

Supporting Information

Mechanistic Insight into Ni-mediated Decarbonylation of Unstrained Ketones: the Origin of Decarbonylation Catalytic Activity

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SI1. Key molecular orbitals (MOs) of INT_{O1}, INTa1 and INTb1.

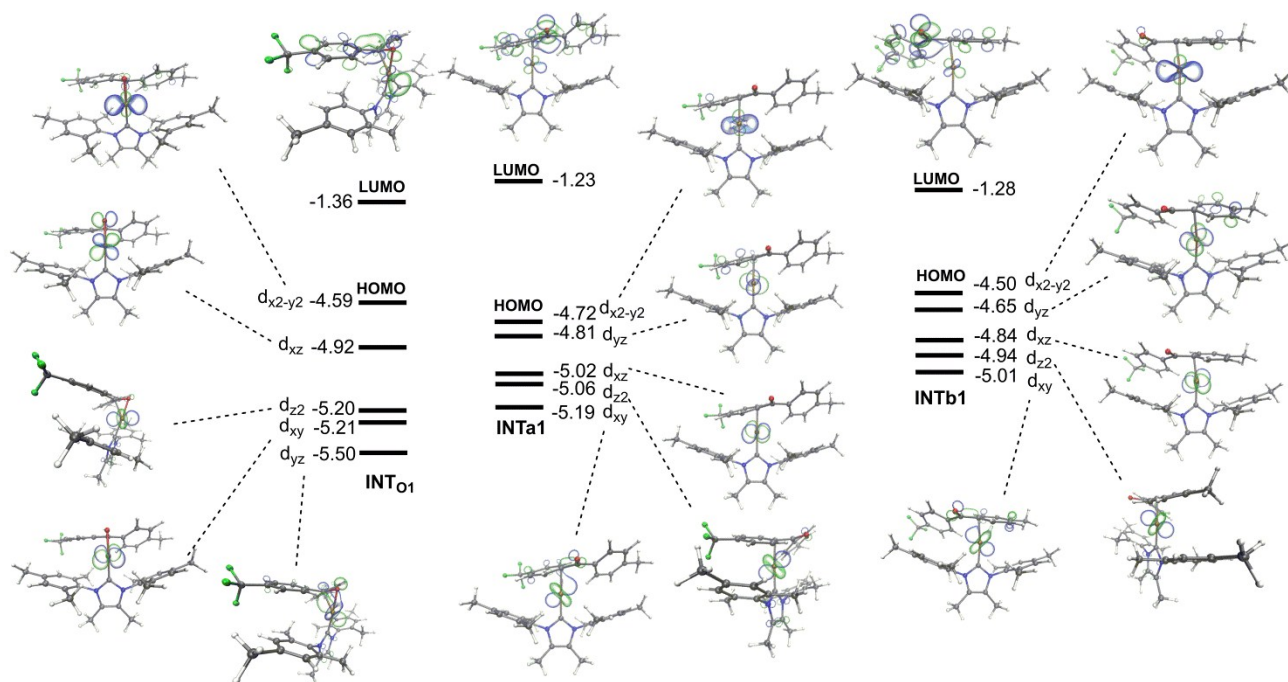
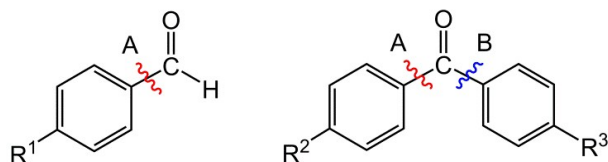


Fig. S1. Selected molecular orbitals (MOs) and MO energies (in eV) of INT_{O1}, INTa1 and INTb1.

SI2. Analysis of the substituent effect on C-C oxidative addition step.

To study the substituent effect on C-C oxidative addition step, we evaluated the oxidative addition barriers for different substituents as shown in Table 1, from which we can see that two CF₃ substituted substrate **CF₃-CF₃** characters are the most favorable oxidative addition transition state (entry 4 in Table S1). To gain more insights into the origins of the relative reactivity, NBO analysis was conducted for the substrates and corresponding oxidative addition transition states (Table S1). The charges transferred from NiL to phenyl and benzoyl moieties were calculated, respectively. Interestingly, a moderate linear correlation was observed between the oxidative addition barriers and the charges transferred from NiL to benzoyl moiety as shown in Fig. S2. The more the electrons transfer, the lower the oxidative addition barriers. When a CF₃ substituent is present on the phenyl

group, the benzoyl moiety was more electron-deficient facilitating the electrons transfer from NiL to benzoyl and promoting the oxidative addition step.



Entry	Label	R ¹	R ²	R ³	cleavage at A	cleavage at B
1	CF ₃	CF ₃			16.4	
2	CH ₃	CH ₃			20.0	
3	CH ₃ -CH ₃		CH ₃	CH ₃	18.4	
4	CF ₃ -CF ₃		CF ₃	CF ₃	14.3	
5	CF ₃ -CH ₃ (A)/CF ₃ -CH ₃ (B)		CF ₃	CH ₃	15.3	16.2
6	CF ₃ -H(A)/CF ₃ -H(B)		CF ₃	H	15.2	15.2
7	CH ₃ -H(A)/CH ₃ -H(B)		CH ₃	H	16.6	16.1

Table S1. Computed activation barriers ($\Delta G^\ddagger$ in kcal/mol) of the oxidative addition step with different substituent.

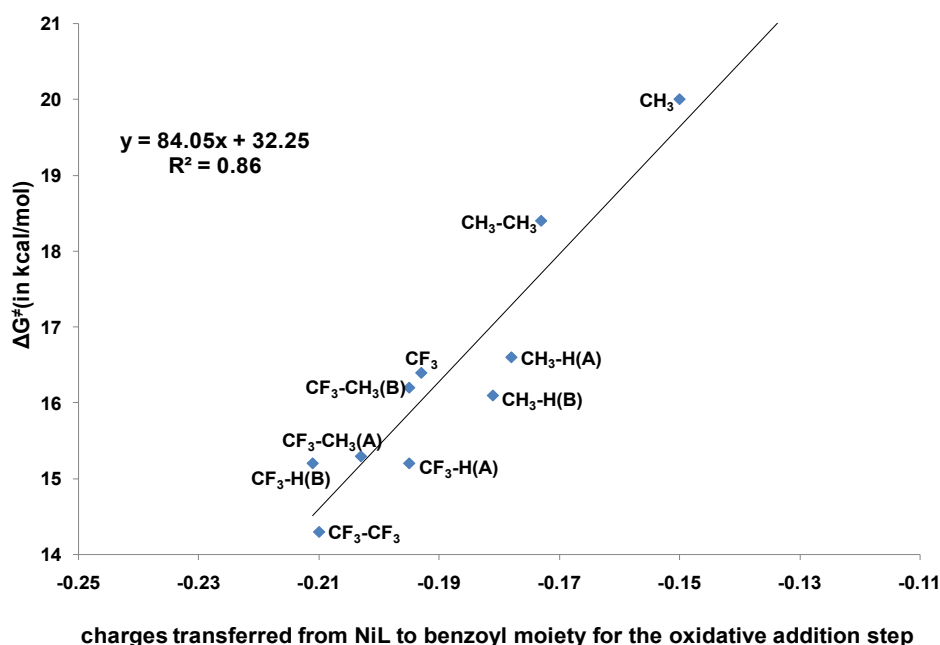


Fig.S2. The linear correlation between the oxidative addition barriers and the charges transferred from NiL to benzoyl moiety in the oxidative addition step.

SI3. Noncovalent interactions analyzation between substrates and IMes^{Me} in TSa7_8 and TSq3_4.

We designed two truncated model systems (**M1**, **M2**) based on the optimized structures of TSa7_8 and TSq3_4 and examined the effect of noncovalent interactions on the energy of TSa7_8 relative to TSq3_4. Figure S2 shows the structures of TSa7_8, TSq3_4 and the corresponding two truncated models **M1** and **M2**. Model **M1** represents the effect of noncovalent interaction between qionolynyl/trifluoromethyl phenyl and IMes^{Me} on NHC ligand and methyl phenyl is reduced to H atom. Model **M2** represents the effect of noncovalent interaction between methyl phenyl and IMes^{Me} on NHC ligand, and qionolynyl/trifluoromethyl phenyl is reduced to H atom. The two models are divided into two parts as Ni-NHC (denoted as A) and substrate (denoted as B). We calculated the single-point energies of the model structures and their corresponding two parts. The noncovalent interaction in every model is calculated as $\Delta E(\mathbf{M})=[E(\mathbf{M})-E(\mathbf{M}_A)-E(\mathbf{M}_B)]$. From the results we can see that the differences of noncovalent interactions between substrates and IMes^{Me} in TSa7_8 and TSq3_4 are negligible. Photoshop and CYLview programs are used to visually depict the noncovalent interactions between the ligand and the substrate.

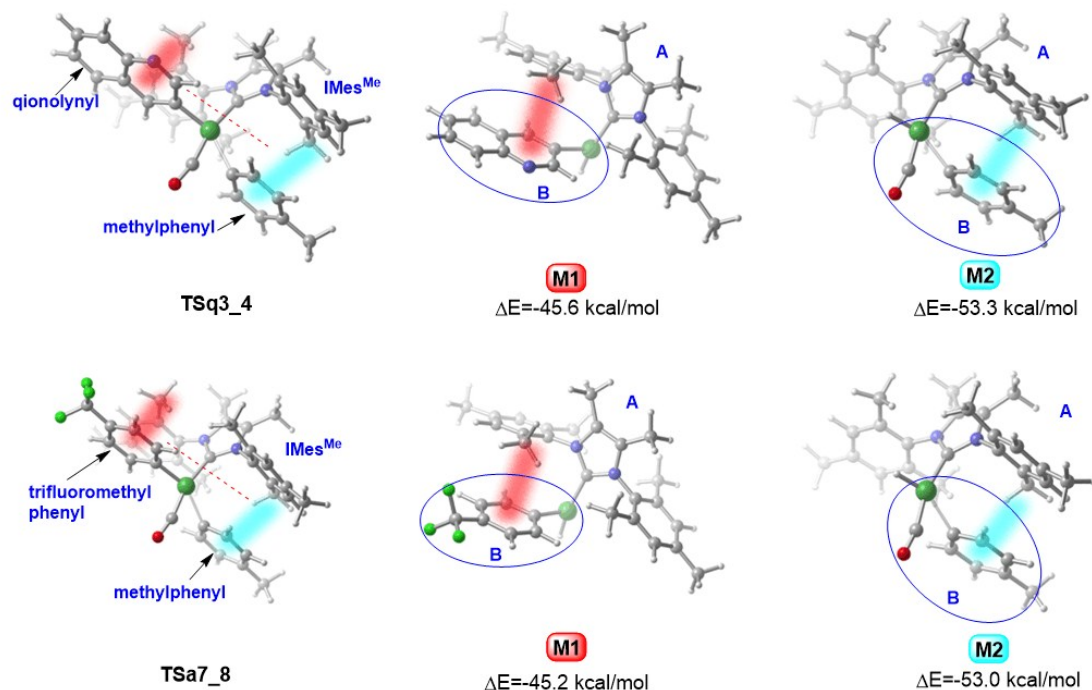


Fig. S3. Noncovalent interactions between substrates and IMes^{Me} in TSa7_8 and TSq3_4.

