18344700	1.24194200
C	1.34665100	1.51205000	3.02180100
O	2.40849600	1.44920800	3.72020800
O	0.19972100	1.01584900	3.55795500
C	0.23225900	0.60613600	4.93776500
H	0.94267000	-0.21931900	5.05550300
H	0.58415600	1.44060100	5.55334000
C	-1.17740100	0.18545200	5.31604300
H	-1.20208300	-0.13962300	6.36223600
H	-1.87781600	1.01844400	5.19705100
H	-1.52040000	-0.64430500	4.68892700
C	0.11811600	0.79734200	-0.05005500
C	-0.06656200	-0.50718500	0.43612200
C	0.41658200	0.95795700	-1.40949600
C	0.04562000	-1.61106700	-0.40900600
H	-0.30186500	-0.64841900	1.48792800
C	0.53331500	-0.14488700	-2.25999300
H	0.55524500	1.96151900	-1.80735400
C	0.34790200	-1.43515000	-1.76265800
H	-0.10864900	-2.61207500	-0.01243300
H	0.76448200	0.00629100	-3.31188100
H	0.43313700	-2.29523900	-2.42202200
C	0.01943400	2.00015300	0.87661700
H	-0.11503500	2.90119400	0.26595900
H	-0.88177900	1.90515300	1.49295900
C	0.10363800	6.04936900	5.49933200
C	0.53058900	5.62471600	4.22833200
C	1.70964900	4.83871000	4.14837700
C	2.42847700	4.56666500	5.32465000
C	1.99646300	5.02449100	6.56702900
C	0.81733200	5.76385900	6.66122300
H	-0.82003600	6.61402600	5.56845500
H	3.33269800	3.96567100	5.23471400
H	2.57597300	4.79185200	7.45723600
H	0.45373100	6.11388900	7.62320100
C	-0.34776900	5.92787900	3.05342200
C	-0.62183200	7.24089800	2.57254400
C	-1.01493500	4.82916300	2.48821800
C	-1.57832800	7.35267000	1.53842300
C	-1.94675500	4.97722600	1.46316600
H	-0.81259000	3.84068100	2.88679400
C	-2.23373500	6.25200400	0.98666000
H	-1.82613500	8.33364300	1.14889200
H	-2.44868000	4.10368000	1.05611700
H	-2.96424600	6.39778300	0.19487400
O	2.20690200	4.36168000	2.95669900
Si	0.06590500	8.91964000	3.21674100
C	-0.91888100	9.40347500	4.77628000
C	-2.21284800	8.88011100	4.97042100
C	-0.45552600	10.33142200	5.72852400
C	-2.99934500	9.25364800	6.06220000

H	-2.61276100	8.16430000	4.25653900
C	-1.23536400	10.70914800	6.82455700
H	0.52952100	10.77586700	5.62119300
C	-2.51039100	10.16854300	6.99643700
H	-3.99299700	8.82905000	6.18287100
H	-0.84501400	11.42520800	7.54371500
H	-3.11857100	10.45964500	7.84917700
C	-0.37574200	10.23091600	1.89383500
C	-1.04299700	11.41893900	2.24415700
C	0.01440600	10.09083400	0.54527400
C	-1.30313200	12.41941800	1.30304600
H	-1.36898300	11.56978000	3.26944800
C	-0.24051100	11.08524800	-0.40004000
H	0.50990400	9.17994100	0.21759800
C	-0.90046900	12.25719100	-0.02222100
H	-1.82340500	13.32436100	1.60777500
H	0.07226700	10.94371800	-1.43183100
H	-1.10202400	13.03327400	-0.75638100
C	1.99769100	9.05183200	3.44921700
C	2.43745100	10.53156700	3.31358200
H	1.98582900	11.17921000	4.07402100
H	3.52828700	10.59880200	3.43983700
H	2.18878800	10.95285500	2.33543400
C	2.68875000	8.25208500	2.32341800
H	2.45975900	7.18233400	2.37248900
H	2.40978400	8.61466200	1.32692400
H	3.77891800	8.37048700	2.41220800
C	2.51294700	8.52827300	4.80661300
H	3.59614300	8.71132000	4.87791300
H	2.04143500	9.03114500	5.65710100
H	2.35168500	7.45629200	4.92669400
H	1.56588900	3.57820500	2.43808500

