

Supporting Information

Nickel-Catalyzed Reductive Arylalkylation of Alkenes: 5-Exo Cyclization vs. 6-Endo Cyclization vs. 1,2-Aryl Migration to 6-Endo Product

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Table of Contents

1. DFT-computed Gibbs free energy barriers for oxidative addition step from ArNi ^{II} LBr species	S2
2. Compare the stability of INT2 and TS2 with different multiplicities... ..	S2
3. Transition states of bromine atom abstraction (² TS6) and oxidative addition (² TS7)	S3
4. Study of the proposed mechanism for the reduction of Ni(II) to Ni(I).....	S3
5. Transition states of 5-exo and 6-endo alkene insertions mediated by Ni(II) and Ni(III) species.	S4
6. Geometrical structures and Gibbs free energy barriers of key transition states.	S5
7. DFT-computed thermodynamics of Ni ^{III} -alkyl species	S5
8. Transition states of HBr departure (² TS17), and hydrogen atom transfer (² TS18).S6	
9. Energies and free energies of calculated structures	S7
10. Cartesian coordinates of the structures	S9

1. DFT-computed Gibbs free energy barriers for oxidative addition step from $\text{ArNi}^{\text{II}}\text{LBr}$ species.

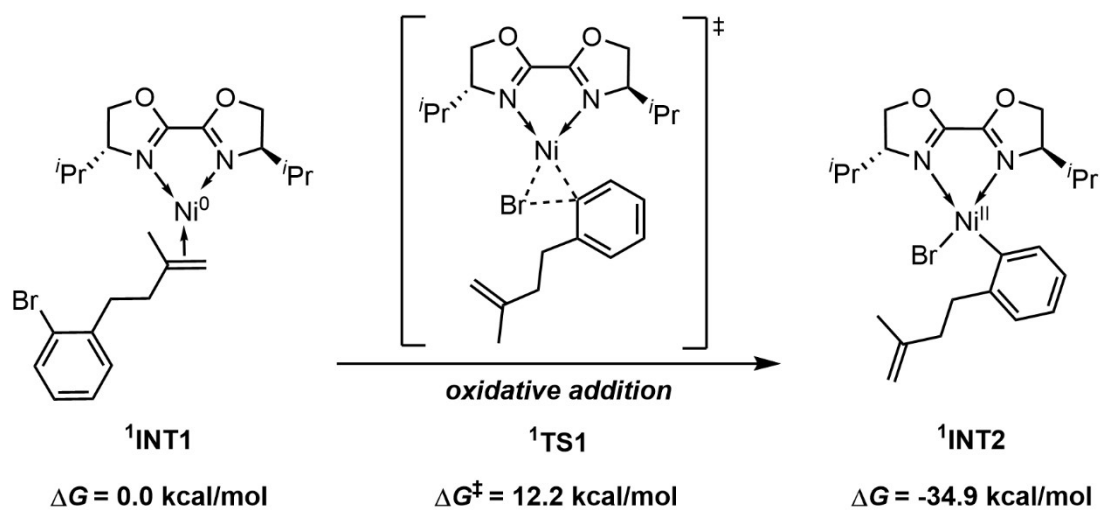


Figure S1. DFT-computed Gibbs free energy barriers for oxidative addition step from $\text{ArNi}^{\text{II}}\text{LBr}$ intermediate.

2. Compare the stability of INT2 and TS2 with different multiplicities.

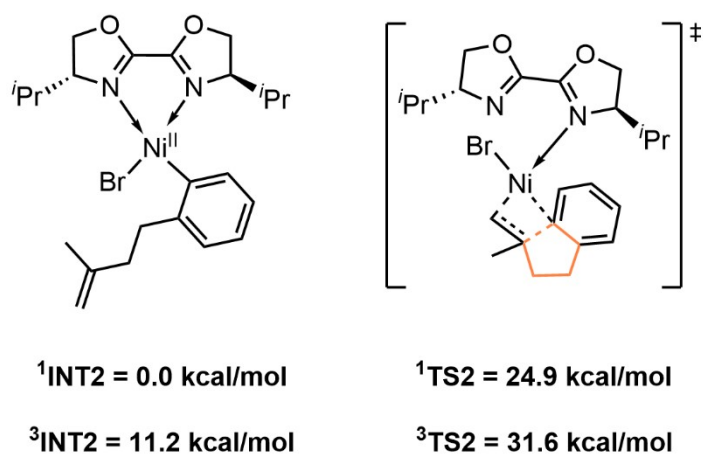


Figure S2. Compare the stability of INT2 and TS2 with different multiplicities.

3. Transition states of bromine atom abstraction (²TS6) and oxidative addition (²TS7).

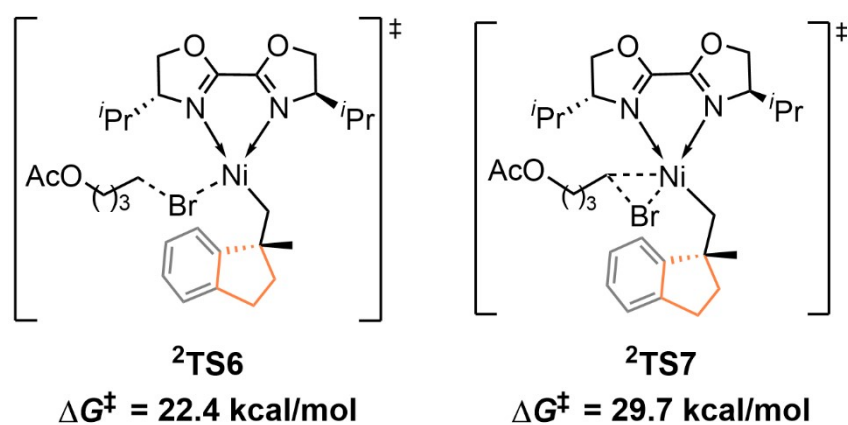


Figure S3. Transition states of bromine atom abstraction (²TS6) and oxidative addition (²TS7).

4. Study of the proposed mechanism for the reduction of Ni(II) to Ni(I).

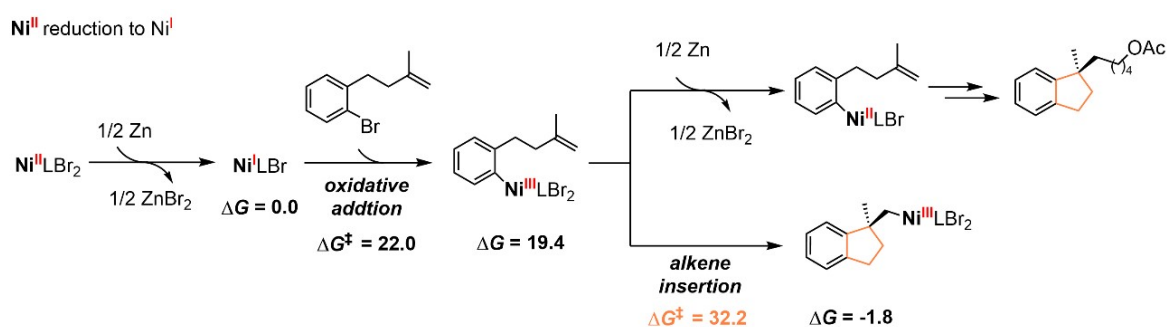


Figure S4. Study of the proposed mechanism for the reduction of Ni(II) to Ni(I).

5. Transition states of 5-exo and 6-endo alkene insertions mediated by Ni(II) and Ni(III) species.

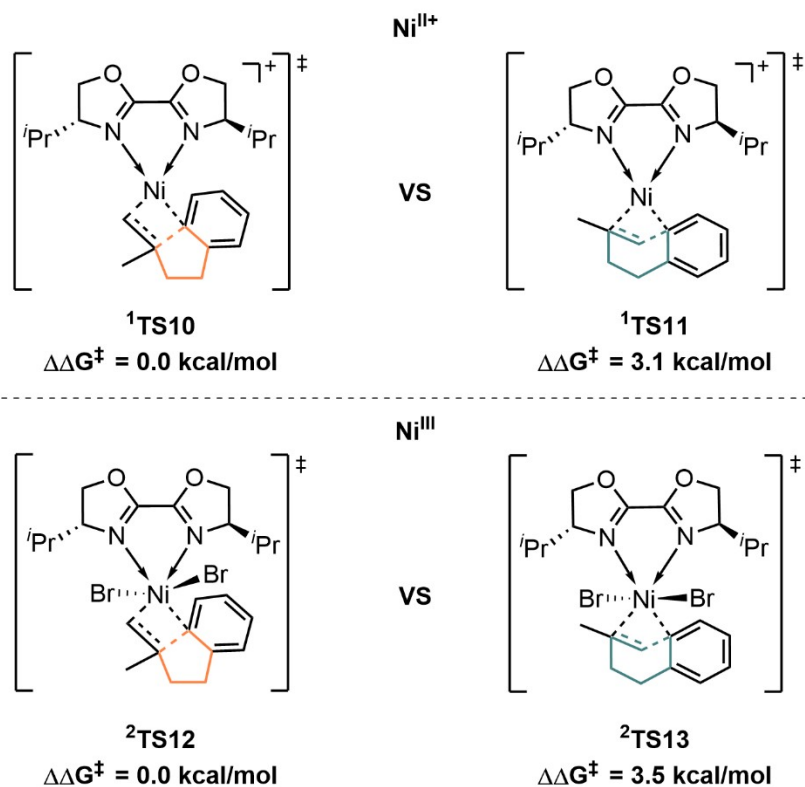


Figure S5. Transition states of 5-exo and 6-endo alkene insertions mediated by Ni(II) and Ni(III) species.

6. Geometrical structures and Gibbs free energy barriers of key transition states.

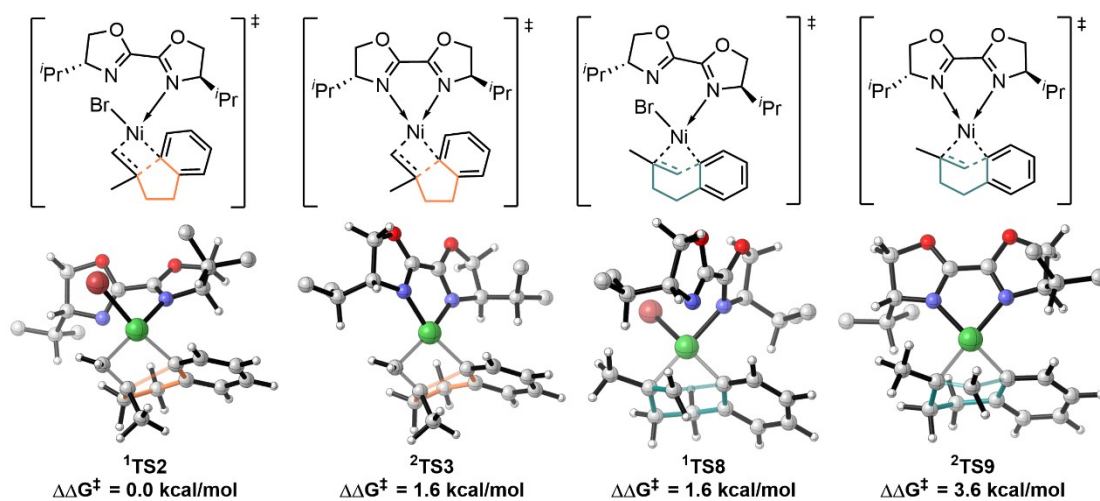


Figure S6. Geometrical structures and Gibbs free energy barriers of key transition states.

7. DFT-computed thermodynamics of Ni^{III}-alkyl species.

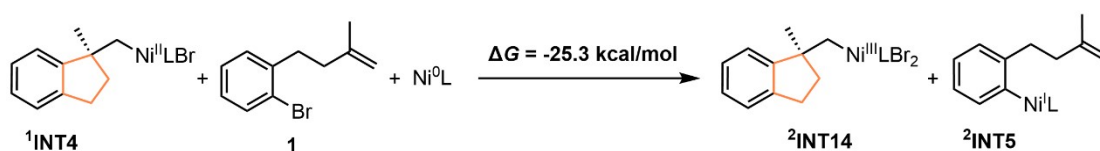
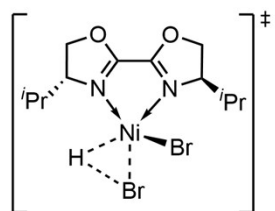


Figure S7. DFT-computed thermodynamics of Ni^{III}-alkyl species.

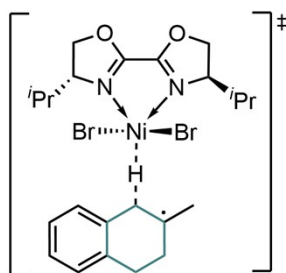
8. Transition states of HBr departure ($^2\text{TS17}$), and hydrogen atom transfer ($^2\text{TS18}$).



${}^2\text{TS17}$

$\Delta G^\ddagger = -7.5 \text{ kcal/mol}$

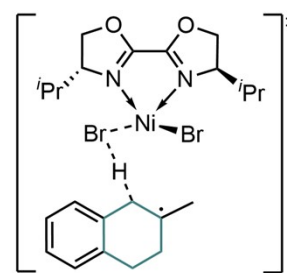
$\Delta\Delta G^\ddagger = 3.0 \text{ kcal/mol}$



${}^2\text{TS16}$

$\Delta G^\ddagger = -0.1 \text{ kcal/mol}$

$\Delta\Delta G^\ddagger = 2.0 \text{ kcal/mol}$



${}^2\text{TS18}$

$\Delta G^\ddagger = 5.6 \text{ kcal/mol}$

$\Delta\Delta G^\ddagger = 7.7 \text{ kcal/mol}$

Figure S8. Transition states of HBr departure (${}^2\text{TS17}$), and hydrogen atom transfer (${}^2\text{TS18}$).

9. Energies and free energies of calculated structures.

Table S1. Electronic Energies and Free Energies (in Hartree) of the Structures Calculated at the (U)B3LYP-D3/def2-TZVP (SMD: N, N-Dimethylacetamide)// (U)B3LYP-D3/6-31G(d)-LANL2DZ Level of Theory

Structures	ZPVE	TCE	TCH	TCG	E_{sol}	$G_{\text{sol}}(E_{\text{sol}}+\text{TCG})$	Imaginary Frequency
1	0.209836	0.221922	0.222866	0.171644	-3001.363127	-3001.191483	—
2	0.167313	0.178188	0.179132	0.129820	-2960.100929	-2959.971109	—
3	0.380165	0.399128	0.400072	0.335732	-813.107120	-812.771388	—
5	0.198712	0.207740	0.208684	0.164917	-426.584394	-426.419477	—
¹ INT1	0.528208	0.559257	0.560201	0.472099	-5239.385878	-5238.913779	—
¹ INT2	0.529567	0.561032	0.561976	0.472693	-5239.442087	-5238.969394	—
³ INT2	0.528048	0.560177	0.561122	0.469033	-5239.420552	-5238.951519	—
¹ INT3	0.528973	0.560603	0.561547	0.463793	-5239.415820	-5238.952027	—
¹ INT4	0.531878	0.561594	0.562538	0.472193	-5239.458371	-5238.986178	—
² INT5	0.525544	0.555575	0.556519	0.462053	-2665.179244	-2664.717191	—
² INT6	0.527170	0.555945	0.556890	0.466990	-2665.192858	-2664.725868	—
² INT7	0.696740	0.737897	0.738841	0.618696	-5625.306914	-5624.688218	—
² INT8	0.695633	0.736854	0.737798	0.620796	-5625.310279	-5624.689483	—
² INT9	0.697163	0.738211	0.739155	0.619376	-5625.325605	-5624.706229	—
¹ INT10	0.530274	0.561187	0.562131	0.467000	-5239.426657	-5238.959657	—
¹ INT11	0.531644	0.561776	0.562720	0.470810	-5239.451897	-5238.981087	—
² INT12	0.526505	0.555879	0.556824	0.464716	-2665.182570	-2664.717854	—
² INT13	0.527715	0.556309	0.557253	0.467858	-2665.189647	-2664.721789	—
² INT14	0.531526	0.564176	0.565120	0.465334	-7813.672628	-7813.207294	—
² INT15	0.207659	0.216908	0.217852	0.173351	-427.113194	-426.939843	—
² INT16	0.207464	0.217447	0.218391	0.170766	-427.143131	-426.972365	—
¹ TS1	0.526186	0.557707	0.558651	0.469308	-5239.363577	-5238.894269	132.30i
¹ TS2	0.528376	0.558867	0.559811	0.472657	-5239.402372	-5238.929715	252.33i
³ TS2	0.527441	0.558125	0.559070	0.470258	-5239.389361	-5238.919103	329.30i
² TS3	0.526339	0.554346	0.555290	0.468258	-2665.140233	-2664.671975	289.44i
² TS4	0.693886	0.735124	0.736068	0.617024	-5625.282872	-5624.665848	261.99i
² TS5	0.696178	0.736324	0.737268	0.621879	-5625.306171	-5624.684292	48.63i
² TS6	0.697677	0.737999	0.738943	0.621204	-5625.317427	-5624.696223	277.06i
² TS7	0.695020	0.735828	0.736772	0.619248	-4282.782249	-4282.163001	337.05i
¹ TS8	0.529134	0.559148	0.560092	0.468682	-5239.401044	-5238.932362	300.32i
² TS9	0.527007	0.554685	0.555629	0.470245	-2665.139578	-2664.669333	334.92i
¹ TS10	0.528922	0.557013	0.557958	0.470524	-2665.036362	-2664.565838	247.34i
¹ TS11	0.528481	0.556592	0.557536	0.470681	-2665.031210	-2664.560529	236.96i
² TS12	0.529766	0.562369	0.563313	0.464541	-7813.616494	-7813.151953	313.00i
² TS13	0.529299	0.562360	0.563304	0.462163	-7813.610047	-7813.147884	300.25i
² TS14	0.529037	0.561736	0.562681	0.463076	-7813.631216	-7813.168140	303.03i
² TS15	0.206844	0.215857	0.216801	0.172595	-427.110500	-426.937905	453.03i
² TS16	0.525345	0.558281	0.559225	0.457174	-7813.666004	-7813.208830	311.26i

² TS17	0.324937	0.347295	0.348239	0.274898	-7387.067226	-7386.792328	99.67 <i>i</i>
² TS18	0.524281	0.557735	0.558679	0.455097	-7813.654819	-7813.199722	649.34 <i>i</i>
Ni ⁰ L	0.315984	0.334070	0.335014	0.272421	-2237.968628	-2237.696206	—
Ni ⁰ LBr	0.318374	0.338784	0.339728	0.270959	-4812.275187	-4812.004228	—
Ni ^{II} LBr ₂	0.321229	0.342885	0.343830	0.272489	-7386.504617	-7386.232128	—
Ni ^{III} LHBr ₂	0.327021	0.349646	0.350590	0.277136	-7387.074259	-7386.797122	—

ZPVE = zero-point vibrational energy; **TCE** = thermal correction to energy; **TCH** = thermal correction to enthalpy; **TCG** = thermal correction to Gibbs free energy.