SI4. Distortion/interaction model analysis of TSa7_8 and TSq3_4.

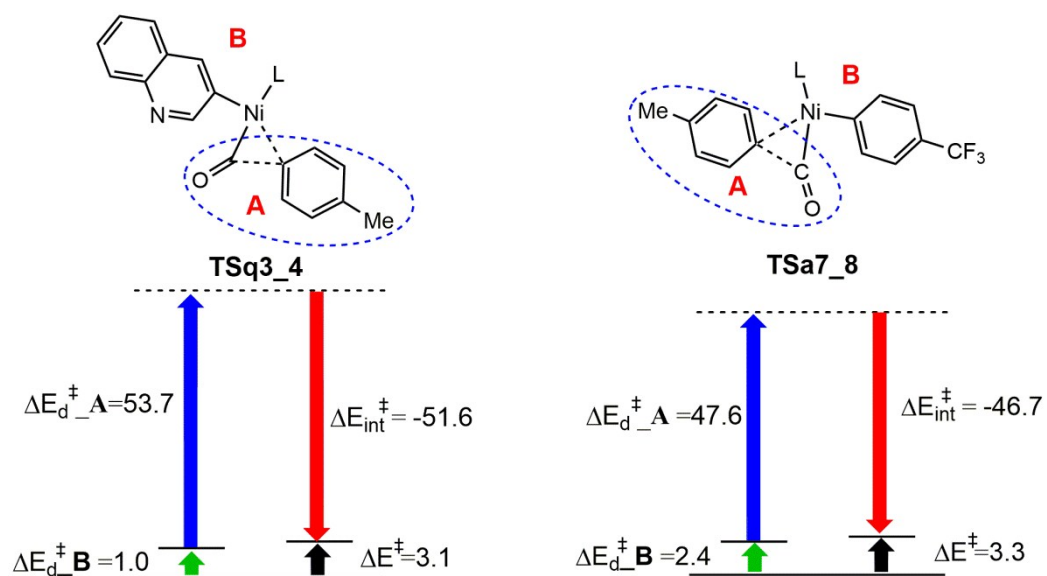


Fig. S4. Distortion, interaction, and activation energies for the TSa7_8 and TSq3_4. (blue: distortion energy of **frag_A**, green: distortion energy of **frag_B**, red: interaction energy, black: activation energy, in kcal/mol).

SI5. Computed free energy profiles for the decarbonylation of 3-quinolinylnyl ketone **2**.

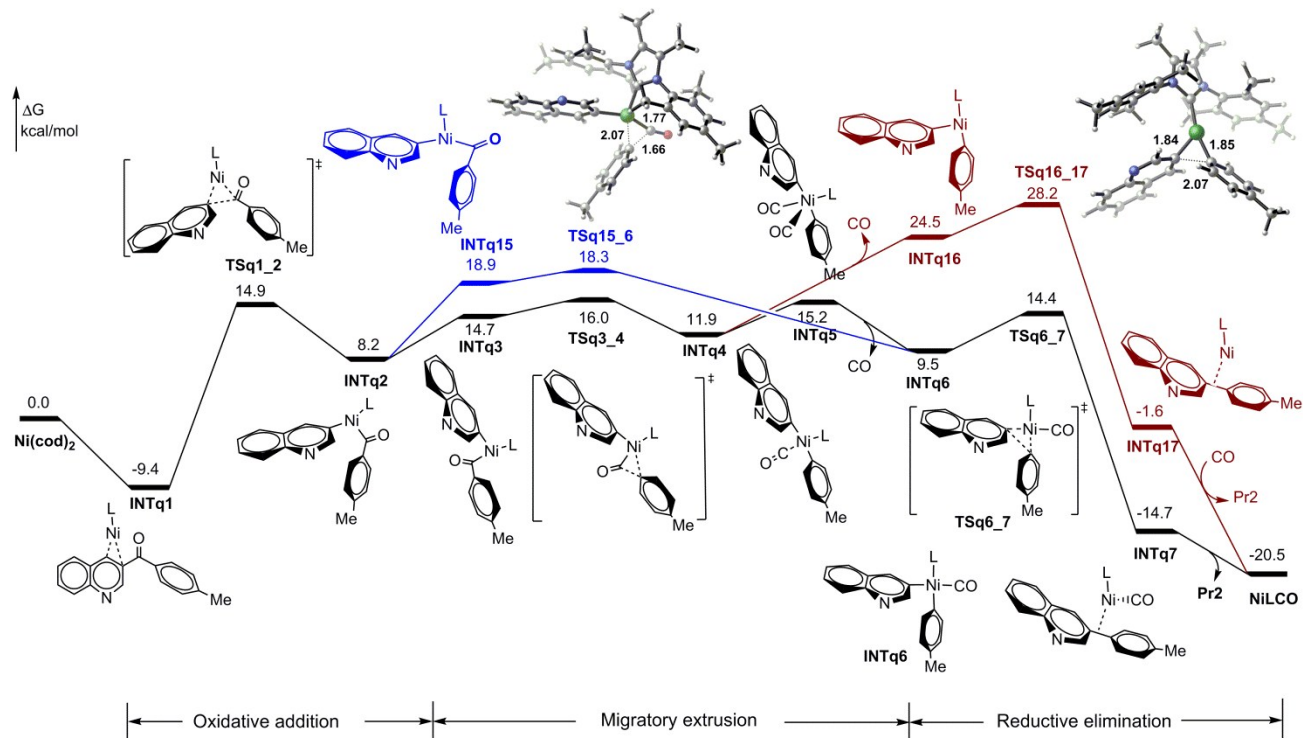


Fig. S5. Computed free energy changes of decarbonylation of 3-quinolinylnyl ketone **2** involving the cleavage of C(quinolinylnyl)-C(O). Free energies are in kcal/mol.

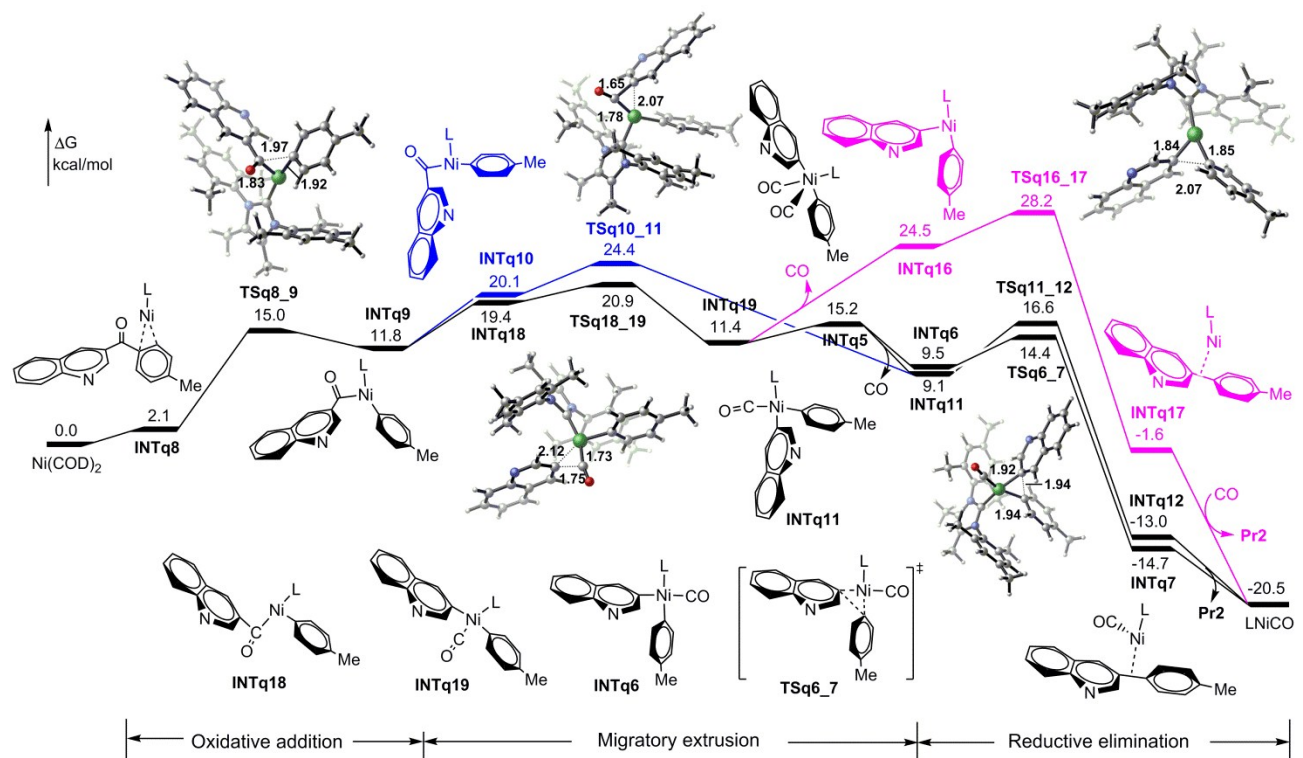
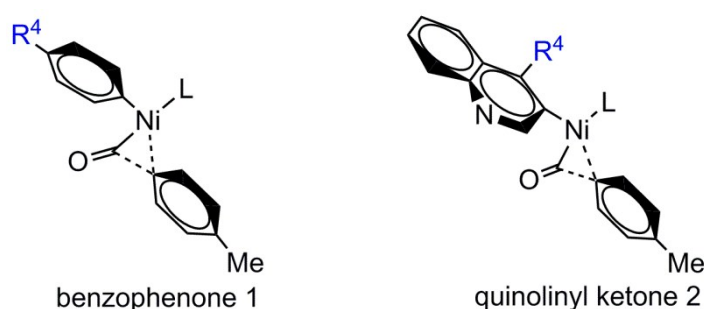


Fig. S6. Computed free energy changes of decarbonylation of 3-quinolinyl ketone **2** involving the cleavage of C(methylphenyl)-C(O). Free energies are in kcal/mol.

