Supporting Information

Mechanistic Study of Palladium-Catalyzed Chemoselective C(sp^3)-H Activation of Carbamoyl Chloride

Qi Zhang,[a] Hai-Zhu Yu,[b] Yao Fu[*a]

Emails: fuyao@ustc.edu.cn

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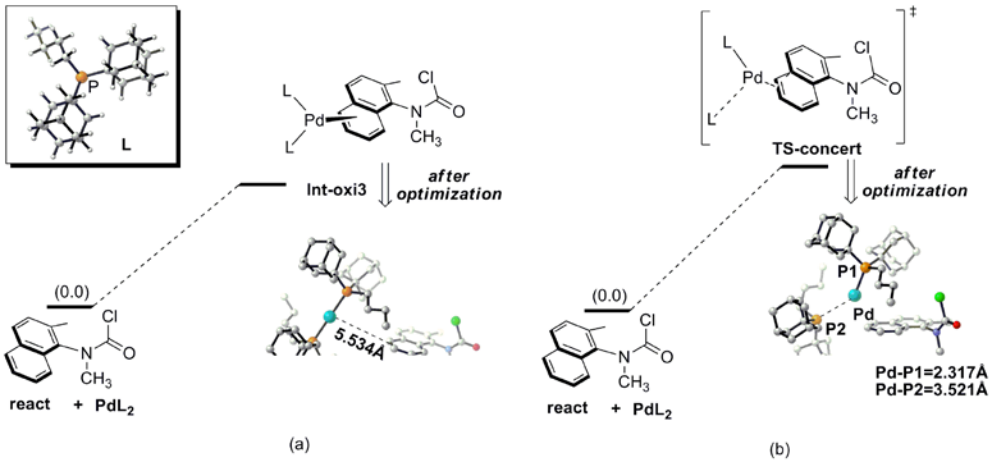
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Other possibilities for the mono-phosphine mechanism oxidative addition



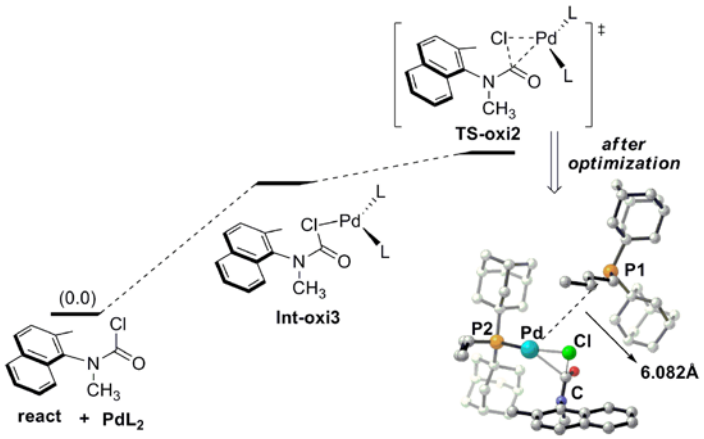
Scheme S1

For the mono-phosphine mechanism, some other possibilities have also been taken into account. (a) It's possible that the coordination of **PdL_2** to **react** occurs before dissociating one ligand(**L**).(Scheme S1a) (b) A concerted process in which the coordination of **PdL_2** to **react** and the ligand dissociation occurs simultaneously has also been examined. (Scheme S1b)

As to (a), due to the steric hindrance of the bulky ligand (Ad_2PBu), intermediate **Int-oxi3** cannot be located because PdL_2 always run away during optimization. As to (b), a concerted transition state **TS-concert** is expected. In **TS-concert** the coordination of **PdL_2** to **react** and the ligand dissociation occur simultaneously. However, due to the steric hindrance of the bulky ligand (Ad_2PBu), one of the phosphine ligands dissociates automatically in the transition state.

Therefore, these two possibilities are all kinetically disfavored.

Details of bis-phosphine mechanism oxidative addition



Scheme S2

We tried to locate the oxidative addition transition state **TS-oxi2** in which bis-ligand coordinated Pd(0) metal center inserts into acylic C-Cl bond. However, a molecule of phosphine on the Pd center automatically dissociated after optimization.(Scheme S2) This phenomenon shows that the system would be more stable by dissociating a large steric hindrance phosphine (Ad_2PBu).

Complete content for Ref (24)

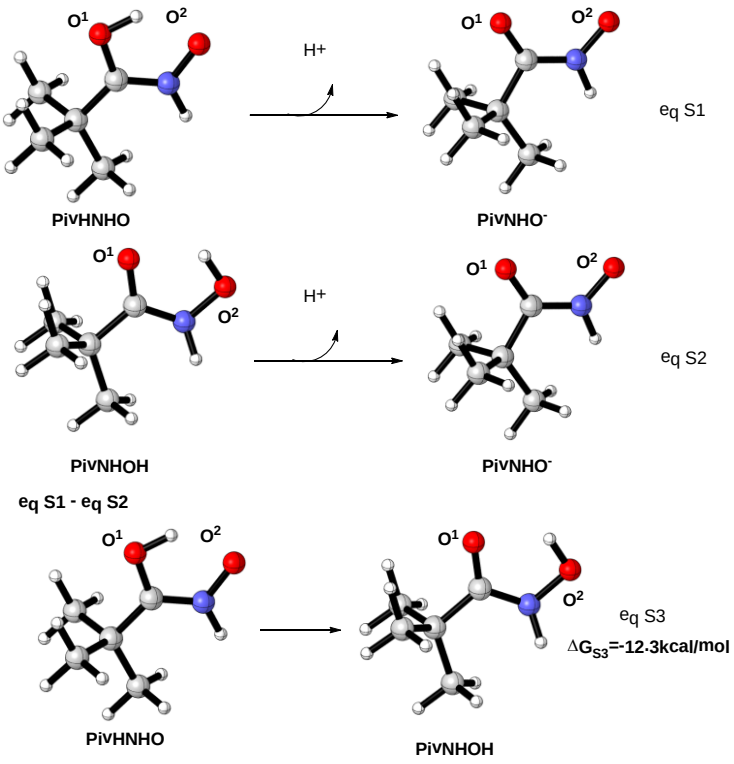
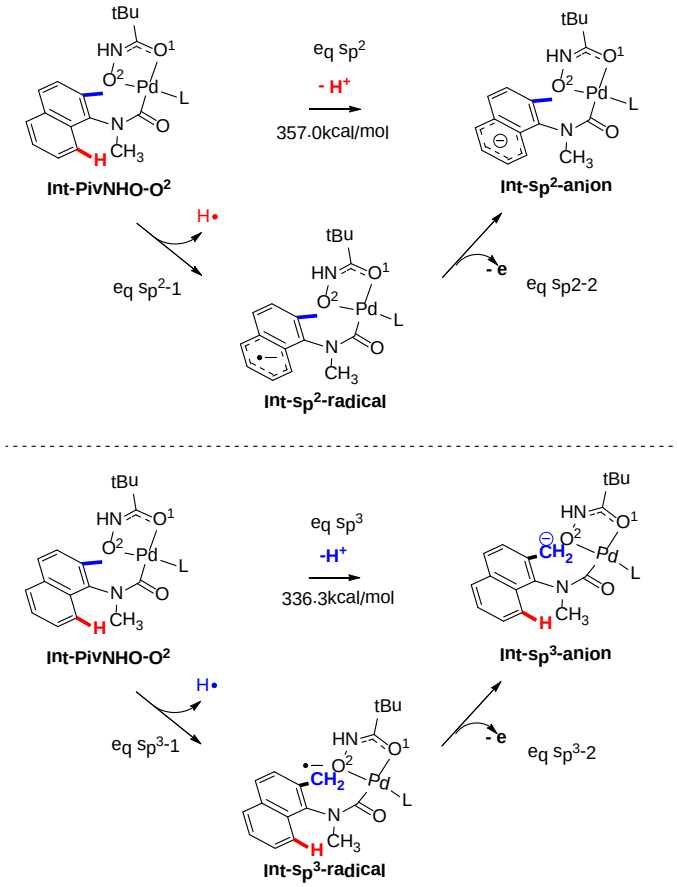


Figure S1. Deprotonation of O^1-H and O^2-H.

As shown in Figure S1, deprotonation process of O^1-H in PivHNHO is shown in eq S1, meanwhile, deprotonation process of O^2-H in PivNHOH is shown in eq S2.

eq S3= eq S1 - eq S3. The Gibbs free energy change of eq S3 is -12.3kcal/mol. This phenomenon indicate that ΔG (eq S1) is lower than ΔG (eq S2), and the acidity of O^2-H is lower than O^1-H. Therefore, the basicity of the carbonyl oxygen O^1 is weaker than the alcohol oxygen O^2.

Complete content for Ref (31)



Scheme S3.

As shown in Scheme S3, eq sp^2 can be decomposed into two eqs : eq sp^2-1 and eq sp^2-2. According to Hess law, ΔG(eq sp^2)= ΔG(eq sp^2-1) + ΔG(eq sp^2-2). In the same way, ΔG(eq sp^3)= ΔG(eq sp^3-1) + ΔG(eq sp^3-2).

Gibbs Free Energy Corrections and Electronic Energies in Solvate of related compounds and Transition States

	Thermal Correction of Gibbs Free Energies (Hartree)	Electronic Energy in solvent (Hartree)
react	0.178824	-1092.524374
Prod-1	0.172804	-631.7262594
Prod-2	0.171057	-631.7258221
PdL_2	1.109647	-2684.752634
PdL	0.541991	-1405.73576
L	0.543433	-1278.950781
Int-oxi1	0.740584	-2498.299214
Int-oxi2	0.739358	-2498.282024
TS-oxi1	0.741354	-2498.279662
Int-Cl	0.741131	-2498.297002
Int-$CsCO_3$	0.752667	-2321.778889
Int-HCO_3	0.769944	-2302.469228
Int-PivNHO-O^2	0.887741	-2439.675188
Int-PivNOH-N	0.88757	-2439.664501
Cs_2CO_3	-0.022207	-303.5737235
CsCl	-0.024995	-480.1384559
PivNHOH	0.130054	-402.1856435
PivNHOCs	0.112915	-421.4891299
Int-PivNHO-O^1	0.887986	-2439.674453

TS-PivNHO-O^2	0.885393	-2439.635012
TS-PivNHO-O^1	0.88532	-2439.627377
Int-PivNHOH	0.885507	-2439.662537
Int-PivHNHO	0.886825	-2439.646127
Int-red1	0.734377	-2037.449071
TS-$CsCO_3$	0.748572	-2321.740804
TS-PivNOH-O^1	0.885333	-2439.625494
TS-PivNOH-N	0.884826	-2439.622375
TS-HCO_3	0.766714	-2302.430282
TS-Cl	0.740637	-2498.257158
Int-PivNHO′-O^2	0.888093	-2439.671474
TS-PivNHO′-O^2	0.882093	-2439.621447
Int-PivNHOH′	0.883716	-2439.642475
Int-red2	0.733316	-2037.444453
Int-$CsCO_3$′	0.752892	-2321.775385
Int-PivNOH′-N	0.88584	-2439.659749
Int-HCO_3′	0.770556	-2302.464529
TS-PivNOH′-O^1	0.882804	-2439.607543
TS-$CsCO_3$′	0.750902	-2321.7285
TS-HCO_3′	0.764285	-2302.418309
TS-Cl′	0.737173	-2498.248861
TS-red1	0.73346	-2037.442254

TS-red2	0.732307	-2037.439887
Int-sp^2-anion	0.874531	-2439.082787
Int-sp^2-radical	0.874527	-2438.992262
Int-sp^3-anion	0.874196	-2439.115437
Int-sp^3-radical	0.875128	-2439.027401
TS-sp^3-A	0.807558	-2438.40484
TS-sp^2-A	0.808326	-2438.404016
TS-sp^3-B	0.836016	-2324.138245
TS-sp^2-B	0.838516	-2324.142206
TS-1p-sp^3	0.945393	-2556.299095
TS-1p-sp^2	0.943665	-2556.296532

Cartesian Coordinates of Intermediates and Transition States

react

N	-1.34645300	-0.37517100	0.73766000
O	-3.25792800	-1.52608200	0.19617000
C	-2.28551800	-0.88625800	-0.10422000
C	-0.37246000	1.80769600	0.22626200
C	0.77627200	2.58680600	-0.07696800
H	0.66065600	3.66271200	-0.17904600
C	2.01468300	2.01319300	-0.23589900
H	2.88006300	2.63189800	-0.46075500
C	2.18939100	0.61063900	-0.10936200
C	3.45764100	-0.00842700	-0.27162300
H	4.31711600	0.61809300	-0.49783400
C	3.59901100	-1.37213200	-0.15013100
H	4.57337800	-1.83514800	-0.27832700
C	2.47004700	-2.17694500	0.13563700
H	2.58560000	-3.25404300	0.21989900
C	1.22593600	-1.60835800	0.29983200
H	0.36456600	-2.23641700	0.50253400
C	1.04840500	-0.20257600	0.18825400
C	-0.22085700	0.43486800	0.34960700
Cl	-1.94318400	-0.52831400	-1.85619900
C	-1.51462600	-0.62498100	2.17707800
H	-0.57493500	-1.00119800	2.59142200
H	-1.78512600	0.30038300	2.69862700
H	-2.30459900	-1.36239700	2.31522800
C	-1.71737100	2.47979200	0.36211600
H	-2.31114800	2.34924900	-0.55163500
H	-2.30650100	2.06869300	1.18793300
H	-1.59966400	3.55444800	0.53085600

Prod-1

C	-0.51278900	0.04197400	0.00017100
C	-0.96031500	1.36022600	0.00011100
C	-2.46239400	1.37080000	0.00014900
H	-2.90201900	1.85537900	-0.88048200
C	0.88074100	-0.26813500	0.00006600
C	1.44154600	-1.57796700	-0.00004500
H	0.79436000	-2.44379900	-0.00014000
C	2.80437200	-1.77424400	-0.00014200
H	3.20057000	-2.78597000	-0.00026900
C	3.69138800	-0.67209500	-0.00011900
H	4.76486600	-0.83977400	-0.00014500
C	3.18851300	0.60695400	-0.00005900
H	3.86049700	1.46196400	-0.00004600
C	1.78764700	0.85554400	0.00001900
C	1.29414300	2.18607900	-0.00001900
C	-0.06160700	2.43721200	0.00002000
N	-1.62914500	-0.82868400	0.00012100
C	-1.66393500	-2.27988000	0.00039400
H	-1.18406000	-2.69235700	-0.89338000
H	-1.18466400	-2.69196700	0.89464000
H	-2.71920800	-2.55972700	0.00007500
C	-2.82592200	-0.11178500	-0.00014700
O	-3.93798300	-0.60863900	-0.00059300
H	2.00743300	3.00582800	-0.00004300
H	-0.43645600	3.45751000	0.00000000
H	-2.90177500	1.85470100	0.88130000

Prod-2

O	0.10023000	3.23194000	0.00241600
C	0.07736700	2.01173600	0.00061400
C	0.86497300	-0.17607500	-0.00256900
C	1.57922600	-1.36365200	-0.00228700
C	0.79553900	-2.56662700	-0.00225600
C	-0.58457500	-2.61158700	-0.00179700
C	-1.32067100	-1.39121100	-0.00121400
C	-2.72818800	-1.19229900	0.00005100
C	-3.26513400	0.09021600	0.00161400
C	-2.45155100	1.25320600	0.00198800
C	-1.08315800	1.07625500	0.00002600
C	-0.55049200	-0.21976500	-0.00195400
H	1.34421300	-3.50579200	-0.00349900
H	-1.10062400	-3.56772200	-0.00288200
H	-3.39302700	-2.05284500	0.00016200
H	-4.34531400	0.20776200	0.00290000
H	-2.89597100	2.24407000	0.00384900
C	3.08852700	-1.46494800	0.00751400
H	3.54720000	-0.90512500	-0.81482000
H	3.52022900	-1.08443500	0.94141600
H	3.40134200	-2.50867000	-0.09279900
N	1.22605600	1.18482100	-0.00021800
C	2.55645400	1.76123600	-0.00541800
H	3.14064800	1.42665200	0.85795200
H	3.10030500	1.51366500	-0.92378400
H	2.42686700	2.84425600	0.04782200

PdL_2

C	-2.74361600	-0.52852200	2.62524500
H	-2.97795900	0.42077400	3.11861900
H	-3.67179000	-1.11080000	2.64618400
C	-1.65313500	-1.24326800	3.44907000
H	-2.13661500	-1.72642300	4.31155100
H	-1.19289400	-2.04741400	2.86120200
C	-0.55488400	-0.30449300	3.96267100
H	-1.02071800	0.52178400	4.52043200
H	-0.04109800	0.14531100	3.10187800
C	0.45893300	-1.01367400	4.86583200
H	1.23246400	-0.32181300	5.21936000
H	0.96205200	-1.83021500	4.33341300
H	-0.02861600	-1.44725500	5.74855600
C	-3.11903500	1.59305400	0.62078600
C	-2.14805400	2.57273900	1.34497800
H	-2.08470500	2.32526800	2.41297800
H	-1.13722400	2.44828600	0.93582700
C	-2.61514800	4.03509100	1.18873400
H	-1.90785400	4.69091400	1.71447900
C	-4.02228700	4.19534500	1.79593300
H	-4.35967700	5.23746100	1.70630100
H	-3.99942600	3.95813700	2.86897100
C	-5.00008500	3.25552300	1.06526400
H	-6.00467700	3.35609600	1.49830300
C	-5.04056900	3.62323800	-0.43167300
H	-5.75477500	2.97698200	-0.96120700
H	-5.39139600	4.65713100	-0.55757200
C	-3.63099500	3.46256300	-1.03540400
H	-3.65676700	3.71086300	-2.10515700
C	-3.17097500	1.99590500	-0.87618000
H	-2.18315100	1.85031600	-1.33298500
H	-3.87379900	1.34941200	-1.41537500
C	-2.65055900	4.40175800	-0.30755300
H	-2.96191600	5.44806600	-0.43622500
H	-1.64568100	4.31086200	-0.74279500
C	-4.53522600	1.78768100	1.22644300
H	-5.26118900	1.13123500	0.73707000
H	-4.54223500	1.52733200	2.29176500
C	-3.29728800	-1.50404200	-0.11956800
C	-4.83949500	-1.46198800	0.01386000
H	-5.22860000	-0.53082400	-0.41311100
H	-5.14337100	-1.48299000	1.06919100
C	-5.48646000	-2.65209200	-0.73382600
H	-6.57689200	-2.59453500	-0.61309800
C	-5.12434000	-2.56752700	-2.22972700
H	-5.50918600	-1.63154500	-2.65882200
H	-5.59968700	-3.39084200	-2.78122400
C	-3.59138400	-2.63508000	-2.38829500
H	-3.32634600	-2.56069300	-3.45192200
C	-3.07647200	-3.96936300	-1.81677600
H	-1.98798900	-4.04066800	-1.94671700
H	-3.52158400	-4.81452800	-2.36068400
C	-3.43754200	-4.04855200	-0.32171400
H	-3.05948000	-4.98886300	0.10219000
C	-2.78957100	-2.86838600	0.43413300
H	-1.69640000	-2.91387400	0.33841300
H	-3.02384100	-2.96287700	1.50141600
C	-2.93556200	-1.45938000	-1.62963200
H	-3.26623400	-0.51569800	-2.07691100
H	-1.84410400	-1.49431800	-1.73780700
C	-4.96865000	-3.98215300	-0.15370300
H	-5.44497200	-4.82897300	-0.66740200
H	-5.23676600	-4.06174500	0.90937600
C	2.39798600	-0.81034000	-2.39909200
H	2.34651100	0.04879500	-3.07698300
H	3.41015200	-1.22193300	-2.50814800
C	1.34806400	-1.83503100	-2.85643600
H	1.33513500	-2.70217300	-2.18494000
H	0.35356900	-1.37871400	-2.77325800
C	1.58172100	-2.31466000	-4.29688800
H	1.59741600	-1.44634500	-4.97159000
H	2.57772000	-2.77491400	-4.37181800
C	0.52163500	-3.31307600	-4.77468800
H	0.71349000	-3.64092500	-5.80300400
H	-0.48096200	-2.86849000	-4.74775900
H	0.50354600	-4.20645900	-4.13806400
C	3.37811300	-1.19123700	0.39514000
C	3.04641100	-2.68274500	0.10166800
H	3.25064500	-2.91736200	-0.94988300
H	1.97608300	-2.86155700	0.27152400
C	3.88861200	-3.62402300	0.99018900
H	3.62693600	-4.66363100	0.75046500
C	5.38571500	-3.38658800	0.70838100
H	5.61302600	-3.61050000	-0.34351000
H	5.99934900	-4.06344000	1.31915800
C	5.73544100	-1.92096300	1.02660800
H	6.79942200	-1.74095100	0.82073500

C	5.43734700	-1.63132600	2.51150500
H	6.05229500	-2.27802700	3.15300500
H	5.70454400	-0.59330700	2.75497600
C	3.93987800	-1.87378200	2.78861800
H	3.71890700	-1.65801000	3.84240600
C	3.08986400	-0.93881000	1.90063700
H	2.02089100	-1.09527600	2.09074800
H	3.30419300	0.10314200	2.16441100
C	3.59125800	-3.34089800	2.47484700
H	4.17575000	-4.01712600	3.11446200
H	2.53072000	-3.53131800	2.69007500
C	4.89043700	-0.97498400	0.14037200
H	5.17097500	0.05881200	0.37041100
H	5.13463000	-1.14710200	-0.91686700
C	2.83582500	1.65998900	-0.88645300
C	4.12573700	1.81246900	-1.73884500
H	4.96694600	1.29174700	-1.27201500
H	3.98895300	1.36575500	-2.73097600
C	4.49264700	3.30610800	-1.90804800
H	5.41059200	3.37702600	-2.50741800
C	4.72768800	3.94077900	-0.52290600
H	5.55956000	3.43570400	-0.01173100
H	5.01495300	4.99579100	-0.63349400
C	3.43996000	3.82504200	0.31750500
H	3.60540700	4.26598400	1.30990600
C	2.29305100	4.56606500	-0.39575500
H	2.53930700	5.63182800	-0.50349400
H	1.37447500	4.50782100	0.20420500
C	2.06273400	3.92900100	-1.78008800
H	1.23523700	4.44058700	-2.29042100
C	1.69358300	2.44093600	-1.60242200
H	1.48678500	1.99879800	-2.58680700
H	0.76985700	2.34259500	-1.01805100
C	3.07316400	2.33402400	0.49069100
H	2.17198800	2.23424600	1.11001300
H	3.88849300	1.83118800	1.02466200
C	3.34669700	4.04622500	-2.62400700
H	3.18383100	3.61540600	-3.62207400
H	3.61116700	5.10278600	-2.77114800
P	-2.31557600	-0.14547400	0.82476700
P	2.16605100	-0.13109200	-0.65612100
Pd	-0.04351100	-0.15414300	0.17103400

PdL

C	-0.00063700	1.33195600	1.79186400
H	-1.04555800	1.39141300	2.11508500
H	0.49922800	0.66616100	2.50626000
C	0.60970300	2.74853200	1.86272400
H	0.88889500	2.94872200	2.90794700
H	1.53763900	2.79703200	1.28115700
C	-0.33597900	3.85617400	1.38299400
H	-1.25599500	3.83231800	1.98586900
H	-0.63146600	3.64051800	0.34587400
C	0.29412400	5.25001200	1.46168400
H	-0.40626800	6.02425000	1.12761900
H	1.18781300	5.31373300	0.82838400
H	0.59748200	5.49588900	2.48759200
C	-1.61713500	-0.54143300	0.19213000
C	-2.78416700	0.45722900	-0.06480800
H	-2.80401700	1.22956000	0.71614900
H	-2.60923000	0.97868300	-1.01485000
C	-4.14326500	-0.27447200	-0.09683000
H	-4.93679500	0.46320900	-0.27689000
C	-4.38360900	-0.97984300	1.25194400
H	-5.35599600	-1.49186200	1.24602200
H	-4.41583900	-0.24105900	2.06499300
C	-3.25105000	-1.99363900	1.50182300
H	-3.40827700	-2.49431400	2.46691200
C	-3.24041100	-3.04079900	0.37029700
H	-2.45159500	-3.78503300	0.54987500
H	-4.19444100	-3.58586300	0.35087300
C	-3.00433800	-2.33205400	-0.97826600
H	-2.98360800	-3.07386400	-1.78797000
C	-1.64424200	-1.60077500	-0.94016600
H	-1.44748200	-1.11315200	-1.90437500
H	-0.85184900	-2.34281000	-0.78635800
C	-4.13512200	-1.31768300	-1.23180100
H	-5.10396500	-1.83428900	-1.28056900
H	-3.98715100	-0.82056900	-2.20030100
C	-1.89046200	-1.25650800	1.54460100
H	-1.09959800	-1.97776500	1.77379500
H	-1.90743000	-0.53284000	2.36842300
C	1.56503400	-0.61815300	0.15665900
C	1.52663900	-1.79310800	1.16437100
H	0.71445200	-2.48232500	0.90916800
H	1.33123300	-1.42768400	2.18175500
C	2.86413800	-2.57263300	1.14175200
H	2.80394400	-3.39602800	1.86633100

C	3.09906400	-3.14026600	-0.27249800
H	2.28692400	-3.82982200	-0.54266900
H	4.03180900	-3.72085700	-0.29593100
C	3.16832500	-1.97915700	-1.28528100
H	3.32253700	-2.37977000	-2.29619600
C	4.33343400	-1.04269700	-0.91363600
H	4.40633000	-0.22250900	-1.64098100
H	5.28718200	-1.58792600	-0.94746600
C	4.09349300	-0.47746100	0.49895000
H	4.90922500	0.20669500	0.76893700
C	2.76214100	0.30418600	0.52846700
H	2.80595800	1.14824300	-0.17268400
H	2.62381200	0.72448400	1.53194000
C	1.84147300	-1.18932000	-1.26117000
H	1.02469500	-1.84654400	-1.57804900
H	1.87317600	-0.35984800	-1.97993000
C	4.02642000	-1.63243500	1.51658800
H	4.97400900	-2.18885000	1.52517300
H	3.88044500	-1.23511800	2.53102500
P	-0.00005500	0.50065200	0.09961500
Pd	0.03019900	1.88274100	-1.67740200

L

C	-0.02330300	2.04091900	1.01271400
H	-1.05901400	2.11790800	1.36231400
H	0.54578500	1.62217100	1.85171300
C	0.47889500	3.46317800	0.68827300
H	0.62213700	4.00591000	1.63492300
H	1.46728700	3.41981300	0.21282500
C	-0.47264500	4.27091600	-0.20410300
H	-1.45481300	4.33830600	0.28684200
H	-0.63475800	3.72714500	-1.14349000
C	0.04395500	5.68137300	-0.50638100
H	-0.65810500	6.23744600	-1.13839800
H	1.00696400	5.64605500	-1.03080400
H	0.19106400	6.25849200	0.41538200
C	-1.58383700	-0.18615000	-0.11186400
C	-2.75463100	0.71839500	-0.60335300
H	-2.79260100	1.64544800	-0.01514300
H	-2.57654000	1.01546500	-1.64500500
C	-4.10990800	-0.01272200	-0.49198500
H	-4.90652700	0.65832300	-0.84086300
C	-4.36568300	-0.40463400	0.97640200
H	-5.33630300	-0.91184600	1.06999700
H	-4.41462600	0.49531800	1.60562200
C	-3.23317000	-1.33024500	1.46122800
H	-3.40613400	-1.60806900	2.50998200
C	-3.19906600	-2.60011200	0.58786100
H	-2.40920500	-3.27922300	0.93876700
H	-4.14969500	-3.14481200	0.67391600
C	-2.94454700	-2.20401400	-0.88056300
H	-2.90762900	-3.10625200	-1.50614200
C	-1.58898900	-1.46881900	-0.98399400
H	-1.38169800	-1.21228400	-2.03212100
H	-0.79385500	-2.14998500	-0.65833200
C	-4.07760700	-1.28045100	-1.36739000
H	-5.04237300	-1.80400400	-1.31361600
H	-3.91864300	-1.00806300	-2.41998300
C	-1.87493000	-0.59482600	1.35692800
H	-1.08446300	-1.24939200	1.73853000
H	-1.89364200	0.28893300	2.00624500
C	1.58207600	-0.18633600	-0.13847800
C	1.58888500	-1.12699500	1.09029800
H	0.79293200	-1.87549600	1.00047600
H	1.39076300	-0.55775500	2.00875200
C	2.94658000	-1.85855700	1.21353400
H	2.91842400	-2.51660300	2.09285200
C	3.18848000	-2.70069500	-0.05603500
H	2.39382100	-3.45189300	-0.16813900
H	4.13625900	-3.25044100	0.03008000
C	3.22171500	-1.77394000	-1.28817600
H	3.38434000	-2.37100600	-2.19572000
C	4.36043100	-0.74915700	-1.12999100
H	4.40733500	-0.09776700	-2.01365200
H	5.32939200	-1.26295400	-1.05863100
C	4.11035800	0.09197200	0.13655500
H	4.90787800	0.83892000	0.24970200
C	2.75524300	0.82450200	0.01884100
H	2.77581700	1.50855600	-0.84108500
H	2.60975000	1.44114200	0.91392300
C	1.87384600	-1.02972500	-1.41328600
H	1.07475000	-1.75912400	-1.58501200
H	1.89066900	-0.37067400	-2.29143700
C	4.08280400	-0.83029300	1.37160300
H	5.04747000	-1.34502100	1.48238200
H	3.93124600	-0.23625100	2.28393800
P	-0.00221100	0.85213700	-0.46022700

Int-oxi1

C	4.60231100	0.62401700	-1.90988100
C	4.47359300	-0.42170100	-1.00177600
C	3.34803900	-1.29500600	-1.00665100
C	2.46555600	-0.01182400	-2.89729700
C	3.56856900	0.81465600	-2.85832400
H	1.69030600	0.14692800	-3.64309400
H	3.66142200	1.62701400	-3.57449900
C	5.78695300	1.55973500	-1.88593400
H	5.73683800	2.23666400	-1.02393500
H	6.73955900	1.02336300	-1.81618800
H	5.81253100	2.17483200	-2.79047900
N	5.55390800	-0.70344900	-0.09049800
C	6.54956900	-1.68798100	-0.53950300
H	7.25187900	-1.87259100	0.27256800
H	7.09093300	-1.30889000	-1.41346900
C	5.74524200	-0.12216900	1.12341400
O	6.65223500	-0.31460200	1.88889500
Cl	4.42906400	1.05911900	1.56545000
C	-2.14337400	-0.16524500	2.50067800
H	-1.52915300	0.59337800	2.99783800
H	-3.18508900	0.10643100	2.71035700
C	-1.81394700	-1.53916300	3.12350200
H	-2.34653200	-1.61497100	4.08320700
H	-2.20172200	-2.34948600	2.49427800
C	-0.31775800	-1.76918900	3.37121500
H	0.06542900	-0.97544600	4.02906200
H	0.22351700	-1.67541600	2.41930300
C	-0.02328800	-3.13767900	3.99323800
H	1.04987300	-3.27046800	4.17235700
H	-0.35462000	-3.94969600	3.33348800
H	-0.53878500	-3.26171600	4.95425800
C	-1.27037400	1.83169100	0.51009500
C	0.20937000	1.84875600	0.99534400
H	0.27078200	1.52992200	2.04455100
H	0.79272100	1.12435600	0.41414800
C	0.81931300	3.25947000	0.85462200
H	1.85873700	3.22835500	1.20680500
C	0.00914200	4.26082900	1.70043000
H	0.44451500	5.26672900	1.62041000
H	0.04929000	3.97958900	2.76208900
C	-1.45121600	4.27389300	1.20872500
H	-2.03998200	4.97780800	1.81253400
C	-1.49035900	4.70176300	-0.27198800
H	-2.52981400	4.73896000	-0.62802900
H	-1.07880500	5.71456400	-0.38337400
C	-0.67524900	3.70107400	-1.11548800
H	-0.71023100	3.99459800	-2.17352700
C	-1.28946300	2.29130200	-0.97063500
H	-0.73527500	1.57187300	-1.58789900
H	-2.31947400	2.31509500	-1.34630400
C	0.78588400	3.68525700	-0.62639500
H	1.23534300	4.68122600	-0.74532300
H	1.38124900	2.98815400	-1.23145100
C	-2.06561800	2.86113200	1.35794400
H	-3.11558000	2.89349500	1.05022400
H	-2.05513000	2.57793700	2.41728800
C	-3.58404400	-0.26733900	-0.11028200
C	-4.64512400	0.82127900	0.18712400
H	-4.32907800	1.78286900	-0.23348200
H	-4.76124600	0.96658600	1.26971200
C	-6.00979300	0.43520000	-0.43438800
H	-6.73813000	1.22394200	-0.20215800
C	-5.85513200	0.30399600	-1.96273500
H	-5.53410100	1.26249000	-2.39434400
H	-6.82347200	0.05667800	-2.41982700
C	-4.82108100	-0.79551800	-2.27885200
H	-4.69636400	-0.88361100	-3.36655500
C	-5.30724700	-2.13800100	-1.70106500
H	-4.58925900	-2.93463000	-1.94000500
H	-6.26660600	-2.42313200	-2.15507300
C	-5.45996600	-2.00344700	-0.17469100
H	-5.78934300	-2.96040800	0.25205400
C	-4.10106100	-1.62310200	0.45192600
H	-3.36165000	-2.40944500	0.24742400
H	-4.22054700	-1.56679100	1.54027900
C	-3.45870400	-0.42346000	-1.65129800
H	-3.09487800	0.50593200	-2.10327100
H	-2.70989900	-1.19540100	-1.87248600
C	-6.49295600	-0.90638200	0.14917000
H	-7.47263300	-1.16989000	-0.27307300
H	-6.62633800	-0.82106600	1.23682300
P	-1.83960700	0.00283800	0.64679900
Pd	-0.27194000	-1.47873000	-0.29645700
H	6.04389800	-2.61832600	-0.81486200
C	2.32068000	-1.07636200	-1.97800800
C	1.19017900	-1.96334100	-2.02440000
C	1.10093800	-3.04642200	-1.13402800