10. Cartesian coordinates of the structures.

1

Br	0.67643100	-1.92202100	-0.00083400
C	1.40872700	-0.14205700	0.02648700
C	2.75331700	0.00032500	-0.31577500
C	3.33186900	1.26935300	-0.31316100
C	2.56137500	2.38035400	0.03201300
C	1.22015700	2.21364800	0.37324500
C	0.60560300	0.95189800	0.38250100
C	-0.86075000	0.82487900	0.71861000
H	-1.02335000	-0.06623100	1.33311700
C	-1.74462500	0.75028500	-0.55317700
C	-3.20897300	0.53874200	-0.23666500
C	-4.10571400	1.52028400	-0.37966800
H	-3.82097400	2.50563900	-0.74183800
H	-5.15748500	1.37505200	-0.14444700
C	-3.59390800	-0.83726100	0.25157000
H	-3.32368400	-1.60064800	-0.49057300
H	-4.66782100	-0.91333400	0.44850500
H	-3.06142100	-1.10241200	1.17423600
H	-1.60758400	1.67497500	-1.12608700
H	-1.37851200	-0.07369600	-1.17969200
H	-1.17709700	1.68789500	1.31519400
H	0.62145500	3.08005900	0.64441200
H	3.00287300	3.37289700	0.03878500
H	4.37907500	1.38264000	-0.57870900
H	3.33697700	-0.87479700	-0.57960400

2

C	-0.19493500	0.28727700	0.48791000
H	0.11055100	-0.68446200	0.08649400
H	-0.25148100	0.17998500	1.57836800
C	-1.58091500	0.62607300	-0.04251800
H	-1.92123200	1.59435100	0.35023800
C	0.83612100	1.35724500	0.11496400
H	0.53632900	2.32614300	0.54417400
C	2.24072700	1.06803300	0.62752100
H	2.93064800	1.88356800	0.40844400
H	2.25339300	0.85732700	1.69857300
O	-2.46282100	-0.42026400	0.38682500
C	-3.78025600	-0.43674900	0.04028500
O	-4.47544000	-1.33386500	0.44959200
C	-4.29346100	0.68046500	-0.85038300

H	-4.13495600	1.66328300	-0.39289000
H	-3.78017500	0.68155000	-1.81859700
H	-5.36028900	0.52307600	-1.00920200
Br	3.04151200	-0.53341700	-0.23690200
H	0.87117600	1.49241600	-0.97334100
H	-1.56449300	0.69132100	-1.13870700

3

C	-0.54716900	1.33037900	0.46566700
C	-2.02035700	1.09625400	0.89873500
C	-2.47134200	-0.30901500	0.51966000
C	-2.07160700	-1.51831900	1.08810500
C	-2.58124800	-2.71605000	0.57730200
C	-3.47890800	-2.70070300	-0.49575600
C	-3.87239900	-1.48826400	-1.07083300
C	-3.36376700	-0.29523600	-0.55861200
C	-3.61329900	1.11928100	-1.03335600
H	-3.09271700	1.29881500	-1.98361900
H	-4.67492900	1.32451400	-1.21509600
C	-3.03136000	1.99034200	0.10963100
H	-2.56786800	2.91442600	-0.25266300
H	-3.84305200	2.28475500	0.78491700
H	-4.56874600	-1.47773800	-1.90633500
H	-3.87310900	-3.63639300	-0.88360700
H	-2.28096600	-3.66323500	1.01763300
H	-1.37468100	-1.53345200	1.92285600
C	-2.12624000	1.34787100	2.41343800
H	-1.42868400	0.71425900	2.97430600
H	-1.89078100	2.39300300	2.65003300
H	-3.13821800	1.13463100	2.77491300
H	-0.24878600	2.34119200	0.78249600
H	0.07643300	0.63038200	1.03765800
C	2.13164900	0.20865700	-0.84474400
H	2.10524000	0.19313800	0.25153300
H	1.75998600	-0.76860600	-1.17753900
C	3.57909900	0.36005300	-1.30434700
H	3.99069300	1.33138100	-1.00600900
H	3.64243100	0.29922600	-2.39516000
C	1.23566400	1.32983100	-1.38898700
H	1.59882000	2.30116700	-1.02057200
H	1.33436500	1.36140700	-2.48327100
C	-0.25146100	1.17019000	-1.03162100
H	-0.82432800	1.91656400	-1.59609800
H	-0.60028800	0.18683900	-1.37227500

O	4.39814600	-0.72125400	-0.83038200
C	5.01172400	-0.69482400	0.38333200
O	5.58291600	-1.68790800	0.76444300
C	4.98467800	0.59832700	1.18323200
H	5.52776200	1.39203900	0.65716800
H	3.96590800	0.95567900	1.36344600
H	5.47506900	0.40667000	2.13772800

5

C	-3.00740400	0.31416100	0.11176700
C	-2.75717900	-1.05901400	0.10341800
C	-1.44628600	-1.52502400	-0.00289600
C	-0.37106200	-0.63007800	-0.09965000
C	-0.62901800	0.75936900	-0.10424900
C	-1.94194400	1.21426400	0.00451100
H	-4.02513000	0.68526100	0.19863600
H	-3.57926700	-1.76553000	0.18235400
H	-1.24741000	-2.59466700	-0.00185900
H	-2.13593400	2.28502000	0.00126500
C	0.54237700	1.69678800	-0.30502000
C	1.82486200	1.17090100	0.35561800
C	1.01495000	-1.10141200	-0.17817000
C	2.06825100	-0.29014100	0.03018000
H	2.68165400	1.78062500	0.04217500
H	1.75732400	1.27937600	1.45078600
H	0.72571000	1.79326400	-1.38692800
H	0.30304300	2.70130500	0.06276800
C	3.49046300	-0.77271500	0.03365500
H	3.97322900	-0.55865100	0.99849600
H	3.55965000	-1.85005000	-0.14957500
H	4.08631600	-0.25509700	-0.73143600
H	1.17275400	-2.16345100	-0.36166500

¹INT1

C	-1.08567100	3.53342500	-0.75761200
H	-1.13346200	3.73786700	-1.83156700
H	-0.77668700	4.43629900	-0.22845400
C	-0.24383200	2.27025700	-0.42117800
N	-1.28207000	1.25556600	-0.17236100
C	-2.40750300	1.88189200	-0.07615000
C	-3.55565100	1.08548900	0.32828600
N	-3.31657900	-0.13000900	0.69595000
C	-4.61813200	-0.77942200	0.91804300
H	-4.65094100	-1.14155500	1.95224700

C	-4.77826100	-1.99711100	-0.01980200
C	-6.10183800	-2.72308900	0.25388700
H	-6.19747300	-3.00347600	1.31019300
H	-6.16844800	-3.63872500	-0.34375000
H	-6.96737400	-2.10039100	-0.00874800
C	-4.61722000	-1.62494600	-1.49900500
H	-5.37920400	-0.90724800	-1.83072400
H	-3.62728400	-1.19161000	-1.67747800
H	-4.71381800	-2.51796700	-2.12634300
H	-3.94508100	-2.66209900	0.24135800
C	-5.63466300	0.38561200	0.71468600
H	-6.14223800	0.68023700	1.63689300
H	-6.37905500	0.19551900	-0.06185500
O	-4.82668000	1.52112800	0.27468200
Ni	-1.43543200	-0.71206000	0.17155100
Br	3.91763400	0.42087200	-1.62077200
C	4.48762000	-0.47852000	-0.01096600
C	5.59120400	0.05796000	0.65161700
C	6.05362600	-0.54999500	1.81865400
C	5.40738400	-1.68665000	2.30631200
C	4.30732600	-2.20516800	1.62523200
C	3.81347700	-1.62207700	0.44679900
C	2.57718100	-2.17527800	-0.21615400
H	2.70691200	-2.17745600	-1.30314100
C	1.32773700	-1.33144900	0.15308200
C	0.03662000	-1.73259400	-0.53947900
C	-0.90726800	-2.59467200	0.11114500
H	-0.66677400	-3.01283700	1.09262400
H	-1.54474400	-3.24617500	-0.49280500
C	0.07862900	-1.66691000	-2.05854200
H	0.43391000	-0.68543700	-2.40078200
H	-0.91798600	-1.82884000	-2.48388700
H	0.74908500	-2.42400900	-2.49517700
H	1.19542900	-1.36472400	1.24195900
H	1.55604600	-0.29078000	-0.10285300
H	2.41940000	-3.21429500	0.09461100
H	3.80434500	-3.08994900	2.00815700
H	5.75930100	-2.16994000	3.21355500
H	6.91341800	-0.13502100	2.33701900
H	6.08101700	0.94044300	0.25452200
O	-2.44108300	3.20590000	-0.31351100
H	0.35393900	1.95234200	-1.28138300
C	0.69299000	2.39591400	0.80370200
C	1.89184300	3.29534000	0.47431400

H	2.57377300	3.35156400	1.32991600
H	1.57772800	4.32098500	0.23829700
H	2.45863800	2.90163400	-0.37717500
C	-0.04267600	2.84954500	2.07137800
H	0.64619000	2.85583500	2.92315200
H	-0.86682300	2.17013200	2.31325600
H	-0.44925700	3.86409900	1.97315500
H	1.06752500	1.38229100	0.98481500

¹INT2

C	-3.53021100	2.54801800	0.52599000
H	-3.56157400	3.18630900	1.41299600
H	-4.46237400	2.64409200	-0.03106400
C	-3.11376700	1.08091500	0.83745800
N	-1.71032600	1.06021100	0.39380800
C	-1.48853000	2.14974800	-0.24376600
C	-0.14249400	2.29918600	-0.80403300
N	0.70856200	1.37417900	-0.52130500
C	2.00597100	1.76958800	-1.11489900
H	2.35940700	0.94327600	-1.73689100
C	3.07485200	2.05355200	-0.03572400
C	4.41282300	2.40773300	-0.69898800
H	4.73080700	1.62060500	-1.39293700
H	5.19231800	2.51327600	0.06275400
H	4.36786100	3.35520500	-1.25250300
C	2.62578500	3.11462100	0.97530300
H	2.44181300	4.08974500	0.50476300
H	1.71114800	2.80211500	1.49066500
H	3.40068800	3.26001700	1.73528100
H	3.20867800	1.11313700	0.50269200
C	1.60309000	2.99575600	-1.98510200
H	1.56846200	2.77565100	-3.05510600
H	2.20909400	3.88524500	-1.81143300
O	0.23175900	3.32092500	-1.57011900
Ni	-0.02196900	-0.09460300	0.61289000
Br	-1.07355100	-1.70599100	1.90004700
C	1.67214100	-0.90552700	0.82546600
C	2.33940300	-0.74093700	2.04423200
C	3.68331800	-1.10726400	2.18287600
C	4.36562200	-1.66147100	1.09827700
C	3.69014800	-1.87100400	-0.10654000
C	2.34353400	-1.50864900	-0.25567200
C	1.59826600	-1.81659000	-1.53611300
H	0.97152200	-0.95719000	-1.80640300

C	0.68633100	-3.06429400	-1.38245800
C	-0.40523400	-3.10852500	-2.42656700
C	-0.34325800	-3.89797200	-3.50387000
H	0.49471600	-4.57208800	-3.66733100
H	-1.12950200	-3.90801400	-4.25575300
C	-1.56933600	-2.18524400	-2.16267700
H	-2.07670800	-2.46947400	-1.23168300
H	-2.29740300	-2.18537500	-2.98050800
H	-1.22699500	-1.15400000	-2.00263300
H	1.30931600	-3.96533800	-1.42322800
H	0.23050800	-3.02621200	-0.38585900
H	2.29161800	-1.97731100	-2.37145700
H	4.21242100	-2.32872700	-0.94568700
H	5.41106800	-1.94474100	1.19258000
H	4.19217500	-0.96007400	3.13302500
H	1.80838700	-0.31098400	2.88938900
O	-2.45268000	3.06800000	-0.33485400
H	-3.12479500	0.87338700	1.91081900
C	-3.93456000	-0.01532800	0.12107500
C	-5.32653700	-0.13096800	0.75647500
H	-5.89424300	-0.94182200	0.28765700
H	-5.90963500	0.79156200	0.62893600
H	-5.25816400	-0.34515000	1.82923000
C	-4.02401400	0.19774900	-1.39525700
H	-4.49302600	-0.67123400	-1.86814500
H	-3.03460300	0.31888800	-1.84633700
H	-4.63004400	1.07557700	-1.65398700
H	-3.38384200	-0.94244300	0.31493300

³INT2

C	3.50430600	2.47496200	-0.81406000
H	3.51807000	2.95347800	-1.79707400
H	4.43402900	2.68863400	-0.28651500
C	3.12179400	0.97006600	-0.86343700
N	1.70888200	0.99717700	-0.43512000
C	1.46790700	2.17025800	0.02015000
C	0.13974400	2.45600700	0.59157800
N	-0.71991100	1.51140200	0.67369100
C	-1.98550500	2.11913500	1.13796400
H	-2.31183900	1.58220800	2.03486400
C	-3.09882200	1.99779200	0.07024800
C	-4.40909600	2.59951300	0.59622500
H	-4.70103600	2.14922100	1.55282900
H	-5.21803700	2.41559600	-0.11835000

H	-4.34057900	3.68611600	0.73952100
C	-2.68946500	2.59678500	-1.27972300
H	-2.48725800	3.67448100	-1.21517300
H	-1.79945100	2.09666100	-1.67485700
H	-3.49250800	2.45251400	-2.00937100
H	-3.25423700	0.92646000	-0.07735400
C	-1.55559800	3.57622000	1.49089200
H	-1.51496300	3.77098100	2.56547900
H	-2.14933000	4.34856600	1.00017300
O	-0.18687000	3.69295700	0.97720700
Ni	0.06169700	-0.36504000	-0.55755800
Br	1.43338000	-2.06834200	-1.67228400
C	-1.76291600	-1.04340000	-0.83141500
C	-2.36749500	-0.90400400	-2.08597200
C	-3.72173400	-1.20319000	-2.28349400
C	-4.48595500	-1.67664300	-1.21662700
C	-3.88893500	-1.85690200	0.03509700
C	-2.53895800	-1.54416200	0.23613300
C	-1.88855700	-1.73095800	1.59117200
H	-1.36905400	-0.79898700	1.85608000
C	-0.86467000	-2.90093900	1.60797000
C	0.19727600	-2.73038500	2.66999800
C	0.20301600	-3.43102100	3.80834800
H	-0.55786500	-4.17913700	4.01880900
H	0.97126500	-3.29188000	4.56584900
C	1.26041300	-1.70789500	2.34494200
H	1.76814700	-1.97410500	1.40809300
H	2.00910800	-1.61290300	3.13790900
H	0.82114000	-0.71056700	2.18457400
H	-1.40476900	-3.84538500	1.73953300
H	-0.37745000	-2.94982900	0.62463200
H	-2.63709100	-1.89554700	2.37585600
H	-4.48189500	-2.23766000	0.86575000
H	-5.53747100	-1.91552900	-1.35729800
H	-4.17389700	-1.07278300	-3.26451300
H	-1.77935500	-0.54570100	-2.93023400
O	2.41589200	3.10476900	-0.04873800
H	3.15260900	0.56833800	-1.87920200
C	3.95658300	0.04234700	0.04858100
C	5.37755100	-0.10424400	-0.51242100
H	5.95371800	-0.81232200	0.09263000
H	5.92234200	0.84976600	-0.50428000
H	5.36028000	-0.47945200	-1.54197000
C	3.96817700	0.49220200	1.51484800

H	4.49321100	-0.24735600	2.12853700
H	2.95418300	0.58813000	1.91571700
H	4.48396700	1.45178900	1.65040900
H	3.46086700	-0.93182500	-0.01918900

¹INT3

C	3.76991300	-1.69490200	-0.70107700
C	1.59001600	-1.32506200	-0.95396200
H	4.41133800	-1.64499100	-1.58640700
H	4.22455100	-2.34891800	0.04394200
N	1.93740000	-0.18556500	-0.50484600
O	2.50641600	-2.30223800	-1.10649600
C	0.18174300	-1.65972200	-1.22227500
C	-2.04603000	-1.73393300	-1.04310000
C	-1.56892200	-2.60891400	-2.22948500
H	-2.71229200	-0.93796200	-1.38337700
H	-1.89307900	-3.64903100	-2.18048100
H	-1.82956900	-2.18716600	-3.20415700
N	-0.78831200	-1.10108500	-0.59486400
O	-0.10992800	-2.59736700	-2.13185400
Ni	-0.50775200	0.31281400	0.76231500
C	-3.67480800	2.92641600	-1.62527800
C	-4.08586100	1.96213800	-0.70414200
C	-3.12717400	1.21311700	-0.00863700
C	-1.75737300	1.41672000	-0.21565100
C	-1.35020500	2.40692100	-1.12872400
C	-2.30982000	3.15018100	-1.82789700
H	-4.40974300	3.50758000	-2.17660600
H	-5.14536300	1.79262500	-0.52439900
H	-3.46116500	0.46414300	0.70796200
H	-1.98640400	3.91620100	-2.53134200
C	0.12194600	2.72684100	-1.22079100
C	0.61857400	3.47678300	0.05255100
C	0.72193300	1.90990000	2.02140100
H	0.39678000	1.58593600	3.00431700
H	1.66816000	1.50970000	1.67116500
C	0.08709800	2.90868500	1.35700600
H	1.71507500	3.45673000	0.06090300
H	0.30865200	4.52696400	-0.01512300
H	0.69643300	1.79883900	-1.30054400
H	0.34841700	3.34183200	-2.10042800
C	3.35980100	-0.30062900	-0.14384300
H	3.38710500	-0.31855100	0.95475900
C	4.18263600	0.90457600	-0.63650100

H	3.74925300	1.77990400	-0.13173800
C	5.64749600	0.77356900	-0.19688500
H	6.21594300	1.67058300	-0.46593900
H	5.73021500	0.63314700	0.88752100
H	6.13488000	-0.08043500	-0.68523100
C	4.05809800	1.13333900	-2.14839500
H	4.48776800	0.30366800	-2.72369800
H	3.00960900	1.24344800	-2.44360300
H	4.59394200	2.04315300	-2.44124200
C	-2.72522000	-2.48810600	0.12121100
H	-2.80415800	-1.75504600	0.93466300
C	-1.89461100	-3.66522700	0.64663000
H	-1.76361900	-4.44783900	-0.11197200
H	-0.91387100	-3.32822100	0.99303400
H	-2.40349400	-4.12436000	1.50114900
C	-4.13967000	-2.91591400	-0.29363700
H	-4.11385900	-3.63944200	-1.11964900
H	-4.65559600	-3.39755100	0.54373600
H	-4.74208900	-2.05764800	-0.61581300
C	-1.12077700	3.59374500	1.94359200
H	-1.90498000	3.73024700	1.19320100
H	-1.53446700	3.03596100	2.78848800
H	-0.82578500	4.59269600	2.29501000
Br	0.45115000	-1.26385000	2.38197700