SI6. Analysis of the substituent effect in decarbonylation step.

In order to study the effect of substituents, decarbonylation transition state free energy barriers when different substituents substituted on phenyl and quinolinyl moieties were calculated. The results are given in Table S2. NBO analysis was conducted to evaluate the correlation between decarbonylation transition state barriers and the transferred charges from substrates to decarbonylation transition states. However, we found no clear correlation between the decarbonylation transition states. However, we found no clear correlation between the decarbonylation barriers and the amount of charges transferred. But the decarbonylation barriers of electron-withdrawing groups substituted reactants are generally lower than those of electron-donating groups substituted reactants indicating that electron-withdrawing groups are beneficial for the decarbonylation step. Additionally, the decarbonylation barriers of quinolinyl ketones are lower than those of benzophenones.



Entry	Label	R ⁴	$\Delta G^\ddagger(1)$	$\Delta G^\ddagger(2)$
1	CH₃-OMe	OMe	25.3	16.2
2	CH₃-NH₂	NH ₂	25.7	21.9
3	CH₃-OH	OH	23.0	15.4
4	CH₃-F	F	20.3	11.8
5	CH₃-CN	CN	16.4	7.7
6	CH₃-NO₂	NO ₂	14.2	7.7
7	CH₃-CCl₃	CCl ₃	18.2	10.8

Table S2. Computed activation barriers ($\Delta G^\ddagger$ in kcal/mol) of the decarbonylation step with different substituents.

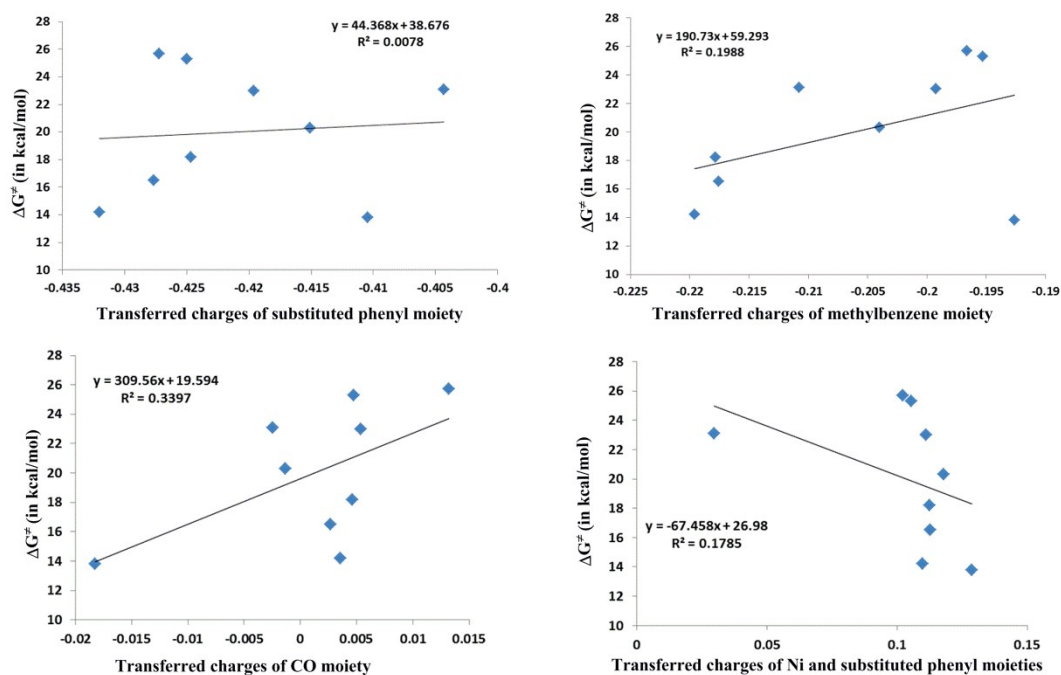


Fig. S7. The relationship between the decarbonylation barriers of benzophenone 1 and the transferred charges of each moiety from substrates to decarbonylation transition states.

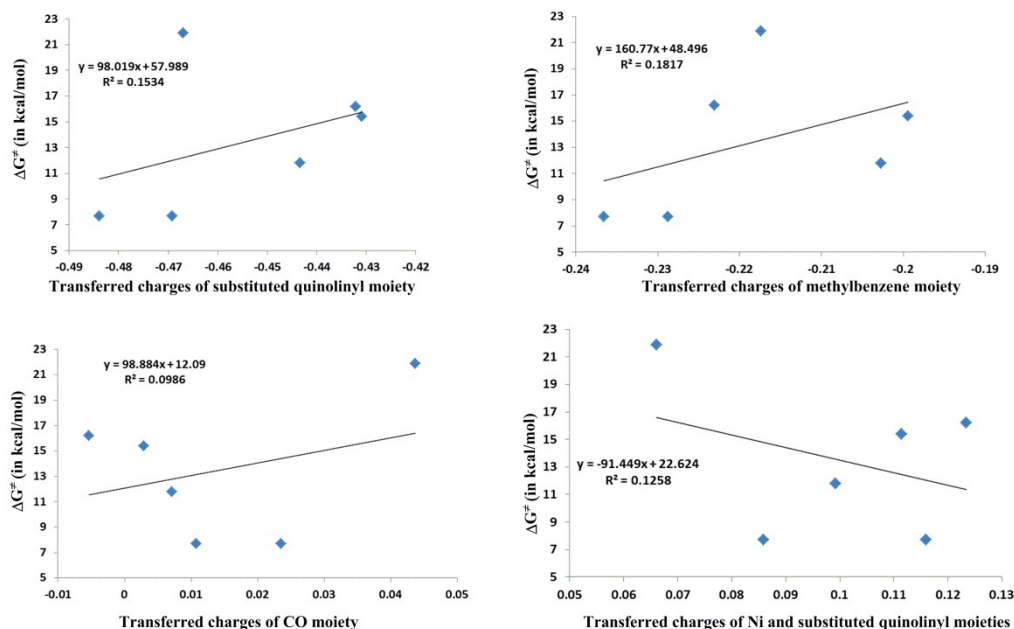


Fig. S8. The relationship between the decarbonylation barriers of quinoliny ketone 2 and the transferred charges of each moiety from substrates to decarbonylation transition states.

SI7. Cartesian coordinates of optimized structures.**Ni(COD)₂**

Ni	0.0000000	0.0000010	-0.0000940
C	2.1924530	-1.8181610	-0.6307450
C	2.5959930	-0.5643260	-1.4151180
C	2.5956010	0.5643610	1.4158670
C	2.1921960	1.8181990	0.6314320
H	1.5997110	-2.4682560	-1.2914370
H	3.0894410	-2.4037350	-0.3657210
H	2.8604450	-0.8578770	-2.4392010
H	3.5099300	-0.1260580	-0.9950230
H	3.5096410	0.1261270	0.9959640
H	2.8598140	0.8578870	2.4400180
H	3.0892230	2.4038320	0.3666660
H	1.5992410	2.4682400	1.2919890
C	1.5022450	-0.4805150	1.4675670
H	0.9623610	-0.5567840	2.4119600
C	1.3560820	-1.5343920	0.5887110
H	0.7346190	-2.3684250	0.9215420
C	1.5026120	0.4805220	-1.4670960
H	0.9630880	0.5568740	-2.4116910
C	1.3561650	1.5344000	-0.5882490
H	0.7348550	2.3684600	-0.9213040
C	-2.1923000	1.8182300	-0.6311940
C	-2.5955640	0.5645230	-1.4159180
C	-2.5959290	-0.5645680	1.4152360
C	-2.1924240	-1.8182640	0.6306210
H	-1.5993760	2.4684440	-1.2916080
H	-3.0893840	2.4037450	-0.3663600
H	-2.8595760	0.8582370	-2.4400680
H	-3.5096920	0.1262240	-0.9963040
H	-3.5099600	-0.1262970	0.9953790
H	-2.8601990	-0.8582810	2.4393210
H	-3.0894250	-2.4037940	0.3655380
H	-1.5996740	-2.4684680	1.2912020
C	-1.5026240	0.4803480	1.4672100
H	-0.9629680	0.5565570	2.4117370
C	-1.3562710	1.5343190	0.5884780
H	-0.7349170	2.3683270	0.9215740
C	-1.5022080	-0.4803590	-1.4676100
H	-0.9623550	-0.5565950	-2.4120220
C	-1.3560570	-1.5343280	-0.5888160
H	-0.7346390	-2.3683490	-0.9217660

NiL(COD)

C	-0.0156470	-0.7362330	-0.0262870
C	0.6337110	-2.9520080	0.0154540
C	-0.7223200	-2.9334820	0.0349530
C	2.3927870	-1.1482640	-0.0237690
C	3.0427460	-0.9311830	1.1971640
C	4.3532360	-0.4556980	1.1684940
H	4.8740040	-0.2847500	2.1119080
C	5.0104820	-0.1887020	-0.0328370
C	4.3286050	-0.4118240	-1.2296220
H	4.8309970	-0.2090740	-2.1767380
C	3.0186460	-0.8875360	-1.2485660
C	2.3340440	-1.1755810	2.4934010
H	2.0164930	-2.2204440	2.6051710
H	1.4225120	-0.5655930	2.5558330
H	2.9741350	-0.9262540	3.3460440
C	6.4069350	0.3551000	-0.0376220
H	6.9630640	0.0337870	-0.9255590
H	6.9678250	0.0364540	0.8481660
H	6.4057970	1.4531380	-0.0397940
C	2.2828800	-1.0956680	-2.5356690
H	1.9161650	-2.1255900	-2.6374440
H	2.9217060	-0.8753230	-3.3971350
H	1.3976800	-0.4456850	-2.5838480
C	-2.4367110	-1.0906560	0.0150620
C	-3.0975340	-0.8881520	-1.2026830
C	-4.3941910	-0.3771150	-1.1704350
H	-4.9196420	-0.2110220	-2.1121210
C	-5.0347900	-0.0762600	0.0322810
C	-4.3431200	-0.2858590	1.2255510
H	-4.8282210	-0.0481760	2.1734460
C	-3.0430510	-0.7895840	1.2405480
C	-2.4164370	-1.1967760	-2.4997360
H	-2.1680310	-2.2625860	-2.5885270
H	-1.4691970	-0.6490750	-2.5850300
H	-3.0493630	-0.9284260	-3.3518950
C	-6.4450100	0.4306220	0.0414320
H	-7.1655930	-0.3981150	0.0377060
H	-6.6595410	1.0449290	-0.8403000
H	-6.6525210	1.0332030	0.9326320
C	-2.2990080	-0.9795290	2.5257630