H	0.37600800	-3.83982600	-1.30028400
C	2.12224500	-3.21968000	-0.14472700
H	2.04026000	-4.04679200	0.55520600
C	3.20541400	-2.37798300	-0.08471900
H	3.96357700	-2.52634500	0.67697200
H	0.52562700	-1.89883500	-2.88169000

Int-oxi2

C	5.71273700	-0.30870900	0.33605900
C	4.57463200	-0.43307000	-0.44609500
C	3.99855000	0.68281700	-1.12928600
C	5.78674100	2.07385300	-0.18419700
C	6.30513400	0.97687600	0.46003500
H	6.26419500	3.04529000	-0.08161300
H	7.19393100	1.08043600	1.07699500
C	6.31017200	-1.47618600	1.08412600
H	5.78580400	-1.64006600	2.03479800
H	6.24891200	-2.41120000	0.51912300
H	7.36258800	-1.28884400	1.31814300
N	3.99959400	-1.73683700	-0.66525900
C	4.45212800	-2.46442600	-1.86292000
H	3.82987700	-3.34893200	-1.99479400
H	5.49938600	-2.76719500	-1.75254100
C	3.12389500	-2.36944800	0.15183600
O	2.67095100	-3.47421600	0.04450300
Cl	2.61584800	-1.31977600	1.59681300
C	-3.13764900	-0.35619100	2.10885600
H	-3.26967200	0.61097600	2.60579600
H	-4.11861300	-0.61364500	1.69169100
C	-2.71982100	-1.39341200	3.17338300
H	-3.62278900	-1.71211900	3.71580500
H	-2.31385700	-2.29208600	2.69416200
C	-1.69768600	-0.86129900	4.18556300
H	-2.11898700	0.01970200	4.69299300
H	-0.80669600	-0.51860300	3.64028600
C	-1.28863200	-1.90780100	5.22649600
H	-0.57245200	-1.49473300	5.94653400
H	-0.81525500	-2.77327900	4.74657500
H	-2.15549800	-2.27403900	5.79198700
C	-2.14414100	1.79335000	0.36122700
C	-1.33590100	2.50411900	1.48738500
H	-1.75694500	2.25893800	2.47188600
H	-0.30585600	2.12577100	1.48473100
C	-1.34670800	4.03536700	1.29625100
H	-0.77122700	4.49747600	2.10973500
C	-2.79879700	4.55098600	1.32774600
H	-2.81833700	5.64342100	1.20731100
H	-3.25829000	4.32850400	2.30106700
C	-3.60021500	3.87800200	0.19686700
H	-4.63990000	4.23242900	0.21794700
C	-2.96129000	4.22785500	-1.16219500
H	-3.53819800	3.77301500	-1.97998600
H	-2.98444700	5.31514500	-1.32144700
C	-1.50744800	3.71527000	-1.18912600
H	-1.05033000	3.95154400	-2.16015000
C	-1.50341200	2.18270700	-0.99601200
H	-0.47695700	1.79575100	-1.04161100
H	-2.06161000	1.72511300	-1.82200200
C	-0.70285000	4.38562200	-0.05931300
H	-0.68554400	5.47555000	-0.20194000
H	0.33963900	4.04011000	-0.08323400
C	-3.59641000	2.34239800	0.39519100
H	-4.20701500	1.88097100	-0.38728500
H	-4.07724100	2.10512100	1.35188400
C	-2.68938700	-1.14965200	-0.72692400
C	-4.06367100	-0.69129900	-1.27543900
H	-3.98084000	0.30694100	-1.72052700
H	-4.80355000	-0.62263000	-0.46637200
C	-4.57286500	-1.67294100	-2.35875200
H	-5.54813700	-1.32172700	-2.72282100
C	-3.56585000	-1.70929800	-3.52577700
H	-3.47107000	-0.70988700	-3.97390800
H	-3.92884900	-2.38032200	-4.31698200
C	-2.19705500	-2.19099300	-3.00449400
H	-1.47250800	-2.20691500	-3.83036200
C	-2.34126900	-3.60608200	-2.41321200
H	-1.36702400	-3.96817700	-2.05800900
H	-2.68455200	-4.30866500	-3.18581300
C	-3.34732000	-3.56484300	-1.24737800
H	-3.44545700	-4.56603700	-0.80656600
C	-2.84473000	-2.59137200	-0.15989000
H	-1.87907300	-2.93247400	0.23640600
H	-3.55623600	-2.59848900	0.67456800
C	-1.68734200	-1.22468500	-1.91280400
H	-1.53715800	-0.23193700	-2.35164700
H	-0.71069600	-1.55356100	-1.53427100
C	-4.71887100	-3.08632700	-1.76256300
H	-5.10312200	-3.77926300	-2.52420800

H	-5.44951200	-3.07766300	-0.94136600
P	-1.92580300	-0.09110200	0.68599700
Pd	0.22849400	-0.68658000	1.07877600
H	4.36221900	-1.81012400	-2.73417600
C	4.62754300	1.96272900	-0.99536800
C	4.07515700	3.08069900	-1.67547900
C	2.94897200	2.94636300	-2.45569400
H	2.53547400	3.80745700	-2.97310700
C	2.32105600	1.68371700	-2.57898700
H	1.42435500	1.58597000	-3.18435300
C	2.82871300	0.57913700	-1.92936500
H	2.32223700	-0.37663500	-2.00968500
H	4.56039700	4.04764500	-1.56683100

TS-oxi1

C	5.21481100	-0.73004800	-0.08273000
C	3.96243800	-0.36053500	-0.55416800
C	3.69548300	0.97238700	-1.00240300
C	6.00821300	1.55409600	-0.41745900
C	6.22966600	0.26287800	-0.00897800
H	6.80433400	2.29258400	-0.36074200
H	7.20586200	-0.02456700	0.37385500
C	5.54672600	-2.12869900	0.37666200
H	5.55765100	-2.18136000	1.47249600
H	4.82626800	-2.87083800	0.02594000
H	6.54207900	-2.42267100	0.02489000
N	2.93518400	-1.35548400	-0.72112000
C	2.88382300	-2.02552200	-2.03214700
H	1.89308800	-2.45293800	-2.18831300
H	3.62952500	-2.82840700	-2.09502600
C	2.19339000	-1.93718200	0.26860100
O	1.62329900	-2.99512700	0.22200400
Cl	2.70101900	-1.19505400	2.06242100
C	-2.89950400	-0.57644600	2.02196400
H	-3.16374900	0.35919700	2.52645800
H	-3.82994000	-0.95021400	1.57830100
C	-2.37538000	-1.56866600	3.08293400
H	-3.24209400	-2.05205500	3.55792700
H	-1.79602100	-2.36894900	2.60838700
C	-1.51905000	-0.91353900	4.17388700
H	-2.10949200	-0.13206500	4.67553200
H	-0.66284800	-0.41026000	3.70205400
C	-1.00611400	-1.91802700	5.20995600
H	-0.41243200	-1.42083700	5.98563500
H	-0.36883000	-2.67541500	4.73775800
H	-1.83437900	-2.43997700	5.70649900
C	-2.20481000	1.69209900	0.28306100
C	-1.52423600	2.51789500	1.41510100
H	-1.90567800	2.20661200	2.39675300
H	-0.44651300	2.30957900	1.41788300
C	-1.77352800	4.02904500	1.22386200
H	-1.28432000	4.57379300	2.04226200
C	-3.28858400	4.31076000	1.24239200
H	-3.47704500	5.38700500	1.12488100
H	-3.71592600	4.01520300	2.21090300
C	-3.96588000	3.52545000	0.10281200
H	-5.04809900	3.71320900	0.11510500
C	-3.37720700	3.97219800	-1.24983700
H	-3.86920400	3.43535300	-2.07331700
H	-3.56557300	5.04299800	-1.40949700
C	-1.86158400	3.69102000	-1.26264700
H	-1.43835600	3.99561600	-2.23009000
C	-1.62029700	2.17629100	-1.06878000
H	-0.54565700	1.95802500	-1.10134100
H	-2.08835300	1.63651900	-1.90087200
C	-1.18007400	4.47658600	-0.12590400
H	-1.33133300	5.55587500	-0.26862700
H	-0.09630800	4.29838400	-0.13937700
C	-3.72497600	2.00895500	0.30004300
H	-4.24612300	1.45823400	-0.48940200
H	-4.17549900	1.70146100	1.25069300
C	-2.27417800	-1.30234900	-0.79643500
C	-3.68127000	-1.03387400	-1.38477400
H	-3.72197000	-0.03346100	-1.83029800
H	-4.44644800	-1.06634300	-0.59744000
C	-4.02228400	-2.07612000	-2.47729600
H	-5.02439800	-1.85862500	-2.87106200
C	-2.98540500	-1.98245000	-3.61476100
H	-3.01132800	-0.98147500	-4.06840800
H	-3.23120900	-2.69976500	-4.41009400
C	-1.58015900	-2.27379500	-3.05088600
H	-0.83656600	-2.19276300	-3.85588400
C	-1.54861300	-3.69316200	-2.45214200
H	-0.54796100	-3.91830800	-2.05929900
H	-1.76787000	-4.43871900	-3.22942200
C	-2.58720900	-3.78233100	-1.31826300
H	-2.56295300	-4.78586800	-0.87314900
C	-2.24763600	-2.74944600	-0.22212800

H	-1.25737700	-2.96301600	0.19896600
H	-2.97658100	-2.84964700	0.59073000
C	-1.23953200	-1.24152100	-1.95308200
H	-1.21504900	-0.23869200	-2.39487900
H	-0.24066100	-1.43517000	-1.54558200
C	-3.99491000	-3.49394000	-1.87495700
H	-4.26130100	-4.23521500	-2.64131300
H	-4.74282000	-3.57979700	-1.07401800
P	-1.71315900	-0.13586500	0.62204200
Pd	0.50315800	-0.43575600	1.23454100
H	3.09025300	-1.28385900	-2.80611900
C	4.74581000	1.94441900	-0.93548600
C	4.50227200	3.26427100	-1.39893100
C	3.27778500	3.61458300	-1.92129100
H	3.10389500	4.62515000	-2.28043100
C	2.23990300	2.65536800	-1.98740100
H	1.27500400	2.93803200	-2.39893400
C	2.43821700	1.36867600	-1.53220100
H	1.62877400	0.64735100	-1.55832200
H	5.30694300	3.99322700	-1.33864400

Int-Cl

N	-3.65637900	0.11641400	1.43406500
O	-1.74067200	0.84015600	2.48919300
C	-2.33605000	0.25704600	1.56371100
C	-4.37986600	-1.92483000	0.29316200
C	-5.06301300	-2.53031200	-0.79593300
H	-5.14736400	-3.61370000	-0.81510800
C	-5.61069200	-1.78297100	-1.80895600
H	-6.13525300	-2.26981800	-2.62754600
C	-5.50063400	-0.36808700	-1.81122900
C	-6.05219300	0.42870300	-2.84920600
H	-6.57685600	-0.06778900	-3.66207800
C	-5.92196800	1.79906100	-2.83531100
H	-6.34589600	2.39799700	-3.63654000
C	-5.22354100	2.43033800	-1.77870700
H	-5.11071700	3.51119900	-1.77901200
C	-4.67920900	1.68659500	-0.75413800
H	-4.13038300	2.18106100	0.04094400
C	-4.80688000	0.27086200	-0.73395100
C	-4.26919700	-0.54557200	0.30742700
Cl	-1.10862800	-1.37873200	-1.18983700
C	-4.56151900	0.62664200	2.48036000
H	-5.32188500	1.26875400	2.02723600
H	-5.05906600	-0.20959600	2.98350500
H	-3.97753700	1.19550700	3.20417600
C	-3.76154800	-2.79583000	1.35781600
H	-2.70198100	-2.96573000	1.12833500
H	-3.81290100	-2.34245900	2.35275700
H	-4.25735000	-3.77079400	1.39996800
C	2.73549100	-0.04127800	2.24464300
H	3.23617500	-1.01209100	2.32013200
H	3.53360100	0.71006400	2.25981700
C	1.81433600	0.12802700	3.47114900
H	2.43617100	0.42532600	4.32821500
H	1.10179400	0.94605200	3.31190800
C	1.04551000	-1.14738100	3.84240000
H	1.76674000	-1.95014800	4.05566800
H	0.45722100	-1.48329700	2.97649600
C	0.11339400	-0.95394000	5.04219100
H	-0.39137600	-1.89056400	5.30671600
H	-0.65657300	-0.20792700	4.81628500
H	0.66712600	-0.61392600	5.92677300
C	2.82799400	-1.31954900	-0.42673000
C	2.24804200	-2.67863000	0.06817100
H	2.43572800	-2.80373400	1.14384400
H	1.16260200	-2.68814300	-0.07739600
C	2.88961000	-3.85442800	-0.70038400
H	2.46164300	-4.79360300	-0.32516500
C	4.41467200	-3.85147300	-0.48040200
H	4.87709800	-4.69628500	-1.00976500
H	4.64526800	-3.97895300	0.58698100
C	4.99931600	-2.52185500	-0.99424500
H	6.08544400	-2.50591300	-0.82983900
C	4.69837000	-2.37511000	-2.49865400
H	5.13469700	-1.44204100	-2.88284700
H	5.16359800	-3.19898800	-3.05772000
C	3.17215100	-2.37797400	-2.71417400
H	2.94776100	-2.26082900	-3.78263700
C	2.54019000	-1.19393800	-1.94711800
H	1.45955600	-1.16457400	-2.12255300
H	2.96642900	-0.25962600	-2.33309100
C	2.58030000	-3.70591500	-2.20300800
H	3.00789500	-4.54984200	-2.76263500
H	1.49539400	-3.72237900	-2.36654300
C	4.36760800	-1.34084700	-0.21889500
H	4.81843000	-0.40442000	-0.56345100
H	4.61845800	-1.44089200	0.84377000

C	2.24816200	1.79327600	-0.06416800
C	3.72915200	2.10454100	-0.39247000
H	4.08053400	1.45356200	-1.20076500
H	4.36961200	1.91078100	0.47894300
C	3.88732700	3.57801600	-0.83662300
H	4.94607100	3.76654900	-1.06001500
C	3.03770800	3.82212000	-2.10022500
H	3.37942600	3.17048700	-2.91648800
H	3.16371400	4.85798600	-2.44462900
C	1.55464800	3.54292100	-1.78270300
H	0.94653400	3.70322800	-2.68252300
C	1.08424600	4.48811800	-0.66090500
H	0.02193700	4.31447800	-0.44092000
H	1.17855700	5.53553700	-0.98013000
C	1.93399700	4.23914800	0.59949100
H	1.59483800	4.89483500	1.41257600
C	1.77588200	2.77089200	1.05236600
H	0.72516400	2.57219200	1.30465600
H	2.35954600	2.61954700	1.96830200
C	1.38713000	2.07589900	-1.32855000
H	1.67187200	1.40759800	-2.14727200
H	0.33198800	1.86537000	-1.11207100
C	3.41791600	4.51854700	0.28974600
H	3.55208400	5.56636700	-0.01239700
H	4.02834800	4.36568500	1.19106800
P	1.88960900	0.02227700	0.56126300
Pd	-0.59135700	-0.13628200	0.75527500

Int-$CsCO_3$

N	-1.63127500	2.30517100	-2.19122000
O	-1.47564500	0.22739200	-3.08542000
C	-1.08094500	1.03078200	-2.23714500
C	-0.17472900	4.23150100	-1.78215300
C	0.22600300	5.29416200	-0.92457300
H	1.02189100	5.95333100	-1.26301500
C	-0.36229200	5.50744800	0.29682500
H	-0.03843100	6.33162100	0.92871000
C	-1.42308300	4.67555500	0.74043000
C	-2.09804200	4.90680700	1.96879700
H	-1.76619500	5.73157700	2.59592200
C	-3.16122800	4.12036000	2.35462500
H	-3.67813200	4.31649900	3.29038600
C	-3.58668300	3.05781000	1.52156900
H	-4.43307800	2.44491800	1.82176100
C	-2.93571200	2.79264100	0.33483000
H	-3.25810300	1.96962700	-0.29371200
C	-1.83819100	3.58768500	-0.09500500
C	-1.16846200	3.36590000	-1.34295200
C	-2.69203000	2.66389200	-3.13981200
H	-3.02405300	1.75116500	-3.63455200
H	-3.52772100	3.13049000	-2.60613900
H	-2.32922900	3.36951100	-3.89804900
C	0.50915200	4.08819200	-3.11773400
H	1.41406500	3.48436300	-2.99166500
H	-0.11962300	3.58097700	-3.85337400
H	0.78640900	5.07187700	-3.51398300
C	0.77276600	-2.66309000	0.04871600
H	1.44984100	-2.44900500	0.88330700
H	0.31614800	-3.63761700	0.26386500
C	1.62123400	-2.73262900	-1.23255100
H	0.99618700	-2.93649900	-2.10819500
H	2.08065600	-1.75173900	-1.39508500
C	2.71429400	-3.80909400	-1.13627600
H	2.25799900	-4.79482000	-0.96632700
H	3.33678800	-3.61723100	-0.24510000
C	3.60583800	-3.87081000	-2.38243700
H	4.38873100	-4.63290300	-2.28468800
H	4.09067000	-2.90436500	-2.57549600
H	3.01633200	-4.11247500	-3.27425100
C	-0.62178300	-0.99145600	2.03248000
C	0.55161900	-0.02037400	2.35293300
H	1.51097100	-0.46985000	2.06942500
H	0.45780300	0.88467100	1.74271200
C	0.56564100	0.35290700	3.85025900
H	1.40943800	1.03198000	4.03476300
C	0.72308200	-0.91983100	4.70438300
H	0.75322100	-0.66284800	5.77269400
H	1.67439600	-1.42068600	4.46951500
C	-0.45644300	-1.86977100	4.42032000
H	-0.34729200	-2.78581100	5.01730600
C	-1.78024500	-1.16912400	4.78232200
H	-2.62708600	-1.84742900	4.60649800
H	-1.79223100	-0.91301800	5.85101600
C	-1.92996800	0.10432400	3.92672100
H	-2.87819600	0.60404900	4.16517300
C	-1.94198300	-0.28276800	2.43006000
H	-2.08766000	0.61365700	1.81803500
H	-2.79715100	-0.94357100	2.24960800

C	-0.75528100	1.05834400	4.21271900
H	-0.75327900	1.34733600	5.27348100
H	-0.86646600	1.97988900	3.62713700
C	-0.46097400	-2.25645200	2.92205300
H	-1.27125200	-2.96835400	2.73678200
H	0.47595300	-2.77753000	2.69308100
C	-2.13916000	-2.20704900	-0.48110900
C	-2.63536600	-3.36673600	0.42316100
H	-2.91316300	-2.99196600	1.41482000
H	-1.84289700	-4.11268300	0.57156900
C	-3.87314900	-4.05249800	-0.20511500
H	-4.19388900	-4.86816800	0.45769100
C	-5.01020600	-3.02162600	-0.34852200
H	-5.29339600	-2.63024500	0.63913200
H	-5.90389900	-3.50336100	-0.76930700
C	-4.54200300	-1.87325900	-1.26278700
H	-5.34168700	-1.12623500	-1.35783200
C	-4.18168300	-2.42821200	-2.65403200
H	-3.85279900	-1.61269600	-3.30967600
H	-5.06393800	-2.89123400	-3.11861400
C	-3.05331000	-3.46568200	-2.50454100
H	-2.78065800	-3.85994500	-3.49262800
C	-1.80720900	-2.79559800	-1.88492000
H	-1.44111100	-1.99902100	-2.54091200
H	-1.02114600	-3.55486400	-1.79345300
C	-3.30120100	-1.18775500	-0.64742900
H	-3.57421200	-0.75353800	0.31996900
H	-2.97816700	-0.37269100	-1.29665700
C	-3.51826300	-4.61779300	-1.59372500
H	-4.39312200	-5.12149700	-2.02850900
H	-2.72605100	-5.37508500	-1.50417000
P	-0.54960800	-1.32248800	0.13098600
Pd	0.44767600	0.50889900	-1.02224500
C	2.88990900	1.26907100	-1.07029000
O	2.49956000	0.26683600	-0.28241600
O	1.91885100	1.80672100	-1.76783500
O	4.07955100	1.63960800	-1.13837100
Cs	5.31763100	-0.53574300	0.32199700

Int-HCO_3

N	1.88435000	-1.06954700	-2.30168500
O	-0.07620300	-2.21532300	-2.24813300
C	0.77675000	-1.57061500	-1.64976700
C	4.05742300	-1.26599400	-1.18534600
C	5.16254500	-0.63423100	-0.54968000
H	5.96618900	-1.26126200	-0.17112600
C	5.23822500	0.72903600	-0.41151500
H	6.09424600	1.18618400	0.07923600
C	4.21700700	1.56578400	-0.93324100
C	4.30271700	2.98229600	-0.87246500
H	5.16271400	3.42995900	-0.37972500
C	3.33209600	3.77613700	-1.44251600
H	3.41634400	4.85868800	-1.40337900
C	2.22650300	3.17746600	-2.09215200
H	1.46936100	3.80634500	-2.55336500
C	2.09911500	1.80502800	-2.14132500
H	1.24384900	1.35294600	-2.63104100
C	3.08384400	0.95771800	-1.56484600
C	3.01077800	-0.47242000	-1.63614000
C	2.04403000	-1.35733400	-3.73422700
H	1.06038400	-1.55679600	-4.15984400
H	2.49890700	-0.49193300	-4.22478200
H	2.68311800	-2.23418500	-3.89767300
C	4.10522900	-2.75921000	-1.39767500
H	4.55088700	-3.25751000	-0.53306600
H	3.11577000	-3.19055100	-1.55069900
H	4.72534900	-2.99563700	-2.27405800
C	-2.28926800	-1.11252900	1.77476100
H	-1.91137400	-0.80876200	2.75639500
H	-3.33625200	-0.78621100	1.72706800
C	-2.19483600	-2.64669300	1.68633900
H	-2.43651600	-3.00117400	0.67863800
H	-1.15889200	-2.94050800	1.88354500
C	-3.12042900	-3.33308100	2.70250100
H	-4.16249100	-3.03685300	2.51091900
H	-2.87966000	-2.97333200	3.71290500
C	-3.00712500	-4.86086400	2.66457700
H	-3.67584500	-5.32945900	3.39582000
H	-1.98407300	-5.18468600	2.89041200
H	-3.26772600	-5.25287300	1.67367900
C	-0.92964700	1.50827600	1.47830700
C	0.28035100	1.21418400	2.41239300
H	0.04805200	0.39862100	3.10570000
H	1.13165200	0.86990800	1.81274400
C	0.68316200	2.47781900	3.20306500
H	1.53236900	2.22422500	3.85064100
C	-0.50311700	2.95638500	4.06127500
H	-0.22009400	3.84643100	4.64024100

H	-0.78451300	2.17930300	4.78530800
C	-1.69486900	3.27934900	3.14057700
H	-2.55182500	3.60919700	3.74336700
C	-1.29651700	4.39159800	2.15014200
H	-2.14775300	4.64588600	1.50248500
H	-1.02780100	5.30544200	2.69779000
C	-0.10497400	3.91016300	1.29981200
H	0.17856100	4.69052600	0.58108600
C	-0.51768100	2.64670900	0.51074400
H	0.31388900	2.32086700	-0.12351200
H	-1.34944100	2.90840900	-0.15316600
C	1.08992000	3.58965400	2.21693300
H	1.39592900	4.49144100	2.76582600
H	1.95154400	3.27072500	1.61573200
C	-2.10884900	2.00739300	2.36156800
H	-2.98908400	2.23271200	1.75226700
H	-2.40575100	1.23548500	3.07996600
C	-2.51752400	0.16373500	-0.93628300
C	-3.69827800	1.10473200	-0.57828300
H	-3.32926300	2.09966300	-0.30996600
H	-4.24848900	0.71913700	0.28994800
C	-4.66342100	1.24578000	-1.78057800
H	-5.48309300	1.91682900	-1.49042200
C	-3.90075600	1.84205900	-2.98073800
H	-3.51378400	2.83915700	-2.72673900
H	-4.58210000	1.97177200	-3.83278400
C	-2.74176200	0.90274900	-3.36345100
H	-2.18548300	1.32779400	-4.20977100
C	-3.29780400	-0.48140100	-3.74884800
H	-2.47696600	-1.15179800	-4.03387500
H	-3.96487400	-0.39320100	-4.61792600
C	-4.06408300	-1.06743600	-2.54806600
H	-4.45344500	-2.06084300	-2.80672300
C	-3.10941200	-1.21868800	-1.34183200
H	-2.30103500	-1.91360000	-1.58901200
H	-3.67650800	-1.64116300	-0.50439100
C	-1.77469500	0.75317200	-2.16725300
H	-1.34365600	1.73058300	-1.92696800
H	-0.95313600	0.09214800	-2.44987300
C	-5.22835800	-0.13423600	-2.16661200
H	-5.92815100	-0.03275300	-3.00761500
H	-5.79620300	-0.56031200	-1.32759300
P	-1.30193400	-0.12273900	0.52119900
Pd	0.67654800	-1.41155100	0.33942000
C	1.93859300	-2.64776700	2.19648400
O	0.97791800	-1.92236700	2.56100600
O	2.61734100	-3.32822200	3.14743600
O	2.30477500	-2.77905400	0.98203000
H	3.30359600	-3.83432600	2.67930900

Int-PivNHO-O^2

N	-0.87432100	-2.12209700	-2.37052800
O	0.46549500	-0.48073100	-3.17126600
C	-0.31644600	-0.85629900	-2.30179400
C	-3.25294200	-2.47283800	-1.89618100
C	-4.26027600	-3.00257600	-1.04338000
H	-5.30070400	-2.86378300	-1.32845100
C	-3.95471500	-3.68214900	0.10947900
H	-4.74519900	-4.07809000	0.74300400
C	-2.60232900	-3.90980300	0.47310200
C	-2.25145100	-4.68151600	1.61285000
H	-3.04893300	-5.07261700	2.24072200
C	-0.93372600	-4.95262500	1.90716400
H	-0.67797100	-5.55917600	2.77173900
C	0.09086700	-4.44803900	1.07077700
H	1.12938800	-4.67656500	1.29635800
C	-0.21609000	-3.66857000	-0.02462400
H	0.57268500	-3.27702400	-0.65710000
C	-1.56578400	-3.37331700	-0.35875600
C	-1.92320100	-2.61451400	-1.52097900
C	-0.51229400	-2.97908700	-3.50856700
H	0.45974600	-2.66267000	-3.88704300
H	-0.46608000	-4.01950500	-3.17340700
H	-1.24482000	-2.90153400	-4.32216700
C	-3.67366200	-1.84196000	-3.20063500
H	-4.61552600	-1.29840100	-3.07910900
H	-2.93261100	-1.13781100	-3.57666500
H	-3.84114400	-2.61906500	-3.96048600
C	1.30166600	2.64665500	0.29826000
H	0.64770100	2.90906100	1.13613800
H	2.31955500	2.94026300	0.58508200
C	0.82961700	3.45801700	-0.92186100
H	1.38508000	3.18508100	-1.82397700
H	-0.21874700	3.21446800	-1.11816400
C	0.97085200	4.96957300	-0.68358600
H	2.02260300	5.21262200	-0.47205900
H	0.40659900	5.25052600	0.21755600
C	0.48380200	5.80498400	-1.87245900

H	0.59212400	6.87865100	-1.67935900
H	-0.57391300	5.60773200	-2.08564100
H	1.05189500	5.56958000	-2.78078000
C	1.16641200	0.27133600	2.06157800
C	-0.32056300	0.33590300	2.51564100
H	-0.72689500	1.34062300	2.36070200
H	-0.92144200	-0.33413300	1.88886000
C	-0.46215100	-0.07182200	3.99908400
H	-1.52190700	-0.00299800	4.27897000
C	0.37189000	0.87518300	4.88301000
H	0.26237800	0.60263500	5.94213100
H	0.01084800	1.90803800	4.77927500
C	1.85150300	0.78761500	4.46282700
H	2.45376000	1.46854700	5.07964200
C	2.35520100	-0.65769100	4.64047400
H	3.41652500	-0.72605800	4.36182300
H	2.28257900	-0.95689900	5.69530100
C	1.51043400	-1.59931700	3.76070500
H	1.87128600	-2.63117800	3.86907000
C	1.65342800	-1.18525600	2.27833500
H	1.07303100	-1.86965900	1.65048000
H	2.70484400	-1.29110600	1.99253200
C	0.03307900	-1.51855900	4.18594700
H	-0.07531500	-1.82512800	5.23614900
H	-0.57146800	-2.20932200	3.58402500
C	1.99404500	1.21333100	2.98245900
H	3.05317700	1.20277900	2.70485600
H	1.64931400	2.24821200	2.88304600
C	2.89616500	0.25600600	-0.60017000
C	4.13349400	0.56122300	0.28776300
H	4.08252200	0.01480900	1.23439300
H	4.17326500	1.63025800	0.53475700
C	5.43820100	0.15650600	-0.44070300
H	6.28746000	0.38206600	0.21865300
C	5.40682500	-1.35309700	-0.75127500
H	5.33496700	-1.93106300	0.18124400
H	6.34212400	-1.65532500	-1.24261600
C	4.20184000	-1.65918200	-1.66159900
H	4.16591000	-2.73550900	-1.87805100
C	4.32385900	-0.86773000	-2.97745300
H	3.46907100	-1.08913400	-3.62887600
H	5.23428600	-1.16401300	-3.51757900
C	4.36237200	0.63770900	-2.65560800
H	4.43474600	1.21368200	-3.58762600
C	3.06475700	1.05441800	-1.92652700
H	2.19799600	0.88980100	-2.57355000
H	3.12916100	2.12490600	-1.70370100
C	2.89287900	-1.25962100	-0.94485200
H	2.78229400	-1.86354200	-0.03902700
H	2.04513100	-1.48157400	-1.59596300
C	5.57450800	0.94589900	-1.75603700
H	6.50946800	0.67205000	-2.26466900
H	5.62788200	2.02383500	-1.54740200
P	1.21914100	0.77170300	0.19206700
Pd	-0.89066400	0.43891400	-0.88196200
C	-3.04319300	2.21415200	-0.06687000
O	-1.84929200	2.04352600	0.34119600
N	-3.51820400	1.50093800	-1.07268900
O	-2.79856800	0.56696700	-1.75658400
C	-3.93885700	3.26049300	0.61212100
C	-4.01645200	2.90811700	2.11378800
C	-5.36306000	3.31491500	0.02752700
C	-3.26023500	4.63728500	0.43860700
H	-4.45712100	1.62592200	-1.42613000
H	-4.59755500	3.66759800	2.65024300
H	-3.01590000	2.86123800	2.55144000
H	-4.50094000	1.93663800	2.26734800
H	-5.88934800	2.35925500	0.14263700
H	-5.36185300	3.59281000	-1.03396500
H	-5.94898300	4.07364500	0.55771000
H	-3.21161400	4.92290600	-0.61900800
H	-3.82624200	5.40916600	0.97348200
H	-2.24075100	4.61539300	0.83271500

