

*Supporting Information*

**Mechanism and Origins of Chemo- and Regioselectivities of  
(NHC)NiH-Catalyzed Cross-Hydroalkenylation of Vinyl  
Ethers with  $\alpha$ -Olefins: A Computational Study**

Hongli Wu,<sup>†</sup> Xiaojie Li,<sup>†</sup> Xiangyang Tang,<sup>†</sup> Genping Huang<sup>†\*</sup>

<sup>†</sup>Department of Chemistry, School of Science and Tianjin Key Laboratory of Molecular Optoelectronic Sciences, Tianjin University,

Tianjin 300072, P. R. China.

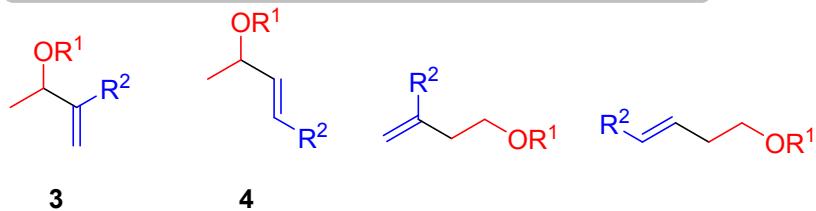
E-mail: gphuang@tju.edu.cn; Web: <http://genpinghuang.weebly.com>

**Table of Contents:**

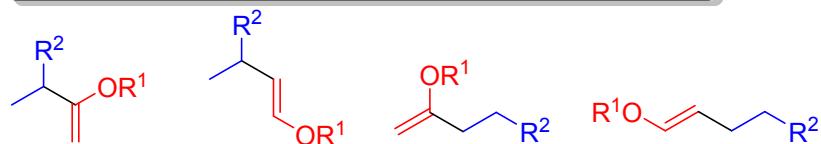
1. All of possible hydroalkenylation products -----	S2
2. Possible complexations between substrates and [L1NiH] <sup>+</sup> -----	S3
3. Other possibilities of the 2,1-hydrometallation of vinyl ether 1a -----	S4
4. $\beta$ -hydride transfer from INT4-----	S5
5. 1a-1a homo-hydroalkenylation from INT2' -----	S6
6. 2a-2a homo-hydroalkenylation reactions -----	S7
7. 2a-1a cross-hydroalkenylation reactions -----	S8
8. $\beta$ -O elimination from INT2' and INT3' -----	S9
9. Validation of computational method-----	S10
10. Table of calculated energies and energy corrections -----	S12
11. Cartesian coordinates -----	S14

## 1. All of possible hydroalkenylation products

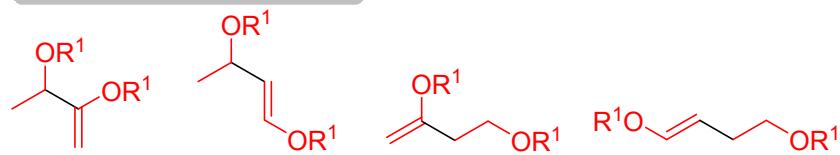
**1-2 cross-hydroalkenylation (1 as acceptor and 2 as donor)**



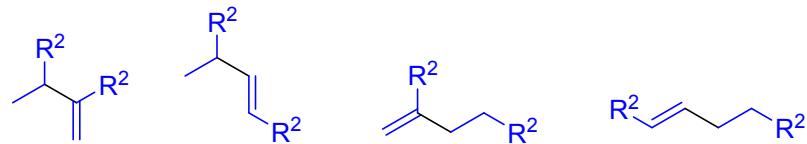
**2-1 cross-hydroalkenylation (1 as donor and 2 as acceptor)**



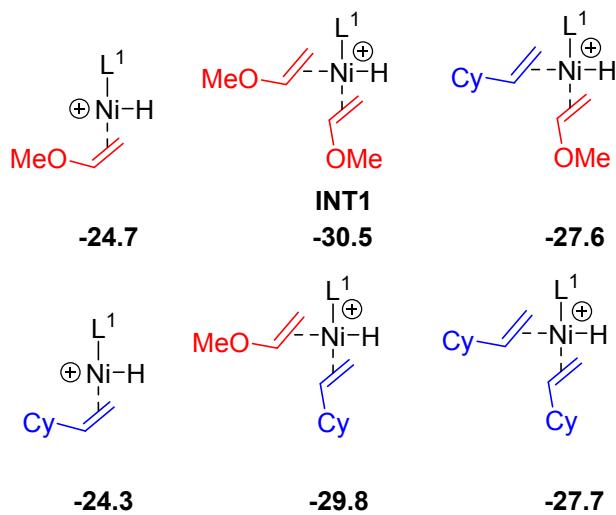
**1-1 homo-hydroalkenylation**



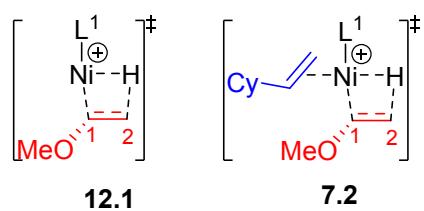
**2-2 homo-hydroalkenylation**



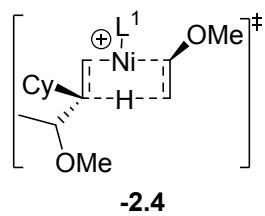
## 2. Possible complexations between substrates and $[L1NiH]^+$



### 3. Other possibilities of the 2,1-hydrometallation of vinyl ether 1a

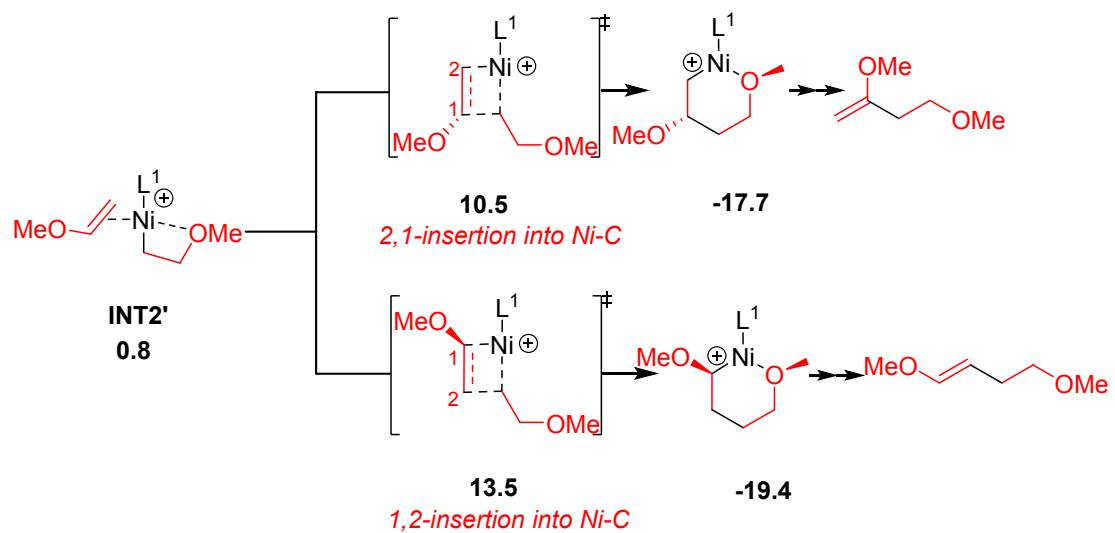


#### 4. $\beta$ -hydride transfer from INT4

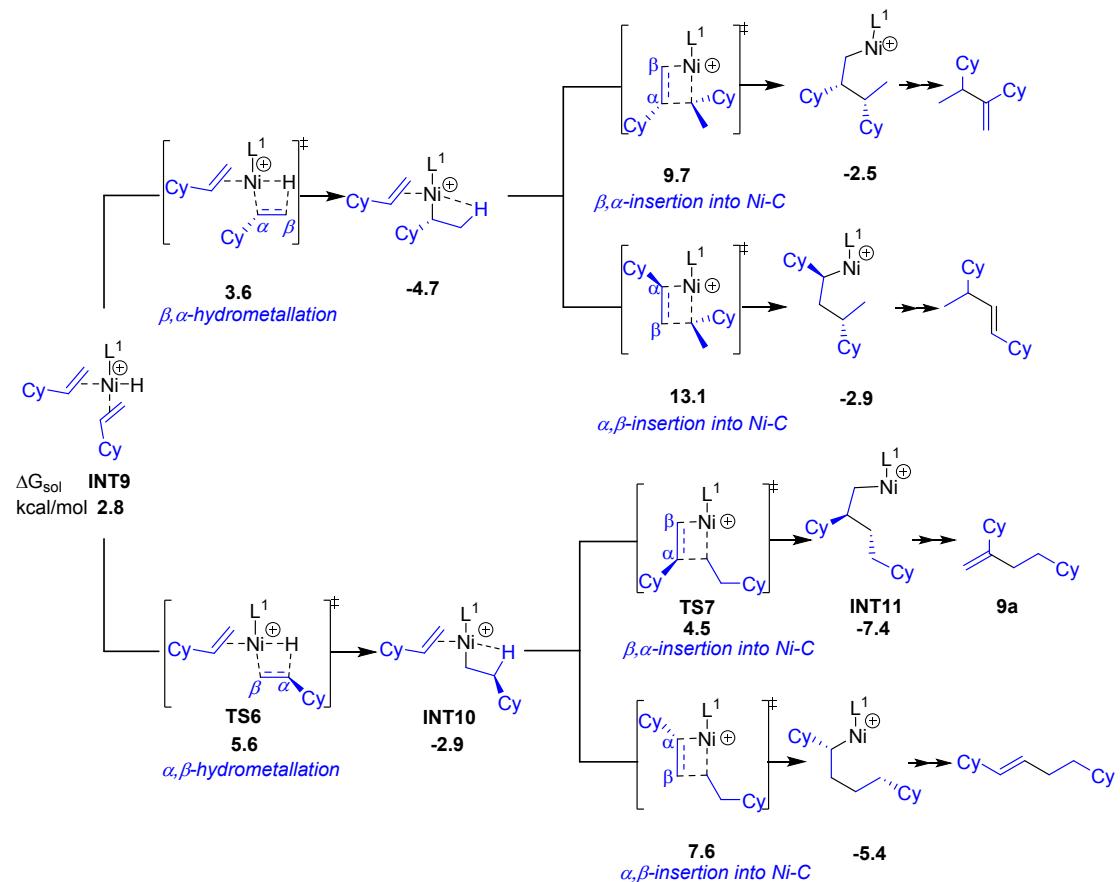


-2.4

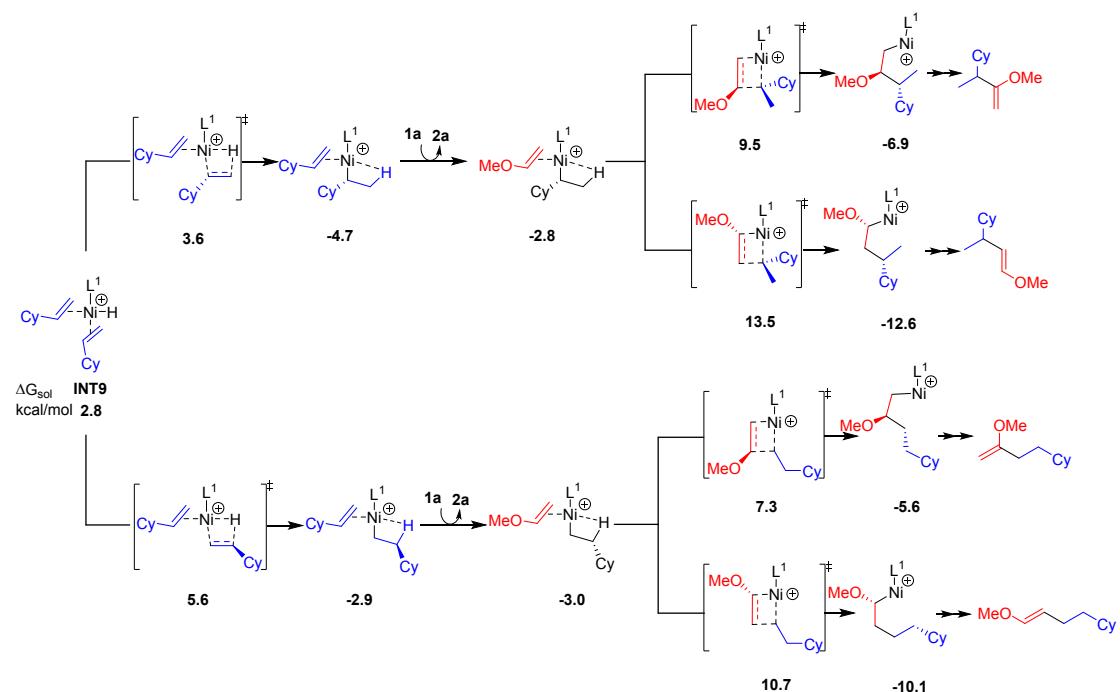
## 5. 1a-1a homo-hydroalkenylation from INT2'



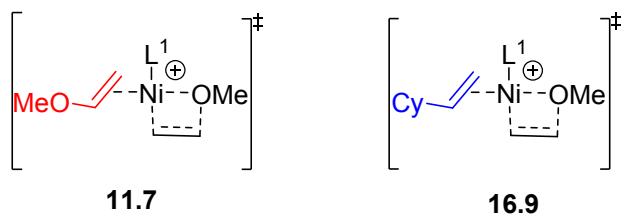
## 6. 2a-2a homo-hydroalkenylation reactions



## 7. 2a-1a cross-hydroalkenylation reactions



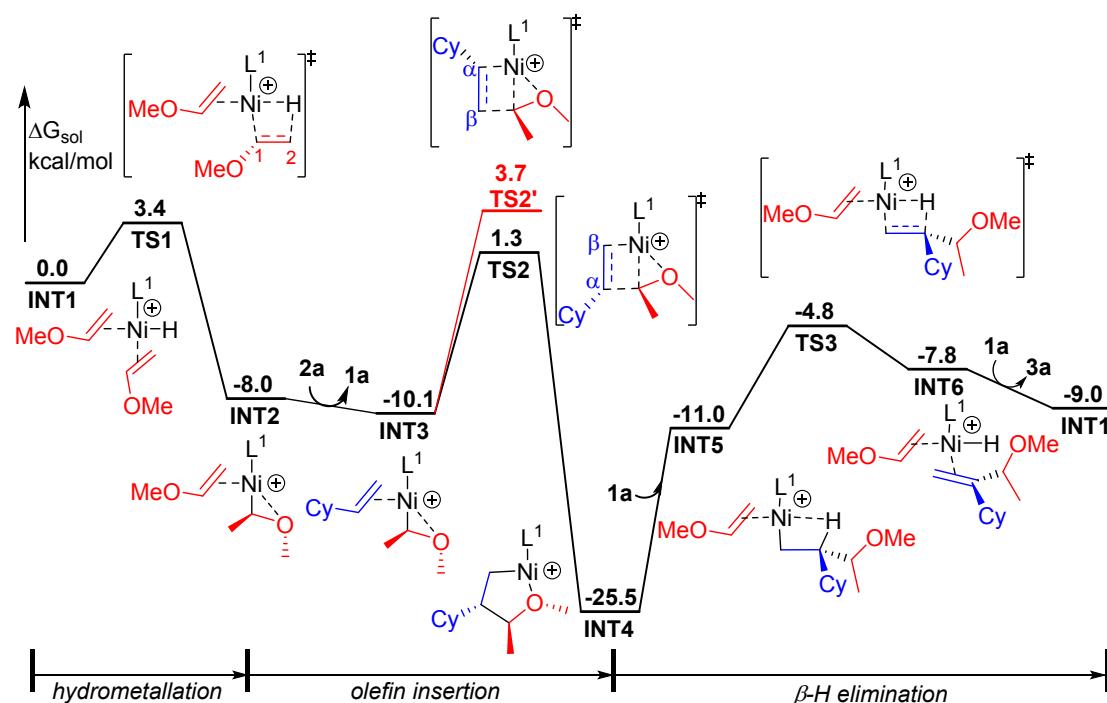
## 8. $\beta$ -O elimination from INT2' and INT3'

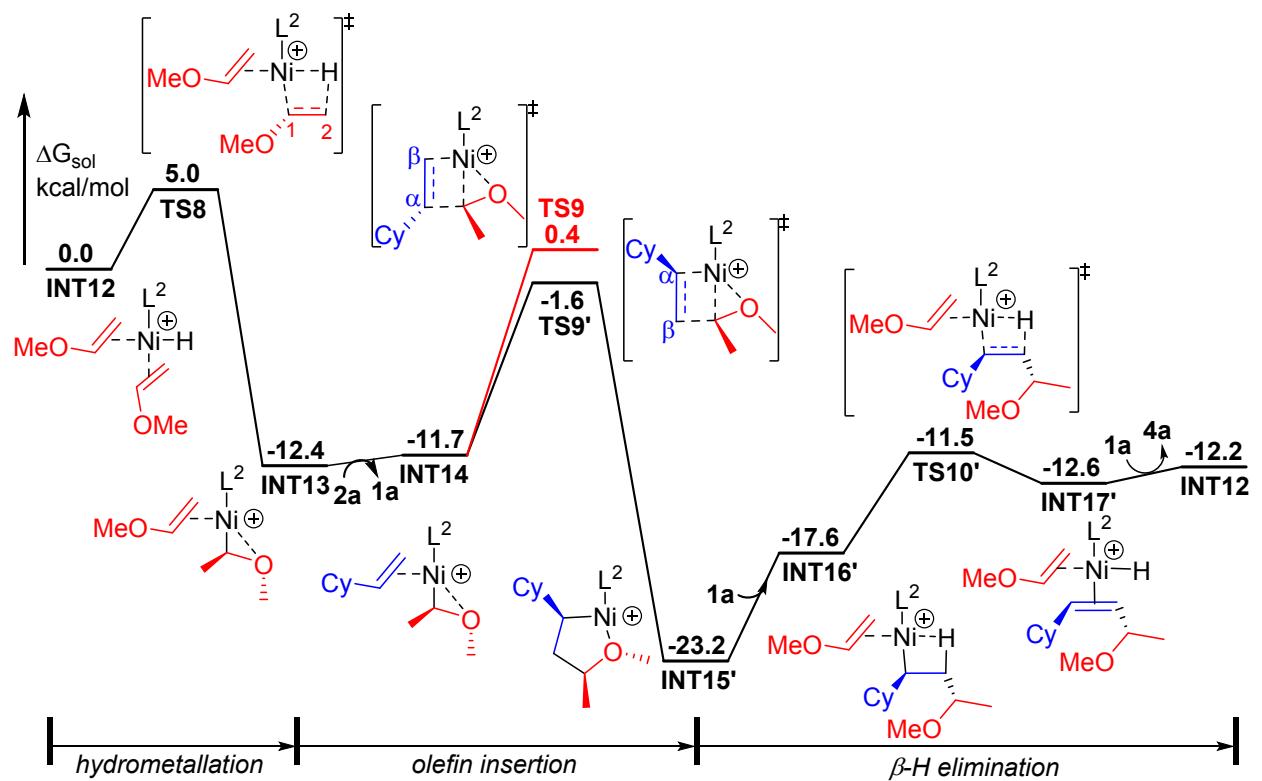


## 9. Validation of the computational method

To further validate our calculated results, the pathways leading to main products for both ligands L<sup>1</sup> and L<sup>2</sup> were re-optimized by including the dispersion corrections using B3LYP-D3(BJ) functional with a mixed basis set of LANL2DZ for Ni and 6-31G(d) for other atoms. Then the energies were calculated using single-point calculations with a larger basis set, which is SDD for Ni and 6-311+G(d,p) for other atoms.

The results show that the energy differences of the optimization with/without dispersion corrections are rather small, being within 1 kcal/mol in most cases. These results indicate that in current study the dispersion effects do not have significant effect on the geometries, and the results presented in the manuscript are reliable.





## 10. Table of calculated energies and energy corrections

Stationary point	Single-point energy-B3LYP-D3(BJ) 6-311+G( <i>d, p</i> ), SDD (a.u.)	Thermal correction to Gibbs free energy at 298.15 K (a.u.)	Optimization energy-B3LYP 6-31G( <i>d</i> ) , LANL2DZ (a.u.)	Solvation energy-toluene (a.u.)
<b>1a</b>	-193.1865028	0.059064	-193.1106971	-0.0023682
<b>2a</b>	-313.3938156	0.171877	-313.2668023	-0.0075766
<b>3a</b>	-506.6116127	0.253339	-506.4065794	-0.0086248
<b>4a</b>	-506.6131772	0.252374	-506.4105001	-0.0106052
<b>INT1</b>	-1718.310315	0.678849	-1716.018681	-0.054446
<b>INT2</b>	-1718.329236	0.683217	-1716.042222	-0.0536205
<b>INT2'</b>	-1718.31638	0.686812	-1716.029755	-0.0551108
<b>TS1</b>	-1718.301235	0.677793	-1716.012176	-0.0541173
<b>TS1'</b>	-1718.304832	0.678213	-1716.015687	-0.0548485
<b>TS5</b>	-1718.306539	0.684877	-1716.025064	-0.0552891
<b>TS5'</b>	-1718.304357	0.686167	-1716.021152	-0.0560712
<b>INT8</b>	-1718.355469	0.684546	-1716.072613	-0.0560713
<b>INT8'</b>	-1718.355806	0.687849	-1716.072916	-0.0555162
<b>INT3</b>	-1838.541601	0.799136	-1836.198561	-0.0588367
<b>INT4</b>	-1838.565145	0.801258	-1836.223722	-0.0607659
<b>INT5</b>	-2031.751411	0.882948	-2029.320053	-0.0574466
<b>INT6</b>	-2031.741142	0.879223	-2029.306641	-0.0565604
<b>TS2</b>	-1838.523378	0.800577	-1836.181764	-0.0593084
<b>TS3</b>	-2031.737119	0.880362	-2029.304348	-0.0567047
<b>TS2'</b>	-1838.520668	0.801287	-1836.176592	-0.0597795
<b>INT3'</b>	-1838.521689	0.794984	-1836.175912	-0.0594419
<b>INT4'</b>	-1838.566362	0.803245	-1836.224035	-0.0597681

<b>TS4</b>	-1838.510043	0.79724	-1836.166498	-0.0597072
<b>TS4'</b>	-1838.510619	0.800117	-1836.165163	-0.0586562
<b>INT7</b>	-1838.56268	0.80326	-1836.221953	-0.05932
<b>INT7'</b>	-1838.560773	0.803497	-1836.215884	-0.0593211
<b>9a</b>	-626.8240444	0.368304	-626.5673598	-0.0140766
<b>INT9</b>	-1958.726137	0.907465	-1956.318872	-0.0621331
<b>INT10</b>	-1958.739616	0.912176	-1956.338002	-0.0625638
<b>TS6</b>	-1958.723055	0.90828	-1956.317114	-0.0615507
<b>TS7</b>	-1958.728886	0.914911	-1956.328165	-0.0641189
<b>INT11</b>	-1958.74757	0.916071	-1956.346948	-0.0656469
<b>INT12</b>	-1328.640749	0.478936	-1326.529248	-0.0533588
<b>INT13</b>	-1328.660182	0.48037	-1326.556821	-0.0544594
<b>TS8</b>	-1328.63192	0.4772	-1326.52189	-0.0527956
<b>INT14</b>	-1448.873903	0.596519	-1446.712081	-0.0576595
<b>INT15'</b>	-1448.894029	0.600361	-1446.731265	-0.0590623
<b>TS9'</b>	-1448.856154	0.598548	-1446.694451	-0.0586812
<b>TS9</b>	-1448.853199	0.5988	-1446.690501	-0.0587747
<b>INT16'</b>	-1642.086611	0.679399	-1639.841928	-0.0579765
<b>TS10'</b>	-1642.072775	0.674604	-1639.824408	-0.057332
<b>INT17'</b>	-1642.075653	0.674134	-1639.825009	-0.0568363
<b>TS2-1</b>	-1366.538711	0.476795	-1364.421991	-0.0586239
<b>TS2'-1</b>	-1366.540658	0.479888	-1364.423514	-0.0593565
<b>TS2-2</b>	-982.9234268	0.381599	-980.9514946	-0.0531634
<b>TS2'-2</b>	-982.9230682	0.381591	-980.951924	-0.0542366
<b>TS9'-1</b>	-1409.517701	0.57176	-1407.375303	-0.0589881
<b>TS9-1</b>	-1409.517539	0.572629	-1407.37348	-0.0588509
<b>TS9'-2</b>	-1370.198947	0.546391	-1368.067205	-0.0604628
<b>TS9-2</b>	-1370.200899	0.547321	-1368.068254	-0.0597331

## 11. Cartesian coordinates

**1a**

C	-1.65431100	-0.08017300	0.01171800
C	-0.32383000	0.05353900	0.00098000
H	-2.34408400	0.75517800	0.04567200
H	-2.08226000	-1.07565900	-0.01484600
H	0.34081300	-0.80575200	-0.03384900
O	0.41153300	1.19400500	0.02895400
C	-0.30832600	2.41575700	0.07725100
H	0.43861200	3.21143500	0.09690800
H	-0.94920000	2.53277300	-0.80685600
H	-0.93176200	2.47221600	0.97951600

**2a**

C	-1.64240300	-0.01553100	-0.07540500
C	-0.31091300	0.06412800	-0.06077200
H	-2.26796500	0.87536800	-0.07565000
H	-2.16054000	-0.97099700	-0.08755900
H	0.27529800	-0.85793800	-0.06090800
C	0.49007900	1.33939300	-0.04301000
C	1.35600600	1.44116900	1.23452100
C	1.38253500	1.45985000	-1.30082300
H	-0.21247900	2.18710500	-0.04417900
C	2.21274700	2.71659700	1.25241400
H	2.01423900	0.56034900	1.28867000
H	0.70949900	1.40115400	2.12006100
C	2.23949100	2.73511900	-1.28220800
H	2.04159100	0.57961600	-1.35422900
H	0.75436100	1.43300800	-2.19995100
C	3.08795200	2.82763600	-0.00510100
H	2.83739800	2.73533400	2.15484000
H	1.55292900	3.59491200	1.31227200
H	2.88294200	2.76665700	-2.17095400
H	1.58108000	3.61441300	-1.34320100
H	3.65634500	3.76652700	0.00776500
H	3.82806000	2.01346500	-0.00318000

**3a**

C	-4.96606600	7.15144300	-2.39456300
C	-3.98688400	7.90855900	-3.30673200
H	-4.55406900	7.06939800	-1.38326500
H	-5.92852600	7.67041200	-2.32633200
H	-3.81145500	8.90927500	-2.87988700
O	-4.51745300	8.05504400	-4.62837900

C	-5.48790100	9.07010200	-4.76469600
H	-5.74396000	9.12299200	-5.82654000
H	-6.40634700	8.86202600	-4.19512800
H	-5.09733500	10.04990400	-4.44487000
H	-5.15217700	6.14218500	-2.77688700
C	-1.59194400	7.65990800	-2.75594900
C	-2.65179400	7.19179000	-3.42333100
H	-1.65048700	8.56758600	-2.15930800
H	-0.62640000	7.16192800	-2.77228800
C	-2.60590800	5.95509100	-4.31274100
C	-1.97293200	6.28110000	-5.68818700
C	-1.88780700	4.75045400	-3.66741500
H	-3.64228000	5.65014300	-4.51277400
C	-1.97182800	5.05649000	-6.61592500
H	-0.94059100	6.62480700	-5.52760300
H	-2.51774500	7.11301100	-6.14668400
C	-1.89588400	3.52519100	-4.59503500
H	-0.84620700	5.01984700	-3.44252800
H	-2.35933200	4.50606000	-2.70687200
C	-1.27892400	3.85029000	-5.96420700
H	-1.48394900	5.30718700	-7.56701100
H	-3.01059000	4.78841600	-6.86024900
H	-1.35823700	2.69293800	-4.12216100
H	-2.93282800	3.18538300	-4.73702500
H	-1.33469800	2.97493800	-6.62440000
H	-0.20972000	4.07519700	-5.83296600

#### 4a

C	-3.45344400	0.49431700	-1.21001500
C	-3.06398300	1.51136800	-2.29438500
H	-2.69732500	0.47404400	-0.41777700
H	-4.41740900	0.74117700	-0.75144400
H	-2.97874900	2.51188700	-1.83730400
O	-4.03988400	1.55486900	-3.34094700
C	-5.21867900	2.25805300	-3.01670700
H	-5.82683700	2.29263200	-3.92517500
H	-5.80605800	1.76941000	-2.22422200
H	-5.00142400	3.29085300	-2.69725200
H	-3.52813100	-0.50906500	-1.64399000
C	-0.62401900	1.85108200	-2.81744300
C	-1.75367900	1.15101000	-2.94164300
H	-0.63457100	2.76997800	-2.22469400
H	-1.76945200	0.23546500	-3.53508100
C	0.70278300	1.49425300	-3.43425900

C	1.16021300	2.57796100	-4.43885100
C	1.78808700	1.27921300	-2.35379500
H	0.58469200	0.54994200	-3.98738600
C	2.53205500	2.25619000	-5.05216100
H	1.21332000	3.54605600	-3.91720500
H	0.40434900	2.68996400	-5.22592000
C	3.16040200	0.95909300	-2.96721500
H	1.86693600	2.19211600	-1.74352700
H	1.47597500	0.47641300	-1.67391600
C	3.59829800	2.03894000	-3.96832800
H	2.83703200	3.06258700	-5.73154100
H	2.44943200	1.34660700	-5.66552400
H	3.90938200	0.84863700	-2.17233600
H	3.10806600	-0.01158600	-3.48254300
H	4.55812500	1.76710600	-4.42609500
H	3.76438700	2.98423800	-3.43029400