H	-1.4096800	-0.3345740	2.5587750	C	-4.6910420	1.5931830	1.6312380
H	-1.9382700	-2.0095340	2.6461570	C	-4.4108040	1.7813790	0.2793080
H	-2.9304890	-0.7389840	3.3873210	H	-5.1965180	1.6131070	-0.4590580
N	-1.0967380	-1.5810300	0.0054620	C	-3.1434250	2.1622400	-0.1605200
N	1.0427330	-1.6097420	-0.0202200	C	-1.2829140	2.3231030	3.1642750
Ni	0.0466550	1.1536420	-0.0434080	H	-0.7411980	3.2706800	3.0504050
C	-1.7281960	3.2737810	-0.7380360	H	-0.5415400	1.5223040	3.0290070
C	-1.3164870	3.6971230	0.6855630	H	-1.6646490	2.2676190	4.1891480
C	1.4273070	3.7274680	-0.6346320	C	-6.0502030	1.1526140	2.0857920
C	1.8389990	3.2457180	0.7688340	H	-6.7896480	1.2210180	1.2798300
H	-2.6153920	2.6253450	-0.6648500	H	-6.4129680	1.7577730	2.9256920
H	-2.0518210	4.1624940	-1.3060780	H	-6.0371830	0.1099840	2.4334740
H	-2.2260510	3.9542550	1.2442340	C	-2.8333380	2.3116740	-1.6162640
H	-0.7195540	4.6160530	0.6557250	H	-2.5457600	3.3404510	-1.8740910
H	0.8302820	4.6444590	-0.5681120	H	-3.6926040	2.0334620	-2.2357780
H	2.3361090	4.0082800	-1.1831680	H	-1.9849370	1.6676670	-1.8886030
H	2.1602360	4.1079890	1.3776460	C	2.4378430	2.1502280	-0.7817910
H	2.7275110	2.6029700	0.6674120	C	2.6289790	1.9115340	-2.1490920
C	0.6876060	2.6673360	-1.4102560	C	3.8776390	1.4593500	-2.5687160
H	1.2931870	2.0901270	-2.1137240	H	4.0405020	1.2634520	-3.6301200
C	-0.6771850	2.4971610	-1.4841970	C	4.9214520	1.2459120	-1.6660740
H	-1.0592240	1.8436710	-2.2716880	C	4.6897890	1.4833160	-0.3134650
C	-0.5751310	2.6092280	1.4187400	H	5.4912020	1.3066810	0.4060000
H	-1.1799290	1.9940140	2.0893770	C	3.4540180	1.9309840	0.1532380
C	0.7875780	2.4343900	1.4754060	C	1.4989390	2.0792350	-3.1150940
H	1.1686710	1.7271270	2.2168490	H	0.9963670	3.0490110	-3.0043820
C	1.6009440	-4.0744660	0.0012300	H	0.7331620	1.3099310	-2.9336810
H	2.1664180	-4.1179080	-0.9398190	H	1.8443530	1.9858170	-4.1500950
H	2.3389420	-3.9930160	0.8098410	C	6.2528570	0.7535030	-2.1488520
H	1.0831200	-5.0318150	0.1180120	H	6.6984410	1.4426900	-2.8776060
C	-1.7200290	-4.0281650	0.0866840	H	6.1651900	-0.2187390	-2.6518210
H	-2.4094840	-3.9077340	0.9327400	H	6.9655980	0.6396030	-1.3241910
H	-2.3372910	-4.0745940	-0.8208390	C	3.2043120	2.1164610	1.6164670
H	-1.2238020	-4.9977150	0.1971130	H	2.4631410	1.3851800	1.9692280
NiL2				H	2.8034290	3.1115070	1.8498110
C	0.1298080	1.8466350	0.0323520	H	4.1246640	1.9737800	2.1937470
C	-0.4179810	4.0788120	0.2076260	N	1.1766700	2.6522040	-0.3343980
C	0.8633920	4.0141780	-0.2379380	N	-0.8416670	2.7543260	0.3691760
C	-2.1461590	2.3606990	0.7996210	Ni	0.0056400	0.0052670	0.0359050
C	-2.3873400	2.1745040	2.1661900	C	1.8364960	5.0754930	-0.5871830
C	-3.6677140	1.7924350	2.5594830	H	2.7378120	5.0273600	0.0385210
H	-3.8713890	1.6397260	3.6209000	H	2.1700560	4.9959180	-1.6304700
				H	1.3897610	6.0658450	-0.4532240
				C	-1.2973880	5.2322720	0.5109770

H	-2.2305870	5.1947500	-0.0667250	H	-2.7579320	-3.1049690	1.8496710
H	-1.5817460	5.2636230	1.5714170	H	-4.0836560	-1.9797890	2.2152650
H	-0.7937250	6.1747460	0.2734330	N	-1.1701070	-2.6391750	-0.3509320
C	-0.1202390	-1.8364180	0.0136450	N	0.8481790	-2.7467670	0.3511000
C	0.4174880	-4.0702510	0.1994170	C	-1.8384170	-5.0621140	-0.5947430
C	-0.8630670	-4.0022100	-0.2473930	H	-2.7398960	-5.0121580	0.0303910
C	2.1514720	-2.3618350	0.7931800	H	-2.1712640	-4.9835160	-1.6383330
C	2.3768250	-2.1679440	2.1618770	H	-1.3929140	-6.0528500	-0.4594710
C	3.6553060	-1.7955570	2.5689700	C	1.2920820	-5.2250130	0.5109480
H	3.8466850	-1.6358290	3.6317210	H	2.2184250	-5.2049890	-0.0786270
C	4.6933130	-1.6143830	1.6526380	H	1.5889800	-5.2376610	1.5683520
C	4.4296130	-1.8115010	0.2990090	H	0.7784040	-6.1678040	0.2973740
H	5.2260400	-1.6562940	-0.4309690				
C	3.1636690	-2.1830090	-0.1542990				
C	1.2558940	-2.2926450	3.1446590	I			
H	0.6781790	-3.2154580	3.0057980	C	0.5109340	-0.3369070	0.6584400
H	0.5478290	-1.4614170	3.0133100	C	0.2164580	0.8703960	0.0225410
H	1.6259880	-2.2692240	4.1750250	C	1.2483370	1.5983980	-0.5795740
C	6.0537100	-1.1984170	2.1264470	C	2.5423600	1.1101100	-0.5798050
H	6.7751020	-1.1544720	1.3025830	C	2.8224390	-0.1033150	0.0507280
H	6.4507400	-1.8951960	2.8756370	C	1.8136580	-0.8212900	0.6796020
H	6.0273390	-0.2087320	2.6023490	H	-0.2744040	-0.8927410	1.1643810
C	2.8719680	-2.3219290	-1.6149670	H	1.0127020	2.5501810	-1.0480990
H	2.3508120	-3.2594850	-1.8486800	H	3.3418010	1.6673380	-1.0635090
H	3.7905820	-2.2829150	-2.2098300	H	2.0417430	-1.7545470	1.1857220
H	2.2118910	-1.5061120	-1.9452210	C	-1.1526420	1.4741960	0.0310480
C	-2.4365940	-2.1373850	-0.7834050	O	-1.2688770	2.6904840	0.0536050
C	-2.6454630	-1.8988450	-2.1477770	C	-2.3536120	0.5997460	0.0111160
C	-3.9023440	-1.4551310	-2.5518170	C	-2.3612040	-0.6765950	-0.5605090
H	-4.0798690	-1.2610760	-3.6112270	C	-3.5524180	1.1204490	0.5127650
C	-4.9379550	-1.2540970	-1.6371140	C	-3.5370030	-1.4130470	-0.6163090
C	-4.6880240	-1.4882640	-0.2869080	H	-1.4523370	-1.0869450	-0.9950780
H	-5.4828040	-1.3175630	0.4420010	C	-4.7158560	0.3728620	0.4725790
C	-3.4430030	-1.9262270	0.1644260	H	-3.5459250	2.1236340	0.9320970
C	-1.5272490	-2.0607990	-3.1283490	C	-4.7281990	-0.9077100	-0.0931750
H	-1.0172470	-3.0271280	-3.0224390	H	-3.5349160	-2.3982000	-1.0801980
H	-0.7644720	-1.2860050	-2.9598990	H	-5.6404940	0.7837740	0.8759760
H	-1.8871570	-1.9721620	-4.1588230	C	-5.9864410	-1.7172510	-0.1212170
C	-6.2827320	-0.7851730	-2.1065020	H	-5.9436340	-2.5019540	-0.8835600
H	-6.7348150	-1.4971920	-2.8089160	H	-6.1607530	-2.2088350	0.8447870
H	-6.2148480	0.1744110	-2.6357890	H	-6.8629300	-1.0915640	-0.3232370
H	-6.9813210	-0.6579180	-1.2717490	C	4.2364090	-0.5948670	0.0313200
C	-3.1713470	-2.1131890	1.6236350	F	5.0666690	0.2802540	0.6158030
H	-2.4302050	-1.3775130	1.9668390	F	4.6761710	-0.7558910	-1.2249380