Int-PivNOH-N

C	-3.81290300	2.74055400	-2.16665300
C	-3.63664200	1.99535800	-0.98557100
C	-4.27030300	2.34626300	0.22176300
C	-5.12683800	3.45327100	0.21144800
C	-5.33907900	4.19046800	-0.95161400
C	-4.68033100	3.83938700	-2.12682800
H	-5.62854500	3.73714100	1.13278800
H	-6.00799800	5.04665500	-0.93811300
H	-4.82557700	4.42818200	-3.02896600
C	-4.02289000	1.58863600	1.50419100
H	-3.00502400	1.76893500	1.87033100
H	-4.72264400	1.91128800	2.28059900
H	-4.13560300	0.50916900	1.36730900

C	-3.08974600	2.40341000	-3.45123500
H	-2.08639700	2.00972500	-3.26419200
H	-3.62980200	1.65045900	-4.04043900
H	-2.99472800	3.29442200	-4.07916200
N	-2.76496900	0.83398700	-1.02238500
C	-3.25114700	-0.41678500	-1.67152600
H	-2.37079600	-1.04173600	-1.83218300
H	-3.65899700	-0.13364900	-2.64563800
C	-4.29232100	-1.15749000	-0.86235200
C	-3.90227700	-2.13341700	0.07189000
C	-5.65597400	-0.89815000	-1.01983400
C	-4.84813000	-2.81154400	0.82958900
H	-2.84733600	-2.37031500	0.18508500
C	-6.62044900	-1.57174700	-0.26412300
H	-5.98279000	-0.15611200	-1.74481000
C	-6.21478700	-2.53238100	0.66957900
H	-4.55586700	-3.57252300	1.54622900
H	-7.66963500	-1.34477700	-0.41496700
C	-1.55502000	0.88278800	-0.47521300
O	-1.00981600	1.83163000	0.11698400
Cl	-0.19384500	-2.26018300	-1.10323500
O	-7.06218200	-3.25277200	1.46057600
C	-8.45589600	-3.02583600	1.33482200
H	-8.81356900	-3.25599300	0.32228900
H	-8.93510200	-3.69971200	2.04747300
H	-8.72133100	-1.98916600	1.58233600
C	2.55926500	-0.98508500	2.41156600
H	3.00566900	-2.00304900	2.37985700
H	3.29454000	-0.35688800	2.95352400
C	1.24221600	-1.02950300	3.19070400
H	1.48168300	-1.20651800	4.26096500
H	0.72432600	-0.04714200	3.17122400
C	0.27001000	-2.12049100	2.70815000
H	0.81765600	-3.05196200	2.47080600
H	-0.22108100	-1.81336700	1.74956800
C	-0.81014300	-2.40562100	3.75006400
H	-1.51679900	-3.15922800	3.38175200
H	-1.39045800	-1.50590100	3.98432800
H	-0.38638700	-2.78268300	4.68665300
C	3.55680400	-1.40584000	-0.33234500
C	3.18719300	-2.88992200	-0.09474800
H	3.30826800	-3.17452800	0.96861100
H	2.12530100	-3.09323400	-0.35428300
C	4.08417500	-3.79812200	-0.96866900
H	3.80650200	-4.86152900	-0.79324800
C	5.56585700	-3.58206500	-0.59366900
H	6.21323800	-4.23911400	-1.19976000
H	5.74079700	-3.86186000	0.45880100
C	5.93537300	-2.10234400	-0.82744300
H	7.00015800	-1.93621100	-0.55059900
C	5.72870000	-1.74796400	-2.31537100
H	6.01826700	-0.70067000	-2.50513200
H	6.38343200	-2.37003800	-2.94994200
C	4.24880500	-1.97309900	-2.69499600
H	4.09694500	-1.71938000	-3.76769300
C	3.34880000	-1.06550800	-1.82441600
H	2.28548200	-1.21589900	-2.12285200
H	3.59200400	-0.00311400	-2.03626900
C	3.86964600	-3.44949200	-2.45648000
H	4.47207700	-4.11239200	-3.09954600
H	2.81252400	-3.61935100	-2.73550500
C	5.03531300	-1.20129100	0.05296500
H	5.34671300	-0.14212800	-0.08098800
H	5.21025500	-1.44847400	1.11617000
C	2.94923300	1.45606300	0.78275500
C	4.33532500	1.63198400	1.42958800
H	5.12102900	1.11374000	0.83728000
H	4.36370600	1.19773400	2.44654700
C	4.69031800	3.13674600	1.50245300
H	5.69415600	3.25341800	1.96804900
C	4.71238300	3.72532100	0.07522200
H	5.48143800	3.22349300	-0.53598500
H	4.99085600	4.79300100	0.10736500
C	3.31978700	3.55804200	-0.57013600
H	3.33398300	3.98050300	-1.59936800
C	2.26522100	4.29973500	0.27795900
H	1.26401800	4.19972000	-0.18252700
H	2.48512200	5.37984900	0.31092600
C	2.24837700	3.70770900	1.70302400
H	1.48279500	4.23593800	2.31440300
C	1.88870400	2.20422700	1.62945300
H	0.86345300	2.11574500	1.18572600
H	1.82127500	1.79964900	2.65583800
C	2.95210300	2.05669200	-0.64089800
H	3.66767700	1.52909600	-1.30594800
H	1.94936200	1.95672100	-1.11644000
C	3.63814100	3.87791100	2.35277000
H	3.89437000	4.94863200	2.43140300

H	3.63041600	3.48553500	3.38376900
P	2.31501500	-0.34430500	0.65726000
Pd	0.14231900	-0.11318300	-0.12382900

CS_2CO_3

C	-0.00008400	1.21676900	0.00037200
O	-1.12419100	1.84768800	-0.00014900
O	1.12409500	1.84781900	-0.00019600
O	0.00000400	-0.11972000	0.00154100
Cs	-2.87890000	-0.32643000	-0.00010900
Cs	2.87892300	-0.32642200	-0.00010600

CsCl

Cl	0.00000000	0.00000000	-2.41778100
Cs	0.00000000	0.00000000	0.74731400

PivNHOH

C	0.51489300	-0.30369100	0.00456000
O	0.90234400	-1.47545300	0.00155900
N	1.44214200	0.69496200	0.11756200
O	2.77926900	0.29465800	-0.04117800
C	-0.96901000	0.08544300	-0.00754400
C	-1.62020800	-0.62632700	-1.21211300
C	-1.19890500	1.60449600	-0.10537300
C	-1.58041900	-0.45193800	1.30633900
H	1.29816500	1.60216500	-0.30492100
H	2.66486200	-0.68544900	-0.07960800
H	-2.70296400	-0.45657100	-1.20720200
H	-1.43162600	-1.70204400	-1.16911500
H	-1.22255800	-0.24831200	-2.16154400
H	-0.80859900	2.01987700	-1.04371200
H	-0.74411300	2.14188200	0.73467500
H	-2.27338300	1.81572900	-0.08592100
H	-1.14366300	0.04731900	2.17884200
H	-2.66203800	-0.27458200	1.31695700
H	-1.40008900	-1.52628500	1.40035800

PivNHOCs

C	-1.33465900	0.11404600	-0.00038800
O	-0.51621100	-0.85035100	-0.00075100
N	-0.95881500	1.39472500	-0.00012700
O	0.30572800	1.84310600	-0.00026900
C	-2.84983400	-0.19736500	0.00006500
C	-3.14126500	-1.04492300	-1.25744000
C	-3.77135500	1.03633500	0.00052900
C	-3.14036000	-1.04514000	1.25764200
H	-1.67568600	2.11412100	0.00016000
H	-4.17812200	-1.40595300	-1.25596000
H	-2.46620200	-1.90441100	-1.29165800
H	-2.98849100	-0.45565200	-2.17060800
H	-3.62184500	1.65955700	-0.88998000
H	-3.62136900	1.65925500	0.89117100
H	-4.82083600	0.71653200	0.00075800
H	-2.98702700	-0.45598700	2.17079300
H	-4.17718800	-1.40625200	1.25678800
H	-2.46521000	-1.90458300	1.29128000
Cs	2.30586200	-0.17271700	0.00007000

Int-PivNHO-O[1]

N	0.82923500	1.54142200	-2.48215700
O	0.65236400	-0.67274300	-2.93238700
C	0.79700700	0.20927600	-2.08922000
C	2.40172100	3.07386100	-1.38512200
C	2.61923300	4.19948600	-0.54341900
H	3.64437100	4.49752700	-0.33774400
C	1.57986700	4.92144400	-0.01029000
H	1.77499900	5.78223600	0.62501700
C	0.23788400	4.58372100	-0.32011700
C	-0.85683500	5.37284400	0.12549900
H	-0.65259300	6.23397000	0.75778400
C	-2.14662200	5.07573900	-0.25490800
H	-2.97348500	5.69769300	0.07702000
C	-2.39300200	3.96109800	-1.09182500
H	-3.41018800	3.73603300	-1.40195200
C	-1.35562600	3.15559100	-1.51126300
H	-1.55162900	2.29623600	-2.14105700
C	-0.01171600	3.43583200	-1.14205300
C	1.09532100	2.65833100	-1.61792100
C	0.72445200	1.84696700	-3.91670300
H	0.26194600	0.99487200	-4.41488200
H	0.11295800	2.74383400	-4.05483300
H	1.71054600	2.02057300	-4.36564100
C	3.58542100	2.41470300	-2.04996900
H	4.52052300	2.82610400	-1.65611900
H	3.59371000	1.33504200	-1.89242900
H	3.57873200	2.60331900	-3.13144800
C	-0.53743600	-2.68175300	1.36783700
H	-0.08298800	-2.30914900	2.29035200

H	-1.46000600	-3.20430900	1.64807100
C	0.46687300	-3.66376800	0.73336900
H	-0.03223100	-4.31783400	0.01018700
H	1.23174400	-3.10794800	0.18154200
C	1.15052500	-4.53159400	1.80017100
H	0.39004600	-5.06310100	2.39115000
H	1.67895600	-3.86753300	2.49676900
C	2.13260500	-5.54469700	1.20254000
H	2.61881600	-6.14129000	1.98349700
H	2.91884600	-5.03833500	0.62863500
H	1.62447300	-6.23895100	0.52191300
C	-1.71796400	-0.03043200	1.87950600
C	-0.52288200	0.65989800	2.59891600
H	0.18881100	-0.08285700	2.97417400
H	0.03186300	1.26820600	1.87461400
C	-1.02098600	1.55458600	3.75511000
H	-0.14883500	2.01219800	4.24081600
C	-1.80017100	0.70512200	4.77729500
H	-2.14250000	1.33263200	5.61221500
H	-1.14696800	-0.06870500	5.20412100
C	-3.00716100	0.05153700	4.07689000
H	-3.56278600	-0.56674700	4.79517200
C	-3.93116000	1.14528400	3.50756100
H	-4.80656500	0.68801800	3.02442900
H	-4.31054400	1.78055500	4.32002400
C	-3.14225900	1.99241900	2.49117300
H	-3.79387200	2.76688200	2.06490800
C	-2.64917500	1.08437300	1.34124600
H	-2.12125800	1.68999500	0.59850000
H	-3.52442400	0.65010900	0.84551700
C	-1.94112300	2.65375300	3.19141300
H	-2.29102500	3.31076200	4.00050900
H	-1.39109600	3.28363300	2.48038500
C	-2.50634000	-0.86142700	2.93222600
H	-3.36297900	-1.36570100	2.47075400
H	-1.86965800	-1.64127900	3.36222700
C	-2.29073000	-1.58668300	-0.84645800
C	-3.60924300	-2.11998800	-0.22379300
H	-4.08485000	-1.35378500	0.39776100
H	-3.40536200	-2.98085000	0.42626000
C	-4.59950700	-2.53997200	-1.33798500
H	-5.51917000	-2.90971900	-0.86439600
C	-4.92363600	-1.32059200	-2.22328200
H	-5.38978500	-0.52789600	-1.62064500
H	-5.65034200	-1.60113500	-2.99833100
C	-3.62509900	-0.80300100	-2.87129800
H	-3.84679900	0.07505900	-3.49317700
C	-2.99373600	-1.90883100	-3.73794500
H	-2.07246100	-1.53939100	-4.20581100
H	-3.68007400	-2.19864600	-4.54613200
C	-2.67781200	-3.12356300	-2.84616600
H	-2.21314500	-3.91464700	-3.44930300
C	-1.68665800	-2.71619800	-1.73223800
H	-0.74029600	-2.38343200	-2.17072300
H	-1.48412300	-3.59828700	-1.11773700
C	-2.62559500	-0.38461700	-1.77020100
H	-3.05214100	0.44183500	-1.19480300
H	-1.70757600	-0.02203600	-2.23776900
C	-3.97649900	-3.65033300	-2.20596900
H	-4.68754100	-3.96241100	-2.98381700
H	-3.76492900	-4.53753700	-1.59250300
P	-0.96791600	-1.09830900	0.45251100
Pd	1.19318100	-0.35421000	-0.19542300
C	3.96410800	-0.83471200	0.46215800
O	3.34124800	-0.32277600	-0.52760300
N	3.30984300	-1.21632400	1.54417600
O	1.96810000	-1.06941000	1.70571300
C	5.48406500	-1.03063900	0.38067300
C	5.77568900	-1.88573300	-0.87261800
C	6.07073900	-1.72897500	1.62288200
C	6.13803600	0.35969400	0.22385300
H	3.78589600	-1.61298500	2.34342400
H	6.85803300	-1.98779300	-1.01582300
H	5.34456100	-1.42335300	-1.76407400
H	5.34875500	-2.89066400	-0.77213600
H	5.64128300	-2.72689600	1.77435100
H	5.92453500	-1.13768800	2.53571200
H	7.15084100	-1.85718600	1.49308300
H	5.94212300	0.98954100	1.09984100
H	7.22413100	0.25404200	0.11623600
H	5.75046100	0.87290900	-0.65911700

TS-PivNHO-O[2]

N	-2.50245200	-0.62293600	-2.30128200
O	-0.57315300	-1.34391700	-3.24499300
C	-1.12061300	-0.67105500	-2.38629000
C	-2.77184900	1.65843200	-1.51202500
C	-3.44214500	2.58439500	-0.65959900

H	-3.14638300	3.62990400	-0.70565100
C	-4.46390900	2.20003500	0.17177900
H	-4.97491000	2.93469100	0.78994700
C	-4.87673800	0.84247600	0.23804800
C	-5.92330200	0.41666900	1.09713400
H	-6.43113800	1.16288200	1.70427300
C	-6.28985100	-0.90932300	1.17131200
H	-7.09326300	-1.22101300	1.83298300
C	-5.60616900	-1.86970400	0.38883600
H	-5.88263300	-2.91844900	0.46154100
C	-4.58956600	-1.48902300	-0.46174800
H	-4.06135000	-2.23959900	-1.03985200
C	-4.20117600	-0.12390900	-0.57935600
C	-3.16888000	0.32159900	-1.46161800
C	-3.24339100	-1.26078800	-3.40236100
H	-2.93048000	-2.30242800	-3.50732500
H	-4.31035600	-1.21496700	-3.18399300
H	-3.04565700	-0.74867800	-4.35196900
C	-1.69790000	2.13029100	-2.44180500
H	-1.76459300	1.64798800	-3.42095100
H	-1.82851400	3.21028700	-2.59431800
H	-0.35972100	2.37671100	-2.29290000
C	1.24814500	-2.68998200	-1.10659700
H	1.66132100	-3.47624300	-0.46110500
H	0.22522100	-2.98254100	-1.35547700
C	2.04227200	-2.61232300	-2.42411100
H	1.74355000	-1.72066100	-2.98040200
H	3.11728000	-2.53544900	-2.22391600
C	1.79097100	-3.84643600	-3.30380600
H	0.72265700	-3.88579800	-3.55129600
H	2.01934400	-4.76089900	-2.73602100
C	2.61445000	-3.82560200	-4.59573800
H	2.40805100	-4.70664800	-5.21444400
H	3.69114400	-3.81299500	-4.38352200
H	2.38247500	-2.93578200	-5.19291600
C	2.84972800	-0.56633500	0.31056200
C	3.35025300	0.25750600	-0.91550900
H	3.31928500	-0.34883200	-1.82601100
H	2.68695800	1.11229600	-1.08591100
C	4.79530500	0.75104400	-0.68326400
H	5.11645700	1.31407500	-1.56928400
C	5.73078600	-0.45457900	-0.46295900
H	6.76520300	-0.11240800	-0.31889800
H	5.72991200	-1.10264200	-1.35048100
C	5.26051300	-1.24573000	0.77297800
H	5.91698400	-2.11239300	0.93001900
C	5.29829200	-0.33319800	2.01312800
H	4.98960800	-0.89423800	2.90672500
H	6.32429000	0.01636100	2.19418100
C	4.35718200	0.86558200	1.78484500
H	4.36096600	1.51359300	2.67205800
C	2.91514600	0.35386500	1.56043200
H	2.23058700	1.19636400	1.43384800
H	2.60302200	-0.19645700	2.45523400
C	4.82981600	1.66453100	0.55563000
H	5.84716000	2.04641100	0.72124200
H	4.17938000	2.53475700	0.39689300
C	3.81902500	-1.76056300	0.54438900
H	3.50415500	-2.34812500	1.41396200
H	3.82068300	-2.44005600	-0.31304800
C	0.11812100	-1.72666900	1.47036100
C	0.93570800	-2.66658600	2.39574000
H	1.83504200	-2.16242300	2.76356700
H	1.26866800	-3.55523400	1.84296000
C	0.08165300	-3.10278900	3.61016700
H	0.68942900	-3.76089900	4.24577800
C	-0.34440100	-1.85460600	4.40923900
H	0.54335700	-1.31932600	4.77494600
H	-0.92311800	-2.15386400	5.29403600
C	-1.18926100	-0.93268200	3.50734500
H	-1.48747100	-0.03779600	4.06974700
C	-2.44237000	-1.68656200	3.02560700
H	-3.06344700	-1.03297900	2.40068100
H	-3.05783600	-1.99130100	3.88364200
C	-2.00486600	-2.92702300	2.22434000
H	-2.89142200	-3.45873600	1.85543700
C	-1.15297700	-2.49793300	1.00799700
H	-1.75170400	-1.86931300	0.33955800
H	-0.87046000	-3.39627700	0.44675400
C	-0.35415300	-0.49058600	2.28643800
H	0.50092700	0.10030800	2.62573200
H	-0.94845000	0.16643100	1.64080300
C	-1.17090700	-3.85765700	3.12505500
H	-1.76826700	-4.18950700	3.98563500
H	-0.87825800	-4.76159200	2.57224200
P	1.05420900	-1.12903200	-0.09236600
Pd	-0.17969400	0.60208700	-1.14553100
C	0.59091700	3.43356700	-0.00252000

O	0.57160700	2.21301600	0.31631900
N	0.72701500	3.82978200	-1.26715700
O	0.81402800	2.95805600	-2.30726100
C	0.49474000	4.50771500	1.09830900
C	-0.72609400	4.16603200	1.97848200
C	0.34466800	5.94017800	0.55019000
C	1.78170700	4.42360500	1.94988700
H	0.70463300	4.80938100	-1.51908800
H	-0.78847900	4.86210700	2.82338800
H	-0.64623300	3.14731600	2.36487000
H	-1.65974100	4.23553300	1.40871200
H	-0.54991200	6.04888500	-0.07505500
H	1.22096500	6.25791000	-0.02879300
H	0.24490200	6.64152100	1.38585900
H	2.67011800	4.65349700	1.34976700
H	1.73417800	5.14364700	2.77544900
H	1.90359200	3.42274500	2.37308100

TS-PivNHO-O[1]

N	1.95474400	-1.20817800	-2.21337300
O	0.25452100	0.12028200	-2.90840400
C	0.73343800	-0.57495500	-2.02210600
C	1.59108700	-3.07720900	-0.71992600
C	2.08057200	-3.96063800	0.28441200
H	1.39458000	-4.69231900	0.70360200
C	3.38815000	-3.92936900	0.69887600
H	3.74424800	-4.63343500	1.44741600
C	4.29897000	-2.98335400	0.15899500
C	5.65458000	-2.93082200	0.57702800
H	5.99788300	-3.65896800	1.30868800
C	6.51850700	-1.97989500	0.08140700
H	7.55354800	-1.95176200	0.41081400
C	6.04704600	-1.02675700	-0.85168100
H	6.72155000	-0.26176200	-1.22784200
C	4.73906600	-1.05645700	-1.28747200
H	4.39601200	-0.30622200	-1.99084300
C	3.82539500	-2.04268600	-0.81684300
C	2.46696900	-2.13139000	-1.25475100
C	2.52016800	-1.13500300	-3.56939500
H	2.79923700	-0.10726500	-3.82286200
H	3.40028300	-1.77604600	-3.62183300
H	1.77838900	-1.46899000	-4.30294700
C	0.18062700	-3.19809500	-1.20686900
H	0.12355000	-3.12770100	-2.29705900
H	-0.18900900	-4.18847900	-0.91379400
H	-1.17697800	-2.85693600	-0.83492500
C	-0.67270100	0.95765000	2.36386200
H	-0.88973800	1.93104600	2.82048000
H	-1.57882400	0.35147500	2.41257800
C	0.40501800	0.20565800	3.16396900
H	0.72148500	-0.68199800	2.60395500
H	1.29463800	0.83240800	3.30346800
C	-0.11315900	-0.23673500	4.54063300
H	-0.97266400	-0.90363000	4.39070000
H	-0.48548300	0.63734100	5.09489100
C	0.95327900	-0.95639900	5.37304500
H	0.55521400	-1.27444400	6.34366600
H	1.81574900	-0.30561600	5.56416100
H	1.32038900	-1.84924300	4.85281600
C	1.15561300	2.30358200	0.37936900
C	2.42317400	1.41057600	0.51480900
H	2.42033700	0.87694100	1.47047900
H	2.42244700	0.64828000	-0.26891900
C	3.70851300	2.26069300	0.40761200
H	4.57274700	1.59352500	0.51442900
C	3.72427400	3.32776400	1.51943400
H	4.64376900	3.92657400	1.45894900
H	3.72141500	2.84637600	2.50744400
C	2.48961400	4.23655900	1.36797000
H	2.48548100	4.99330600	2.16419400
C	2.52506900	4.92902800	-0.00836100
H	1.66023800	5.59842400	-0.11915400
H	3.42525100	5.55343300	-0.09285700
C	2.51357500	3.85710400	-1.11619200
H	2.52385800	4.34247000	-2.10125700
C	1.22324100	3.01422200	-1.00009700
H	1.17756200	2.27821200	-1.81060100
H	0.36524700	3.68301100	-1.12501000
C	3.74940500	2.95105400	-0.96835800
H	4.66912300	3.54405900	-1.07163700
H	3.76145300	2.19799700	-1.76810000
C	1.20356900	3.38564100	1.49475300
H	0.32853400	4.04190400	1.43937300
H	1.18739200	2.91597400	2.48456700
C	-1.97841000	2.02749800	-0.08235300
C	-2.16646300	3.47067500	0.45562900
H	-1.34638600	4.11539900	0.12248300
H	-2.15659100	3.47854400	1.55387600

C	-3.49972700	4.06893800	-0.05371500	O	-0.40520300	-0.84498800	-2.90003900
H	-3.59836000	5.08947300	0.34036300	C	-1.02296400	-0.12094200	-2.12917600
C	-3.48962600	4.10337200	-1.59514400	C	-2.58302000	2.18062900	-1.18279200
H	-2.66223600	4.73155100	-1.95357500	C	-3.31443200	3.08628900	-0.36455100
H	-4.41890900	4.55680300	-1.96729300	H	-2.87165500	4.05585300	-0.14781800
C	-3.34034400	2.66819800	-2.13850200	C	-4.56279800	2.77888000	0.11721000
H	-3.32012000	2.68843500	-3.23581500	H	-5.11667000	3.49977400	0.71443400
C	-4.52459800	1.81072700	-1.65693100	C	-5.14512600	1.51006200	-0.13930200
H	-4.43831500	0.79194500	-2.05876400	C	-6.41305700	1.15387900	0.39111000
H	-5.47368400	2.22429600	-2.02589200	H	-6.95962700	1.89914300	0.96517500
C	-4.52297900	1.77765400	-0.11773900	C	-6.93745300	-0.10556300	0.20596500
H	-5.35054400	1.15025400	0.24281100	H	-7.90692700	-0.36494500	0.62258200
C	-3.19375600	1.17695900	0.39220100	C	-6.19559000	-1.07100700	-0.51487100
H	-3.08514400	0.14751900	0.03152300	H	-6.59270400	-2.07578400	-0.63497500
H	-3.23110300	1.13656300	1.48695700	C	-4.97201400	-0.75200100	-1.06382800
C	-2.01429800	2.05504600	-1.63701900	H	-4.41525200	-1.51384700	-1.59675800
H	-1.18130000	2.63937900	-2.03490000	C	-4.41264200	0.55117900	-0.92019800
H	-1.88320400	1.04382700	-2.03359700	C	-3.15399900	0.93855000	-1.47631800
C	-4.68018100	3.20768800	0.43354500	C	-2.98474100	-0.57576800	-3.47867300
H	-5.63075100	3.64290400	0.09544800	H	-2.98961800	-1.66888900	-3.41135800
H	-4.70939000	3.19040300	1.53234400	H	-4.00613200	-0.21502200	-3.60050400
P	-0.37759200	1.15191500	0.52725800	H	-2.38867800	-0.30172900	-4.35507000
Pd	-0.26803000	-1.07028200	-0.34108400	C	-1.21777500	2.49393200	-1.66786400
C	-3.14747600	-2.87638800	0.15425200	H	-1.12856400	2.42123100	-2.75708400
O	-2.41521900	-3.18106300	-0.85161400	H	-0.88006100	3.48162200	-1.33908200
N	-2.66902200	-2.24535000	1.20908900	C	1.42855700	-0.26855000	2.23792900
O	-1.39156700	-1.85548400	1.39512500	H	1.96239600	-1.03793800	2.80951400
C	-4.62748700	-3.27393600	0.10644300	H	2.12832100	0.55561700	2.07276100
C	-5.24980200	-2.63526500	-1.15514400	C	0.25249200	0.28676700	3.05716100
C	-5.42177500	-2.83311000	1.35064900	H	-0.30721400	1.00434900	2.44406200
C	-4.68339100	-4.81458700	-0.01459800	H	-0.44936200	-0.51249500	3.32320500
H	-3.28877000	-2.02560800	1.97981500	C	0.71954900	0.97329800	4.35002200
H	-6.28703500	-2.97015100	-1.27194300	H	1.41260500	1.78806700	4.09637800
H	-4.68766200	-2.91822200	-2.04860200	H	1.29766100	0.25930300	4.95438800
H	-5.25238900	-1.54103800	-1.08580100	C	-0.44015700	1.52795700	5.18399100
H	-5.42755200	-1.74284200	1.47295300	H	-0.07972300	2.01370300	6.09819000
H	-5.03725800	-3.29148100	2.27052700	H	-1.13150400	0.72975900	5.48114700
H	-6.46468200	-3.15116000	1.24663600	H	-1.01730200	2.26820600	4.61623000
H	-4.25538600	-5.29576800	0.87286400	C	-0.02434600	-2.47780900	0.80098200
H	-5.72362100	-5.14593800	-0.11330700	C	-1.50832600	-2.02556500	0.95269800
H	-4.12366700	-5.15337000	-0.89018100	H	-1.62020900	-1.33578800	1.79632800
				H	-1.82032800	-1.47501100	0.05982200
Int-PivNHOH				C	-2.43745400	-3.24185700	1.16504900
N	-2.39913900	0.03698000	-2.27715800	H	-3.46694400	-2.87697700	1.27428000

C	-2.01182800	-4.00632100	2.43351800
H	-2.67713400	-4.86506500	2.60020400
H	-2.10161900	-3.35731100	3.31597600
C	-0.55665500	-4.48861300	2.27350200
H	-0.24249800	-5.02700000	3.17816700
C	-0.45691400	-5.42206400	1.05143500
H	0.57247100	-5.79080800	0.93882700
H	-1.09746700	-6.30305800	1.19697000
C	-0.88746300	-4.65342500	-0.21315300
H	-0.80456700	-5.30865000	-1.09069500
C	0.04641200	-3.43849700	-0.41793600
H	-0.22282100	-2.90498400	-1.33665400
H	1.06822300	-3.81030600	-0.54762200
C	-2.34262100	-4.17612000	-0.05538800
H	-3.01311700	-5.03794100	0.07146100
H	-2.66692100	-3.64717600	-0.96208800
C	0.37497900	-3.26836500	2.07604200
H	1.41415900	-3.61077000	2.00944800
H	0.30842800	-2.62650700	2.96236800
C	2.76432800	-1.31310800	-0.19248100
C	3.50299200	-2.48163600	0.51034100
H	2.92629600	-3.40921600	0.42769800
H	3.62202900	-2.27197700	1.58211000
C	4.89497400	-2.70499400	-0.12925700
H	5.38734100	-3.54208000	0.38445500
C	4.72592100	-3.03879500	-1.62526400
H	4.13370000	-3.95732000	-1.74267600
H	5.70773600	-3.23188000	-2.07993800
C	4.02743200	-1.86319900	-2.33842600
H	3.89400100	-2.10295800	-3.40155400
C	4.88021600	-0.58950400	-2.19523400
H	4.39598800	0.24919100	-2.71282300
H	5.86603300	-0.73309100	-2.66014800
C	5.04112300	-0.26369600	-0.69941400
H	5.63121100	0.65542100	-0.58038800
C	3.65279500	-0.03907800	-0.05928300
H	3.15978800	0.81404200	-0.53771200
H	3.79931700	0.21705100	0.99641300
C	2.63632500	-1.63041700	-1.71010100
H	2.02331700	-2.52034700	-1.86942600
H	2.11538200	-0.81438900	-2.22093000
C	5.74906600	-1.43102100	0.01527500
H	6.74589500	-1.59419700	-0.41794000
H	5.89731600	-1.19168800	1.07798600
P	1.02585700	-0.88911600	0.51375100
Pd	-0.07088500	0.97359900	-0.73847800
C	1.64677000	3.60889100	0.07289500
O	1.15983200	2.55087900	0.51333400
N	2.07091000	3.73362600	-1.19532000
O	2.16077300	2.67215900	-2.08439600
C	1.76282300	4.85380200	0.97483200
C	0.34740000	5.17631900	1.49979700
C	2.34325400	6.09026600	0.26148200
C	2.68126700	4.46474500	2.15512200
H	2.46337200	4.57724700	-1.58105500
H	0.39584400	5.99737000	2.22415600
H	-0.09139800	4.30262200	1.98780300
H	-0.31808900	5.48237800	0.68397600
H	1.71748400	6.41499100	-0.57915300
H	3.36564600	5.91987000	-0.09905400
H	2.39033700	6.92675400	0.96665400
H	3.69494200	4.22860800	1.81030700
H	2.74862400	5.29784900	2.86382600
H	2.28531300	3.59174600	2.68030000
H	1.31636400	2.15277200	-1.96228900

Int-PivHNHO

N	2.04694000	-1.21328800	-2.13624700
O	0.31479600	0.06770100	-2.83413800
C	0.80320200	-0.61189300	-1.93755000
C	1.78495700	-2.99800500	-0.52923200
C	2.34891000	-3.86661900	0.44689600
H	1.69096500	-4.57560800	0.94482500
C	3.69017200	-3.85377300	0.73991300
H	4.10360500	-4.54920500	1.46694700
C	4.55743900	-2.92062300	0.11401000
C	5.93844300	-2.85682700	0.43757300
H	6.33557600	-3.57893600	1.14795500
C	6.75850900	-1.89755700	-0.11279100
H	7.81247800	-1.85832400	0.14885800
C	6.21540800	-0.94570400	-1.00778200
H	6.85300000	-0.16661600	-1.41795400
C	4.88397700	-0.99312400	-1.36190200
H	4.48733200	-0.24252700	-2.03545700
C	4.01268200	-1.99227400	-0.83835100
C	2.62801200	-2.09239400	-1.18157300
C	2.59707800	-1.10732900	-3.49510300
H	2.91079600	-0.08331500	-3.72428500