¹INT4

C	-2.95514800	-2.85300600	0.69818800
C	-0.87235500	-2.12219500	0.49720000
H	-3.58493900	-2.89891100	1.58701600
H	-3.20659800	-3.67627200	0.02367000
N	-1.49239100	-1.24288900	-0.20060700
O	-1.56669200	-3.06709800	1.13727700
C	0.58543300	-2.01493100	0.50466400
C	2.54577500	-1.28115500	-0.24135500
C	2.74357000	-2.35743600	0.85150600
H	3.07653800	-0.36762200	0.02314100
H	3.39391300	-3.18583000	0.57065400
H	3.06193100	-1.92230500	1.80287200
N	1.09455400	-1.02714200	-0.14949400
O	1.39838700	-2.91128500	1.06270300
Ni	-0.20096300	0.18459000	-0.99183700
C	1.72228900	0.71361400	3.58267100
C	2.87600000	0.85963000	2.80604800
C	2.81313900	1.50694900	1.56407300

C	1.59086400	1.99016000	1.10139800
C	0.44475900	1.88842400	1.90570600
C	0.50262700	1.24202700	3.13901900
H	1.77824800	0.21739200	4.54830200
H	3.82932100	0.49010800	3.17745400
H	3.71690700	1.64052500	0.97290000
H	-0.38454500	1.16595900	3.76369600
C	-0.73276300	2.55624800	1.22997000
C	-0.07327100	3.37312000	0.09510200
C	1.10770400	1.57827000	-1.35624000
H	2.07866900	1.08667400	-1.51138600
H	0.83046000	2.07657200	-2.29050600
C	1.26613800	2.64656700	-0.23642400
H	-0.71765000	3.45732900	-0.78246600
H	0.15230000	4.38321100	0.46067200
H	-1.41441300	1.80972800	0.80639900
H	-1.32106600	3.17337800	1.91953300
C	-2.93497200	-1.46602700	-0.00648400
H	-3.40611100	-1.50258400	-0.99226700
C	-3.56806500	-0.30488000	0.79481400
H	-3.33067800	0.59336700	0.21409100
C	-5.09375100	-0.46221000	0.84110800
H	-5.54968400	0.39331600	1.35090700
H	-5.51948900	-0.51769500	-0.16749900
H	-5.39495600	-1.36576100	1.38861100
C	-2.97055000	-0.15683800	2.20020600
H	-3.22477900	-1.00622400	2.84746800
H	-1.88062800	-0.06482000	2.16975300
H	-3.36225500	0.74641600	2.68035900
C	2.92905600	-1.69486800	-1.68112800
H	2.59485200	-0.86843900	-2.32033900
C	2.21385200	-2.96717400	-2.15497800
H	2.47385400	-3.83812900	-1.54020200
H	1.12615600	-2.84164000	-2.13462800
H	2.49922500	-3.19684800	-3.18704300
C	4.45437100	-1.81673400	-1.80491900
H	4.84700000	-2.63780200	-1.19098800
H	4.73920500	-2.02183200	-2.84224400
H	4.95685300	-0.89285900	-1.49419200
C	2.34759200	3.65315400	-0.67544100
H	2.53775900	4.39697900	0.10862100
H	3.29530700	3.14957700	-0.90330400
H	2.02834700	4.18117600	-1.58123800
Br	-1.90327300	1.23795300	-2.19382100

²INT5

C	4.33234900	0.01829300	-0.18085100
C	2.40718900	1.11969200	0.05069400
H	4.94155700	-0.26709500	0.68032200
H	4.97770300	0.14335400	-1.05333400
N	1.96130800	-0.05449500	-0.25911800
O	3.73608700	1.31693600	0.11811600
C	1.41915200	2.13733500	0.36418900
C	-0.63387200	2.93868400	0.66227900
C	0.41002800	4.09840900	0.68342000
H	-1.14968500	2.87193900	1.62703000
H	0.26945400	4.83663200	-0.10989600
H	0.46687200	4.61006900	1.64714100
N	0.20063800	1.74239000	0.49948800
O	1.70085500	3.45010800	0.45221600
Ni	-0.02462200	-0.32980000	0.04361400
C	-4.23949500	-1.83237500	1.84212200
C	-3.76852900	-0.54896900	2.12189400
C	-2.52428200	-0.14605300	1.62372300
C	-1.70133600	-0.97724800	0.83644000
C	-2.20391500	-2.28217900	0.58544300
C	-3.45062300	-2.69391600	1.07566900
H	-5.20311300	-2.16430300	2.22249000
H	-4.36594500	0.13090700	2.72792700
H	-2.17689500	0.85867900	1.86376700
H	-3.81011100	-3.70084100	0.86158300
C	-1.39896700	-3.23788100	-0.27244300
C	-1.59064600	-3.03402500	-1.80180900
C	0.03391500	-1.25820400	-2.46806600
H	0.29506700	-0.26193600	-2.81327200
H	0.85806900	-1.95341600	-2.32371500
C	-1.24285400	-1.63635900	-2.27918700
H	-0.96807200	-3.76888700	-2.32901200
H	-2.63491300	-3.25681100	-2.05383400
H	-0.33017100	-3.11269900	-0.04798500
H	-1.65524100	-4.28014000	-0.03927600
C	3.12539000	-0.93525500	-0.43619300
H	3.13257700	-1.28819800	-1.47495500
C	3.02222300	-2.17007900	0.48603300
H	2.10685600	-2.68826100	0.16709500
C	4.21452000	-3.11058900	0.26692300
H	4.08944100	-4.03092300	0.84724100
H	4.32101900	-3.38971300	-0.78874700

H	5.15644600	-2.64811600	0.58984000
C	2.84230800	-1.79202400	1.96149200
H	1.93942100	-1.18714200	2.09631900
H	2.73745200	-2.69541400	2.57196200
H	3.70294900	-1.23179900	2.34980100
C	-1.70700700	2.99121700	-0.44789600
H	-2.28488900	2.06641500	-0.32194200
C	-1.09522000	2.97185600	-1.85400400
H	-0.48680000	3.86407700	-2.05211300
H	-0.46446300	2.08722100	-1.98921000
H	-1.88627400	2.94181100	-2.61129600
C	-2.64357900	4.18847000	-0.24327800
H	-2.11191400	5.14244600	-0.35930600
H	-3.45287400	4.17489000	-0.98134000
H	-3.09902500	4.17464000	0.75428700
C	-2.39736100	-0.69395100	-2.49323600
H	-2.97291000	-0.60215800	-1.56478000
H	-2.06256500	0.30333700	-2.79488600
H	-3.07510700	-1.08488400	-3.26449900

²INT6

C	1.33223600	-2.90892800	1.10417500
H	1.60603500	-3.93576600	0.84603300
H	1.80425700	-2.62546500	2.04751700
O	-0.11833600	-2.89012700	1.31457500
C	-0.58096100	-1.99079400	0.43191600
N	0.24773100	-1.37451600	-0.33697300
C	1.59371200	-1.88629200	-0.04223600
H	2.19512200	-1.04889600	0.31358500
C	2.27585400	-2.47658700	-1.29092500
C	2.30614200	-1.44971800	-2.43102900
H	2.85616100	-0.55320600	-2.12300700
H	2.80008200	-1.87197200	-3.31406900
H	1.29770100	-1.13099800	-2.71046000
C	3.69755900	-2.94002700	-0.93750700
H	4.19363700	-3.36677100	-1.81617000
H	4.29665600	-2.09041000	-0.58778700
H	3.70665500	-3.70397200	-0.15001900
H	1.68385000	-3.34744600	-1.61294600
Ni	-0.64352200	0.32298500	-1.18984700
C	0.43869700	1.94704100	-1.57273900
C	1.13681200	2.69907100	-0.40588700
C	2.16965100	1.81818000	0.28931600
C	3.44588900	1.46640300	-0.15054300

C	4.26749600	0.67737500	0.66575000
C	3.81468000	0.24054600	1.91584700
C	2.52685000	0.57875000	2.35273600
C	1.71369900	1.36293000	1.53560200
C	0.29857800	1.83289800	1.77468600
H	-0.39639200	1.01607100	1.53403300
H	0.10587400	2.12929500	2.81266800
C	0.14515100	2.99543400	0.76557600
H	-0.87963300	3.10438200	0.39723500
H	0.42600600	3.93367900	1.26222000
H	2.17145900	0.24334100	3.32523700
H	4.46435000	-0.35823900	2.54944900
H	5.26847200	0.41467100	0.33191900
H	3.80899700	1.81511700	-1.11415000
C	1.78087200	4.00627400	-0.91323700
H	2.47777600	3.80577100	-1.73587500
H	1.00632100	4.68150400	-1.29744800
H	2.33098800	4.53103200	-0.12015400
H	-0.20498500	2.68283500	-2.08909500
H	1.21089800	1.67093100	-2.31189700
N	-2.28853000	-0.71006300	-0.54833100
C	-1.98683700	-1.63688200	0.30189000
O	-2.96554800	-2.20561300	1.02555600
C	-4.19767400	-1.56119300	0.58007700
H	-4.66342600	-1.10451100	1.45660000
H	-4.85436200	-2.34147900	0.18870900
C	-3.74938900	-0.53091200	-0.50214400
H	-4.15154600	-0.81241800	-1.48357100
C	-4.13654000	0.94001800	-0.23845700
C	-5.66008000	1.11397500	-0.30381000
H	-5.93151700	2.17006100	-0.20110600
H	-6.06858600	0.75194000	-1.25524000
H	-6.16075900	0.56887700	0.50740600
C	-3.55322200	1.48322200	1.07049000
H	-3.79439900	2.54611800	1.17993400
H	-2.46509000	1.38320500	1.07837400
H	-3.95739300	0.96485000	1.94944800
H	-3.68298700	1.50757100	-1.06287500
²INT7			
C	-2.85698000	2.95529300	1.16878900
C	-2.84007200	1.44107500	0.83112400
C	-0.81267700	2.14306500	1.38262400
H	-2.92742800	3.59194600	0.28205200

H	-3.60705900	3.24589100	1.90464200
H	-3.29348300	0.86342300	1.64915200
N	-1.39691200	1.13427400	0.84230900
O	-1.53735200	3.20241400	1.75776000
C	0.63046500	2.03726300	1.59199800
C	2.60119100	1.00754800	1.61346800
C	2.71185700	2.41120100	2.27572500
H	3.28173000	0.92420700	0.76082500
H	3.08245600	2.39726500	3.30254900
H	3.30127500	3.11574900	1.68317900
N	1.21474000	0.99281300	1.12345600
O	1.33937100	2.91593600	2.31234100
C	2.84277500	-0.21027200	2.53331800
H	2.59888700	-1.08191300	1.91185600
C	1.90933600	-0.23186500	3.75015500
H	2.08022000	-1.13809900	4.34143700
H	2.07631100	0.62732300	4.41255800
H	0.85947600	-0.22894700	3.43909300
C	4.32116000	-0.29845100	2.93245700
H	4.50545400	-1.19639400	3.53234900
H	4.96622800	-0.34587300	2.04728200
H	4.62947000	0.56580600	3.53574300
C	-3.52922900	1.00077300	-0.46880900
H	-3.44483300	-0.08871100	-0.48118000
C	-5.01700200	1.37028000	-0.43703300
H	-5.16375400	2.45906300	-0.45229300
H	-5.53210900	0.95398200	-1.30944500
H	-5.50661100	0.96822800	0.45732500
C	-2.82990700	1.52484000	-1.72452700
H	-3.32539500	1.13323400	-2.62055400
H	-2.84479900	2.61912400	-1.78197900
H	-1.78893900	1.18565200	-1.73236300
C	2.44141600	0.81312500	-2.23999000
H	2.30589800	0.57319100	-1.18374500
H	3.29111700	1.50418700	-2.32314200
C	1.17172800	1.50316400	-2.70680900
H	0.33514400	0.79468800	-2.68092000
H	1.28403800	1.90521800	-3.72110600
C	2.71178900	-0.48130900	-3.00897700
H	1.86020200	-1.16031400	-2.89165800
H	2.81803500	-0.27340800	-4.08560600
C	3.98872300	-1.18937100	-2.57979600
H	4.15721700	-2.10819200	-3.14200300
H	4.86762200	-0.54613100	-2.65604900

O	0.90322700	2.56091200	-1.76205500
C	-0.11024200	3.43832100	-1.94671300
O	-0.50643800	4.07860000	-0.99729900
C	-0.66002100	3.59946000	-3.35028200
H	0.13327600	3.90362600	-4.04254500
H	-1.08615100	2.66184800	-3.71978200
H	-1.43645500	4.36417500	-3.32826200
Br	3.93456800	-1.76349900	-0.67002000
Ni	-0.00165600	-0.29078900	0.08126900
C	-0.35750100	-1.86682400	-1.09862800
C	-1.10543000	-3.08551300	-0.48117400
C	-2.55957100	-2.73204000	-0.20031800
C	-3.62744100	-2.67729200	-1.09621700
C	-4.90328800	-2.33418200	-0.63135100
C	-5.10618600	-2.03570700	0.72000800
C	-4.03351700	-2.08373200	1.61977200
C	-2.76869500	-2.44206900	1.15641200
C	-1.47712800	-2.58537300	1.92847100
H	-1.04150400	-1.59313100	2.11836400
H	-1.61048100	-3.07285300	2.90213900
C	-0.58485900	-3.39875800	0.95853400
H	0.47806500	-3.15374300	1.05620800
H	-0.70897400	-4.46901300	1.17293400
H	-4.19310200	-1.86592800	2.67428900
H	-6.10052200	-1.77486300	1.07413700
H	-5.74130800	-2.30069900	-1.32350200
H	-3.47368400	-2.90894800	-2.14743700
C	-0.98473100	-4.32441800	-1.38958800
H	-1.34298700	-4.10349700	-2.40268400
H	0.06689200	-4.62652700	-1.47287200
H	-1.55745200	-5.17944400	-1.00458200
H	0.63976400	-2.24100300	-1.40007900
H	-0.86627300	-1.59751200	-2.04131300

²INT8

C	-3.46632900	2.17511400	1.11681900
C	-2.85933700	1.75223300	-0.23920600
C	-1.43829100	1.34750000	1.42029800
H	-3.84940600	3.19460000	1.15372900
H	-4.21973500	1.46451600	1.46760500
H	-3.52486100	1.06339100	-0.75731100
N	-1.65925300	1.01088800	0.19587100
O	-2.33648500	2.09603900	2.05491800
C	-0.16171100	0.92444900	1.99567100

C	1.81036600	-0.09578700	1.98842400
C	1.67161600	0.83247600	3.22584300
H	2.66631900	0.20381100	1.38476700
H	1.85121900	0.34913900	4.18665100
H	2.26963600	1.74006800	3.12563600
N	0.59263100	0.22986500	1.22765200
O	0.26093300	1.25999700	3.21089900
C	1.89649800	-1.61172900	2.26563900
H	1.85817300	-2.07866300	1.27421100
C	0.71904100	-2.13548900	3.09781900
H	0.77515000	-3.22584300	3.18996100
H	0.72009900	-1.72044800	4.11400600
H	-0.24104600	-1.89172100	2.63145000
C	3.24764900	-1.95577700	2.90704000
H	3.34774900	-3.03901300	3.03633700
H	4.08209500	-1.61170500	2.28423300
H	3.35499000	-1.49674800	3.89891400
C	-2.46694700	2.90414000	-1.19269000
H	-1.84047600	2.43895700	-1.96522400
C	-3.72404500	3.47501500	-1.86416200
H	-4.40153900	3.92563700	-1.12670300
H	-3.45644200	4.25833500	-2.58138800
H	-4.28023300	2.69857900	-2.40310000
C	-1.64258900	4.00548400	-0.51095100
H	-1.32302300	4.74381000	-1.25565800
H	-2.23119200	4.54604400	0.24068900
H	-0.74296300	3.61632800	-0.02471700
C	4.98275700	0.30717500	-0.46221300
H	4.29555800	-0.44079000	-0.05035100
H	5.58506700	0.70646300	0.36259400
C	4.14257500	1.41706100	-1.07256800
H	3.49445700	0.99623700	-1.84306400
H	4.76908500	2.20781900	-1.50610300
C	5.88554000	-0.36889500	-1.50790700
H	5.24120200	-0.72272400	-2.33525800
H	6.56559800	0.37014700	-1.95635200
C	6.66497600	-1.50999100	-0.94514200
H	6.20588500	-2.17701300	-0.22059700
H	7.61373600	-1.81014300	-1.37806800
O	3.34827000	1.99298500	-0.00882300
C	2.18044800	2.62751700	-0.24727300
O	1.54343900	3.03052900	0.70770600
C	1.71653300	2.77217900	-1.67900600
H	2.51575400	3.11342400	-2.34377700

H	1.36807400	1.79389500	-2.03396100
H	0.88785700	3.47854100	-1.70588100
Ni	-0.27457600	-0.11943400	-0.61572400
C	-1.38354200	-0.63490400	-2.12841400
C	-2.19386700	-1.94656700	-1.90575100
C	-3.05983000	-1.85255000	-0.65287400
C	-4.29665700	-1.23240700	-0.48870100
C	-4.89140800	-1.20086800	0.78047100
C	-4.25254900	-1.79612300	1.87287600
C	-3.03124500	-2.46044900	1.69851500
C	-2.44878600	-2.49930100	0.43338500
C	-1.17346300	-3.18237300	-0.00937800
H	-0.29174500	-2.61831500	0.31806800
H	-1.07443400	-4.19447300	0.40084400
C	-1.28444000	-3.16364800	-1.55213100
H	-0.30973900	-3.10059200	-2.03979800
H	-1.78126100	-4.08346200	-1.88694600
H	-2.55595300	-2.96046000	2.53952800
H	-4.72066400	-1.77161000	2.85367600
H	-5.86262800	-0.72910100	0.91226300
H	-4.80588400	-0.78514000	-1.33993800
C	-3.02301800	-2.22573200	-3.17441600
H	-3.67034600	-1.37605600	-3.42466000
H	-2.36007700	-2.39889700	-4.02997900
H	-3.65842500	-3.11107800	-3.04565200
H	-0.74427100	-0.75673000	-3.00955600
H	-2.08609900	0.18568800	-2.33287300
Br	1.67058100	-1.12510700	-1.49258100