### 9a

C	-1.25003100	-0.33847300	-1.94711000
C	-0.24725300	-0.24207500	-1.06619400
H	-1.74773800	0.52880600	-2.37023300
H	-1.61192500	-1.30776500	-2.28331900
C	0.27068500	1.08325900	-0.52355100
C	0.04193900	2.30016800	-1.43942800
C	-0.31725400	1.37331400	0.88171900
H	1.36081200	0.97867600	-0.39368500
C	0.64341400	3.58085300	-0.83876000
H	-1.03695100	2.45267300	-1.58497500
H	0.46690500	2.10425700	-2.43176800
C	0.26930800	2.65530400	1.49317400
H	-1.40810900	1.47233700	0.78620200
H	-0.13982900	0.52331100	1.55262000
C	0.08232300	3.86358300	0.56342500
H	0.45166800	4.43282600	-1.50373700
H	1.73675900	3.47395100	-0.77705600
H	-0.19402300	2.85080800	2.46903600
H	1.34291000	2.50615800	1.68238700
H	0.56024200	4.75307900	0.99384300
H	-0.99064200	4.09327500	0.48246900
C	0.44463200	-1.49004600	-0.54534800
C	1.76238600	-1.79691600	-1.28900900
H	-0.23533800	-2.34447800	-0.63505200
H	0.66511400	-1.37636800	0.52625100
H	1.53094100	-2.01699200	-2.34098500

H	2.38808100	-0.89298400	-1.29943600
C	2.58924800	-2.95148200	-0.69203600
C	1.85538400	-4.30699900	-0.74010400
C	3.95663500	-3.06775300	-1.39482200
H	2.78104700	-2.71441500	0.36836400
C	2.70909700	-5.45208600	-0.17104400
H	1.59664900	-4.53191900	-1.78691300
H	0.90710000	-4.24999100	-0.19176400
C	4.81555400	-4.20845800	-0.82682900
H	3.78979700	-3.24105500	-2.46935800
H	4.49629500	-2.11418800	-1.31581500
C	4.07003100	-5.55063600	-0.87481300
H	2.16647700	-6.40257300	-0.25573700
H	2.87027200	-5.28098100	0.90391700
H	5.76262700	-4.27728400	-1.37761500
H	5.07823600	-3.97820500	0.21659000
H	4.67884500	-6.34254200	-0.41966300
H	3.91385500	-5.83966300	-1.92494300

### INT1

Ni	-0.72207300	1.08316500	-0.79737000
C	-0.74696900	-0.19549200	3.16928000
C	0.41846200	0.49091200	3.10072000
N	0.51267300	0.99478100	1.80930500
N	-1.35339400	-0.08717600	1.91961400
C	-0.57765500	0.64406200	1.06468300
C	-2.65523500	-0.65287900	1.63634500
C	-3.79651100	-0.00303700	2.16294300
C	-2.73348700	-1.85421500	0.90136000
C	-5.04566700	-0.57589700	1.88803800
C	-4.01183000	-2.37374300	0.65314300
C	-5.15568600	-1.74234400	1.13375400
H	-5.94370400	-0.10823500	2.27965300
H	-4.10915900	-3.29965300	0.09441200
H	-6.13475700	-2.17162000	0.93984700
C	1.64620100	1.76823600	1.34166800
C	2.79615400	1.07667700	0.90559600
C	1.57726900	3.17619100	1.40081600
C	3.89056700	1.84742700	0.49396600
C	2.70262700	3.89266400	0.97364600
C	3.84509500	3.23857600	0.52084700
H	4.79530200	1.35088200	0.15738500
H	2.68979600	4.97726500	1.00933900
H	4.70827600	3.81530800	0.20087700

C	-1.50399400	-2.63247400	0.44113100
C	-1.52108100	-2.91350800	-1.07259900
C	-1.36493900	-3.94305400	1.24446200
H	-0.61660500	-2.02762100	0.64614200
H	-1.58028600	-1.98532100	-1.65154900
H	-0.60408200	-3.43797200	-1.36471100
H	-2.36484400	-3.55059000	-1.36090500
H	-1.31188500	-3.74932200	2.32138900
H	-2.21359000	-4.61340100	1.06751200
H	-0.45269200	-4.47388700	0.94988200
C	2.90306400	-0.44603900	0.91961000
C	3.78886500	-0.91990900	2.09149600
C	3.42328600	-1.01516100	-0.41346200
H	1.90075500	-0.85791400	1.07497800
H	3.40421900	-0.57287200	3.05690100
H	3.83383600	-2.01448000	2.11940000
H	4.81281800	-0.54335800	1.98843700
H	2.81169800	-0.67477100	-1.25611400
H	4.46003200	-0.72083500	-0.60947700
H	3.39547400	-2.11031300	-0.38951600
C	-3.71828900	1.24544000	3.04299100
C	-4.00906600	0.88857600	4.51702700
C	-4.65921500	2.37397300	2.57728100
H	-2.69666000	1.63672200	2.99514400
H	-3.33002600	0.11602700	4.89331400
H	-3.89872000	1.77442800	5.15212200
H	-5.03230100	0.51504500	4.63624000
H	-4.46743200	2.66815000	1.54006100
H	-5.71341200	2.08766600	2.65617100
H	-4.51682400	3.25866000	3.20733000
C	0.37473800	3.92233900	1.97346400
C	-0.05364500	5.12240900	1.10837000
C	0.65757900	4.37430500	3.42232100
H	-0.47101000	3.22694000	2.00924000
H	-0.21879000	4.83160600	0.06502500
H	-0.98396000	5.55228600	1.49629400
H	0.69639700	5.92028800	1.11588400
H	0.90011500	3.52498300	4.07033400
H	1.50211300	5.07165800	3.45680900
H	-0.21700200	4.88331100	3.84329000
H	-1.20603400	-0.74350700	3.97627700
H	1.18568200	0.66827600	3.83735700
C	0.13738900	1.70625500	-2.66942800
C	-0.86713300	0.96016600	-3.22826000

H	1.17085900	1.38265900	-2.66825800
H	-0.03718500	2.76900300	-2.53379700
H	0.36349200	0.10703200	-0.79375100
C	-2.32912800	2.66883100	-0.75723200
C	-3.26976500	1.71182500	-0.99041600
H	-2.08289400	3.38929700	-1.53148100
H	-2.10739500	2.93567500	0.26916200
H	-3.64123600	1.06572500	-0.19700400
O	-3.80824300	1.52939200	-2.19725800
C	-4.63587500	0.36431200	-2.38505900
H	-5.26190200	0.57456400	-3.25192000
H	-4.00705600	-0.51009700	-2.57907800
H	-5.25963600	0.18933700	-1.50340000
H	-1.86454300	1.36603900	-3.36385300
O	-0.80321400	-0.28180900	-3.71182100
C	0.47656800	-0.92888600	-3.77406500
H	0.88111600	-1.06753500	-2.76646500
H	0.29548800	-1.89534500	-4.24302000
H	1.16952500	-0.34036300	-4.38437800

### INT2

Ni	-1.14809500	1.34985400	-0.90695600
C	-0.71537300	-0.00914200	3.14977300
C	0.40234900	0.74225300	3.02112200
N	0.39634200	1.24436300	1.72544700
N	-1.38555700	0.06292300	1.93338800
C	-0.70965900	0.83895000	1.02377300
C	-2.61568800	-0.66714900	1.71793800
C	-3.81252800	-0.15512500	2.26990600
C	-2.55896000	-1.90192700	1.03703300
C	-4.98082600	-0.90582900	2.08082000
C	-3.76154700	-2.60334900	0.87281500
C	-4.96009900	-2.11281500	1.38463900
H	-5.91794100	-0.54544900	2.49346900
H	-3.75377100	-3.55857600	0.35600100
H	-5.87748800	-2.68097900	1.25805600
C	1.50223400	2.03875100	1.23449800
C	2.69690300	1.36817400	0.89058700
C	1.38509700	3.44422600	1.21981300
C	3.78961300	2.15731600	0.50676300
C	2.50793300	4.17947000	0.81531000
C	3.69776000	3.54679700	0.46479100
H	4.72696400	1.67655600	0.24277900
H	2.45656600	5.26401500	0.79776300

H	4.55971500	4.13851400	0.16967400
C	-1.25646000	-2.51601300	0.53039600
C	-1.28846400	-2.76161700	-0.98937800
C	-0.92590300	-3.81432600	1.29488100
H	-0.44528500	-1.80828900	0.72293700
H	-1.47912500	-1.82903400	-1.53318800
H	-0.32669500	-3.16022500	-1.33044000
H	-2.06346100	-3.48403200	-1.26972200
H	-0.86086700	-3.63746300	2.37393500
H	-1.68684000	-4.58483600	1.12840600
H	0.03556600	-4.21756700	0.95798500
C	2.84542100	-0.15202900	0.93479900
C	3.89075700	-0.58077800	1.98452200
C	3.18316200	-0.73859800	-0.45031500
H	1.88579100	-0.58247700	1.23636200
H	3.64222300	-0.19944000	2.98125200
H	3.94347600	-1.67356100	2.04307500
H	4.89090800	-0.21330500	1.72926000
H	2.40850000	-0.49705900	-1.18624200
H	4.14178000	-0.36468800	-0.82764300
H	3.26026000	-1.82985700	-0.38654800
C	-3.86927600	1.13943200	3.08095500
C	-4.03500200	0.83418300	4.58529200
C	-4.98257600	2.09508400	2.60829400
H	-2.91591500	1.66371700	2.95484100
H	-3.22630800	0.20101200	4.96532600
H	-4.03648800	1.76434400	5.16411000
H	-4.98083300	0.31596300	4.77932200
H	-4.89668900	2.32983000	1.54203300
H	-5.98070000	1.67795600	2.77997700
H	-4.92557300	3.03607900	3.16623400
C	0.12740600	4.17789800	1.67784700
C	-0.40102600	5.15123700	0.60701600
C	0.37476900	4.90940600	3.01340800
H	-0.65502200	3.43332900	1.85467100
H	-0.60373000	4.63277800	-0.33745300
H	-1.33313800	5.61765700	0.94563600
H	0.31112900	5.95773600	0.40159000
H	0.70721300	4.21602900	3.79363800
H	1.14163800	5.68480000	2.90776300
H	-0.54531700	5.39396300	3.35917700
H	-1.09406300	-0.58890600	3.97625900
H	1.19875200	0.96229000	3.71429100
C	-1.38338400	0.62391700	-3.76456000

C	-0.86169500	1.61498500	-2.75484600
H	-2.41883000	0.86382600	-4.01757900
H	-0.78887800	0.66232500	-4.68848700
H	-1.33842600	-0.40261000	-3.38578600
C	-2.87101400	2.48498400	-0.76672000
C	-3.54466000	1.30163700	-0.98193200
H	-2.88256700	3.24869100	-1.53870800
H	-2.74045500	2.81455900	0.25835900
H	-3.73911600	0.60065300	-0.17375400
O	-4.10246700	1.01649200	-2.15631000
C	-4.69111700	-0.28865700	-2.30645000
H	-5.37192400	-0.21653100	-3.15436000
H	-3.91241500	-1.02850400	-2.51422100
H	-5.24305800	-0.56882400	-1.40405700
H	-0.89273000	2.66025500	-3.08030200
O	0.40514200	1.26361400	-2.23773500
C	1.44211600	2.26614700	-2.34720900
H	1.07452400	3.24311400	-2.02069100
H	2.26301400	1.94699200	-1.71048200
H	1.76350200	2.31115700	-3.39179600

### INT2'

Ni	-0.67667700	1.48016500	-0.85395500
C	-1.26506300	0.19742700	3.23753100
C	-0.09794300	0.88210600	3.29154400
N	0.15829800	1.33729000	2.00362400
N	-1.70263000	0.25530700	1.91720800
C	-0.82634900	0.95658100	1.13022500
C	-2.98772100	-0.28257900	1.51324300
C	-4.14538500	0.49280000	1.75734400
C	-3.04813100	-1.57871900	0.95687400
C	-5.37791800	-0.04634000	1.36289800
C	-4.30829100	-2.06251300	0.58083700
C	-5.46030500	-1.30325800	0.77031800
H	-6.28667500	0.52154600	1.53437400
H	-4.39267300	-3.05434300	0.14951900
H	-6.42722200	-1.70240400	0.47710300
C	1.28769700	2.19870800	1.69243000
C	2.54247500	1.61229700	1.41803100
C	1.10346000	3.59813100	1.76109900
C	3.61291500	2.47515600	1.15228700
C	2.21133300	4.40882400	1.48210400
C	3.45029100	3.85711600	1.17234000
H	4.59080200	2.05940300	0.93441100

H	2.10611300	5.48793100	1.52430100
H	4.29612900	4.50590700	0.96350100
C	-1.82000700	-2.47711200	0.84465200
C	-1.80700200	-3.33458000	-0.43337900
C	-1.70434300	-3.38153100	2.09201600
H	-0.93495800	-1.83336400	0.82301300
H	-1.96221700	-2.72940400	-1.33379400
H	-0.84497900	-3.84996200	-0.52831100
H	-2.58054300	-4.10954900	-0.41454900
H	-1.63509900	-2.79417300	3.01346700
H	-2.57649000	-4.03938700	2.17828700
H	-0.81045500	-4.01217100	2.02616600
C	2.77975400	0.10574000	1.47166200
C	3.32363400	-0.31317800	2.85544200
C	3.72830200	-0.39304300	0.36590700
H	1.81359900	-0.39117000	1.33030300
H	2.63995700	-0.04107600	3.66597200
H	3.47592500	-1.39787000	2.89425900
H	4.28668300	0.16975200	3.05620000
H	3.42253300	-0.02792500	-0.61903400
H	4.76075200	-0.07175500	0.54007300
H	3.73634300	-1.48865700	0.34599400
C	-4.11218200	1.83825900	2.48302800
C	-4.55407600	1.66508600	3.95296300
C	-4.97030900	2.92156300	1.80132400
H	-3.07763300	2.19811000	2.49235500
H	-3.92804200	0.94201000	4.48566000
H	-4.49292800	2.62141300	4.48407000
H	-5.59023100	1.31325000	4.00970300
H	-4.70626400	3.05554200	0.74726400
H	-6.03938900	2.68960700	1.85231300
H	-4.82636400	3.88153900	2.30898400
C	-0.20362200	4.24599600	2.21265600
C	-0.60212700	5.46475900	1.35944600
C	-0.11879100	4.64101400	3.70346600
H	-1.00419900	3.50430800	2.12070900
H	-0.60712100	5.22930500	0.29005100
H	-1.60395300	5.80773100	1.64133900
H	0.07844000	6.30913800	1.51096500
H	0.09317400	3.77540400	4.34025400
H	0.67493500	5.37837700	3.86766100
H	-1.06441900	5.08359800	4.03701200
H	-1.82422400	-0.31756100	4.00215600
H	0.56506700	1.09272200	4.11523800

C	0.80864100	0.85162300	-2.83269700
C	-0.07704900	2.05246400	-2.60237600
H	0.38055300	0.13885300	-3.54750200
H	1.85005300	1.05295000	-3.11205700
C	-2.12403600	2.94098500	-0.86739900
C	-2.89449000	1.88849000	-1.33606100
H	-1.86526700	3.74623300	-1.54725600
H	-2.19233600	3.18454200	0.18535400
H	-3.33582500	1.16165600	-0.65477000
O	-3.25230100	1.79031300	-2.60928000
C	-3.86861800	0.56061800	-3.03015300
H	-4.42749400	0.79387100	-3.93602900
H	-3.09397600	-0.18102700	-3.25067200
H	-4.54407600	0.18063200	-2.25655800
H	0.47570000	2.98116600	-2.41940200
H	-0.85145300	2.20155400	-3.35433900
O	0.80606600	0.22891100	-1.50195400
C	0.94060600	-1.19205700	-1.51632900
H	0.11511100	-1.65644800	-2.06834500
H	1.89322500	-1.46418300	-1.98390400
H	0.93322600	-1.53438900	-0.48184200

### INT3

Ni	-1.08491100	0.75939100	-0.89863400
C	-1.54238200	-0.35264900	3.09848400
C	-0.32154300	0.21687300	3.23797100
N	0.04674600	0.69494400	1.98379200
N	-1.89140900	-0.22278900	1.75958100
C	-0.91717000	0.42554600	1.05053700
C	-3.15790800	-0.69347400	1.23120400
C	-4.24587200	0.20504500	1.18871200
C	-3.27222700	-2.04714200	0.84657500
C	-5.46635800	-0.28393100	0.70373300
C	-4.51852100	-2.47870000	0.37599800
C	-5.60237100	-1.60815700	0.29735000
H	-6.32638200	0.37674000	0.66033800
H	-4.64544600	-3.51256400	0.07245300
H	-6.56026500	-1.96729500	-0.06821100
C	1.29426400	1.40417400	1.76860200
C	2.40471700	0.69236300	1.26448400
C	1.36909900	2.76362200	2.14727200
C	3.60284600	1.39928600	1.10144300
C	2.59608200	3.41556600	1.96245000
C	3.69824600	2.74665400	1.43940200

H	4.47863700	0.88706000	0.71770700
H	2.69236500	4.45963800	2.24229900
H	4.63979400	3.27253200	1.30897400
C	-2.12259300	-3.04247700	0.98306500
C	-2.01559800	-4.00480100	-0.21496300
C	-2.24881800	-3.84926400	2.29407300
H	-1.18790000	-2.47238500	1.03327600
H	-2.01728300	-3.46446800	-1.16639700
H	-1.09023600	-4.58796200	-0.14435000
H	-2.84189100	-4.72340400	-0.23504000
H	-2.25656200	-3.20071000	3.17589700
H	-3.17558800	-4.43407600	2.30233900
H	-1.40935200	-4.54631300	2.39697800
C	2.35616100	-0.80830600	0.98500200
C	2.77698900	-1.60446100	2.24029800
C	3.21468800	-1.23434400	-0.21942700
H	1.31793300	-1.07459200	0.75811700
H	2.13192200	-1.38395800	3.09685700
H	2.72392800	-2.68212900	2.04714900
H	3.80730600	-1.36270800	2.52487300
H	3.00277100	-0.63034400	-1.10895900
H	4.28610700	-1.15091500	-0.00916700
H	3.02260600	-2.28580700	-0.46172400
C	-4.16080600	1.63547100	1.71487400
C	-4.81105700	1.73642000	3.11158400
C	-4.78716600	2.66350600	0.75374000
H	-3.10332600	1.89536700	1.82880300
H	-4.33572300	1.05675600	3.82717500
H	-4.72268500	2.75636700	3.50269200
H	-5.87631400	1.48323700	3.06787100
H	-4.37289300	2.57849000	-0.25751000
H	-5.87300300	2.54335000	0.67649400
H	-4.60129100	3.68046500	1.11711800
C	0.20805700	3.51519300	2.80051300
C	0.00024100	4.93254100	2.23210100
C	0.40756100	3.59486900	4.33051400
H	-0.71278800	2.95116900	2.61492000
H	-0.10878600	4.93070200	1.14284700
H	-0.90644400	5.37301500	2.66115200
H	0.83110400	5.59991300	2.48438300
H	0.49698000	2.60374600	4.78663300
H	1.31688300	4.15521800	4.57547200
H	-0.44028500	4.10655100	4.79951900
H	-2.19236300	-0.82904400	3.81470200

H	0.31684100	0.32911600	4.09920600
C	-2.97588100	0.08318600	-3.01014400
C	-1.51478300	0.09677100	-2.64098600
H	-3.24681400	1.01524900	-3.51551100
H	-3.19389400	-0.74526700	-3.69827300
H	-0.80866400	0.25442200	-3.45826500
O	-1.15448400	-0.99999500	-1.83185200
C	0.08336600	-1.67618900	-2.15528900
H	0.35825400	-2.25837400	-1.27725400
H	-0.10010400	-2.33818700	-3.00584300
H	0.86995300	-0.95571300	-2.39419900
H	-3.61321800	-0.03492400	-2.12773000
C	-1.09724000	2.78189000	-0.64380600
C	-1.05843400	2.66613900	-2.02287500
H	-0.19799000	3.00422700	-0.08145900
H	-2.04008800	2.97651200	-0.14086300
H	-2.01020700	2.71298500	-2.54940700
C	0.15036600	2.91399600	-2.90099800
C	0.07995100	4.37243200	-3.43268700
C	1.51444700	2.65392300	-2.23960100
H	0.07089800	2.26027300	-3.78342400
C	1.24205400	4.67395400	-4.39266300
H	0.11672200	5.06162400	-2.57725200
H	-0.88078100	4.54381600	-3.93505400
C	2.67377800	2.95079000	-3.20453000
H	1.62200400	3.28844400	-1.34949000
H	1.56984100	1.61543600	-1.88405900
C	2.60342900	4.38776700	-3.74288100
H	1.18572700	5.71935200	-4.71840500
H	1.13236200	4.05902900	-5.29768800
H	3.62963400	2.78003100	-2.69494000
H	2.63766800	2.24474800	-4.04758100
H	3.41080000	4.56157200	-4.46392600
H	2.76602900	5.09294300	-2.91484800

### INT3'

Ni	-1.03348400	0.54188300	-0.97639500
C	-1.59153000	-0.18422700	3.10822900
C	-0.38719300	0.41576300	3.25465900
N	0.03545400	0.79309600	1.98295200
N	-1.87901700	-0.17716600	1.74827000
C	-0.87683700	0.42135000	1.02984700
C	-3.14597600	-0.66313500	1.22553200
C	-4.19033900	0.26662600	1.02093600

C	-3.32048300	-2.05085600	1.03160000
C	-5.41220100	-0.22807000	0.54673600
C	-4.56741600	-2.48521400	0.56441400
C	-5.59941200	-1.58650800	0.31196500
H	-6.23577700	0.45842400	0.37903500
H	-4.73644400	-3.54494700	0.40433600
H	-6.55801100	-1.94813200	-0.04905600
C	1.25302000	1.56581200	1.79644300
C	2.45001700	0.89632500	1.46526800
C	1.20796500	2.95756100	2.04802800
C	3.60698300	1.67264500	1.31953600
C	2.39809200	3.67966100	1.88789100
C	3.58237100	3.04997000	1.51678300
H	4.54437500	1.19010700	1.06391300
H	2.39924800	4.74950100	2.06911200
H	4.49278100	3.63116200	1.40120300
C	-2.24573200	-3.08017300	1.37038900
C	-2.12638200	-4.18927700	0.30834800
C	-2.50694100	-3.70895800	2.75676600
H	-1.28273000	-2.56026500	1.41850300
H	-2.04411000	-3.77048400	-0.69883300
H	-1.24104700	-4.80400200	0.50598400
H	-2.99035500	-4.86213600	0.32320900
H	-2.52832300	-2.95754600	3.55271000
H	-3.46881600	-4.23362100	2.77026200
H	-1.72330200	-4.43508800	3.00115600
C	2.53737100	-0.62312300	1.36426000
C	2.99657100	-1.22339300	2.71147800
C	3.45399500	-1.10620000	0.22611200
H	1.53113600	-1.00298300	1.16362700
H	2.31862200	-0.95130400	3.52730300
H	3.03186800	-2.31735100	2.65249400
H	3.99855900	-0.86718000	2.97571400
H	3.19732500	-0.63806200	-0.73078700
H	4.50808000	-0.89033800	0.43004500
H	3.37059200	-2.19287600	0.11233300
C	-4.07434600	1.74490800	1.38380200
C	-4.75090900	2.01844300	2.74478100
C	-4.65070000	2.67728400	0.30134600
H	-3.01335000	1.98728600	1.49635700
H	-4.30857100	1.41340900	3.54359700
H	-4.64390000	3.07383900	3.02053500
H	-5.82125700	1.78750700	2.70433800
H	-4.23271300	2.45953200	-0.68811900

H	-5.73966900	2.59116900	0.22497900
H	-4.42919400	3.72203000	0.54734400
C	-0.04427100	3.67888400	2.54964700
C	-0.30137500	5.02461100	1.84342000
C	0.03775500	3.90446500	4.07597700
H	-0.91023100	3.03632500	2.35677600
H	-0.32181300	4.92466200	0.75366100
H	-1.26653000	5.43116300	2.16483300
H	0.45975000	5.77010200	2.09714000
H	0.16086500	2.96592100	4.62565100
H	0.88596600	4.55084500	4.32795500
H	-0.87515000	4.39024300	4.43839800
H	-2.26882900	-0.60770200	3.83214700
H	0.20734100	0.61407800	4.13173100
C	-1.74479500	0.15569500	-2.78934600
H	-1.58225000	0.70796100	-3.71211000
C	-0.98864000	2.59485000	-0.76388100
C	-0.93969200	2.51549600	-2.14266600
H	-0.08428900	2.76454000	-0.19310100
H	-1.92467200	2.84502200	-0.27563800
H	-1.88121800	2.63146600	-2.67374300
C	0.29219200	2.68182900	-2.99973500
C	0.39573300	4.17880300	-3.40994200
C	1.61378700	2.20686600	-2.37264500
H	0.13394500	2.11308900	-3.92767000
C	1.58383000	4.41206000	-4.35744500
H	0.52003800	4.78707300	-2.50295700
H	-0.53782500	4.50539300	-3.88543000
C	2.79718900	2.43667500	-3.32713100
H	1.80191300	2.74791100	-1.43534800
H	1.53769700	1.14226100	-2.10930200
C	2.90126000	3.90984300	-3.75008400
H	1.65494800	5.47973700	-4.59644800
H	1.39537200	3.89142800	-5.30733000
H	3.72762500	2.11164000	-2.84621500
H	2.67084000	1.80869000	-4.22139500
H	3.72124000	4.04038800	-4.46594200
H	3.15259200	4.52116700	-2.87102100
H	-2.81232300	0.15041200	-2.53504100
C	-1.12928600	-1.22105700	-2.81935700
H	-1.77946900	-2.03959800	-3.15792300
H	-0.20255200	-1.23895600	-3.40542700
O	-0.79459300	-1.43269200	-1.41489000
C	0.34158500	-2.27655200	-1.21333700

H	1.24234400	-1.82734800	-1.64611900
H	0.46779000	-2.40473200	-0.13935800
H	0.15423200	-3.25057800	-1.67785000

#### INT4

Ni	-0.50912900	0.12127500	-0.62547000
C	-1.67345700	0.09041400	3.30861700
C	-0.41157300	0.56538500	3.46680100
N	0.12293200	0.71793100	2.19528400
N	-1.88535300	-0.03902800	1.94385700
C	-0.77444700	0.33430000	1.23980300
C	-3.11672700	-0.54824500	1.37155700
C	-4.20793500	0.33500300	1.21812700
C	-3.18531800	-1.91488300	1.03346300
C	-5.38215900	-0.19128200	0.66512300
C	-4.38356100	-2.38050500	0.47620500
C	-5.46832600	-1.52939400	0.28755700
H	-6.24455500	0.45403100	0.53311600
H	-4.47194900	-3.42757800	0.20211200
H	-6.39048900	-1.91276100	-0.13981100
C	1.46567900	1.20757800	1.95222900
C	2.49187800	0.27235700	1.71007300
C	1.69811000	2.59761800	2.02316900
C	3.77844800	0.77451300	1.47654400
C	3.00682100	3.03925700	1.79182800
C	4.03412800	2.14214100	1.51027800
H	4.59311200	0.08357100	1.28147000
H	3.22620700	4.10118100	1.83880100
H	5.04060500	2.50996500	1.33258700
C	-2.04330800	-2.89557400	1.28675100
C	-1.52323500	-3.51950800	-0.02222200
C	-2.45921600	-3.98913600	2.29161800
H	-1.21060300	-2.34625700	1.73757700
H	-1.19887700	-2.74441300	-0.72793300
H	-0.67142900	-4.17899700	0.17927400
H	-2.29539800	-4.11660200	-0.51983600
H	-2.79970400	-3.55321400	3.23695400
H	-3.27242100	-4.60932100	1.89874100
H	-1.61179800	-4.64950600	2.50763700
C	2.25997500	-1.23595800	1.71842000
C	3.14870500	-1.94600800	2.75854600
C	2.46370100	-1.84059400	0.31644400
H	1.22021300	-1.42266300	2.00651600
H	2.99525900	-1.53259900	3.76089500

H	2.91235700	-3.01546700	2.79186200
H	4.21261100	-1.84965200	2.51673600
H	1.81446300	-1.34827400	-0.42086400
H	3.49576200	-1.71593200	-0.02968300
H	2.23462600	-2.91237200	0.31786900
C	-4.16772000	1.78944300	1.68509700
C	-4.86429000	1.93519900	3.05588700
C	-4.78695400	2.77154700	0.67280700
H	-3.11815300	2.07711800	1.81337900
H	-4.40986900	1.29191400	3.81701700
H	-4.80237600	2.97089300	3.40821700
H	-5.92408300	1.66570200	2.98488700
H	-4.33095200	2.67820200	-0.31829200
H	-5.86627100	2.62138100	0.56283100
H	-4.63835300	3.80063400	1.01759200
C	0.61033300	3.60332300	2.39482800
C	0.55711900	4.80675700	1.43629600
C	0.79072300	4.08637100	3.85013300
H	-0.35956500	3.09799300	2.33209800
H	0.45113500	4.48687700	0.39500400
H	-0.29621200	5.44678500	1.68640000
H	1.45806200	5.42594200	1.50601400
H	0.78000000	3.25406000	4.56249000
H	1.74384900	4.61311200	3.97230900
H	-0.01345100	4.77783800	4.12548400
H	-2.43090100	-0.17094500	4.03016800
H	0.15370900	0.80338700	4.35367800
C	-2.52314900	-0.19361900	-3.56759800
C	-1.18846300	0.52138200	-3.37736200
H	-3.16220700	0.40212700	-4.22799400
H	-2.39887300	-1.17450100	-4.03707200
H	-0.67913400	0.62343400	-4.34405500
O	-0.28450300	-0.26806600	-2.52882800
C	0.24214800	-1.46705700	-3.11317300
H	1.02263600	-1.83504900	-2.44610700
H	-0.53287500	-2.23068600	-3.23017300
H	0.68273900	-1.23049200	-4.08759300
H	-3.04499300	-0.33006600	-2.61447500
C	-1.47444000	1.67260000	-1.16472200
C	-1.29517800	1.88753300	-2.67987800
H	-1.14570200	2.52096000	-0.56213300
H	-2.50161200	1.41001600	-0.89826900
H	-2.23250500	2.33742400	-3.04573600
C	-0.17222400	2.87614200	-3.10145700