TS_{I-A}

C	-1.04855000	-1.57808700	-1.64698100
C	-2.02244200	-1.58910900	-0.63316800
C	-3.34315100	-1.94181900	-1.01951900
C	-3.63497100	-2.22027200	-2.36177600
C	-2.64066700	-2.19208100	-3.33702200
C	-1.33286800	-1.87411500	-2.97727700
H	-0.02957600	-1.33778600	-1.37547700
H	-4.65702800	-2.44432300	-2.64381100
H	-2.89535400	-2.41923500	-4.36896300
H	-0.53579200	-1.85547500	-3.71454000
C	-1.61153900	-1.27144000	0.76972600
C	-0.66159900	-0.24951700	1.07464400
C	-2.12393200	-2.06853500	1.81135800
C	-0.30337600	-0.09494400	2.43529800
C	-1.75932500	-1.86692700	3.14183300
H	-2.81006600	-2.87129200	1.57184300
C	-0.84440900	-0.86460000	3.46468100
H	0.44604200	0.65308400	2.68607800
H	-2.17561200	-2.50694300	3.91656400
H	-0.54114200	-0.70272700	4.49655600
O	-4.34188800	-1.96196700	-0.07436200

Si	-5.91103900	-2.59299300	0.01683300	C	-3.55082800	2.48078300	-0.97273400
C	-7.02261700	-1.96264300	-1.38895500	C	-4.68284800	2.29173400	1.24472500
C	-7.54888600	-0.65815100	-1.29734900	C	-4.63994900	1.72602100	-0.18292900
C	-7.36026800	-2.70976400	-2.53417200	H	-5.31502800	1.68177600	1.90172400
C	-8.35965900	-0.12317000	-2.30007400	H	-5.11219900	3.30396900	1.24086400
H	-7.33100600	-0.05205500	-0.42237100	H	-4.39589000	0.65803700	-0.14284000
C	-8.17375100	-2.18335600	-3.53965500	H	-5.60873500	1.81319700	-0.69061000
H	-6.98651400	-3.72211500	-2.65380500	P	0.63230300	3.85069300	-0.35169300
C	-8.67466000	-0.88567000	-3.42591600	P	-2.15358400	2.76121200	0.28116600
H	-8.74906100	0.88683300	-2.19924100	Rh	-0.16823200	1.77252700	0.08725300
H	-8.41671200	-2.78784400	-4.40982400	C	-3.11874600	1.80281800	-2.27344200
H	-9.30825800	-0.47348200	-4.20700300	H	-2.39918200	2.41928100	-2.82360500
C	-6.56791300	-1.84807500	1.62228600	H	-2.64879500	0.83513500	-2.08046000
C	-5.70808900	-1.31550200	2.60123000	H	-3.98843100	1.63903300	-2.92279700
C	-7.94870900	-1.85678900	1.90191300	H	-3.93096700	3.48485100	-1.20490200
C	-6.20617600	-0.81736000	3.80805300	C	-3.00459800	3.13818500	3.04386900
H	-4.63867100	-1.28577400	2.41705800	H	-1.96010400	3.07778000	3.36851300
C	-8.45042200	-1.36361000	3.10807000	H	-3.25694000	4.19584200	2.91330100
H	-8.64963000	-2.23898800	1.16314800	H	-3.62856800	2.74400300	3.85578500
C	-7.57824500	-0.84238800	4.06566700	H	-2.92877800	1.29121700	1.96963000
H	-5.51971600	-0.41228100	4.54761000	C	2.43947600	3.61238200	1.88612000
H	-9.52086700	-1.38155800	3.29709600	H	1.60996200	3.59693900	2.60111000