F	4.3850310	-1.7649260	0.6585340	C	-4.1422120	1.5851310	0.6868860
				H	-4.7320980	1.3699640	1.5791020
				C	-4.7582760	1.5566450	-0.5642140
2				C	-3.9805460	1.7889830	-1.6978830
C	-5.2578030	-1.0041270	0.0559450	H	-4.4450420	1.7419670	-2.6838160
C	-4.1019880	-1.5543910	-0.4375880	C	-2.6157030	2.0597790	-1.6079870
C	-2.8834650	-0.8407180	-0.3622050	C	-2.1340610	1.8566140	2.1768060
C	-2.8776480	0.4555930	0.2306180	H	-1.4758380	2.7223850	2.3272020
C	-4.0863560	0.9974030	0.7311150	H	-1.5075570	0.9593650	2.2944390
C	-5.2518330	0.2808970	0.6457380	H	-2.8837960	1.8497290	2.9740970
H	-6.1915470	-1.5581570	-0.0053920	C	-6.2250500	1.2762250	-0.6808630
H	-4.0818330	-2.5396350	-0.8970470	H	-6.8225660	2.1552260	-0.4050890
C	-1.6496890	1.1419260	0.2804730	H	-6.5292010	0.4610640	-0.0127610
H	-4.0690980	1.9885830	1.1810180	H	-6.5027080	1.0013210	-1.7048450
H	-6.1790890	0.6981550	1.0305040	C	-1.7813400	2.2383450	-2.8391000
C	-0.5069270	0.5411140	-0.1972830	H	-1.3102500	3.2286140	-2.8897980
C	-0.6305840	-0.7530540	-0.7704230	H	-2.3866950	2.1129420	-3.7425800
H	-1.5954380	2.1463430	0.6985640	H	-0.9667720	1.5019410	-2.8725560
H	0.2527250	-1.2335370	-1.1950680	C	2.7320920	1.5663580	0.3068430
N	-1.7569590	-1.4177370	-0.8637810	C	3.5217820	1.1414400	-0.7679390
C	0.7717940	1.3094890	-0.1790620	C	4.7459420	0.5425450	-0.4793520
O	0.7426210	2.5289560	-0.2643050	H	5.3684910	0.1910290	-1.3029680
C	2.0643320	0.5880390	-0.0540650	C	5.1833460	0.3596130	0.8336490
C	2.1835230	-0.6401610	0.6055190	C	4.3647920	0.7928080	1.8768240
C	3.2171590	1.1988780	-0.5567010	H	4.6893930	0.6493160	2.9081730
C	3.4253140	-1.2408430	0.7498270	C	3.1301920	1.3967650	1.6364710
H	1.3045240	-1.1180850	1.0333390	C	3.0400950	1.2787710	-2.1783150
C	4.4509970	0.5814840	-0.4304230	H	2.6987460	2.2972810	-2.4028860
H	3.1209020	2.1624780	-1.0516720	H	2.1867160	0.6124470	-2.3642360
C	4.5767330	-0.6460630	0.2267710	H	3.8301300	1.0180020	-2.8894070
H	3.5085740	-2.1913420	1.2751560	C	6.4788680	-0.3408400	1.1071490
H	5.3401400	1.0558520	-0.8432150	H	7.2711090	-0.0055520	0.4276320
C	5.9131610	-1.2986790	0.3942050	H	6.3721290	-1.4240030	0.9603260
H	6.2979460	-1.1534080	1.4118840	H	6.8202120	-0.1781510	2.1349980
H	5.8561360	-2.3801900	0.2264570	C	2.2283690	1.7917860	2.7642540
H	6.6534790	-0.8852710	-0.2983790	H	1.3262800	1.1617920	2.7738720
				H	1.8812670	2.8299100	2.6819830
				H	2.7311490	1.6775820	3.7299580
INTa1				N	1.4616100	2.1713530	0.0457440
C	0.3051420	1.4567960	-0.0225560	N	-0.6476280	2.4104790	-0.2126460
C	-0.1025260	3.6993830	-0.2403330	Ni	0.1084550	-0.3906700	0.2952970
C	1.2382520	3.5473720	-0.0792130	C	2.3397440	4.5360940	-0.0200430
C	-2.0424830	2.1142270	-0.3327060	H	2.8867960	4.4782900	0.9297420
C	-2.7856070	1.8685040	0.8292780	H	3.0725860	4.3801000	-0.8224000

H	1.9463440	5.5523240	-0.1206010	H	-6.1238800	0.4566070	-1.2015950
C	-0.9416330	4.9121510	-0.3795500	C	-5.8103510	0.7164880	0.9115890
H	-1.5019980	4.9241680	-1.3234730	C	-4.9645540	0.4253060	1.9823460
H	-1.6787380	4.9848490	0.4308030	H	-5.1895710	0.8316710	2.9694780
H	-0.3202850	5.8125270	-0.3480920	C	-3.8273540	-0.3651300	1.8235320
C	-0.0709730	-2.9094020	-0.5551800	C	-3.9933080	-1.0750440	-1.9181020
C	-0.1353430	-2.2925520	0.7325510	H	-3.9050350	-2.1687890	-1.9605060
C	1.0889140	-1.8128060	1.3045320	H	-3.0141370	-0.6678640	-2.2110130
C	2.3139700	-2.0196320	0.6275590	H	-4.7334170	-0.7651830	-2.6630330
C	2.3332010	-2.6502130	-0.5969020	C	-7.0450080	1.5410110	1.1141620
C	1.1317040	-3.0906490	-1.1982280	H	-7.8917990	0.9155820	1.4270580
H	-0.9806340	-3.2950990	-1.0095760	H	-7.3470860	2.0508280	0.1921230
H	1.0969380	-1.5062300	2.3499880	H	-6.9038280	2.3006960	1.8917050
H	3.2414550	-1.6742050	1.0807220	C	-2.8892040	-0.6109520	2.9630820
H	1.1646060	-3.5882220	-2.1648450	H	-2.6177640	-1.6696550	3.0606330
C	-1.3590570	-2.2093260	1.5689850	H	-3.3231840	-0.2781560	3.9114550
O	-1.2747360	-2.0959080	2.7896880	H	-1.9515700	-0.0599610	2.8065640
C	-2.7074510	-2.2611940	0.9285630	C	1.0164640	-2.1319440	-0.4348570
C	-2.9826510	-1.7638960	-0.3485680	C	1.9890830	-2.1198610	0.5706610
C	-3.7615380	-2.7900960	1.6831170	C	3.3225280	-1.9750820	0.1900750
C	-4.2723190	-1.8275520	-0.8653710	H	4.0912110	-1.9387680	0.9630950
H	-2.1894520	-1.2922200	-0.9305990	C	3.6930980	-1.8333090	-1.1470370
C	-5.0408700	-2.8626910	1.1581180	C	2.6923870	-1.8376140	-2.1190420
H	-3.5489440	-3.1449580	2.6890620	H	2.9629970	-1.7037060	-3.1672000
C	-5.3160600	-2.3930510	-0.1318900	C	1.3475840	-1.9897170	-1.7881560
H	-4.4730100	-1.4314320	-1.8608560	C	1.6081760	-2.1938750	2.0174050
H	-5.8482430	-3.2938890	1.7500050	H	1.1174150	-3.1415110	2.2760720
C	-6.6960750	-2.5085720	-0.7034850	H	0.9009240	-1.3961550	2.2824890
H	-6.9414690	-3.5528230	-0.9375010	H	2.4902820	-2.0938940	2.6585320
H	-7.4569450	-2.1578040	0.0046440	C	5.1339100	-1.6892120	-1.5316800
H	-6.8010910	-1.9322870	-1.6291480	H	5.5677650	-2.6569530	-1.8174040
C	3.5996960	-2.7920820	-1.3685230	H	5.7320280	-1.2971570	-0.7017140
F	4.6958560	-2.6278480	-0.6154600	H	5.2541190	-1.0192890	-2.3912720
F	3.6743010	-1.8880830	-2.3656720	C	0.2879350	-1.9285160	-2.8425950
F	3.7005430	-3.9968180	-1.9529240	H	-0.2343300	-0.9619450	-2.7917670
INTb1				H	-0.4746890	-2.7086020	-2.7161210
C	-1.1831360	-1.1489370	0.0093650	H	0.7226920	-2.0268440	-3.8423180
C	-2.3316920	-3.0724990	0.4817540	N	-0.3648310	-2.2349760	-0.0675100
C	-1.0465200	-3.4252950	0.2081880	N	-2.3865380	-1.6799170	0.3622530
C	-3.5562270	-0.8771810	0.5506970	Ni	-0.8357600	0.6195800	-0.5213450
C	-4.3650670	-0.5879010	-0.5532480	C	-0.3852610	-4.7493480	0.1354980
C	-5.4883350	0.2121360	-0.3487530	H	0.0351980	-4.9321500	-0.8621430
				H	0.4415020	-4.8397570	0.8518900
				H	-1.1007900	-5.5497070	0.3472630