²INT9

C	2.96988800	2.69605300	-2.03198600
H	2.90428800	3.25982600	-2.96344000
H	3.79028700	3.08453900	-1.42187600
O	3.30298800	1.31194500	-2.37785900
C	2.45720700	0.57091100	-1.64504700
N	1.54579500	1.13859100	-0.95242800
C	1.63837900	2.58427700	-1.23896700
H	1.71578900	3.10977400	-0.28946600
C	0.37767300	3.09455800	-1.97120500
C	0.39159100	4.62853600	-2.03391300
H	1.23212300	4.99738900	-2.63669400
H	-0.52880800	5.00425500	-2.49394900
H	0.47666600	5.06326000	-1.03196500
C	0.19391300	2.47670000	-3.36390000

H	-0.77532900	2.76780800	-3.78313900
H	0.96618600	2.81955900	-4.06365900
H	0.22593000	1.38339500	-3.33094900
H	-0.46644100	2.78836200	-1.33990800
Ni	0.13755900	-0.62358000	0.04975300
C	-1.07842400	0.52760100	1.07686000
C	-0.42702800	1.05471100	2.39073300
C	0.50678300	2.23566100	2.14576800
C	0.17474900	3.56626600	1.89442600
C	1.19544300	4.52062700	1.78761400
C	2.53656700	4.13882500	1.91046400
C	2.87044700	2.79740500	2.14082900
C	1.85176900	1.85451500	2.26534000
C	1.94327700	0.37484700	2.56056200
H	2.14501300	-0.18761300	1.63336500
H	2.74740500	0.11540100	3.25805100
C	0.53420100	0.05602700	3.10852900
H	0.23731900	-0.98364600	2.96550400
H	0.52184200	0.27517100	4.18351900
H	3.91200500	2.50181200	2.24686000
H	3.32114500	4.88754700	1.83635000
H	0.94374600	5.56458700	1.61873300
H	-0.86591500	3.86917900	1.80913800
C	-1.59854800	1.44231000	3.32196800
H	-2.29816300	2.12456400	2.82517900
H	-2.15580200	0.54652500	3.61749100
H	-1.22564600	1.93493200	4.22817300
H	-1.92035800	-0.12696300	1.31432400
H	-1.43099400	1.38116900	0.49022500
N	1.80371300	-1.59423400	-0.88884700
C	2.58692600	-0.89452200	-1.62309900
O	3.52989300	-1.51222900	-2.34143300
C	3.25154900	-2.94372900	-2.15796300
H	4.20859200	-3.44301500	-2.00631200
H	2.78913400	-3.30077300	-3.08319000
C	2.29787400	-2.98686600	-0.93836800
H	1.44142600	-3.64538900	-1.09851200
C	2.96877900	-3.37348200	0.40218700
C	3.30252400	-4.87139500	0.40583400
H	3.72102500	-5.16587900	1.37426300
H	2.40474200	-5.47501700	0.23126100
H	4.04474900	-5.12962700	-0.36197800
C	4.19880100	-2.51881600	0.73653100
H	4.57962800	-2.78780300	1.72769000

H	3.95739100	-1.45059400	0.75953800
H	5.01835800	-2.66726900	0.02170500
H	2.20043800	-3.19412700	1.16098800
C	-3.65021300	-0.06688100	-1.13957600
H	-3.45380800	0.60302900	-0.29728800
H	-3.74394600	0.56430700	-2.03277800
C	-4.97595900	-0.76887400	-0.89098000
H	-4.91992100	-1.36504000	0.02880600
H	-5.21978500	-1.44537500	-1.72165500
C	-2.50107600	-1.06966900	-1.31063200
H	-2.48187100	-1.76914100	-0.46732800
H	-2.69939400	-1.68783100	-2.20110800
C	-1.13337700	-0.41163500	-1.45759800
H	-0.49460300	-0.92692600	-2.18594300
H	-1.19351300	0.64681300	-1.71297100
O	-5.98650200	0.24817500	-0.77188000
C	-7.27669600	-0.05541500	-0.47271600
O	-8.08531300	0.83982100	-0.40654100
C	-7.62539600	-1.51325300	-0.23008300
H	-7.36890900	-2.13718300	-1.09318500
H	-7.07960300	-1.90993800	0.63341500
H	-8.69675400	-1.57821600	-0.03962600
Br	-0.50749000	-2.80684500	1.15772100

¹INT10

C	4.05897800	1.67687700	-1.14347300
C	3.42690700	0.31948300	-1.57636600
C	2.00329700	1.43312700	-0.31278500
H	4.98005600	1.57567500	-0.56537700
H	4.22973400	2.36184000	-1.97858000
H	3.32531600	0.27342500	-2.66784000
N	2.07278600	0.36112300	-0.99706600
O	3.05873100	2.27930100	-0.27497900
C	0.83096200	1.81529600	0.49595500
C	-1.10396500	1.76353400	1.62891500
C	-0.28280100	3.02047600	2.02091500
H	-1.16592600	1.06650100	2.47133000
H	-0.78579900	3.96442600	1.80183100
H	0.04729700	3.01266700	3.06158800
N	-0.22751600	1.10443400	0.63600600
O	0.91145300	2.95922800	1.18717600
Ni	-0.47712600	-0.75899200	0.15443100
C	-3.05926600	0.72855600	-3.52876000
C	-1.69630800	1.01899200	-3.45285700

C	-0.94315000	0.54749400	-2.37302500
C	-1.52477600	-0.23037800	-1.36293700
C	-2.89083600	-0.55268200	-1.46243000
C	-3.64515700	-0.06099600	-2.53955900
H	-3.65933600	1.10361400	-4.35398100
H	-1.22039600	1.61874900	-4.22594100
H	0.11211000	0.78927400	-2.31086700
H	-4.70388500	-0.30762300	-2.60402000
C	-3.52305300	-1.51985900	-0.48945300
C	-2.87149200	-2.92260000	-0.64147900
C	-1.53842100	-3.02991700	0.06775200
C	-1.62838700	-3.52423100	1.48829100
C	-0.34349000	-2.83978200	-0.57616400
Br	0.82314900	-1.23905300	2.20989500
H	-1.97251400	-4.56830300	1.46608200
H	-0.67686400	-3.46031700	2.01311300
H	-2.37409700	-2.95203600	2.05355900
H	-3.54304500	-3.67706600	-0.21350100
H	-2.76425600	-3.14061600	-1.70894100
H	-3.39944100	-1.18553000	0.54995300
H	-4.60007000	-1.60153800	-0.67591500
C	-2.52319000	2.02755500	1.09006400
H	-2.90166600	1.04914700	0.77463500
C	-2.55032800	2.94761000	-0.13578700
H	-2.22928400	3.96813000	0.10975500
H	-1.91332200	2.56105300	-0.93495700
H	-3.56979700	3.01245100	-0.53051800
C	-3.41983000	2.55344700	2.21995900
H	-4.45037700	2.67105200	1.86783000
H	-3.43049900	1.87044200	3.07807300
H	-3.08364100	3.53641100	2.57604600
C	4.18339100	-0.94782100	-1.11534900
H	3.55962400	-1.79199400	-1.43963900
C	5.53990100	-1.04786000	-1.82831600
H	5.42960700	-1.01725700	-2.91959100
H	6.20917200	-0.22852100	-1.53446500
H	6.04254400	-1.98526800	-1.56648400
C	4.32963000	-1.03165100	0.40933800
H	3.35605000	-1.01453700	0.90868700
H	4.83350400	-1.96479100	0.68609900
H	4.93836800	-0.20798600	0.80520800
H	-0.31522100	-2.68402600	-1.65102900
H	0.59530400	-3.06396000	-0.07739300

¹INT11

C	-2.98468600	-1.15487300	-2.25049500
C	-2.77043000	-0.77906200	-0.76004300
C	-0.81910900	-1.03388900	-1.78292600
H	-3.57938200	-2.05573600	-2.40888700
H	-3.39390700	-0.33150700	-2.84139000
H	-3.26078500	0.17082100	-0.54805600
N	-1.30490000	-0.59028000	-0.67491500
O	-1.64025700	-1.42656700	-2.75720200
C	0.62970300	-1.20625700	-1.88014200
C	2.71380000	-1.20973100	-1.11063500
C	2.67512400	-1.68907800	-2.59280500
H	3.12526200	-1.97291800	-0.44459400
H	3.28847400	-1.09565700	-3.27220500
H	2.91372900	-2.74901700	-2.71190700
N	1.28559100	-1.06499600	-0.79221600
O	1.27430100	-1.51421800	-3.00951600
Ni	0.11911300	-0.39559300	0.81564200
C	-0.67814300	3.98598800	-1.90636200
C	-1.99775700	3.53527000	-1.82259000
C	-2.39132600	2.77101400	-0.72478700
C	-1.49082800	2.43379800	0.29536200
C	-0.16569800	2.90373100	0.22065900
C	0.21908500	3.67443100	-0.88571200
H	-0.35376900	4.58345900	-2.75448500
H	-2.71418700	3.78202800	-2.60219100
H	-3.42518200	2.43680900	-0.64749100
H	1.24458900	4.03460700	-0.94165900
C	0.85382900	2.57091600	1.29705400
C	0.26029900	1.85686600	2.52173000
C	-0.78706200	0.80307000	2.12647600
C	-1.29095200	0.02150900	3.33454200
C	-1.93254800	1.57981700	1.46703000
H	-0.47314900	-0.50770300	3.82771900
H	-1.76112400	0.69914900	4.06900600
H	-2.04699700	-0.72171100	3.05094000
C	3.46448000	0.11521600	-0.84860100
H	3.28903200	0.32191500	0.21364300
C	2.91276600	1.28453400	-1.67353300
H	3.42256900	2.21356600	-1.39537400
H	3.06921400	1.13945400	-2.75064000
H	1.84262800	1.43546700	-1.50100400
C	4.97163700	-0.07554600	-1.06297100
H	5.51309400	0.83985500	-0.80098700

H	5.36344300	-0.88765200	-0.43952100
H	5.20876000	-0.30510600	-2.11073600
C	-3.23007200	-1.82622700	0.27764700
H	-2.93849500	-1.41474100	1.25112600
C	-4.75760400	-1.97041900	0.25429700
H	-5.11190200	-2.39996900	-0.69170700
H	-5.08988000	-2.63653000	1.05736100
H	-5.25473900	-1.00256100	0.39297800
C	-2.51562200	-3.17429700	0.11568000
H	-2.86183100	-3.87853500	0.87937900
H	-2.71266500	-3.62921400	-0.86397800
H	-1.43305100	-3.06122400	0.23638300
H	-2.37574300	2.24068900	2.23595100
H	-2.74993600	0.91638600	1.17212600
H	1.62920700	1.92763400	0.85886400
H	1.36973600	3.49039900	1.60603000
H	-0.23532400	2.60304800	3.16932400
H	1.06471600	1.40577200	3.10505000
Br	1.82348300	-1.14006200	2.30038200

²INT12

C	-3.43418700	-1.69451400	-1.22514500
C	-2.89789200	-0.34318400	-0.65944500
C	-1.33865400	-1.92091000	-0.50109400
H	-4.30856300	-2.08189400	-0.69747000
H	-3.64284100	-1.66110100	-2.29709600
H	-2.85320000	0.42082800	-1.44363700
N	-1.51838200	-0.67018400	-0.28239800
O	-2.34274000	-2.64882400	-1.02119900
C	-0.02988300	-2.48786500	-0.17817600
C	2.09873300	-2.47847500	0.43703100
C	1.72752700	-3.85182400	-0.19577000
H	2.48152900	-2.61328600	1.45491400
H	2.33686300	-4.12886400	-1.05785700
H	1.72581300	-4.67167600	0.52824900
N	0.80277500	-1.78039300	0.49931500
O	0.35684900	-3.67836300	-0.66908200
Ni	0.08875400	0.39494300	0.56742300
C	0.70899900	3.94134500	-2.66938800
C	0.07951100	2.73991400	-2.99850900
C	-0.09519100	1.76752500	-2.00933800
C	0.34741000	1.93000600	-0.67807300
C	0.99202300	3.15351900	-0.37806000
C	1.15676000	4.14082300	-1.36269400

H	0.84580300	4.71833700	-3.41858800
H	-0.27621300	2.56720200	-4.01338300
H	-0.58877200	0.83529600	-2.28858100
H	1.64691200	5.08038800	-1.10636300
C	1.55380800	3.43588300	1.00697600
C	0.77388800	2.81170000	2.17858200
C	0.89023100	1.30702300	2.33953100
C	2.28664600	0.75836400	2.55034700
C	-0.21677800	0.54665200	2.68346100
H	2.95641100	1.02677000	1.72692200
H	2.72535100	1.16933800	3.47249600
H	2.27257200	-0.33245700	2.63602500
C	3.11886300	-1.62727300	-0.35817700
H	3.21215300	-0.68951100	0.20254100
C	2.62281400	-1.27080200	-1.76613000
H	3.38671700	-0.69391500	-2.29837100
H	2.40980400	-2.16589100	-2.36563500
H	1.72148700	-0.65134900	-1.71891800
C	4.49123200	-2.31428900	-0.38168900
H	5.23585900	-1.66186200	-0.84996100
H	4.84163000	-2.55284900	0.63033700
H	4.46932100	-3.24745800	-0.95937300
C	-3.65932300	0.25127300	0.54499900
H	-3.08134200	1.14114900	0.82832400
C	-5.06842100	0.69303400	0.12902100
H	-5.68782500	-0.16438200	-0.16629000
H	-5.57793400	1.19039700	0.96145400
H	-5.03702700	1.39370700	-0.71386400
C	-3.68598100	-0.69507600	1.75174400
H	-4.17107700	-0.20762600	2.60468600
H	-4.24803200	-1.61401500	1.54016100
H	-2.67061000	-0.97106600	2.05247900
H	-1.19319500	1.00961300	2.81115700
H	-0.10465800	-0.45773800	3.08657600
H	2.60003600	3.09714600	1.05474200
H	1.59658800	4.52162900	1.16693500
H	-0.28491400	3.07925000	2.08183600
H	1.13979800	3.27192300	3.11151600

²INT13

C	-1.48281300	2.84923200	1.12478700
C	-1.73046900	1.66362700	0.14419400
C	0.45678400	1.98583600	0.45023500
H	-1.89202000	3.80378200	0.78664700

H	-1.83574300	2.64117300	2.13806300
H	-2.28749400	0.86638300	0.64005500
N	-0.36902800	1.17644200	-0.12761200
O	-0.02841400	2.99821700	1.18870300
C	1.87015900	1.73789000	0.25275800
C	3.65830600	0.61506200	-0.46810200
C	4.08904300	1.82590600	0.41049300
H	4.09452800	0.69396200	-1.47033600
H	4.71541600	1.56049700	1.26421600
H	4.57939900	2.61522600	-0.16701200
N	2.19913900	0.78981500	-0.57171400
O	2.84225800	2.37182200	0.93469700
Ni	0.62247800	-0.46306700	-0.92199200
C	-4.13356400	-0.86245700	1.84848900
C	-4.56434900	-0.93318200	0.52049500
C	-3.70031900	-1.42906700	-0.45607900
C	-2.40567000	-1.86659600	-0.14063700
C	-1.97213000	-1.79379900	1.19749000
C	-2.84682900	-1.29219100	2.17280000
H	-4.79504500	-0.48188000	2.62280800
H	-5.56529300	-0.60717500	0.24852300
H	-4.03294600	-1.48338000	-1.49113500
H	-2.50601400	-1.24044600	3.20574100
C	-0.56589900	-2.20497500	1.59264700
C	0.16144800	-3.00357400	0.50345900
C	-0.00973100	-2.37105300	-0.88181200
C	0.78030800	-3.17543100	-1.92245400
C	-1.50627600	-2.43287100	-1.22355100
H	1.85808900	-3.16403400	-1.70740100
H	0.46585500	-4.23838000	-1.94646900
H	0.64466300	-2.77600900	-2.93626700
C	3.99953000	-0.78405100	0.09728100
H	3.52537800	-1.49580500	-0.59278900
C	3.39794100	-1.02263700	1.48775000
H	3.61481200	-2.04228800	1.82364300
H	3.80920900	-0.33445300	2.23723500
H	2.31024800	-0.90531400	1.46491400
C	5.51545200	-1.02095900	0.07982700
H	5.74784200	-2.04283800	0.39824600
H	5.93533800	-0.87685800	-0.92320700
H	6.03778900	-0.34012400	0.76475800
C	-2.45983500	2.01186000	-1.17166100
H	-2.50617100	1.06550300	-1.72686400
C	-3.89687200	2.46785400	-0.88560500

H	-3.91652800	3.42107300	-0.34084000
H	-4.44591400	2.61864000	-1.82185600
H	-4.43436800	1.72214000	-0.29058300
C	-1.69397200	3.03095100	-2.02461700
H	-2.22054100	3.21097900	-2.96850600
H	-1.59936400	3.99906200	-1.51519300
H	-0.68743000	2.67005800	-2.26075800
H	-1.80739200	-3.49138500	-1.38579600
H	-1.71627600	-1.92132400	-2.17297600
H	0.00607600	-1.28761800	1.79841100
H	-0.59907900	-2.76690600	2.53668200
H	-0.23450900	-4.04012400	0.49775800
H	1.22511800	-3.08262200	0.76502300

²INT14

C	-0.62086300	3.81051900	-1.53083300
C	-1.58926200	2.02312100	-0.62866800
H	-0.65964000	4.82717100	-1.13683200
H	-0.53035600	3.83746000	-2.61887800
N	-0.36160500	1.76756400	-0.38574400
O	-1.91040800	3.17546800	-1.22383200
C	-2.58416600	1.00124800	-0.27593800
C	-3.33123900	-0.95961100	0.47105500
C	-4.52215900	0.00390500	0.17523800
H	-3.24245500	-1.14314800	1.54887800
H	-5.17263200	-0.33833500	-0.63252500
H	-5.12210400	0.24189200	1.05495300
N	-2.16608500	-0.15430500	0.08088600
O	-3.89567200	1.25156300	-0.27387200
Ni	-0.03951400	-0.21731700	0.21412100
C	4.30873400	0.30760100	-1.08961400
C	3.74127000	0.76788200	0.09981700
C	2.90737900	-0.06527600	0.86053900
C	2.65729700	-1.36265200	0.40752200
C	3.23273300	-1.82503700	-0.78385400
C	4.05723400	-0.99563600	-1.53560300
H	4.95714600	0.96048000	-1.66843000
H	3.96231100	1.77232000	0.45153000
H	2.46923000	0.29060100	1.78674900
H	4.49798900	-1.35237300	-2.46317600
C	2.77282900	-3.23075100	-1.08345800
C	2.25285000	-3.71699300	0.28693100
C	0.28394500	-2.19031600	0.70713300
H	-0.40897900	-2.34262000	1.53427800