H	3.45146300	-1.77798600	-3.58792600
H	1.82749500	-1.38540100	-4.22259000
C	0.32998000	-2.98497300	-0.81195800
H	0.09832100	-3.14046800	-1.87081900
H	-0.21260200	-3.71856700	-0.20624700
H	-2.10603400	-1.82969400	-0.90376400
C	-0.96216900	1.22503300	2.38373000
H	-1.22956300	2.21418700	2.77638300
H	-1.85947400	0.60197800	2.42520900
C	0.08929300	0.55850300	3.28713300
H	0.43227400	-0.37448200	2.82291700
H	0.97188600	1.20030300	3.39753700
C	-0.47115900	0.24681500	4.68341800
H	-1.32948000	-0.43110200	4.57714200
H	-0.86166200	1.16965300	5.13671600
C	0.56841000	-0.38108500	5.61802300
H	0.13943700	-0.60541300	6.60169800
H	1.42068300	0.29214800	5.77267500
H	0.95991800	-1.31743800	5.20164100
C	0.93786800	2.50093600	0.41961100
C	2.20969400	1.62859800	0.64550000
H	2.17959700	1.15059400	1.63037700
H	2.24008500	0.82096000	-0.09230400
C	3.49163300	2.48132700	0.53117500
H	4.35865000	1.83074300	0.70378800
C	3.46183800	3.60824200	1.58137500
H	4.37847000	4.21153500	1.51895100
H	3.42927700	3.18184700	2.59397200
C	2.22584000	4.49739900	1.33922100
H	2.19224500	5.29926000	2.08946400
C	2.30502600	5.10951300	-0.07330000
H	1.44056900	5.76470800	-0.25149400
H	3.20413700	5.73500500	-0.16342100
C	2.33622600	3.97729000	-1.11888800
H	2.37616600	4.40732200	-2.12875400
C	1.04919200	3.13049600	-0.99635800
H	1.03656800	2.34653300	-1.76215900
H	0.19033200	3.78254200	-1.18908300
C	3.57280300	3.09110400	-0.88071000
H	4.49198300	3.68429200	-0.98871300
H	3.61514100	2.29151900	-1.63277100
C	0.93957700	3.64590500	1.46787500
H	0.06326800	4.29067700	1.33659600
H	0.88361100	3.23783100	2.48374800
C	-2.16394000	2.12297100	-0.16738800
C	-2.41756200	3.59510500	0.24794200
H	-1.59802900	4.23873200	-0.08996100
H	-2.46478900	3.68321400	1.34175900
C	-3.73925200	4.11286600	-0.37093100
H	-3.88566800	5.15711100	-0.06257200
C	-3.65516000	4.03079200	-1.90845300
H	-2.82924300	4.65543600	-2.27656300
H	-4.57797800	4.42552200	-2.35652200
C	-3.43847400	2.56354600	-2.33192900
H	-3.36394500	2.50170500	-3.42558500
C	-4.61859000	1.70487200	-1.84202500
H	-4.48005400	0.66089100	-2.15492400
H	-5.56000900	2.05340300	-2.29031900
C	-4.69644000	1.79190600	-0.30725800
H	-5.52392300	1.16894200	0.05984700
C	-3.38103300	1.27947700	0.31942200
H	-3.23002300	0.22213400	0.07333900
H	-3.47493300	1.34086300	1.40934300
C	-2.12354600	2.03590300	-1.71948600
H	-1.28794200	2.61729300	-2.11709200
H	-1.94028300	1.00353000	-2.03403000
C	-4.92153000	3.25581200	0.11985400
H	-5.86302100	3.63517600	-0.30150000
H	-5.01091200	3.32191700	1.21349200
P	-0.57154700	1.31760300	0.55262200
Pd	-0.21964900	-1.02524200	-0.25090700
C	-3.04270800	-3.12733100	0.15455800
O	-2.91040300	-2.43543600	-0.96431600
N	-2.41952000	-2.75235100	1.24017000
O	-1.66974600	-1.66761200	1.38195200
C	-3.95007800	-4.34204500	0.09672100
C	-5.35176700	-3.86610800	-0.35666200
C	-4.06600600	-5.04422800	1.46277200
C	-3.37306900	-5.32761700	-0.94727700
H	-2.52068400	-3.32117200	2.07730900
H	-6.01804200	-4.73020600	-0.45543300
H	-5.30101700	-3.35604900	-1.32211700
H	-5.79161200	-3.17727800	0.37350600
H	-4.48362500	-4.38378000	2.23266100
H	-3.10165000	-5.43439800	1.81131300
H	-4.74255700	-5.89935800	1.36963000
H	-2.38352400	-5.68925600	-0.64622200
H	-4.03868800	-6.19244800	-1.04477000

H	-3.27854400	-4.85056500	-1.92619300

Int-red1

N	2.37763700	-1.36701600	-1.76801200
O	0.22676500	-1.39550600	-2.50172300
C	1.00978100	-1.43103600	-1.56717800
C	3.05925700	-2.38548500	0.31081200
C	3.98681900	-2.49233600	1.38452100
H	3.78267700	-3.21535400	2.17075000
C	5.13226400	-1.73652200	1.42452500
H	5.84399600	-1.85766400	2.23791600
C	5.39694400	-0.76712500	0.42159000
C	6.54506100	0.06597000	0.47914400
H	7.25614500	-0.09114300	1.28732400
C	6.75153500	1.06406100	-0.44658900
H	7.63235300	1.69738000	-0.38592300
C	5.79542900	1.27730300	-1.46721600
H	5.93655800	2.08912800	-2.17618600
C	4.68237600	0.47075900	-1.56831800
H	3.95398000	0.67079300	-2.34544000
C	4.45510600	-0.59619600	-0.65081400
C	3.32664500	-1.47054100	-0.71080200
C	2.80448600	-1.42359800	-3.17619900
H	2.53549500	-0.50839900	-3.71325800
H	3.88417000	-1.56448300	-3.21352900
H	2.30419300	-2.26113700	-3.67257500
C	1.78914900	-3.14455800	0.28855800
H	1.66700600	-3.77331200	-0.59935100
H	1.63852100	-3.75052800	1.19050400
C	-1.75603200	0.33530600	2.44322000
H	-2.50888600	1.11868800	2.59241400
H	-2.21914100	-0.60220500	2.76830600
C	-0.53784900	0.59012600	3.34762900
H	0.25952400	-0.12683500	3.10532700
H	-0.12041400	1.58600100	3.15692800
C	-0.88766800	0.47945100	4.83978900
H	-1.28499100	-0.52499800	5.04420700
H	-1.69916800	1.18254600	5.07609700
C	0.30998300	0.75224900	5.75591300
H	0.03310100	0.65793500	6.81204500
H	0.70396900	1.76465200	5.60384900
H	1.12686000	0.04691800	5.56022500
C	-0.89058500	1.84549300	-0.01111500
C	0.64159300	1.97859300	0.24073900
H	0.86700300	1.87050300	1.30727600
H	1.17380300	1.16893800	-0.27036200
C	1.16423800	3.34383300	-0.25665300
H	2.24111000	3.40084800	-0.05168600
C	0.42978500	4.48132500	0.47945000
H	0.80760100	5.45703500	0.14356700
H	0.62214200	4.42057700	1.55989400
C	-1.08263900	4.37544900	0.20199600
H	-1.61421800	5.17832900	0.73052400
C	-1.33513200	4.49393200	-1.31392200
H	-2.41277900	4.44264600	-1.52437600
H	-0.98558300	5.46938900	-1.67960500
C	-0.59640500	3.35506700	-2.04399900
H	-0.78561100	3.42336300	-3.12356800
C	-1.12879700	1.99526600	-1.53803500
H	-0.64636300	1.17333500	-2.08073000
H	-2.20051000	1.94405900	-1.75833900
C	0.91535200	3.46318400	-1.77222200
H	1.30073000	4.42139800	-2.14785200
H	1.45360800	2.66804300	-2.30580200
C	-1.60878100	3.01346500	0.71537800
H	-2.69247600	2.95721300	0.55805300
H	-1.44059200	2.95579100	1.79742900
C	-3.11417300	-0.44931600	-0.06812600
C	-4.25040900	0.59335400	0.08104800
H	-4.00584700	1.50752700	-0.47246700
H	-4.37427600	0.88031800	1.13416400
C	-5.58202500	0.01935500	-0.45890400
H	-6.36624600	0.77991200	-0.34438600
C	-5.41942000	-0.34159900	-1.94967400
H	-5.16176800	0.55577100	-2.52959900
H	-6.37065400	-0.71778400	-2.35119700
C	-4.31519700	-1.40745000	-2.10356000
H	-4.18661900	-1.65568200	-3.16517300
C	-4.70478200	-2.67153900	-1.31742300
H	-3.93433700	-3.44469700	-1.44036000
H	-5.64527400	-3.08969500	-1.70285400
C	-4.85733400	-2.30550800	0.16994300
H	-5.11416600	-3.20170300	0.75067100
C	-3.52719000	-1.73551400	0.71052400
H	-2.73177400	-2.48969700	0.62563800
H	-3.65947400	-1.52117700	1.77704600
C	-2.97920000	-0.84953700	-1.56613600
H	-2.69224500	0.01225900	-2.17281600

H	-2.17631500	-1.58462900	-1.68624300
C	-5.96450500	-1.24494700	0.33473300
H	-6.92390100	-1.64110800	-0.02546800
H	-6.09951000	-0.99942700	1.39769400
P	-1.40436200	0.09852300	0.61149300
Pd	0.29761600	-1.67106000	0.30245700

TS-$CsCO_3$

N	1.28953600	-1.99534500	-2.24866500
O	1.21223200	0.16824900	-2.90705200
C	0.89410900	-0.67293800	-2.07009000
C	-0.56049700	-3.14523900	-1.15856400
C	-1.01351800	-4.19272900	-0.30386400
H	-2.08042100	-4.26402100	-0.10461800
C	-0.15291900	-5.10997200	0.24265900
H	-0.53019000	-5.91230000	0.87308000
C	1.24429700	-5.02686300	0.00137200
C	2.15792600	-5.95435900	0.56619300
H	1.76283800	-6.76084800	1.18047600
C	3.51432900	-5.83900200	0.35552800
H	4.20234400	-6.55572200	0.79582200
C	4.01094000	-4.77087700	-0.42761100
H	5.08249700	-4.66605500	-0.57826500
C	3.14914700	-3.85783100	-0.99859800
H	3.54887900	-3.03518900	-1.58114700
C	1.74010700	-3.96044900	-0.82038600
C	0.80839800	-3.04756000	-1.41024200
C	1.91464800	-2.32452700	-3.53841400
H	2.80651700	-1.71177200	-3.69641400
H	2.18740300	-3.38019000	-3.54265700
H	1.22198600	-2.12533200	-4.36546900
C	-1.54958800	-2.18264800	-1.73012900
H	-1.24923900	-1.78328000	-2.70153500
H	-2.49913800	-2.71197700	-1.89747900
H	-2.29358200	-1.35284400	-0.97931700
C	0.36007000	1.34928900	2.28912700
H	0.82171500	2.20124900	2.80347800
H	-0.71505600	1.52154800	2.21752400
C	0.54028700	0.05220000	3.09674200
H	0.25563600	-0.80253300	2.47323900
H	1.58935800	-0.08957600	3.38878300
C	-0.34225300	0.05628300	4.35399000
H	-1.38857000	0.13977800	4.03470700
H	-0.12037200	0.94867000	4.95827900
C	-0.16042800	-1.19993400	5.21250500
H	-0.81341000	-1.17995800	6.09328500
H	0.87378500	-1.29769600	5.56743400
H	-0.40052800	-2.10413900	4.63973100
C	2.81268100	1.14290400	0.54069600
C	3.12505200	-0.37488000	0.68293900
H	2.67198900	-0.77557900	1.59577600
H	2.68080000	-0.92323100	-0.15182300
C	4.64909400	-0.62172400	0.71610100
H	4.82159500	-1.70079400	0.81769800
C	5.27090800	0.12514000	1.91165200
H	6.35421100	-0.05649800	1.95305400
H	4.84782800	-0.24940600	2.85415100
C	4.99280800	1.63363500	1.76631100
H	5.42004500	2.17417100	2.62209900
C	5.62426600	2.14805000	0.45815500
H	5.45496600	3.22932200	0.35438800
H	6.71260300	1.99604100	0.47931500
C	5.00275000	1.39656900	-0.73502000
H	5.43679300	1.76726100	-1.67341300
C	3.47880100	1.65148500	-0.76609200
H	3.03022400	1.16193400	-1.63633800
H	3.31280500	2.72840600	-0.88022900
C	5.27904200	-0.11211700	-0.59421600
H	6.36198500	-0.30119700	-0.59607100
H	4.85630000	-0.65257700	-1.45226800
C	3.46448700	1.88069500	1.74503700
H	3.27404500	2.95839100	1.69306300
H	3.03617500	1.52592100	2.68893700
C	0.34577400	3.04654500	-0.14290800
C	1.11669200	4.23310400	0.49277400
H	2.18646900	4.16344200	0.26817200
H	1.01445700	4.21479200	1.58599200
C	0.58067000	5.57807000	-0.05438300
H	1.14843000	6.39624600	0.40970000
C	0.76508900	5.61823400	-1.58489100
H	1.83082300	5.53468400	-1.84058100
H	0.41769000	6.58338900	-1.98030500
C	-0.02667700	4.46131600	-2.22724300
H	0.11258700	4.47891800	-3.31636600
C	-1.52122500	4.60981300	-1.89088600
H	-2.09390400	3.79908500	-2.36185800
H	-1.91251300	5.55710400	-2.28942900
C	-1.69576400	4.56248000	-0.36149900

H	-2.76070100	4.64564700	-0.10447800
C	-1.16514000	3.22268500	0.19408200
H	-1.74054800	2.38184000	-0.20694700
H	-1.31869100	3.21590900	1.27764700
C	0.49252200	3.11070600	-1.68912700
H	1.53508700	2.98359700	-1.98998400
H	-0.05342100	2.28116300	-2.14879600
C	-0.91488600	5.72383700	0.28444000
H	-1.29197500	6.68927100	-0.08180800
H	-1.05935300	5.71638300	1.37399500
P	0.89879300	1.32329500	0.50470700
Pd	-0.39731000	-0.33432200	-0.54915300
C	-3.09531000	-0.21319100	0.73276800
O	-1.83631000	0.01403200	0.98653400
O	-4.00173300	0.13012700	1.53516700
O	-3.39966200	-0.82330000	-0.40856000
Cs	-6.31632700	-0.74535900	0.07466800

TS-PivNOH-O[1]

N	2.22904900	-0.57026400	-2.26029700
O	0.46753900	0.70022700	-2.91857500
C	0.93732700	-0.08849500	-2.10976300
C	1.89439600	-2.75763200	-1.27263000
C	2.35833700	-3.80270800	-0.42159200
H	1.72628100	-4.67768500	-0.28951800
C	3.58406500	-3.74424500	0.19335200
H	3.92563300	-4.56821000	0.81582200
C	4.42942100	-2.61513500	0.02672500
C	5.69635600	-2.52810000	0.66117800
H	6.02982700	-3.36703200	1.26814400
C	6.48729000	-1.40909500	0.52348300
H	7.45482600	-1.35616300	1.01499100
C	6.02845300	-0.31881800	-0.25285900
H	6.64385400	0.57241700	-0.34562200
C	4.80735400	-0.37446800	-0.89078200
H	4.46449600	0.47713300	-1.46814100
C	3.97557200	-1.52595300	-0.79006000
C	2.71158500	-1.63969300	-1.44741900
C	2.92077100	-0.21938500	-3.51086200
H	3.91716400	-0.66131100	-3.50137200
H	2.36406000	-0.59614300	-4.37696700
H	2.99979400	0.86694200	-3.60860100
C	0.57250100	-2.87979800	-1.96631000
H	0.60910500	-2.50397800	-2.99171000
H	0.31174600	-3.94462600	-2.01159300
H	-0.79020800	-2.75102000	-1.58465500
C	-0.93389100	0.70374500	2.29108400
H	-1.33368900	1.60205400	2.77673900
H	-1.72249800	-0.05173300	2.29868000
C	0.24364600	0.14359900	3.10650200
H	0.71091200	-0.68741400	2.55846700
H	1.03045500	0.89610600	3.22923100
C	-0.19904800	-0.33338000	4.49955700
H	-0.98654100	-1.09136900	4.38975000
H	-0.66203200	0.50678300	5.03610500
C	0.95529600	-0.89818100	5.33433100
H	0.60824700	-1.23138900	6.31884000
H	1.73670600	-0.14507500	5.49349700
H	1.42434100	-1.75749900	4.83853200
C	0.64442300	2.50586800	0.47460700
C	2.06467000	1.87892000	0.58646800
H	2.15558500	1.27823700	1.49781400
H	2.23713600	1.19888000	-0.25170700
C	3.15035700	2.97850600	0.59145300
H	4.13075200	2.49241000	0.67829900
C	2.92829200	3.92717500	1.78496400
H	3.70681900	4.70242700	1.80415900
H	3.00706700	3.37294700	2.73089400
C	1.53695000	4.57767000	1.66275800
H	1.36254200	5.24582400	2.51695500
C	1.45807300	5.37925500	0.34918700
H	0.47784300	5.86862000	0.26171300
H	2.21439700	6.17629800	0.34838200
C	1.68370500	4.42646400	-0.84032300
H	1.61300600	4.98573000	-1.78253100
C	0.59121300	3.33232400	-0.84003100
H	0.71378600	2.67623500	-1.70665700
H	-0.38406900	3.81925700	-0.94167300
C	3.07537400	3.77709400	-0.72355800
H	3.85760900	4.54881100	-0.74559400
H	3.25422100	3.11348200	-1.58082400
C	0.44819000	3.47769600	1.67309000
H	-0.54028500	3.94774300	1.63504500
H	0.50760200	2.93718600	2.62407700
C	-2.36741500	1.64975900	-0.12738400
C	-2.82592500	3.00749000	0.46562100
H	-2.12953100	3.80592900	0.19082300
H	-2.84733800	2.96069600	1.56268700

C	-4.23423000	3.37671500	-0.06078000
H	-4.52442200	4.34424400	0.37071200
C	-4.19639800	3.48090300	-1.59865600
H	-3.48964300	4.26385000	-1.90782100
H	-5.18438600	3.77493700	-1.97926700
C	-3.77706600	2.12178800	-2.19427100
H	-3.73716400	2.19436100	-3.28884600
C	-4.79144700	1.03999900	-1.78036000
H	-4.50950100	0.07246500	-2.21671900
H	-5.79238100	1.28673100	-2.16158200
C	-4.81795800	0.94215600	-0.24412800
H	-5.52158300	0.15834000	0.06751200
C	-3.41393600	0.57248100	0.28487700
H	-3.11228500	-0.40662100	-0.10170600
H	-3.46948600	0.48582800	1.37584100
C	-2.37300400	1.73820400	-1.67965800
H	-1.64441900	2.47188500	-2.03328500
H	-2.06404500	0.77820000	-2.10568800
C	-5.24808700	2.29451300	0.35585700
H	-6.25379600	2.56426100	0.00522800
H	-5.29964900	2.22458600	1.45166900
P	-0.63643600	1.06345400	0.47958500
Pd	-0.14037700	-0.98234900	-0.64052800
C	-2.16457100	-3.16266300	-0.08832000
O	-2.00355900	-3.13854800	-1.37185700
N	-1.39159700	-2.34958300	0.60604300
O	-1.55388400	-2.41944300	2.02448400
C	-3.21960000	-4.12876400	0.48655100
C	-3.94130300	-4.83633400	-0.67732000
C	-4.26618900	-3.35481000	1.31972000
C	-2.51973600	-5.19817100	1.35815800
H	-0.63478000	-2.45089500	2.33661600
H	-4.69040800	-5.52653800	-0.27090600
H	-3.24341800	-5.40690500	-1.29604400
H	-4.44958400	-4.11960800	-1.32889800
H	-4.77634900	-2.60453600	0.70370600
H	-3.81571900	-2.85145600	2.17665400
H	-5.02679100	-4.05360500	1.68885300
H	-2.02222800	-4.75077400	2.22048700
H	-3.26278600	-5.91856100	1.72115700
H	-1.77669100	-5.75338900	0.77296400

TS-PivNOH-N

N	-2.29457900	0.28213700	-2.24825900
O	-0.44000600	-0.84268800	-2.92240700
C	-0.96307700	-0.07974700	-2.12083800
C	-2.17914500	2.53308400	-1.33944500
C	-2.75011100	3.55863700	-0.53063000
H	-2.21793900	4.50300900	-0.44510300
C	-3.95512600	3.39147700	0.10385400
H	-4.38056800	4.19899300	0.69526500
C	-4.66845400	2.16751200	0.00165300
C	-5.91066100	1.96840900	0.65901200
H	-6.32830600	2.79071400	1.23586500
C	-6.57407800	0.76394100	0.58081900
H	-7.52387900	0.62549900	1.08997300
C	-6.00566100	-0.30095900	-0.15697700
H	-6.51933300	-1.25785200	-0.20365600
C	-4.80487500	-0.13825400	-0.81520900
H	-4.37625000	-0.97069100	-1.36253700
C	-4.10381300	1.10050200	-0.77407100
C	-2.86743100	1.32502800	-1.45534300
C	-2.97202400	-0.14320800	-3.48417600
H	-4.02583000	0.12855300	-3.42412500
H	-2.52301300	0.34274100	-4.35927300
H	-2.87373500	-1.22416300	-3.61027200
C	-0.87529000	2.76309000	-2.03126500
H	-0.82289900	2.28444700	-3.01201100
H	-0.75067800	3.84366600	-2.19517800
H	0.40252100	2.88511800	-1.49852400
C	1.09458100	-0.49928600	2.22968200
H	1.58422500	-1.31994900	2.76880600
H	1.81161300	0.31938500	2.14208900
C	-0.10446600	0.03161800	3.03223300
H	-0.60529400	0.81764500	2.45407000
H	-0.84528700	-0.75819400	3.20229100
C	0.32837300	0.59494700	4.39485700
H	1.06425200	1.39413000	4.23634000
H	0.84470100	-0.19011600	4.96655300
C	-0.84742200	1.13528400	5.21536600
H	-0.51081100	1.53311100	6.17964200
H	-1.58574100	0.34959700	5.41871300
H	-1.36305300	1.94307200	4.68195400
C	-0.38009600	-2.54607000	0.57221400
C	-1.83905800	-2.01558500	0.68887200
H	-1.95160500	-1.37843600	1.57205300
H	-2.07689500	-1.39057200	-0.17559400
C	-2.84378200	-3.18557500	0.77368600

H	-3.85387800	-2.76498600	0.85949200
C	-2.52950900	-4.05213800	2.00826000
H	-3.24862200	-4.87941700	2.08646500
H	-2.62824600	-3.45533400	2.92579500
C	-1.09748600	-4.60749600	1.88588300
H	-0.85908200	-5.21660900	2.76835300
C	-0.98856600	-5.47003400	0.61355000
H	0.02198500	-5.89377400	0.52731300
H	-1.68562700	-6.31737000	0.67302900
C	-1.30684400	-4.59995900	-0.61790400
H	-1.21608600	-5.20231500	-1.53149500
C	-0.29566900	-3.43371900	-0.69962800
H	-0.48530900	-2.83332700	-1.59482600
H	0.70966400	-3.85556700	-0.80096900
C	-2.73839000	-4.04400700	-0.50086800
H	-3.46492000	-4.86797100	-0.46768500
H	-2.97932500	-3.43892200	-1.38575900
C	-0.08860900	-3.43584600	1.81527000
H	0.92983900	-3.83776700	1.77712400
H	-0.16480400	-2.84810000	2.73707900
C	2.53759200	-1.49715800	-0.16726200
C	3.12444900	-2.77184900	0.49477700
H	2.48938700	-3.63999700	0.29075400
H	3.16929300	-2.65409000	1.58575000
C	4.54428600	-3.05704900	-0.05090800
H	4.92712800	-3.96669200	0.43128100
C	4.47493300	-3.26585600	-1.57711800
H	3.82835900	-4.12285200	-1.81252500
H	5.47362300	-3.50241100	-1.96979100
C	3.92773500	-1.98833000	-2.24483700
H	3.86542500	-2.13632300	-3.33084300
C	4.85992300	-0.80352100	-1.93266400
H	4.48857900	0.10694500	-2.42237700
H	5.86772300	-0.99395900	-2.32763500
C	4.91665100	-0.59994700	-0.40758600
H	5.56094000	0.25737200	-0.17004300
C	3.50045700	-0.31089400	0.13904200
H	3.10709800	0.61232400	-0.30069000
H	3.57564000	-0.14592300	1.21959800
C	2.51043800	-1.68696600	-1.71072900
H	1.83786000	-2.50022300	-1.99399100
H	2.10892600	-0.78625800	-2.18638500
C	5.47305200	-1.86966300	0.26484900
H	6.48915700	-2.07826200	-0.09747400
H	5.54526600	-1.72294400	1.35180300
P	0.78456900	-1.01965300	0.46152400
Pd	0.07811700	0.91577400	-0.71175000
C	1.77201300	3.24099000	0.21145600
O	1.24662400	2.19469100	0.71775100
N	1.60389500	3.41022700	-1.10007800
O	1.91396000	4.70523900	-1.62140800
C	2.54006900	4.21453400	1.13002500
C	2.67455500	3.59419700	2.53231100
C	1.74630200	5.53773900	1.24514400
C	3.95448000	4.48188100	0.56822400
H	2.39613400	4.49334400	-2.43765900
H	3.20978100	4.29152300	3.18800700
H	3.23540100	2.65430300	2.50346500
H	1.69564700	3.38672200	2.97252600
H	0.74503300	5.35621500	1.65388500
H	1.64302700	6.03058900	0.27681400
H	2.26746400	6.21897800	1.92923400
H	3.91205400	4.95536400	-0.41366300
H	4.50116500	5.14513900	1.24953700
H	4.52488000	3.54902300	0.48220600

TS-HCO_3

N	2.11121200	-0.10966000	-2.21097200
O	-0.03600800	0.19668200	-2.87338400
C	0.74580300	-0.25444100	-2.04836300
C	2.85786000	-2.13971500	-1.10887400
C	3.80285100	-2.80430300	-0.27380600
H	3.65488400	-3.86230200	-0.06993000
C	4.89487300	-2.15415200	0.24256300
H	5.61437100	-2.69142700	0.85614500
C	5.10534500	-0.77211500	-0.00915300
C	6.21719600	-0.07498700	0.53128900
H	6.93315100	-0.63072200	1.13283300
C	6.38845800	1.27400200	0.31233200
H	7.24361600	1.79539900	0.73341000
C	5.43572100	1.98370900	-0.45553200
H	5.55943500	3.05211700	-0.61324300
C	4.34980700	1.33447600	-1.00443000
H	3.62244200	1.89924800	-1.57707400
C	4.15364700	-0.06312000	-0.81566500
C	3.05509300	-0.78594000	-1.37721900
C	2.54683300	0.45002500	-3.50245100
H	2.14402100	1.45784800	-3.63680800

H	3.63576400	0.48305500	-3.52396900
H	2.18373800	-0.17131100	-4.32909000
C	1.67925600	-2.88082900	-1.64382900
H	1.37264200	-2.55226700	-2.63893300
H	1.95648800	-3.93863600	-1.76123100
H	0.69830500	-3.59751300	-0.80893400
C	-1.32294700	-0.17460500	2.30978300
H	-2.03265500	0.49133200	2.81607000
H	-1.75834800	-1.17487200	2.29878800
C	-0.00424900	-0.26192500	3.09815700
H	0.75313000	-0.77317500	2.49109400
H	0.38717200	0.74009300	3.31351800
C	-0.18161500	-1.02348300	4.42097500
H	-0.53135000	-2.03973000	4.19722400
H	-0.97244200	-0.54516500	5.01698400
C	1.10929100	-1.09222100	5.24348000
H	0.95834800	-1.64863500	6.17563000
H	1.46770400	-0.08944900	5.50796200
H	1.90825400	-1.59188900	4.68212200
C	-0.59685600	2.11258600	0.48665500
C	0.95337300	2.09168800	0.61964400
H	1.25510600	1.58345300	1.54128100
H	1.38984900	1.52251000	-0.20548600
C	1.52226900	3.52795800	0.61643700
H	2.61334800	3.46600700	0.71595900
C	0.93197200	4.32669600	1.79432600
H	1.34541500	5.34466600	1.80914500
H	1.20843100	3.85617500	2.74825700
C	-0.60149200	4.37913100	1.65277800
H	-1.03389900	4.93451400	2.49599400
C	-0.97371800	5.07101900	0.32740000
H	-2.06626500	5.13607600	0.22643500
H	-0.59091400	6.10101100	0.31977800
C	-0.37784100	4.27145000	-0.84727500
H	-0.64973300	4.75002400	-1.79741700
C	-0.95540700	2.83758600	-0.83929700
H	-0.57696700	2.27280000	-1.69756300
H	-2.04280700	2.90437100	-0.95252200
C	1.15553900	4.22012000	-0.71003100
H	1.57305000	5.23631700	-0.73785800
H	1.59038400	3.67097400	-1.55668200
C	-1.17103400	2.94024700	1.67215900
H	-2.26446200	2.98258100	1.62341700
H	-0.91165900	2.47267800	2.62853700
C	-3.00938800	0.11380600	-0.12434600
C	-3.99165000	1.15853800	0.46668900
H	-3.68356800	2.17376800	0.19441900
H	-3.99561400	1.10567500	1.56353100
C	-5.42384500	0.91309300	-0.06788900
H	-6.09172900	1.67037500	0.36448300
C	-5.42598300	1.03227600	-1.60520600
H	-5.10736100	2.03968200	-1.90749700
H	-6.44516600	0.89070800	-1.99077900
C	-4.47762500	-0.02686500	-2.20196700
H	-4.46443600	0.06294900	-3.29601400
C	-4.95641200	-1.43354400	-1.79990500
H	-4.29869000	-2.19575600	-2.23934200
H	-5.96809200	-1.61963100	-2.18692300
C	-4.94684400	-1.54449400	-0.26465700
H	-5.26526100	-2.55081300	0.03861900
C	-3.51899000	-1.30380600	0.27400100
H	-2.83593300	-2.06798500	-0.11349000
H	-3.53884500	-1.41786400	1.36319400
C	-3.04321700	0.20177900	-1.67641700
H	-2.68462600	1.17520000	-2.02004800
H	-2.35991500	-0.53718100	-2.10613700
C	-5.90035600	-0.49449800	0.33762100
H	-6.92570600	-0.66257200	-0.01968100
H	-5.92406300	-0.58711500	1.43256700
P	-1.19991900	0.28766000	0.50235700
Pd	0.14439800	-1.41433300	-0.51971300
C	-0.46685600	-4.03067000	0.80352100
O	-0.60051600	-2.82393100	1.07874000
O	-1.01326100	-4.93086300	1.64498100
O	0.14769600	-4.51043200	-0.21801400
H	-0.80700100	-5.81203900	1.28794300

TS-Cl

N	2.18565900	-0.50034500	-2.18525200
O	0.03465300	-0.22516000	-2.85892200
C	0.82023100	-0.60419500	-2.00686800
C	2.93601600	-2.30354600	-0.74844200
C	3.89233000	-2.82464500	0.16946500
H	3.73847500	-3.82722300	0.56100700
C	5.00082700	-2.10618500	0.54067000
H	5.73051600	-2.53576000	1.22294200
C	5.20779700	-0.78715300	0.05734900
C	6.32356900	-0.01065600	0.46606600