C	-3.5212100	-3.8816330	0.8371940	C	5.5198350	-0.0342020	-0.0755180
H	-3.9680380	-3.5483090	1.7826860	C	4.7856750	-0.2177730	1.0936850
H	-4.3053760	-3.8177010	0.0712670	H	5.1632620	-0.8933450	1.8630550
H	-3.2508220	-4.9360230	0.9483670	C	3.5655250	0.4246280	1.3024030
C	2.1610070	1.4021170	0.6222230	C	3.2439940	2.3516540	-1.9804670
C	2.2554010	1.7454970	-0.7306470	H	2.8455680	3.2968960	-1.5899650
C	3.5220150	1.8543560	-1.3132400	H	2.4149240	1.8490510	-2.5012560
C	4.6702370	1.6635560	-0.5604210	H	4.0126710	2.5834730	-2.7247880
C	4.5604730	1.3368770	0.7898290	C	6.8246460	-0.7392580	-0.2901370
C	3.3074440	1.1932550	1.3781910	H	7.6376130	-0.0285660	-0.4855680
H	1.1807450	1.2528680	1.0744360	H	6.7798130	-1.4092700	-1.1586110
H	3.5840920	2.0868080	-2.3733440	H	7.1097890	-1.3370240	0.5827450
H	5.6524080	1.7646370	-1.0165650	C	2.7694710	0.1765440	2.5456830
H	3.2271670	0.9148650	2.4268030	H	2.5901510	1.0925560	3.1227670
C	1.0687690	1.9150820	-1.6391650	H	3.2828310	-0.5334470	3.2021200
O	1.2028680	1.6411690	-2.8308740	H	1.7832350	-0.2400570	2.3009520
C	-0.2250510	2.3944810	-1.1001840	C	-1.6544310	2.2717420	0.1160560
C	-0.3908720	3.1643580	0.0891870	C	-2.4979170	1.4715110	0.8934850
C	-1.4049380	2.0536680	-1.8334810	C	-3.8511980	1.4345580	0.5603890
C	-1.6362230	3.6068190	0.4798420	H	-4.5186590	0.7969470	1.1429610
H	0.4838790	3.4503330	0.6701750	C	-4.3622390	2.1509050	-0.5205580
C	-2.6666150	2.5236380	-1.4023350	C	-3.4835110	2.9156450	-1.2890400
H	-1.2980100	1.6097690	-2.8229310	H	-3.8636810	3.4640590	-2.1518990
C	-2.8012810	3.2870060	-0.2569910	C	-2.1244270	2.9911500	-0.9894370
H	-1.7314680	4.2143750	1.3797070	C	-1.9595190	0.6060300	1.9891480
H	-3.5526290	2.2761680	-1.9885940	H	-1.2889490	1.1479920	2.6678820
C	-4.1355380	3.7752600	0.2134630	H	-1.3776710	-0.2219870	1.5576300
H	-4.9512230	3.3596370	-0.3891870	H	-2.7728220	0.1686850	2.5782440
H	-4.3131180	3.4901860	1.2593760	C	-5.8221260	2.0853720	-0.8519070
H	-4.2037910	4.8703550	0.1658070	H	-6.3769800	2.9076950	-0.3811600
C	5.7886960	1.0428880	1.5875160	H	-6.2699150	1.1505010	-0.4951790
F	6.8614510	1.6985820	1.1319010	H	-5.9952510	2.1565110	-1.9316920
F	6.0992470	-0.2697690	1.5518600	C	-1.1851330	3.7706650	-1.8570610
F	5.6431120	1.3595080	2.8791270	H	-0.5188510	3.0947130	-2.4118610
INTol				H	-0.5369070	4.4412600	-1.2793300
C	0.6743470	1.4875040	-0.0443030	H	-1.7333820	4.3739630	-2.5874570
C	1.6419610	3.0686090	1.2963840	N	-0.2614180	2.3463680	0.4452150
C	0.3050330	3.3236360	1.2687330	N	1.8388250	1.9392000	0.4980620
C	3.0933690	1.2768200	0.2990770	Ni	0.4703970	0.1407380	-1.3338750
C	3.7936000	1.4774630	-0.8963820	C	-0.5053790	4.3812880	1.9177820
C	5.0059810	0.8119290	-1.0595030	H	-1.0409760	4.9956460	1.1831100
H	5.5652610	0.9579730	-1.9849070	H	-1.2614230	3.9596620	2.5924190
				H	0.1326700	5.0451810	2.5086520
				C	2.7647550	3.7966490	1.9344160

H	3.3260270	3.1721660	2.6407080	C	3.6656590	3.4084730	-0.7211300
H	3.4825470	4.1538950	1.1840770	H	3.6645210	4.0557600	-1.5994580
H	2.3942090	4.6682480	2.4820620	C	3.4821020	2.0362940	-0.8962270
C	-1.6161870	-2.9250530	0.1796470	C	3.6019090	0.8523850	2.7256130
C	-1.2913080	-2.0010240	-0.8244490	H	4.2976270	0.0071470	2.6428990
C	-2.3376140	-1.2695470	-1.4085810	H	2.5976870	0.4176800	2.8317760
C	-3.6398020	-1.3935700	-0.9582470	H	3.8367130	1.4021730	3.6426960
C	-3.9307930	-2.2646140	0.0897540	C	3.9997880	5.4492910	0.7153650
C	-2.9196430	-3.0447230	0.6436760	H	4.7735380	5.6924690	1.4530560
H	-0.8476750	-3.5675180	0.5993190	H	3.0659670	5.9056190	1.0737390
H	-2.1021670	-0.5758790	-2.2121070	H	4.2635650	5.9422140	-0.2269690
H	-4.4318840	-0.8020970	-1.4104070	C	3.2248570	1.4538270	-2.2497560
H	-3.1540910	-3.7522090	1.4365520	H	3.8577600	0.5812680	-2.4570700
C	0.0964480	-1.7527220	-1.3250340	H	3.3884500	2.1951720	-3.0384650
O	0.2222010	-1.2721710	-2.5275320	H	2.1835240	1.1081680	-2.3156100
C	1.2917320	-2.3855100	-0.6967130	C	1.8018310	-3.3227330	-0.1760950
C	1.4396620	-2.5625460	0.6861190	C	1.2961090	-3.7137120	-1.4194000
C	2.3772680	-2.7229610	-1.5158420	C	0.4597630	-4.8290150	-1.4643870
C	2.6112660	-3.0883770	1.2162360	H	0.0541210	-5.1454070	-2.4261630
H	0.6468890	-2.2455810	1.3623950	C	0.1296420	-5.5450630	-0.3150910
C	3.5424530	-3.2501330	-0.9804380	C	0.6483810	-5.1180140	0.9089360
H	2.2852300	-2.5511450	-2.5855640	H	0.3901050	-5.6636440	1.8179100
C	3.6813810	-3.4498870	0.3960030	C	1.4875420	-4.0112040	1.0022470
H	2.7040650	-3.2075540	2.2965570	C	1.6024150	-2.9251040	-2.6541620
H	4.3720730	-3.5038290	-1.6412480	H	2.6798290	-2.7725290	-2.7985860
C	4.9385540	-4.0283830	0.9695910	H	1.1523990	-1.9243850	-2.5895050
H	4.9027390	-5.1260200	0.9983380	H	1.2059970	-3.4202710	-3.5464330
H	5.8157230	-3.7539570	0.3712790	C	-0.7572310	-6.7517160	-0.3796850
H	5.1092570	-3.6874340	1.9981020	H	-0.1960470	-7.6726080	-0.1739090
C	-5.2929150	-2.3140300	0.6930470	H	-1.2203360	-6.8612940	-1.3661090
F	-6.2235960	-1.7356170	-0.0773140	H	-1.5598410	-6.6974190	0.3655250
F	-5.3251910	-1.6723440	1.8799150	C	1.9979850	-3.5329170	2.3256480
F	-5.6970720	-3.5678550	0.9374810	H	1.5102060	-2.5885240	2.6035410
INTo2				H	3.0768950	-3.3318630	2.3095750
C	2.2475450	-0.9105350	0.0854350	H	1.7968930	-4.2646940	3.1148050
C	4.5380180	-1.0106150	-0.1071170	N	2.6798510	-2.1965250	-0.1072300
C	4.0702100	-2.2804920	-0.2267890	N	3.4154040	-0.1956830	0.0790130
C	3.5002500	1.2215240	0.2398080	Ni	0.5102440	-0.3618040	0.2832310
C	3.6561090	1.7479300	1.5279390	C	4.7692680	-3.5693940	-0.4412660
C	3.8249820	3.1252530	1.6564450	H	4.5740160	-4.2781650	0.3739460
H	3.9500480	3.5522150	2.6527320	H	4.4474140	-4.0570550	-1.3704580
C	3.8463760	3.9679430	0.5427690	H	5.8511020	-3.4152870	-0.4995720
				C	5.9133120	-0.4613900	-0.1525090
				H	6.0350070	0.2634490	-0.9681960

H	6.1752460	0.0600940	0.7776530	H	-3.0745150	-3.4600890	1.5839260
H	6.6429720	-1.2627130	-0.3044290	C	-1.0891850	-3.0136230	0.9006930
C	-4.4466610	1.6845640	0.3396800	C	0.1532670	-3.0642260	-2.7053370
C	-3.4979390	0.6734550	0.1192930	H	1.1009610	-3.6062270	-2.5908610
C	-3.9427810	-0.6483780	-0.0272620	H	0.4187570	-2.0078900	-2.8525410
C	-5.2939040	-0.9520110	0.0172810	H	-0.3383170	-3.4226060	-3.6154860
C	-6.2232050	0.0648220	0.2210350	C	-4.3444720	-4.1443690	-0.7277970
C	-5.7973740	1.3817730	0.3910020	H	-4.4135200	-5.1901690	-1.0540400
H	-4.1220020	2.7096260	0.4985420	H	-4.8441860	-3.5392670	-1.4946470
H	-3.2053290	-1.4315890	-0.1800180	H	-4.9171400	-4.0444070	0.1996720
H	-5.6268340	-1.9782620	-0.1081350	C	-0.5705420	-2.6373760	2.2524900
H	-6.5290320	2.1672820	0.5695140	H	0.3573670	-3.1677280	2.5028100
C	-2.0459270	0.9328160	0.0864420	H	-1.3089190	-2.8484050	3.0325340
O	-1.2822050	-0.0326820	0.3206730	H	-0.3336280	-1.5644500	2.2835790
C	-1.4999190	2.2671080	-0.2065400	C	3.9691600	-0.5530370	0.1775620
C	-2.1095190	3.1501390	-1.1076340	C	4.2786030	0.0128410	1.4189440
C	-0.2851680	2.6500610	0.3852420	C	5.2922030	0.9685370	1.4680990
C	-1.5229420	4.3742730	-1.4042710	H	5.5442210	1.4204460	2.4285180
H	-3.0299840	2.8624260	-1.6117380	C	5.9898400	1.3569810	0.3241720
C	0.2759630	3.8837010	0.1047600	C	5.6390180	0.7828650	-0.8979840
H	0.2123270	1.9584320	1.0670880	H	6.1634060	1.0904090	-1.8037660
C	-0.3276450	4.7655550	-0.7978760	C	4.6297020	-0.1732930	-0.9958700
H	-1.9975810	5.0382570	-2.1255980	C	3.5136190	-0.3734930	2.6456410
H	1.2145550	4.1662080	0.5823730	H	3.4686550	-1.4623740	2.7796610
C	0.3086850	6.0876370	-1.0935560	H	2.4734080	-0.0258740	2.5734170
H	0.3085830	6.7377340	-0.2086580	H	3.9592270	0.0649630	3.5444600
H	1.3573760	5.9619930	-1.3931480	C	7.1069260	2.3526200	0.4081490
H	-0.2104000	6.6206250	-1.8973270	H	8.0709730	1.8557650	0.5811450
C	-7.6919260	-0.2115170	0.2659810	H	6.9572120	3.0608360	1.2306380
F	-7.9769220	-1.5110850	0.1429260	H	7.2043110	2.9276960	-0.5194750
F	-8.3420050	0.4340480	-0.7150420	C	4.2255770	-0.7432470	-2.3191480
F	-8.2368940	0.2089300	1.4175420	H	3.2043950	-0.4275950	-2.5736660
INTo3				H	4.2216520	-1.8408310	-2.3185200
C	1.6451190	-1.3599800	-0.0760960	H	4.8960750	-0.4045100	-3.1155640
C	2.1011900	-3.6051870	0.1446650	N	2.9830020	-1.5853580	0.1138500
C	3.2825430	-2.9439130	0.2532310	N	1.1209910	-2.6255870	-0.0546170
C	-0.2633570	-2.9378150	-0.2250510	Ni	0.8365590	0.2734140	-0.2553010
C	-0.7383200	-3.2190020	-1.5127090	C	4.6634140	-3.4297570	0.4820430
C	-2.0686310	-3.6099320	-1.6487830	H	5.3364240	-3.1475680	-0.3380700
H	-2.4549100	-3.8339070	-2.6444700	H	5.0925880	-3.0146280	1.4036070
C	-2.9174870	-3.7227920	-0.5445260	H	4.6776780	-4.5206160	0.5676560
C	-2.4151280	-3.4086420	0.7169950	C	1.7762190	-5.0493260	0.2098510
				H	1.0487750	-5.2651790	1.0031580
				H	1.3415550	-5.4154640	-0.7296080