H	-0.05309000	-2.64630800	-0.22152000
C	1.76051700	-2.43398900	1.04349700
H	1.47201000	-4.48138500	0.21208000
H	3.08158700	-4.14942200	0.86167900
C	0.44549000	2.90124700	-0.84783100
H	1.15850100	2.50904700	-1.58100300
C	1.22542500	3.53303600	0.32541300
H	1.81827500	2.71238200	0.74539900
C	2.18542500	4.60921400	-0.19847600
H	2.79479100	5.01072900	0.61839500
H	2.86353700	4.20506200	-0.96007200
H	1.64218000	5.45338600	-0.64382700
C	0.31150000	4.05848900	1.43915600
H	-0.34671700	4.86445000	1.08898800
H	-0.30015600	3.25135400	1.85271700
H	0.91658900	4.46680500	2.25607400
C	-3.36805800	-2.31809700	-0.25897100
H	-2.45919300	-2.84452200	0.05956200
C	-3.31455700	-2.17673100	-1.78530100
H	-4.18576300	-1.63535000	-2.17711100
H	-2.40609900	-1.65482900	-2.10155100
H	-3.31536100	-3.16814800	-2.25193900
C	-4.58149500	-3.13534400	0.20759700
H	-5.52511900	-2.66585400	-0.10004400
H	-4.56011800	-4.13746200	-0.23348900
H	-4.60002200	-3.24711000	1.29870700
C	1.96177400	-2.55893000	2.56076400
H	3.02504200	-2.68215100	2.79526500
H	1.58594400	-1.67520500	3.08131700
H	1.42157900	-3.43361500	2.94385200
Br	0.32048000	-0.67885000	-2.16961400
Br	-0.21223200	0.37456600	2.58783300
H	1.96361300	-3.18753700	-1.82428100
H	3.56204200	-3.87339100	-1.48984700

²INT15

C	2.73816700	0.07434500	-0.27256300
C	2.23543000	-1.24392900	-0.14556000
C	0.91168800	-1.48734300	0.13204400
C	-0.00885500	-0.36807200	0.35101400
C	0.53393800	0.98990800	0.13679800
C	1.85542200	1.18005200	-0.16394200
H	3.78760400	0.23677800	-0.49753100
H	2.91536500	-2.08299000	-0.27584100

H	0.53952900	-2.50354600	0.23239700
H	2.22498900	2.18445500	-0.36238200
C	-0.59806300	1.98448000	0.08905800
C	-1.78644300	1.14863600	-0.46279100
C	-1.15593500	-0.49746900	1.39051300
C	-1.52437500	-0.29953100	-0.03954600
H	-2.75922900	1.51303200	-0.10961700
H	-1.79435200	1.19583500	-1.55929700
H	-0.83702500	2.36614200	1.09259800
H	-0.37067100	2.85666300	-0.53235900
C	-2.20029400	-1.40027400	-0.82055500
H	-1.98452300	-1.30982800	-1.89210900
H	-1.86658200	-2.39068800	-0.49220700
H	-3.28983800	-1.35736900	-0.69059700
H	-1.28809000	0.30249600	2.11610300
H	-1.28125100	-1.49579500	1.80403100

²INT16

C	2.99670300	0.32436600	-0.24082200
C	2.75122900	-1.04962400	-0.21922300
C	1.45487800	-1.51871100	0.00323100
C	0.39804300	-0.62878100	0.21369400
C	0.64529200	0.75566000	0.19345700
C	1.94358900	1.21873800	-0.03930900
H	4.00104900	0.69880100	-0.42081400
H	3.56295000	-1.75378400	-0.38231400
H	1.25993300	-2.58923200	0.01084200
H	2.12948200	2.29053900	-0.06417900
C	-0.52120700	1.68988800	0.41646000
C	-1.76211600	1.22192300	-0.37155300
C	-1.01471300	-1.11465400	0.47287800
C	-2.06765100	-0.22909400	-0.13484500
H	-2.62943700	1.84572700	-0.10618200
H	-1.58514200	1.40583100	-1.44717500
H	-0.77555900	1.70973900	1.48718500
H	-0.25332200	2.71595700	0.13908700
C	-3.46618900	-0.73393500	-0.28433200
H	-4.00674300	-0.19896900	-1.07638800
H	-3.49228400	-1.80567400	-0.52157000
H	-4.05864400	-0.60252300	0.64065100
H	-1.16906400	-1.18371600	1.57050300
H	-1.13037200	-2.14734700	0.11253400

¹TS1

C	4.81819500	0.49775300	0.37640700
H	5.50445200	1.03707700	-0.28230300
H	5.38513700	0.00960900	1.17116300
C	3.85284900	-0.44989400	-0.39336300
N	2.56883900	0.26848200	-0.32243000
C	2.72663100	1.24963600	0.50083300
C	1.53537200	1.99749200	0.87746100
N	0.39231400	1.48692800	0.56719600
C	-0.61997000	2.52263900	0.85078900
H	-1.40917600	2.08351500	1.46849000
C	-1.25261600	3.02109100	-0.46995200
C	-2.38831200	4.01193500	-0.18307800
H	-3.13975600	3.57649700	0.48706000
H	-2.89231600	4.29490400	-1.11359700
H	-2.01798500	4.93609200	0.27999600
C	-0.21486600	3.59345300	-1.44406800
H	0.29918600	4.47268100	-1.03434800
H	0.53494200	2.83685300	-1.69792100
H	-0.70372000	3.90248100	-2.37432200
H	-1.68066400	2.13068900	-0.94131700
C	0.18591200	3.58273800	1.65463900
H	-0.01374600	3.54628800	2.72970500
H	0.06604500	4.60651200	1.29613100
O	1.58526100	3.21099800	1.45413300
Ni	0.66139500	-0.20140900	-0.66344200
Br	-0.50336700	-2.32763700	0.55544700
C	-0.90624300	-0.99197800	-1.14795900
C	-0.14367600	-1.36020600	-2.30181300
C	-0.63207900	-0.94931600	-3.57110400
C	-1.83658700	-0.27941100	-3.67218000
C	-2.61444800	-0.02597100	-2.51550100
C	-2.19744000	-0.39655000	-1.24727300
C	-3.02766700	-0.14083300	-0.01569300
H	-2.35464000	0.00479400	0.83521000
C	-4.00263900	-1.30631800	0.29292600
C	-4.65626100	-1.15420500	1.64878100
C	-5.90535400	-0.69550100	1.78324900
H	-6.51499000	-0.44036200	0.91900200
H	-6.36754000	-0.56481600	2.75921600
C	-3.80401700	-1.53552100	2.83538900
H	-3.56206500	-2.60629600	2.80360900
H	-4.30483500	-1.32193800	3.78533900
H	-2.83990100	-1.01154900	2.82411200
H	-4.75874100	-1.34783100	-0.49993900

H	-3.43734100	-2.24505800	0.25584600
H	-3.61392500	0.77947900	-0.13257800
H	-3.56248700	0.50043600	-2.61706400
H	-2.21504300	0.02395300	-4.64457800
H	-0.07774900	-1.22123400	-4.46667700
H	0.61658000	-2.13354400	-2.25211000
O	3.94669200	1.48847300	1.00710900
H	4.14802500	-0.53296000	-1.44485900
C	3.69392500	-1.87576600	0.18388400
C	4.98969900	-2.67741800	0.00288300
H	4.84729600	-3.71317500	0.32893200
H	5.81030000	-2.25839600	0.60019200
H	5.31164700	-2.69523700	-1.04566100
C	3.21460800	-1.87453900	1.64112200
H	3.09426400	-2.90343200	1.99596800
H	2.24144800	-1.38317200	1.73061700
H	3.92997300	-1.37692000	2.30904000
H	2.90231900	-2.34270100	-0.41818500

¹TS2

C	3.86435700	-1.45257700	-0.20516100
C	1.75075500	-1.06844700	-0.78821300
H	4.65288500	-1.67480700	-0.92938000
H	4.10802900	-1.90730800	0.75639700
N	2.10506000	0.13014900	-0.54718500
O	2.63849800	-2.07739300	-0.68327200
C	0.36070800	-1.44555100	-1.11239600
C	-1.86661100	-1.58956800	-1.06345600
C	-1.29750600	-2.45358900	-2.21936300
H	-2.51312300	-0.79927300	-1.45273900
H	-1.56621600	-3.50981800	-2.16421000
H	-1.54768800	-2.06373100	-3.20966700
N	-0.65447600	-0.94797300	-0.51133600
O	0.15233500	-2.36050000	-2.07105300
Ni	-0.49993800	0.42430000	0.95456000
C	-4.00310100	1.63401700	-1.79903700
C	-4.22376800	1.18712200	-0.49228700
C	-3.15814800	1.12687700	0.41382200
C	-1.87000100	1.47640200	-0.00694000
C	-1.66005900	1.99059100	-1.29314100
C	-2.72517300	2.05175100	-2.19375100
H	-4.83086000	1.69022800	-2.50109500
H	-5.22238200	0.89528300	-0.17660600
H	-3.32721200	0.78816900	1.43346800

H	-2.56702800	2.44657200	-3.19551100
C	-0.26745200	2.51401300	-1.54637800
C	0.29654900	3.08448400	-0.20986100
C	0.06566200	1.95226000	2.06247200
H	-0.38852300	1.95884300	3.05198000
H	1.14330500	1.81312100	2.05609600
C	-0.54919400	2.69211900	1.01297200
H	1.31569800	2.71814900	-0.06899800
H	0.33398900	4.18067000	-0.25221600
H	0.38461200	1.69113500	-1.86435100
H	-0.25917700	3.26465800	-2.34433300
C	3.50590500	0.05985800	-0.09308100
H	3.50333700	0.36093000	0.96253600
C	4.40949400	1.03224500	-0.87763900
H	3.98741400	2.03177800	-0.70142800
C	5.84042900	1.01123800	-0.32212900
H	6.46231800	1.76293400	-0.82087300
H	5.85613600	1.21935900	0.75449200
H	6.31686300	0.03533500	-0.48239700
C	4.38264400	0.77552500	-2.39001200
H	4.80923900	-0.20288800	-2.64455400
H	3.35818000	0.80831500	-2.77468900
H	4.97149900	1.53418500	-2.91774800
C	-2.63159700	-2.35490200	0.03629100
H	-2.82380400	-1.61153700	0.81984100
C	-1.81118400	-3.48806600	0.66407500
H	-1.56097200	-4.26901000	-0.06599100
H	-0.88738600	-3.10295400	1.10594900
H	-2.38819800	-3.96621300	1.46349300
C	-3.98134800	-2.83982300	-0.50950400
H	-3.85002600	-3.57521200	-1.31468700
H	-4.56379600	-3.32523600	0.28102900
H	-4.57300700	-2.00541300	-0.90575100
C	-1.62308900	3.69780500	1.41294800
H	-2.21339000	4.03917300	0.55860700
H	-2.29993100	3.28241400	2.16403300
H	-1.11260600	4.56529300	1.85482100
Br	0.62742000	-1.06538100	2.43884700

³TS2

C	-3.98724400	0.65164000	0.93317900
C	-2.24802800	0.88303100	-0.42767900
H	-4.95231700	1.16055100	0.88323900
H	-3.73867800	0.40258500	1.96636700

N	-2.61866300	-0.27386100	-0.79648200
O	-2.97158200	1.58903300	0.46725100
C	-0.97369300	1.51488800	-0.83479000
C	1.20292800	1.97701600	-0.99975300
C	0.36372600	3.11171700	-1.63556700
H	1.91024300	1.55540400	-1.71851100
H	0.56303900	4.10281900	-1.22648700
H	0.43471700	3.14252600	-2.72678600
N	0.17249900	0.95353900	-0.69534200
O	-1.01458200	2.76872000	-1.29977700
Ni	0.46944200	-0.79139400	0.39495000
C	5.00554900	0.05768900	0.64640400
C	4.20377900	-0.49564500	1.64864000
C	2.99712600	-1.12155400	1.31154900
C	2.56980800	-1.14903500	-0.02609000
C	3.41901100	-0.67416700	-1.03283100
C	4.62564800	-0.05219900	-0.69420400
H	5.93978100	0.54874300	0.90591300
H	4.51215900	-0.43967200	2.68963800
H	2.38132000	-1.54159800	2.10589900
H	5.28044200	0.32623100	-1.47767200
C	3.03196700	-1.00727200	-2.45737400
C	1.61285500	-1.59536000	-2.45770100
C	-0.06242400	-2.43487300	-0.79354500
H	-0.39990700	-3.24518900	-0.14985400
H	-0.82757700	-1.95625000	-1.39890700
C	1.30614900	-2.39244400	-1.19243600
H	0.87321600	-0.79230300	-2.53289200
H	1.46632200	-2.25349700	-3.32396700
H	3.10230300	-0.14059700	-3.12778900
H	3.74958300	-1.74389000	-2.84566900
C	-3.84341600	-0.56964000	-0.02218900
H	-3.63620300	-1.47385800	0.56143700
C	-5.04245400	-0.84656900	-0.95356700
H	-4.73037900	-1.68250400	-1.59455200
C	-6.26666100	-1.29433800	-0.14238500
H	-7.09337200	-1.56909900	-0.80710500
H	-6.03538600	-2.16232400	0.48664600
H	-6.62834300	-0.49187000	0.51347800
C	-5.37150700	0.34474800	-1.86319500
H	-5.70528200	1.21626000	-1.28605800
H	-4.49808300	0.64280800	-2.45210600
H	-6.17829700	0.08533700	-2.55798500
C	1.97637200	2.36729000	0.28048700

H	2.43157800	1.44157400	0.64475200
C	1.06143800	2.90583600	1.38857200
H	0.53340500	3.81854800	1.08298300
H	0.32239600	2.15779000	1.69339700
H	1.65874700	3.15527600	2.27228900
C	3.11244700	3.33945900	-0.06394800
H	2.73322700	4.30591900	-0.42158800
H	3.72070900	3.53680800	0.82493300
H	3.77310600	2.92244100	-0.83315900
C	2.13154500	-3.64846100	-0.94906300
H	3.20181400	-3.49727700	-1.11133900
H	1.98664900	-4.01152000	0.07244800
H	1.77892000	-4.42893200	-1.63777900
Br	-0.77175100	-0.56521500	2.41703100

²TS3

C	3.90775900	1.38267800	-1.10040400
C	1.90786700	1.52306100	-0.14636200
H	4.93501800	1.49472000	-0.74992600
H	3.83822300	1.73671400	-2.13699200
N	1.93347500	0.25127700	-0.57054200
O	3.06949100	2.22061500	-0.27265800
C	0.70950500	2.00570500	0.38297300
C	-1.48737500	1.93617300	0.86369800
C	-0.82567200	3.21195200	1.44203300
H	-2.04540800	1.40544800	1.64476200
H	-1.35663400	4.13892600	1.21719000
H	-0.67050400	3.13626200	2.52605800
N	-0.31033700	1.14993800	0.47401800
O	0.47053300	3.27989700	0.79858700
Ni	0.25051100	-0.64551900	-0.18843200
C	-4.37608500	-0.95346600	-0.73469600
C	-3.51086100	-0.97048200	-1.83320900
C	-2.13783300	-1.15915800	-1.64054500
C	-1.63147800	-1.30396300	-0.34328200
C	-2.50697000	-1.33565000	0.75028200
C	-3.87483000	-1.14419400	0.55970200
H	-5.44325800	-0.81470000	-0.88581500
H	-3.90493900	-0.83790200	-2.83771600
H	-1.46623200	-1.18412900	-2.49560800
H	-4.55331000	-1.16980400	1.40991100
C	-1.82633800	-1.70199600	2.04538000
C	-0.80518300	-2.82172500	1.70167200
C	0.98584300	-2.46123000	-0.08615300

H	1.41538700	-2.83380200	-1.01711500
H	1.68885900	-2.38617900	0.74026500
C	-0.37426000	-2.78368600	0.21701900
H	0.07809700	-2.74221800	2.34255600
H	-1.25818700	-3.80257000	1.89301800
H	-1.28513100	-0.82666600	2.42848000
H	-2.53296100	-2.02079400	2.81917900
C	3.32268000	-0.04629700	-0.94583200
H	3.33979100	-0.56570700	-1.91229400
C	4.07999700	-0.93127900	0.07822200
H	3.55891200	-1.89425800	0.08732600
C	5.52017900	-1.20606400	-0.38152400
H	5.99762100	-1.94546100	0.27155200
H	5.54730100	-1.59723500	-1.40655800
H	6.13947500	-0.30122800	-0.35160200
C	4.03504000	-0.35564900	1.49892400
H	2.99987900	-0.22504300	1.83100400
H	4.54200000	-1.02501800	2.20383900
H	4.52871700	0.62212700	1.55201700
C	-2.45685500	2.19699700	-0.31332900
H	-2.74061600	1.21055600	-0.68284300
C	-1.79911700	2.95372400	-1.47417000
H	-1.48565500	3.96373700	-1.18315600
H	-0.91604300	2.41731900	-1.83633800
H	-2.50221000	3.05204000	-2.30975400
C	-3.73630400	2.89200400	0.17199600
H	-3.53880900	3.90591100	0.54408400
H	-4.45965400	2.98098900	-0.64675700
H	-4.21473400	2.32282500	0.97885500
C	-1.02359800	-3.85236900	-0.65896000
H	-2.10827000	-3.89306600	-0.53047900
H	-0.80250200	-3.68789900	-1.71682000
H	-0.59733800	-4.82248200	-0.36658500

²TS4

C	-0.59766400	3.11116000	1.21998000
C	-0.98143300	2.37654000	-0.09544600
C	0.13199200	1.01254800	1.25822200
H	0.17326200	3.87459900	1.10782400
H	-1.46274300	3.50911800	1.75110600
H	-2.05450000	2.18576400	-0.11364300
N	-0.32245700	1.06662300	0.05395100
O	-0.01477200	2.06067300	2.06544900
C	0.75343500	-0.24145600	1.68985100

C	1.43783100	-2.35013000	1.46523900
C	1.98788600	-1.73686700	2.78558000
H	2.24068300	-2.46300000	0.72765400
H	1.56675100	-2.18899000	3.68719900
H	3.07694500	-1.73708400	2.85259200
N	0.56374600	-1.28183600	0.95741100
O	1.55567400	-0.33654100	2.75689500
C	0.71488300	-3.70430600	1.56713000
H	0.31392100	-3.87578700	0.55973900
C	-0.45480400	-3.69881400	2.55814500
H	-1.02539000	-4.62992200	2.47205000
H	-0.11165300	-3.62562200	3.59808300
H	-1.13750600	-2.86828700	2.36456000
C	1.72104900	-4.81775800	1.88967200
H	1.22675800	-5.79514000	1.89850500
H	2.52840300	-4.85610000	1.14856200
H	2.17452500	-4.67130400	2.87976400
C	-0.62061000	3.07058500	-1.41962600
H	-0.98032900	2.39053000	-2.20465600
C	-1.38958700	4.39392400	-1.53991600
H	-1.05886600	5.11364800	-0.77932700
H	-1.22293000	4.85347700	-2.52051700
H	-2.46698500	4.23748200	-1.41290100
C	0.88618100	3.26413300	-1.61980300
H	1.08730300	3.66828500	-2.61863800
H	1.30118100	3.96333700	-0.88517500
H	1.41192300	2.31045800	-1.51857600
C	3.45674500	-0.00439900	-0.62677500
H	2.36649200	-0.00315100	-0.69741200
H	3.72207300	-0.56633200	0.27866400
C	3.94009100	1.42827300	-0.48309600
H	3.79541100	1.97264900	-1.42497200
H	5.00565700	1.46484000	-0.22417700
C	4.03962300	-0.68628600	-1.87392200
H	3.70407800	-0.14384600	-2.76847400
H	5.14295600	-0.59418300	-1.85785500
C	3.66099800	-2.13268900	-2.00124400
H	3.88471000	-2.62260800	-2.94474500
H	3.81169200	-2.76284800	-1.12664200
O	3.15038600	2.05079800	0.55157400
C	3.32113500	3.35760000	0.87461100
O	2.50737600	3.89409900	1.59176400
C	4.53300800	4.07738600	0.31583500
H	5.46230700	3.56957300	0.59558300