C	-0.53265500	4.33112600	-2.73645900
C	1.24474800	2.52949800	-2.60089500
H	-0.14205400	2.83473900	-4.20293900
C	0.51245500	5.33006900	-3.25882200
H	-0.61030800	4.43244600	-1.64435600
H	-1.52349700	4.57924900	-3.14104700
C	2.29020700	3.53023500	-3.12387600
H	1.25757700	2.53347600	-1.50093000
H	1.52126400	1.51417600	-2.90889000
C	1.92492600	4.97832800	-2.76935300
H	0.24213500	6.34755500	-2.95141600
H	0.49782900	5.32333100	-4.35837900
H	3.27917700	3.27635600	-2.72256000
H	2.36391100	3.43417600	-4.21711200
H	2.65855700	5.67066500	-3.19968400
H	1.97571700	5.10875500	-1.67817200

#### INT4'

Ni	-0.83004400	0.24784100	-0.55476100
C	-1.91964400	-1.15851800	3.10366800
C	-0.70659100	-0.67551800	3.47510200
N	-0.17198900	-0.02801600	2.36968100
N	-2.09979400	-0.79947000	1.77709000
C	-1.01982100	-0.10730800	1.30055700
C	-3.28391700	-1.13631800	1.01101600
C	-4.39987700	-0.27582100	1.08609400
C	-3.28878200	-2.33300600	0.26533200
C	-5.53833100	-0.63945200	0.35611200
C	-4.45551000	-2.64207000	-0.44604600
C	-5.56695300	-1.80522700	-0.40564500
H	-6.41892900	-0.00583200	0.39203000
H	-4.49738900	-3.55688100	-1.02944300
H	-6.46373200	-2.06826600	-0.95940600
C	1.11535800	0.63790700	2.40410700
C	2.23380100	-0.01333500	1.84498000
C	1.20374000	1.88513700	3.06089700
C	3.46434100	0.65298700	1.91288600
C	2.46300000	2.49691300	3.10530400
C	3.57959100	1.89571200	2.52947000
H	4.34844400	0.18152700	1.49443900
H	2.57234100	3.45410800	3.60553500
H	4.54616200	2.38901200	2.57812900
C	-2.10846200	-3.30062400	0.23553600
C	-1.61597900	-3.56313600	-1.20101400

C	-2.45562900	-4.62310000	0.94860500
H	-1.27643800	-2.84652300	0.78447400
H	-1.37555000	-2.62581700	-1.71728900
H	-0.71820200	-4.19154000	-1.18692400
H	-2.37133000	-4.08205600	-1.80112700
H	-2.76122300	-4.44999700	1.98613400
H	-3.27545900	-5.14515600	0.44293900
H	-1.58758100	-5.29187700	0.95736300
C	2.17149000	-1.41646100	1.24757000
C	2.93376500	-2.42316500	2.13398400
C	2.69040600	-1.45875800	-0.20208600
H	1.12430300	-1.73491400	1.22479400
H	2.54294100	-2.43051600	3.15722700
H	2.84127300	-3.43657800	1.72715600
H	4.00075400	-2.18014600	2.18676100
H	2.13913200	-0.75837800	-0.84089900
H	3.75206200	-1.19595000	-0.26444900
H	2.57809300	-2.46789700	-0.61556000
C	-4.42242900	0.97586500	1.96048800
C	-5.24288900	0.72617700	3.24397900
C	-4.95220800	2.21579300	1.21586900
H	-3.39406300	1.19891700	2.26513300
H	-4.84529300	-0.11546800	3.82174000
H	-5.22948700	1.61401300	3.88611800
H	-6.28792800	0.49988900	3.00413200
H	-4.38952900	2.40618300	0.29554100
H	-6.00895200	2.11286800	0.94707900
H	-4.86588000	3.10064300	1.85608900
C	0.01745600	2.54312500	3.76544000
C	-0.18164500	4.01712200	3.36610100
C	0.16269800	2.42253200	5.29797100
H	-0.89360100	2.00864600	3.47609500
H	-0.31367000	4.12885700	2.28571500
H	-1.07337900	4.41857100	3.86023000
H	0.66528900	4.64246200	3.66833700
H	0.26655400	1.38059800	5.62023400
H	1.04614600	2.96562700	5.65198300
H	-0.71482400	2.84585000	5.79930900
H	-2.66133200	-1.71944400	3.65005800
H	-0.17625100	-0.72998600	4.41229000
C	-2.56049500	1.00521300	-4.13731700
C	-1.51755300	1.40790600	-3.10342200
H	-3.06071800	1.90297700	-4.51663300
H	-2.11944000	0.49118700	-4.99667500

H	-0.71736000	1.98674800	-3.57698100
O	-0.87746500	0.22182800	-2.51729000
C	0.09031800	-0.43316400	-3.35133000
H	0.48797900	-1.27477900	-2.78202900
H	-0.38799800	-0.80907100	-4.25983900
H	0.90083200	0.25719600	-3.60959400
H	-3.31741300	0.35407400	-3.68709600
C	-1.21516200	2.13291400	-0.65240200
C	-2.10035400	2.16687200	-1.91114100
H	-1.83769800	2.35829100	0.21843400
H	-3.07474900	1.72726400	-1.66436100
H	-2.30073800	3.20353400	-2.21965500
C	0.05120500	2.99994100	-0.58056400
C	1.20397200	2.66942000	-1.55200700
C	-0.30886500	4.50788800	-0.69869000
H	0.45335700	2.85300700	0.43127400
C	2.43158400	3.55857800	-1.29267200
H	0.88063800	2.82257400	-2.59103500
H	1.48301300	1.61215900	-1.45347900
C	0.91487800	5.40673000	-0.45448500
H	-0.70458000	4.71086400	-1.70414400
H	-1.11027800	4.75994500	0.00849500
C	2.07668700	5.04915300	-1.39188500
H	3.22833600	3.30893300	-2.00446000
H	2.82631900	3.34073800	-0.29020000
H	0.62993900	6.45828900	-0.58211200
H	1.24275700	5.29615700	0.58895100
H	2.95386800	5.66511700	-1.16019500
H	1.79449400	5.28683500	-2.42823800

### INT5

Ni	-0.35940800	1.23478800	-1.49617600
C	0.03913400	-1.40990100	1.85564500
C	0.83927000	-0.40929700	2.28873100
N	0.84560900	0.55804700	1.29081500
N	-0.43821700	-1.02714200	0.60880900
C	0.04832500	0.19684400	0.22824500
C	-1.29449500	-1.91388000	-0.15192900
C	-2.65333000	-2.01562200	0.21779000
C	-0.70795700	-2.73514500	-1.13643600
C	-3.43481700	-2.95692300	-0.46449800
C	-1.54337200	-3.64642400	-1.79489800
C	-2.89062500	-3.75825400	-1.46550000
H	-4.48178900	-3.07162800	-0.20052500

H	-1.12519500	-4.29400600	-2.55944700
H	-3.51631400	-4.48334100	-1.97835000
C	1.66955900	1.74410700	1.41898900
C	3.05473900	1.63174700	1.15759100
C	1.07807600	2.94070800	1.88323200
C	3.83629300	2.78383500	1.32012600
C	1.91118600	4.05909000	2.01993000
C	3.27277100	3.98618100	1.73563500
H	4.90252400	2.73597000	1.12423300
H	1.49275500	4.99747800	2.36672100
H	3.89817100	4.86655200	1.85294500
C	0.78726300	-2.72570100	-1.44369200
C	1.07924900	-2.45380600	-2.93074700
C	1.44782800	-4.04059900	-0.98002900
H	1.24762500	-1.91329600	-0.87321200
H	0.62641300	-1.51048700	-3.25075600
H	2.16142500	-2.40177300	-3.09924600
H	0.68764200	-3.25186000	-3.57184200
H	1.28107400	-4.21829200	0.08815000
H	1.04974800	-4.90256600	-1.52702800
H	2.52949300	-4.00616300	-1.15372500
C	3.73006700	0.31652500	0.76700800
C	4.43184300	-0.31745100	1.98858900
C	4.74145000	0.46906900	-0.38676400
H	2.95444500	-0.38218400	0.43322600
H	3.73752600	-0.49858900	2.81507800
H	4.88459500	-1.27622000	1.71240000
H	5.22806000	0.33675900	2.36116100
H	4.30319200	0.96432400	-1.25933000
H	5.62157100	1.04598800	-0.08308800
H	5.09750300	-0.51872000	-0.69895400
C	-3.26789600	-1.20337300	1.35718400
C	-3.51719500	-2.09490400	2.59260600
C	-4.57019500	-0.48999000	0.94832800
H	-2.55293800	-0.42640400	1.64759100
H	-2.59796400	-2.57782600	2.94107400
H	-3.91934600	-1.49869900	3.41943100
H	-4.24031600	-2.88657600	2.36631900
H	-4.41845200	0.16094300	0.08146400
H	-5.36566300	-1.20069200	0.69903700
H	-4.93372900	0.12778500	1.77706300
C	-0.38843200	3.01892100	2.30228800
C	-1.03769900	4.38048700	1.99943700
C	-0.53452900	2.68588700	3.80400600

H	-0.94221000	2.26009600	1.73885900
H	-0.89690100	4.67771500	0.95467600
H	-2.11359400	4.32726900	2.19574200
H	-0.63695500	5.17749200	2.63523800
H	-0.15066100	1.68820100	4.04036300
H	0.01231500	3.41097400	4.41755900
H	-1.58901600	2.71998600	4.10053600
H	-0.23367600	-2.35090000	2.30525100
H	1.40229800	-0.29062400	3.20013800
C	-4.10342300	-0.42079600	-3.23739700
C	-2.88848600	0.43324900	-3.59839400
H	-5.01066600	0.18590200	-3.15787800
H	-4.28563400	-1.16751800	-4.01655300
H	-3.11347900	1.01050600	-4.50917900
O	-1.73957800	-0.37474400	-3.85169300
C	-1.71539100	-0.97782600	-5.13609100
H	-0.75848900	-1.49618800	-5.22469300
H	-2.52313100	-1.70938300	-5.26936500
H	-1.79103000	-0.22208900	-5.93267200
H	-3.94594200	-0.95190300	-2.29444500
C	-1.21384900	2.17963600	-2.92003600
C	-2.45984600	1.46081100	-2.51347300
H	-0.83781000	1.91525900	-3.90694700
H	-1.17457200	3.25224000	-2.72257000
H	-2.17586500	0.79104000	-1.60077300
C	-3.61606600	2.35031300	-1.97196900
C	-3.20547100	3.18151500	-0.74338900
C	-4.21677100	3.26596900	-3.06189500
H	-4.41284900	1.67227000	-1.63788800
C	-4.38454000	4.00290400	-0.19549200
H	-2.39247800	3.86987000	-1.01214200
H	-2.80992700	2.51673200	0.03796300
C	-5.38782500	4.10163300	-2.51805100
H	-3.43212200	3.93756400	-3.43929400
H	-4.55886700	2.67348300	-3.91918700
C	-4.98238700	4.91158600	-1.27928200
H	-4.05536400	4.60074600	0.66297900
H	-5.16106500	3.31978900	0.17802300
H	-5.76184300	4.76711000	-3.30529600
H	-6.21982200	3.43148700	-2.25697800
H	-5.84670800	5.45699500	-0.88229600
H	-4.23900400	5.66939300	-1.56724500
C	1.56665300	1.53280700	-2.23384000
C	1.49294800	2.83994100	-1.78996400

H	1.60144000	1.30268700	-3.29377300
H	2.01913600	0.80798600	-1.56934300
H	1.57556200	3.08187400	-0.73592100
O	1.37807200	3.94634400	-2.51238400
C	1.57564100	3.88975400	-3.93793200
H	1.57966100	4.92744700	-4.26943200
H	2.53776100	3.41854300	-4.16278600
H	0.76477200	3.34617200	-4.42516100

### INT6

Ni	-0.45170300	1.24611100	-1.17274900
C	0.12391600	-1.48915800	1.88556000
C	0.95062800	-0.50473800	2.30714100
N	0.90545100	0.50038500	1.34483500
N	-0.42937100	-1.06457600	0.68236900
C	0.04526800	0.16748700	0.33040700
C	-1.39295900	-1.87486000	-0.03380000
C	-2.72680300	-1.88656500	0.42700600
C	-0.94359100	-2.69360500	-1.09029700
C	-3.62479600	-2.73982800	-0.22638300
C	-1.88784300	-3.52650300	-1.70477800
C	-3.21356100	-3.55066900	-1.28108700
H	-4.65801400	-2.77978500	0.10476100
H	-1.57573500	-4.17595400	-2.51707500
H	-3.92617900	-4.21145000	-1.76666000
C	1.72501700	1.69346800	1.43413000
C	3.11697400	1.56986100	1.21811800
C	1.11588500	2.91599000	1.79893200
C	3.89017700	2.73459600	1.32611300
C	1.94087700	4.04522600	1.87633900
C	3.31066900	3.96029500	1.63674700
H	4.96216800	2.67759900	1.16654700
H	1.51032900	5.00337400	2.14492000
H	3.92930500	4.85022200	1.70963600
C	0.51283300	-2.74449700	-1.54256700
C	0.65750700	-2.51348100	-3.05900700
C	1.17334200	-4.07311500	-1.12019800
H	1.05445900	-1.93758300	-1.03906700
H	0.17269000	-1.58104200	-3.36720900
H	1.71818000	-2.46294400	-3.33175300
H	0.21355600	-3.33178200	-3.63700200
H	1.12476600	-4.21853500	-0.03532200
H	0.67981400	-4.92952600	-1.59325600
H	2.22809300	-4.08778400	-1.41797000

C	3.81521700	0.23888800	0.93248900
C	4.55861500	-0.26306600	2.19018800
C	4.79448800	0.30819300	-0.25624800
H	3.05214000	-0.50644100	0.68177700
H	3.89015200	-0.36968300	3.05087600
H	5.01916400	-1.23825000	1.99687400
H	5.35421200	0.43377300	2.47692100
H	4.31007400	0.67496400	-1.16614900
H	5.64901300	0.95962100	-0.04424500
H	5.19433700	-0.69055600	-0.46328900
C	-3.20288000	-1.05670600	1.61726100
C	-3.47989000	-1.95665900	2.84000400
C	-4.44222000	-0.20792700	1.27959500
H	-2.40401000	-0.36089000	1.89207300
H	-2.59477500	-2.53399100	3.12898000
H	-3.78290800	-1.34943200	3.70037800
H	-4.28583800	-2.66929700	2.63163500
H	-4.25116700	0.44544400	0.42236000
H	-5.31336500	-0.82947500	1.04516800
H	-4.71044800	0.42157200	2.13557200
C	-0.35698300	3.00884600	2.19598100
C	-0.99528100	4.37147200	1.87594500
C	-0.52114200	2.68638000	3.69822800
H	-0.91066400	2.25346600	1.62965300
H	-0.83601900	4.66224200	0.83173300
H	-2.07484200	4.32311900	2.05391600
H	-0.60280300	5.17127700	2.51361700
H	-0.14392600	1.68831300	3.94477100
H	0.02272000	3.41262500	4.31320600
H	-1.57861400	2.72705100	3.98355800
H	-0.12681600	-2.44423900	2.31833900
H	1.56700300	-0.41989700	3.18715900
C	-3.16262000	-0.24574200	-3.43083500
C	-2.42770800	1.03955900	-3.83251600
H	-4.21774100	-0.05210400	-3.21808300
H	-3.12555000	-0.97162400	-4.24795900
H	-2.98157300	1.51835900	-4.65729100
O	-1.10875100	0.75609400	-4.29959700
C	-1.05675000	0.30031500	-5.64621600
H	-0.00089900	0.16608900	-5.89280400
H	-1.57114300	-0.65947400	-5.78177300
H	-1.49591300	1.03847500	-6.33289600
H	-2.70276700	-0.69459200	-2.54690900
C	-1.20108100	2.78929300	-2.52938500

C	-2.35513900	2.08361200	-2.71715400
H	-0.40919300	2.70239500	-3.25474900
H	-1.16910200	3.64081900	-1.85621800
H	-1.74844100	1.02384900	-0.54563200
C	-3.67019400	2.42922600	-2.02852500
C	-3.54607300	3.40730800	-0.84667800
C	-4.67850200	3.00442300	-3.06953900
H	-4.10528300	1.49657100	-1.64586400
C	-4.90967900	3.70084800	-0.20110400
H	-3.11583700	4.35566100	-1.19831400
H	-2.85232500	2.99911500	-0.10277000
C	-6.03960300	3.32114600	-2.42814800
H	-4.25071300	3.91887000	-3.50466700
H	-4.82899900	2.30152500	-3.89643200
C	-5.90677300	4.26120200	-1.22387800
H	-4.77694600	4.40652700	0.62817900
H	-5.31470300	2.77753400	0.23739000
H	-6.70128400	3.75812600	-3.18563100
H	-6.51193000	2.38117600	-2.10708200
H	-6.88599000	4.41889900	-0.75663600
H	-5.56047100	5.24687900	-1.56684500
C	1.62971000	1.10430500	-2.20539900
C	1.93452200	2.42213500	-2.05287100
H	1.39626000	0.67047700	-3.17068900
H	1.90914000	0.42509900	-1.41225700
H	2.20637100	2.83750400	-1.08687700
O	1.94747600	3.37227700	-2.99009100
C	1.96272200	2.97871400	-4.37360200
H	2.10194800	3.90101900	-4.93692600
H	2.79825700	2.29418000	-4.55455800
H	1.02327400	2.50178300	-4.66614600

#### INT7

Ni	-1.81915600	1.02074500	-0.70892900
C	-1.31434400	-0.17674800	3.24439400
C	-0.14826500	0.41927700	2.89270600
N	-0.31731000	0.85878200	1.58708000
N	-2.17003900	-0.08991400	2.14924500
C	-1.56001200	0.54847700	1.11114900
C	-3.51360900	-0.63577500	2.19318500
C	-4.54533000	0.16674300	2.72274400
C	-3.71327100	-1.96669100	1.77377600
C	-5.82253400	-0.40345700	2.80123800
C	-5.01272500	-2.48074400	1.87417700

C	-6.05678900	-1.70960600	2.37869200
H	-6.64265600	0.17984000	3.20801300
H	-5.20608300	-3.50337600	1.56557800
H	-7.05462500	-2.13231500	2.45423000
C	0.67772500	1.56195600	0.80652000
C	1.57918600	0.80786000	0.02044700
C	0.73403700	2.97187700	0.90035900
C	2.54812000	1.51836700	-0.70126600
C	1.72332100	3.62386500	0.15313100
C	2.62164400	2.90762500	-0.63646300
H	3.26412500	0.97398800	-1.30932200
H	1.79973800	4.70593600	0.20062600
H	3.38862700	3.43534600	-1.19648700
C	-2.58022800	-2.86004100	1.27461700
C	-2.89825500	-3.51515800	-0.08287600
C	-2.22595900	-3.92997100	2.32882400
H	-1.69176900	-2.23697100	1.12932000
H	-3.14166000	-2.76581000	-0.84420300
H	-2.03297900	-4.08851500	-0.43405700
H	-3.74279700	-4.20936800	-0.01442700
H	-1.94417900	-3.47564800	3.28526400
H	-3.07431700	-4.59789100	2.51595300
H	-1.38575900	-4.54350200	1.98435900
C	1.55898900	-0.71724600	-0.03468800
C	2.82721000	-1.30949200	0.61349300
C	1.37768500	-1.23872200	-1.47367700
H	0.70090200	-1.06949800	0.54623700
H	2.94134100	-0.97590600	1.65070600
H	2.77711500	-2.40383100	0.61223500
H	3.73074300	-1.01586900	0.06766100
H	0.46261500	-0.84210900	-1.92948500
H	2.22183800	-0.96338200	-2.11590800
H	1.30913700	-2.33207700	-1.47206500
C	-4.30758500	1.57981600	3.25151500
C	-4.30831500	1.58906700	4.79507400
C	-5.32251700	2.60227600	2.70639200
H	-3.31540000	1.90564100	2.92092900
H	-3.55343800	0.90936000	5.20552000
H	-4.09731600	2.59627400	5.17173400
H	-5.28269100	1.27984200	5.18977500
H	-5.34066300	2.61204200	1.61136800
H	-6.33979900	2.39598400	3.05609800
H	-5.05934800	3.60860400	3.05061100
C	-0.21986100	3.78500600	1.77142600

C	-1.14698900	4.66877900	0.91282000
C	0.54264200	4.62786400	2.81291200
H	-0.85798100	3.08777900	2.32306000
H	-1.74255800	4.06230200	0.21995200
H	-1.83867000	5.22702500	1.55328000
H	-0.57769100	5.39757200	0.32434400
H	1.18864000	4.00398300	3.44011500
H	1.17158900	5.38826800	2.33730800
H	-0.16582900	5.14771700	3.46681800
H	-1.62220500	-0.65396000	4.16103100
H	0.77050700	0.57307500	3.43676100
C	-3.49382400	0.31549100	-3.28649400
H	-3.14739700	-0.67260900	-2.95879500
C	-3.71124000	0.74472100	-0.79482900
C	-4.30985800	1.00794300	-2.17190500
H	-3.82206000	-0.29731000	-0.48483800
H	-4.11202700	1.39949400	-0.01785300
H	-4.27735100	2.09171400	-2.36296300
C	-2.31294600	1.15761700	-3.72837700
H	-1.66638600	0.62929000	-4.44014900
H	-2.65891100	2.09008100	-4.19406400
H	-4.11289300	0.15164600	-4.17774800
O	-1.50816900	1.52132300	-2.58148400
C	-0.51870200	2.51936300	-2.88443700
H	0.04791000	2.71558000	-1.97453800
H	0.15506900	2.14460300	-3.66246100
H	-1.00828000	3.43847000	-3.22611600
C	-5.82530900	0.61939800	-2.25344400
C	-6.11799400	-0.88552400	-2.08534100
C	-6.70312800	1.44405100	-1.29253600
H	-6.12967000	0.89421500	-3.27732800
C	-7.61271300	-1.18975500	-2.28852900
H	-5.82452500	-1.21122800	-1.07745900
H	-5.52327300	-1.47663900	-2.79417000
C	-8.19764800	1.14574900	-1.49524800
H	-6.43275700	1.20880500	-0.25335900
H	-6.50903100	2.51645100	-1.43536700
C	-8.49256200	-0.35423900	-1.34737600
H	-7.79817300	-2.26011300	-2.13535300
H	-7.88803900	-0.97271000	-3.33090600
H	-8.79502700	1.72554100	-0.78083000
H	-8.50189200	1.47912400	-2.49804800
H	-9.55319400	-0.55438800	-1.54167500
H	-8.30042900	-0.65935700	-0.30775400

**INT7'**

Ni	-2.68063700	0.37759700	-0.72812900
C	-0.27502000	-0.58684400	2.50452000
C	0.55884500	0.14565900	1.72435500
N	-0.20201900	0.61473100	0.66428600
N	-1.52944400	-0.54692800	1.90921000
C	-1.49950700	0.18744200	0.75581900
C	-2.68099000	-1.20401000	2.49683400
C	-3.27653200	-0.61155500	3.63167200
C	-3.11014000	-2.43858600	1.96493900
C	-4.36053700	-1.28373500	4.21140000
C	-4.20217800	-3.05904000	2.58506900
C	-4.82524200	-2.48820400	3.69194400
H	-4.84317400	-0.86038700	5.08667200
H	-4.56047900	-4.01153000	2.20833500
H	-5.66592200	-2.99231300	4.16001600
C	0.33660900	1.43581500	-0.40181200
C	0.85605500	0.79841300	-1.54763300
C	0.36377800	2.83580400	-0.22437200
C	1.38627600	1.61778700	-2.55295300
C	0.90809400	3.60204300	-1.26279200
C	1.40855900	3.00304900	-2.41674200
H	1.79995000	1.16359800	-3.44820500
H	0.94990100	4.68205300	-1.16311100
H	1.83091500	3.61823600	-3.20621600
C	-2.38214900	-3.14555400	0.82382700
C	-3.33840600	-3.77348400	-0.20666100
C	-1.41488300	-4.21075000	1.38397100
H	-1.77733800	-2.40395100	0.29082900
H	-4.07059400	-3.04488800	-0.57393900
H	-2.76828100	-4.15584600	-1.06119500
H	-3.89515900	-4.61959000	0.20942500
H	-0.68021500	-3.76844300	2.06562300
H	-1.96188200	-4.98230600	1.93740700
H	-0.86949500	-4.70151700	0.56970400
C	0.90233900	-0.71934500	-1.70638400
C	2.35412400	-1.23628200	-1.63423900
C	0.21735100	-1.19049400	-3.00392600
H	0.35682200	-1.16994600	-0.87033000
H	2.83542800	-0.94833500	-0.69333600
H	2.37461500	-2.32955100	-1.70547100
H	2.96012000	-0.83522800	-2.45435200
H	-0.81552900	-0.82791000	-3.06374500

H	0.74653000	-0.83571400	-3.89506600
H	0.20142100	-2.28544500	-3.04715400
C	-2.76264900	0.67743500	4.27291200
C	-2.03056400	0.37111500	5.59743800
C	-3.87673800	1.71412400	4.51022900
H	-2.03764200	1.13681800	3.59262300
H	-1.19889500	-0.32774200	5.45565300
H	-1.62737600	1.29225400	6.03272500
H	-2.71361200	-0.07507000	6.32884600
H	-4.40547200	1.95731100	3.58387400
H	-4.61601000	1.36158600	5.23746900
H	-3.44507300	2.63887800	4.90899200
C	-0.11661300	3.51416400	1.05639000
C	-1.03262800	4.72285700	0.78845000
C	1.08503300	3.93145200	1.93122000
H	-0.70308000	2.78641400	1.62733100
H	-1.88668000	4.45147000	0.15851000
H	-1.42003200	5.11380100	1.73566800
H	-0.49782300	5.54189700	0.29563800
H	1.71852400	3.07467900	2.18605700
H	1.71173900	4.66555200	1.41244200
H	0.73790000	4.38555000	2.86602400
H	-0.09916400	-1.12830100	3.42012200
H	1.60897900	0.37229600	1.81954500
C	-3.21751100	2.72304800	-2.44669900
H	-2.17636200	2.75651500	-2.10335900
C	-3.87455100	1.77011700	-0.08428200
C	-4.19803600	2.71747100	-1.25591600
H	-5.19891800	2.50272800	-1.65050400
H	-4.24527300	3.73826900	-0.85269700
C	-3.43712700	1.52654000	-3.35682500
H	-4.43953800	1.56120500	-3.80310900
H	-2.69365600	1.46892200	-4.16110900
O	-3.34981900	0.31300500	-2.57180300
C	-3.88578500	-0.84663100	-3.22893800
H	-3.36856000	-1.00303900	-4.18185000
H	-3.71608800	-1.70160800	-2.57447200
H	-4.95943200	-0.71683000	-3.40191800
H	-3.37779400	3.62158100	-3.05587600
C	-5.08916400	1.14112100	0.61154400
C	-6.05645700	2.23888600	1.13997500
C	-5.87583500	0.12190100	-0.24162600
H	-4.71483100	0.59903600	1.48929800
C	-7.24193600	1.63472500	1.91046900

H	-6.44415800	2.82241300	0.29388800
H	-5.50774000	2.94405000	1.77829300
C	-7.07258700	-0.47139200	0.52035400
H	-6.23715800	0.60220500	-1.16307400
H	-5.20336700	-0.68950300	-0.55182800
C	-8.01057700	0.62097300	1.05181400
H	-7.90992100	2.43772800	2.24577400
H	-6.87090000	1.13600700	2.81737900
H	-7.62186200	-1.16257300	-0.13133400
H	-6.69600900	-1.06742800	1.36378800
H	-8.82552400	0.17139500	1.63179000
H	-8.48111300	1.14306400	0.20571000
H	-3.25425600	2.28909300	0.65272400