H	7.05100900	-0.46409800	1.13569700
C	6.48102000	1.29038000	0.04345300
H	7.33783500	1.87420700	0.36811600
C	5.50923300	1.87215300	-0.80418900
H	5.61752900	2.90774000	-1.11610800
C	4.42354900	1.14032900	-1.23617500
H	3.68199300	1.61291600	-1.87043500
C	4.24351100	-0.21644700	-0.84049300
C	3.14227500	-1.02301900	-1.26376700
C	2.61295200	-0.05704100	-3.52473000
H	2.28030000	0.96664200	-3.72066400
H	3.69956700	-0.10754000	-3.58258300
H	2.17264300	-0.70622900	-4.28884900
C	1.71303000	-3.07045400	-1.09111900
H	1.46050100	-3.07339600	-2.15389500
H	1.81408600	-4.12054700	-0.78803800
H	0.58370800	-3.46244200	0.18344600
C	-1.44417100	-0.24540300	2.34121100
H	-2.19517200	0.41547000	2.79190600
H	-1.84908400	-1.26064500	2.38318000
C	-0.15140300	-0.23268500	3.17542400
H	0.62751000	-0.80570300	2.65629900
H	0.23033900	0.78967200	3.28248200
C	-0.36789600	-0.82958100	4.57470400
H	-0.72143500	-1.86434400	4.47082300
H	-1.16943600	-0.27833100	5.08742900
C	0.90138100	-0.80561800	5.43264500
H	0.72129900	-1.24340500	6.42104100
H	1.26136400	0.21984100	5.58284300
H	1.70910700	-1.37493400	4.95718800
C	-0.72318600	1.95274100	0.40182000
C	0.82737000	1.96334900	0.54555100
H	1.13279400	1.50920500	1.49380900
H	1.27729800	1.35752100	-0.24707300
C	1.37649000	3.40452300	0.46808800
H	2.46736700	3.36552100	0.58274000
C	0.75897900	4.25845400	1.59256700
H	1.15857100	5.28130200	1.55676600
H	1.02862700	3.84449700	2.57430600
C	-0.77350400	4.28244900	1.42972800
H	-1.22284800	4.88198000	2.23283200
C	-1.13648600	4.89020600	0.06078800
H	-2.22828700	4.93546900	-0.05722200
H	-0.76562400	5.92255400	-0.00388900
C	-0.51567500	4.03056800	-1.05781500
H	-0.78359900	4.44768300	-2.03757500
C	-1.07405700	2.59122800	-0.97032500
H	-0.67474600	1.98033600	-1.78750400
H	-2.16088000	2.63461600	-1.10021200
C	1.01630800	4.01258100	-0.90064900
H	1.41738600	5.03235900	-0.98364000
H	1.47143700	3.42193000	-1.70779000
C	-1.32655500	2.84077800	1.52497200
H	-2.41995900	2.86421200	1.45225700
H	-1.08134000	2.43354500	2.51220600
C	-3.07252000	-0.14353500	-0.13912000
C	-4.11601900	0.86895800	0.39966300
H	-3.85486900	1.88986000	0.09763600
H	-4.13559800	0.85370400	1.49762900
C	-5.52432700	0.53027100	-0.14674200
H	-6.23930100	1.26429100	0.24872100
C	-5.50771300	0.59590100	-1.68741900
H	-5.23809900	1.60786000	-2.02096700
H	-6.51176700	0.38747000	-2.08237200
C	-4.49614000	-0.43138700	-2.23413600
H	-4.46971900	-0.37703600	-3.33030200
C	-4.90767400	-1.84718700	-1.79231700
H	-4.20408400	-2.58797000	-2.19557900
H	-5.90160700	-2.09800700	-2.18837400
C	-4.91807300	-1.90695800	-0.25433200
H	-5.18892700	-2.91763900	0.07840400
C	-3.51388600	-1.57308200	0.29587900
H	-2.78505000	-2.31376000	-0.05688800
H	-3.55047800	-1.65325100	1.38761400
C	-3.08453800	-0.10895000	-1.69522600
H	-2.77847500	0.87304200	-2.06505300
H	-2.35470400	-0.82241700	-2.09153500
C	-5.93210400	-0.88687100	0.30016200
H	-6.94255400	-1.11971900	-0.06274500
H	-5.96546600	-0.94396000	1.39729300
P	-1.28616900	0.12034100	0.50789100
Pd	0.17975700	-1.58958800	-0.36933600
Cl	-0.26099500	-3.76818000	1.31199200

Int-PivNHO′-O[2]

N	1.68124400	-2.23179600	-1.35555900
O	-0.00339300	-1.18486300	-2.45228800
C	0.76642800	-1.19864700	-1.49592500

C	2.82227700	-2.74509700	0.75999800	H	-3.87571500	4.75649900	-2.43501700
C	4.02845500	-2.79272400	1.51447900	H	-3.23079900	4.61928000	-0.79662600
H	3.99207400	-3.20370700	2.52102000	C	-4.43615900	2.91402200	-1.41573500
C	5.22213700	-2.36029800	0.99603100	H	-5.36388600	3.33197800	-1.00134200
H	6.13456000	-2.42406200	1.58480100	C	-4.74715100	2.14507400	-2.71517100
C	5.28874400	-1.83543400	-0.32173000	H	-5.47335400	1.34397000	-2.51589300
C	6.51442300	-1.39557600	-0.88965300	H	-5.20949300	2.81874000	-3.45008700
H	7.42088800	-1.47251200	-0.29307000	C	-3.44185800	1.55081600	-3.28085900
C	6.55823400	-0.88353700	-2.16665600	H	-3.65718200	0.99466900	-4.20299400
H	7.50192200	-0.55387500	-2.59351800	C	-2.82993600	0.57360600	-2.25186700
C	5.36682200	-0.77965100	-2.92365900	H	-1.91344200	0.12180000	-2.64493000
H	5.40085600	-0.35905300	-3.92531700	H	-3.54507800	-0.23969400	-2.08496500
C	4.16280900	-1.19453700	-2.39813800	C	-2.44659200	2.68708400	-3.58137800
H	3.25234000	-1.07556800	-2.97436600	H	-2.86784400	3.37303700	-4.32991800
C	4.08542200	-1.74591500	-1.09072600	H	-1.52090800	2.27520700	-4.00436800
C	2.85305500	-2.21095400	-0.51863400	C	-3.82538100	1.94962200	-0.37138200
C	1.63066600	-3.32845200	-2.33598700	H	-4.56582600	1.18499900	-0.12101400
H	0.61977000	-3.38808600	-2.73898000	H	-3.62111500	2.50840000	0.54918500
H	2.32996400	-3.17088900	-3.16628400	C	-2.60134200	-1.51219000	0.53828300
H	1.89374800	-4.26391900	-1.83313400	C	-4.14139300	-1.31515900	0.57004400
C	1.56718800	-3.29272200	1.38937900	H	-4.49355900	-0.88231100	-0.36993300
H	1.18536300	-2.60680100	2.15623600	H	-4.42227500	-0.62000100	1.37189700
H	0.77704300	-3.43488300	0.65053300	C	-4.86543300	-2.66546100	0.78125100
H	1.76524100	-4.25257600	1.88199500	H	-5.94799800	-2.48020200	0.79557300
C	-1.87603800	1.03904200	1.95612900	C	-4.51427400	-3.61454300	-0.38103700
H	-1.77706500	2.10141600	1.70857600	H	-4.84026400	-3.17900100	-1.33580200
H	-2.91260800	0.88704300	2.28485300	H	-5.04750300	-4.56836500	-0.26592500
C	-0.89805400	0.74032100	3.10752200	C	-2.99212400	-3.85175200	-0.39848000
H	-0.91429100	-0.32051100	3.37772100	H	-2.73122500	-4.51953300	-1.23011400
H	0.11727100	0.96802800	2.77191300	C	-2.55333200	-4.48547300	0.93508300
C	-1.22429400	1.57499100	4.35612500	H	-1.47328300	-4.68508400	0.92194200
H	-2.25432600	1.36782800	4.68179500	H	-3.05486600	-5.45187200	1.08494900
H	-1.19684200	2.64256600	4.09439500	C	-2.90468600	-3.52526300	2.08647700
C	-0.26000200	1.30879700	5.51726500	H	-2.57486200	-3.95338900	3.04261400
H	-0.51009200	1.91798200	6.39366400	C	-2.19443100	-2.16563600	1.88976100
H	0.77362700	1.53999500	5.23267000	H	-1.10777100	-2.29883500	1.93433600
H	-0.29008300	0.25582700	5.82402400	H	-2.47557800	-1.51172900	2.72184100
C	-2.51893900	1.31051600	-0.92100000	C	-2.24907200	-2.51157800	-0.59612700
C	-1.52788100	2.46745700	-1.24932400	H	-2.49085200	-2.09336600	-1.57666100
H	-1.24801000	3.00800600	-0.33702000	H	-1.17139500	-2.69472600	-0.60017200
H	-0.60074600	2.04733700	-1.65572800	C	-4.42780700	-3.29672700	2.11596400
C	-2.14080100	3.44567000	-2.27546100	H	-4.95256200	-4.24883900	2.27546400
H	-1.41321300	4.24472400	-2.47149300	H	-4.69670400	-2.63822800	2.95392600
C	-3.44088200	4.05054600	-1.71353100	P	-1.61975500	0.13941500	0.32811900

Pd	0.71897200	0.30083600	-0.16661700
C	2.13491900	2.63211800	0.82204100
O	0.95591400	2.18448200	1.00753900
N	2.98698300	1.97934200	0.05223200
O	2.70084600	0.80973900	-0.58579200
C	2.56569200	3.94593200	1.48923000
C	1.61218500	5.05478500	0.99176600
C	4.01993800	4.34156800	1.17160300
C	2.40353200	3.77181100	3.01517000
H	3.93135200	2.30122900	-0.11205100
H	1.83358300	6.00111300	1.49949500
H	0.57199300	4.78552000	1.19316400
H	1.72088400	5.21358300	-0.08767600
H	4.17652500	4.50012300	0.09740500
H	4.73608400	3.58982600	1.52577600
H	4.26263100	5.28335500	1.67582700
H	3.07823300	2.99662000	3.39770200
H	2.63710300	4.71107000	3.53033800
H	1.37830000	3.48376500	3.26216100

TS-PivNHO′-O[2]

N	-0.19390100	3.17605800	-1.16588900
O	0.42193100	1.47645100	-2.52805900
C	0.02260300	1.84596900	-1.43589300
C	0.28135500	4.82556600	0.54984500
C	-0.04028000	5.42791600	1.79422600
H	0.52736600	6.30093000	2.10753500
C	-1.01837900	4.91775300	2.60948800
H	-1.24135900	5.38477600	3.56596500
C	-1.73029200	3.75120900	2.22990900
C	-2.69186100	3.16761200	3.09483000
H	-2.89087200	3.64943200	4.04968200
C	-3.34420000	2.00673500	2.74341600
H	-4.07105600	1.56023300	3.41791700
C	-3.06502900	1.39671200	1.50218100
H	-3.57688600	0.47386100	1.24762000
C	-2.16334700	1.94047600	0.58398900
H	-2.53544700	1.64888900	-0.64867900
C	-1.46392100	3.13634600	0.95981600
C	-0.45740500	3.72219500	0.12576200
C	-0.27605100	4.04695300	-2.35356900
H	0.70928600	4.24464500	-2.78647900
H	-0.89379100	3.55291600	-3.10750900
H	-0.74524600	4.98702700	-2.06144000
C	1.44529500	5.38267800	-0.23848100
H	2.13223800	5.91323600	0.42880500
H	2.00605300	4.58686400	-0.73927200
H	1.13311000	6.09572800	-1.01252400
C	0.80171100	-2.51312000	-1.42839200
H	1.73977100	-3.04246200	-1.64300300
H	0.15668900	-3.22697700	-0.90382800
C	0.09499500	-2.08624700	-2.72651100
H	-0.85969200	-1.61882600	-2.46073800
H	0.67112500	-1.31467600	-3.24773800
C	-0.14895800	-3.27359000	-3.66926800
H	-0.72745400	-4.04591100	-3.14122300
H	0.81183200	-3.74017100	-3.93271400
C	-0.88761500	-2.86905500	-4.94959200
H	-1.05482900	-3.73119200	-5.60591000
H	-0.31822500	-2.12161900	-5.51520800
H	-1.86459800	-2.42812400	-4.71685500
C	2.91671500	-0.53810100	-0.57299500
C	3.09108900	-0.36550300	-2.11137300
H	2.96340700	-1.33218300	-2.61385300
H	2.32748800	0.31095600	-2.50343500
C	4.49874200	0.18038400	-2.44264300
H	4.57833300	0.29542600	-3.53175000
C	5.56668700	-0.81071900	-1.94364100
H	6.57347900	-0.44405800	-2.18806400
H	5.44875000	-1.78045300	-2.44735500
C	5.42153500	-0.98168500	-0.42009500
H	6.16757700	-1.69960200	-0.05306000
C	5.62615200	0.38051000	0.27222900
H	5.54865300	0.26696700	1.36280800
H	6.63517300	0.76114800	0.06191600
C	4.56436000	1.37585300	-0.23536500
H	4.69955000	2.34613100	0.26114200
C	3.15305800	0.84357300	0.09729300
H	2.39670100	1.55547800	-0.24887200
H	3.03888100	0.77053000	1.18456700
C	4.70157800	1.54657700	-1.76041100
H	5.69220500	1.95189000	-2.01012000
H	3.95678300	2.26482500	-2.12888300
C	4.01143300	-1.52249200	-0.08158500
H	3.94556700	-1.66442700	1.00172400
H	3.87363400	-2.50848600	-0.54548300
C	0.97949200	-1.97651600	1.49235300
C	1.64101900	-3.37829200	1.58640700

H	2.71892700	-3.31519500	1.41204100
H	1.23293700	-4.04535900	0.81757400
C	1.38992200	-4.00129900	2.98069800
H	1.88005800	-4.98354600	3.01771700
C	1.97993000	-3.08525100	4.07178100
H	3.06489900	-2.97877400	3.93106500
H	1.83020100	-3.53451200	5.06332100
C	1.29663300	-1.70455600	4.00540700
H	1.72051500	-1.04410800	4.77360700
C	-0.21739400	-1.86791000	4.23694900
H	-0.71233000	-0.88753100	4.21216500
H	-0.40436900	-2.29768100	5.23101100
C	-0.79895000	-2.78236100	3.14166300
H	-1.88260100	-2.88905400	3.28352900
C	-0.54545900	-2.14567100	1.75866200
H	-1.03878100	-1.16495100	1.72493200
H	-1.01634200	-2.75229300	0.97688800
C	1.55022100	-1.07256900	2.61782900
H	2.62889500	-0.93114000	2.48915300
H	1.08700900	-0.07828000	2.56864200
C	-0.12471500	-4.16596200	3.20924800
H	-0.31243600	-4.63301100	4.18611900
H	-0.55185700	-4.83351400	2.44790400
P	1.11999100	-1.11456200	-0.22209700
Pd	-0.72644000	0.45114500	-0.24419400
C	-3.68412000	-0.85004000	-1.12275300
O	-2.60825300	-1.14091800	-0.54222800
N	-3.91934300	0.33075500	-1.70589900
O	-3.01976900	1.34033200	-1.83148500
C	-4.82178100	-1.89838000	-1.15873400
C	-4.25551500	-3.15775200	-1.85026000
C	-6.08858800	-1.43923100	-1.90594000
C	-5.18835400	-2.23536600	0.30283200
H	-4.80832800	0.51020900	-2.15325600
H	-4.99327000	-3.96880200	-1.82679100
H	-3.34680400	-3.49421800	-1.34482600
H	-4.00746500	-2.95442800	-2.89897800
H	-5.88480200	-1.20997900	-2.95913000
H	-6.55206800	-0.56231800	-1.43666300
H	-6.83383500	-2.24263300	-1.88984400
H	-5.61473600	-1.36336400	0.81415500
H	-5.93201200	-3.04077800	0.33330700
H	-4.30165100	-2.55639900	0.85585000

Int-PivNHOH′

N	-1.03990200	3.48149000	-0.75721400
O	0.42028100	2.22356600	-1.93639900
C	-0.34837700	2.31443400	-0.98803900
C	-2.08243900	5.03690800	0.80477700
C	-3.15616800	5.31746800	1.69214300
H	-3.28002200	6.34206600	2.03570400
C	-4.02745100	4.34585400	2.11364000
H	-4.86003600	4.59187600	2.76837500
C	-3.81133400	2.99293300	1.74634200
C	-4.63646200	1.94900700	2.24232300
H	-5.48125800	2.21019100	2.87569800
C	-4.35548200	0.63461600	1.94955500
H	-4.98813000	-0.16150000	2.33625600
C	-3.21160400	0.31109000	1.17957500
H	-2.96318700	-0.73798000	1.02940500
C	-2.38757600	1.29932900	0.65381000
H	-2.59202000	0.21102000	-1.42720200
C	-2.71497000	2.66536100	0.88035100
C	-1.93511600	3.73545000	0.32373500
C	-1.03255800	4.41560600	-1.90302100
H	-0.13171900	5.03543500	-1.92435600
H	-1.06435400	3.83336200	-2.82585900
H	-1.91499700	5.05184200	-1.84347100
C	-1.12621500	6.16667500	0.48205000
H	-1.07404000	6.85190100	1.33488400
H	-0.11473400	5.79606800	0.29199400
H	-1.42878000	6.76338800	-0.38818600
C	1.42235900	-1.95949900	-1.47141200
H	2.40914300	-2.36481700	-1.73216400
H	0.86053200	-2.77503800	-1.00290400
C	0.65403100	-1.52360300	-2.73022800
H	-0.32443100	-1.13458900	-2.43156700
H	1.17186500	-0.70307600	-3.23813900
C	0.45338400	-2.68589800	-3.71354500
H	-0.08833400	-3.49550800	-3.20396400
H	1.42896500	-3.10344900	-4.00427900
C	-0.31843400	-2.26509400	-4.96909600
H	-0.47616600	-3.11211500	-5.64762300
H	0.22267300	-1.48898600	-5.52436800
H	-1.29936700	-1.85310400	-4.70374200
C	3.26362600	0.23268400	-0.51507700
C	3.30775000	0.55313500	-2.03788100
H	3.31397600	-0.38038300	-2.61376100

H	2.41483400	1.11551200	-2.32581300
C	4.57971000	1.35540600	-2.39020300
H	4.57057400	1.56820900	-3.46753700
C	5.82578100	0.52268600	-2.03415900
H	6.74140900	1.07124600	-2.29602500
H	5.83597700	-0.41103000	-2.61407000
C	5.80881000	0.20950800	-0.52587300
H	6.68650000	-0.39624000	-0.26188400
C	5.82800700	1.52820400	0.27342600
H	5.83983900	1.31710000	1.35229500
H	6.74494700	2.09100000	0.04929800
C	4.58673800	2.36679000	-0.09110200
H	4.59286200	3.30423100	0.48122800
C	3.30459300	1.58044700	0.25931100
H	2.42210600	2.17548700	-0.00013000
H	3.26610600	1.40525300	1.34094300
C	4.59708900	2.67840200	-1.60029700
H	5.48975700	3.26442500	-1.86118600
H	3.72122400	3.28512000	-1.86541000
C	4.53203200	-0.58840600	-0.16852400
H	4.55942800	-0.83010400	0.89924600
H	4.52832500	-1.54112100	-0.71516300
C	1.68194600	-1.67860400	1.46155100
C	2.52646900	-2.97716700	1.37707900
H	3.57554300	-2.74402600	1.16812100
H	2.17167500	-3.61015900	0.55534200
C	2.43376800	-3.77040000	2.70187100
H	3.04721100	-4.67723900	2.61354900
C	2.95725100	-2.90047900	3.86169000
H	4.00978200	-2.63434300	3.68999200
H	2.92036000	-3.46412600	4.80422300
C	2.09783200	-1.62475600	3.97449700
H	2.47332000	-0.99645600	4.79323900
C	0.63295600	-2.01531300	4.24867400
H	0.01326800	-1.11439600	4.35523400
H	0.55970300	-2.56867500	5.19540000
C	0.11379600	-2.88036800	3.08422800
H	-0.93652300	-3.14856800	3.25904400
C	0.20731900	-2.07788700	1.76787000
H	-0.40649200	-1.16693700	1.86693700
H	-0.22730900	-2.65628100	0.94539800
C	2.18793100	-0.82442700	2.65458800
H	3.22839900	-0.51893600	2.49709000
H	1.59303600	0.09568900	2.73418300
C	0.96656100	-4.15920000	2.96897600
H	0.89275400	-4.74680700	3.89469700
H	0.58940900	-4.79402600	2.15520800
P	1.59980900	-0.64084100	-0.14884500
Pd	-0.56166700	0.65854800	0.07417800
C	-3.21870400	-2.38316500	-1.32812200
O	-2.11928100	-2.40723300	-0.77458400
N	-3.68886400	-1.26600000	-1.94863800
O	-2.82109700	-0.22812600	-2.27968100
C	-4.17768700	-3.59462400	-1.26779300
C	-3.40490900	-4.79971000	-1.84685300
C	-5.49287800	-3.40411400	-2.04716900
C	-4.49382900	-3.84823200	0.22207300
H	-4.48658800	-1.28214100	-2.56540300
H	-4.00466600	-5.71246100	-1.75146400
H	-2.46124200	-4.94099200	-1.31374300
H	-3.17764100	-4.65317400	-2.90963300
H	-5.31887300	-3.25172000	-3.12013200
H	-6.08441600	-2.56537200	-1.66091100
H	-6.10888200	-4.30492800	-1.94991400
H	-5.05516300	-3.01142500	0.65484900
H	-5.09957800	-4.75558900	0.33086200
H	-3.57017200	-3.97355900	0.79362300

Int-red2

N	-2.45215000	-1.23766800	-1.90280900
O	-0.37961200	-2.13969600	-1.73611500
C	-1.28333300	-1.49078400	-1.22506300
C	-4.50270100	0.06867800	-2.16487100
C	-5.77421700	0.42609900	-1.63652300
H	-6.47295200	0.94054800	-2.29267300
C	-6.14265600	0.12263800	-0.35013200
H	-7.13779600	0.36694800	0.01403100
C	-5.20624800	-0.47158800	0.53655400
C	-5.52057700	-0.74909700	1.89342300
H	-6.52723600	-0.54197800	2.24944100
C	-4.56511200	-1.25939700	2.74365200
H	-4.81614600	-1.48159600	3.77849400
C	-3.23692400	-1.45146100	2.28796300
H	-2.48380700	-1.77506700	3.00537900
C	-2.88529500	-1.18779900	0.97223700
C	-3.89255600	-0.78110800	0.05595600
C	-3.61190500	-0.61750100	-1.34284200
C	-2.60832500	-2.01428000	-3.15153800

H	-2.13468500	-1.51602300	-4.00274800
H	-2.13267300	-2.98758300	-3.01902100
H	-3.67029000	-2.15025500	-3.35253300
C	-4.18080300	0.48893900	-3.58367700
H	-4.67673000	1.44070900	-3.80396800
H	-3.10616700	0.63250100	-3.72868700
H	-4.52281400	-0.23030800	-4.33943700
C	1.90191200	0.33119300	2.41107400
H	2.54464600	-0.52375800	2.64698200
H	2.52226100	1.22712500	2.53937600
C	0.72610900	0.33960700	3.40370200
H	0.04188000	1.16746600	3.18140700
H	0.14129700	-0.58413500	3.27092800
C	1.17996000	0.43669400	4.86781200
H	1.75530100	1.36317700	5.00646000
H	1.87213000	-0.38854600	5.08762900
C	0.01135900	0.40423700	5.85875200
H	0.36406500	0.47832700	6.89364400
H	-0.55897300	-0.52814000	5.76669000
H	-0.68238800	1.23505700	5.68155900
C	2.78762400	-0.92828400	-0.12146300
C	2.46894300	-2.38614800	0.32738100
H	2.47234200	-2.45654800	1.42458800
H	1.46639800	-2.66084800	-0.01672000
C	3.50773100	-3.37229000	-0.24914100
H	3.25633700	-4.38543900	0.09150700
C	4.91699700	-2.99111600	0.24277500
H	5.66102100	-3.69866400	-0.14890300
H	4.96584200	-3.05168400	1.33938000
C	5.25040900	-1.56098600	-0.22569500
H	6.25034300	-1.27762100	0.13015300
C	5.20976700	-1.50259800	-1.76542600
H	5.47081800	-0.49277500	-2.11288600
H	5.95650200	-2.18883200	-2.18844500
C	3.79825800	-1.88445700	-2.25201600
H	3.75713000	-1.83174300	-3.34816600
C	2.76570000	-0.88996900	-1.67369000
H	1.76454800	-1.13859200	-2.03977700
H	3.01307400	0.11768200	-2.02974300
C	3.45931600	-3.31457900	-1.78845900
H	4.17513500	-4.02993400	-2.21735900
H	2.46074800	-3.59848300	-2.14369900
C	4.21901700	-0.56657900	0.36031300
H	4.48548200	0.45143400	0.05547700
H	4.28147700	-0.59641400	1.45477800
C	1.37220400	1.91915400	-0.08808800
C	2.75773700	2.59254200	-0.25355600
H	3.38177900	2.01804100	-0.94711500
H	3.28802100	2.61920800	0.70841500
C	2.59669200	4.03105000	-0.80094200
H	3.59316100	4.47976300	-0.91007800
C	1.89551700	3.98014500	-2.17405800
H	2.49938700	3.39937700	-2.88534800
H	1.80361900	4.99420500	-2.58699600
C	0.50154900	3.34109600	-2.01516300
H	0.00290100	3.29407200	-2.99235100
C	-0.34402000	4.18201200	-1.03993900
H	-1.34669200	3.74570600	-0.93588000
H	-0.47583700	5.20076900	-1.43002800
C	0.36049200	4.22592000	0.32954100
H	-0.24240300	4.80805800	1.03912100
C	0.52044000	2.79127200	0.87941400
H	-0.46844900	2.33359700	1.01927100
H	0.99729500	2.84320600	1.86624100
C	0.64735500	1.90640200	-1.46379700
H	1.19710900	1.29100400	-2.18361700
H	-0.34315900	1.44924000	-1.34820600
C	1.75198600	4.87093800	0.17626500
H	1.65340000	5.89943500	-0.19751600
H	2.25143900	4.93306100	1.15341800
P	1.38253900	0.14164300	0.61392700
Pd	-0.93909200	-0.80847200	0.60680000

Int-$CsCO_3'$

N	0.31265000	3.11401200	-1.49620200
O	1.44100900	1.63221400	-2.79639300
C	0.65929400	1.81373400	-1.86342600
C	0.17757900	3.85125600	0.83182400
C	-0.60611900	4.24711100	1.95131200
H	-0.09328900	4.52480500	2.86982700
C	-1.97650300	4.30361600	1.88981200
H	-2.55500300	4.61595100	2.75680900
C	-2.65733400	3.98922700	0.68536800
C	-4.06838200	4.10704600	0.57280800
H	-4.63587500	4.42234800	1.44614200
C	-4.70239600	3.84817500	-0.62200600
H	-5.78201600	3.95034100	-0.70177100
C	-3.94825800	3.45217300	-1.75102000

H	-4.45225000	3.23465100	-2.68810600
C	-2.58023200	3.31097200	-1.66929200
H	-2.01760700	2.96852200	-2.52653600
C	-1.89325700	3.57044900	-0.45412200
C	-0.46454700	3.46891800	-0.34171800
C	0.80543600	4.23583700	-2.30352500
H	1.24695500	3.82490400	-3.21150600
H	-0.02531300	4.90306000	-2.55930300
H	1.56715200	4.81734400	-1.76772600
C	1.68105800	3.93848800	0.94657900
H	2.01312400	3.71098000	1.96571000
H	2.18587300	3.25944600	0.25926500
H	2.02734400	4.95692400	0.72031900
C	1.11642000	-2.67980000	-0.23552100
H	2.05438400	-3.22200400	-0.05885500
H	0.41858200	-3.02271500	0.53691100
C	0.52203200	-3.05697900	-1.60441100
H	-0.45188200	-2.56673800	-1.70416900
H	1.14671600	-2.68054000	-2.42133900
C	0.36104300	-4.57727600	-1.75776500
H	-0.27561900	-4.96127400	-0.94441600
H	1.33582100	-5.07195900	-1.63358600
C	-0.24183800	-4.97565700	-3.10984800
H	-0.36138300	-6.06264500	-3.19411700
H	0.39754200	-4.64547400	-3.93722200
H	-1.22565000	-4.51276800	-3.25687500
C	3.24518300	-0.59467800	-0.37789600
C	3.35137100	-1.04842900	-1.86457200
H	3.11025100	-2.11365900	-1.95052100
H	2.63413300	-0.48587600	-2.47290700
C	4.78361500	-0.83786100	-2.40109500
H	4.81439000	-1.16925600	-3.44750400
C	5.76799900	-1.67394200	-1.56056500
H	6.79220600	-1.55876400	-1.94209000
H	5.51782700	-2.74203100	-1.63541700
C	5.69959400	-1.21354700	-0.09172500
H	6.39145900	-1.81074200	0.51824600
C	6.08168300	0.27699100	-0.00494800
H	6.06465600	0.61164000	1.04232600
H	7.10747500	0.42502300	-0.37071900
C	5.09050900	1.10322800	-0.84612400
H	5.34158600	2.17000300	-0.77267900
C	3.65352400	0.90253200	-0.31103500
H	2.96429800	1.49625300	-0.91353000
H	3.60181900	1.26960900	0.71952000
C	5.15537500	0.65363900	-2.31806000
H	6.16507000	0.81798200	-2.72076000
H	4.45785700	1.24647200	-2.92230100
C	4.26580400	-1.40691000	0.46083000
H	4.24921900	-1.07358300	1.50500400
H	4.01576700	-2.47576700	0.45847000
C	1.13391500	-0.78402800	2.01391500
C	1.77151700	-1.94894700	2.82017500
H	2.85945800	-1.95203700	2.70555600
H	1.41220500	-2.91739100	2.45152400
C	1.42649600	-1.82052700	4.32284500
H	1.89715500	-2.65284200	4.86372900
C	1.96174000	-0.47995000	4.86501500
H	3.05456600	-0.43865300	4.75575300
H	1.74462600	-0.39245800	5.93871100
C	1.30620700	0.68087900	4.09110400
H	1.69241800	1.63897400	4.46444500
C	-0.22238500	0.62991000	4.27888000
H	-0.69654100	1.46441800	3.74564700
H	-0.47731400	0.73719700	5.34284800
C	-0.75013700	-0.71277600	3.73752500
H	-1.84308800	-0.75164500	3.85493600
C	-0.40731600	-0.82832300	2.23725200
H	-0.88393400	-0.01695700	1.67555800
H	-0.81985400	-1.76260100	1.83424600
C	1.65361500	0.55636800	2.59104900
H	2.74170200	0.62134300	2.47619200
H	1.21483900	1.39077500	2.03282700
C	-0.10158600	-1.87618500	4.51231800
H	-0.35454900	-1.81222800	5.58010000
H	-0.49121100	-2.83898000	4.14915400
P	1.40200000	-0.84767900	0.10866000
Pd	-0.33559400	0.25147300	-1.06586700
C	-2.69460600	-0.49793400	-1.69895500
O	-1.98213700	-1.17098100	-0.79005900
O	-2.07523600	0.54257900	-2.19866800
O	-3.85060800	-0.83990400	-2.01997000
Cs	-4.34505900	-2.74345700	0.10313500