H	2.6777300	-5.6360860	0.4118660	C	-3.0255700	0.2614910	-2.3849990
C	-2.0526920	4.7738500	-0.5955640	C	-3.6590270	0.6677610	1.3586350
C	-0.9161870	4.0409820	-0.2247300	H	-3.7249970	1.7575980	1.4718300
C	0.2643220	4.7450660	0.0621340	H	-2.6776310	0.3646620	1.7518140
C	0.2939630	6.1271150	0.0050340	H	-4.4258810	0.2089930	1.9913330
C	-0.8434050	6.8616920	-0.3516250	C	-5.8189480	-2.3070500	-2.0680090
C	-2.0102550	6.1594630	-0.6601520	H	-6.7314370	-1.8743860	-2.4989730
H	-2.9694080	4.2554170	-0.8672540	H	-6.1206430	-2.8791160	-1.1825750
H	1.1544740	4.1825300	0.3319250	H	-5.4191910	-3.0115640	-2.8063700
H	1.2166720	6.6573670	0.2388190	C	-2.0750910	0.7736520	-3.4225110
H	-2.8992800	6.7117240	-0.9622680	H	-2.0133680	1.8692110	-3.4280560
C	-0.8939670	2.5713290	-0.1851110	H	-2.3697710	0.4426440	-4.4234350
O	0.2086140	1.9873710	-0.2937890	H	-1.0574220	0.4051690	-3.2331260
C	-2.1317600	1.7837790	-0.0166320	C	1.0829430	3.0283690	0.3009170
C	-3.1887000	2.2263490	0.7898750	C	2.1129760	3.1477060	-0.6370190
C	-2.2253120	0.5252260	-0.6302970	C	3.3983980	3.4112450	-0.1634390
C	-4.3133610	1.4349640	0.9797410	H	4.2140410	3.5101840	-0.8805980
H	-3.1171610	3.1844810	1.2993950	C	3.6629040	3.5510650	1.1981800
C	-3.3593380	-0.2516940	-0.4657050	C	2.6085990	3.4101440	2.1022840
H	-1.3911420	0.1630490	-1.2342410	H	2.8045750	3.5035440	3.1711970
C	-4.4026900	0.2013800	0.3405720	C	1.3090680	3.1425360	1.6779850
H	-5.1209070	1.7756030	1.6219450	C	1.8507430	2.9541180	-2.0980170
H	-3.4291040	-1.2181850	-0.9609120	H	0.9852230	3.5310270	-2.4480050
C	-5.5890540	-0.6851490	0.5449390	H	1.6334940	1.8984980	-2.3142310
C	-0.8082170	8.3574030	-0.3854670	H	2.7201610	3.2447360	-2.6962450
F	-5.3108970	-1.7027730	1.3784910	C	5.0519170	3.8240610	1.6906670
F	-6.0000270	-1.2408080	-0.6050330	H	5.7136140	4.1422090	0.8779690
F	-6.6331910	-0.0319440	1.0669090	H	5.4949250	2.9280280	2.1442260
H	0.1474150	8.7295110	-0.7724040	H	5.0588660	4.6053690	2.4598220
H	-1.6106910	8.7667650	-1.0085520	C	0.2039220	2.9239590	2.6622710
H	-0.9303280	8.7797120	0.6209390	H	-0.0325650	1.8522950	2.7226370
TSa1_2				H	-0.7192750	3.4474160	2.3832190
C	-0.7617620	1.5303690	-0.3299030	H	0.4985670	3.2567380	3.6626820
C	-2.3245610	3.1285820	-0.8161340	N	-0.2510450	2.7800610	-0.1592360
C	-1.1857240	3.7762520	-0.4500650	N	-2.0377210	1.7620590	-0.7386380
C	-2.9747770	0.7315770	-1.0673580	Ni	0.2378790	-0.0484190	-0.0242090
C	-3.8070580	0.2269830	-0.0634460	C	-0.8656730	5.2180770	-0.3340650
C	-4.7284480	-0.7570560	-0.4176330	H	-0.5969880	5.4919560	0.6942190
H	-5.3774780	-1.1706250	0.3559960	H	-0.0167060	5.4956230	-0.9719040
C	-4.8194240	-1.2461800	-1.7197020	H	-1.7244530	5.8278840	-0.6307040
C	-3.9548190	-0.7322980	-2.6875490	C	-3.6535880	3.6334290	-1.2319920
H	-4.0024520	-1.1165640	-3.7072940	H	-3.9165230	3.3040170	-2.2454800
				H	-4.4485580	3.2787290	-0.5633940
				H	-3.6681770	4.7273060	-1.2203550

C	1.4382660	-2.6876030	-0.4375060	C	-3.9976140	0.4274310	1.1973070
C	1.5187590	-1.4629450	0.2356260	H	-4.3830500	1.4545580	1.1407750
C	2.7883920	-0.8987280	0.4535090	H	-3.0048520	0.4821780	1.6660850
C	3.9271290	-1.4864390	-0.0697990	H	-4.6516000	-0.1430170	1.8649710
C	3.8203260	-2.6901220	-0.7728550	C	-5.4356430	-3.1818640	-1.9918300
C	2.5830860	-3.2990180	-0.9448960	H	-6.4814340	-2.8897010	-2.1524280
H	0.4752250	-3.1746870	-0.5790930	H	-5.4331030	-3.9030920	-1.1650870
H	2.8624050	0.0049530	1.0570760	H	-5.0968530	-3.7024870	-2.8934630
H	4.9046980	-1.0278660	0.0724610	C	-1.8203420	0.0502260	-3.3340500
H	2.5111320	-4.2438620	-1.4774840	H	-1.8058970	1.1414690	-3.4473870
C	0.2915940	-0.9845210	1.5837450	H	-1.9982700	-0.3937300	-4.3188210
O	0.8522490	-0.4979060	2.5627620	H	-0.8098910	-0.2488360	-3.0170660
C	-0.8738560	-1.9126630	1.7487290	C	0.6509360	3.1584330	0.1743230
C	-1.6571270	-2.3346810	0.6709640	C	1.6792860	3.2794150	-0.7657960
C	-1.2551800	-2.2831680	3.0417410	C	2.9173060	3.7409840	-0.3203310
C	-2.7827820	-3.1189050	0.8836700	H	3.7296190	3.8473760	-1.0400770
H	-1.3989990	-2.0047810	-0.3378110	C	3.1417690	4.0590270	1.0180690
C	-2.3872780	-3.0581280	3.2502290	C	2.0926060	3.9082880	1.9266600
H	-0.6492340	-1.9369950	3.8761010	H	2.2583350	4.1446920	2.9784460
C	-3.1693630	-3.4900260	2.1745970	C	0.8369140	3.4556710	1.5298550
H	-3.3888730	-3.4358480	0.0345020	C	1.4780730	2.8820290	-2.1957700
H	-2.6778060	-3.3337310	4.2638880	H	0.5093790	3.2105990	-2.5927180
C	-4.3811750	-4.3437520	2.3895200	H	1.5115920	1.7874890	-2.3027090
H	-4.1605280	-5.4032300	2.2037680	H	2.2674490	3.2940980	-2.8325040
H	-4.7562440	-4.2648850	3.4157250	C	4.4874530	4.5255320	1.4831240
H	-5.1950650	-4.0656000	1.7081400	H	5.1095370	4.8619370	0.6469420
C	5.0728750	-3.2998830	-1.3111820	H	5.0304020	3.7176140	1.9903850
F	5.9358550	-3.6125690	-0.3312980	H	4.4038080	5.3506260	2.2001200
F	5.7224770	-2.4477610	-2.1216980	C	-0.2626300	3.2533180	2.5245760
F	4.8496790	-4.4174670	-2.0118660	H	-0.4270530	2.1798690	2.6925370
INTa2				H	-1.2159100	3.6814150	2.1908430
C	-0.9614340	1.3896450	-0.3709800	H	-0.0050030	3.7051100	3.4877630
C	-2.7044020	2.7105250	-1.0257510	N	-0.6373140	2.7039730	-0.2639700
C	-1.6847070	3.5362510	-0.6645010	N	-2.2380210	1.4063620	-0.8318980
C	-3.0102250	0.2336970	-1.1142890	Ni	0.3313560	-0.0120280	-0.1180230
C	-3.9149550	-0.2239930	-0.1478650	C	-1.5731920	5.0137270	-0.6693900
C	-4.6918810	-1.3361710	-0.4589940	H	-1.4321040	5.4212350	0.3397680
H	-5.3920910	-1.7157820	0.2874540	H	-0.7222130	5.3523180	-1.2735340
C	-4.5771850	-1.9929000	-1.6856320	H	-2.4798250	5.4630430	-1.0858190
C	-3.6442550	-1.5236110	-2.6083000	C	-4.0629900	2.9959780	-1.5414940
H	-3.5307850	-2.0366070	-3.5640340	H	-4.2320390	2.5253050	-2.5185280
C	-2.8469260	-0.4086010	-2.3449270	H	-4.8425310	2.6227800	-0.8645720
				H	-4.2096280	4.0737800	-1.6578090
				C	1.9250230	-2.2934610	-0.9529510