#### INT8

Ni	-1.46963200	0.47045800	-0.45504300
C	-1.50031400	-0.27585600	3.46157800
C	-0.35139300	0.44364100	3.53716800
N	-0.05425000	0.88705500	2.25042700
N	-1.88021600	-0.25366900	2.12708500
C	-0.99734900	0.45777300	1.37047300
C	-3.02246500	-0.91172900	1.52840200
C	-4.25058100	-0.21310800	1.46228600
C	-2.86264400	-2.23219800	1.04633400
C	-5.33096400	-0.87387000	0.86532400
C	-3.98207800	-2.83836300	0.45851700
C	-5.20036900	-2.16900300	0.36734900
H	-6.29117500	-0.37146000	0.800111000
H	-3.90115200	-3.85446200	0.08438000
H	-6.05677700	-2.66392900	-0.08203200
C	1.14482300	1.64087800	1.94056200
C	2.28996600	0.93086500	1.52635000
C	1.12511500	3.04081600	2.10822900
C	3.43733400	1.68182200	1.23773400
C	2.30613400	3.73528200	1.81769300
C	3.44706300	3.06707700	1.37958000
H	4.33892900	1.17170100	0.91186900
H	2.33383900	4.81377400	1.93778900
H	4.35081900	3.62773800	1.15832500
C	-1.55991000	-3.01705500	1.18054300
C	-0.99642400	-3.43711000	-0.19103800
C	-1.74465200	-4.23942300	2.10316000
H	-0.81450000	-2.36760400	1.64965400
H	-0.79905800	-2.56549500	-0.82673300

H	-0.05211700	-3.97671600	-0.06077100
H	-1.68387400	-4.10070900	-0.72769300
H	-2.11426100	-3.94460700	3.09133800
H	-2.45581500	-4.95851700	1.68199900
H	-0.78888400	-4.75733100	2.23859900
C	2.32789800	-0.59010500	1.40012600
C	3.41164400	-1.20393900	2.30879200
C	2.51142600	-1.03404300	-0.06421500
H	1.36487300	-0.98572300	1.73882000
H	3.26892900	-0.91461600	3.35574800
H	3.37804600	-2.29757200	2.25057300
H	4.41736000	-0.88866000	2.01013100
H	1.71294200	-0.64325900	-0.70406000
H	3.47029300	-0.68925200	-0.46815900
H	2.50036600	-2.12807400	-0.13234900
C	-4.43803400	1.18762800	2.03692900
C	-5.40555400	1.16500200	3.23830900
C	-4.90903800	2.19024100	0.96564400
H	-3.46897900	1.53844100	2.40548600
H	-5.05895000	0.48110300	4.02086700
H	-5.48932500	2.16609600	3.67514100
H	-6.41025800	0.84667100	2.93866800
H	-4.20714800	2.23212000	0.12483100
H	-5.89601800	1.92714400	0.56909700
H	-4.98445000	3.19438600	1.39716700
C	-0.10021300	3.79644000	2.61676200
C	-0.46051200	5.00395600	1.73055000
C	0.09967900	4.23886600	4.08170500
H	-0.95617100	3.11327300	2.59298200
H	-0.59533300	4.70901100	0.68416700
H	-1.39353300	5.45922000	2.08050800
H	0.31206500	5.77965200	1.76267100
H	0.29622100	3.38505200	4.73974000
H	0.94603300	4.92888700	4.17262100
H	-0.79462800	4.75274500	4.45175800
H	-2.07194100	-0.79314100	4.21630300
H	0.28691700	0.67856500	4.37409000
C	-2.70294300	2.48432300	-3.35621300
C	-1.68134900	1.36646700	-3.19117400
H	-2.34604800	3.21232700	-4.09241900
H	-3.66041100	2.09434400	-3.71530500
H	-1.48959800	0.85922000	-4.14237600
O	-2.18442300	0.35807800	-2.25731000
C	-2.99668600	-0.68457400	-2.81249100

H	-3.32639500	-1.31124000	-1.98218900
H	-3.87119300	-0.25804600	-3.31389900
H	-2.40852400	-1.27887000	-3.52001800
H	-2.87843700	3.00501900	-2.40927100
C	-0.45933200	1.95907500	-1.07721600
C	-0.34329500	1.80565700	-2.59482800
H	0.51407400	2.00217800	-0.59060900
H	-1.05980300	2.82818100	-0.78316400
H	-0.06401200	2.77358700	-3.04903400
O	0.61744400	0.82352400	-2.95944500
C	1.95206500	1.30671000	-3.01828000
H	2.57318000	0.47112800	-3.34699200
H	2.04306900	2.12865500	-3.74390500
H	2.31280700	1.65403300	-2.04036100

#### INT8'

Ni	-1.42899500	0.28351400	-0.64943500
C	-2.08195500	-0.62395700	3.22365000
C	-0.88991500	-0.01610600	3.44713100
N	-0.45196400	0.49456300	2.22794400
N	-2.34954900	-0.47611800	1.86988400
C	-1.34743700	0.20662100	1.23691500
C	-3.46377800	-1.07655900	1.16320300
C	-4.66397500	-0.34435100	1.02637300
C	-3.30559400	-2.38679800	0.65777200
C	-5.70896300	-0.95276600	0.32061000
C	-4.38501600	-2.93837700	-0.04698400
C	-5.57046700	-2.22964800	-0.21956600
H	-6.64788600	-0.42324900	0.19681100
H	-4.30112400	-3.94497600	-0.44578000
H	-6.39730700	-2.68009700	-0.76134300
C	0.85287900	1.10874100	2.05929000
C	1.91290700	0.30603500	1.58681700
C	1.02793500	2.46127300	2.43073300
C	3.16537000	0.91669300	1.43565800
C	2.30638200	3.01017200	2.26880400
C	3.36171200	2.25317400	1.76615400
H	4.00204200	0.32895000	1.07024900
H	2.48020900	4.04561200	2.54144000
H	4.34283800	2.70382000	1.64687300
C	-2.05684400	-3.23319500	0.89986700
C	-1.38713700	-3.67875400	-0.41369000
C	-2.38621500	-4.44968300	1.79033600
H	-1.32675600	-2.62591300	1.44328100

H	-1.07933200	-2.81672900	-1.01765700
H	-0.49166400	-4.27259600	-0.19927400
H	-2.05477900	-4.29903700	-1.02213100
H	-2.83375900	-4.14065800	2.74121500
H	-3.08943900	-5.12988200	1.29724600
H	-1.47441900	-5.01514700	2.01187500
C	1.77699900	-1.18788900	1.30374800
C	2.62181400	-2.01085100	2.29876900
C	2.13864900	-1.54266900	-0.15092200
H	0.73229600	-1.47493100	1.45274100
H	2.34802300	-1.78854100	3.33591400
H	2.47084300	-3.08299700	2.12929500
H	3.69158200	-1.80351500	2.18528600
H	1.48643400	-1.01698400	-0.85753500
H	3.17633900	-1.28356900	-0.38829600
H	2.02120000	-2.61933400	-0.31817600
C	-4.86429100	1.02577900	1.66629300
C	-5.63770800	0.89086100	2.99611100
C	-5.56800000	2.02776100	0.73259100
H	-3.87567800	1.43508000	1.90160800
H	-5.12157400	0.22950300	3.70066600
H	-5.75121600	1.87072100	3.47321500
H	-6.63936800	0.47993700	2.82644300
H	-5.05835700	2.10793500	-0.23370100
H	-6.60934200	1.74754600	0.54112700
H	-5.58383100	3.02052300	1.19577400
C	-0.09168600	3.30823600	3.03396600
C	-0.07211000	4.77098800	2.54875500
C	-0.03341700	3.28560500	4.57770200
H	-1.04900200	2.87013600	2.72753300
H	0.01768800	4.84472500	1.46019200
H	-0.99467200	5.27698100	2.85314900
H	0.75955700	5.33332900	2.98686300
H	-0.12102500	2.27305600	4.98280300
H	0.91423800	3.70534600	4.93339400
H	-0.84762500	3.88638600	4.99830800
H	-2.75098700	-1.14753500	3.88833400
H	-0.30636800	0.08871300	4.34725100
C	-1.41502900	1.73754700	-4.34843300
C	-0.61891200	0.86694200	-3.38156200
H	-0.72364800	2.40247300	-4.87702300
H	-1.92735300	1.13875800	-5.10757600
H	0.05041700	0.20567500	-3.94800700
O	-1.48490900	-0.00794900	-2.58699200

C	-2.30378100	-0.94406400	-3.29845100
H	-2.78898100	-1.57262600	-2.54979000
H	-3.06586400	-0.42680500	-3.88782800
H	-1.67973600	-1.56445200	-3.95246100
H	-2.14356500	2.35157200	-3.81455600
C	-0.66094700	1.98800900	-1.09760300
C	0.18175100	1.64363900	-2.32502900
H	1.03607800	1.04665200	-1.98984200
O	-1.70050100	2.83357300	-1.44570200
C	-2.26953000	3.60559000	-0.39413900
H	-2.65998000	2.95956200	0.40101700
H	-1.52731400	4.29443700	0.02496200
H	-3.08730600	4.17849900	-0.83410600
H	-0.06709600	2.36763100	-0.25941800
H	0.58155200	2.56598900	-2.76828200

#### INT9

Ni	-0.93976700	0.82179400	-0.95873300
C	-0.77047400	-0.09115100	3.10714900
C	0.35401100	0.64920400	2.96542000
N	0.41411800	1.03836500	1.63329500
N	-1.39150900	-0.12611800	1.86244900
C	-0.66574800	0.57124900	0.93656800
C	-2.63454800	-0.83955900	1.64673500
C	-3.82317700	-0.29638400	2.18758200
C	-2.59870900	-2.07939100	0.97310700
C	-5.00603500	-1.02094900	1.99077900
C	-3.81747100	-2.74875400	0.79754800
C	-5.00834000	-2.22695900	1.29400300
H	-5.93777800	-0.63774100	2.39468900
H	-3.82884800	-3.70555900	0.28470900
H	-5.93839800	-2.77079100	1.15506400
C	1.54749100	1.76200400	1.09156800
C	2.71693700	1.03027000	0.78931500
C	1.46837100	3.16426700	0.96502700
C	3.81684900	1.75164800	0.30847700
C	2.60012700	3.82998600	0.47528600
C	3.75985300	3.13384800	0.14561700
H	4.73600400	1.22507200	0.07125000
H	2.57948500	4.91026500	0.37021400
H	4.62887900	3.67227700	-0.22189300
C	-1.30481600	-2.74785300	0.51446700
C	-1.34686900	-3.16241800	-0.96776500
C	-0.97850100	-3.95704500	1.41645700

H	-0.48735400	-2.02989200	0.62047500
H	-1.55711500	-2.30274700	-1.61335500
H	-0.38008200	-3.58295400	-1.26642200
H	-2.10869800	-3.92570800	-1.16064100
H	-0.89767000	-3.66213200	2.46854500
H	-1.75360800	-4.72830800	1.34498700
H	-0.02665700	-4.40927600	1.11603600
C	2.84454200	-0.47324900	1.02938900
C	3.73205600	-0.75017000	2.26207800
C	3.37848000	-1.23542100	-0.19720000
H	1.84836900	-0.87339600	1.24333600
H	3.34655200	-0.25770800	3.16150900
H	3.78310500	-1.82647200	2.46098800
H	4.75413100	-0.38961300	2.10053300
H	2.74281200	-1.07785900	-1.07410900
H	4.39786900	-0.93203700	-0.45918800
H	3.40375500	-2.31004800	0.01522800
C	-3.86352300	0.99900300	2.99997700
C	-4.06683300	0.69441900	4.50029000
C	-4.94425300	1.98444000	2.51302000
H	-2.89722500	1.50363000	2.89350500
H	-3.29095300	0.02992400	4.89546100
H	-4.04702700	1.62197100	5.08298800
H	-5.03400500	0.20951700	4.67380200
H	-4.82489600	2.23088000	1.45359900
H	-5.95469900	1.58648300	2.65539400
H	-4.87989700	2.91580900	3.08644600
C	0.25029500	3.97027800	1.40682200
C	-0.22622500	4.96144300	0.32862800
C	0.53539100	4.70277000	2.73519900
H	-0.57107900	3.27127600	1.59579000
H	-0.41310200	4.45642500	-0.62569700
H	-1.15454300	5.44890600	0.64702800
H	0.50951000	5.75241100	0.14817500
H	0.82052500	4.00127000	3.52688000
H	1.35062400	5.42600300	2.62176600
H	-0.35412100	5.24850100	3.06977500
H	-1.19110500	-0.59233700	3.96373000
H	1.11567600	0.93216900	3.67418600
C	-0.95812300	0.35922400	-3.09128400
C	-0.38860100	1.59830800	-3.02915600
H	-2.03180500	0.24310700	-3.19982800
H	-0.35957500	-0.53176900	-3.24682400
H	0.27662200	0.03657300	-0.92713200

C	-2.72970300	2.43131200	-0.79357600
C	-3.54308400	1.37810700	-1.03069000
H	-2.60338400	3.23225400	-1.51583300
H	-2.31444500	2.60509600	0.19429300
H	-3.68412700	0.65237200	-0.23178800
H	-1.05391800	2.46120800	-3.01712800
C	1.07415400	1.94345100	-3.18661300
C	1.96690600	0.75966700	-3.59609800
C	1.20408000	3.10182900	-4.21113400
H	1.43401400	2.33227700	-2.22023700
C	3.43041600	1.18947700	-3.78533600
H	1.58834800	0.33894300	-4.53923800
H	1.90523800	-0.03789400	-2.84598000
C	2.66849900	3.52670400	-4.39806800
H	0.79005900	2.77372900	-5.17561600
H	0.60009100	3.95894300	-3.88371100
C	3.55544000	2.33836200	-4.79621900
H	4.02701400	0.32854700	-4.11010200
H	3.83977600	1.50851600	-2.81626900
H	2.72750300	4.31940400	-5.15331200
H	3.03895300	3.95971800	-3.45742200
H	4.60096300	2.65815900	-4.88007700
H	3.25725500	1.98036000	-5.79222600
C	-4.40542100	1.13333400	-2.24341600
C	-5.88354100	1.00748400	-1.77857600
C	-4.28881100	2.17481400	-3.37027800
H	-4.13261200	0.14369100	-2.64870000
C	-6.81597400	0.67765700	-2.95453300
H	-6.19038700	1.95846800	-1.32036100
H	-5.96380000	0.23881100	-0.99981700
C	-5.22398000	1.84229800	-4.54555400
H	-4.54963100	3.16490800	-2.96898500
H	-3.25465800	2.24448300	-3.73093800
C	-6.68316900	1.70406000	-4.08848700
H	-7.85204800	0.63282600	-2.59829100
H	-6.57284600	-0.32445300	-3.33696700
H	-5.13631000	2.61798700	-5.31529000
H	-4.89706300	0.90171800	-5.01274300
H	-7.31845300	1.41767200	-4.93477000
H	-7.04847300	2.68077200	-3.73959100

#### INT10

Ni	-1.68377100	0.34867700	-0.54515400
C	-0.11134100	2.10036200	3.05847100

C	-1.35212700	2.64004400	3.00034800
N	-1.93329600	2.17003900	1.83035500
N	0.03274700	1.30109900	1.92992500
C	-1.09213400	1.32923500	1.14783300
C	1.26708400	0.59062400	1.66079900
C	1.52576300	-0.60476000	2.36852700
C	2.19220700	1.15921300	0.75847200
C	2.73890600	-1.25560900	2.10803000
C	3.38511400	0.45811200	0.53604200
C	3.65448200	-0.73814600	1.19573000
H	2.97321100	-2.17693000	2.63183900
H	4.12213000	0.86399300	-0.14945200
H	4.58931800	-1.25987000	1.01144200
C	-3.23750700	2.60744300	1.37723900
C	-3.33953100	3.88376000	0.77976700
C	-4.35399200	1.77030500	1.58597800
C	-4.60635000	4.28470900	0.33632600
C	-5.59404200	2.22486500	1.11676100
C	-5.71949100	3.46201000	0.48982600
H	-4.72532300	5.26029900	-0.12495800
H	-6.47681200	1.61005500	1.26122500
H	-6.69224600	3.79554900	0.13967000
C	1.97936900	2.52066500	0.10055000
C	2.31988600	2.52493300	-1.40081400
C	2.79046700	3.60363600	0.84473700
H	0.92107300	2.78382100	0.19095700
H	1.77474200	1.74317400	-1.94040200
H	2.05367400	3.49274200	-1.84013000
H	3.38982900	2.37415400	-1.58030000
H	2.51376600	3.65902300	1.90331100
H	3.86520000	3.39603500	0.79104800
H	2.61493000	4.58812800	0.39631000
C	-2.15947700	4.84958700	0.66882800
C	-2.31764300	6.00669900	1.67880200
C	-1.96158400	5.40450800	-0.75374300
H	-1.24437400	4.30905800	0.93070000
H	-2.41810000	5.63947000	2.70603700
H	-1.44627300	6.66985300	1.63966500
H	-3.20671200	6.60667000	1.45468800
H	-1.79333700	4.60230500	-1.47944700
H	-2.82397400	5.98956800	-1.09123600
H	-1.08956800	6.06739200	-0.77702300
C	0.57257600	-1.17546900	3.41804900
C	1.09929000	-0.89462600	4.84217900

C	0.31356600	-2.68414500	3.23897100
H	-0.39184700	-0.66490500	3.31798700
H	1.23832000	0.17631900	5.02425200
H	0.39604000	-1.27573500	5.59098700
H	2.06501300	-1.38581400	5.00632800
H	-0.03892300	-2.92141700	2.23006000
H	1.21413800	-3.27831100	3.42699500
H	-0.44733000	-3.01786000	3.95316200
C	-4.27014600	0.46215000	2.36873600
C	-5.01061700	-0.69972100	1.68133000
C	-4.79447900	0.66619300	3.80659500
H	-3.21552100	0.17871700	2.44400700
H	-4.66836500	-0.84199100	0.65019900
H	-4.83837100	-1.63193200	2.23109700
H	-6.09347300	-0.53767200	1.65464100
H	-4.23544900	1.44838000	4.33169600
H	-5.85095500	0.95707200	3.80206000
H	-4.70259600	-0.26162200	4.38246000
H	0.67890500	2.20643300	3.78417900
H	-1.86990000	3.31150800	3.66664500
C	-2.61241500	-0.02396300	-2.18236500
C	-2.94124400	1.42414700	-2.10609400
H	-1.94170900	-0.33637900	-2.98212900
H	-2.31719500	1.88875700	-1.22974900
H	-3.43815800	-0.72067100	-2.03545900
C	-2.62551700	2.33575300	-3.31770000
C	-1.14451700	2.33845500	-3.72972300
C	-3.52697300	1.97178200	-4.51547400
H	-2.88491300	3.35934100	-3.01137500
C	-0.89408100	3.27791300	-4.92188900
H	-0.83688200	1.32167500	-4.01199200
H	-0.51634700	2.63230300	-2.87657400
C	-3.27659500	2.90596600	-5.71033000
H	-3.32457800	0.93263700	-4.81324600
H	-4.58274400	2.01255900	-4.21656900
C	-1.79500200	2.92254500	-6.11445900
H	0.16215800	3.23461000	-5.21383800
H	-1.09090200	4.31476000	-4.61287400
H	-3.90068700	2.59795900	-6.55767100
H	-3.59295900	3.92519500	-5.44492800
H	-1.63378800	3.63310700	-6.93372900
H	-1.51198300	1.93202800	-6.50007000
H	-3.96539400	1.58965500	-1.75582100
C	-1.71902500	-1.64835200	0.08352000

C	-0.48674900	-1.53489400	-0.51905200
H	-2.52614100	-2.18846200	-0.40451000
H	-1.84000900	-1.46020400	1.14601500
H	0.33933500	-1.15519600	0.07871000
C	-0.08752200	-2.18094600	-1.81771800
C	0.89117600	-1.31860400	-2.64123400
C	0.56971200	-3.55143200	-1.48248800
H	-0.98650200	-2.38390800	-2.41534500
C	1.36866700	-2.04271900	-3.90976100
H	1.75825400	-1.07279100	-2.01032400
H	0.41966500	-0.36387100	-2.90584000
C	1.04718900	-4.27304600	-2.75325800
H	1.42580800	-3.38118300	-0.81353200
H	-0.14392100	-4.17709500	-0.93262900
C	2.00329300	-3.40090700	-3.57856000
H	2.08146100	-1.40845900	-4.45026300
H	0.51328800	-2.19547900	-4.58427100
H	1.53290600	-5.21553000	-2.47356100
H	0.17462100	-4.54187600	-3.36582700
H	2.28887900	-3.92100600	-4.50030300
H	2.93044900	-3.23852700	-3.00988300

#### INT11

Ni	-2.96965700	-0.38057100	-0.31362100
C	-1.97664000	0.76804300	3.53569700
C	-0.80880100	0.89866900	2.85640300
N	-1.08019100	0.55769800	1.54009700
N	-2.93909500	0.35275000	2.62298300
C	-2.39117500	0.21144200	1.38307800
C	-4.30751400	0.07457900	3.01878300
C	-5.18970000	1.16327300	3.19521700
C	-4.66914800	-1.25989600	3.29438200
C	-6.48769100	0.86839700	3.63135200
C	-5.98413000	-1.49090000	3.72031200
C	-6.88478000	-0.44251000	3.88435400
H	-7.19479800	1.67737600	3.78363700
H	-6.29952700	-2.50501900	3.94591200
H	-7.89597600	-0.64549600	4.22516000
C	-0.09264000	0.50539500	0.48015700
C	0.58537500	-0.71413700	0.26688900
C	0.16386800	1.67139600	-0.27060900
C	1.52223900	-0.75223100	-0.77358300
C	1.11938900	1.57404600	-1.29050500
C	1.78462400	0.37720100	-1.54581500

H	2.06369200	-1.67162400	-0.97210600
H	1.35149200	2.45009800	-1.88808000
H	2.52250700	0.32826200	-2.34150800
C	-3.68766300	-2.42726000	3.22113700
C	-4.17835900	-3.54850000	2.28621900
C	-3.39046000	-2.97736800	4.63193200
H	-2.74215100	-2.05802200	2.81184600
H	-4.34860600	-3.17463600	1.27064300
H	-3.43314300	-4.35042000	2.23493900
H	-5.11444000	-3.99379800	2.64024100
H	-3.00145500	-2.19595700	5.29402200
H	-4.29252300	-3.38909900	5.09777600
H	-2.64596700	-3.77976500	4.57914600
C	0.32359400	-1.95504400	1.11818000
C	1.62338300	-2.63258000	1.59229400
C	-0.57480100	-2.96143100	0.37351200
H	-0.21570300	-1.64248800	2.01851100
H	2.27766200	-1.92359200	2.11014300
H	1.38752000	-3.44669800	2.28610900
H	2.18895100	-3.06726300	0.76113700
H	-1.54337900	-2.51430300	0.09975800
H	-0.10217400	-3.31152600	-0.55018900
H	-0.78472900	-3.83402500	1.00210000
C	-4.76821300	2.61814400	2.99003700
C	-4.52424100	3.31109700	4.34842100
C	-5.78076300	3.42836500	2.15801100
H	-3.82011100	2.62540400	2.44043100
H	-3.76769500	2.79041100	4.94547700
H	-4.18297000	4.34102400	4.19542800
H	-5.44533300	3.34681100	4.94092700
H	-5.98689200	2.95550700	1.19255200
H	-6.73478900	3.55111900	2.68170400
H	-5.38494400	4.43203000	1.96785000
C	-0.51293700	3.00775800	0.02013900
C	-1.10559800	3.65849700	-1.24396800
C	0.46715300	3.97142200	0.72240900
H	-1.34478300	2.82747800	0.70944200
H	-1.79713900	2.98169000	-1.75855800
H	-1.65517000	4.56713400	-0.97474700
H	-0.32844400	3.94913400	-1.95907000
H	0.85527300	3.54500300	1.65418700
H	1.32448700	4.20042200	0.07952700
H	-0.03344600	4.91545500	0.96458300
H	-2.21472600	0.92097700	4.57603000

H	0.17808000	1.18990100	3.18017300
C	-4.43245300	0.14257600	-2.96938500
C	-4.33559600	0.93060500	-0.53657300
C	-5.24523400	0.60937200	-1.73328500
H	-4.87234000	1.02845200	0.40582200
H	-3.73028100	1.82861600	-0.71244000
H	-5.67748100	1.58902400	-2.00250500
H	-5.10402900	-0.37128700	-3.66804900
C	-6.48396400	-0.28605300	-1.44253800
C	-6.18602400	-1.74381200	-1.04134800
C	-7.44690400	0.36025600	-0.42484600
H	-7.02854900	-0.32841400	-2.39983000
C	-7.47494200	-2.56357700	-0.85175200
H	-5.60830800	-1.75085300	-0.10391000
H	-5.56709100	-2.23544200	-1.80342300
C	-8.74131400	-0.45260100	-0.26363600
H	-6.96065400	0.43674500	0.55754300
H	-7.68330700	1.38585800	-0.74079300
C	-8.43857200	-1.90177200	0.14250900
H	-7.22296200	-3.57977800	-0.52349900
H	-7.97504000	-2.66744300	-1.82555800
H	-9.39150400	0.02524900	0.47940800
H	-9.29628900	-0.44700700	-1.21285100
H	-9.36681000	-2.48180700	0.21138600
H	-7.98675200	-1.90805600	1.14534800
C	-3.25154800	-0.78269200	-2.62632200
H	-2.39841500	-0.16226300	-2.27894500
H	-3.57236500	-1.48968100	-1.81956800
C	-2.71942700	-1.67106100	-3.77247700
C	-2.20118600	-0.82880900	-4.95594200
C	-1.62921100	-2.64123200	-3.28286900
H	-3.56960500	-2.27248200	-4.13123400
C	-1.66121500	-1.71204000	-6.09294300
H	-1.39694900	-0.16763100	-4.59533800
H	-2.99563400	-0.17723600	-5.33891200
C	-1.08785000	-3.52383400	-4.41920000
H	-0.80061000	-2.05795600	-2.85111100
H	-2.02632800	-3.27257900	-2.47553600
C	-0.57706900	-2.67746500	-5.59417500
H	-1.27012900	-1.07871100	-6.89810700
H	-2.49094000	-2.28907300	-6.52608400
H	-0.28995000	-4.17319200	-4.03844100
H	-1.88900900	-4.18970100	-4.77060100
H	-0.24193300	-3.32722300	-6.41121600

H	0.30261700	-2.10052100	-5.27189200
H	-4.04358400	1.01592500	-3.50512800

**TS1**

Ni	-0.91024000	1.10283400	-0.78403600
C	-0.73301500	-0.11684400	3.21527900
C	0.42216100	0.57958400	3.09449400
N	0.47533500	1.04525600	1.78652900
N	-1.37443400	-0.04889700	1.98055700
C	-0.63297600	0.66863300	1.08225100
C	-2.65034000	-0.68368700	1.73015600
C	-3.82046500	-0.07626700	2.24246200
C	-2.67299700	-1.91030800	1.03228600
C	-5.04017500	-0.72022300	1.99448600
C	-3.92442900	-2.50036700	0.80689200
C	-5.09597600	-1.91296600	1.27679400
H	-5.95895800	-0.28512000	2.37472900
H	-3.97816900	-3.44588100	0.27535600
H	-6.05360600	-2.39510900	1.10110100
C	1.60152200	1.79244000	1.26357000
C	2.74889400	1.07594300	0.86017100
C	1.52909400	3.19963200	1.23109000
C	3.84030300	1.82091900	0.39733500
C	2.65273600	3.89014300	0.75886900
C	3.79476900	3.21163500	0.34386400
H	4.74212600	1.30513600	0.08209300
H	2.63574500	4.97511700	0.72500100
H	4.65610400	3.76843100	-0.01405300
C	-1.41066900	-2.63403700	0.57100700
C	-1.41208800	-2.88899200	-0.94791100
C	-1.21836800	-3.95119400	1.35134300
H	-0.54897200	-1.99753800	0.78939000
H	-1.51329400	-1.94899900	-1.50318800
H	-0.47284600	-3.36351500	-1.25330500
H	-2.22927500	-3.55376900	-1.24978000
H	-1.17679900	-3.77312000	2.43129900
H	-2.03572200	-4.65561900	1.16038600
H	-0.28296600	-4.43616100	1.05074600
C	2.85372800	-0.44520900	0.94742800
C	3.79611400	-0.86493900	2.09509600
C	3.30233300	-1.08317100	-0.38125800
H	1.86013400	-0.84544800	1.17456200
H	3.46442300	-0.46332600	3.05903900
H	3.83571900	-1.95684400	2.17873200

H	4.81580900	-0.50407900	1.91979100
H	2.63765600	-0.80250400	-1.20565200
H	4.32049600	-0.78690600	-0.65572700
H	3.29309600	-2.17551600	-0.29477500
C	-3.79998000	1.20509800	3.07545300
C	-4.00675500	0.88566600	4.57222500
C	-4.84117800	2.24289500	2.61131100
H	-2.81114800	1.66511500	2.97107400
H	-3.25152200	0.18966000	4.95196900
H	-3.95073500	1.80333400	5.16801500
H	-4.98983100	0.43278000	4.74334600
H	-4.74299000	2.47691300	1.54621000
H	-5.86638000	1.89900100	2.78526300
H	-4.71363400	3.17310400	3.17557100
C	0.31428200	3.98048300	1.72325900
C	-0.19466500	4.98083100	0.66789700
C	0.61730400	4.68999200	3.05896000
H	-0.49535200	3.26764300	1.91105900
H	-0.37900500	4.48190800	-0.28958300
H	-1.12685300	5.44737700	1.00708900
H	0.52668800	5.78635700	0.49214100
H	0.92584900	3.97638100	3.83101200
H	1.42175700	5.42522500	2.94508900
H	-0.27119000	5.21938400	3.42175900
H	-1.15935500	-0.65190500	4.04843500
H	1.20796800	0.78543500	3.80374700
C	0.13923600	0.67391900	-2.64630400
C	-0.66707700	1.77905400	-2.83734100
H	-0.23607400	-0.30342500	-2.92985800
H	1.21702100	0.79686600	-2.61531200
H	0.31285700	0.29602900	-0.88022600
C	-2.68306100	2.37730200	-0.64335600
C	-3.37449500	1.28339300	-1.08199800
H	-2.52913100	3.22929300	-1.29597600
H	-2.61388900	2.54863800	0.42306600
H	-3.68108300	0.49154800	-0.40066000
O	-3.77020000	1.15442600	-2.35322500
C	-4.39579900	-0.09158100	-2.71316100
H	-4.83123100	0.06433400	-3.69972000
H	-3.65102400	-0.89319900	-2.75429200
H	-5.18104700	-0.34755600	-1.99520800
H	-1.67085900	1.69977100	-3.24972400
O	-0.13367200	3.02842600	-2.74923900
C	-0.78011400	4.03901700	-3.53239200