H	4.49546900	4.11731300	-0.77847400
H	4.53790900	5.09250700	0.71276400
Br	1.18854800	-2.21176900	-2.13558700
Ni	-0.43608600	-0.87860100	-0.85451600
C	-2.22402900	-1.40657600	-1.60632000
C	-3.52457100	-1.33250500	-0.77455400
C	-3.84786500	0.08586300	-0.31902500
C	-4.35951300	1.14180600	-1.07376300
C	-4.65026900	2.36134600	-0.44770300
C	-4.42241700	2.52584200	0.92370300
C	-3.88870300	1.47315600	1.67866000
C	-3.60630400	0.26049300	1.05131300
C	-3.02450900	-1.00123600	1.64333500
H	-1.93740100	-0.89344400	1.73502100
H	-3.41274500	-1.22982600	2.64297700
C	-3.37636100	-2.07884400	0.59037200
H	-2.62335000	-2.86972600	0.52472900
H	-4.33116000	-2.54630500	0.86343900
H	-3.70767300	1.59825900	2.74417300
H	-4.66289100	3.47119700	1.40371700
H	-5.06658700	3.18110300	-1.02814900
H	-4.54966300	1.01564900	-2.13673200
C	-4.69583800	-1.92481700	-1.58927300
H	-4.80515700	-1.41043000	-2.55136000
H	-4.50821700	-2.98425300	-1.80169400
H	-5.64857700	-1.84482800	-1.04890600
H	-2.12101200	-2.43011300	-1.99352100
H	-2.32447300	-0.75346200	-2.49227500

²TS5

C	-1.24698200	3.42800100	1.62705700
H	-1.14449900	3.99915000	2.54943800
H	-1.47293500	4.09287400	0.79034600
O	-2.40212300	2.52951400	1.79245200
C	-2.00141800	1.37558900	1.25754800
N	-0.77341700	1.24788000	0.88760000
C	-0.06776100	2.47860000	1.31064700
H	0.50456600	2.85200700	0.46637200
C	0.89913400	2.18705000	2.48112000
C	1.89179400	3.34811200	2.63367500
H	1.37374000	4.28171000	2.89143400
H	2.61164700	3.13961400	3.43239500
H	2.44811100	3.51770300	1.70546800
C	0.18348700	1.88823600	3.80650700

H	0.89665200	1.49929900	4.54112800
H	-0.26548600	2.79130400	4.23738800
H	-0.61039400	1.14325900	3.69025200
H	1.45718900	1.29112500	2.18288900
Ni	-0.31700600	-0.52218000	0.06682300
C	1.38103900	0.09255700	-0.68269600
C	1.33588900	0.80660200	-2.07079300
C	1.11331400	2.30008700	-1.88959600
C	2.03058300	3.26437800	-1.47064600
C	1.60426300	4.58781200	-1.30099600
C	0.27174000	4.93837800	-1.54934600
C	-0.64457300	3.97139400	-1.98392300
C	-0.21605500	2.65598000	-2.15883500
C	-0.99974200	1.44145500	-2.60267900
H	-1.60929400	1.06459700	-1.76969600
H	-1.68363700	1.64707300	-3.43434900
C	0.11154300	0.42881100	-2.96302800
H	-0.18793100	-0.61136700	-2.82770600
H	0.39165600	0.57208300	-4.01466000
H	-1.67528700	4.24949600	-2.19541400
H	-0.04863600	5.96952000	-1.42238800
H	2.31215600	5.34784800	-0.98036100
H	3.06366600	2.98941500	-1.27239900
C	2.66074500	0.48854000	-2.79450800
H	3.53121800	0.67335600	-2.15527800
H	2.68160300	-0.57182600	-3.07105600
H	2.76334100	1.08555700	-3.70922400
H	1.99829700	-0.79811200	-0.78204200
H	1.85610700	0.75175900	0.05505600
N	-2.35842300	-0.81987100	0.53774600
C	-2.87981800	0.21917200	1.07770100
O	-4.16108600	0.19262200	1.45913800
C	-4.58152400	-1.19699400	1.22713600
H	-5.54020200	-1.16213100	0.70880700
H	-4.70999100	-1.66002000	2.20935900
C	-3.42445600	-1.82579600	0.39556400
H	-3.06772000	-2.75777300	0.84487500
C	-3.74589400	-2.09832300	-1.09223200
C	-4.74211700	-3.25969800	-1.21153200
H	-4.91640200	-3.50471600	-2.26464700
H	-4.36509800	-4.16214800	-0.71598500
H	-5.71676000	-3.01100900	-0.76973900
C	-4.23752300	-0.85114900	-1.83690100
H	-4.37337400	-1.07980400	-2.89935000

H	-3.51453800	-0.03282800	-1.76790100
H	-5.20219100	-0.49120500	-1.45564500
H	-2.79247500	-2.40890100	-1.53232600
C	2.50136100	-1.84225800	2.02965000
H	2.32419900	-1.30813100	1.09667900
H	2.75303700	-1.08166100	2.78104200
C	3.70074100	-2.76182900	1.81769000
H	3.41698900	-3.64920900	1.24083100
H	4.13240300	-3.10363100	2.76294300
C	1.20151600	-2.56436300	2.39742000
H	1.01477700	-3.36715200	1.67462300
H	1.30548400	-3.04692100	3.38802200
C	0.03206000	-1.62949800	2.39298000
H	-0.96642100	-2.05477900	2.36686400
H	0.12902200	-0.68659100	2.92135600
O	4.75629200	-2.03194700	1.16480200
C	4.72799700	-1.83058000	-0.18406400
O	5.37399800	-0.91724600	-0.64466700
C	3.94487100	-2.80991200	-1.03999200
H	4.29527800	-3.83440900	-0.86744300
H	2.86726600	-2.79049500	-0.84184000
H	4.11137700	-2.54230900	-2.08360800
Br	-0.08398300	-2.66235200	-0.95612400

²TS6

C	-4.29538200	-0.27186800	-2.62763900
H	-4.19097600	-0.59862800	-3.66455300
H	-5.35518000	-0.13370400	-2.39813200
O	-3.64590500	1.02778900	-2.50803300
C	-2.76053900	0.88866900	-1.49571500
N	-2.63781500	-0.23733600	-0.91359000
C	-3.55089600	-1.17085600	-1.59536800
H	-4.24755700	-1.56050000	-0.84498100
C	-2.77106700	-2.37321800	-2.17491700
C	-3.74214800	-3.42949300	-2.71946500
H	-4.32638600	-3.04247600	-3.56477000
H	-3.19514900	-4.30860600	-3.07689400
H	-4.44517500	-3.76205900	-1.94624500
C	-1.73624900	-1.96009800	-3.23028500
H	-1.12790100	-2.82330200	-3.52138000
H	-2.21301600	-1.57791300	-4.14156900
H	-1.05891700	-1.18762500	-2.85332400
H	-2.23813100	-2.80804000	-1.31920900
Ni	0.32987100	0.57349300	0.26008100

C	1.02081200	-0.64291600	1.75909700
C	0.01949000	-0.99937200	2.88378000
C	-0.94934700	-2.11055400	2.49525000
C	-0.69703900	-3.47724800	2.37252200
C	-1.71913500	-4.32628600	1.93505700
C	-2.98583700	-3.81134900	1.63593900
C	-3.24177100	-2.44333400	1.77710100
C	-2.21954100	-1.59817700	2.20584600
C	-2.24700500	-0.10022800	2.39097500
H	-2.22083500	0.38306000	1.40717500
H	-3.15085000	0.25631700	2.89896100
C	-0.95807600	0.17739500	3.19676900
H	-0.51123000	1.15040900	2.96787500
H	-1.19136600	0.16943800	4.26788700
H	-4.23153200	-2.04454400	1.56598000
H	-3.77723100	-4.48004700	1.30675600
H	-1.53101900	-5.39196500	1.83511600
H	0.28519600	-3.88143700	2.60591000
C	0.85776900	-1.36353600	4.12774000
H	1.52667400	-2.20805600	3.92666000
H	1.47774600	-0.51403600	4.43753300
H	0.20523200	-1.63842900	4.96448800
H	1.54760600	0.28963400	2.01026000
H	1.79066500	-1.40485300	1.66397900
N	-0.89981200	2.08023800	-0.43070100
C	-1.98289600	2.08784000	-1.12215400
O	-2.47233900	3.26423300	-1.53459900
C	-1.52354400	4.27963000	-1.08516900
H	-2.08779300	5.02530300	-0.52137200
H	-1.09796600	4.74364600	-1.97813400
C	-0.48519200	3.49545600	-0.24719200
H	0.51944900	3.58005900	-0.66590800
C	-0.40235700	3.84905900	1.25119400
C	0.20304200	5.24731000	1.42987400
H	0.32393700	5.48064900	2.49329800
H	1.18789300	5.31219000	0.95444900
H	-0.44116500	6.02422100	0.99627000
C	-1.74318000	3.70675900	1.98150900
H	-1.60730400	3.85942900	3.05773800
H	-2.17621200	2.71201100	1.83831000
H	-2.47536900	4.44954800	1.63950100
H	0.30599400	3.12031000	1.66777000
C	2.88911000	-1.78803700	-0.76759300
H	3.19036600	-1.00082700	-0.07086100

H	2.89788300	-2.74190400	-0.22363700
C	3.91160500	-1.85866200	-1.89634500
H	3.96406500	-0.90132000	-2.42627700
H	3.63853300	-2.63043700	-2.62418800
C	1.48432300	-1.47745600	-1.29113400
H	1.51862000	-0.55881500	-1.88730700
H	1.16345600	-2.28430700	-1.97287100
C	0.42294400	-1.37915100	-0.20206400
H	-0.58746300	-1.16969600	-0.58153600
H	0.34940800	-2.30185600	0.36278900
O	5.19699100	-2.26042600	-1.39944400
C	6.10756700	-1.36395600	-0.92055700
O	7.08812900	-1.79513000	-0.36070900
C	5.86509800	0.11353400	-1.16008600
H	5.85174800	0.33172500	-2.23477800
H	4.91503800	0.46755900	-0.74571900
H	6.68745400	0.66113900	-0.69882400
Br	2.44878300	1.79113500	-0.27994300

²TS7

C	-0.99415600	-2.95883400	2.36937800
H	-1.61470800	-2.96334400	3.26943000
H	-0.88704200	-3.97563100	1.98838700
O	0.34167000	-2.49841700	2.76216200
C	0.51226900	-1.34313900	2.10308000
N	-0.39914300	-0.91043400	1.31606100
C	-1.45787300	-1.93872500	1.28960500
H	-1.40277700	-2.39621300	0.29771500
C	-2.87055700	-1.35758800	1.46297200
C	-3.92250200	-2.46587100	1.31738100
H	-3.86619500	-3.18120600	2.14902900
H	-4.92514100	-2.03049500	1.30928300
H	-3.78364100	-3.02460600	0.38303200
C	-3.05843300	-0.55928800	2.75740100
H	-4.03501600	-0.06540600	2.74577100
H	-3.01998900	-1.20559100	3.64376500
H	-2.28454400	0.20876700	2.86246500
H	-2.99454700	-0.66526400	0.62208800
Ni	0.52802200	0.63417700	-0.14272000
C	-0.83439700	0.43652600	-1.61711200
C	-0.43613800	-0.41282700	-2.85745200
C	-0.08577900	-1.82259000	-2.40043200
C	-0.94698500	-2.86767900	-2.06951300
C	-0.41777500	-4.07706400	-1.59750800

C	0.96444700	-4.23581300	-1.45918900
C	1.83176600	-3.19405600	-1.81431000
C	1.30262500	-1.99595300	-2.29086900
C	2.02510100	-0.74434100	-2.74060500
H	2.40456900	-0.18680500	-1.87473000
H	2.89064100	-0.95896100	-3.37951700
C	0.92060500	0.06339600	-3.46438500
H	1.05314300	1.14305600	-3.34941600
H	0.94650300	-0.17276100	-4.53638800
H	2.90832500	-3.32963400	-1.73634100
H	1.36895400	-5.17835200	-1.09874700
H	-1.08509300	-4.89838000	-1.34594400
H	-2.02295900	-2.74757900	-2.17679600
C	-1.55259400	-0.40158100	-3.91747800
H	-2.50323800	-0.74708900	-3.49157400
H	-1.71054800	0.61957600	-4.28580000
H	-1.31358000	-1.04240700	-4.77707100
H	-1.14367400	1.43106600	-1.98503400
H	-1.73700000	-0.03425500	-1.18953600
N	2.03308700	0.29720700	1.31421700
C	1.78223800	-0.61100100	2.18616600
O	2.69928300	-0.89252500	3.11903000
C	3.76505200	0.09017400	2.90956600
H	4.71156300	-0.45204000	2.90807300
H	3.73995100	0.77985600	3.75797800
C	3.41053300	0.76780800	1.55618600
H	3.38910800	1.85820100	1.64335200
C	4.32834800	0.39745000	0.36906100
C	5.72707000	0.99658300	0.56777400
H	6.35321100	0.80235200	-0.30961600
H	5.67950700	2.08239100	0.71272500
H	6.23900300	0.55953500	1.43545100
C	4.38336600	-1.11313900	0.10914000
H	4.97537400	-1.31751600	-0.78965200
H	3.38476800	-1.52970500	-0.05342900
H	4.85228200	-1.65714100	0.93926700
H	3.87211400	0.88035900	-0.50211700
C	-2.34897900	2.51311800	0.79296700
H	-2.10588800	1.48206700	0.51728500
H	-2.42955300	2.54654400	1.88617000
C	-3.70058300	2.89449500	0.20161600
H	-3.67907500	2.84984500	-0.89173200
H	-3.98243400	3.91253100	0.48941200
C	-1.22087100	3.43041300	0.30859300

H	-1.17339100	3.40308300	-0.78602800
H	-1.43295700	4.47531900	0.57897200
C	0.11878600	3.03775900	0.88923200
H	0.72585500	3.84305000	1.28667400
H	0.12740800	2.17352300	1.55215000
O	-4.72942000	2.05103500	0.74946600
C	-5.16430400	0.92299400	0.13297800
O	-5.86413900	0.16261200	0.76517300
C	-4.78271200	0.68844100	-1.31590600
H	-5.16204500	1.49364700	-1.95549300
H	-3.69771500	0.63613500	-1.45566700
H	-5.22991300	-0.25591000	-1.62727000
Br	1.71810300	2.79861100	-0.84665800

¹TS8

C	3.92498900	2.06417300	-1.13710000
C	3.39625200	0.69216700	-1.64092800
C	1.80528400	1.73724800	-0.53409600
H	4.82000300	2.00470600	-0.51514000
H	4.09169200	2.78279500	-1.94563900
H	3.49498600	0.61240400	-2.72957600
N	1.96266300	0.72404500	-1.29323900
O	2.84488800	2.57299100	-0.30673800
C	0.55992500	2.03018600	0.19910600
C	-1.44239500	1.84768100	1.16640900
C	-0.72029300	3.12368200	1.65978500
H	-1.65605900	1.17589900	2.00117400
H	-1.29385400	4.04453900	1.54824500
H	-0.35629600	3.03100900	2.68654300
N	-0.39236700	1.18827200	0.35478700
O	0.45301000	3.22880400	0.79484900
Ni	-0.26308000	-0.81606500	0.18066200
C	-4.01758700	-0.36115700	-2.45126900
C	-2.87244100	0.30744200	-2.89884000
C	-1.63891200	0.04454800	-2.30429400
C	-1.55298500	-0.87776000	-1.25587300
C	-2.68837700	-1.59070500	-0.81906100
C	-3.92017900	-1.30249600	-1.42333000
H	-4.98176300	-0.15943300	-2.91034000
H	-2.94434500	1.03623700	-3.70242600
H	-0.73837800	0.55756700	-2.62935200
H	-4.81225800	-1.82572400	-1.08408300
C	-2.57041000	-2.60293900	0.30580800
C	-1.32601100	-3.52717000	0.21571100

C	-0.02716400	-2.79881900	-0.10971100
C	1.23879500	-3.36258400	0.49787900
C	0.03929000	-2.17049700	-1.39151900
Br	0.35399400	-0.86477900	2.48934500
H	1.43086000	-4.36258400	0.07703200
H	2.10285700	-2.73035200	0.27609200
H	1.15559700	-3.45105200	1.58249300
H	-1.21836900	-4.04504700	1.17429800
H	-1.50910900	-4.30031200	-0.54650700
H	-2.50668800	-2.06751000	1.26222700
H	-3.47720800	-3.21886800	0.34664500
C	-2.73292600	2.08113900	0.35160300
H	-3.00648700	1.10629500	-0.06547600
C	-2.53936300	3.05819100	-0.81512100
H	-2.34369100	4.07988900	-0.46588800
H	-1.71204800	2.74907700	-1.46016600
H	-3.44293900	3.08752900	-1.43304700
C	-3.86547000	2.53678800	1.28273400
H	-4.80086700	2.64553100	0.72284400
H	-4.03571300	1.81308100	2.08866800
H	-3.64510800	3.50884400	1.74385000
C	4.06383000	-0.55055500	-1.00045400
H	3.50238800	-1.41445300	-1.38348200
C	5.51948100	-0.68252400	-1.47098000
H	5.59149700	-0.70395100	-2.56547600
H	6.13604100	0.15037900	-1.10912600
H	5.96487900	-1.60597600	-1.08535700
C	3.95771900	-0.56187300	0.53124100
H	2.91935900	-0.52257000	0.87587800
H	4.40201800	-1.48011300	0.93135800
H	4.49884700	0.28066100	0.98042700
H	-0.55908100	-2.53413700	-2.21981500
H	0.98411100	-1.73285400	-1.71438600