H	-7.96584100	-0.45627700	5.00509600	H	2.64706800	2.57844400	1.59556500
C	-5.84424300	-4.51602500	0.15988500	H	3.32285500	4.01052900	2.40217600
C	-7.28221000	-5.08416800	0.19071500	H	1.82033200	5.47897600	1.01361000
H	-7.83801700	-4.87333100	-0.72940600	C	0.51328600	4.87934500	-3.08180000
H	-7.24799400	-6.17618500	0.31330300	H	1.06716800	5.03556100	-4.01604500
H	-7.86044000	-4.68165000	1.03087800	H	-0.31902400	4.20046300	-3.29945500
C	-5.15034400	-4.89354500	1.48974300	H	0.08847600	5.84226900	-2.77918100
H	-4.10491000	-4.56619700	1.51314100	H	1.81729500	3.33662500	-2.36516200
H	-5.65870400	-4.46402200	2.35936000	C	3.71460600	-1.69632600	-2.18019800
H	-5.14980700	-5.98647000	1.60952400	C	3.17180300	-1.19813600	-0.98515800
C	-5.05178400	-5.18035900	-0.98881700	C	2.22797600	-0.13978800	-1.07144500
H	-5.01171800	-6.26755700	-0.82835700	C	1.88706900	0.38071300	-2.33033600
H	-5.50670400	-5.01889200	-1.97211500	C	2.45602800	-0.12368300	-3.49997100
H	-4.02072900	-4.81601400	-1.04044300	C	3.37540200	-1.16977700	-3.42713600
C	-3.02441400	5.50884500	0.47112600	H	4.40876200	-2.52762800	-2.12645300
C	-1.96808800	4.61097300	0.24865100	H	1.13563300	1.16552000	-2.36095500
C	-0.68772200	5.11342000	-0.04334200	H	2.17004600	0.29445700	-4.46221300
C	-0.48444900	6.50181400	-0.09329700	H	3.81892900	-1.58305300	-4.32856200
C	-1.53791000	7.38446100	0.14084800	C	3.49780600	-1.87282600	0.31057500
C	-2.81209200	6.88592100	0.42223900	C	4.81041300	-1.99644700	0.85061600
H	-4.02093800	5.13506000	0.68533600	C	2.41871400	-2.49149800	0.96509600
H	0.50077100	6.90196500	-0.31505300	C	4.94845700	-2.79120400	2.01110800
H	-1.36667200	8.45687200	0.10104800	C	2.58903600	-3.24669600	2.12170500
H	-3.63785200	7.56853800	0.60442900	H	1.42479300	-2.39620600	0.54042800
C	1.44010200	4.30363300	-2.00921800	C	3.86931500	-3.40941200	2.64211600
C	2.10435800	4.47618400	0.66774900	H	5.93260800	-2.92991100	2.44431400
C	2.66296200	5.17424500	-1.65795100	H	1.72799000	-3.70818100	2.59782800
C	3.25363700	4.62693500	-0.35052400	H	4.03458800	-4.00854900	3.53414000
H	3.39636000	5.16266500	-2.47441900	O	1.66551100	0.38061200	0.05883200
H	2.35608100	6.22150900	-1.52402400	Si	6.44446100	-1.22371600	0.19115200
H	3.70978600	3.64602900	-0.53685200	C	7.07891500	-2.27879200	-1.26564000
H	4.04333800	5.27584400	0.04905200	C	6.72773500	-3.64231600	-1.33326600
C	-3.23325000	2.32503900	1.76843900	C	7.95466500	-1.79470200	-2.25600200