H	-1.86184300	4.05528600	-3.35035700
H	-0.34300900	4.98981000	-3.22702800
H	-0.59279800	3.87349100	-4.59935300

### TS1'

Ni	-0.75745900	1.46624000	-0.79309900
C	-0.65018200	-0.22744800	3.06651100
C	0.49203500	0.49956300	3.04607800
N	0.55820400	1.10571100	1.79695400
N	-1.26844300	-0.03904400	1.83287600
C	-0.52810900	0.78480500	1.03024300
C	-2.54726600	-0.63618500	1.50987000
C	-3.71739000	-0.05316300	2.04989200
C	-2.57385600	-1.80779300	0.72378300
C	-4.94127500	-0.65977800	1.73675000
C	-3.82840800	-2.36588700	0.44213200
C	-5.00001800	-1.79755900	0.93543000
H	-5.86047500	-0.24126300	2.13414500
H	-3.88725000	-3.27062100	-0.15488200
H	-5.96032900	-2.25385800	0.71204500
C	1.65176500	1.96861800	1.39569300
C	2.84880900	1.37305200	0.94088200
C	1.50053300	3.36453300	1.53599400
C	3.89878500	2.22964300	0.58731500
C	2.58449600	4.16993300	1.16197500
C	3.76815400	3.61241100	0.68792500
H	4.83612500	1.80921300	0.23717600
H	2.50621700	5.24812600	1.25896000
H	4.59765600	4.25664400	0.41054500
C	-1.30703900	-2.51761800	0.25359800
C	-1.35082800	-2.88969900	-1.23932900
C	-1.04241900	-3.76602800	1.12242100
H	-0.46238000	-1.83589500	0.39024400
H	-1.49412300	-2.00491900	-1.86964400
H	-0.40807200	-3.36617200	-1.53094900
H	-2.15155100	-3.60237600	-1.46441500
H	-0.95776800	-3.50641400	2.18330200
H	-1.85195100	-4.49782800	1.02187900
H	-0.10924100	-4.25285300	0.81726100
C	3.04864800	-0.13966200	0.88227900
C	3.85953400	-0.63254700	2.10048000
C	3.72439800	-0.60498400	-0.42085000
H	2.06276500	-0.61527500	0.92432400
H	3.37510300	-0.37122400	3.04701000

H	3.97315200	-1.72209800	2.06967500
H	4.86151000	-0.18883000	2.10744800
H	3.20349200	-0.22292800	-1.30504200
H	4.76791400	-0.27846800	-0.48214200
H	3.72709200	-1.69962600	-0.47100000
C	-3.69384200	1.15730900	2.98351400
C	-3.92562400	0.71752500	4.44570700
C	-4.71554500	2.24302600	2.59243800
H	-2.69862100	1.61199100	2.93032000
H	-3.18465900	-0.01848600	4.77463200
H	-3.86569100	1.58087200	5.11755400
H	-4.91675100	0.26582700	4.56564900
H	-4.59079400	2.57180900	1.55556400
H	-5.74735300	1.89600100	2.71220700
H	-4.59289100	3.11775100	3.24033700
C	0.25715700	4.00611600	2.14606400
C	-0.25487500	5.21025500	1.33386500
C	0.52602300	4.41314000	3.61081900
H	-0.54158100	3.25730500	2.15788400
H	-0.41292900	4.94871500	0.28193000
H	-1.20637000	5.56481000	1.74603800
H	0.44329900	6.05342300	1.36660900
H	0.83371600	3.55465000	4.21793100
H	1.32122400	5.16474400	3.66909200
H	-0.37626300	4.84177500	4.06166700
H	-1.08263800	-0.85410300	3.82982200
H	1.25491900	0.64752100	3.79343200
C	0.44978400	1.07160500	-2.71858400
C	-0.46879800	2.13690900	-2.65104300
H	1.52190300	1.25955400	-2.63894100
H	0.49099200	0.64087900	-1.11219000
C	-2.41683100	2.80690000	-0.55856900
C	-3.17418200	1.76462500	-1.03113800
H	-2.24980400	3.67676700	-1.18544800
H	-2.34698500	2.93937500	0.51442100
H	-3.50010000	0.95591200	-0.37854300
O	-3.61097000	1.72092100	-2.28577400
C	-4.19056700	0.48533500	-2.74473300
H	-4.83214400	0.74437400	-3.58671500
H	-3.39628200	-0.19197600	-3.07365600
H	-4.78110900	0.01660100	-1.95102300
H	-0.04849000	3.13291800	-2.52032900
H	-1.38519200	2.06380700	-3.22905900
O	0.09428300	-0.05634400	-3.36492400

C	1.07768300	-1.09550000	-3.39371300
H	2.02192500	-0.72464400	-3.80939400
H	1.24341800	-1.49178300	-2.38528300
H	0.67782400	-1.87823400	-4.03809100

### TS2

Ni	-1.04255400	0.70986100	-0.72342200
C	-1.55807100	-0.27909000	3.20779400
C	-0.33530900	0.29520300	3.32025600
N	0.02490800	0.73456200	2.04982700
N	-1.92077200	-0.18694700	1.86936600
C	-0.94673800	0.43220500	1.13919300
C	-3.17167300	-0.69573700	1.34297100
C	-4.29007200	0.16520100	1.30846000
C	-3.23229600	-2.04540300	0.93779900
C	-5.49279200	-0.36596700	0.82513400
C	-4.46330500	-2.52015100	0.46678800
C	-5.58009400	-1.69159700	0.40636600
H	-6.37703800	0.26228900	0.78843600
H	-4.55016500	-3.55544400	0.15213300
H	-6.52601900	-2.08290200	0.04260900
C	1.28056900	1.40608600	1.77608300
C	2.37642800	0.63414000	1.33525000
C	1.37296600	2.79276600	2.02575100
C	3.58619500	1.30412000	1.11157300
C	2.60922800	3.40650100	1.78395900
C	3.70204500	2.67471100	1.32723000
H	4.45360900	0.74420800	0.77751100
H	2.72133600	4.47029100	1.96645800
H	4.65198500	3.17203900	1.15269100
C	-2.04265900	-2.99576900	1.04314700
C	-1.79069400	-3.77053000	-0.26420800
C	-2.22486400	-3.96870200	2.22712300
H	-1.14608400	-2.39952800	1.24292200
H	-1.69693400	-3.08960100	-1.11638300
H	-0.86776200	-4.35588500	-0.18020500
H	-2.59992500	-4.47529000	-0.48436700
H	-2.34541300	-3.43348200	3.17541500
H	-3.11060600	-4.59835400	2.08593900
H	-1.35420800	-4.62782300	2.31869300
C	2.30225200	-0.88346300	1.18214700
C	2.84229100	-1.57913500	2.45052000
C	3.03678800	-1.40379900	-0.06645200
H	1.24882000	-1.16356900	1.07685400

H	2.28815100	-1.27496900	3.34481400
H	2.76017600	-2.66797200	2.35590600
H	3.89789700	-1.33264600	2.61166100
H	2.70884900	-0.88512400	-0.97397000
H	4.12233800	-1.28193900	0.01283000
H	2.84432800	-2.47524500	-0.19301100
C	-4.24290600	1.59918400	1.83015500
C	-4.85331400	1.68099200	3.24595500
C	-4.93513200	2.60208900	0.88838000
H	-3.19236900	1.89903700	1.90615900
H	-4.33127500	1.02396600	3.94998700
H	-4.79273300	2.70533800	3.63066600
H	-5.90882000	1.38646800	3.23530000
H	-4.54427100	2.53474300	-0.13328600
H	-6.01764300	2.44209400	0.84115300
H	-4.77616400	3.62449600	1.24867800
C	0.21774600	3.60926600	2.60425900
C	0.05283300	4.99039800	1.94172600
C	0.38800300	3.78092600	4.13002100
H	-0.71089000	3.05344600	2.43331700
H	-0.02620900	4.91892300	0.85197200
H	-0.85682500	5.47287400	2.31539600
H	0.88912500	5.65850700	2.17378600
H	0.44005100	2.81788300	4.64810700
H	1.30762000	4.33125400	4.35880100
H	-0.45478100	4.34307500	4.54775700
H	-2.19850500	-0.74275900	3.94113600
H	0.31080500	0.43140400	4.17243800
C	-3.04917800	0.28999500	-2.85880900
C	-1.53889900	0.45308000	-2.80080500
H	-3.51920500	1.14129300	-3.35917000
H	-3.29067500	-0.61641100	-3.42514400
H	-1.08408100	0.58067100	-3.78285600
O	-0.99079600	-0.72518900	-2.18915700
C	0.16768100	-1.30436700	-2.82303000
H	0.49095500	-2.11959100	-2.17602900
H	-0.12172300	-1.69886900	-3.80228400
H	0.97243300	-0.57283300	-2.93321600
H	-3.48664000	0.18756700	-1.86018500
C	-1.24401500	2.56252300	-0.84308200
C	-1.10697500	2.25898600	-2.28358000
H	-0.41767100	3.08103500	-0.36444700
H	-2.22265900	2.89698600	-0.49883200
H	-1.98372600	2.57758300	-2.85000400

C	0.18076700	2.69448500	-3.00214100
C	0.12521700	4.21653400	-3.28158000
C	1.49462400	2.34292000	-2.27950300
H	0.20075000	2.19976600	-3.98640300
C	1.35012400	4.68669100	-4.08330000
H	0.08386500	4.75560700	-2.32444200
H	-0.79732700	4.46559300	-3.82255000
C	2.71935000	2.79572000	-3.09161300
H	1.52297900	2.83207900	-1.29779200
H	1.55022200	1.26443700	-2.08068300
C	2.66466200	4.30163300	-3.38892600
H	1.29902300	5.77194700	-4.23048200
H	1.32046000	4.23526200	-5.08559700
H	3.63595500	2.54749300	-2.54341000
H	2.75867500	2.23767700	-4.03884300
H	3.52017300	4.59721800	-4.00752200
H	2.75325400	4.85834600	-2.44460400

### TS2'

Ni	-1.12322200	0.64739800	-0.67901900
C	-1.77654000	-1.32744600	2.82332400
C	-0.56659600	-0.83047000	3.17366500
N	-0.12773900	-0.04029300	2.11417900
N	-2.05223700	-0.84236500	1.55093900
C	-1.03645100	-0.04536100	1.09357400
C	-3.29018300	-1.12013600	0.84775600
C	-4.35662000	-0.20315500	0.97732700
C	-3.40109400	-2.32268000	0.11720000
C	-5.55412000	-0.51448500	0.32071900
C	-4.62512500	-2.58084100	-0.51294200
C	-5.68845100	-1.68732300	-0.41781100
H	-6.39893500	0.16190900	0.40159300
H	-4.75053600	-3.49710900	-1.08055900
H	-6.63020000	-1.91183000	-0.91074400
C	1.10400300	0.72043000	2.19702100
C	2.26244600	0.22451700	1.56073500
C	1.11106500	1.88390100	2.99729800
C	3.44454900	0.95900500	1.71590400
C	2.32604800	2.57189400	3.11992000
C	3.47811900	2.12103800	2.48368500
H	4.35713100	0.61107900	1.24411900
H	2.37073100	3.46828300	3.73076000
H	4.40990800	2.66783500	2.59717600
C	-2.27168700	-3.34696600	0.04033800

C	-2.09931100	-3.94053200	-1.37073800
C	-2.48473000	-4.47991300	1.06734900
H	-1.33707700	-2.83572900	0.29830100
H	-2.03630300	-3.15582600	-2.13082900
H	-1.18572100	-4.54472600	-1.41290800
H	-2.92942100	-4.60274800	-1.63926800
H	-2.54072400	-4.09919200	2.09230500
H	-3.41540000	-5.02090000	0.86185800
H	-1.65923900	-5.19927200	1.02051000
C	2.27356900	-1.10367500	0.80614200
C	2.61629800	-2.26532700	1.76512400
C	3.22905900	-1.11435400	-0.40010600
H	1.26288600	-1.28124700	0.42244700
H	1.90264900	-2.33288200	2.59279900
H	2.60309700	-3.22220000	1.23036200
H	3.61600900	-2.13219800	2.19389200
H	3.06164100	-0.25705100	-1.06220100
H	4.27986100	-1.09636200	-0.09238600
H	3.08628900	-2.03282500	-0.98058000
C	-4.26887100	1.04506200	1.85204400
C	-4.92675000	0.78873600	3.22532200
C	-4.88171200	2.29243300	1.18879300
H	-3.21060300	1.26178700	2.02921800
H	-4.45953500	-0.05403900	3.74610300
H	-4.83580500	1.67398400	3.86501000
H	-5.99310400	0.56205700	3.11313500
H	-4.45803200	2.47363200	0.19441200
H	-5.96805800	2.20878200	1.07812100
H	-4.68902900	3.17646800	1.80665500
C	-0.11209700	2.37811500	3.77085900
C	-0.41373800	3.87006800	3.53266400
C	0.05565000	2.10598300	5.28157500
H	-0.98701100	1.81543400	3.42956100
H	-0.56331600	4.08966200	2.47096900
H	-1.32571600	4.15478000	4.06917200
H	0.39239100	4.51492800	3.89865200
H	0.22568500	1.04421700	5.48987200
H	0.90726400	2.66219500	5.68909000
H	-0.84151100	2.41840200	5.82749600
H	-2.46304100	-1.97001800	3.35079100
H	0.02160900	-0.95370500	4.06862600
C	-2.60553300	0.49072800	-3.68028500
C	-1.36945700	0.62762400	-2.81553400
H	-2.86387100	1.43822600	-4.16107000

H	-2.41529600	-0.24990700	-4.46563000
H	-0.48948000	0.98590400	-3.35178600
O	-1.07024800	-0.64353300	-2.22473100
C	0.17429200	-1.24802500	-2.64541400
H	0.31365700	-2.12262300	-2.01088700
H	0.08750700	-1.55562600	-3.69184900
H	1.01014700	-0.55395200	-2.52055100
H	-3.45871700	0.14755000	-3.08700000
C	-1.24869600	2.54968800	-0.51755800
C	-1.82149700	2.26994400	-1.83537400
H	-1.98706500	2.78994000	0.24837600
H	-2.90742400	2.21212900	-1.86829600
H	-1.41107900	2.83361500	-2.67189400
C	0.04154100	3.35447100	-0.40136600
C	1.15896600	2.92407200	-1.37367000
C	-0.25052600	4.86958700	-0.56174900
H	0.42701200	3.20481200	0.61489300
C	2.42823800	3.77573600	-1.20520100
H	0.80986000	3.02147900	-2.41370600
H	1.39585500	1.86243900	-1.21349300
C	1.01927900	5.71930500	-0.39499500
H	-0.68063200	5.04867100	-1.55882100
H	-1.01314700	5.18046200	0.16441900
C	2.12778300	5.27390000	-1.35920600
H	3.18548100	3.46176000	-1.93442600
H	2.85387600	3.58797700	-0.20985600
H	0.77894000	6.77791100	-0.55099900
H	1.37968300	5.62998100	0.64011300
H	3.03802900	5.86106500	-1.18880100
H	1.81408900	5.47853200	-2.39354900

### TS3

Ni	-0.42727700	1.25461300	-1.41209600
C	-0.01298000	-1.39886600	1.83045000
C	0.79851000	-0.40428800	2.25237600
N	0.80164300	0.56314300	1.25355200
N	-0.50918500	-1.01539500	0.59025400
C	-0.01581500	0.20380200	0.20428900
C	-1.39852800	-1.90238600	-0.13186800
C	-2.73990100	-1.99809400	0.29910100
C	-0.85817400	-2.73719000	-1.13186600
C	-3.54988500	-2.95339800	-0.32804100
C	-1.72029600	-3.66515700	-1.73041100
C	-3.05002000	-3.77604800	-1.33430000

H	-4.58494200	-3.05948500	-0.01814200
H	-1.33681200	-4.32494500	-2.50265500
H	-3.69608900	-4.51327000	-1.80262900
C	1.64561400	1.73733900	1.37198200
C	3.03540000	1.58962700	1.15183000
C	1.06997400	2.95561600	1.79884600
C	3.83641900	2.72954200	1.30551300
C	1.92238100	4.06059900	1.92521200
C	3.28831300	3.95381100	1.67393000
H	4.90604000	2.65449600	1.13875000
H	1.51632800	5.01499000	2.24146700
H	3.92871800	4.82437100	1.78333200
C	0.61656300	-2.71779300	-1.52449100
C	0.81245900	-2.52693200	-3.03991300
C	1.33190000	-3.99077900	-1.02695100
H	1.08942800	-1.86351000	-1.03067800
H	0.29124500	-1.63081500	-3.38992700
H	1.87988300	-2.43022000	-3.27155600
H	0.43441200	-3.38452600	-3.60810300
H	1.23964100	-4.10621400	0.05876700
H	0.91432100	-4.88979200	-1.49421900
H	2.39889400	-3.95055400	-1.27477200
C	3.69906900	0.25230000	0.81772300
C	4.37672300	-0.34457800	2.07135400
C	4.72988700	0.34957100	-0.32504000
H	2.92029500	-0.44947900	0.49803800
H	3.67239600	-0.48184400	2.89768600
H	4.81650500	-1.32055400	1.83777000
H	5.17995200	0.31049400	2.42690200
H	4.30992200	0.81464300	-1.22213200
H	5.61184400	0.92769100	-0.02906400
H	5.07900500	-0.65363300	-0.59273100
C	-3.31315200	-1.15025500	1.43355600
C	-3.52742800	-1.99935700	2.70452200
C	-4.62510200	-0.44631500	1.03912700
H	-2.58774400	-0.36615800	1.67381600
H	-2.59880600	-2.47028000	3.04428500
H	-3.90701900	-1.37537700	3.52148300
H	-4.25612200	-2.79810600	2.52574900
H	-4.49536400	0.16664500	0.14176200
H	-5.43186900	-1.16135300	0.84437700
H	-4.95823400	0.20722000	1.85319000
C	-0.39761000	3.06823900	2.20617600
C	-1.01423500	4.44425200	1.90121400

C	-0.55947200	2.73850800	3.70720800
H	-0.96483100	2.32184700	1.64040700
H	-0.85981600	4.74030700	0.85810000
H	-2.09240600	4.41477300	2.08989100
H	-0.60072300	5.23067200	2.54192300
H	-0.19947900	1.73236500	3.94520100
H	0.00026800	3.45110900	4.32377200
H	-1.61460000	2.79626000	3.99794300
H	-0.28517500	-2.33819800	2.28347700
H	1.37330400	-0.28818200	3.15645700
C	-3.54309700	-0.46807600	-3.17549000
C	-2.63247100	0.64880100	-3.68306200
H	-4.54623300	-0.09567000	-2.94619900
H	-3.65493900	-1.23875900	-3.94365700
H	-3.13548000	1.15510700	-4.52471000
O	-1.39081800	0.13638400	-4.15881000
C	-1.43894700	-0.38638600	-5.47948100
H	-0.42385700	-0.70357900	-5.72862200
H	-2.10661800	-1.25399500	-5.56187600
H	-1.76449800	0.38000800	-6.19825700
H	-3.12446800	-0.93433400	-2.28183300
C	-1.16210600	2.49670100	-2.87078700
C	-2.33892600	1.77506300	-2.67684600
H	-0.56207400	2.25517700	-3.73750000
H	-1.04502100	3.48944300	-2.44488300
H	-1.83737500	0.79907400	-1.23326900
C	-3.55165200	2.37631800	-1.96078800
C	-3.20540300	3.32831100	-0.80325300
C	-4.46428100	3.11053000	-2.98401900
H	-4.13961100	1.55189600	-1.54046800
C	-4.47091400	3.86898900	-0.11942300
H	-2.62216000	4.17852800	-1.18253600
H	-2.56919700	2.80403500	-0.07929300
C	-5.72580000	3.67180200	-2.30730800
H	-3.89218800	3.92919400	-3.44322100
H	-4.75961600	2.43661900	-3.79639900
C	-5.38567000	4.58553600	-1.12283900
H	-4.18961100	4.55084100	0.69221600
H	-5.01832900	3.03663100	0.34654400
H	-6.32504900	4.21299600	-3.04920400
H	-6.34713200	2.83555200	-1.95551700
H	-6.30448400	4.92177100	-0.62816600
H	-4.88019100	5.48937000	-1.49287000
C	1.66141500	1.46994700	-2.16980400

C	1.71576300	2.80250800	-1.87224500
H	1.64144200	1.10790700	-3.19240600
H	1.98015200	0.76908200	-1.41177300
H	1.79536100	3.15261400	-0.84835700
O	1.68779500	3.83460900	-2.71443700
C	1.95612900	3.61049500	-4.10936900
H	2.05933100	4.60248300	-4.54825600
H	2.88801100	3.04725500	-4.22416200
H	1.13614800	3.07732800	-4.59560800

#### TS4

Ni	-2.57482300	0.59354100	-0.74207500
C	-1.33967500	-0.06854700	3.18412100
C	-0.24733200	0.54345700	2.66026100
N	-0.55276300	0.83567700	1.33821700
N	-2.29044000	-0.13276600	2.17310500
C	-1.81378400	0.41843600	1.01840900
C	-3.58337500	-0.76795100	2.33739300
C	-4.62439200	-0.03934400	2.95465100
C	-3.73049100	-2.10542000	1.91683400
C	-5.85897300	-0.68519200	3.09821700
C	-4.99090600	-2.69539000	2.08222500
C	-6.04561100	-1.99384200	2.65823100
H	-6.68390800	-0.16061900	3.56946200
H	-5.14284200	-3.72408600	1.76933700
H	-7.01240700	-2.47349500	2.78192100
C	0.38208100	1.44261700	0.41250600
C	1.28411600	0.60208900	-0.27498500
C	0.38266500	2.84618100	0.26832600
C	2.19904100	1.21358900	-1.14227400
C	1.32447700	3.39995600	-0.60854500
C	2.22182700	2.59579700	-1.30788800
H	2.91056000	0.59876300	-1.68517800
H	1.36352000	4.47720900	-0.73613700
H	2.94783900	3.04937400	-1.97673900
C	-2.58048500	-2.93647400	1.35264700
C	-2.86979300	-3.43782600	-0.07476100
C	-2.23969100	-4.11347700	2.29036300
H	-1.69049700	-2.30171800	1.29802400
H	-3.06861100	-2.60267400	-0.75637400
H	-2.01143300	-3.99857800	-0.46189800
H	-3.73923500	-4.10365200	-0.10335200
H	-1.99703900	-3.76356600	3.29962600
H	-3.07581100	-4.81642700	2.37331000

H	-1.37619800	-4.66745400	1.90540700
C	1.32112800	-0.91266300	-0.08627400
C	2.63244600	-1.35481200	0.59558500
C	1.11329500	-1.66483100	-1.41508700
H	0.49912600	-1.19792900	0.57805600
H	2.77159100	-0.85492200	1.56040000
H	2.62395700	-2.43613400	0.77204400
H	3.50432500	-1.12483100	-0.02678200
H	0.16638300	-1.38319200	-1.89124900
H	1.91818500	-1.45999200	-2.12918800
H	1.09518400	-2.74612100	-1.23997800
C	-4.42829900	1.36783200	3.51816600
C	-4.20612500	1.31053000	5.04572900
C	-5.59240300	2.32367500	3.19464100
H	-3.52349300	1.79181500	3.06806800
H	-3.34890200	0.68324000	5.31194700
H	-4.02619600	2.31528800	5.44415400
H	-5.08658600	0.89915100	5.55200100
H	-5.80066100	2.37169800	2.12057800
H	-6.51715700	2.02835500	3.70169800
H	-5.34715900	3.33521100	3.53601700
C	-0.55920100	3.75776100	1.04932100
C	-1.26844300	4.78159200	0.14176600
C	0.19131900	4.46928700	2.19451400
H	-1.33592100	3.13370000	1.50352900
H	-1.76590700	4.29494400	-0.70504400
H	-2.02277300	5.33273700	0.71450100
H	-0.56949200	5.52107300	-0.26435900
H	0.64734900	3.75107400	2.88479500
H	0.99037200	5.10973900	1.80423000
H	-0.49629400	5.10085500	2.76800900
H	-1.52668600	-0.46867000	4.16774200
H	0.70949600	0.78862600	3.09366000
C	-2.69557100	0.52815400	-2.69556700
H	-2.27661400	-0.47214900	-2.41292900
C	-4.00170000	1.81095900	-0.31947900
C	-4.32588900	1.57764700	-1.68903600
H	-4.60979700	1.35693200	0.45800500
H	-3.53210700	2.75477200	-0.04760400
H	-4.05964700	2.37549500	-2.37835700
C	-1.61336200	1.47344000	-3.18858700
H	-0.85256000	1.67236300	-2.41372000
H	-1.08318800	0.97802400	-4.02496900
H	-3.43468200	0.34195100	-3.47206500

O	-2.20772500	2.67442000	-3.62359800
C	-1.28129300	3.56581600	-4.22897200
H	-1.83932400	4.46057000	-4.51093600
H	-0.47821500	3.84144100	-3.52998600
H	-0.83314200	3.12095900	-5.12921900
C	-5.55840100	0.78503800	-2.09852500
C	-5.76248700	-0.55404500	-1.36895900
C	-6.80053100	1.69854000	-1.91567400
H	-5.48310700	0.57365800	-3.17475500
C	-7.04933000	-1.25660500	-1.83291900
H	-5.81920300	-0.38614700	-0.28517800
H	-4.89792900	-1.20873400	-1.54001600
C	-8.08500500	0.99169900	-2.37932800
H	-6.89288400	1.96799200	-0.85378200
H	-6.66197900	2.63624400	-2.46878600
C	-8.27952600	-0.35289700	-1.66469000
H	-7.18063300	-2.18968100	-1.27204500
H	-6.94750400	-1.53955800	-2.89075900
H	-8.94603700	1.64758400	-2.20445800
H	-8.03425300	0.82558300	-3.46490500
H	-9.17448800	-0.85773600	-2.04690200
H	-8.45442600	-0.17339100	-0.59367500

#### TS4\*

Ni	-2.59735900	1.29743900	-0.54134700
C	-0.27593700	-0.65441000	2.40604800
C	0.61757100	0.00999000	1.63221500
N	-0.12285800	0.67624800	0.66830300
N	-1.54115600	-0.37589300	1.89984200
C	-1.46577600	0.44818800	0.81368500
C	-2.73530700	-0.92792100	2.50727200
C	-3.24785800	-0.30217200	3.66353900
C	-3.27761500	-2.11599100	1.97256800
C	-4.36903800	-0.88857700	4.26605300
C	-4.39864100	-2.65346800	2.61789800
C	-4.94236000	-2.04643600	3.74791000
H	-4.79128000	-0.43955800	5.15965000
H	-4.84455900	-3.56848400	2.24220400
H	-5.80719300	-2.48739400	4.23551900
C	0.44703000	1.50228500	-0.37539600
C	0.89719700	0.87626600	-1.55918100
C	0.55387000	2.89328900	-0.15351100
C	1.42056800	1.70504500	-2.56043400
C	1.08480700	3.66815800	-1.19240900

C	1.50439000	3.08456300	-2.38569900
H	1.78002700	1.26276100	-3.48428700
H	1.18522300	4.74096600	-1.05999500
H	1.91806400	3.70550200	-3.17531200
C	-2.63933900	-2.85281500	0.79686600
C	-3.66772000	-3.44627700	-0.18164300
C	-1.68981000	-3.95758200	1.31082300
H	-2.03822100	-2.13444200	0.23007900
H	-4.37422200	-2.68772400	-0.53395400
H	-3.14837700	-3.86347700	-1.05185500
H	-4.24248100	-4.26332700	0.26760600
H	-0.90148900	-3.55029400	1.95297100
H	-2.24082900	-4.70598100	1.89160200
H	-1.20820800	-4.47009500	0.47022700
C	0.89135600	-0.63909900	-1.75112900
C	2.32752000	-1.19660000	-1.65290300
C	0.22524800	-1.07149300	-3.07079200
H	0.31064900	-1.08586800	-0.93739300
H	2.79895600	-0.93643400	-0.69864200
H	2.31811400	-2.28870800	-1.74002800
H	2.96130000	-0.80112600	-2.45459000
H	-0.81169100	-0.72531500	-3.12499600
H	0.76475900	-0.69235100	-3.94581200
H	0.22180300	-2.16510500	-3.14188100
C	-2.59762100	0.92432300	4.30212300
C	-1.82514800	0.52510900	5.57804300
C	-3.60563900	2.04465300	4.61997500
H	-1.87135100	1.33598300	3.59290100
H	-1.06057000	-0.23145200	5.37126000
H	-1.32736300	1.39910600	6.01276900
H	-2.50260500	0.11278600	6.33416100
H	-4.16765400	2.35050100	3.73115000
H	-4.32921100	1.74062800	5.38390700
H	-3.07736600	2.92367400	5.00545800
C	0.18440200	3.55040800	1.17416900
C	-0.75552900	4.75761300	1.00022600
C	1.45782500	3.95639700	1.94605500
H	-0.34689700	2.81352900	1.78473700
H	-1.66937800	4.47788900	0.46400900
H	-1.04454600	5.15325600	1.98012500
H	-0.27895500	5.57400600	0.44695100
H	2.11261200	3.09589200	2.12159000
H	2.03457900	4.70659200	1.39347000
H	1.19339600	4.38585100	2.91886600