²TS9

C	-2.43930000	-2.48209400	-1.45866000
C	-2.53477900	-1.27232700	-0.49579500
C	-0.43589000	-2.07073000	-0.58983200
H	-3.19464700	-3.25427300	-1.29795300
H	-2.46375700	-2.16439300	-2.50862500
H	-3.00587900	-0.42134300	-1.00013400
N	-1.12446700	-0.98307800	-0.24173900
O	-1.14297800	-3.06907000	-1.18810800
C	0.92307200	-2.08845800	-0.27876300

C	2.88235100	-1.18599400	0.37025900
C	3.04742300	-2.68422000	0.00805000
H	3.28955300	-1.01043800	1.37182900
H	3.86461900	-2.89443800	-0.68553400
H	3.16833600	-3.30539600	0.90439700
N	1.42387900	-1.03139800	0.38115800
O	1.81117200	-3.05250400	-0.64163500
Ni	0.07560200	0.38253400	0.56229200
C	-2.45773700	3.58013400	-1.68411200
C	-3.16318800	2.72806700	-0.82947700
C	-2.46904200	1.90507700	0.05554700
C	-1.06667700	1.89824500	0.07895500
C	-0.34830100	2.79963400	-0.74028700
C	-1.06320500	3.61594100	-1.62596800
H	-2.98976900	4.22806300	-2.37545100
H	-4.25025000	2.70937500	-0.84733000
H	-3.01539800	1.26651000	0.74072100
H	-0.51458800	4.29356900	-2.27746400
C	1.16441300	2.87336900	-0.67210100
C	1.72530600	2.83545900	0.77119000
C	1.11913900	1.72540800	1.62434500
C	2.01763600	1.10178400	2.67150600
C	-0.27508300	1.89733700	1.93529300
H	2.99145700	0.83415700	2.25282400
H	2.20439100	1.81146500	3.49248200
H	1.56939400	0.19863200	3.09819900
C	3.57232500	-0.20151800	-0.60386200
H	3.27556100	0.79639900	-0.25968500
C	3.08202600	-0.36030500	-2.04872200
H	3.53062000	0.40422900	-2.69377600
H	3.34975000	-1.34078300	-2.46079600
H	1.99338200	-0.25851700	-2.10379800
C	5.10124100	-0.29621700	-0.50549500
H	5.57886900	0.47628500	-1.11889800
H	5.44609800	-0.16591800	0.52822200
H	5.46989200	-1.26681200	-0.86090600
C	-3.31379700	-1.55278400	0.81560100
H	-3.14711000	-0.67193300	1.45117500
C	-4.82055800	-1.66790100	0.54671700
H	-5.05093700	-2.54229100	-0.07542900
H	-5.37845900	-1.77947000	1.48346300
H	-5.20389300	-0.77968300	0.02866200
C	-2.77654300	-2.76865900	1.58260900
H	-3.30595400	-2.88380100	2.53570000

H	-2.90944600	-3.69793400	1.01610100
H	-1.70923800	-2.65387900	1.79687900
H	-0.71322700	2.88952900	1.97176700
H	-0.72485700	1.23606600	2.68102000
H	1.58956300	2.02495700	-1.22222400
H	1.51328500	3.78261300	-1.17710100
H	1.54571300	3.81185100	1.24788600
H	2.81365600	2.71509200	0.71964900

¹TS10

C	3.98062300	1.54570200	-0.90170200
C	1.89846200	1.59621800	-0.13163000
H	4.87368000	1.67788500	-0.29128300
H	4.16429100	1.92080800	-1.90999700
N	1.99614300	0.34132300	-0.40502800
O	2.93400700	2.39428600	-0.31390600
C	0.60016700	2.08242200	0.35556200
C	-1.57968300	1.98508900	0.80319500
C	-0.95829500	3.30223600	1.35441100
H	-2.02338200	1.39051400	1.60737200
H	-1.42862200	4.21113100	0.98068100
H	-0.89757200	3.33737500	2.44437700
N	-0.38591400	1.26020900	0.30281000
O	0.42729100	3.29605300	0.85247700
Ni	0.24959400	-0.61838200	-0.20129500
C	-4.33930400	-1.10997400	-0.60917200
C	-3.52039400	-1.05638400	-1.74210400
C	-2.13290800	-1.18075500	-1.60780100
C	-1.58008600	-1.33536400	-0.33151500
C	-2.40146400	-1.44355300	0.79805300
C	-3.78334800	-1.30949200	0.66194200
H	-5.41686700	-1.02782300	-0.71726100
H	-3.96047900	-0.92648400	-2.72669000
H	-1.49723900	-1.15681200	-2.48974200
H	-4.42905700	-1.40084600	1.53178500
C	-1.66460700	-1.87265700	2.04579300
C	-0.74904600	-3.04331700	1.60625000
C	1.03428600	-2.40248800	-0.11235700
H	1.51797200	-2.67905500	-1.05083900
H	1.70944700	-2.28888800	0.73574900
C	-0.27526100	-2.89656200	0.14436200
H	0.11827600	-3.13140800	2.26860200
H	-1.31124500	-3.98070500	1.67799300
H	-1.05078400	-1.04347600	2.42533700

H	-2.33690200	-2.17656700	2.85350400
C	3.38921000	0.10237000	-0.86727700
H	3.33850800	-0.31605600	-1.87770700
C	4.16071900	-0.88600100	0.03721100
H	3.65384400	-1.85122600	-0.06360800
C	5.59612100	-1.06963400	-0.48087800
H	6.10363600	-1.85429500	0.08871300
H	5.61034000	-1.36089900	-1.53773500
H	6.19314400	-0.15622100	-0.37262000
C	4.12991500	-0.47924600	1.51587400
H	4.61709100	0.48910300	1.68488100
H	3.10310300	-0.41108400	1.89282200
H	4.66306600	-1.21795600	2.12254800
C	-2.63614100	2.17706900	-0.30550000
H	-2.90642000	1.17130100	-0.63138600
C	-2.09336700	2.93746400	-1.52194000
H	-1.79978400	3.96539500	-1.27542100
H	-1.22660200	2.42866900	-1.95861700
H	-2.86380100	3.00029000	-2.29698700
C	-3.89576400	2.83584300	0.27409500
H	-3.70678900	3.86052300	0.61800400
H	-4.67717700	2.89092400	-0.49048000
H	-4.29442900	2.26131200	1.11849100
C	-0.85410700	-3.90035100	-0.83555100
H	-1.93854100	-3.98973200	-0.74415000
H	-0.60208800	-3.65125900	-1.86917600
H	-0.40362000	-4.87498700	-0.59988400

¹TS11

C	1.46108200	-3.71921900	-0.06453900
C	1.91121500	-2.28978100	0.34490500
C	-0.23353500	-2.29689000	-0.25412500
H	2.05231100	-4.16964700	-0.86130600
H	1.38405200	-4.41010400	0.77808800
H	2.32577100	-2.28854300	1.35726000
N	0.62851100	-1.54961200	0.34527400
O	0.09920900	-3.53200000	-0.59157300
C	-1.52785600	-1.69678400	-0.60916400
C	-3.04082800	-0.08424700	-0.81179700
C	-3.65460200	-1.46160200	-1.20529800
H	-3.08766000	0.60736400	-1.65923200
H	-4.51452900	-1.75976800	-0.60472600
H	-3.90010300	-1.54261900	-2.26587700
N	-1.62121400	-0.41646600	-0.55734000

O	-2.58342400	-2.43144800	-0.93466300
Ni	0.10647700	0.37262300	0.47981900
C	1.20612600	3.59105100	-2.39376700
C	-0.14326800	3.24368500	-2.27689100
C	-0.57712800	2.51435500	-1.16994600
C	0.35424100	2.11333600	-0.20432200
C	1.69213000	2.55532000	-0.23801300
C	2.10468600	3.25961300	-1.38058200
H	1.55108100	4.14852500	-3.25938600
H	-0.85412400	3.53265800	-3.04569300
H	-1.61801300	2.23472300	-1.07466300
H	3.13999800	3.58496600	-1.45122400
C	2.62488600	2.47135800	0.95949100
C	2.41106100	1.30776800	1.94344800
C	0.96246300	0.92481400	2.16276900
C	0.70637200	-0.15052800	3.19662500
C	-0.06063100	1.88699600	1.87152500
H	1.34920800	-1.02075300	3.03442600
H	0.92901600	0.24033800	4.19960700
H	-0.33552800	-0.48549800	3.19419800
H	2.94890100	0.41549600	1.60151900
H	2.86760000	1.57198700	2.90976200
H	3.66514000	2.47143600	0.61737500
H	2.50210000	3.41589200	1.51118400
C	-3.66601300	0.60571000	0.42321600
H	-3.07504800	1.51917600	0.58036300
C	-3.55648800	-0.24664700	1.69468100
H	-3.96307000	0.29899100	2.55225800
H	-4.12094700	-1.18324300	1.61109100
H	-2.51354700	-0.49861300	1.91935100
C	-5.11526400	1.01978000	0.13210300
H	-5.52602500	1.58770200	0.97272100
H	-5.18313700	1.64827200	-0.76343000
H	-5.76284100	0.14712400	-0.01693100
C	2.91898100	-1.60722400	-0.61227300
H	3.03891300	-0.58438500	-0.23247500
C	4.28145800	-2.31090100	-0.54169400
H	4.23059500	-3.33447500	-0.93255800
H	5.01862400	-1.77177100	-1.14477600
H	4.65906900	-2.36045800	0.48649900
C	2.39689700	-1.50000600	-2.05173400
H	3.13572700	-0.99222900	-2.67946800
H	2.21270200	-2.48456600	-2.49856400
H	1.47033000	-0.91740900	-2.09985200

H	0.15866800	2.94840900	1.83158800
H	-1.07985200	1.68794400	2.20458400

²TS12

C	0.86004600	3.38680200	-1.75096100
C	-0.62007700	2.18048700	-0.63220200
H	1.21360500	4.40535300	-1.59030700
H	0.85859400	3.14999800	-2.81804100
N	0.44593800	1.51349800	-0.39019600
O	-0.53442100	3.33378700	-1.29923400
C	-1.90520800	1.62708300	-0.19801800
C	-3.30488700	0.11153900	0.63882400
C	-3.97572200	1.51875000	0.60181300
H	-3.17019100	-0.22003800	1.67470700
H	-4.88099200	1.56281500	-0.00577700
H	-4.17545800	1.92624000	1.59482700
N	-1.95897700	0.38879100	0.11225500
O	-2.98550500	2.39364000	-0.03084400
Ni	-0.03996800	-0.48262900	0.13071300
C	4.63813300	-0.97717500	-0.29607000
C	4.05176000	-0.32452200	0.78822100
C	2.68933700	-0.50276500	1.06518900
C	1.93588400	-1.31001900	0.21694200
C	2.52935800	-2.07716800	-0.79323700
C	3.88417100	-1.86597400	-1.06796500
H	5.69429300	-0.83730100	-0.51093400
H	4.64320400	0.32829200	1.42516300
H	2.21576300	0.00293600	1.89902200
H	4.35909500	-2.44225200	-1.85838000
C	1.74229200	-3.22062800	-1.37285900
C	1.12300000	-3.94025400	-0.16285400
C	-0.75130000	-2.40759800	0.56232100
H	-1.38456400	-2.09914500	1.38911500
H	-1.22476900	-2.62440300	-0.39135300
C	0.50670300	-2.97307100	0.84686000
H	0.34689100	-4.64557500	-0.48694500
H	1.90004100	-4.51779200	0.35056500
C	1.58004500	2.31031800	-0.89509600
H	2.20129000	1.65844800	-1.51615900
C	2.42495000	2.87690100	0.27083700
H	2.79428000	2.00635600	0.81658500
C	3.64330100	3.63376500	-0.27629900
H	4.29212400	3.95448200	0.54604700
H	4.23723700	3.00123600	-0.94754800

H	3.35379400	4.53608000	-0.83004700
C	1.59979100	3.71891800	1.25334600
H	1.12582500	4.58050600	0.76568100
H	0.82350700	3.10949400	1.72762600
H	2.24722300	4.10863000	2.04674600
C	-4.03560100	-0.98701200	-0.16224900
H	-3.41803100	-1.88851200	-0.06720100
C	-4.15261100	-0.65891400	-1.65612700
H	-4.74504200	0.24910900	-1.82912800
H	-3.16447300	-0.52591300	-2.10718500
H	-4.65783900	-1.47783800	-2.18066100
C	-5.40042300	-1.28383900	0.47698600
H	-6.07942900	-0.42521400	0.39537200
H	-5.88384100	-2.12680000	-0.02828500
H	-5.30367600	-1.53643400	1.54015400
C	0.94467600	-3.11473100	2.28190200
H	2.03033400	-3.21330200	2.35950800
H	0.60898400	-2.26706600	2.88353600
H	0.49059000	-4.03432000	2.68060200
Br	-0.33901600	-0.74147800	-2.46010100
Br	-0.25732200	0.25864200	2.67565000
H	0.96567400	-2.84018200	-2.04233800
H	2.38185700	-3.90579000	-1.93873200

²TS13

C	-1.41138600	-2.60123000	-0.88095900
C	0.78466300	-2.28596200	-0.75064000
H	-0.91101300	-4.68002300	-1.53981700
H	-0.74313700	-3.44512200	-2.82360700
H	-2.12953800	-2.02640300	-1.47282700
N	-0.32009600	-1.69937600	-0.46956000
O	0.75301500	-3.45656100	-1.39262900
C	2.04881300	-1.65974900	-0.34427600
C	3.36358300	-0.11019900	0.55694300
C	4.16504300	-1.42420700	0.30192500
H	3.23879900	0.06561500	1.63202500
H	4.97573700	-1.31197700	-0.42089700
H	4.54672700	-1.88589200	1.21424900
N	2.02735000	-0.44617500	0.04671600
O	3.19098600	-2.35491700	-0.27859400
Ni	-0.01883400	0.30756700	0.16011400
C	-4.63741200	0.55618300	-0.54521800
C	-4.07301700	-0.14822200	0.51977700
C	-2.81450200	0.22052500	1.00238500

C	-2.10034300	1.25081600	0.37527800
C	-2.70426000	2.04846400	-0.62762700
C	-3.96418500	1.65139200	-1.09389300
H	-5.61908700	0.28259500	-0.92309300
H	-4.61100100	-0.97145700	0.98397400
H	-2.36347600	-0.29458900	1.84391600
H	-4.43544400	2.22737000	-1.88733300
C	-2.06097800	3.30242000	-1.16001400
C	-1.61798000	4.29180800	-0.02715300
C	-0.79726600	3.54387600	0.97620000
C	0.67979400	3.41314000	0.74896500
C	-1.46189000	2.73561900	1.86993700
H	0.87795200	3.05702100	-0.27388500
H	1.18159300	4.38499900	0.85087600
H	1.13243400	2.70911200	1.45595900
C	3.93534400	1.16714000	-0.08978600
H	3.20670400	1.95679500	0.13675400
C	4.05777200	1.07072000	-1.61526600
H	4.41967200	2.02239000	-2.02072900
H	4.77455600	0.29736900	-1.92103900
H	3.08770400	0.85726900	-2.07274600
C	5.27003300	1.53667600	0.57360500
H	5.64452800	2.48762700	0.17975100
H	5.16817700	1.63684000	1.66112500
H	6.03872000	0.77778700	0.37507600
C	-2.12725900	-3.19292900	0.35700000
H	-2.52119400	-2.33382300	0.90427500
C	-3.31710900	-4.05739300	-0.08232800
H	-2.99547500	-4.95129000	-0.63208800
H	-3.88044900	-4.40159900	0.79177400
H	-4.00366000	-3.49371100	-0.72595100
C	-1.17457300	-3.93878700	1.30097300
H	-1.73435600	-4.34838900	2.14888000
H	-0.67052400	-4.77851000	0.80550200
H	-0.41688000	-3.25860200	1.70340900
H	-2.50231200	2.93689500	2.10627400
H	-0.92478300	2.09839000	2.56264200
H	-1.17935900	3.02701400	-1.74427700
H	-2.75104500	3.82440200	-1.83240500
H	-2.51089200	4.71724900	0.44546200
H	-1.05446000	5.11120100	-0.48782000
Br	0.27376700	0.99868400	-2.22228800
Br	0.30826000	-0.19212300	2.59762600

²TS14

C	3.84485400	-1.36677400	-1.40978500
C	2.58412000	0.28483000	-0.62222700
H	4.77845800	-1.75030200	-0.99602300
H	3.84432500	-1.48294300	-2.49627300
N	1.82187100	-0.71720000	-0.39390500
O	3.80194200	0.07156200	-1.13049500
C	2.08762000	1.63149700	-0.31136200
C	0.65710200	3.16034600	0.43099300
C	2.05704700	3.79979300	0.18550100
H	0.44903900	3.09316000	1.50660600
H	2.06660900	4.53178300	-0.62572600
H	2.50356600	4.23556700	1.08035800
N	0.85123800	1.77754700	-0.02599400
O	2.91148300	2.68294100	-0.22732400
Ni	-0.12765900	-0.13520600	0.08773600
C	-1.68120200	-3.26084200	-1.34038100
C	-0.98553400	-3.00521400	-0.16336100
C	-1.38080800	-1.99071600	0.72355900
C	-2.54702600	-1.19676900	0.38768200
C	-3.28035000	-1.52684600	-0.82549200
C	-2.85915300	-2.53499500	-1.64757400
H	-1.34241000	-4.04307000	-2.01247100
H	-0.12371000	-3.61234300	0.09626900
H	-0.95486900	-1.93807500	1.71889400
H	-3.43767400	-2.79421300	-2.53007200
C	-4.54901500	-0.71916800	-0.89741200
C	-4.82664200	-0.36605200	0.58527200
C	-2.45617400	0.55332500	0.63534500
C	-3.45210200	-0.34180000	1.27207700
H	-5.35533900	0.58532500	0.70952600
H	-5.43318800	-1.15180300	1.05248700
H	-4.38336300	0.18673500	-1.49725000
H	-5.37256300	-1.26456200	-1.36841500
C	2.56213300	-1.93678800	-0.73625500
H	1.96034800	-2.50224900	-1.45575400
C	2.79810200	-2.80236700	0.52316800
H	1.79949800	-3.00908800	0.92848500
C	3.45229700	-4.13543800	0.13469000
H	3.54302600	-4.78760300	1.00982400
H	2.86684900	-4.66807100	-0.62535700
H	4.46373400	-3.98628900	-0.26523000
C	3.58218800	-2.06449500	1.61614100
H	4.58087500	-1.76321000	1.27411100