Int-PivNOH′-N

N	1.56913300	-2.04310000	-1.50765900
O	0.07905000	-0.67642400	-2.54165700
C	0.75447400	-0.91323300	-1.54633200

C	2.55152500	-2.91031800	0.57784000
C	3.70528400	-3.11861800	1.38583200
H	3.58532300	-3.64974100	2.32718200
C	4.94836300	-2.68955300	0.99901500
H	5.81681700	-2.87371500	1.62672500
C	5.12268500	-2.01033100	-0.23578800
C	6.40118800	-1.57770700	-0.67725900
H	7.26264600	-1.77419400	-0.04334000
C	6.55346400	-0.91964600	-1.87752000
H	7.53683600	-0.59407400	-2.20459800
C	5.42035900	-0.65813900	-2.68306200
H	5.53825400	-0.12716100	-3.62364700
C	4.16223200	-1.06311100	-2.28098500
H	3.29979500	-0.83754600	-2.89879700
C	3.97348800	-1.76007200	-1.05344300
C	2.68318600	-2.21775400	-0.61603400
C	1.49675600	-2.99257200	-2.62893700
H	0.54725700	-2.84274600	-3.14248100
H	2.31126200	-2.84690600	-3.34934900
H	1.55890400	-4.01349100	-2.23845500
C	1.23908500	-3.47191700	1.05850200
H	0.85056300	-2.88307900	1.89843800
H	0.48582500	-3.46346800	0.26963500
H	1.36539800	-4.50163900	1.41439900
C	-1.97131100	0.68471100	2.17620500
H	-1.84911600	1.77282000	2.15599900
H	-3.01767900	0.49296100	2.44928900
C	-1.01696000	0.12820200	3.24886600
H	-1.04953500	-0.96704200	3.27511700
H	0.00657900	0.41490300	2.99009800
C	-1.35683600	0.67165200	4.64544100
H	-2.38906400	0.39760100	4.90995400
H	-1.32748200	1.76996400	4.62038700
C	-0.39841600	0.16223700	5.72727900
H	-0.65635400	0.56617700	6.71314700
H	0.63483800	0.45442000	5.50486100
H	-0.42558800	-0.93249700	5.79846600
C	-2.44331400	1.58992200	-0.60475200
C	-1.38085700	2.73021600	-0.60649500
H	-1.14242700	3.04200400	0.41774800
H	-0.44655500	2.35983700	-1.04477700
C	-1.87569600	3.94439900	-1.42414000
H	-1.10103800	4.72214000	-1.39264400
C	-3.18447600	4.48648700	-0.82124700
H	-3.53367000	5.35784000	-1.39270900
H	-3.01601500	4.82668800	0.21013900
C	-4.24784000	3.37330100	-0.84613400
H	-5.18430800	3.74354300	-0.40702200
C	-4.49594300	2.92689000	-2.30076800
H	-5.27023800	2.14693000	-2.33019600
H	-4.87173200	3.77168400	-2.89462000
C	-3.18146200	2.39405200	-2.90343300
H	-3.35362200	2.06722700	-3.93758400
C	-2.69137700	1.17897600	-2.08159100
H	-1.77310300	0.76573700	-2.51215200
H	-3.45543800	0.39503900	-2.13806300
C	-2.11736000	3.50777000	-2.88178700
H	-2.45299500	4.36372000	-3.48403400
H	-1.18185600	3.14524100	-3.32785400
C	-3.75630600	2.16971100	-0.00651000
H	-4.54371400	1.41233000	0.02283000
H	-3.59436800	2.50228600	1.02560900
C	-2.77323500	-1.46291000	0.22760800
C	-4.30079900	-1.18635000	0.20578300
H	-4.56437600	-0.55609700	-0.64805800
H	-4.60658400	-0.64823400	1.11269200
C	-5.09628100	-2.50923500	0.09788100
H	-6.16790600	-2.26931700	0.08227000
C	-4.70485300	-3.23070300	-1.20646300
H	-4.94579100	-2.60046100	-2.07364600
H	-5.28433700	-4.15801900	-1.31359100
C	-3.19652600	-3.54477700	-1.18066000
H	-2.90794600	-4.05116600	-2.11118900
C	-2.88083000	-4.45035600	0.02498900
H	-1.81178400	-4.70305500	0.03901600
H	-3.43189700	-5.39789100	-0.05284100
C	-3.27232600	-3.71779100	1.32204300
H	-3.03012900	-4.34426700	2.19096400
C	-2.48826900	-2.39009300	1.44266800
H	-1.41484100	-2.59586900	1.51621600
H	-2.78721300	-1.89506100	2.37296500
C	-2.38598000	-2.23483700	-1.06228100
H	-2.54450200	-1.61672600	-1.95049900
H	-1.31857600	-2.47324700	-1.04093500
C	-4.78219500	-3.41293400	1.30431000
H	-5.35820100	-4.34627600	1.23930700
H	-5.08075500	-2.91727900	2.23869800
P	-1.69353500	0.12632200	0.40662500

Pd	0.68229300	0.28815200	0.05082600
C	2.23567600	2.15556400	0.99772400
O	1.14637900	1.86214700	1.61670600
N	2.60623200	1.23547500	0.11189600
O	3.54662400	1.65546200	-0.85800900
C	2.97620000	3.46498500	1.30502700
C	2.34808500	4.10933600	2.55508600
C	2.82553800	4.43252700	0.10730600
C	4.47004600	3.18163100	1.57930900
H	4.02352300	0.83512000	-1.07303600
H	2.87449100	5.04336300	2.78660800
H	2.42070200	3.44830300	3.42463000
H	1.28994900	4.33595300	2.39860700
H	1.76772900	4.64240600	-0.09308200
H	3.27290600	4.01966100	-0.79928200
H	3.31790400	5.38547900	0.33854700
H	4.95265500	2.72539900	0.71333500
H	4.98673200	4.12035100	1.81499500
H	4.58828300	2.50951400	2.43769200

Int-HCO_3'

N	-2.14301500	0.96104900	-1.80147600
O	-0.33493000	-0.23127500	-2.49373600
C	-1.07601800	0.11176200	-1.58070500
C	-3.27494200	2.19421900	-0.00156900
C	-4.42439200	2.36895500	0.81981600
H	-4.43360200	3.19554600	1.52660700
C	-5.51205500	1.53926800	0.72386600
H	-6.38451600	1.70079400	1.35279500
C	-5.52305600	0.46405100	-0.20369100
C	-6.64367300	-0.39814600	-0.33563300
H	-7.51283600	-0.22113800	0.29395700
C	-6.63451200	-1.43548000	-1.24079700
H	-7.49897700	-2.08700400	-1.33684100
C	-5.49179300	-1.65731800	-2.04508200
H	-5.48189600	-2.48528000	-2.74892700
C	-4.38765700	-0.84035400	-1.93664500
H	-3.50825900	-1.04052100	-2.53891900
C	-4.37064700	0.24797500	-1.02369900
C	-3.24835700	1.13403500	-0.89433300
C	-2.33528500	1.50410600	-3.15537700
H	-1.39424300	1.41660600	-3.69798200
H	-3.11398600	0.95888200	-3.70211600
H	-2.63322300	2.55468600	-3.08057300
C	-2.14970400	3.18929800	0.12860200
H	-1.65606900	3.09245600	1.10368200
H	-1.39283000	3.04848400	-0.64466300
H	-2.53037500	4.21617100	0.06163900
C	1.80276400	-0.14428200	2.30104400
H	1.85667000	-1.21484800	2.52491400
H	2.80167500	0.26682500	2.49813500
C	0.76433300	0.47667700	3.25463500
H	0.63128800	1.54532800	3.05466000
H	-0.20301700	-0.00565600	3.08653500
C	1.16981800	0.28930800	4.72513700
H	2.14812600	0.76008800	4.90333200
H	1.30199700	-0.78254500	4.92736400
C	0.13793200	0.86701100	5.69966500
H	0.44600800	0.71920100	6.74113300
H	-0.83835200	0.38580600	5.56753500
H	0.00208500	1.94449900	5.54218700
C	2.47166600	-1.55101200	-0.22292500
C	1.59570700	-2.81742100	0.01776600
H	1.36912800	-2.94041300	1.08387200
H	0.63229600	-2.69861900	-0.49218400
C	2.30269600	-4.08186200	-0.51751900
H	1.65649600	-4.94785600	-0.32340800
C	3.65362400	-4.26876700	0.19784200
H	4.15457500	-5.17582000	-0.16766100
H	3.49608400	-4.40237100	1.27714900
C	4.53690600	-3.03378100	-0.06140400
H	5.49957900	-3.14970700	0.45473200
C	4.77314300	-2.87563700	-1.57603300
H	5.42187200	-2.00956900	-1.77039400
H	5.29497300	-3.75875200	-1.96999200
C	3.41812300	-2.69565200	-2.28817100
H	3.57996800	-2.57261400	-3.36730300
C	2.71441000	-1.42705000	-1.75196800
H	1.76178000	-1.26778100	-2.26700700
H	3.35001400	-0.56060600	-1.96884700
C	2.53432300	-3.93153300	-2.03329000
H	3.01919800	-4.83264400	-2.43431900
H	1.57360200	-3.82289600	-2.55387900
C	3.83534300	-1.77044200	0.49228900
H	4.49433500	-0.90766600	0.35649900
H	3.68980300	-1.89496800	1.57136700
C	2.24031400	1.62646700	-0.09623900
C	3.79336600	1.63479100	-0.05617600

H	4.20031800	0.88736900	-0.74337700
H	4.15284000	1.38055400	0.94939500
C	4.34189700	3.02398600	-0.46022300
H	5.43880000	2.98816000	-0.42112000
C	3.88130500	3.35553400	-1.89308400
H	4.26625600	2.60546400	-2.59780300
H	4.28930900	4.32649700	-2.20594000
C	2.34147300	3.38541500	-1.93641800
H	2.00428000	3.61021700	-2.95679300
C	1.81837100	4.46148500	-0.96618700
H	0.72178800	4.50849900	-1.00968400
H	2.19252900	5.45305100	-1.25606000
C	2.28084500	4.11860100	0.46235400
H	1.89626600	4.86653600	1.16846400
C	1.74275400	2.73062200	0.87862800
H	0.64700400	2.74375200	0.90556200
H	2.08908600	2.51906900	1.89554800
C	1.77386300	2.00800000	-1.52667700
H	2.07509800	1.24855800	-2.25371900
H	0.68162600	2.04636900	-1.55693500
C	3.82061700	4.09776100	0.51275500
H	4.22357500	5.08295900	0.24068100
H	4.16452200	3.88351700	1.53441600
P	1.47206000	-0.04984200	0.45670600
Pd	-0.81487000	-0.61844700	0.26221900
C	-2.23017000	-2.15284000	1.73458800
O	-1.05934700	-1.93253900	2.14149000
O	-3.02796100	-2.94962400	2.47777300
O	-2.70535300	-1.66176300	0.65775000
H	-3.87772100	-2.99272400	2.00488200

TS-PivNOH′-O[1]

N	-0.76979400	2.78454800	-1.64998400
O	-0.13345600	0.91159700	-2.74014600
C	-0.42567100	1.45730200	-1.68293100
C	-0.40559500	4.78058100	-0.33015400
C	-0.72824100	5.58745800	0.79042800
H	-0.27075600	6.57062700	0.87064200
C	-1.57532400	5.14031300	1.77058500
H	-1.80864700	5.76541800	2.62919200
C	-2.12991200	3.83682900	1.70140100
C	-2.93434300	3.34806200	2.76188200
H	-3.13836100	4.00636600	3.60347700
C	-3.42968200	2.06556500	2.73261900
H	-4.04329000	1.69142500	3.54848700
C	-3.13522600	1.23396600	1.63343700
H	-3.52651200	0.22150200	1.62832200
C	-2.38423300	1.65822900	0.53535800
H	-2.91069200	0.89121900	-0.49016100
C	-1.85735600	2.99601900	0.56542600
C	-1.00906100	3.53014600	-0.46083400
C	-1.04798100	3.39888500	-2.96193600
H	-0.12942600	3.62232300	-3.51301600
H	-1.64222300	2.70172000	-3.55767500
H	-1.61492000	4.31684400	-2.80429700
C	0.62185400	5.30008300	-1.31122500
H	1.27480800	6.02696200	-0.81741700
H	1.24859100	4.49111200	-1.69977100
H	0.17215100	5.80704100	-2.17461300
C	1.08648600	-2.76069900	-0.69585200
H	2.09620800	-3.17762200	-0.80917500
H	0.59428600	-3.34650400	0.08866700
C	0.27721700	-2.93355300	-1.99242900
H	-0.73658800	-2.55416200	-1.82786100
H	0.70337600	-2.33076100	-2.80101800
C	0.22037700	-4.40501400	-2.43019100
H	-0.26419700	-4.99740800	-1.64114700
H	1.24365100	-4.79832800	-2.52439100
C	-0.52347200	-4.60761200	-3.75458000
H	-0.54602600	-5.66555000	-4.04121400
H	-0.04122400	-4.05107600	-4.56769400
H	-1.55963300	-4.25814800	-3.68334400
C	2.81124800	-0.28839500	-0.80895500
C	2.76712300	-0.56893100	-2.34034200
H	2.78308100	-1.65060500	-2.51933400
H	1.84108600	-0.17560600	-2.76887800
C	3.98873300	0.05893400	-3.04753900
H	3.91187600	-0.15007000	-4.12269000
C	5.27976900	-0.56507900	-2.48585500
H	6.16078600	-0.14558800	-2.99120100
H	5.28942800	-1.64803300	-2.67311700
C	5.35578100	-0.28593400	-0.97325000
H	6.26393600	-0.74127800	-0.55544400
C	5.37947700	1.23654600	-0.73397700
H	5.46299300	1.45096900	0.34090400
H	6.26106900	1.68014900	-1.21704000
C	4.08983300	1.86004000	-1.30187700
H	4.09334100	2.94372800	-1.12291300

C	2.85981400	1.24952600	-0.59408900
H	1.94708600	1.70889600	-0.98287000
H	2.89977300	1.48863000	0.47425900
C	4.00168200	1.58166300	-2.81444900
H	4.85496000	2.03819300	-3.33540900
H	3.08997300	2.03160500	-3.22938200
C	4.12732700	-0.89839000	-0.25653300
H	4.22210800	-0.70287900	0.81633900
H	4.13170800	-1.98843800	-0.38918800
C	1.42956500	-1.30745700	1.86032900
C	2.39325700	-2.46865400	2.23209100
H	3.40275700	-2.27602100	1.86055600
H	2.05752400	-3.40402000	1.76838800
C	2.44937500	-2.65719500	3.76710000
H	3.15119700	-3.47123500	3.99267200
C	2.93374200	-1.35404400	4.43390200
H	3.94340600	-1.10052200	4.08122900
H	3.00165100	-1.48986400	5.52209700
C	1.95186800	-0.21285000	4.10144200
H	2.29655900	0.72019300	4.56643600
C	0.54953500	-0.56936200	4.62982200
H	-0.15505900	0.24516700	4.41436700
H	0.57586600	-0.69293900	5.72127900
C	0.07504800	-1.87254700	3.95855000
H	-0.93366500	-2.12486900	4.31336000
C	0.02420500	-1.66433000	2.42917400
H	-0.68364800	-0.85869400	2.19698500
H	-0.35325200	-2.57339900	1.94424800
C	1.90060000	-0.01036000	2.57000100
H	2.89860500	0.27674500	2.22182100
H	1.22166100	0.81569700	2.32153400
C	1.04867800	-3.01690200	4.29647800
H	1.08234600	-3.17866500	5.38267300
H	0.70309700	-3.95696000	3.84367400
P	1.20480700	-1.01266000	-0.03258700
Pd	-0.90647500	0.19141900	-0.22389000
C	-3.58990700	-1.14323200	-0.76214500
O	-3.72792200	0.08742200	-1.13608100
N	-2.55256300	-1.44912200	0.00351300
O	-2.43983400	-2.84686700	0.32302000
C	-4.67996000	-2.13147100	-1.24394700
C	-5.71643000	-1.36822300	-2.09227500
C	-5.40542100	-2.74782500	-0.02531500
C	-4.05406400	-3.24072300	-2.11823900
H	-2.30898600	-2.82506200	1.28458900
H	-6.48684700	-2.07031500	-2.43425800
H	-5.25473100	-0.90581700	-2.96893500
H	-6.20076900	-0.57424600	-1.51717100
H	-5.85213800	-1.96496000	0.59967400
H	-4.72722500	-3.34289600	0.58832300
H	-6.21752400	-3.39811000	-0.37320900
H	-3.32986100	-3.83666800	-1.56089700
H	-4.84451700	-3.90713200	-2.48577500
H	-3.55258200	-2.80686800	-2.99161200

TS-$CsCO_3'$

N	1.11654800	1.87601600	2.23592700
O	1.92263700	-0.17597700	1.76977200
C	1.12557200	0.73273600	1.47940200
C	-0.43878800	3.53049900	3.06802900
C	-1.18904300	4.71966000	2.88211000
H	-1.72008600	5.13931900	3.73330300
C	-1.26625000	5.32458200	1.65454900
H	-1.84871400	6.23345800	1.52173700
C	-0.62277100	4.75489800	0.52568400
C	-0.78079000	5.34264100	-0.75540100
H	-1.37071500	6.25315100	-0.83749300
C	-0.22081500	4.76100200	-1.86953300
H	-0.35436300	5.20801600	-2.85163100
C	0.51842000	3.56900200	-1.73253700
H	0.92672800	3.08857100	-2.61531000
C	0.75902900	2.96591200	-0.49789400
H	1.83223600	2.22618500	-0.75118400
C	0.17079700	3.56159700	0.67179500
C	0.26610600	2.99844700	1.99064400
C	2.20474800	2.01576500	3.21687600
H	2.09433400	1.30780200	4.04390900
H	3.16518000	1.82040500	2.72821100
H	2.20568200	3.03484900	3.60224300
C	-0.46193500	2.87157800	4.42937400
H	-1.39404600	3.11669000	4.94914500
H	-0.39417900	1.78216000	4.34849600
H	0.36131500	3.20261100	5.07675900
C	-0.31542800	-2.49972200	-1.66558600
H	-0.77342600	-3.47272600	-1.44365700
H	-0.70655700	-2.18351300	-2.63775000
C	1.20964600	-2.61238000	-1.80209600
H	1.59382200	-1.62765400	-2.08054900

H	1.66181800	-2.90252600	-0.84266600
C	1.63546400	-3.61545500	-2.88403800
H	1.12826500	-3.35745800	-3.82359200
H	1.30627600	-4.63128900	-2.61906800
C	3.15045800	-3.58900600	-3.11927300
H	3.44812000	-4.27167300	-3.92363900
H	3.69561800	-3.89932300	-2.21417700
H	3.46353700	-2.57354400	-3.38892900
C	-1.25872900	-2.21558400	1.17536900
C	0.05612100	-2.98343200	1.50508300
H	0.28195300	-3.69832500	0.70459800
H	0.88889000	-2.27480900	1.56984000
C	-0.08103400	-3.76136600	2.83238300
H	0.86433700	-4.28517100	3.03096400
C	-1.22524700	-4.78526600	2.70685800
H	-1.32420300	-5.36382100	3.63591700
H	-1.00319100	-5.50377600	1.90517000
C	-2.54000700	-4.04114300	2.40575300
H	-3.36038600	-4.76414800	2.30235200
C	-2.84892500	-3.06427500	3.55794600
H	-3.79934100	-2.54519300	3.37056000
H	-2.96733100	-3.61805400	4.49967400
C	-1.70122700	-2.04305500	3.67938900
H	-1.92236000	-1.33339000	4.48803200
C	-1.56521400	-1.25486000	2.35764300
H	-0.76771000	-0.51306000	2.45019400
H	-2.49084100	-0.70020100	2.17216000
C	-0.38154800	-2.77874900	3.98002900
H	-0.45664000	-3.31965400	4.93394700
H	0.43912800	-2.05578400	4.07851500
C	-2.41156800	-3.24979700	1.08146400
H	-3.36232500	-2.74328400	0.88454200
H	-2.23996400	-3.94713300	0.25101400
C	-2.58051700	-0.64539400	-1.25734500
C	-3.41690300	-1.78777200	-1.90090800
H	-3.72893000	-2.51951800	-1.14910200
H	-2.82104500	-2.33003700	-2.64372000
C	-4.67426500	-1.21154700	-2.59490000
H	-5.24520600	-2.04493600	-3.02649700
C	-5.54252800	-0.46821300	-1.56065100
H	-5.87119100	-1.16103300	-0.77270500
H	-6.45022800	-0.07772900	-2.04119800
C	-4.72752300	0.68758200	-0.94678700
H	-5.33655100	1.21458600	-0.19997400
C	-4.30370000	1.66560200	-2.05883500
H	-3.73854900	2.50460800	-1.63140700
H	-5.19294100	2.09037000	-2.54558000
C	-3.43687400	0.91464900	-3.08819700
H	-3.11122200	1.60717800	-3.87499700
C	-2.18258500	0.35469700	-2.38448000
H	-1.60753300	1.18382900	-1.95841500
H	-1.52178600	-0.12198900	-3.11765400
C	-3.47610900	0.11356900	-0.24342100
H	-3.80502100	-0.56078400	0.55554600
H	-2.90447200	0.92377300	0.22720800
C	-4.24982000	-0.23647800	-3.70907900
H	-5.13665600	0.15721400	-4.22518800
H	-3.64749100	-0.76205400	-4.46298100
P	-0.93820500	-1.22589600	-0.43651800
Pd	0.44878800	0.71410300	-0.38959700
C	2.40697800	0.72824700	-2.32895500
O	2.85483500	1.55443600	-1.37581800
O	1.10124300	0.62753800	-2.49298800
O	3.22111800	0.01759500	-2.96483900
Cs	4.40387500	-0.71504300	-0.23380100

TS-HCO_3'

N	2.58400500	1.95668700	0.47313000
O	0.95094900	1.82683800	2.03839400
C	1.48676200	1.36930000	1.04467600
C	3.55123300	2.49136800	-1.69080600
C	4.27422000	2.08191400	-2.84327100
H	4.55678900	2.83910700	-3.57067500
C	4.59807800	0.76725000	-3.06207200
H	5.14727100	0.47348700	-3.95343500
C	4.18884700	-0.23333300	-2.14274400
C	4.44860800	-1.60666400	-2.38509000
H	4.99977000	-1.87891400	-3.28266300
C	4.00257500	-2.57801500	-1.51444100
H	4.20852800	-3.62722100	-1.71136900
C	3.27603900	-2.20337100	-0.36510200
H	2.91989400	-2.97143100	0.31765700
C	3.01744600	-0.86810600	-0.04850400
H	3.00897100	-0.79836100	1.31954800
C	3.47998600	0.14300300	-0.95286000
C	3.20714300	1.53367500	-0.74067700
C	3.25443900	2.96837300	1.31609900
H	2.70434500	3.91398000	1.32806000

H	3.31745600	2.58961300	2.33899200
H	4.25993500	3.13126000	0.92835900
C	3.15472700	3.94541200	-1.56957800
H	3.08541300	4.39996600	-2.56318200
H	2.18321700	4.05574300	-1.07759300
H	3.87961400	4.53706200	-0.99547500
C	-2.27526900	-0.62371000	1.97867900
H	-3.27744600	-0.17752700	2.02062700
H	-2.42282100	-1.70922000	1.95816300
C	-1.45388800	-0.26990200	3.23002500
H	-0.48201300	-0.76907200	3.15525300
H	-1.23850500	0.80295300	3.26289000
C	-2.14578400	-0.70289800	4.52992300
H	-2.36014600	-1.78110600	4.48686800
H	-3.12093900	-0.20189000	4.62094300
C	-1.29282000	-0.39959100	5.76727800
H	-1.77794200	-0.74915000	6.68604700
H	-1.11608400	0.67781000	5.86981000
H	-0.31068800	-0.88310500	5.69594900
C	-2.22943800	1.49738100	-0.16295900
C	-2.20288400	2.44812600	1.07026500
H	-2.81719300	2.03436000	1.87898300
H	-1.18312600	2.54107500	1.45565600
C	-2.75552600	3.84057400	0.69229100
H	-2.71812800	4.48244500	1.58222100
C	-4.21231800	3.70211700	0.21058600
H	-4.62656600	4.68803100	-0.04192500
H	-4.83893700	3.28871300	1.01328800
C	-4.25219600	2.78059500	-1.02283500
H	-5.28854800	2.66453800	-1.36743900
C	-3.39455300	3.39101000	-2.14948300
H	-3.43508300	2.75416100	-3.04439100
H	-3.79575800	4.37214900	-2.43809800
C	-1.93859100	3.53423000	-1.66297000
H	-1.32038300	3.95826600	-2.46530700
C	-1.37567200	2.14474700	-1.28841000
H	-0.33561500	2.24011900	-0.95558100
H	-1.36109000	1.50473600	-2.17804900
C	-1.89563200	4.45534000	-0.42858000
H	-2.26936200	5.45557400	-0.68809100
H	-0.85979900	4.57835800	-0.08406800
C	-3.69619800	1.38472300	-0.65464500
H	-3.75603800	0.73875400	-1.53734000
H	-4.32639300	0.92983900	0.12139800
C	-1.96192000	-1.61062400	-0.80642800
C	-3.43755900	-2.07717100	-0.68916400
H	-4.12157200	-1.27282700	-0.97689100
H	-3.67642800	-2.34139200	0.34775400
C	-3.68720700	-3.30658500	-1.59449700
H	-4.73862100	-3.60731700	-1.49453200
C	-3.38918600	-2.93586200	-3.06094800
H	-4.05264400	-2.12288700	-3.38816000
H	-3.58978600	-3.79435900	-3.71638700
C	-1.91471200	-2.50347500	-3.19004100
H	-1.69960900	-2.22677000	-4.23061600
C	-0.99785900	-3.66498700	-2.76067800
H	0.05668200	-3.37744900	-2.87024300
H	-1.16233500	-4.53588700	-3.41000800
C	-1.29847100	-4.03113900	-1.29429700
H	-0.63776200	-4.84505900	-0.96934000
C	-1.03952200	-2.80036400	-0.39902200
H	0.01838900	-2.50873900	-0.50636400
H	-1.18086400	-3.06781100	0.65470600
C	-1.65882900	-1.27219900	-2.29044100
H	-2.29300200	-0.44610600	-2.63255500
H	-0.61631300	-0.94252300	-2.39376000
C	-2.77065900	-4.46609600	-1.15829700
H	-2.96062400	-5.35304200	-1.77818600
H	-2.98707000	-4.75022900	-0.11915100
P	-1.45542800	-0.17114900	0.35437100
Pd	0.92705600	-0.44601500	0.45573100
C	2.25885300	-1.78141900	2.98377900
O	3.16945600	-0.97584800	2.58420300
O	2.31798300	-2.04767100	4.32093300
O	1.35963200	-2.31777100	2.30082200
H	1.59002900	-2.67174100	4.48322100

TS-Cl′

N	-2.84791700	-1.68073000	0.10566800
O	-1.12606200	-2.18002400	1.49987700
C	-1.67700000	-1.39800400	0.75167500
C	-4.04568500	-1.41310000	-1.99603100
C	-4.79940800	-0.58935100	-2.87548700
H	-5.24662500	-1.05008500	-3.75307700
C	-4.96287200	0.75426200	-2.65076400
H	-5.54966300	1.36283600	-3.33454200
C	-4.33846500	1.37130700	-1.53577100
C	-4.43455000	2.76795700	-1.30405900

H	-5.03066400	3.36753500	-1.98842600
C	-3.78428900	3.35962700	-0.24064700
H	-3.87629700	4.42931400	-0.06982300
C	-2.99733000	2.57191200	0.62479300
H	-2.50140300	3.05147600	1.46698400
C	-2.88111500	1.18818900	0.46634500
H	-3.05820100	0.59996000	1.77584800
C	-3.57440300	0.57140100	-0.62532900
C	-3.48925300	-0.83913300	-0.85608000
C	-3.59748800	-2.82072700	0.68161700
H	-3.13734700	-3.77564400	0.41244500
H	-3.60627000	-2.71579500	1.76884900
H	-4.62094600	-2.78358000	0.31109500
C	-3.85391300	-2.86773800	-2.36056600
H	-3.90601300	-2.99126200	-3.44722800
H	-2.88217900	-3.24100700	-2.02256600
H	-4.62281600	-3.51957000	-1.92593300
C	2.28074000	-0.09072500	2.16395300
H	3.24087900	-0.61728700	2.08942900
H	2.52100500	0.93707300	2.45934800
C	1.39685400	-0.71817800	3.25620400
H	0.45263200	-0.16230700	3.31954300
H	1.11270800	-1.73954000	2.98442800
C	2.08917000	-0.71832300	4.62674000
H	2.36476300	0.31192800	4.89669400
H	3.03399900	-1.27822000	4.56098700
C	1.21230100	-1.31925500	5.73069100
H	1.72504100	-1.30296600	6.69943000
H	0.95291900	-2.36055800	5.50537600
H	0.27379400	-0.76285000	5.83564300
C	2.14551100	-1.50192800	-0.49969900
C	1.97231800	-2.75300100	0.41096100
H	2.59204400	-2.65262400	1.31028600
H	0.93343600	-2.83879300	0.74256300
C	2.39862900	-4.03388900	-0.33962400
H	2.25868200	-4.89185800	0.33070700
C	3.88137300	-3.92266300	-0.74247900
H	4.20657900	-4.83545400	-1.26037400
H	4.51045000	-3.82205900	0.15306600
C	4.06575100	-2.69987300	-1.66114900
H	5.12231400	-2.60331000	-1.94482800
C	3.20097900	-2.87140400	-2.92628100
H	3.34197400	-2.01544300	-3.60136600
H	3.51516700	-3.76756700	-3.47861300
C	1.71814300	-2.99039600	-2.52041900
H	1.09662000	-3.10244600	-3.41863600
C	1.27974200	-1.71081500	-1.77372600
H	0.22230600	-1.78473000	-1.49325200
H	1.36672600	-0.84965800	-2.44607500
C	1.53075200	-4.21189900	-1.60048600
H	1.81342900	-5.13267700	-2.12925900
H	0.47398900	-4.31430900	-1.31886200
C	3.63557500	-1.41264600	-0.91842800
H	3.79806200	-0.55590800	-1.58157100
H	4.27356000	-1.26507500	-0.03650900
C	2.18236400	1.66865400	-0.21754300
C	3.68943200	1.93271700	0.04360000
H	4.30598300	1.18072500	-0.45828200
H	3.91266200	1.86233500	1.11487400
C	4.08715300	3.33823000	-0.46602800
H	5.15744400	3.49036900	-0.27381800
C	3.81226100	3.43555500	-1.97982000
H	4.41024100	2.68965000	-2.52187100
H	4.11592500	4.42191900	-2.35618600
C	2.31000200	3.20740600	-2.24305800
H	2.10923000	3.26401400	-3.32090400
C	1.48955000	4.28230900	-1.50453600
H	0.41764600	4.14496400	-1.70180500
H	1.75755600	5.28191300	-1.87290900
C	1.76822100	4.18365900	0.00780400
H	1.17465700	4.93367800	0.54636300
C	1.36527300	2.77961200	0.50976900
H	0.28692800	2.63549000	0.32343600
H	1.50987500	2.72046400	1.59620100
C	1.90718100	1.80274900	-1.73884000
H	2.47568300	1.04938600	-2.29580800
H	0.84403800	1.61975800	-1.94582900
C	3.26859900	4.41144500	0.27709300
H	3.56368200	5.41438800	-0.06001200
H	3.47199600	4.36475600	1.35593800
P	1.49684000	0.01484000	0.46414600
Pd	-0.89954000	0.43333500	0.58985200
Cl	-3.54827200	0.12848900	3.16579000