H	-0.13770000	-1.29375700	3.26309400
H	1.69376600	0.06920300	1.67307700
C	-2.89463400	2.02957200	-2.34184300
H	-1.79297800	1.85005500	-2.28899100
C	-4.18479700	1.94728600	0.47016600
C	-4.11361900	2.73676400	-0.71220300
H	-4.92766500	2.67540200	-1.42819000
H	-3.64736600	3.71691800	-0.65098900
C	-3.58022400	1.01949500	-3.22931400
H	-4.66882100	1.18747300	-3.25495000
H	-3.21254900	1.14226400	-4.26431400
O	-3.28815200	-0.28244100	-2.75458500
C	-3.83499100	-1.30747400	-3.57686200
H	-3.44242400	-1.24276900	-4.60141100
H	-3.54007100	-2.26084200	-3.13623500
H	-4.93199000	-1.24622600	-3.60960700
H	-3.02493200	3.04108900	-2.72710500
C	-5.33046700	0.99410600	0.76219900
C	-6.46391300	1.78792600	1.47316800
C	-5.90268300	0.23729200	-0.45046600
H	-4.96350600	0.24900000	1.47768000
C	-7.62571200	0.86831400	1.88053900
H	-6.83279800	2.56867100	0.79166900
H	-6.06673700	2.30480900	2.35571000
C	-7.05893000	-0.68871600	-0.03657000
H	-6.28237200	0.95520700	-1.19323400
H	-5.10765600	-0.33558800	-0.94178800
C	-8.17541600	0.08411200	0.68095200
H	-8.42033400	1.46551100	2.34408300
H	-7.27248700	0.16439900	2.64731100
H	-7.45835700	-1.20101700	-0.92059000
H	-6.67018700	-1.47049400	0.63142500
H	-8.96370800	-0.60461600	1.00759400
H	-8.64547600	0.78319900	-0.02622300
H	-3.72917200	2.37969500	1.36060000

### TS5

Ni	-1.11990200	0.74566200	-0.72196800
C	-1.53060000	-0.34579600	3.19636600
C	-0.31990300	0.25543100	3.30134800
N	0.00595200	0.73552700	2.03692400
N	-1.91885500	-0.22951100	1.86737600
C	-0.97583500	0.43542600	1.13744800
C	-3.18109700	-0.72363000	1.35523900

C	-4.29200800	0.14655000	1.35547400
C	-3.25892200	-2.06553000	0.92664600
C	-5.50804300	-0.36597300	0.88442200
C	-4.50209000	-2.52168700	0.47032500
C	-5.61352000	-1.68316000	0.44498500
H	-6.38742000	0.27071300	0.87601200
H	-4.60361000	-3.54971100	0.13748700
H	-6.56867800	-2.06105900	0.09138700
C	1.22594600	1.47137900	1.76760500
C	2.33830900	0.77560500	1.24834800
C	1.26585000	2.84387100	2.09505700
C	3.50994800	1.51148300	1.03012900
C	2.46689300	3.52516400	1.85652600
C	3.57444300	2.87073200	1.32561000
H	4.38860200	1.01311600	0.63431700
H	2.53819500	4.58107900	2.09759700
H	4.49607400	3.41907500	1.15239300
C	-2.07143400	-3.02225800	0.99488100
C	-1.89420900	-3.84136100	-0.29738400
C	-2.19231900	-3.95693800	2.21724200
H	-1.16208100	-2.42552600	1.12601800
H	-1.85843000	-3.19211500	-1.17818000
H	-0.96328400	-4.41788400	-0.24895900
H	-2.70810900	-4.55989800	-0.44309700
H	-2.25149500	-3.39335100	3.15475400
H	-3.09068200	-4.58056200	2.14693600
H	-1.32378100	-4.62240000	2.27745900
C	2.32045500	-0.73106300	1.00102000
C	2.87193900	-1.48599700	2.23026300
C	3.08605300	-1.14737800	-0.26778400
H	1.27841600	-1.04043200	0.86524700
H	2.29417400	-1.26586000	3.13424200
H	2.83740100	-2.56867000	2.06315700
H	3.91410300	-1.20691500	2.42272300
H	2.76374400	-0.57271300	-1.14302300
H	4.16733500	-1.01170700	-0.15918000
H	2.91890900	-2.21124100	-0.47125400
C	-4.22664100	1.57372100	1.89340300
C	-4.94559200	1.67499300	3.25501000
C	-4.79265200	2.60485400	0.89905200
H	-3.17508500	1.82958400	2.05801700
H	-4.51437900	0.98534800	3.98895600
H	-4.86449400	2.69153900	3.65613100
H	-6.01060300	1.43558100	3.15892100

H	-4.28675600	2.54389500	-0.07130500
H	-5.86494400	2.46296600	0.72604100
H	-4.65777800	3.61905000	1.29133500
C	0.09150100	3.58025900	2.73888500
C	-0.21117400	4.93498900	2.07035200
C	0.33862500	3.77976100	4.24999400
H	-0.80353200	2.95850800	2.62903500
H	-0.37435400	4.83150600	0.99271500
H	-1.11481400	5.37218800	2.50941100
H	0.60006700	5.65569700	2.21898400
H	0.50211900	2.82821000	4.76704300
H	1.22137900	4.40587000	4.42186300
H	-0.52093300	4.27437300	4.71610300
H	-2.14866700	-0.83892900	3.92963300
H	0.33727400	0.39051500	4.14523800
C	-3.18901700	0.44888500	-2.74824400
C	-1.67408500	0.44526800	-2.74610500
H	-3.57671100	1.38094200	-3.16936000
H	-3.54899000	-0.38196000	-3.36580400
H	-1.21722900	0.56210500	-3.72815000
O	-1.20541300	-0.74965600	-2.13881700
C	0.03477300	-1.27835100	-2.67714400
H	0.32700400	-2.09119500	-2.01344400
H	-0.15816000	-1.66568700	-3.68210500
H	0.80479200	-0.50526700	-2.70546900
H	-3.60065600	0.32092100	-1.74180900
C	-0.97502900	2.61413200	-0.88480200
C	-0.95573100	2.21015300	-2.28975200
H	-0.02987800	2.95298600	-0.46561200
H	-1.85297600	3.15758300	-0.53583500
H	-1.72610300	2.66267500	-2.92463900
O	0.29001400	2.12447800	-2.91297200
C	0.78812200	3.38973900	-3.36011300
H	1.73348700	3.18655300	-3.86504200
H	0.08876900	3.85675500	-4.06746300
H	0.96097800	4.07053200	-2.51782100

### TSS'

Ni	-1.14705500	0.68356600	-0.83134100
C	-2.03177700	-0.78006500	2.89674600
C	-0.81536900	-0.26081800	3.19155500
N	-0.33338300	0.32996700	2.02715900
N	-2.27113600	-0.50243100	1.55668400
C	-1.22479700	0.17963200	1.00306100

C	-3.45862000	-0.94527100	0.85025700
C	-4.58388400	-0.09238100	0.80757900
C	-3.45598400	-2.23932600	0.28646100
C	-5.71844100	-0.56708000	0.13659600
C	-4.62277800	-2.65910600	-0.36545600
C	-5.73896900	-1.83207100	-0.44632600
H	-6.60346800	0.05717200	0.07876600
H	-4.66020300	-3.64956500	-0.80766800
H	-6.63431400	-2.17862200	-0.95481600
C	0.97063800	0.96262400	1.95721300
C	2.07218200	0.19343400	1.52044500
C	1.10116900	2.29550000	2.40482400
C	3.32736100	0.81512900	1.51207000
C	2.38327800	2.86007000	2.37654300
C	3.48310100	2.13318300	1.93196900
H	4.19856300	0.25817900	1.18419300
H	2.52405700	3.88174700	2.71315300
H	4.46773400	2.59191400	1.92213700
C	-2.27335000	-3.19638600	0.41724900
C	-1.92300400	-3.89895200	-0.90790400
C	-2.53927300	-4.23928900	1.52403100
H	-1.39526900	-2.61397900	0.71652300
H	-1.78261200	-3.17590300	-1.71749700
H	-0.99917700	-4.47722900	-0.79029400
H	-2.70298200	-4.60315000	-1.21695100
H	-2.72924700	-3.76478900	2.49267800
H	-3.41185100	-4.85520500	1.27870700
H	-1.67700300	-4.90607600	1.63766600
C	1.94611700	-1.28093300	1.14081500
C	2.18945400	-2.18330600	2.37075800
C	2.88633500	-1.69669900	-0.00528000
H	0.91954600	-1.45568700	0.79920900
H	1.48348800	-1.96983200	3.17936100
H	2.08009400	-3.23944800	2.09870900
H	3.20275700	-2.03873700	2.76227500
H	2.81268600	-1.01857300	-0.86258900
H	3.93449900	-1.71849700	0.31121900
H	2.63725100	-2.70930200	-0.34254200
C	-4.61706500	1.25968800	1.51717800
C	-5.17509400	1.10188800	2.94900400
C	-5.41944300	2.32739600	0.75349400
H	-3.58946900	1.62914800	1.58958000
H	-4.58074500	0.40371600	3.54755900
H	-5.17760700	2.06843600	3.46571600

H	-6.20555900	0.72907300	2.92645100
H	-5.07127500	2.42611100	-0.27865600
H	-6.49294200	2.10871900	0.74081800
H	-5.29858800	3.29743100	1.24852300
C	-0.07415300	3.10192200	2.95590400
C	-0.04117800	4.58235400	2.53017500
C	-0.13114000	3.01408400	4.49721000
H	-0.99899500	2.66701200	2.55972000
H	0.10219400	4.69795500	1.45045700
H	-0.98332000	5.06867400	2.80581800
H	0.76171700	5.13435200	3.03068000
H	-0.23554000	1.98323600	4.84863000
H	0.78053100	3.42789000	4.94293100
H	-0.98381300	3.58631700	4.87975400
H	-2.74056100	-1.32066900	3.50314300
H	-0.24671000	-0.25901900	4.10709500
C	-2.90986900	0.43299200	-3.08388500
C	-1.40843100	0.47336800	-2.88753800
H	-3.27972400	1.39185000	-3.45536600
H	-3.15489400	-0.34470100	-3.81697200
H	-0.84557500	0.69398100	-3.79448100
O	-0.96588400	-0.75119100	-2.33185200
C	0.34273500	-1.19474500	-2.75563000
H	0.57504900	-2.07176400	-2.15325900
H	0.30161900	-1.46657700	-3.81476400
H	1.09402000	-0.41674800	-2.59041300
H	-3.43360700	0.19796200	-2.15184200
C	-1.20299500	2.58120400	-0.78525400
C	-0.85954300	2.26829100	-2.16643200
H	0.19972100	2.30591300	-2.41794000
O	-2.47438300	3.07872600	-0.54184100
C	-2.55542800	4.50776400	-0.54174500
H	-1.89488200	4.94179300	0.21877900
H	-2.29126900	4.91943500	-1.52532200
H	-3.59157000	4.75915700	-0.31056900
H	-0.41924700	2.98830400	-0.14147200
H	-1.50069400	2.71141800	-2.92568200

### TS6

Ni	-2.05537200	1.43073000	-0.35825700
C	-0.38829600	0.14534300	3.26475500
C	-1.58470800	0.60496300	3.69567600
N	-2.27707600	1.03952800	2.57070000
N	-0.35820000	0.32174400	1.88545800

C	-1.52838100	0.86966400	1.43228400
C	0.86850500	0.08462000	1.14727000
C	1.04829600	-1.14457700	0.47839200
C	1.88533700	1.05958800	1.24002700
C	2.28437100	-1.36155000	-0.14338900
C	3.10436400	0.77971800	0.60829800
C	3.30245900	-0.41279900	-0.07994600
H	2.46219700	-2.29335000	-0.66914600
H	3.91117700	1.50415000	0.66469200
H	4.25711900	-0.61122700	-0.55881900
C	-3.58040600	1.66576900	2.68309900
C	-3.66383400	3.07347000	2.59706700
C	-4.70289000	0.85142800	2.95757300
C	-4.93375100	3.65076700	2.72837100
C	-5.94279400	1.49009700	3.08944100
C	-6.06249800	2.87115800	2.96353400
H	-5.03669200	4.72942000	2.66669400
H	-6.82755700	0.89713200	3.29729900
H	-7.03546800	3.34273100	3.06748900
C	1.73268000	2.36018500	2.02776000
C	2.02531100	3.60631000	1.17035000
C	2.62546700	2.34797000	3.28641800
H	0.69436400	2.44154800	2.36318800
H	1.37390800	3.64837000	0.29135300
H	1.86063000	4.51441000	1.76135300
H	3.06325300	3.62804500	0.82056800
H	2.40464800	1.49109900	3.93225100
H	3.68690500	2.29640300	3.01949400
H	2.47162300	3.26156100	3.87139100
C	-2.43930600	3.97716600	2.46544600
C	-2.10156800	4.61418900	3.83081900
C	-2.60440600	5.06179400	1.38520200
H	-1.58470700	3.36239500	2.17094300
H	-1.91550000	3.85112200	4.59465000
H	-1.20455800	5.23870900	3.74950200
H	-2.92196000	5.24836600	4.18532900
H	-2.85185900	4.62382100	0.41170400
H	-3.39067600	5.78084000	1.63817100
H	-1.67141900	5.62633200	1.27819300
C	-0.00966600	-2.24498800	0.49453900
C	0.20755400	-3.18872500	1.69818300
C	-0.05872200	-3.05864300	-0.81048400
H	-0.98798300	-1.76831900	0.62182500
H	0.16347800	-2.65154500	2.65132000

H	-0.56162600	-3.96939200	1.71621900
H	1.18520200	-3.67971700	1.63455400
H	-0.14053000	-2.41248400	-1.69147000
H	0.83052900	-3.68557000	-0.93643200
H	-0.92219500	-3.73231400	-0.79687800
C	-4.61395600	-0.66174300	3.15647000
C	-5.67978200	-1.43747000	2.35746400
C	-4.71880000	-1.02316300	4.65452100
H	-3.63206900	-0.99735500	2.80400700
H	-5.66046200	-1.18058000	1.29400800
H	-5.50363600	-2.51462600	2.45317600
H	-6.69039400	-1.24223900	2.73156400
H	-3.94845100	-0.52777300	5.25491900
H	-5.69298500	-0.72702400	5.05936900
H	-4.61150700	-2.10464900	4.79346300
H	0.44843400	-0.27483300	3.79910500
H	-2.01006300	0.67116500	4.68379700
C	-1.12514300	2.79651600	-2.02272500
C	-2.48617000	2.56107400	-2.06400800
H	-0.76649200	3.69515100	-1.52216600
H	-0.71836100	2.04788600	-0.28829700
C	-4.23511300	0.78065900	-0.60260200
C	-3.60055500	-0.41957200	-0.64543100
H	-4.68914900	1.21035800	-1.48820900
H	-4.48252000	1.25020200	0.34422500
H	-3.28725700	-0.86323200	0.29795700
H	-3.18493000	3.27744200	-1.63526600
C	-3.42915000	-1.32755300	-1.84257800
C	-3.95183900	-2.73969800	-1.46066200
C	-4.10349200	-0.84820400	-3.14107100
H	-2.34810500	-1.43023500	-2.03185400
C	-3.77328000	-3.74768700	-2.60589100
H	-5.01818200	-2.66217400	-1.20404100
H	-3.43751400	-3.09507100	-0.55807400
C	-3.91681000	-1.85923200	-4.28517300
H	-5.17767200	-0.70555400	-2.95481500
H	-3.70585800	0.12617600	-3.44877200
C	-4.43196500	-3.25310900	-3.90089600
H	-4.19133500	-4.71694800	-2.30907600
H	-2.69978200	-3.90952700	-2.78120700
H	-4.43025000	-1.49551000	-5.18289600
H	-2.84871800	-1.92335600	-4.54059300
H	-4.24664000	-3.96306900	-4.71537100
H	-5.52203600	-3.21255400	-3.76277800

H	-2.88274200	1.89120200	-2.82032800
C	-0.16351500	2.14949400	-2.99149700
C	-0.09915100	3.05680000	-4.25376700
C	1.24963700	1.91966600	-2.42919000
H	-0.58304000	1.18062700	-3.29965800
C	0.85761000	2.48476000	-5.31163900
H	0.24314200	4.05861600	-3.95494600
H	-1.10454600	3.17955400	-4.67419500
C	2.20318400	1.35271500	-3.49161900
H	1.64565300	2.87834200	-2.06177100
H	1.20080300	1.24714200	-1.56762300
C	2.26130800	2.24480500	-4.73934800
H	0.90295600	3.16885600	-6.16734400
H	0.45053400	1.53625100	-5.69110500
H	3.20301700	1.23207900	-3.05809100
H	1.86617900	0.34549400	-3.77858200
H	2.90763000	1.79285900	-5.50104700
H	2.71668300	3.21051400	-4.47560400

### TS7

Ni	-3.00240400	0.27034500	-0.49677100
C	-1.86160800	0.29094300	3.49325100
C	-0.71900100	0.68507900	2.87977500
N	-0.98337900	0.69701500	1.51592800
N	-2.80752700	0.08080900	2.49479000
C	-2.27330400	0.32412800	1.26204300
C	-4.16527100	-0.34102500	2.78153500
C	-5.09040800	0.62774900	3.22844300
C	-4.48834100	-1.70984900	2.66327600
C	-6.38714900	0.18729600	3.52514300
C	-5.80103800	-2.08796000	2.97336100
C	-6.74245100	-1.15185900	3.39337000
H	-7.12602200	0.90188800	3.87329900
H	-6.08855400	-3.13134900	2.89850400
H	-7.75302300	-1.47035500	3.63298100
C	-0.00073300	1.04360000	0.50796200
C	0.93721500	0.06215800	0.11917200
C	0.01096100	2.35803000	-0.00721300
C	1.88270600	0.42521700	-0.84863400
C	0.97849800	2.65961500	-0.97423300
C	1.89989100	1.70500300	-1.39669600
H	2.62264600	-0.30129000	-1.16893400
H	1.02174200	3.66131500	-1.38982200
H	2.64518600	1.96474700	-2.14313800

C	-3.45028200	-2.77065600	2.30171900
C	-4.00333300	-3.87789900	1.38714600
C	-2.84535700	-3.38473500	3.58319800
H	-2.63718100	-2.27988100	1.75625800
H	-4.48354100	-3.46437400	0.49342200
H	-3.18776000	-4.53476700	1.06503900
H	-4.73646500	-4.50910400	1.90071300
H	-2.37681500	-2.62239900	4.21482200
H	-3.61864600	-3.88366200	4.17824500
H	-2.08233400	-4.12899800	3.32817300
C	0.99525100	-1.32576300	0.75449000
C	2.14897300	-1.40371600	1.77809900
C	1.12648300	-2.45691100	-0.28171000
H	0.05985900	-1.49341900	1.29938000
H	2.05454700	-0.64088500	2.55842400
H	2.16295900	-2.38542900	2.26456600
H	3.11783600	-1.25656000	1.28765800
H	0.32798700	-2.41569200	-1.02937600
H	2.08470700	-2.41979500	-0.81093000
H	1.07119200	-3.42961300	0.21930000
C	-4.71820600	2.09277000	3.45644200
C	-4.50291400	2.36861100	4.96089300
C	-5.75568600	3.08012500	2.88759700
H	-3.76914300	2.28818700	2.94505600
H	-3.73130800	1.72140600	5.39100700
H	-4.19702800	3.40896900	5.11829600
H	-5.42742100	2.20033300	5.52458700
H	-5.95149200	2.90386500	1.82502100
H	-6.71122500	3.02085000	3.41946300
H	-5.38905100	4.10655200	2.99868900
C	-0.92146300	3.45377100	0.50287300
C	-1.55830200	4.27512200	-0.63359400
C	-0.17581800	4.37769900	1.48954000
H	-1.73845300	2.97754300	1.05393700
H	-2.07011900	3.63113500	-1.35806600
H	-2.29147400	4.97869100	-0.22337200
H	-0.81625900	4.86648100	-1.18065500
H	0.23653800	3.81467600	2.33398800
H	0.65507500	4.89387600	0.99544300
H	-0.85515700	5.13916600	1.88941200
H	-2.09365300	0.13929700	4.53502100
H	0.24736100	0.95208800	3.27650700
C	-3.16923100	0.30565900	-2.55532300
C	-4.38386800	1.53460600	-0.28863500

C	-4.67813100	1.13317300	-1.66297900
H	-5.05426100	1.19953100	0.49806100
H	-3.98361800	2.53597300	-0.13421400
H	-4.57485700	1.95995600	-2.36719300
H	-3.79317800	0.15206300	-3.43187300
C	-5.94457900	0.31760300	-1.94825300
C	-6.17914700	-0.88790200	-1.01889300
C	-7.17463000	1.25750600	-1.91400100
H	-5.86837200	-0.06645400	-2.97673800
C	-7.45859600	-1.64767100	-1.40714900
H	-6.27231000	-0.54800100	0.02091100
H	-5.31460700	-1.56427700	-1.04615100
C	-8.46409700	0.50837000	-2.28764900
H	-7.27509000	1.68112300	-0.90430000
H	-7.02060000	2.10374000	-2.59647800
C	-8.68447900	-0.72272700	-1.39585800
H	-7.61019000	-2.48992300	-0.72135600
H	-7.33587200	-2.07962200	-2.41121700
H	-9.31963500	1.19042800	-2.21679400
H	-8.40510000	0.19154100	-3.33895800
H	-9.57591700	-1.27142400	-1.72190100
H	-8.87867600	-0.39428700	-0.36431800
C	-2.34717200	-0.97880800	-2.30004000
H	-1.34424300	-0.81198600	-2.71306500
H	-2.10698200	-1.18101700	-1.20722200
C	-2.95023600	-2.27930800	-2.87346500
C	-2.88919700	-2.29718100	-4.41595000
C	-2.24465000	-3.52740900	-2.30938800
H	-4.00748900	-2.32737600	-2.57479000
C	-3.47771700	-3.59403500	-4.99547900
H	-1.83770600	-2.20294000	-4.72743900
H	-3.41635100	-1.43245500	-4.83948100
C	-2.82886100	-4.82913600	-2.88073600
H	-1.17390500	-3.47354800	-2.55774500
H	-2.31332200	-3.53345300	-1.21298800
C	-2.78832200	-4.83729800	-4.41567500
H	-3.38944500	-3.58227600	-6.08824700
H	-4.55351900	-3.63462000	-4.77023000
H	-2.28054000	-5.68950300	-2.47874800
H	-3.86981100	-4.93665700	-2.54233300
H	-3.26066200	-5.74781700	-4.80266000
H	-1.74124200	-4.86120200	-4.75077300
H	-2.51975900	1.16648000	-2.73662100

**INT12**

Ni	-1.13866900	1.67647400	-0.29473700
C	0.39446000	-0.85801000	2.57370800
C	1.19888500	0.21599700	2.76843900
N	0.78643800	1.19872700	1.87675800
N	-0.50117700	-0.51022500	1.56661600
C	-0.25891900	0.76036300	1.13223800
C	-1.49612900	-1.39328500	1.01443000
C	-2.54116500	-1.88245300	1.81761300
C	-1.39237500	-1.74685000	-0.33447000
C	-3.47171900	-2.73503600	1.20614300
C	-2.33754000	-2.59229900	-0.90761400
C	-3.39323300	-3.10666500	-0.14122600
H	-4.29087500	-3.11942900	1.80934800
H	-2.24708900	-2.86441900	-1.95585000
C	-2.69060100	-1.52083100	3.27843900
H	-2.05122600	-2.14095400	3.91927500
H	0.38046300	-1.82920900	3.04172600
H	2.01724300	0.36116000	3.45521300
C	-1.33609200	3.40275200	-1.93895700
C	-1.85423300	2.16791100	-2.24002600
H	0.09859300	1.24159000	-0.94119500
H	-2.90872900	1.98848500	-2.05940100
H	-3.72146500	-1.67786700	3.60799400
H	-2.42557500	-0.47670900	3.47578500
H	-0.56419800	-1.36205900	-0.92088300
C	-4.40133100	-4.05299100	-0.74748000
H	-5.30963000	-4.11636200	-0.14110900
H	-4.68602500	-3.74102100	-1.75794000
H	-3.98644900	-5.06600800	-0.82648000
C	1.43933300	2.51524700	1.70774500
C	1.40024600	3.34075100	3.00426100
C	2.87329300	2.35309300	1.17677100
H	0.83910800	3.02300400	0.94427300
C	2.07128800	4.70988300	2.79682900
H	1.92742800	2.79665200	3.80028600
H	0.36166300	3.46234400	3.33680000
C	3.53707500	3.72569800	0.97622500
H	3.46195800	1.76441400	1.89405200
H	2.85393700	1.78654300	0.23799900
C	3.50427300	4.56212000	2.26395600
H	2.06651000	5.26440900	3.74188200
H	1.47609700	5.30079600	2.08536900
H	4.56874000	3.58597800	0.63420100

H	3.01275700	4.26761200	0.17547200
H	3.94166900	5.55055500	2.08306100
H	4.12943900	4.07885500	3.02848000
C	-2.80131000	2.59142200	1.04663800
C	-3.61061000	1.59314500	0.59561400
H	-2.97114500	3.63213900	0.79078000
H	-2.18437200	2.39707700	1.91497700
H	-3.48880000	0.56509600	0.92627100
O	-0.16902900	3.92539600	-2.30496600
C	0.66957800	3.18112000	-3.20243800
H	0.13660100	2.97457300	-4.13615100
H	1.53011800	3.81995300	-3.39674600
H	0.98863600	2.24553500	-2.73141300
H	-1.36341200	1.49938600	-2.93729600
H	-1.90390700	4.13157300	-1.36696900
O	-4.62008700	1.68387600	-0.27425500
C	-5.13181800	2.98394700	-0.61007600
H	-5.36604200	3.54559600	0.29985400
H	-4.41848700	3.54540000	-1.22237200
H	-6.03944800	2.80206900	-1.18461600

### INT13

Ni	-1.14364900	0.62992300	-0.99794200
C	-1.53149200	-0.35416700	3.03978000
C	-0.28488900	0.17868200	3.10107600
N	0.03640100	0.59896600	1.81562500
N	-1.94172600	-0.24878900	1.71607200
C	-0.97739100	0.33765300	0.94919400
C	-3.23937800	-0.65707100	1.23386600
C	-3.46117200	-1.98459000	0.83141300
C	-4.26542200	0.28939200	1.20603100
C	-4.74870700	-2.31390800	0.39069900
C	-5.53529100	-0.07127800	0.76146000
C	-5.79726100	-1.38469800	0.34900800
H	-4.94028600	-3.33692900	0.07494700
H	-6.32977700	0.66994800	0.74587300
H	-2.16114200	-0.78437800	3.80295100
H	0.38527200	0.29407200	3.93793600
C	-2.66580600	-0.17152100	-3.35735000
C	-1.27979500	-0.01060900	-2.78594900
H	-2.98208500	0.76389200	-3.83257800
H	-2.69728000	-0.96001600	-4.12227000
H	-0.49439200	0.23313800	-3.50685000
O	-0.89613600	-1.08695200	-1.94408100

C	0.41927700	-1.65592000	-2.12726200
H	0.64561000	-2.21669600	-1.21995100
H	0.38922900	-2.32891700	-2.98843900
H	1.16756300	-0.87246100	-2.28325300
H	-3.39344500	-0.42422000	-2.57932000
C	-1.79980700	2.55754700	-0.79842400
C	-0.94157300	2.73198100	-1.86533600
H	-1.52814900	2.94457900	0.17686400
H	-2.85908000	2.43818200	-1.01104700
H	-1.28176100	2.65990400	-2.89601100
C	1.30027900	1.26686100	1.44217800
C	1.49042400	2.58127500	2.21847300
C	2.50792600	0.33005700	1.61335800
H	1.18300200	1.50791900	0.38017500
C	2.79301900	3.27969400	1.79450100
H	1.52718800	2.36855300	3.29580300
H	0.62693200	3.23665000	2.05209200
C	3.81037500	1.03453800	1.19611900
H	2.58196600	0.02043600	2.66504700
H	2.35279300	-0.58327600	1.02526000
C	4.00842100	2.35471200	1.95621900
H	2.92529700	4.19457500	2.38287900
H	2.70672400	3.59409500	0.74415100
H	4.65983100	0.36263200	1.36296500
H	3.78131800	1.23789700	0.11517000
H	4.91644100	2.85846800	1.60547700
H	4.16308100	2.13999000	3.02324800
C	-2.36339200	-3.02071600	0.85701800
H	-1.56855200	-2.76824300	0.14580400
H	-1.89990200	-3.10295500	1.84671600
H	-2.75491900	-4.00527100	0.58767600
H	-4.06356200	1.30239700	1.54229500
C	-7.18040600	-1.79965200	-0.09294500
H	-7.77283100	-2.15176500	0.76148600
H	-7.72558600	-0.96440800	-0.54373100
H	-7.14269700	-2.61644200	-0.82056400
O	0.30506400	3.19163200	-1.68215200
C	1.12065800	3.32592400	-2.85638000
H	2.02266200	3.84928100	-2.54048300
H	1.38561700	2.34021300	-3.25547400
H	0.60408900	3.91492300	-3.62170000