C	7.21625000	-4.47694500	-2.34055400
H	6.05534500	-4.05975400	-0.58736000
C	8.44604200	-2.62278500	-3.26859700
H	8.26708100	-0.75462900	-2.24584500
C	8.07627800	-3.96751100	-3.31529700
H	6.92349200	-5.52380900	-2.36451200
H	9.11713900	-2.21537100	-4.02093600
H	8.45629400	-4.61324100	-4.10297100
C	7.75388200	-1.41970500	1.57508000
C	9.01143900	-1.98879900	1.30270000
C	7.54242100	-0.93335300	2.88248900
C	10.00912300	-2.06681300	2.27873200
H	9.21959300	-2.37971800	0.31083700
C	8.53353500	-1.00651400	3.86225700
H	6.57985600	-0.50486100	3.15110100
C	9.77428700	-1.57391300	3.56196200
H	10.96909000	-2.51528900	2.03412200
H	8.33602500	-0.62368200	4.86069500
H	10.54803100	-1.63349500	4.32336700
C	6.38001000	0.68816700	-0.19835700
C	7.80217300	1.29125200	-0.08483300
H	8.50521200	0.85612300	-0.80506200
H	7.75515300	2.37070200	-0.29050800
H	8.23135000	1.15999200	0.91252500
C	5.48798200	1.37508700	0.86013900
H	4.45307700	1.01980600	0.82155100
H	5.86167900	1.21886100	1.87880600
H	5.47746200	2.46128400	0.68765900
C	5.83090400	1.03336900	-1.59927200
H	5.91168600	2.11900800	-1.76349900
H	6.38821200	0.54042700	-2.40234300
H	4.78105500	0.75938900	-1.71150100
H	0.62668200	-0.08775000	0.38189600

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C	3.05618800	-2.89952100	-0.31097100
C	2.40965900	-1.65283000	-0.35118200
C	0.99589400	-1.64018000	-0.30176100
C	0.28470100	-2.84631800	-0.24072100
C	0.95685400	-4.06751700	-0.20492300
C	2.35053600	-4.09866800	-0.23544500
H	4.14144000	-2.91617500	-0.36275800
H	-0.79939800	-2.82129400	-0.22940000
H	0.38522400	-4.99065200	-0.15896900
H	2.88384000	-5.04466900	-0.21369900
C	3.22869300	-0.41310600	-0.44094600
C	2.96320000	0.58169000	-1.39746000

C	4.33735700	-0.24172400	0.40538900
C	3.78411500	1.70443000	-1.50560400
C	5.15589800	0.88341000	0.30042100
H	4.54876700	-0.99358100	1.16113300
C	4.88337300	1.86114500	-0.65759100
H	3.56563000	2.45694800	-2.25905700
H	6.00426100	0.99657300	0.97051700
H	5.52041300	2.73752700	-0.74300500
O	0.35016200	-0.43380700	-0.33900600
Si	-1.04691200	0.17029200	0.40529800
C	-2.55415500	-0.63942000	-0.40375700
C	-2.45157000	-1.05748800	-1.74603300
C	-3.80189600	-0.79616900	0.22842100
C	-3.53989300	-1.60936700	-2.42283600
H	-1.50238700	-0.95669100	-2.26668700
C	-4.89618200	-1.34559900	-0.44439600
H	-3.93319800	-0.48896500	1.26221700
C	-4.76711400	-1.75476200	-1.77219800
H	-3.43003700	-1.92614400	-3.45688900
H	-5.84727500	-1.45595400	0.07040900
H	-5.61662900	-2.18450600	-2.29669900
C	-1.01575500	1.99552600	-0.05997600
C	0.19390300	2.71186600	-0.13921400
C	-2.21132000	2.69938000	-0.29665900
C	0.20658300	4.07591000	-0.43645700
H	1.13701100	2.19609200	0.01390200
C	-2.20316000	4.06438900	-0.59047300
H	-3.16335300	2.17449900	-0.26275700
C	-0.99241500	4.75610500	-0.65979500
H	1.15392900	4.60597300	-0.49668800
H	-3.14013500	4.58522800	-0.77148600
H	-0.98318500	5.81823700	-0.89161500
C	-0.93436900	-0.05095800	2.31541300
C	-1.92665600	0.90411700	3.02056800
H	-2.97341900	0.67861700	2.78418100
H	-1.81691400	0.81014200	4.11054200
H	-1.74507700	1.95176200	2.75798200
C	0.49663900	0.32965300	2.76189100
H	1.25520900	-0.32638300	2.32243400
H	0.74771900	1.36213300	2.49186400
H	0.57860100	0.24760500	3.85527800
C	-1.22913900	-1.50076900	2.76044200
H	-1.17328600	-1.57325400	3.85640100
H	-2.23005700	-1.83154400	2.46028200
H	-0.50583700	-2.21168300	2.34777300
H	2.11379000	0.46718200	-2.06221600