H	3.03643800	-1.17888200	1.95509100
H	3.71980900	-2.72018500	2.48293200
C	-0.53327700	3.85021000	-0.26301300
H	-1.41491700	3.25571300	0.01339900
C	-0.42681300	3.84117600	-1.79283500
H	0.44452300	4.40893100	-2.14468000
H	-0.35884500	2.81822000	-2.17610100
H	-1.31461100	4.31156900	-2.23112600
C	-0.71851400	5.26745100	0.29867500
H	0.13072800	5.91364700	0.03982000
H	-1.61790500	5.73216400	-0.11944500
H	-0.81689600	5.26126300	1.39123100
C	-3.41053900	-0.49377600	2.77877300
H	-3.87957700	-1.43699600	3.08211700
H	-2.38161600	-0.47131200	3.15149800
H	-3.95892300	0.32978700	3.25187000
H	-2.67020600	1.09871700	-0.27609300
H	-1.69502300	0.95653600	1.30003900
Br	-0.63157400	0.00050900	-2.37554100
Br	0.47069500	0.12205800	2.62547300

²TS15

C	2.69454100	0.13671800	-0.41138800
C	2.27935000	-1.18069400	-0.14469900
C	1.00577700	-1.45049100	0.32257200
C	0.07141000	-0.37580500	0.53968100
C	0.51211600	0.97708100	0.23751800
C	1.78393200	1.20216900	-0.23803700
H	3.69929700	0.33185400	-0.77361200
H	2.97764700	-2.00166100	-0.29125900
H	0.70747900	-2.46838400	0.56074900
H	2.07652600	2.21308100	-0.51550500
C	-0.63819000	1.94708400	0.20950700
C	-1.78465300	1.14094100	-0.47098000
C	-1.21185200	-0.57580900	1.31664600
C	-1.60592600	-0.31504600	-0.08920400
H	-2.77536100	1.52088800	-0.18071200
H	-1.70518200	1.24017800	-1.56100300
H	-0.94204500	2.24468800	1.22314600
H	-0.40058200	2.86685300	-0.33384400
C	-2.11570500	-1.40832200	-0.97847100
H	-1.88450100	-1.20589000	-2.03125300
H	-1.67058000	-2.37502800	-0.71583800
H	-3.20860800	-1.51648200	-0.89493500

H	-1.46358800	0.15952900	2.08391800
H	-1.35530300	-1.59657300	1.67127800

²TS16

C	0.17662600	3.57469700	-1.64926600
C	-1.28787200	2.18202900	-0.71930900
H	0.51266400	4.45486600	-1.09647500
H	0.23511500	3.76987600	-2.72121100
N	-0.21372500	1.49586400	-0.58956400
O	-1.23651200	3.37375800	-1.31831800
C	-2.55315000	1.62503900	-0.21989900
C	-3.90468900	0.11935400	0.69865400
C	-4.67141700	1.45389800	0.43890900
H	-3.81676600	-0.07673700	1.77359700
H	-5.49714900	1.35853500	-0.26918100
H	-5.02422400	1.93871200	1.35112700
N	-2.55527200	0.42282600	0.20800000
O	-3.67902900	2.34694300	-0.17033400
Ni	-0.56647800	-0.39849100	0.25479400
C	5.44425100	0.76352000	0.09680400
C	4.90599500	0.73311100	1.38483200
C	3.83343200	-0.11451100	1.66896900
C	3.29954900	-0.93626500	0.66952100
C	3.82752700	-0.89307700	-0.63726800
C	4.90052000	-0.04432900	-0.90812800
H	6.28168700	1.41802100	-0.12984000
H	5.31893400	1.36552700	2.16595000
H	3.39775000	-0.13790600	2.66431900
H	5.31418400	-0.01157100	-1.91377700
C	3.15072000	-1.73460100	-1.69531900
C	2.68466200	-3.09296900	-1.14614600
C	2.18710200	-1.85932400	0.95676300
C	1.95844500	-2.96103000	0.16542700
H	2.03641200	-3.58643400	-1.87805500
H	3.54891600	-3.76027000	-0.98413100
H	2.25434700	-1.20616700	-2.04989600
H	3.80801500	-1.87768800	-2.56010000
C	0.88405100	2.25717300	-1.20866300
H	1.21863900	1.68588900	-2.08312000
C	2.08009600	2.43145800	-0.25337200
H	2.47609800	1.42552800	-0.09201000
C	3.17627600	3.26795900	-0.92722100
H	4.06565100	3.29934900	-0.29152400
H	3.47451200	2.83741600	-1.89091900

H	2.85357600	4.30352100	-1.09949800
C	1.67483100	2.99258700	1.11423300
H	1.23004200	3.99411700	1.03700900
H	0.96226200	2.32959300	1.61551400
H	2.56055800	3.07617800	1.75314000
C	-4.48054500	-1.13875700	0.01423700
H	-3.78685300	-1.95051700	0.27131000
C	-4.51038800	-1.02395500	-1.51493900
H	-5.14966500	-0.19752700	-1.85315900
H	-3.50207900	-0.88170100	-1.91446000
H	-4.91446800	-1.94447700	-1.95043800
C	-5.86013900	-1.47390900	0.59845900
H	-6.59886200	-0.69809500	0.35666100
H	-6.23301900	-2.41640700	0.18361900
H	-5.82345000	-1.57645300	1.68991700
C	0.94188200	-3.99185000	0.52556700
H	1.34386000	-5.00435700	0.38573300
H	0.58793800	-3.88245800	1.55472700
H	0.08321300	-3.88514900	-0.15242200
H	0.86913100	-1.05592500	0.38735200
H	1.76246000	-1.82685800	1.95652200
Br	-0.65317200	-1.62344500	-1.82748300
Br	-0.44475200	-0.15188600	2.64212800

²TS17

C	-2.40950600	2.53472400	1.33593900
C	-0.50693000	1.83291000	0.42209000
H	-3.20221800	3.09101300	0.83419600
H	-2.37882100	2.80755300	2.39349600
N	-1.09894400	0.71288200	0.61263600
O	-1.13565500	2.96499300	0.74335100
C	0.83442100	1.81595800	-0.18328700
C	2.67174600	0.93723800	-1.07323900
C	2.80285200	2.48877100	-0.97319800
H	2.69995500	0.61318900	-2.11943100
H	3.62629800	2.82675800	-0.34128100
H	2.85947700	2.98367300	-1.94490100
N	1.31445500	0.69134600	-0.56284400
O	1.55807400	2.92922300	-0.33381700
Ni	-0.04989000	-0.91303400	-0.12009300
C	-2.45807200	0.99558400	1.09766600
H	-2.60183100	0.45895400	2.04127400
C	-3.50873100	0.49814700	0.07778700
H	-3.30901700	-0.57399600	-0.04646700

C	-4.92277700	0.67897700	0.64647400
H	-5.66401300	0.24978800	-0.03555500
H	-5.03486100	0.18499700	1.61937700
H	-5.17529800	1.74009700	0.77509300
C	-3.35216700	1.15128700	-1.30113600
H	-3.48190400	2.24109700	-1.26059900
H	-2.37574400	0.91845900	-1.73482700
H	-4.11035000	0.75710400	-1.98554700
C	3.71153800	0.11431600	-0.28000600
H	3.42368500	-0.93527200	-0.42824500
C	3.66895700	0.39992000	1.22666900
H	3.90460800	1.44815400	1.45311900
H	2.68663200	0.16187700	1.64540700
H	4.40889700	-0.21847700	1.74579500
C	5.11469400	0.32005000	-0.86762300
H	5.46118700	1.35320800	-0.73304600
H	5.83780100	-0.33209100	-0.36679200
H	5.14133200	0.09154200	-1.93988000
H	-0.64743300	-2.07043900	0.73358700
Br	0.56701500	-2.00362000	2.04238200
Br	-1.00803000	-1.76274700	-2.08054700

²TS18

C	-0.35936100	3.89889300	-1.30853800
C	-1.69471700	2.36965300	-0.39021900
H	-0.07468900	4.80221800	-0.76328500
H	-0.34228400	4.10156300	-2.38124200
N	-0.56302900	1.76839800	-0.29602100
O	-1.74428600	3.58945000	-0.94555600
C	-2.88400700	1.64709000	0.05847500
C	-4.02821700	-0.11422100	0.79871700
C	-4.99929600	1.04455000	0.40981600
H	-4.08315400	-0.32603000	1.87260900
H	-5.67053900	0.79728900	-0.41607100
H	-5.58236400	1.42609200	1.25080500
N	-2.70742100	0.46171600	0.51960600
O	-4.13066200	2.13310800	-0.04957900
Ni	-0.75992100	-0.24578900	0.25833800
C	4.30366400	1.40495900	2.02427400
C	3.20621900	0.80827500	2.64893600
C	2.54552800	-0.25891700	2.03615000
C	2.99217400	-0.73392100	0.79791200
C	4.08325900	-0.12299400	0.15463000
C	4.73651000	0.94105900	0.77781300

H	4.82162600	2.23223800	2.50228900
H	2.85996100	1.17383900	3.61147400
H	1.67978700	-0.72461700	2.49912900
H	5.58563700	1.41106800	0.28651900
C	4.47157400	-0.64294000	-1.21250700
C	4.36363700	-2.17886400	-1.28195900
C	2.31668900	-1.88414700	0.12953100
C	3.04543800	-2.67536500	-0.77835200
H	4.55378100	-2.54546100	-2.29765400
H	5.13877800	-2.63366600	-0.63870600
H	3.79196100	-0.21927500	-1.96642600
H	5.48568000	-0.32851100	-1.48080800
C	0.45690300	2.63564300	-0.89930400
H	0.83311300	2.10863400	-1.78397200
C	1.63596700	2.86512900	0.06480200
H	2.04348900	1.86807700	0.26243400
C	2.73079300	3.70207700	-0.60790400
H	3.60701500	3.77432300	0.04450400
H	3.05398100	3.25025800	-1.55388300
H	2.38877000	4.72405800	-0.82003300
C	1.19919400	3.46099000	1.40774200
H	0.78081500	4.46996400	1.29677300
H	0.44718100	2.82706800	1.88893100
H	2.05880100	3.53224300	2.08151300
C	-4.20781100	-1.44770700	0.03995200
H	-3.42651400	-2.10355600	0.44398700
C	-3.96499200	-1.30596600	-1.46799300
H	-4.66717600	-0.60281700	-1.93690100
H	-2.94333600	-0.96865700	-1.67105000
H	-4.09721000	-2.27535100	-1.96103000
C	-5.57948200	-2.06000300	0.35230000
H	-6.39974000	-1.44559100	-0.04354000
H	-5.66786000	-3.05171200	-0.10428900
H	-5.73290000	-2.17369800	1.43255600
C	2.41134000	-3.87410900	-1.38294100
H	3.14269400	-4.55174300	-1.83438800
H	1.77725700	-4.41000600	-0.67008500
H	1.74125800	-3.50969400	-2.18272100
H	1.54008800	-1.43796800	-0.72221900
H	1.53720700	-2.38565400	0.72045100
Br	0.18757200	-0.88761300	-2.05104200
Br	-0.75033300	-2.14636000	1.76443800

Ni⁰L

C	-2.62092300	1.49344600	1.08709600
H	-3.45632400	2.02867300	0.62968100
H	-2.57280200	1.74586000	2.15335000
O	-1.40552500	1.95040300	0.45168800
C	-0.63981800	0.83349200	0.28867000
N	-1.22757500	-0.32622900	0.62876700
C	-2.64263200	-0.04170200	0.86523100
H	-2.97749000	-0.54676900	1.78033000
C	-3.53863400	-0.53117000	-0.30024800
C	-5.02695400	-0.33750700	0.02256100
H	-5.28805200	0.72662700	0.08580200
H	-5.65569200	-0.77975800	-0.75853100
H	-5.29661900	-0.80553200	0.97765200
C	-3.16030200	0.10532700	-1.64407100
H	-3.77836100	-0.30499200	-2.45105700
H	-3.30913500	1.19190300	-1.63153200
H	-2.11027200	-0.08958000	-1.88436500
H	-3.34425300	-1.61219300	-0.37696600
Ni	-0.00000600	-1.71473900	0.00015300
N	1.22752900	-0.32629000	-0.62865600
C	0.63973400	0.83346600	-0.28874800
O	1.40540500	1.95037600	-0.45194400
C	2.62082000	1.49335600	-1.08727400
H	3.45619800	2.02868300	-0.62993400
H	2.57269900	1.74560500	-2.15356700
C	2.64257700	-0.04175900	-0.86517400
H	2.97742900	-0.54696400	-1.78019900
C	3.53861900	-0.53102700	0.30036100
C	5.02694700	-0.33791100	-0.02274400
H	5.65567400	-0.78008000	0.75840200
H	5.29632700	-0.80634500	-0.97771600
H	5.28835100	0.72612200	-0.08639000
C	3.16067300	0.10610000	1.64399300
H	3.77877500	-0.30404100	2.45103600
H	2.11063900	-0.08845800	1.88454800
H	3.30976300	1.19263600	1.63098400
H	3.34396000	-1.61196900	0.37752200

Ni^ILBr

C	3.22396400	-1.88975600	0.78580300
H	4.00251300	-2.15131400	0.06620900
H	3.49632100	-2.27258700	1.77172300
O	2.00097500	-2.58171000	0.37084100
C	1.08448400	-1.61718300	0.23069900

N	1.41554000	-0.39313500	0.46179600
C	2.84969700	-0.37580900	0.79207400
H	2.96373900	0.04493400	1.79746100
C	3.62070700	0.52418000	-0.19917100
C	5.10702100	0.59104400	0.17658100
H	5.59849800	-0.38323900	0.05507000
H	5.63303100	1.30255700	-0.46851000
H	5.24654300	0.91266600	1.21574500
C	3.41147400	0.10449600	-1.65980200
H	3.94189500	0.79032300	-2.32872300
H	3.79386800	-0.90565200	-1.85675900
H	2.34939300	0.13121400	-1.92500600
H	3.18411600	1.52471800	-0.07562300
Ni	-0.03972200	0.94324000	0.02234500
N	-0.97061700	-0.81170500	-0.53422900
C	-0.28541400	-1.85330400	-0.22267000
O	-0.86369600	-3.05935300	-0.26607600
C	-2.24479700	-2.80028500	-0.69258100
H	-2.90127700	-3.22353800	0.07048300
H	-2.39621600	-3.32675200	-1.63737100
C	-2.34354400	-1.24806700	-0.82334900
H	-2.58382300	-0.96205300	-1.85357800
C	-3.33947200	-0.53464900	0.11921100
C	-4.78114400	-0.93101100	-0.22423600
H	-5.48947100	-0.35654300	0.38187500
H	-5.01133700	-0.74049900	-1.27956400
H	-4.96818600	-1.99467900	-0.02370100
C	-3.01417800	-0.76357400	1.60051300
H	-3.72219500	-0.21329800	2.22885100
H	-2.00893000	-0.39968300	1.83781700
H	-3.07989200	-1.82334300	1.88140600
H	-3.20415900	0.53597800	-0.08379000
Br	-1.01936200	3.01217000	-0.00083500

Ni^{II}LBr₂

C	2.75190800	2.53728000	-0.84199300
C	0.70425200	1.98134900	-0.20020500
H	3.52705600	3.04412300	-0.26750900
H	2.83469200	2.80509700	-1.89833100
N	1.22776000	0.81818700	-0.36527800
O	1.45549200	3.06264700	-0.37055800
C	-0.70410000	1.98147900	0.19964200
C	-2.67221000	1.00389900	0.59883900
C	-2.75168200	2.53813200	0.84102600

H	-2.94682100	0.43268000	1.48847500
H	-3.52660200	3.04450300	0.26580700
H	-2.83489600	2.80683900	1.89709000
N	-1.22770600	0.81844900	0.36529700
O	-1.45510000	3.06296500	0.36966800
Ni	-0.00013700	-0.68823100	-0.00033800
C	2.67231200	1.00335300	-0.59861300
H	2.94725200	0.43132500	-1.48761800
C	3.49422200	0.47748600	0.60198400
H	3.25026500	-0.58822300	0.66098300
C	4.99498800	0.61644700	0.31282300
H	5.57827000	0.15661800	1.11738400
H	5.26845400	0.11891100	-0.62498400
H	5.30761300	1.66720100	0.24542300
C	3.09922900	1.13663400	1.92941900
H	3.27425000	2.22078900	1.92574800
H	2.04399100	0.95755600	2.16341100
H	3.69166900	0.71420700	2.74756700
C	-3.49463100	0.47718600	-0.60101300
H	-3.25086500	-0.58860900	-0.65928700
C	-3.09987000	1.13513000	-1.92913900
H	-3.27444600	2.21936800	-1.92632600
H	-2.04478400	0.95542000	-2.16329400
H	-3.69275300	0.71230500	-2.74675900
C	-4.99529900	0.61649400	-0.31155500
H	-5.30792800	1.66730500	-0.24512000
H	-5.57880500	0.15585800	-1.11549200
H	-5.26849700	0.11988900	0.62682600
Br	1.51845200	-2.24676500	-0.80166700
Br	-1.51820800	-2.24675700	0.80181500

Ni^{III}LBr₂

C	2.75190800	-2.53728000	0.84199300
C	0.70425200	-1.98134900	0.20020500
H	3.52705600	-3.04412300	0.26750900
H	2.83469200	-2.80509700	1.89833100
N	1.22776000	-0.81818700	0.36527800
O	1.45549200	-3.06264700	0.37055800
C	-0.70410000	-1.98147900	-0.19964200
C	-2.67221000	-1.00389900	-0.59883900
C	-2.75168200	-2.53813200	-0.84102600
H	-2.94682100	-0.43268000	-1.48847500
H	-3.52660200	-3.04450300	-0.26580700
H	-2.83489600	-2.80683900	-1.89709000

N	-1.22770600	-0.81844900	-0.36529700
O	-1.45510000	-3.06296500	-0.36966800
Ni	-0.00013700	0.68823100	0.00033800
C	2.67231200	-1.00335300	0.59861300
H	2.94725200	-0.43132500	1.48761800
C	3.49422200	-0.47748600	-0.60198400
H	3.25026500	0.58822300	-0.66098300
C	4.99498800	-0.61644700	-0.31282300
H	5.57827000	-0.15661800	-1.11738400
H	5.26845400	-0.11891100	0.62498400
H	5.30761300	-1.66720100	-0.24542300
C	3.09922900	-1.13663400	-1.92941900
H	3.27425000	-2.22078900	-1.92574800
H	2.04399100	-0.95755600	-2.16341100
H	3.69166900	-0.71420700	-2.74756700
C	-3.49463100	-0.47718600	0.60101300
H	-3.25086500	0.58860900	0.65928700
C	-3.09987000	-1.13513000	1.92913900
H	-3.27444600	-2.21936800	1.92632600
H	-2.04478400	-0.95542000	2.16329400
H	-3.69275300	-0.71230500	2.74675900
C	-4.99529900	-0.61649400	0.31155500
H	-5.30792800	-1.66730500	0.24512000
H	-5.57880500	-0.15585800	1.11549200
H	-5.26849700	-0.11988900	-0.62682600
Br	1.51845200	2.24676500	0.80166700
Br	-1.51820800	2.24675700	-0.80181500