#### INT14

Ni	-0.85135400	0.55108100	-0.91287600
----	-------------	------------	-------------

C	-1.60392600	-0.31099400	3.09474600
C	-0.32075500	0.10424200	3.24098100
N	0.13277300	0.46189500	1.97632700
N	-1.90534500	-0.19681400	1.74286200
C	-0.83672500	0.28140000	1.04095200
C	-3.19306600	-0.51818300	1.17454600
C	-3.44338100	-1.80546400	0.67161900
C	-4.18549100	0.46498000	1.17647800
C	-4.71947400	-2.05096700	0.14749000
C	-5.44414800	0.18673000	0.65018000
C	-5.73048200	-1.08126400	0.12512600
H	-4.93388800	-3.04240800	-0.24495600
H	-6.21104200	0.95664300	0.65594500
H	-2.32354100	-0.67122300	3.81329000
H	0.29565100	0.17388300	4.12289000
C	-2.06333900	-0.54526400	-3.37237400
C	-0.77648100	-0.19549200	-2.67222400
H	-2.39971300	0.29826300	-3.98296500
H	-1.92385500	-1.40598200	-4.04076100
H	0.05579800	0.11425100	-3.30782900
O	-0.38717400	-1.17487500	-1.72981200
C	0.99347400	-1.60867300	-1.72097800
H	1.17561000	-2.03925600	-0.73623900
H	1.11849200	-2.36812600	-2.49715400
H	1.66855500	-0.76658800	-1.89960400
H	-2.85474300	-0.79469200	-2.65790300
C	-1.40489000	2.50642200	-0.63630900
C	-1.26592800	2.40637600	-2.01000000
H	-0.64171500	2.97890400	-0.02467100
H	-2.38878400	2.42065400	-0.18409900
H	-2.16940000	2.18614500	-2.57634100
C	-0.13513900	2.98156100	-2.83796700
C	-0.53106100	4.41225400	-3.29640400
C	1.24371200	3.00556900	-2.15601700
H	-0.04540400	2.37527600	-3.75201200
C	0.54146000	5.02303600	-4.21265000
H	-0.66257600	5.04318900	-2.40609400
H	-1.50018700	4.38689100	-3.81055000
C	2.31622200	3.61055200	-3.07708200
H	1.18991800	3.59985200	-1.23263300
H	1.52965300	1.98594200	-1.85762200
C	1.92464800	5.01994300	-3.54627000
H	0.25127800	6.04444800	-4.48538100
H	0.58485000	4.45033800	-5.15042400

H	3.28177800	3.63541100	-2.55750400
H	2.44968100	2.95908500	-3.95323500
H	2.67981100	5.40935000	-4.23890100
H	1.91364800	5.69926800	-2.68152300
C	1.47682500	1.00884900	1.69811100
C	1.68289900	2.36223100	2.40034800
C	2.58534400	0.00772200	2.06499200
H	1.49132200	1.16904800	0.61444300
C	3.07379800	2.93835500	2.08654800
H	1.58173200	2.22673800	3.48599500
H	0.89348700	3.06050000	2.09548400
C	3.97410200	0.59084400	1.75061200
H	2.52511200	-0.22658400	3.13670200
H	2.42565900	-0.93531900	1.52696700
C	4.18895400	1.94461700	2.44370100
H	3.20972100	3.88076900	2.62882200
H	3.13191200	3.18390300	1.01585300
H	4.74715400	-0.12382000	2.05455700
H	4.07766900	0.71722700	0.66266300
H	5.16559100	2.35777100	2.16720600
H	4.20954100	1.79642700	3.53281900
C	-2.39362200	-2.89090400	0.69015200
H	-1.58254000	-2.66853200	-0.01225600
H	-1.94472500	-3.00507700	1.68336900
H	-2.82939900	-3.85277100	0.40678000
H	-3.96758900	1.44159800	1.59981200
C	-7.10398400	-1.40453200	-0.41287800
H	-7.78918400	-1.67054700	0.40230400
H	-7.54143300	-0.54779800	-0.93588800
H	-7.07643300	-2.25063000	-1.10608800

#### INT15'

Ni	-1.22835500	0.10273100	-0.91739900
C	-2.18451100	-1.86880400	2.51260100
C	-0.94364500	-1.47004300	2.89341400
N	-0.41237600	-0.73042200	1.84580600
N	-2.38789800	-1.35882000	1.23831700
C	-1.29925700	-0.64471900	0.81929700
C	-3.56347700	-1.60019100	0.43956900
C	-3.50148100	-2.48353100	-0.65271800
C	-4.75993300	-0.97490000	0.79785700
C	-4.68015100	-2.68323400	-1.38393400
C	-5.91429800	-1.20395700	0.05484800
C	-5.89141900	-2.06185900	-1.05384900
H	-4.65508800	-3.36909900	-2.22771600

H	-6.84035200	-0.71201700	0.33958200
H	-2.92838400	-2.46570900	3.01678800
H	-0.40127700	-1.65516800	3.80661200
C	-0.79996500	2.81347000	-3.91859900
C	-0.18513800	1.70886900	-3.06554500
H	-0.03929500	3.57593600	-4.11772100
H	-1.13955300	2.43758400	-4.88880900
H	0.63790700	1.24183200	-3.62247800
O	-1.15813300	0.64281300	-2.79488800
C	-1.47410800	-0.22861100	-3.88876400
H	-2.19240700	-0.96007600	-3.51333600
H	-1.93404700	0.33583600	-4.70417700
H	-0.57135300	-0.73746500	-4.24748100
H	-1.64416600	3.29385200	-3.41742400
C	-0.72773400	1.93363300	-0.55417400
C	0.31004100	2.14139700	-1.67316300
H	0.63192500	3.19121000	-1.71379700
C	0.96975700	-0.20152900	1.82809800
C	1.20193500	0.82086400	2.95232000
C	2.00035900	-1.34378500	1.87813800
H	1.06265300	0.30042700	0.86152500
C	2.63699800	1.37277700	2.89551900
H	1.03835700	0.33686600	3.92515400
H	0.46768200	1.63205900	2.87436100
C	3.43147100	-0.78337100	1.82073000
H	1.87000100	-1.91397500	2.80821300
H	1.81990100	-2.03881700	1.04883300
C	3.68003700	0.24524900	2.93380700
H	2.79250200	2.06980400	3.72652400
H	2.76394600	1.95661600	1.97204800
H	4.14924100	-1.60828100	1.89113300
H	3.59631500	-0.31026900	0.84152100
H	4.68907900	0.66303900	2.84276400
H	3.63694000	-0.25753200	3.91054500
C	-2.23873900	-3.23491800	-1.01575900
H	-1.43723000	-2.57695100	-1.38127900
H	-1.82767400	-3.77200300	-0.15324400
H	-2.44142300	-3.96717900	-1.80195600
H	-4.77726800	-0.30657300	1.65356600
C	-7.14748000	-2.33383500	-1.84626000
H	-7.70694400	-1.41154300	-2.03615100
H	-6.92377000	-2.80159400	-2.80949800
H	-7.81597100	-3.00974200	-1.29809600
H	1.20572500	1.56016200	-1.42545500

C	-1.95828100	2.84866600	-0.52615100
C	-2.94619200	2.47482200	0.59987300
C	-1.52689300	4.33344100	-0.35852000
H	-2.49890600	2.76517400	-1.47948000
C	-4.14752600	3.43021600	0.67333000
H	-2.40973200	2.48660800	1.56164600
H	-3.29857900	1.44836500	0.44992100
C	-2.73176200	5.28567900	-0.28901700
H	-0.93525300	4.42597400	0.56469300
H	-0.87060600	4.63879300	-1.18179200
C	-3.70628400	4.89121300	0.82783400
H	-4.80136900	3.13851100	1.50490000
H	-4.74634300	3.32665300	-0.24366800
H	-2.37587000	6.31289700	-0.14346900
H	-3.25938000	5.27276200	-1.25402100
H	-4.57832900	5.55591600	0.82467600
H	-3.21551300	5.02294200	1.80324900
H	-0.22726800	1.96951300	0.41806100

#### INT16'

Ni	-1.93119600	0.21979000	-0.13456800
C	-1.79472200	-3.56245600	1.70502600
C	-0.66554600	-3.69474300	0.96570900
N	-0.51094100	-2.51306200	0.25057100
N	-2.30120800	-2.29832600	1.42926400
C	-1.51327900	-1.63625700	0.52692100
C	-3.53580000	-1.77825600	1.95535300
C	-3.69425000	-1.56021200	3.33488200
C	-4.56780200	-1.49217800	1.05673200
C	-4.92413700	-1.04449000	3.76433900
C	-5.77583200	-0.97619800	1.51880100
C	-5.97528800	-0.74915200	2.88716700
H	-5.06197800	-0.86251500	4.82777600
H	-6.57352900	-0.76223900	0.81245500
H	-2.28835600	-4.24831200	2.37501300
H	0.02332900	-4.52048800	0.88680600
C	-1.74729700	-0.64583300	-4.37217400
C	-1.54985500	0.55553800	-3.44419800
H	-2.76832100	-0.65801300	-4.76871600
H	-1.06774200	-0.61273200	-5.22876600
H	-1.74643000	1.48315800	-4.00443000
O	-0.22562100	0.61843100	-2.90928200
C	0.76174700	1.02140900	-3.85199500
H	1.70192500	1.12289400	-3.30440500

H	0.90278500	0.28119800	-4.64926300
H	0.50494100	1.98882600	-4.30678800
H	-1.57415000	-1.58539400	-3.83427200
C	-2.54595300	1.65944300	-1.28519900
C	-2.52863800	0.51908400	-2.25686900
C	0.59390800	-2.25424300	-0.69637300
C	1.94824400	-2.18360700	0.03048900
C	0.61747000	-3.30014400	-1.82470500
H	0.36800900	-1.27764800	-1.13727400
C	3.09098600	-1.90180600	-0.95976200
H	2.13698700	-3.13799300	0.54128800
H	1.91110300	-1.41361200	0.81245300
C	1.75943100	-3.00908800	-2.81245500
H	0.75674700	-4.30224200	-1.39640700
H	-0.35110700	-3.30751400	-2.33954100
C	3.11716000	-2.93214100	-2.09869600
H	4.04715400	-1.89548100	-0.42424300
H	2.96299300	-0.89451800	-1.38336800
H	1.77727400	-3.78177300	-3.58930600
H	1.55831700	-2.05560300	-3.32115800
H	3.90765300	-2.68122200	-2.81531100
H	3.37012000	-3.92028300	-1.68864100
C	-2.60320100	-1.85294000	4.34001200
H	-2.57496800	-2.91544600	4.61312300
H	-1.60888200	-1.59438800	3.96027100
H	-2.77110200	-1.28928000	5.26188300
H	-4.42379600	-1.70084400	0.00060100
C	-7.29482900	-0.23021400	3.40625300
H	-7.16912600	0.32336600	4.34187600
H	-7.77963400	0.43061500	2.68065300
H	-7.98764900	-1.05774500	3.60683400
H	-2.25653200	-0.47790600	-1.71260100
C	-3.90201300	2.34892900	-1.11390700
C	-4.00329300	3.29643400	0.09747500
C	-4.23197800	3.13306100	-2.41688400
H	-4.67482800	1.57134700	-0.99420700
C	-5.34381700	4.04939900	0.15428900
H	-3.17549500	4.02069400	0.06039900
H	-3.88753200	2.72416500	1.02313800
C	-5.57952100	3.86718400	-2.34887000
H	-3.42917200	3.86508100	-2.59251400
H	-4.22475500	2.45087300	-3.27710400
C	-5.63899300	4.81215200	-1.14267300
H	-5.34103100	4.73460300	1.01078500

H	-6.15269700	3.32652500	0.33827400
H	-5.74282100	4.42062400	-3.28181200
H	-6.39278500	3.13012800	-2.27621800
H	-6.62075200	5.29702900	-1.08429100
H	-4.89925200	5.61556600	-1.27236400
H	-1.72140300	2.36618300	-1.40894400
H	-3.53736100	0.28387100	-2.61421900
C	-1.54527500	1.25976300	1.61301500
C	-0.31393400	1.42680700	1.01415000
H	-2.18062400	2.12801200	1.73304100
H	-1.66790400	0.44761900	2.31990600
H	0.44884500	0.64689100	1.04146200
O	0.05577600	2.59299900	0.49556300
C	1.27002900	2.60863800	-0.27451500
H	1.50467300	3.65882600	-0.44589500
H	2.08515700	2.13517000	0.28427900
H	1.10331100	2.09461400	-1.22409000

#### INT17'

Ni	-1.90150300	-0.05730800	-0.59453100
C	-1.98281200	-3.42528100	1.77217700
C	-0.80776100	-3.64315900	1.13255900
N	-0.61521300	-2.57152300	0.26613400
N	-2.48811700	-2.22340400	1.28606100
C	-1.64475200	-1.68997000	0.35645500
C	-3.74932300	-1.65601800	1.69738000
C	-3.87222900	-1.05528300	2.96179500
C	-4.83970300	-1.75164400	0.83085800
C	-5.13095200	-0.55068100	3.31164600
C	-6.07746900	-1.23935500	1.21135100
C	-6.24349800	-0.63385800	2.46432100
H	-5.24569100	-0.07939200	4.28515900
H	-6.92294600	-1.32163300	0.53356400
H	-2.50969400	-4.00762600	2.51147100
H	-0.10566400	-4.45709400	1.21639700
C	-1.45483100	-0.91656000	-4.10899600
C	-1.38931900	0.50470700	-3.53889000
H	-2.43333500	-1.08780800	-4.57095800
H	-0.69935000	-1.07666700	-4.88321600
H	-1.52611800	1.21298700	-4.37743700
O	-0.14066400	0.80060100	-2.90959700
C	0.95595100	0.89176000	-3.81227000
H	1.81179800	1.25329500	-3.23688700
H	1.21627300	-0.07958000	-4.25046200

H	0.74541000	1.60175700	-4.62523900
H	-1.31583400	-1.65819200	-3.31711000
C	-2.57756300	1.76304600	-1.61310600
C	-2.52119100	0.78140200	-2.56888600
C	0.54620200	-2.41296500	-0.63283600
C	1.85279500	-2.24490900	0.16268700
C	0.64455700	-3.57847400	-1.63222600
H	0.34460500	-1.48933800	-1.18706700
C	3.05132600	-2.06014900	-0.78346300
H	2.01701100	-3.13480100	0.78588000
H	1.76401600	-1.39314700	0.84926700
C	1.84542400	-3.39053300	-2.57428000
H	0.76106200	-4.52262500	-1.08247100
H	-0.28966600	-3.65669000	-2.20118100
C	3.15622100	-3.21251400	-1.79372100
H	3.97269200	-1.97790000	-0.19580000
H	2.94157600	-1.10948200	-1.32688600
H	1.91530100	-4.24829100	-3.25260600
H	1.67353600	-2.50676700	-3.20621100
H	3.98727700	-3.03338600	-2.48554800
H	3.39087900	-4.14387200	-1.25902100
C	-2.71240000	-0.95747200	3.92532000
H	-2.47630900	-1.92844800	4.37841800
H	-1.79934200	-0.60488300	3.43368200
H	-2.94571800	-0.26676300	4.74015100
H	-4.71196300	-2.23272300	-0.13376300
C	-7.59151900	-0.11544900	2.90577800
H	-7.49176700	0.71317000	3.61378800
H	-8.18695300	0.23112700	2.05517100
H	-8.16786500	-0.90450000	3.40613200
H	-2.73215700	-1.01337900	-1.31170000
C	-3.90273300	2.27762800	-1.08030300
C	-3.88543400	2.66307600	0.41318200
C	-4.32603200	3.49775900	-1.94322800
H	-4.65947800	1.49121100	-1.21955400
C	-5.21894800	3.27840600	0.86908500
H	-3.07142000	3.38256900	0.58801900
H	-3.66900500	1.77589300	1.02040300
C	-5.66080700	4.10127100	-1.48030000
H	-3.53935900	4.26468700	-1.88117900
H	-4.38821200	3.19707900	-2.99672900
C	-5.62079700	4.48157600	0.00577300
H	-5.14675000	3.57062900	1.92391100
H	-6.00506500	2.51135000	0.81160300

H	-5.90061500	4.97707900	-2.09533800
H	-6.46590000	3.37122500	-1.64889800
H	-6.59551900	4.86922000	0.32531300
H	-4.89649400	5.29580900	0.15441000
H	-1.71167100	2.39958100	-1.45580200
H	-3.46160400	0.32549600	-2.87521000
C	-0.67835600	1.08419800	1.01501000
C	0.19093100	1.75098600	0.20902900
H	-1.49829100	1.61520600	1.48681400
H	-0.32078300	0.17686400	1.48266100
H	1.09647300	1.27520600	-0.16856900
O	0.00365200	3.01880600	-0.14885300
C	0.94141800	3.59442900	-1.07705400
H	0.77361100	4.67062200	-1.04438600
H	1.96901700	3.37316000	-0.77014500
H	0.74959100	3.21102600	-2.08184700

### TS2-1

Ni	-1.01570300	0.66663700	-0.69628100
C	-1.61317800	-0.20355100	3.25534100
C	-0.39070300	0.37134700	3.35997800
N	-0.00862100	0.73874600	2.07171200
N	-1.95526800	-0.17168700	1.90627700
C	-0.96854600	0.40732200	1.16228300
C	-3.19291000	-0.68808700	1.38441600
C	-4.13556300	0.18741800	0.83964000
C	-3.44643700	-2.05894300	1.46493300
C	-5.34175200	-0.32365300	0.35614700
C	-4.65778000	-2.55901500	0.98420400
C	-5.60306000	-1.69441800	0.42730900
H	-6.08361300	0.35228800	-0.05879900
H	-4.86022800	-3.62398100	1.04442600
H	-6.54552900	-2.08683200	0.05753800
C	1.25640600	1.35336200	1.76971800
C	2.21933800	0.63905300	1.05403000
C	1.51958200	2.64102500	2.24238100
C	3.45902200	1.22895000	0.80108100
C	2.76343100	3.22132300	1.98704000
C	3.73195900	2.51766000	1.26675300
H	4.21638700	0.67490000	0.25455400
H	2.97434400	4.22138100	2.35345900
H	4.70079800	2.96943500	1.07627400
H	-2.27312400	-0.61829300	4.00089200
H	0.24821300	0.53972900	4.21246400

C	-2.87102900	0.23363100	-3.09689000
C	-1.38517500	0.41997900	-2.83542200
H	-3.26919500	1.04252500	-3.71591700
H	-3.02654200	-0.71184600	-3.62750100
H	-0.79970700	0.52066200	-3.74914100
O	-0.92441500	-0.74979900	-2.12823200
C	0.26085800	-1.39956900	-2.62978700
H	0.46070900	-2.22560700	-1.94645700
H	0.05983000	-1.78944900	-3.63244700
H	1.11457000	-0.71638000	-2.65351800
H	-3.44013600	0.19318000	-2.16259100
C	-1.22227600	2.50999600	-0.82524100
C	-1.09134200	2.21153800	-2.27950000
H	-0.40532700	3.05706100	-0.35733600
H	-2.20372600	2.84687200	-0.48823500
H	-1.99195700	2.51502600	-2.81510300
C	0.15415800	2.74305100	-3.01089000
C	0.03396200	4.27612400	-3.18755400
C	1.50546700	2.39133300	-2.36407100
H	0.15125200	2.31440100	-4.02577900
C	1.20810900	4.84232100	-4.00241600
H	0.01174600	4.75272300	-2.19740900
H	-0.91779500	4.52318500	-3.67618400
C	2.68100600	2.94634000	-3.18621200
H	1.55306600	2.80961200	-1.35045900
H	1.60825500	1.30364800	-2.25038300
C	2.56088600	4.46496300	-3.38168100
H	1.11223300	5.93184000	-4.07763900
H	1.15644600	4.45364200	-5.02983300
H	3.62713800	2.69890200	-2.68990800
H	2.70449600	2.45248000	-4.16871800
H	3.38144600	4.83124000	-4.00963400
H	2.66547100	4.96381300	-2.40701100
H	-3.93157500	1.25308400	0.81797500
H	-2.70145100	-2.72312500	1.89319300
H	0.75845400	3.17902700	2.79988200
H	2.00309300	-0.37188200	0.72265800

#### TS2'-1

Ni	-0.87040700	0.37046800	-0.81186200
C	-1.89561100	-0.38422500	3.08603800
C	-0.57618600	-0.14948900	3.28145000
N	-0.02074800	0.09008100	2.02585300
N	-2.12089400	-0.28217200	1.71588000

C	-0.96896800	0.02040800	1.04691100
C	-3.40742000	-0.45353100	1.10236900
C	-4.49770800	0.27358600	1.58708500
C	-3.55969900	-1.35609000	0.04593900
C	-5.75254200	0.09697800	1.00211200
C	-4.81745700	-1.51684000	-0.53816700
C	-5.91356000	-0.79333000	-0.06204300
H	-6.60184300	0.66031900	1.37641700
H	-4.94323700	-2.22448400	-1.35232100
H	-6.89178100	-0.92910300	-0.51312400
C	1.37125400	0.37544600	1.82274700
C	2.13468100	-0.44921900	0.99328500
C	1.95542400	1.45083500	2.49628100
C	3.49320400	-0.17863200	0.82049200
C	3.31700500	1.70682400	2.32568000
C	4.08526200	0.89825000	1.48491800
H	4.09431200	-0.82374900	0.18632100
H	3.77499100	2.54081400	2.84862400
H	5.14431900	1.09986600	1.35662600
H	-2.68099600	-0.64748300	3.77670600
H	0.02490200	-0.16496000	4.17678100
C	-1.40886700	-0.04359700	-4.15590500
C	-0.57997300	0.22143300	-2.91543500
H	-1.55376500	0.86767400	-4.74249700
H	-0.89094500	-0.77392100	-4.78847900
H	0.39958000	0.65717000	-3.12958400
O	-0.40103100	-1.00548600	-2.18857700
C	0.87477000	-1.65719300	-2.36374000
H	0.86754800	-2.51686400	-1.69247500
H	0.96992500	-1.99868800	-3.39867200
H	1.69751600	-0.98132400	-2.10862600
H	-2.38717200	-0.45539200	-3.89041600
C	-1.47007900	2.18149100	-0.81642700
C	-1.54244700	1.78927700	-2.22592000
H	-2.44203900	2.20034400	-0.31904500
H	-2.53746000	1.54080800	-2.58747700
H	-0.98270500	2.40407800	-2.92916600
C	-0.53487300	3.28813200	-0.34247100
C	0.89281100	3.22211000	-0.92091200
C	-1.16478500	4.67751300	-0.62217600
H	-0.45061600	3.18739700	0.75034200
C	1.77348100	4.37265000	-0.40503800
H	0.85174900	3.28164100	-2.01952300
H	1.35164900	2.25651300	-0.66978300

C	-0.28126300	5.82417900	-0.10656700
H	-1.31154600	4.78994800	-1.70701800
H	-2.16186900	4.73091900	-0.16615500
C	1.13924900	5.74309200	-0.68308600
H	2.76848000	4.31143100	-0.86248800
H	1.92077300	4.25187900	0.67780600
H	-0.74197500	6.78737700	-0.35637100
H	-0.23219400	5.77729500	0.99121300
H	1.76506000	6.54089000	-0.26575800
H	1.10114500	5.91263200	-1.76920200
H	1.67127900	-1.30941000	0.52189600
H	1.34863300	2.08339400	3.13739900
H	-4.36192100	0.97752200	2.40294000
H	-2.71033600	-1.93988400	-0.29395600

### TS2-2

Ni	-1.02979300	0.62854100	-0.73090100
C	-1.55524700	-0.03043900	3.27634200
C	-0.21780100	0.19665300	3.26905500
N	0.13642800	0.45002600	1.95196000
N	-1.98762400	0.08997600	1.96405300
C	-0.94916000	0.38276800	1.13456500
C	-3.37499400	-0.09711900	1.54775800
C	1.50180300	0.73696500	1.52171400
H	-2.22879700	-0.26358200	4.08668600
H	0.50349700	0.20130200	4.07178700
C	-2.82576800	0.12082400	-3.18568900
C	-1.35625700	0.35478000	-2.87552500
H	-3.22370100	0.90348400	-3.83749000
H	-2.93875500	-0.84116200	-3.69662700
H	-0.74557300	0.47432200	-3.77005900
O	-0.87654800	-0.79347600	-2.14705800
C	0.32085300	-1.43431800	-2.63601200
H	0.53534500	-2.24156800	-1.93515000
H	0.12542100	-1.84832000	-3.62977100
H	1.16209600	-0.73617700	-2.67522000
H	-3.43046500	0.08997800	-2.27324900
C	-1.34209100	2.45552400	-0.86932900
C	-1.14390200	2.16079400	-2.31664900
H	-0.58399900	3.06645200	-0.38148400
H	-2.35439000	2.72557100	-0.56304300
H	-2.03260800	2.42870900	-2.88969300
C	0.11314000	2.72892100	-2.99828400
C	-0.03424200	4.25983600	-3.17347100

C	1.44868500	2.40365700	-2.30418300
H	0.16027200	2.30501000	-4.01374700
C	1.15668500	4.85360500	-3.94360000
H	-0.10299200	4.73260500	-2.18364500
H	-0.97268000	4.48754900	-3.69569800
C	2.64182400	2.98708800	-3.08086300
H	1.44830700	2.82505200	-1.28911600
H	1.56850600	1.31613600	-2.19340900
C	2.49423800	4.50347800	-3.27546400
H	1.04012500	5.94090300	-4.01866700
H	1.15040500	4.46771200	-4.97320200
H	3.57569900	2.75788000	-2.55379700
H	2.70892600	2.49696100	-4.06288400
H	3.32864300	4.88875300	-3.87263500
H	2.55413200	5.00183000	-2.29691800
H	-3.67570800	-1.14002400	1.68335800
H	-4.03084500	0.55040400	2.13580100
H	-3.45865400	0.16880100	0.49393300
H	2.14353600	-0.13257000	1.69160700
H	1.48734900	0.97570700	0.45854900
H	1.89673000	1.59182100	2.07753800

#### TS2'-2

Ni	-1.11071700	0.49308700	-0.87389500
C	-1.54268100	-0.57813500	3.06507700
C	-0.18765000	-0.55667000	3.00910900
N	0.15196200	-0.20417800	1.71062400
N	-1.99872600	-0.23628200	1.80074400
C	-0.96016300	-0.00071600	0.95219200
C	-3.41336600	-0.16590300	1.44306800
C	1.52929800	-0.07256800	1.24613400
H	-2.21355900	-0.80864100	3.87841700
H	0.55520400	-0.76226300	3.76448600
C	-2.18529600	0.35110800	-4.11846700
C	-1.15320400	0.40173400	-3.01097900
H	-2.23985500	1.30097700	-4.65725700
H	-1.90610900	-0.42950400	-4.83545600
H	-0.14927000	0.65603700	-3.36082400
O	-1.11069300	-0.86134100	-2.33090800
C	-0.00913400	-1.73508500	-2.66641100
H	-0.05279100	-2.55897800	-1.95376500
H	-0.14387700	-2.11324000	-3.68371300
H	0.94769500	-1.20871600	-2.58239400
H	-3.17543600	0.10917700	-3.72066200

C	-1.35189000	2.37619600	-0.74859800
C	-1.68165500	2.07892700	-2.14943200
H	-2.23034800	2.55226100	-0.12308700
H	-2.74485900	2.05137700	-2.37750700
H	-1.11129700	2.62052300	-2.90227200
C	-0.17926800	3.27501300	-0.36962900
C	1.09943000	3.07192000	-1.20605800
C	-0.60445400	4.76580300	-0.41159500
H	0.07000600	3.04607900	0.67797000
C	2.23815200	3.99470200	-0.73915600
H	0.88907500	3.28752700	-2.26448500
H	1.42167000	2.02159300	-1.16042900
C	0.52992400	5.69559500	0.04771800
H	-0.89836800	5.02389500	-1.44009200
H	-1.49359900	4.91523600	0.21430600
C	1.81257700	5.47020300	-0.76559200
H	3.12353200	3.84056700	-1.36754200
H	2.52918500	3.71863600	0.28524300
H	0.20646100	6.74021200	-0.03105000
H	0.73583900	5.51279200	1.11245900
H	2.62171500	6.10237200	-0.38174300
H	1.64280000	5.77922300	-1.80728700
H	1.51685900	0.10929200	0.17194400
H	2.02353100	0.76525700	1.74639400
H	2.08223500	-0.99338900	1.45135900
H	-3.88610400	-1.14228900	1.58159200
H	-3.92319900	0.57588700	2.06424700
H	-3.49123300	0.12387600	0.39492500

### TS8

Ni	-1.23754800	1.59881800	-0.39381900
C	0.37413500	-0.82007100	2.56985000
C	1.13699200	0.28545200	2.75358000
N	0.70987500	1.22958100	1.82668800
N	-0.50823100	-0.52800700	1.53390400
C	-0.30281300	0.73892000	1.06773300
C	-1.46944600	-1.45379800	0.99287200
C	-2.54654600	-1.90254000	1.77573100
C	-1.29769300	-1.89560100	-0.32291900
C	-3.44224600	-2.80123700	1.17710300
C	-2.20771600	-2.78541500	-0.88487600
C	-3.29972700	-3.25431600	-0.13937500
H	-4.28333700	-3.15866800	1.76642900
H	-2.06092000	-3.13049400	-1.90501700