TS-red1

N	-2.88755200	-1.80226000	0.86622100
O	-1.18983400	-3.16158700	1.62577500
C	-1.62908800	-2.42785600	0.75695800

C	-2.94378600	-2.00020200	-1.47273900
C	-3.44410200	-1.68850200	-2.75558900
H	-2.99769000	-2.16101100	-3.62704200
C	-4.50626200	-0.82389000	-2.89837600
H	-4.91291500	-0.60701100	-3.88290900
C	-5.07424300	-0.18061400	-1.76782500
C	-6.13615800	0.75372500	-1.91106300
H	-6.53987000	0.92509800	-2.90641600
C	-6.63456200	1.44331900	-0.83010500
H	-7.44295500	2.15768400	-0.95998300
C	-6.07569500	1.23514000	0.45334000
H	-6.44625900	1.80429600	1.30173200
C	-5.06275500	0.31906800	0.63660900
H	-4.64240500	0.18952900	1.62626700
C	-4.54533400	-0.43875700	-0.45355200
C	-3.50231200	-1.40713600	-0.34137900
C	-3.63992600	-2.06995800	2.09539400
H	-3.50061000	-1.28027900	2.84293100
H	-4.70311600	-2.15923300	1.86393400
H	-3.26832500	-3.00695700	2.51740900
C	-1.77955300	-2.87840200	-1.18315900
H	-2.03331400	-3.89255100	-0.86381400
H	-1.06421300	-2.96834100	-2.01495100
C	2.01910000	-0.47869800	2.10487800
H	2.74722000	0.24909300	2.48607300
H	1.14008800	-0.41642200	2.75334500
C	2.57066600	-1.90950300	2.22421500
H	1.86212900	-2.60782600	1.76089400
H	3.51873100	-2.00600000	1.68036900
C	2.79941100	-2.31806400	3.68788400
H	1.84756100	-2.24550600	4.23181800
H	3.48462400	-1.60352600	4.16709100
C	3.35927700	-3.73779800	3.82657400
H	3.50598800	-4.00772500	4.87874300
H	4.32783600	-3.83449000	3.31999600
H	2.67751900	-4.47382200	3.38417400
C	2.96578100	0.19633400	-0.67539400
C	3.25555700	-1.22820400	-1.23876300
H	3.41186200	-1.94152200	-0.42318800
H	2.37862900	-1.58385100	-1.79679800
C	4.49523700	-1.21805600	-2.15935400
H	4.67383900	-2.23984700	-2.51978600
C	5.72408000	-0.72301900	-1.37074700
H	6.61426400	-0.72945100	-2.01477800
H	5.93259200	-1.39982200	-0.53053200
C	5.45619600	0.70246600	-0.84951400
H	6.32617400	1.05921400	-0.28191100
C	5.19009200	1.64415300	-2.04053800
H	5.01545200	2.66847500	-1.68216800
H	6.07041700	1.68177800	-2.69689100
C	3.96357500	1.13937200	-2.82640900
H	3.76042100	1.81526300	-3.66789800
C	2.72958100	1.12662000	-1.89610800
H	1.84569700	0.79075200	-2.45496200
H	2.53206800	2.15228300	-1.56750400
C	4.23717200	-0.28108800	-3.35407900
H	5.10455600	-0.27457800	-4.02875300
H	3.37907000	-0.64009200	-3.93904600
C	4.22538700	0.68602100	0.08717200
H	4.06370300	1.69045400	0.49535300
H	4.43500700	0.02718700	0.93808400
C	0.60119100	1.75762800	0.76728900
C	1.60126900	2.87811900	1.15176900
H	2.32549300	3.04539300	0.34650600
H	2.17489500	2.58778300	2.04249200
C	0.85022400	4.20211700	1.42875100
H	1.58475900	4.97547100	1.69137400
C	0.07734600	4.62725600	0.16408500
H	0.77538600	4.78670000	-0.67012000
H	-0.43238300	5.58487400	0.33911000
C	-0.95120100	3.53674800	-0.20127700
H	-1.49700100	3.83129100	-1.10732800
C	-1.94006900	3.34882800	0.96338700
H	-2.69381500	2.59420600	0.70259200
H	-2.47907000	4.28629600	1.16016700
C	-1.15897300	2.91454200	2.21672400
H	-1.85414000	2.75405100	3.05192800
C	-0.40824800	1.59184200	1.94293400
H	-1.12177700	0.79100400	1.70906200
H	0.11478100	1.30372900	2.86120700
C	-0.21930900	2.20470800	-0.47621100
H	0.42930500	2.32757400	-1.34865800
H	-0.94274300	1.41871100	-0.72866200
C	-0.13775100	4.00671800	2.59431800
H	-0.65558600	4.95080400	2.81307700
H	0.40479800	3.72089400	3.50652100
P	1.38895600	0.04044400	0.41576000
Pd	-0.18109500	-1.51778300	-0.40141100

TS-red2

N	-2.38479600	-0.77163700	-1.96146000
O	-0.92246600	-2.53881000	-1.68092600
C	-1.56874300	-1.62550100	-1.19666300
C	-4.37379500	0.73762800	-1.85029800
C	-5.58700700	1.00154200	-1.14510600
H	-6.26281900	1.74048400	-1.57009500
C	-5.94435300	0.35061900	0.01255800
H	-6.90269300	0.55055900	0.48541900
C	-5.04874000	-0.58361300	0.60142200
C	-5.31888300	-1.33822400	1.77421600
H	-6.27370400	-1.20689000	2.27827600
C	-4.39350000	-2.24317000	2.25774500
H	-4.62643500	-2.83283200	3.14143800
C	-3.12266300	-2.39066300	1.64226600
H	-2.39502400	-3.06841700	2.08142000
C	-2.80817300	-1.62916100	0.52597300
C	-3.80206000	-0.80109300	-0.04310300
C	-3.52003800	-0.21833200	-1.31502800
C	-2.44498900	-1.05308900	-3.40328200
H	-1.74950600	-1.86775400	-3.60401700
H	-3.45584800	-1.36364600	-3.69016300
H	-2.15810500	-0.18048100	-3.99545800
C	-4.08412900	1.52770800	-3.10817600
H	-4.66300700	2.45725300	-3.10490600
H	-3.02526900	1.79787300	-3.17875900
H	-4.34760100	0.98814000	-4.02662800
C	2.03722900	0.12374000	2.40412000
H	2.66888000	-0.76621800	2.49932800
H	2.70244700	0.98626200	2.53950300
C	0.97243200	0.08139300	3.51350800
H	0.29267200	0.93805500	3.42731100
H	0.34900000	-0.81314400	3.37144800
C	1.58248200	0.06058600	4.92283100
H	2.19858100	0.96018600	5.06485000
H	2.26781400	-0.79475200	5.00933700
C	0.52551300	-0.01566800	6.02978100
H	0.98783900	-0.02430300	7.02342800
H	-0.08100400	-0.92473500	5.93571300
H	-0.15665300	0.84230200	5.98643300
C	2.62892300	-0.94995700	-0.28831300
C	2.32228100	-2.42722200	0.10340200
H	2.44642200	-2.56859600	1.18630500
H	1.27912600	-2.66035200	-0.13715200
C	3.25832900	-3.39777100	-0.64898700
H	3.01699500	-4.42428000	-0.34313900
C	4.72537700	-3.08054000	-0.30292300
H	5.39825400	-3.77738200	-0.82180700
H	4.89825600	-3.21249600	0.77469800
C	5.04369200	-1.63087500	-0.71701300
H	6.08597400	-1.39262500	-0.46475500
C	4.82589600	-1.47086900	-2.23512400
H	5.07330200	-0.44622300	-2.54758400
H	5.49899200	-2.14315400	-2.78507000
C	3.35788700	-1.79222400	-2.57680800
H	3.19325300	-1.66799100	-3.65554900
C	2.42662700	-0.81713400	-1.82128900
H	1.38214800	-1.02762300	-2.07969200
H	2.64971500	0.20649100	-2.14596700
C	3.03347700	-3.24119900	-2.16583200
H	3.67376400	-3.94274600	-2.71895000
H	1.99238900	-3.48038800	-2.41675800
C	4.11602500	-0.65352600	0.04473500
H	4.37944700	0.37422600	-0.22647100
H	4.29881600	-0.75376400	1.12155400
C	1.34977700	1.94031900	0.11278400
C	2.74415000	2.57423500	-0.12133300
H	3.27197900	2.04405700	-0.92199200
H	3.36300700	2.49020500	0.78252100
C	2.60182300	4.06283200	-0.51890300
H	3.60432200	4.48235300	-0.67794100
C	1.78178900	4.16800700	-1.82103900
H	2.29468400	3.63578600	-2.63446200
H	1.69885500	5.21921400	-2.13006000
C	0.38009800	3.56710900	-1.59355300
H	-0.20359400	3.62936900	-2.52189900
C	-0.33852000	4.34493900	-0.47491000
H	-1.34677500	3.93784300	-0.31909900
H	-0.45759100	5.39960900	-0.75965400
C	0.48364000	4.23529600	0.82307200
H	-0.02793500	4.77181400	1.63330200
C	0.62494200	2.75106400	1.22611300
H	-0.36737000	2.31860200	1.41340200
H	1.18636200	2.69459800	2.16686800
C	0.51149600	2.08273200	-1.18924500
H	0.97753200	1.52487800	-2.00845100
H	-0.48055800	1.64096700	-1.03382400
C	1.88532900	4.83812600	0.60333000

H	1.80356600	5.90073700	0.33609900
H	2.46982700	4.78630700	1.53269600
P	1.34190400	0.10797000	0.65823000
Pd	-0.86216800	-0.85681000	0.55799100

Int-sp^3-anion

N	-1.14997200	-0.84819000	-2.89101400
O	0.69847100	0.44030100	-3.27346900
C	-0.21440200	0.07843700	-2.53146900
C	-3.50109200	-1.12820700	-2.10806900
C	-4.38996700	-1.92748200	-1.27261100
H	-5.44431000	-1.65153300	-1.27481000
C	-3.97832900	-2.99005300	-0.53081200
H	-4.69744100	-3.55360500	0.06420800
C	-2.61444300	-3.43007000	-0.54969800
C	-2.19761100	-4.59893900	0.11142300
H	-2.93525500	-5.14669600	0.69872900
C	-0.89730900	-5.08000000	0.00342200
H	-0.59676400	-5.99631300	0.50559500
C	0.01524700	-4.36178200	-0.79676500
H	1.03293400	-4.73216600	-0.91674700
C	-0.35226600	-3.18874600	-1.43292400
H	0.37714700	-2.66017900	-2.03763400
C	-1.67899800	-2.65800800	-1.33622000
C	-2.10303600	-1.48132900	-2.00563700
C	-1.12189000	-1.36669000	-4.26450000
H	-0.52370900	-0.70129700	-4.88897400
H	-0.68914700	-2.37636500	-4.29195100
H	-2.15057200	-1.40983000	-4.63590500
C	-4.05323100	-0.13855500	-2.90931100
H	-5.13358500	-0.08849500	-3.02896300
H	-3.44248200	0.47909600	-3.55693800
C	1.66470600	2.29893600	1.32256800
H	1.09219900	2.27648000	2.25582800
H	2.72095900	2.38697400	1.61034300
C	1.21486000	3.54344600	0.53663100
H	1.68769800	3.57744800	-0.45116200
H	0.13591000	3.47676600	0.36023100
C	1.52971100	4.84257700	1.29428700
H	2.61263000	4.91121200	1.48044000
H	1.05143500	4.81023600	2.28425400
C	1.05988800	6.09380400	0.54369200
H	1.28615700	7.00982800	1.10398000
H	-0.02227700	6.06211800	0.37050000
H	1.54634200	6.17159200	-0.43664700
C	1.10282500	-0.49467700	2.05014400
C	-0.38718600	-0.28869000	2.45126600
H	-0.58817200	0.76470100	2.68123500
H	-1.03064100	-0.53911500	1.60088600
C	-0.75558700	-1.17341900	3.66103200
H	-1.80751700	-0.99114900	3.92002200
C	0.14378700	-0.82060000	4.86154000
H	-0.12517100	-1.43450900	5.73390300
H	-0.00361700	0.23003200	5.15113800
C	1.61751700	-1.06128200	4.48009800
H	2.26757000	-0.80275500	5.32891600
C	1.81613600	-2.54353600	4.10510100
H	2.87098200	-2.73124500	3.85551100
H	1.57194500	-3.18555700	4.96433700
C	0.91325200	-2.88764000	2.90446300
H	1.05473700	-3.93626600	2.61249100
C	1.29745200	-1.99251400	1.70467300
H	0.69612300	-2.26545100	0.83161700
H	2.34679600	-2.18985500	1.45111900
C	-0.56096000	-2.65475900	3.28500300
H	-0.83724100	-3.30140400	4.13160100
H	-1.21056700	-2.92553700	2.44413400
C	1.99334200	-0.16041300	3.27893100
H	3.05300400	-0.30212300	3.03979500
H	1.87296800	0.88737300	3.57659500
C	3.04668800	0.24052400	-0.35477300
C	4.26238000	0.09028300	0.59518700
H	4.11683700	-0.76107000	1.26978900
H	4.37886100	0.98364100	1.22391400
C	5.56088600	-0.13790600	-0.21639000
H	6.40246300	-0.23394000	0.48503300
C	5.42381300	-1.43033500	-1.04587600
H	5.27150200	-2.29177300	-0.37964800
H	6.35175800	-1.61846600	-1.60601200
C	4.23271400	-1.28867200	-2.01303000
H	4.11862800	-2.21248900	-2.59648900
C	4.47288200	-0.10139400	-2.96478700
H	3.62915300	-0.00489000	-3.65855700
H	5.38061000	-0.26935300	-3.56395600
C	4.61524700	1.18664800	-2.13195500
H	4.77560400	2.04409200	-2.80015800
C	3.32126600	1.42759300	-1.32420600
H	2.47197400	1.54557000	-2.00628300

H	3.43477100	2.35874900	-0.75621500
C	2.93113700	-1.04903000	-1.21495100
H	2.72808600	-1.91991500	-0.58453100
H	2.09760300	-0.94492800	-1.91189300
C	5.80616600	1.05317100	-1.16291500
H	6.74102000	0.90208500	-1.72277300
H	5.92735600	1.97902100	-0.58156600
P	1.37534200	0.62139500	0.50516600
Pd	-0.55952900	1.04129700	-0.80942300
C	-3.08468600	2.10640100	0.25160100
O	-1.96804000	2.13396300	0.84641100
N	-3.17735000	2.04010700	-1.07739000
O	-2.04407700	2.03165100	-1.84367200
C	-4.38703500	2.14631100	1.07051600
C	-4.42488300	0.87691600	1.95042900
C	-5.65162300	2.20545800	0.19425000
C	-4.32801400	3.39817400	1.97190100
H	-3.92703400	1.50875300	-1.55174700
H	-5.31118100	0.88797800	2.59883900
H	-3.53201600	0.82287100	2.58034100
H	-4.45998100	-0.02805000	1.33282700
H	-5.75861600	1.30987900	-0.42846500
H	-5.63876700	3.07879900	-0.46714100
H	-6.54137700	2.27264100	0.83328500
H	-4.33489600	4.31542300	1.37011500
H	-5.19500500	3.42552300	2.64497300
H	-3.41387700	3.39241200	2.57171800

Int-sp^3-radical

N	0.37558300	1.95979800	-2.59391100
O	-0.58594800	0.01060400	-3.25971800
C	0.09369700	0.61034700	-2.43310700
C	2.60729200	2.81755800	-1.97257900
C	3.39650400	3.65469100	-1.10003100
H	4.47176200	3.68000100	-1.25954300
C	2.83188100	4.40801400	-0.11594900
H	3.45032900	5.03545600	0.52185700
C	1.41492500	4.42143200	0.07782100
C	0.80551000	5.26084300	1.03708700
H	1.44169700	5.88578800	1.65993700
C	-0.57015900	5.31088200	1.17334300
H	-1.02469200	5.97261600	1.90538800
C	-1.38322800	4.50349600	0.34811700
H	-2.46476500	4.54939100	0.44693800
C	-0.81684100	3.65201800	-0.57983500
H	-1.44670300	3.02515300	-1.19997400
C	0.59418900	3.57974700	-0.74862000
C	1.20665200	2.74282900	-1.72785800
C	-0.10355700	2.64641800	-3.80356300
H	-0.76542800	1.96590500	-4.33847400
H	-0.64484900	3.55849000	-3.52912100
H	0.73861300	2.92190300	-4.44987800
C	3.22602800	2.15026900	-3.03363800
H	4.29751100	2.23920800	-3.18280200
H	2.67745500	1.50732400	-3.70643900
C	-0.70244500	-2.78959000	0.67317300
H	-0.00574300	-2.81342900	1.51712300
H	-1.64472200	-3.22536400	1.02946200
C	-0.09820400	-3.65751400	-0.44561500
H	-0.69443700	-3.60364000	-1.36129900
H	0.89073800	-3.26356000	-0.69653700
C	0.02974800	-5.12672800	-0.01370200
H	-0.96285500	-5.52294100	0.24647200
H	0.63140400	-5.18486900	0.90493000
C	0.66272900	-6.00891000	-1.09524800
H	0.74384900	-7.05130400	-0.76572800
H	1.67060300	-5.65855600	-1.34976900
H	0.06737900	-5.99457800	-2.01639000
C	-0.94586900	-0.21461200	2.10596600
C	0.55153100	0.00753600	2.46445900
H	1.10525700	-0.93563900	2.41444200
H	1.01085700	0.66712800	1.71865600
C	0.69655000	0.62963100	3.86938100
H	1.76574500	0.75981000	4.08424300
C	0.06440700	-0.30273400	4.92036100
H	0.17938800	0.12315300	5.92690500
H	0.57822000	-1.27440400	4.92286300
C	-1.42871200	-0.49512700	4.59322300
H	-1.88691700	-1.16796700	5.33089500
C	-2.14273400	0.87022500	4.62001300
H	-3.21459600	0.74207600	4.41200000
H	-2.06323200	1.31865600	5.62018600
C	-1.50178700	1.79707600	3.56869400
H	-2.01409900	2.76839500	3.56702800
C	-1.65237400	1.16455900	2.16571600
H	-1.23148200	1.83724000	1.41108200
H	-2.72088600	1.05947200	1.94777600
C	-0.01115300	1.99766800	3.89825200

H	0.09709200	2.46277000	4.88844300
H	0.44706500	2.67922300	3.16971600
C	-1.57368300	-1.13477800	3.19172900
H	-2.63413700	-1.31439300	2.98630000
H	-1.08157000	-2.11321000	3.20312800
C	-2.74630300	-0.88269900	-0.42866200
C	-3.87489100	-1.29508800	0.55516000
H	-3.90720200	-0.61885100	1.41582300
H	-3.69687800	-2.30569300	0.94567300
C	-5.25128300	-1.25658300	-0.15364700
H	-6.02264000	-1.55255300	0.57039100
C	-5.53083900	0.17320200	-0.65662400
H	-5.55727900	0.87478200	0.18953000
H	-6.51825800	0.21631300	-1.13694500
C	-4.43218700	0.58351100	-1.65582400
H	-4.61601400	1.60758300	-2.00817500
C	-4.42438500	-0.38513500	-2.85338200
H	-3.64623500	-0.09097700	-3.56878400
H	-5.38812700	-0.34551400	-3.38058600
C	-4.15540000	-1.81261700	-2.34256800
H	-4.13578200	-2.51115600	-3.18952000
C	-2.78311700	-1.86653800	-1.63482100
H	-1.98393200	-1.62120400	-2.34191400
H	-2.62399200	-2.89054300	-1.27994200
C	-3.05401100	0.54511500	-0.95771800
H	-3.04387100	1.27133400	-0.13873200
H	-2.28320500	0.84164700	-1.67110800
C	-5.25698400	-2.22823600	-1.34843500
H	-6.24055100	-2.21541300	-1.83846900
H	-5.08605200	-3.25716400	-1.00143300
P	-0.98029900	-0.96306200	0.32508100
Pd	0.96404100	-0.40665100	-0.94480100
C	3.47447400	-1.62214800	-0.11979800
O	2.31141300	-1.58110500	0.39624900
N	3.71320300	-1.05314700	-1.28908100
O	2.76565000	-0.42703200	-2.04304200
C	4.61458600	-2.32572700	0.63049300
C	4.80772300	-1.59310200	1.97685300
C	5.94513900	-2.32902200	-0.14546000
C	4.17064900	-3.78137100	0.89299700
H	4.62364900	-1.07999100	-1.72763600
H	5.56959900	-2.10224500	2.57909400
H	3.87230500	-1.57208600	2.54223500
H	5.13318100	-0.55800700	1.81918400
H	6.31689700	-1.31296200	-0.32761500
H	5.85840400	-2.85123300	-1.10634100
H	6.71019700	-2.85137600	0.43915100
H	4.05162100	-4.33421200	-0.04654700
H	4.91960700	-4.30221200	1.50119900
H	3.21443700	-3.80086700	1.42240400

Int-sp^2-anion

N	0.23266900	1.82524000	-2.76830100
O	-0.58283500	-0.24185800	-3.27672800
C	0.00975700	0.50601000	-2.50534600
C	1.94761200	3.25394800	-1.78391900
C	2.31413500	4.25896900	-0.84938300
H	3.34912900	4.59851200	-0.83072100
C	1.39058400	4.82129700	0.00101700
H	1.69438400	5.60293100	0.69892400
C	0.02599500	4.43405700	-0.04726200
C	-0.95931700	5.07894400	0.74858400
H	-0.65344800	5.86573600	1.43854600
C	-2.28404000	4.72116100	0.60537300
H	-3.04647600	5.23275400	1.19882200
C	-2.65605800	3.70018300	-0.31117700
H	-3.72999500	3.47755700	-0.36494100
C	-1.76867300	2.97703000	-1.11448000
C	-0.39480200	3.39107100	-0.95549300
C	0.63192500	2.80125800	-1.77728100
C	-0.46301200	2.38822300	-3.93439400
H	-0.51276500	1.63053600	-4.71842100
H	-1.46891000	2.69280100	-3.61668300
H	0.09898800	3.25846400	-4.28807800
C	2.96683600	2.76498200	-2.78760100
H	3.95987400	3.16962000	-2.55165400
H	2.71401700	3.09932500	-3.80453600
C	-0.08415100	-2.72091000	0.95249400
H	0.66504700	-2.45328900	1.70515600
H	-0.87187800	-3.28052400	1.47306500
C	0.61969800	-3.62784300	-0.07203300
H	-0.08452800	-4.00235200	-0.82174500
H	1.36903900	-3.04200900	-0.61311000
C	1.29993100	-4.82615900	0.60781400
H	0.55495700	-5.40180600	1.17797300
H	2.02983800	-4.45721100	1.34192000
C	2.00532200	-5.75313500	-0.38836500
H	2.49245700	-6.59592400	0.11815400

H	2.77392200	-5.21005100	-0.95209100
H	1.29584900	-6.16586100	-1.11676200
C	-0.87266000	-0.13660400	2.09321200
C	0.53235900	0.48560100	2.33711500
H	1.30564800	-0.29183700	2.34084600
H	0.77711100	1.15907400	1.50794100
C	0.56351900	1.26627200	3.66825700
H	1.57227000	1.67925000	3.80829600
C	0.22370600	0.31991500	4.83650700
H	0.26468500	0.86284100	5.79256500
H	0.96330800	-0.49224600	4.89636800
C	-1.18576900	-0.26579500	4.62102500
H	-1.43223700	-0.95122400	5.44552600
C	-2.21629000	0.87811000	4.56779700
H	-3.22875200	0.46751400	4.44007400
H	-2.21350200	1.43322100	5.51783100
C	-1.86800800	1.81499300	3.39430000
H	-2.60423400	2.62586700	3.32536600
C	-1.90921400	1.01458400	2.07214300
H	-1.73711600	1.68130500	1.22190700
H	-2.91952000	0.60565900	1.95718500
C	-0.46518900	2.41094000	3.61171300
H	-0.44179400	2.99012900	4.54762200
H	-0.22529400	3.10085100	2.79438700
C	-1.21263600	-1.06360800	3.29483200
H	-2.20336500	-1.51580000	3.16480900
H	-0.49401700	-1.88636600	3.37493500
C	-2.49945400	-1.43201600	-0.32570000
C	-3.47184900	-2.12549000	0.66609600
H	-3.67698200	-1.47415000	1.52388500
H	-3.03550700	-3.05308700	1.06214900
C	-4.81169900	-2.45653400	-0.04058800
H	-5.47881200	-2.94440500	0.68557800
C	-5.46406600	-1.15931700	-0.56050700
H	-5.68180100	-0.48174900	0.27728200
H	-6.42568300	-1.39350700	-1.04225600
C	-4.50806000	-0.47508200	-1.55821700
H	-4.95116900	0.46389700	-1.91448700
C	-4.24363600	-1.41099000	-2.75113500
H	-3.56239900	-0.92489400	-3.45998500
H	-5.18167600	-1.62889100	-3.28494500
C	-3.61089700	-2.71470500	-2.23234300
H	-3.40793700	-3.39156100	-3.07443100
C	-2.27598000	-2.39756500	-1.52672500
H	-1.57100400	-1.95457400	-2.23642000
H	-1.85364900	-3.34209300	-1.16754400
C	-3.18191100	-0.13684100	-0.84570000
H	-3.40622300	0.53492400	-0.01469600
H	-2.52711800	0.44321700	-1.50092600
C	-4.56012400	-3.40222800	-1.23165100
H	-5.51467500	-3.65563400	-1.71664300
H	-4.11867400	-4.34670500	-0.87975500
P	-0.76087300	-1.04976200	0.39052200
Pd	1.03410700	-0.31264900	-0.98785100
C	3.79689900	-1.00064300	-0.15385700
O	2.67909900	-1.14062400	0.42547000
N	3.87799400	-0.59092600	-1.41185100
O	2.80512500	-0.33009400	-2.20728400
C	5.09445800	-1.28606900	0.62442100
C	5.14888700	-0.29860100	1.81081400
C	6.37253900	-1.13690000	-0.22187800
C	5.00467400	-2.73014100	1.16180100
H	4.76805000	-0.47094400	-1.87606400
H	6.01652500	-0.51320400	2.44791400
H	4.24058800	-0.37725200	2.41380200
H	5.22993500	0.73594600	1.45715300
H	6.50197700	-0.11170300	-0.59051700
H	6.37719300	-1.82164700	-1.07919100
H	7.25091200	-1.37319000	0.39045300
H	4.99356100	-3.45689300	0.34026000
H	5.86541800	-2.95439600	1.80461600
H	4.08732700	-2.86073300	1.74139000
H	3.01948300	1.67225400	-2.80505100

Int-sp^2-radical

N	0.62917300	2.21815300	-2.39029100
O	-0.48420500	0.41228200	-3.19169000
C	0.22617600	0.89595800	-2.31570700
C	2.85669500	2.99479900	-1.69944000
C	3.65587300	3.69443200	-0.75209700
H	4.72642400	3.75811000	-0.93334700
C	3.12133000	4.29533500	0.36159000
H	3.76170500	4.82672100	1.06202100
C	1.72202900	4.26643800	0.59412900
C	1.10676600	4.95477400	1.67622400
H	1.74323900	5.48747700	2.37866700
C	-0.26277600	4.97969100	1.82797500
H	-0.71597600	5.52744400	2.65053500

C	-1.09725000	4.29397700	0.89733300
H	-2.17880700	4.31968100	1.00286400
C	-0.48023300	3.61309800	-0.10595500
C	0.90053900	3.54176900	-0.34027100
C	1.49521700	2.87399600	-1.45546400
C	0.17458100	3.03849900	-3.52048800
H	-0.56042000	2.46134400	-4.08059100
H	-0.27953300	3.96381200	-3.14963700
H	1.01115000	3.29534800	-4.18188800
C	3.51106600	2.48381800	-2.95845300
H	4.50766600	2.08629100	-2.74224700
H	3.63754100	3.30718100	-3.67643600
C	-0.94086800	-2.81756900	0.22998900
H	-0.28421700	-3.03335400	1.07923700
H	-1.92479200	-3.23678200	0.47745200
C	-0.34965900	-3.52400000	-1.00348200
H	-0.93049400	-3.30340400	-1.90476600
H	0.65729300	-3.13376800	-1.18033300
C	-0.28348900	-5.04659800	-0.80729100
H	-1.29445700	-5.43973100	-0.62475300
H	0.29900100	-5.27169400	0.09795200
C	0.33672400	-5.77252800	-2.00607700
H	0.37156000	-6.85625600	-1.84425200
H	1.36204000	-5.42778300	-2.18804100
H	-0.23928500	-5.58943400	-2.92139800
C	-1.06020200	-0.49411000	2.05915600
C	0.42689400	-0.45763600	2.51390800
H	0.90714200	-1.42599300	2.34001000
H	0.97759400	0.26688100	1.90258600
C	0.53745700	-0.07062000	4.00475000
H	1.59948600	-0.06418600	4.28482500
C	-0.22177100	-1.09523500	4.86927000
H	-0.13358300	-0.83535500	5.93358900
H	0.21782500	-2.09503500	4.74667000
C	-1.70321100	-1.11184000	4.44729000
H	-2.25296800	-1.84839500	5.04896200
C	-2.31389400	0.28796400	4.65416800
H	-3.37762400	0.28151900	4.37665000
H	-2.26308900	0.56917000	5.71525600
C	-1.54516400	1.30951700	3.79381200
H	-1.98257500	2.30868300	3.92302100
C	-1.65921600	0.91365500	2.30461900
H	-1.14274200	1.65314200	1.68421800
H	-2.71695200	0.93679700	2.02248500
C	-0.06454600	1.33129400	4.21674700
H	0.02386700	1.62850800	5.27141300
H	0.48452200	2.07520100	3.62431700
C	-1.81172600	-1.51725100	2.95776700
H	-2.86797400	-1.58231400	2.67954100
H	-1.38830900	-2.52038000	2.83561300
C	-2.80160200	-0.60101800	-0.59380900
C	-3.99141700	-1.06088400	0.29210100
H	-3.99864800	-0.52387800	1.24581900
H	-3.90644400	-2.13067500	0.52456100
C	-5.33762300	-0.79510000	-0.42480500
H	-6.15226800	-1.12955800	0.23212600
C	-5.47911300	0.71458900	-0.70208800
H	-5.47019300	1.27501300	0.24386600
H	-6.44478900	0.91985100	-1.18483000
C	-4.31968600	1.17706200	-1.60560600
H	-4.40720200	2.25495400	-1.79762600
C	-4.35760600	0.40608100	-2.93891300
H	-3.53518900	0.73565300	-3.58619900
H	-5.29777800	0.61017800	-3.47083100
C	-4.22607700	-1.10117600	-2.65172600
H	-4.23820300	-1.65966200	-3.59715300
C	-2.88599600	-1.38523300	-1.93728600
H	-2.04850200	-1.10877000	-2.58442600
H	-2.82549300	-2.46146600	-1.74001800
C	-2.97069700	0.91323700	-0.90065300
H	-2.92613400	1.50160600	0.02060600
H	-2.15510400	1.25411600	-1.54070600
C	-5.38992400	-1.56661200	-1.75669300
H	-6.35287300	-1.39133500	-2.25675300
H	-5.31772300	-2.64794000	-1.57236100
P	-1.07311800	-0.94341600	0.17769900
Pd	0.97050300	-0.31560700	-0.90261700
C	3.36162400	-1.77956700	-0.13481000
O	2.15860200	-1.79730300	0.27982000
N	3.72151100	-0.98099800	-1.12510000
O	2.87021700	-0.14109200	-1.78114200
C	4.40849600	-2.68433500	0.53107100
C	4.49566800	-2.27689300	2.01879800
C	5.80446700	-2.57714900	-0.11073500
C	3.90478900	-4.14003600	0.42246500
H	4.66537000	-0.96055700	-1.48687000
H	5.18493400	-2.94133900	2.55340700
H	3.51293700	-2.33862900	2.49392700

H	4.86102300	-1.24864800	2.12584100
H	6.21772100	-1.56413400	-0.02810400
H	5.79247100	-2.86936600	-1.16798500
H	6.49827300	-3.25083700	0.40379700
H	3.85607400	-4.46401600	-0.62400200
H	4.58263200	-4.81634300	0.95657500
H	2.90495600	-4.23360500	0.85420500
H	2.93196200	1.69037300	-3.42817600