C	-2.75868400	-1.45616800	3.20469900
H	-2.12294700	-2.01374600	3.90391000
H	0.38242700	-1.77930900	3.06245200
H	1.93571800	0.47558700	3.45247400
C	-1.98739100	2.48849200	-2.16575600
C	-0.81526200	1.82275400	-2.51168900
H	0.00836800	1.25662000	-1.11464600
H	-0.91341900	0.82542400	-2.92898000
H	-3.79527100	-1.62464100	3.50962700
H	-2.53119600	-0.39388600	3.34370200
H	-0.43725100	-1.55094700	-0.88814800
C	-4.29142300	-4.21802000	-0.74585000
H	-5.00169700	-4.58638500	-0.00039100
H	-4.86666400	-3.73990300	-1.54836200
H	-3.78343600	-5.08377300	-1.18572900
C	1.31383500	2.56620900	1.64627400
C	1.22270900	3.41242000	2.92684200
C	2.76135500	2.45433900	1.13922700
H	0.70326500	3.03859100	0.86764200
C	1.84058000	4.80383300	2.70376500
H	1.76034400	2.90442600	3.73947000
H	0.17547400	3.49687000	3.24265900
C	3.37411800	3.84812000	0.92345500
H	3.36103100	1.90251200	1.87627100
H	2.78169500	1.86987600	0.21121200
C	3.28630400	4.70661900	2.19405200
H	1.79902200	5.37480100	3.63801500
H	1.23169600	5.35749100	1.97382700
H	4.41584200	3.74364100	0.60011600
H	2.84350000	4.35453100	0.10320600
H	3.68555900	5.70879400	2.00089300
H	3.91919400	4.26395800	2.97648500
C	-2.87236400	2.44085500	0.83139100
C	-3.67670700	1.45171800	0.33242600
H	-3.01038900	3.47940600	0.54944500
H	-2.34154600	2.24454700	1.75445400
H	-3.58202700	0.42004500	0.66279000
O	-2.15100700	3.83630200	-2.03295200
C	-1.04409500	4.69106800	-2.32548100
H	-0.70861200	4.55430300	-3.36024300
H	-1.41120000	5.70899700	-2.19277000
H	-0.20733200	4.51384900	-1.63886300
H	0.08164900	2.35932200	-2.80360000
O	-4.65475500	1.56527400	-0.56580700

C	-5.18893600	2.87501300	-0.85632100
H	-5.47897200	3.36899100	0.07640100
H	-4.46662200	3.49106200	-1.39703900
H	-6.06739700	2.69479200	-1.47513400
H	-2.94449900	1.98474000	-2.25676600

### TS9

Ni	-0.88374600	0.50539600	-0.74438800
C	-0.21970800	0.56112100	3.31151800
C	-1.31108800	-0.24214900	3.25571900
N	-1.65819400	-0.35841900	1.91624600
N	0.07899600	0.92245400	2.00250800
C	-0.80662600	0.35569100	1.13180600
C	1.18711700	1.77815300	1.65510900
C	2.41734900	1.21781100	1.27496200
C	1.02409500	3.15998100	1.76847600
C	3.46721000	2.10220000	0.99731900
C	2.08976500	4.01215700	1.48742500
C	3.33304200	3.49335100	1.09984300
H	4.42894300	1.68718700	0.70444500
H	1.95618300	5.08667300	1.57961800
H	0.37005100	0.90663800	4.14602900
H	-1.86030500	-0.73202100	4.04367900
C	-2.54470300	-0.36681300	-3.21060700
C	-1.13322100	0.08610100	-2.87377100
H	-3.01870600	0.31471800	-3.92255200
H	-2.50739600	-1.36310300	-3.66402500
H	-0.51955900	0.25290600	-3.75855000
O	-0.51640700	-0.95416700	-2.08524800
C	0.76883600	-1.43789000	-2.52685800
H	1.08647300	-2.16790500	-1.78160900
H	0.65373000	-1.92700300	-3.49904000
H	1.50064500	-0.62801900	-2.59392400
H	-3.17492600	-0.42426900	-2.31701200
C	-1.44975700	2.26248800	-0.96949200
C	-1.20577200	1.93264700	-2.39974400
H	-0.77343300	2.97830800	-0.50615800
H	-2.49046400	2.40669800	-0.67428600
H	-2.12216200	2.03395500	-2.98257900
C	-0.04356000	2.64393400	-3.11328500
C	-0.40398300	4.13271100	-3.33711100
C	1.32592800	2.52694300	-2.42030400
H	0.05321800	2.19712100	-4.11586000
C	0.69163300	4.86201800	-4.13160400

H	-0.53766900	4.62301000	-2.36286300
H	-1.36541000	4.21000200	-3.86182600
C	2.42304100	3.24864400	-3.22118800
H	1.27427400	2.96256400	-1.41456800
H	1.59811500	1.47138100	-2.28278200
C	2.06505700	4.72309500	-3.45916400
H	0.42424700	5.91958800	-4.24119000
H	0.73952200	4.44623900	-5.14836500
H	3.37936800	3.16804300	-2.69079900
H	2.55882500	2.74601900	-4.19002400
H	2.83661000	5.20550300	-4.07064900
H	2.05275900	5.25216000	-2.49494100
C	-2.80575800	-1.14420300	1.41516300
C	-2.64547800	-2.64012500	1.73337400
C	-4.13932000	-0.58871200	1.94239000
H	-2.77490500	-1.01166000	0.32752800
C	-3.83581500	-3.44423600	1.18344400
H	-2.58729000	-2.77629400	2.82217200
H	-1.70004600	-3.00687600	1.31508500
C	-5.32396500	-1.40084900	1.39191600
H	-4.14486300	-0.63784400	3.04009600
H	-4.23101800	0.47005200	1.67074200
C	-5.17526500	-2.89817300	1.70045700
H	-3.71951500	-4.49943100	1.45504500
H	-3.82361400	-3.40283100	0.08430100
H	-6.25876700	-1.01192500	1.81094800
H	-5.38823700	-1.25660500	0.30315700
H	-6.00667000	-3.45875000	1.25815600
H	-5.23699300	-3.05337000	2.78713700
C	2.61877200	-0.27625500	1.18303600
H	2.42213900	-0.77029800	2.14203800
H	1.94373700	-0.73042400	0.44799200
H	3.64574600	-0.51145600	0.89102600
H	0.06328700	3.55969500	2.08043300
C	4.50672300	4.40679300	0.83709500
H	4.18806800	5.34832400	0.37800200
H	5.01979600	4.66081800	1.77359900
H	5.24384400	3.93705500	0.17869900

### TS9'

Ni	-0.96753400	0.49105700	-1.11800300
C	-2.22613400	-1.81722100	2.01378600
C	-1.00188100	-1.49456500	2.50205700
N	-0.39193700	-0.67582700	1.55973900

N	-2.33912700	-1.18929100	0.77988400
C	-1.20909300	-0.47725700	0.49196200
C	-3.48936600	-1.29853900	-0.08482000
C	-3.62456400	-2.41460000	-0.92843000
C	-4.46167400	-0.29773000	-0.04504500
C	-4.77065800	-2.47768600	-1.72980000
C	-5.58914100	-0.39026400	-0.85884800
C	-5.76365800	-1.48868700	-1.71164300
H	-4.89347500	-3.33345800	-2.38973700
H	-6.34414800	0.39045600	-0.82064400
H	-3.02136600	-2.41933800	2.42468700
H	-0.52260500	-1.77456000	3.42641000
C	-2.49083600	0.94643000	-3.55618700
C	-1.02244600	0.82560200	-3.19661800
H	-2.75062800	1.98292500	-3.78691600
H	-2.69428000	0.33324500	-4.44140300
H	-0.35152600	1.18001000	-3.97958000
O	-0.72990200	-0.53282900	-2.89844000
C	0.59536500	-0.98824200	-3.25138800
H	0.67826400	-2.00409900	-2.86503800
H	0.69497500	-0.99367400	-4.34106900
H	1.36518000	-0.35288100	-2.80202500
H	-3.13766200	0.59595700	-2.74563500
C	-0.82472100	2.33102900	-0.61847900
C	-0.47669200	2.31702300	-2.04600800
H	-1.06135600	2.98023800	-2.68182400
C	0.97891000	-0.13779100	1.68457900
C	1.12757700	0.76039300	2.92354600
C	2.02425100	-1.26674600	1.67557300
H	1.11654500	0.47286500	0.78637700
C	2.55360700	1.33065500	3.01204400
H	0.91640000	0.17348700	3.82813200
H	0.38487100	1.56611200	2.88670700
C	3.44769300	-0.69185900	1.76829500
H	1.84488500	-1.93502800	2.52907100
H	1.90549000	-1.87177900	0.76795700
C	3.61129700	0.21664400	2.99603500
H	2.64816300	1.93753600	3.91944700
H	2.72569800	2.01029600	2.16432900
H	4.17263300	-1.51307500	1.79771900
H	3.66610600	-0.11627600	0.85650200
H	4.61712100	0.65155000	3.01157200
H	3.51793800	-0.38717800	3.91004600
C	-2.58342000	-3.50743300	-0.97949700

H	-1.59209900	-3.10620000	-1.22050300
H	-2.49283000	-4.02961800	-0.01956000
H	-2.84129500	-4.25084500	-1.73826600
H	-4.33451100	0.54333200	0.62924400
C	-7.00337800	-1.62211900	-2.56348200
H	-7.39241900	-0.64378800	-2.86317800
H	-6.80929300	-2.20594900	-3.46867100
H	-7.80185800	-2.13367800	-2.01059800
H	0.58679600	2.37020500	-2.27651800
C	-2.04750600	3.10371500	-0.13715500
C	-2.35784400	2.83053300	1.34745200
C	-1.85253900	4.62915100	-0.34955600
H	-2.92102900	2.79798800	-0.73475500
C	-3.56745600	3.63519200	1.84885500
H	-1.47359800	3.10229400	1.94506300
H	-2.51889300	1.75812900	1.50562500
C	-3.06159400	5.43894400	0.14525000
H	-0.95011100	4.94720300	0.19365200
H	-1.66827500	4.84300000	-1.41028800
C	-3.37915300	5.14115700	1.61713600
H	-3.73514500	3.43001700	2.91319400
H	-4.47220600	3.29805000	1.32025500
H	-2.87026700	6.50946300	0.00413000
H	-3.93752000	5.19471600	-0.47376100
H	-4.27545800	5.68916300	1.93078500
H	-2.55423500	5.50389900	2.24745900
H	0.03456100	2.43189900	0.04909600

### TS9-1

Ni	-0.88752800	0.52268200	-0.72993200
C	-0.21510900	0.54729500	3.33026600
C	-1.31032900	-0.25079500	3.26672900
N	-1.65970400	-0.34995700	1.92678700
N	0.08366600	0.92148300	2.02510900
C	-0.80489500	0.36783500	1.15002200
C	1.19288700	1.77770700	1.68245600
C	2.42068800	1.21781700	1.29399600
C	1.03211400	3.15898200	1.80543800
C	3.47102700	2.10245500	1.01892600
C	2.09822700	4.01131500	1.52653700
C	3.33939000	3.49310300	1.13132700
H	4.43108000	1.68797300	0.71987600
H	1.96677400	5.08538800	1.62661300
H	0.37646900	0.88154500	4.16809000

H	-1.86074300	-0.74707100	4.04984800
C	-1.16947000	0.08294100	-2.78039500
H	-0.71424100	0.21007800	-3.76175900
O	-0.53661000	-0.98350400	-2.07034600
C	0.75529700	-1.41172700	-2.55153300
H	1.09742600	-2.17481200	-1.85194400
H	0.63768200	-1.84754100	-3.54831400
H	1.46703700	-0.58213900	-2.58031500
C	-1.45323200	2.28798200	-0.96307100
C	-1.20197100	1.94087000	-2.38063300
H	-0.77671500	2.99971600	-0.49464200
H	-2.49508900	2.42413200	-0.66881900
H	-2.11553900	1.99826900	-2.97943800
C	-0.03465300	2.62362000	-3.10910300
C	-0.40484200	4.09730400	-3.40649500
C	1.32478900	2.55226300	-2.39072600
H	0.08065000	2.12937000	-4.08684000
C	0.69588200	4.79829400	-4.21930000
H	-0.55609100	4.63011200	-2.45724200
H	-1.35925000	4.14193400	-3.94736200
C	2.42708500	3.24292900	-3.21144900
H	1.25598800	3.03797900	-1.40908700
H	1.60277300	1.50731500	-2.19537600
C	2.06168400	4.70145900	-3.52458300
H	0.42173800	5.84745700	-4.38027900
H	0.75944600	4.33708800	-5.21541800
H	3.37653900	3.19547800	-2.66503500
H	2.57987600	2.69487500	-4.15281400
H	2.83731400	5.15951600	-4.14940400
H	2.03437500	5.27635900	-2.58728800
C	-2.80909400	-1.12756800	1.41531700
C	-2.63188600	-2.63206100	1.67919600
C	-4.13905700	-0.60121800	1.97975500
H	-2.79583700	-0.95705600	0.33226800
C	-3.82314600	-3.42652900	1.11749400
H	-2.55698400	-2.80449400	2.76190800
H	-1.68945300	-2.97540700	1.23512400
C	-5.32461000	-1.40375000	1.41716500
H	-4.12994000	-0.68840800	3.07505900
H	-4.24265700	0.46543300	1.74598200
C	-5.15962000	-2.90967400	1.67093700
H	-3.69509900	-4.48947700	1.35084700
H	-3.82591100	-3.34700000	0.02039400
H	-6.25640500	-1.03774200	1.86260900

H	-5.40493900	-1.22179100	0.33526300
H	-5.99246300	-3.46114400	1.21999800
H	-5.20564100	-3.10382600	2.75215000
C	2.61900400	-0.27595300	1.19061400
H	2.42807100	-0.77623900	2.14751800
H	1.93832600	-0.72439700	0.45722000
H	3.64358700	-0.51089800	0.89016800
H	0.07304700	3.55801400	2.12360100
C	4.51355100	4.40645300	0.87053500
H	4.19493900	5.35069800	0.41703300
H	5.02904200	4.65505900	1.80714800
H	5.24861600	3.93919800	0.20808800
H	-2.22654800	-0.17432000	-2.85423200

### TS9'-1

Ni	-0.98755700	0.50862200	-1.12712200
C	-2.19480700	-1.85089000	1.98188500
C	-0.98133500	-1.50875300	2.48431500
N	-0.38310300	-0.66158300	1.56001000
N	-2.31269100	-1.20693400	0.75749400
C	-1.19678900	-0.46581200	0.48963600
C	-3.45289100	-1.32081700	-0.12009300
C	-3.61588700	-2.47281900	-0.90858900
C	-4.38305900	-0.28033400	-0.15559700
C	-4.74747200	-2.53167500	-1.73040700
C	-5.49677500	-0.37066800	-0.98783100
C	-5.69935000	-1.50452600	-1.78568800
H	-4.89026200	-3.41383000	-2.35042600
H	-6.21949800	0.44070800	-1.00705000
H	-2.98036300	-2.47404300	2.37971200
H	-0.50293400	-1.79205900	3.40809600
C	-1.09195100	0.81733700	-3.15870500
H	-0.48012400	1.14646800	-3.99778100
O	-0.90882300	-0.55838800	-2.89570700
C	0.35299300	-1.12060500	-3.32453800
H	0.36253900	-2.14837500	-2.96213700
H	0.39520300	-1.10887100	-4.41770100
H	1.19677500	-0.56501800	-2.90337800
C	-0.81225900	2.35551500	-0.63154500
C	-0.51724000	2.33489400	-2.06506300
H	-1.15336900	2.96032600	-2.69299800
C	0.97599500	-0.09822000	1.70281800
C	1.10575900	0.75854100	2.97300300
C	2.04600500	-1.20245500	1.65306000

H	1.09923500	0.54672500	0.82697000
C	2.51882200	1.35674300	3.08185400
H	0.90903600	0.13534000	3.85634700
H	0.34533700	1.54835100	2.96523300
C	3.45636400	-0.59950600	1.76612800
H	1.88220900	-1.90554400	2.48144100
H	1.94000000	-1.77641900	0.72393200
C	3.60077500	0.26792400	3.02566100
H	2.60042700	1.93210300	4.01078300
H	2.67489000	2.07074300	2.25965500
H	4.19941700	-1.40489500	1.76606900
H	3.66097500	0.01298200	0.87542400
H	4.59672900	0.72413100	3.05682300
H	3.52162500	-0.37049000	3.91727900
C	-2.61955800	-3.60792900	-0.88529000
H	-1.59417400	-3.24910800	-1.03201200
H	-2.63555800	-4.14673800	0.06991800
H	-2.84216700	-4.33152400	-1.67391900
H	-4.23620600	0.58811900	0.47884100
C	-6.92494800	-1.63293200	-2.65839000
H	-7.27378700	-0.65597900	-3.00776800
H	-6.73179800	-2.26081900	-3.53384700
H	-7.75191500	-2.09389100	-2.10283600
H	0.53264200	2.40131100	-2.34556800
C	-2.02568300	3.12093900	-0.11776900
C	-2.30695100	2.84120400	1.37125300
C	-1.83547000	4.64746500	-0.32854600
H	-2.90989800	2.81666200	-0.70055500
C	-3.50767000	3.64309500	1.89805400
H	-1.41149800	3.11176400	1.95240500
H	-2.46469700	1.76819100	1.52879300
C	-3.03554100	5.45411700	0.19246200
H	-0.92307500	4.96390800	0.19869800
H	-1.67176500	4.86452000	-1.39195900
C	-3.32512600	5.15011600	1.66884800
H	-3.65526100	3.43318000	2.96436000
H	-4.42167800	3.30687600	1.38523300
H	-2.84713200	6.52519500	0.05195900
H	-3.92260000	5.21195300	-0.41117500
H	-4.21610000	5.69574600	2.00108200
H	-2.48918100	5.51155800	2.28522700
H	0.06715000	2.45572300	0.00871500
H	-2.15558300	0.98838100	-3.32467900

**TS9-2**

Ni	-0.15308900	0.37393600	-0.70101900
C	-0.13485700	0.65243100	3.36382900
C	-1.34057400	0.04154300	3.23745900
N	-1.55699600	-0.15936500	1.88034400
N	0.36110100	0.81395900	2.07712700
C	-0.51478100	0.31803600	1.15355600
C	1.64380600	1.38862900	1.75364500
C	2.77051400	0.55568800	1.62634200
C	1.73849200	2.77081000	1.58324600
C	3.98492900	1.17089100	1.29244200
C	2.96465600	3.35067000	1.26367900
C	4.10978700	2.55647800	1.11199800
H	4.86999000	0.54637400	1.19297000
H	3.03246500	4.42786400	1.13799700
H	0.40962400	0.98367400	4.23429400
H	-2.05005500	-0.26431700	3.98938200
C	0.76647800	0.01768000	-2.55019000
H	1.30512100	0.51309900	-3.35473400
O	1.64516900	-0.25625400	-1.44698300
C	-1.62654700	1.23812900	-1.46721900
C	-0.72759900	1.21962500	-2.63969400
H	-1.82398300	2.20304400	-1.00326200
H	-2.51066600	0.60257500	-1.52597300
H	-1.12459600	0.60285500	-3.45085900
C	-0.17530800	2.55015300	-3.17051700
C	-1.32486100	3.39441300	-3.76995700
C	0.62390500	3.37438500	-2.14469400
H	0.50467400	2.31456900	-4.00460900
C	-0.79693800	4.70000100	-4.38633500
H	-2.05021200	3.63179300	-2.97962800
H	-1.86406300	2.80850800	-4.52564400
C	1.15070400	4.68118900	-2.76197800
H	-0.01448700	3.61340100	-1.28318000
H	1.46446800	2.78494000	-1.74865400
C	0.01350100	5.51637700	-3.36936000
H	-1.63746500	5.29117700	-4.76780000
H	-0.16398000	4.46324300	-5.25359300
H	1.68705700	5.25957200	-2.00021600
H	1.88395400	4.44000600	-3.54527600
H	0.42089000	6.41631100	-3.84433900
H	-0.65226600	5.86166900	-2.56497100
C	-2.75306800	-0.82338300	1.31669300
C	-2.92945800	-2.24095900	1.88620700

C	-4.01507800	0.03233700	1.51588500
H	-2.54220200	-0.90376600	0.24680900
C	-4.15942500	-2.92360100	1.26349300
H	-3.06101600	-2.18662300	2.97560500
H	-2.02180800	-2.82871200	1.70228000
C	-5.24287900	-0.65862600	0.89833000
H	-4.18425200	0.18478200	2.59100300
H	-3.86129300	1.02472300	1.07458300
C	-5.42947500	-2.07978200	1.45024500
H	-4.28835600	-3.91693100	1.70762500
H	-3.98021300	-3.08369100	0.19025600
H	-6.13595900	-0.05201100	1.08569700
H	-5.12201900	-0.70464000	-0.19414700
H	-6.28007300	-2.56580000	0.95901100
H	-5.67635100	-2.02515700	2.52022900
C	2.69107600	-0.93759400	1.84250000
H	2.23757200	-1.18018700	2.81007500
H	2.08663200	-1.42789000	1.07039700
H	3.68877400	-1.38381500	1.81951400
H	0.84979400	3.38371300	1.70224400
C	5.45116100	3.17836200	0.80453700
H	5.95475800	3.48972600	1.72870700
H	6.11556100	2.47420700	0.29421700
H	5.34695500	4.06922700	0.17693700
H	0.36712600	-0.94664200	-2.86099200
H	2.29549900	0.46180100	-1.33471300

#### TS9'-2

Ni	-0.98954700	0.51025700	-1.12124500
C	-2.19267800	-1.84974900	1.98676500
C	-0.97886000	-1.50763100	2.48870500
N	-0.38243300	-0.65756200	1.56605900
N	-2.31283200	-1.20298600	0.76427500
C	-1.19800800	-0.46059000	0.49791000
C	-3.45266700	-1.31669800	-0.11435200
C	-3.61352600	-2.46743900	-0.90530600
C	-4.38333700	-0.27659300	-0.14867900
C	-4.74417300	-2.52499700	-1.72838600
C	-5.49599900	-0.36589500	-0.98254100
C	-5.69668800	-1.49830800	-1.78284900
H	-4.88533700	-3.40571900	-2.35073900
H	-6.21933800	0.44493200	-1.00089000
H	-2.97710700	-2.47478500	2.38384600
H	-0.49899200	-1.79289100	3.41111800

C	-1.07187400	0.82441300	-3.14851500
H	-0.42342200	1.12302300	-3.96967200
O	-0.95007300	-0.57323800	-2.87616200
C	-0.81169700	2.35701500	-0.62072800
C	-0.50714300	2.33547600	-2.05116200
H	-1.13365000	2.96412000	-2.68578200
C	0.97756800	-0.09523100	1.70717700
C	1.10985400	0.75997600	2.97810500
C	2.04665000	-1.20015500	1.65394800
H	1.10009100	0.55043500	0.83171000
C	2.52344500	1.35732200	3.08496600
H	0.91444000	0.13572100	3.86098000
H	0.34975000	1.55017900	2.97288300
C	3.45748500	-0.59791300	1.76509300
H	1.88399700	-1.90420200	2.48170900
H	1.93867800	-1.77288800	0.72426200
C	3.60468300	0.26799400	3.02537700
H	2.60701500	1.93150700	4.01443200
H	2.67828600	2.07227000	2.26334100
H	4.19996400	-1.40377400	1.76273300
H	3.66076900	0.01525600	0.87458800
H	4.60088000	0.72371200	3.05514300
H	3.52695500	-0.37134200	3.91644700
C	-2.61553300	-3.60108600	-0.88488800
H	-1.59251000	-3.24209500	-1.04625700
H	-2.62069600	-4.13361600	0.07386600
H	-2.84535300	-4.32975500	-1.66663600
H	-4.23843400	0.59029800	0.48838200
C	-6.92084900	-1.62613400	-2.65761200
H	-7.27727700	-0.64801100	-2.99575900
H	-6.72230500	-2.24231400	-3.54017200
H	-7.74422900	-2.10027900	-2.10786900
H	0.54600500	2.39241800	-2.32183900
C	-2.02910600	3.11956600	-0.11262300
C	-2.31325600	2.84268300	1.37643600
C	-1.84143200	4.64613200	-0.32682700
H	-2.91083600	2.81173100	-0.69718100
C	-3.51704700	3.64328500	1.89814800
H	-1.41981900	3.11658300	1.95903600
H	-2.46923200	1.76977500	1.53628100
C	-3.04470600	5.45114100	0.18931000
H	-0.93107400	4.96579600	0.20187900
H	-1.67576400	4.86116500	-1.39036900
C	-3.33712400	5.15010400	1.66572200

H	-3.66659600	3.43558300	2.96456700
H	-4.42906400	3.30371800	1.38405500
H	-2.85811500	6.52219900	0.04655200
H	-3.92964100	5.20549900	-0.41595900
H	-4.23012100	5.69454700	1.99432100
H	-2.50354600	5.51491700	2.28327000
H	0.06413500	2.45462400	0.02436800
H	-2.12223300	1.01653600	-3.35964800
H	-0.04541900	-0.87493000	-3.07471900

**TS10'**

Ni	-1.88881400	0.03890200	-0.47732800
C	-1.90606300	-3.45855000	1.71800800
C	-0.73275700	-3.64767800	1.06662100
N	-0.54789700	-2.54434400	0.23843700
N	-2.41444200	-2.23970700	1.27942800
C	-1.57730700	-1.66755200	0.36546100
C	-3.67824600	-1.68798200	1.70063100
C	-3.84235000	-1.20836900	3.01065300
C	-4.73294000	-1.66480800	0.78398000
C	-5.10251300	-0.69997700	3.35411400
C	-5.97134100	-1.15243500	1.15901800
C	-6.17703900	-0.66442800	2.45749100
H	-5.24708900	-0.31910300	4.36248300
H	-6.78752900	-1.14276500	0.44134800
H	-2.42996900	-4.07300700	2.43296700
H	-0.02785100	-4.46179500	1.11787700
C	-1.68529900	-1.02546100	-4.08269400
C	-1.56873700	0.38717900	-3.50233400
H	-2.70272100	-1.19808800	-4.45066300
H	-1.00755300	-1.17025800	-4.92851300
H	-1.76144000	1.10835500	-4.31795700
O	-0.27704800	0.66331600	-2.95987700
C	0.75209800	0.76604100	-3.93816300
H	1.65378200	1.09500400	-3.41596900
H	0.96197200	-0.19483500	-4.42400600
H	0.49490700	1.50530200	-4.71046100
H	-1.46131400	-1.77806100	-3.32044700
C	-2.60295900	1.72353400	-1.53623100
C	-2.62490900	0.67587400	-2.44924600
C	0.61439700	-2.34895800	-0.65207700
C	1.90668400	-2.12963300	0.15464600
C	0.76427000	-3.51724500	-1.64160900
H	0.38415200	-1.43865000	-1.21633700

C	3.10806100	-1.91060500	-0.78069700
H	2.09364300	-3.00855700	0.78705400
H	1.78040200	-1.27673500	0.83436800
C	1.96667400	-3.29352200	-2.57396700
H	0.91030200	-4.45361400	-1.08587700
H	-0.16101800	-3.63284100	-2.21881400
C	3.26249900	-3.06551900	-1.78141700
H	4.02026900	-1.79310600	-0.18473900
H	2.97174200	-0.96803200	-1.33225400
H	2.07300400	-4.15261200	-3.24584300
H	1.77069000	-2.41988900	-3.21276500
H	4.09405500	-2.86251300	-2.46599000
H	3.52350500	-3.98467600	-1.23785500
C	-2.72891700	-1.23711800	4.03196000
H	-2.59818900	-2.23810300	4.46228500
H	-1.76502700	-0.94748300	3.60053600
H	-2.94785900	-0.55614600	4.85904300
H	-4.57566400	-2.05820100	-0.21544100
C	-7.53031000	-0.14890300	2.88617100
H	-7.45146200	0.51960800	3.74852300
H	-8.02863600	0.39386100	2.07617700
H	-8.18991300	-0.97846600	3.17269700
H	-2.55192400	-0.85256600	-1.44410300
C	-3.91109400	2.33426200	-1.05088100
C	-3.91129700	2.82350500	0.41072400
C	-4.27603100	3.50378300	-2.00617100
H	-4.69908700	1.57133600	-1.14495000
C	-5.23033200	3.51651200	0.79058400
H	-3.07408500	3.52195900	0.55852200
H	-3.74657300	1.97248700	1.08139900
C	-5.59503400	4.18915400	-1.61769400
H	-3.46185600	4.24360800	-1.98181100
H	-4.32983600	3.13196800	-3.03753600
C	-5.56890500	4.67136700	-0.16144600
H	-5.17155300	3.87686800	1.82493200
H	-6.04301400	2.77544700	0.76479000
H	-5.78659200	5.02781400	-2.29798600
H	-6.42580400	3.48128600	-1.75328100
H	-6.53334900	5.11709000	0.10967300
H	-4.81527000	5.46509000	-0.05378800
H	-1.72595600	2.36432300	-1.50127600
H	-3.60520100	0.28700700	-2.72610300
C	-0.92446900	1.14975000	1.20567700
C	0.04342900	1.66261300	0.39241200

H	-1.70516600	1.79826500	1.58500900
H	-0.67782100	0.26425200	1.77565800
H	0.91999000	1.07812200	0.10871700
O	0.00324100	2.91150800	-0.06126300
C	1.02231200	3.31518100	-0.99451500
H	0.98734600	4.40390900	-1.02471900
H	2.00910700	2.98819100	-0.64991500
H	0.80298100	2.90066200	-1.98100800