TS-sp^3-A

N	0.98421900	-1.63338200	-2.39198200
O	0.82316400	0.58400100	-2.88637800
C	0.58204800	-0.33047000	-2.09943400
C	-0.77805900	-2.86784300	-1.21762200
C	-1.15108100	-3.94573400	-0.39885300
H	-2.19811300	-4.05473000	-0.12536100
C	-0.21427000	-4.86835400	0.05519400
H	-0.52769300	-5.69890500	0.68317900
C	1.12724100	-4.72122600	-0.28997000
C	1.55104100	-3.65380200	-1.09274000
C	0.58881600	-2.73866900	-1.56850600
C	1.52397900	-1.89879600	-3.74661900
H	2.03198900	-0.98188900	-4.05142500
H	2.26501000	-2.69697100	-3.67435300
C	-1.80349600	-1.87872300	-1.67763500
H	-1.59918700	-1.48506300	-2.67512300
H	-2.77092300	-2.39684000	-1.74202600
H	-2.48492900	-1.01365100	-0.90031900
C	0.38071700	1.34468900	2.42596800
H	0.83471700	2.18025400	2.97312800
H	-0.70583100	1.44011200	2.47428000
C	0.72765300	-0.00256700	3.08190600
H	0.41792800	-0.81520400	2.41442900
H	1.81054900	-0.10152800	3.23499400
C	0.00964200	-0.17180900	4.42935900
H	-1.07152200	-0.11390200	4.25207200
H	0.26775900	0.66629300	5.09385200
C	0.35051600	-1.49626800	5.12036600
H	-0.18523800	-1.59998000	6.07140600
H	1.42468300	-1.57234600	5.33345400
H	0.07673500	-2.34964800	4.48802800
C	2.64558100	1.46620100	0.43505000
C	3.07644700	-0.02957000	0.43691400
H	2.74373000	-0.52559300	1.35440600
H	2.59122300	-0.55014300	-0.39319100
C	4.61060300	-0.16049900	0.31096500
H	4.87188700	-1.22707200	0.32348300
C	5.29480100	0.55530700	1.49133600
H	6.38659600	0.45299400	1.41675300
H	4.99387800	0.09249300	2.44164500
C	4.89931900	2.04418100	1.47773500
H	5.37225200	2.56163100	2.32366300
C	5.35720100	2.68499800	0.15304500
H	5.10236800	3.75421000	0.14057300
H	6.45024200	2.61651900	0.05945900
C	4.67432000	1.96207900	-1.02436600
H	4.98607300	2.42190400	-1.97178400
C	3.13966000	2.09784600	-0.89591700
H	2.64591900	1.61867400	-1.74722700
H	2.88199200	3.16179000	-0.93236600
C	5.07127400	0.47393700	-1.01476600
H	6.15963800	0.36995000	-1.12945200
H	4.60684200	-0.04459900	-1.86456700
C	3.36392300	2.17236200	1.62046500
H	3.09340100	3.23255600	1.66541800
H	3.05829500	1.72448500	2.57282500
C	0.02225300	3.24349400	0.16882800
C	0.83641100	4.43575700	0.73778000
H	1.85867500	4.43383800	0.34541900
H	0.90973600	4.36243000	1.83122600
C	0.16777800	5.77786300	0.35302400
H	0.77060100	6.59917200	0.76433500
C	0.10324200	5.89785100	-1.18296400
H	1.11647500	5.87624200	-1.60822100
H	-0.34108300	6.86293300	-1.46531500
C	-0.73510600	4.73580500	-1.75227500
H	-0.77413100	4.81084200	-2.84723600
C	-2.16122900	4.79488800	-1.17475400
H	-2.76722700	3.97790300	-1.59052100
H	-2.65061400	5.73843700	-1.45722600
C	-2.08564500	4.67124200	0.35827900
H	-3.09780000	4.69087600	0.78534200
C	-1.41849600	3.33538100	0.75320400
H	-2.01807600	2.48569800	0.41379700
H	-1.39123500	3.27853000	1.84629100
C	-0.08313700	3.38799100	-1.37572500
H	0.90165800	3.31702700	-1.84493000
H	-0.66904300	2.55777600	-1.78386400

C	-1.25917000	5.83992700	0.92961300
H	-1.72688000	6.80137100	0.67407400
H	-1.22813600	5.77974700	2.02655500
P	0.73241900	1.51091000	0.60324300
Pd	-0.58949000	-0.12348500	-0.46536500
C	-3.20722800	0.00689800	0.90571000
O	-1.93293200	0.07338100	1.18465300
O	-4.08608400	0.34169600	1.74056700
O	-3.55229000	-0.42077500	-0.30552200
Cs	-6.44595800	-0.01818300	0.12877400
H	1.86589800	-5.43058100	0.07628300
C	3.02606100	-3.51911200	-1.39949400
H	3.62294300	-3.94245300	-0.58456400
H	3.31240700	-4.05644600	-2.31457700
H	3.32086400	-2.47415300	-1.52955600
C	0.46814200	-2.27792100	-4.76761800
C	0.20416400	-3.62257200	-5.05811600
C	-0.26219500	-1.28618800	-5.44073300
C	-0.76729500	-3.97418600	-5.99776500
H	0.76425400	-4.40034900	-4.54387100
C	-1.23161300	-1.63559500	-6.38154800
H	-0.06323900	-0.24283100	-5.21378700
C	-1.48717800	-2.98045200	-6.66326300
H	-0.95775000	-5.02289600	-6.21212500
H	-1.78457600	-0.85632100	-6.90053800
H	-2.23926800	-3.25149500	-7.40012600

TS-sp^2-A

C	3.37561600	-3.04709600	2.18546900
C	2.88037100	-2.89699000	0.87165600
C	3.61109800	-3.37381600	-0.23752700
C	4.84124600	-4.00087900	0.00051600
C	5.34014300	-4.15941400	1.29088800
C	4.60717300	-3.68462800	2.37590300
H	5.41064800	-4.37254200	-0.84827200
H	6.29705700	-4.65005400	1.45010100
H	4.99294300	-3.79872500	3.38640700
C	3.11788400	-3.22368000	-1.65529300
H	3.28034100	-2.20018500	-2.00834500
H	3.64556200	-3.91453400	-2.32133900
H	2.04435300	-3.41876800	-1.73457000
C	2.60625200	-2.53165500	3.38038500
H	2.15529300	-1.55639400	3.17385200
H	1.78947900	-3.20811600	3.66715900
H	3.26464200	-2.43249700	4.24931400
N	1.59942100	-2.25878100	0.70455100
C	0.38133400	-2.99704800	1.10551700
H	-0.18593100	-2.40681000	1.83545500
H	0.70770900	-3.92407900	1.58297500
C	-0.46562300	-3.26842800	-0.11737300
C	-1.23865900	-2.19992800	-0.61608500
C	-0.37511200	-4.47577100	-0.81857300
C	-1.84952200	-2.35650900	-1.87801800
H	-1.98610400	-1.51491100	0.17569600
C	-1.01942600	-4.61890000	-2.05025900
H	0.21895200	-5.29576400	-0.41879400
C	-1.74316200	-3.55032500	-2.59170600
H	-2.43451300	-1.53008200	-2.27497800
H	-0.94357000	-5.55760300	-2.59432800
C	1.48074700	-1.03642300	0.05310800
O	2.45669100	-0.51017500	-0.47598700
Pd	-0.33396700	-0.17197300	-0.07262500
H	-2.22411500	-3.65702200	-3.56162800
C	-3.28572000	0.19449800	0.06555900
O	-4.41327900	0.75165900	0.04290100
O	-2.25628500	0.67722800	-0.57357700
O	-3.10481700	-0.93383600	0.75591200
Cs	-5.99046100	-1.37068800	1.20293200
C	2.32585800	2.21711000	1.11873200
H	2.86458700	2.22173100	0.16619000
H	2.40720400	3.23275500	1.52759300
C	3.05803600	1.23071500	2.04612800
H	2.51828100	1.07509200	2.98557100
H	3.12857100	0.26268200	1.54903900
C	4.47834900	1.72572300	2.36687900
H	4.42797100	2.70904800	2.85790500
H	5.02538300	1.88112700	1.42632700
C	5.26051900	0.75050700	3.25376900
H	6.27351400	1.11851700	3.45542800
H	5.34855000	-0.23255400	2.77631400
H	4.76089500	0.60648400	4.22040400
C	0.42608900	3.11939900	-0.92006900
C	0.96484400	2.25436000	-2.09869300
H	1.99177700	1.92377700	-1.90239400
H	0.36249700	1.34190600	-2.18452400
C	0.90553000	3.04124200	-3.42553800
H	1.29989700	2.40344100	-4.22807400
C	1.75523800	4.32197400	-3.31413100

H	1.73076300	4.87787400	-4.26215800
H	2.80610300	4.06401700	-3.12091600
C	1.20509900	5.19698200	-2.17198900
H	1.81335800	6.10721400	-2.07618500
C	-0.25801400	5.57642600	-2.47280900
H	-0.65302800	6.22254200	-1.67570100
H	-0.31232000	6.15266900	-3.40757700
C	-1.10212000	4.29211400	-2.58254300
H	-2.15007800	4.55230300	-2.78320900
C	-1.03998600	3.51480300	-1.24787400
H	-1.67237700	2.62251700	-1.28754500
H	-1.44381100	4.15791100	-0.45660700
C	-0.55833600	3.41616800	-3.72747000
H	-0.62306300	3.95701500	-4.68285800
H	-1.16758500	2.50820600	-3.82697800
C	1.28397000	4.41309300	-0.83946500
H	0.94180000	5.05773200	-0.02294800
H	2.33439000	4.17426400	-0.63975600
C	-0.45688500	2.74615300	2.12120800
C	-0.30425000	4.28435700	2.25796100
H	-0.68401100	4.78771000	1.36406400
H	0.75389400	4.56082700	2.35872200
C	-1.08873900	4.80172600	3.48734100
H	-0.96012800	5.89097600	3.55093700
C	-2.58267700	4.46206000	3.31757000
H	-2.97868300	4.94235100	2.41230100
H	-3.15737900	4.85633900	4.16805500
C	-2.74774800	2.93317100	3.22021700
H	-3.80786900	2.68246700	3.08056600
C	-2.21657400	2.27345200	4.50675800
H	-2.35352200	1.18411300	4.45499600
H	-2.77542200	2.62898900	5.38486800
C	-0.72264400	2.61238900	4.66113000
H	-0.32051100	2.12922000	5.56229400
C	0.07281300	2.10624900	3.43573600
H	0.01344600	1.01137800	3.37181600
H	1.12465400	2.36844500	3.58578600
C	-1.96262200	2.38877200	2.00766000
H	-2.39782000	2.76721700	1.08044100
H	-2.06981200	1.30097700	1.97124800
C	-0.55245700	4.14014300	4.77101900
H	-1.09430600	4.52115600	5.64819900
H	0.50737000	4.39402800	4.91487000
P	0.52019900	1.98716600	0.64088200

TS-sp^3-B

N	-2.85948900	1.07500400	-0.54939100
O	-2.37679100	-0.93142800	-1.52170900
C	-1.97999000	0.09701700	-0.98582400
C	-1.38801600	3.01849500	-0.71309700
C	-0.87799700	4.19630400	-0.14407600
H	-0.12627900	4.75885500	-0.69294300
C	-1.33701800	4.66253200	1.08415000
H	-0.93586100	5.58274400	1.50156400
C	-2.31413800	3.95097700	1.77578200
C	-2.84158100	2.75971000	1.25836400
C	-2.37694300	2.30566200	0.00795900
C	-4.28238400	0.95595000	-0.95825600
H	-4.48747400	-0.11415800	-1.02462300
H	-4.90097900	1.37676200	-0.16406400
C	-0.92253500	2.55295700	-2.06078500
H	-1.76591600	2.23520800	-2.68023200
H	-0.43392100	3.40271200	-2.55562700
H	0.05211400	1.75179600	-2.55948300
Pd	-0.03207300	0.58979900	-0.84343500
C	2.57801400	2.07769900	-1.71493500
O	2.13668800	1.31765000	-0.80626100
N	2.08184200	2.08071000	-2.95080300
O	1.02873000	1.31834800	-3.34158300
C	3.76683500	3.01179600	-1.41177000
C	3.43683600	3.78599600	-0.11822800
C	4.06862100	4.01648300	-2.54105900
C	5.00932900	2.12266300	-1.18278700
H	2.42508600	2.73006600	-3.64672200
H	4.29196000	4.40412400	0.17960400
H	3.19982700	3.09540700	0.69427800
H	2.57254900	4.44518500	-0.26057100
H	3.20784300	4.66003300	-2.75986500
H	4.38305700	3.51969100	-3.46753500
H	4.89396300	4.66930200	-2.23614100
H	5.26545200	1.56046100	-2.08870200
H	5.87292800	2.74071600	-0.90982800
H	4.82834200	1.40687700	-0.37694800
H	-2.66925800	4.30936800	2.73909400
C	-3.87653100	2.01213400	2.06917100
H	-3.72628600	2.19597000	3.13822000
H	-4.89925500	2.33706900	1.83227400
H	-3.82995100	0.93311900	1.90111900
C	-4.60072900	1.64255600	-2.27179300

C	-5.13798000	2.93593100	-2.28889500
C	-4.35861200	0.99472400	-3.49312800
C	-5.42477400	3.57419400	-3.49739500
H	-5.33342500	3.44742400	-1.34900500
C	-4.64491700	1.63098800	-4.70134400
H	-3.94092800	-0.00802800	-3.48678200
C	-5.17882200	2.92236200	-4.70686800
H	-5.84161900	4.57807100	-3.49304600
H	-4.45401200	1.11657500	-5.63961400
H	-5.40391600	3.41611400	-5.64865200
P	0.44335100	-1.50189500	0.14406800
C	0.30031500	-2.72126700	-1.28339100
C	2.10875900	-1.67750200	1.00555000
C	-0.80994300	-2.14851000	1.41550100
H	-0.76914600	-2.61254700	-1.51253800
C	1.06110900	-2.25961700	-2.54963900
C	0.58456800	-4.20720700	-0.97991200
H	2.06620600	-2.64422900	1.52625000
C	2.28178400	-0.56336100	2.06451600
C	3.33414000	-1.71604500	0.06888300
C	-0.30144200	-3.25191300	2.37229600
C	-1.47162500	-1.02770200	2.24686100
H	-1.59184200	-2.58206500	0.77490400
H	2.14414500	-2.31831900	-2.38537100
H	0.83736500	-1.21155200	-2.77356900
C	0.69946700	-3.14652500	-3.75227200
C	0.25746400	-5.09285700	-2.19826100
H	-0.00907800	-4.55290400	-0.12740800
H	1.64138600	-4.34196300	-0.70788400
H	1.42845000	-0.54247200	2.75167000
H	2.29897600	0.40453100	1.54919000
C	3.57757200	-0.75259500	2.87168900
C	4.63542300	-1.89291700	0.87511200
H	3.37046600	-0.79001900	-0.51488500
H	3.24729700	-2.54437100	-0.64099700
C	-1.45411000	-3.82326000	3.21787000
H	0.45066400	-2.82670200	3.05039100
H	0.19187400	-4.06333000	1.82899900
C	-2.62443100	-1.58091600	3.10275800
H	-0.72407000	-0.56588300	2.90654200
H	-1.83394100	-0.23414000	1.59016100
H	1.25868100	-2.81137000	-4.63489400
H	-0.36663400	-3.01713600	-3.98826200
C	0.98521100	-4.62739400	-3.46665400
H	-0.82771000	-5.06332000	-2.37449400
H	0.50921000	-6.13705800	-1.97029700
H	3.51015800	-1.68166000	3.45803500
H	3.68270800	0.06525500	3.59628600
C	4.80722700	-0.81783900	1.95659100
H	5.49302500	-1.88505800	0.18991100
H	4.62942400	-2.88450800	1.35278300
C	-2.16266200	-2.72264700	4.01875400
H	-1.06717300	-4.59826900	3.89217400
H	-2.17829900	-4.31819900	2.55426300
H	-3.06341700	-0.77098200	3.69897800
H	-3.42095900	-1.94706900	2.43779400
H	2.06888000	-4.76909600	-3.33632600
H	0.68933300	-5.25008600	-4.32092700
H	4.95045000	0.16119400	1.47849800
H	5.71280200	-1.01349200	2.54541800
H	-3.01503400	-3.14027700	4.56960000
H	-1.46819700	-2.32261600	4.77251900

TS-sp^2-B

C	4.68910800	-1.36267900	1.35614500
C	3.97647400	-1.62527700	0.16792000
C	4.65113900	-1.89703900	-1.04103600
C	6.05157500	-1.89364200	-1.03191400
C	6.76991400	-1.63637000	0.13306300
C	6.08843500	-1.37457000	1.31844200
H	6.58060200	-2.10228100	-1.95879300
H	7.85671000	-1.64021400	0.11663300
H	6.64229500	-1.16844800	2.23132700
C	3.92005100	-2.17896200	-2.33069500
H	3.55431200	-1.24749600	-2.77618400
H	4.58409000	-2.67000600	-3.04941400
H	3.04829200	-2.82129500	-2.17312200
C	3.97968000	-1.07538800	2.65920000
H	3.10141700	-0.44129300	2.50916100
H	3.63014400	-1.99475200	3.14805200
H	4.65203100	-0.57255700	3.36139600
N	2.53248700	-1.65311400	0.22812000
C	1.89627600	-2.79570200	0.92130900
H	1.25331600	-2.42922000	1.72999600
H	2.70053700	-3.38861700	1.36080500
C	1.08602500	-3.59906000	-0.06261200
C	-0.15370100	-3.04202600	-0.43529900
C	1.56222500	-4.76783100	-0.65706400

C	-0.87224900	-3.66443400	-1.47672700
H	-0.79584400	-2.57801600	0.56858500
C	0.81632700	-5.38506100	-1.66689000
H	2.51679000	-5.19026200	-0.34981800
C	-0.39271900	-4.82532000	-2.08782700
H	-1.81332500	-3.23688200	-1.80703500
H	1.18544500	-6.29611800	-2.13147600
C	1.79409700	-0.71887800	-0.47629400
O	2.36978700	0.15393900	-1.12027800
Pd	-0.24296500	-0.78979800	-0.42980200
C	-3.27275900	-1.78795700	0.10042000
O	-2.57274300	-0.94452800	-0.53216700
N	-2.82764300	-2.43322900	1.17654100
O	-1.57421000	-2.30891900	1.67036900
C	-4.71321500	-2.09663500	-0.36930300
C	-5.54634000	-0.80450200	-0.23930300
C	-5.40279000	-3.21555900	0.43735900
C	-4.65040700	-2.51243800	-1.85465700
H	-3.39746800	-3.13948100	1.62398800
H	-6.57370000	-0.98294700	-0.57890500
H	-5.11874000	-0.00427000	-0.84717600
H	-5.58691400	-0.46199900	0.80141700
H	-5.52985300	-2.94697700	1.49338800
H	-4.85775500	-4.16546300	0.37596400
H	-6.40464000	-3.39145300	0.03014600
H	-4.12897700	-3.46911400	-1.97615800
H	-5.66380700	-2.62924400	-2.25668000
H	-4.12468500	-1.75700100	-2.44434400
H	-0.95974200	-5.29741400	-2.88664400
P	-0.25116900	1.63150000	-0.67863300
C	0.38929400	2.05577000	-2.40908500
C	-1.86680900	2.57423100	-0.46586000
C	0.97307200	2.48622800	0.48895000
H	1.46920200	1.92696200	-2.27812000
C	-0.04904900	1.00043600	-3.45108800
C	0.13131000	3.48264700	-2.94102300
H	-1.60184800	3.63354700	-0.60242000
C	-2.46358900	2.41145600	0.94945900
C	-2.94109400	2.21796300	-1.51658300
C	0.82050500	4.01411300	0.66130800
C	1.04087000	1.80529500	1.87509100
H	1.93175900	2.28935900	-0.00781800
H	-1.13746200	1.03698300	-3.59652800
H	0.18459800	-0.00122900	-3.07429500
C	0.64943200	1.22825000	-4.80176800
C	0.83683200	3.69909800	-4.29347400
H	0.48178400	4.23829900	-2.23097400
H	-0.94490900	3.65308200	-3.07334200
H	-1.72741500	2.65951600	1.71986700
H	-2.73440200	1.35860100	1.09937800
C	-3.69891600	3.31134400	1.13243600
C	-4.18677300	3.10925500	-1.34890400
H	-3.20337300	1.16048400	-1.40410800
H	-2.55362000	2.34176200	-2.53249800
C	1.96657300	4.59322400	1.51194000
H	-0.13336100	4.24250500	1.15535400
H	0.80055500	4.52253300	-0.30757000
C	2.18339300	2.38622300	2.72574100
H	0.09234200	1.94061700	2.41100800
H	1.16787000	0.72484100	1.75323700
H	0.29762900	0.48603000	-5.53006400
H	1.72890200	1.05884200	-4.67749800
C	0.41631800	2.65014600	-5.33177500
H	1.92485400	3.64415000	-4.14258600
H	0.62226800	4.71095000	-4.66182300
H	-3.38597700	4.36483000	1.07260200
H	-4.11512700	3.16805700	2.13809900
C	-4.77108700	3.03793500	0.06963600
H	-4.94742800	2.82242700	-2.08705500
H	-3.91400000	4.15124200	-1.57509900
C	2.05928500	3.90814700	2.88165900
H	1.82378400	5.67506200	1.63283200
H	2.91641200	4.46011900	0.97386800
H	2.19405500	1.90153500	3.71057600
H	3.14472800	2.14825100	2.24774100
H	-0.65097800	2.78080800	-5.56611100
H	0.96354500	2.80461200	-6.27069300
H	-5.19457400	2.03945400	0.23826000
H	-5.60018400	3.75005400	0.17374000
H	2.91019000	4.30587000	3.44943600
H	1.15619100	4.14167300	3.46526900

TS-1p-sp^3

N	-2.89702600	1.00755200	-0.63959100
O	-2.10779400	-0.61075100	-2.03571000
C	-1.87526800	0.26707100	-1.21735600
C	-1.68072300	3.10025100	-0.31540000
C	-1.38009400	4.20500900	0.49708100

H	-0.67881000	4.94954200	0.12786600	H	3.36479300	-1.06203900	1.65066000
C	-1.98065000	4.37328600	1.74135400	C	5.08277900	-0.86231100	-1.35495900
H	-1.74043400	5.24259200	2.34837900	H	6.11258400	-1.08700900	-1.66711300
C	-2.89264000	3.42852600	2.20642500	H	4.91651700	0.20781200	-1.53611500
C	-3.21589400	2.30021500	1.43891500	C	2.72030000	-3.17527600	-0.00479900
C	-2.61172100	2.15090000	0.17462100	H	2.59228800	-3.43948900	1.05012000
C	-4.26522500	0.83121000	-1.19187100	H	2.02549600	-3.79985100	-0.57452700
H	-4.31730400	-0.20363900	-1.53448500	C	0.34409100	-1.10916300	2.10534000
H	-4.97973500	0.96004300	-0.37733200	C	0.99576500	-2.26966200	2.90225600
C	-1.05109900	2.94944000	-1.66998000	H	2.08146900	-2.27050400	2.76510700
H	-1.78319000	2.64126800	-2.42096200	H	0.62480400	-3.23870500	2.54270900
H	-0.65963000	3.93245100	-1.96483300	C	0.68970500	-2.12727300	4.41169700
H	0.10047000	2.41659500	-2.15357700	H	1.16796600	-2.95969600	4.94530200
C	-0.42113300	-2.65006300	-0.31730200	C	1.25467600	-0.78691800	4.92329800
H	-0.18450200	-3.49905300	0.33725400	H	2.34392600	-0.75642000	4.77952900
H	-1.44871800	-2.35113500	-0.09501100	H	1.07259000	-0.68918200	6.00250400
C	-0.37226600	-3.08543600	-1.79450300	C	0.58446700	0.37446500	4.16241400
H	-0.40985900	-2.20302200	-2.43777200	H	0.98945500	1.33157600	4.51695500
H	0.56376300	-3.61400100	-2.00933700	C	-0.93744100	0.33644300	4.39564600
C	-1.55287300	-4.00233100	-2.14733000	H	-1.41689000	1.17517900	3.87448400
H	-2.48484300	-3.44587700	-1.98604900	H	-1.16259400	0.44762300	5.46580700
H	-1.57409500	-4.86235800	-1.46129700	C	-1.49156600	-1.00344400	3.87622400
C	-1.50077600	-4.50193500	-3.59484400	H	-2.58018500	-1.03641900	4.01745100
H	-2.35800200	-5.14503200	-3.82575000	C	-1.18922800	-1.15207500	2.36789200
H	-0.58887900	-5.08220200	-3.78495900	H	-1.68191200	-0.35154600	1.80408300
H	-1.51372900	-3.66204300	-4.29960900	H	-1.61004900	-2.10340300	2.02246500
C	2.42579600	-1.66571700	-0.23383100	C	0.87541800	0.24663500	2.65130700
C	2.64120600	-1.33619800	-1.74354000	H	1.95108600	0.33993000	2.47691000
H	1.93065500	-1.89073700	-2.36409300	H	0.40115100	1.07141700	2.10625900
H	2.45284000	-0.27248400	-1.92602200	C	-0.83287100	-2.16696200	4.64251600
C	4.08071600	-1.69592100	-2.17475600	H	-1.05501300	-2.08921000	5.71575700
H	4.19071400	-1.46425000	-3.24223400	H	-1.24312100	-3.12772100	4.30050000
C	4.34176700	-3.19676200	-1.93729300	P	0.61647700	-1.18315600	0.20690700
H	5.35780800	-3.46142500	-2.26205400	Pd	-0.02025600	0.89622600	-0.75802900
H	3.64760900	-3.80227500	-2.53663500	C	2.40653900	2.89523300	-0.85575500
C	4.16606100	-3.51340700	-0.43972000	O	1.96893800	1.90721100	-0.20140700
H	4.34035600	-4.58361000	-0.26355000	N	2.08990300	3.09359700	-2.13384500
C	5.16776800	-2.68058300	0.38330100	O	1.24537400	2.28380300	-2.82403500
H	5.06768300	-2.91537800	1.45263000	C	3.36225800	3.89301200	-0.17238600
H	6.19710300	-2.93613500	0.09570800	C	2.67882400	4.38243400	1.12212400
C	4.89969300	-1.18277400	0.14042800	C	3.71851200	5.10755500	-1.05172800
H	5.59834600	-0.58050800	0.73718700	C	4.65841400	3.13335100	0.18849500
C	3.45816500	-0.84019700	0.58188900	H	2.41614500	3.91000000	-2.63474300
H	3.26227600	0.22661200	0.44702100	H	3.35822100	5.03418500	1.68422800

H	2.39973100	3.53489100	1.75264400
H	1.76797300	4.95031400	0.90026900
H	2.82977200	5.68420000	-1.33577900
H	4.25712700	4.81671400	-1.96228300
H	4.37699300	5.78142900	-0.49270400
H	5.16366500	2.76025200	-0.71027200
H	5.35146800	3.80057600	0.71460100
H	4.44252900	2.28116800	0.83859000
H	-3.35910700	3.55461600	3.18062300
C	-4.18705700	1.28724400	2.00405900
H	-4.14126200	1.28524300	3.09806600
H	-5.22670900	1.51458400	1.73060000
H	-3.97150100	0.27400100	1.65261700
C	-4.60255800	1.78456200	-2.32116300
C	-5.29960700	2.97240700	-2.06562100
C	-4.22159000	1.49435500	-3.64039200
C	-5.60959900	3.85574900	-3.10164800
H	-5.60184700	3.20733900	-1.04746900
C	-4.53093700	2.37589800	-4.67684700
H	-3.67859800	0.57589800	-3.84404800
C	-5.22585900	3.55860600	-4.41040700
H	-6.15211600	4.77278300	-2.88644100
H	-4.23199800	2.13740000	-5.69426800
H	-5.46873800	4.24314300	-5.21901300

TS-1p-sp^2

C	4.61572400	-1.39946200	1.42430900
C	3.93415600	-1.70731100	0.22916900
C	4.63703700	-1.96064300	-0.96678100
C	6.03637100	-1.90176900	-0.93524900
C	6.72477700	-1.60611500	0.23844200
C	6.01457900	-1.35728400	1.41010200
H	6.58828900	-2.09620300	-1.85178600
H	7.81104800	-1.56809400	0.23937600
H	6.54508700	-1.11815500	2.32868800
C	3.93768200	-2.27279200	-2.26706600
H	3.52840900	-1.35838800	-2.70989800
H	4.63542200	-2.72238100	-2.98088200
H	3.09897100	-2.96096900	-2.12585200
C	3.86799200	-1.10697100	2.70439800
H	3.04857100	-0.40118700	2.53566200
H	3.42402300	-2.01115200	3.14110800
H	4.54118800	-0.68020100	3.45441700
N	2.49065200	-1.79469600	0.27422200
C	1.89414300	-2.98698300	0.91595100
H	1.24133900	-2.68113600	1.74193400
H	2.71923100	-3.57284000	1.32620000
C	1.10351700	-3.77020400	-0.10182400
C	-0.15000100	-3.22677000	-0.45056200
C	1.59786300	-4.90976300	-0.73599100
C	-0.86738100	-3.83093500	-1.50391900
H	-0.78872200	-2.83927700	0.59062600
C	0.85663900	-5.50690900	-1.76169300
H	2.56082600	-5.32584200	-0.44678400
C	-0.36792400	-4.96048700	-2.15587500
H	-1.82532600	-3.41670500	-1.80558700
H	1.24044400	-6.39472700	-2.25827000
C	1.72618800	-0.87361400	-0.41969800
O	2.27505800	0.00356000	-1.07406800
C	-2.45407800	1.78359000	-0.61688300
H	-3.04457500	1.07571100	-0.03292300
H	-2.72416000	2.79547000	-0.29041800
C	-2.82577600	1.58078700	-2.09425100
H	-2.27324000	2.27353200	-2.73712600
H	-2.53994400	0.56674800	-2.39882400
C	-4.32611900	1.79178200	-2.35205300
H	-4.61096000	2.80659600	-2.03851100
H	-4.90665800	1.10368700	-1.72385500
C	-4.70878100	1.58487700	-3.82153500
H	-5.78132300	1.74395400	-3.98217500
H	-4.46826600	0.56699200	-4.15267200
H	-4.16710600	2.28040000	-4.47446100
C	-0.71813400	1.78108700	1.78205100
C	-1.86480500	0.92844100	2.40568200
H	-2.83535600	1.25113800	2.01161700
H	-1.73649700	-0.12831900	2.14384400
C	-1.89017100	1.08612000	3.94302600
H	-2.71074200	0.47315200	4.33934000
C	-2.12289500	2.56546400	4.30488100
H	-2.16270700	2.68993700	5.39613800
H	-3.09002500	2.90590900	3.90861900
C	-0.97971700	3.41422600	3.71739500
H	-1.13905500	4.47335800	3.96154800
C	0.36554900	2.94272000	4.30517600
H	1.18727900	3.55495500	3.90753700
H	0.36702100	3.07569000	5.39596200
C	0.58772800	1.45891200	3.95032300
H	1.55108300	1.12225800	4.35669700

C	0.61391700	1.29060300	2.41516700
H	0.76122600	0.23415900	2.16147700
H	1.46661000	1.83944600	2.00332100
C	-0.55319500	0.60872500	4.53889700
H	-0.57060700	0.69991500	5.63416600
H	-0.39698800	-0.45225700	4.30354700
C	-0.94878000	3.26296800	2.17771900
H	-0.15068000	3.89865100	1.78013100
H	-1.89334600	3.63005900	1.75516400
C	0.34698500	2.76586900	-1.06066200
C	-0.39491800	4.12691600	-1.19589500
H	-0.60099500	4.55862700	-0.21062700
H	-1.36205500	3.99524200	-1.69329800
C	0.45277000	5.12514300	-2.02240900
H	-0.09867200	6.07294200	-2.09218200
C	1.80922500	5.36090200	-1.33058600
H	1.65597800	5.79503900	-0.33213900
H	2.40369500	6.08495400	-1.90532800
C	2.55965400	4.02066700	-1.21882000
H	3.52106900	4.17552300	-0.71086400
C	2.80328000	3.44201700	-2.62567900
H	3.34987200	2.49364100	-2.55232000
H	3.42252500	4.13280500	-3.21563900
C	1.44619900	3.21697600	-3.31883000
H	1.60789800	2.79551700	-4.32013400
C	0.61101700	2.21202000	-2.49499800
H	1.13826100	1.25950500	-2.42257200
H	-0.33425700	2.02669400	-3.01422400
C	1.71951300	3.03027000	-0.38110600
H	1.57106800	3.46205000	0.61528000
H	2.26423700	2.09059900	-0.26521200
C	0.69173100	4.55534900	-3.43410400
H	1.27055000	5.27022100	-4.03570000
H	-0.26768400	4.40720100	-3.94999100
P	-0.68172100	1.43657500	-0.11241000
Pd	-0.29898600	-0.99007400	-0.34319600
C	-3.30533000	-2.10608400	0.28995500
O	-2.64435400	-1.24339200	-0.35439000
N	-2.79632400	-2.79483500	1.31023900
O	-1.51767200	-2.67679400	1.74190700
C	-4.78917200	-2.35652200	-0.06152600
C	-5.59968000	-1.14655400	0.45645700
C	-5.36085200	-3.64666000	0.56177600
C	-4.91040500	-2.44689500	-1.59619800
H	-3.33422000	-3.52562700	1.75744100
H	-6.65633500	-1.25225200	0.18276000
H	-5.22654400	-0.21330900	0.02606800
H	-5.53687200	-1.06788300	1.54815300
H	-5.40291900	-3.59968300	1.65724500
H	-4.78542900	-4.53257200	0.26820800
H	-6.38978400	-3.79316700	0.21498100
H	-4.38434500	-3.32828600	-1.98240200
H	-5.96427800	-2.53024300	-1.88637800
H	-4.48319300	-1.56193900	-2.07291000
H	-0.93149900	-5.42101700	-2.96376800