C	1.8357100	-1.1460290	-0.1478980	H	1.6542180	4.0023420	1.5525510
C	3.0247040	-0.6847500	0.4450240	H	1.2828940	2.5086580	2.4038610
C	4.2441600	-1.3053830	0.2151210	H	0.7563390	4.0602600	3.0793740
C	4.3016570	-2.4358500	-0.6027280	C	-4.0520850	4.4331630	1.8457380
C	3.1401560	-2.9351680	-1.1840070	H	-3.9806840	5.5230480	1.9537120
H	1.0280870	-2.7027000	-1.4223840	H	-4.2343540	4.0269350	2.8478950
H	2.9836910	0.1763010	1.1151790	H	-4.9320040	4.2180460	1.2307600
H	5.1571790	-0.9274760	0.6739610	C	-1.6983950	2.1650630	-1.9809570
H	3.1847190	-3.8219420	-1.8123690	H	-1.0799090	2.7170320	-2.7014800
C	0.1284370	-0.4949760	1.6221360	H	-2.7225450	2.1444100	-2.3678510
O	0.6947440	0.1013840	2.5148530	H	-1.3306680	1.1311860	-1.9593270
C	-0.8903500	-1.5550490	1.8788600	C	3.1573360	-0.1835240	-1.0196090
C	-1.3640730	-2.3863160	0.8620040	C	2.8971320	-1.1518710	-1.9949950
C	-1.4227860	-1.6797650	3.1654300	C	3.6668180	-2.3161550	-1.9805920
C	-2.3482280	-3.3260520	1.1281640	H	3.4738280	-3.0844260	-2.7301370
H	-0.9598200	-2.2719360	-0.1447490	C	4.6775370	-2.5146670	-1.0416480
C	-2.4200180	-2.6104520	3.4216420	C	4.9317260	-1.5046510	-0.1110860
H	-1.0450980	-1.0284280	3.9510250	H	5.7359130	-1.6363560	0.6141390
C	-2.8976430	-3.4476350	2.4088950	C	4.1953960	-0.3221970	-0.0872840
H	-2.7150550	-3.9686520	0.3271090	C	1.8674070	-0.9250730	-3.0588960
H	-2.8409640	-2.6959590	4.4231290	H	2.2320670	-0.2093060	-3.8093400
C	-3.9707510	-4.4572860	2.6775760	H	0.9325200	-0.5180150	-2.6569920
H	-3.5727800	-5.4797890	2.6497030	H	1.6347600	-1.8566260	-3.5855950
H	-4.4310850	-4.3092000	3.6602560	C	5.5018760	-3.7663340	-1.0409870
H	-4.7638890	-4.4071310	1.9207690	H	5.1380210	-4.4907000	-1.7771810
C	5.6326680	-3.0570700	-0.8568530	H	5.4919840	-4.2527710	-0.0580920
F	6.3273550	-3.2404840	0.2785320	H	6.5516790	-3.5502930	-1.2763470
F	6.4044820	-2.2795790	-1.6389070	C	4.5388440	0.7791510	0.8669190
F	5.5473500	-4.2489060	-1.4630510	H	3.6544650	1.2140410	1.3438850
INTa3				H	5.0703880	1.5913970	0.3515220
C	1.2039220	1.0592860	-0.2118320	H	5.1968300	0.4134930	1.6618540
C	1.5547010	3.0156990	-1.3281310	N	2.3301010	0.9829950	-0.9684710
C	2.5633000	2.1739740	-1.6672520	N	0.7285510	2.3076620	-0.4434660
C	-0.4740970	2.8375960	0.1255710	C	3.7141800	2.3337930	-2.5861110
C	-0.4149480	3.4107180	1.4028100	H	4.6768670	2.2257480	-2.0702710
C	-1.5966740	3.9129040	1.9430850	H	3.6931050	1.5848060	-3.3889250
H	-1.5724210	4.3637780	2.9363530	H	3.6942290	3.3233110	-3.0524560
C	-2.8038640	3.8650100	1.2417790	C	1.2762860	4.4207750	-1.7046950
C	-2.8142900	3.2992190	-0.0315270	H	0.3010910	4.5326780	-2.1953390
H	-3.7511860	3.2493150	-0.5878000	H	1.2710180	5.0783650	-0.8255090
C	-1.6581480	2.7799130	-0.6160730	H	2.0428450	4.7896090	-2.3928170
C	0.8809370	3.4982940	2.1483150	C	-1.0923340	-1.7559970	-1.2374450
				C	-1.0190430	-0.8357530	-0.1794490
				C	-2.2452280	-0.2926090	0.2518920

C	-3.4566580	-0.6204720	-0.3439790	H	-1.1144130	-2.0377060	2.7681050
C	-3.4815720	-1.5167560	-1.4140110	H	-0.6695300	-3.5332240	3.6081200
C	-2.2942830	-2.0919990	-1.8583420	C	4.1829830	-3.9144750	2.5354580
H	-0.1788930	-2.2368720	-1.5984980	H	4.1896930	-4.9881570	2.7638490
H	-2.2561320	0.4312160	1.0715310	H	4.2841940	-3.3858450	3.4906610
H	-4.3875920	-0.1735020	0.0071940	H	5.0730270	-3.6994770	1.9348420
H	-2.3124580	-2.7998040	-2.6848000	C	1.8265130	-2.4585620	-1.6661830
C	1.5925490	-0.1930500	2.3752330	H	1.3139830	-3.1907190	-2.3043210
O	2.2897670	0.4554200	3.1176020	H	2.8624150	-2.3817950	-2.0133890
C	0.7505070	-1.4023160	2.6721190	H	1.3471770	-1.4854430	-1.8362420
C	-0.3418570	-1.2939930	3.5616930	C	-3.1926280	-0.1613920	-1.0224970
C	0.8100660	-2.5076890	1.8038100	C	-2.9814760	0.7070300	-2.1003890
C	-1.2851290	-2.2955430	3.6258550	C	-3.8193440	1.8153930	-2.2157390
H	-0.4126390	-0.4157870	4.2026160	H	-3.6642230	2.5101020	-3.0421720
C	-0.1535020	-3.5177970	1.8877300	C	-4.8495220	2.0544240	-1.3051980
H	1.6481620	-2.6047250	1.1099110	C	-5.0477580	1.1441850	-0.2669190
C	-1.2092550	-3.4224480	2.7832400	H	-5.8591520	1.3091700	0.4431140
H	-2.1127200	-2.2193290	4.3306490	C	-4.2339200	0.0234840	-0.1051080
H	-0.0917050	-4.3773470	1.2221530	C	-1.9218700	0.4341720	-3.1240110
C	-2.2795670	-4.4656250	2.8390920	H	-2.2523310	-0.3301720	-3.8409550
H	-2.5141700	-4.7453910	3.8730680	H	-0.9909820	0.0691420	-2.6743500
H	-3.2081430	-4.0887870	2.3906650	H	-1.6918090	1.3368420	-3.6998500
H	-1.9936310	-5.3706830	2.2936840	C	-5.7517020	3.2402060	-1.4640550
C	-4.7928530	-1.8263030	-2.0467420	H	-5.2455260	4.0661000	-1.9757270
F	-5.6489640	-2.4046950	-1.1838520	H	-6.1088160	3.6084080	-0.4959010
F	-4.6862420	-2.6491930	-3.0985050	H	-6.6389000	2.9866870	-2.0592310
F	-5.4139150	-0.7141190	-2.4830360	C	-4.4690870	-0.9337180	1.0224920
Ni	0.5447000	-0.3155450	0.8597590	H	-3.8486790	-0.6827390	1.8923420
TSa3_4				H	-4.2310450	-1.9683930	0.7494360
C	-1.1676360	-1.1783100	-0.0882760	H	-5.5149080	-0.8981210	1.3456390
C	-1.4153300	-3.2821740	-0.9333410	N	-2.2968400	-1.2620300	-0.8370300
C	-2.4688610	-2.5456810	-1.3705440	N	-0.6256630	-2.4197450	-0.1590980
C	0.5825320	-2.8036320	0.5067780	C	-3.6386700	-2.9045400	-2.2061710
C	0.5232330	-3.1185780	1.8707390	H	-4.5780620	-2.8670930	-1.6393070
C	1.7110440	-3.4687380	2.5085500	H	-3.7524870	-2.2261870	-3.0605830
H	1.6866900	-3.7174310	3.5705710	H	-3.5289320	-3.9191530	-2.6006100
C	2.9264310	-3.5181560	1.8215090	C	-1.0729840	-4.7114010	-1.1201640
C	2.9394000	-3.2013490	0.4648190	H	-0.1109930	-4.8454330	-1.6303740
H	3.8841860	-3.2156540	-0.0798960	H	-1.0016660	-5.2377660	-0.1596390
C	1.7780060	-2.8377840	-0.2182920	H	-1.8409310	-5.2117240	-1.7175590
C	-0.7726940	-3.0709420	2.6211830	C	1.0395900	1.4811690	-1.4132030
H	-1.5784560	-3.5886020	2.0843400	C	1.0287230	0.7218670	-0.2326890
				C	2.2840500	0.2862420	0.2321610
				C	3.4616790	0.5374090	-0.4587530

C	3.4231570	1.2558360	-1.6554820	H	-0.6154920	3.4869650	3.7808450
C	2.2085050	1.7441950	-2.1264480	C	-5.3599270	2.3005390	2.7853910
H	0.1014390	1.8858130	-1.8016340	H	-5.7280710	1.2688830	2.8503300
H	2.3469960	-0.2891310	1.1595050	H	-6.1368630	2.8814260	2.2739590
H	4.4162280	0.1650230	-0.0842530	H	-5.2695230	2.6843370	3.8069870
H	2.1789440	2.3229220	-3.0476720	C	-2.7548630	1.7794200	-1.4804380
C	-1.5988690	0.6803380	2.2227470	H	-2.4504040	2.6293660	-2.1054670
O	-2.3636350	0.6070480	3.1307180	H	-3.7368030	1.4454370	-1.8306720
C	-0.4721290	1.9247580	2.1226580	H	-2.0404760	0.9658130	-1.6671470
C	0.6175820	1.9266730	2.9969790	C	2.7064010	1.3006860	-1.1326590
C	-0.7969700	3.0869900	1.4139280	C	2.7169830	0.4119130	-2.2136320
C	1.3822760	3.0742940	3.1481260	C	3.8389610	-0.4020160	-2.3729190
H	0.8709040	1.0166110	3.5423160	H	3.8604680	-1.1120050	-3.2002000
C	-0.0251780	4.2280350	1.5652910	C	4.9263450	-0.3335980	-1.5019890
H	-1.6466100	3.0763840	0.7288660	C	4.8977890	0.6051940	-0.4694760
C	1.0761850	4.2352040	2.4305000	H	5.7513270	0.6853900	0.2047430
H	2.2398820	3.0759980	3.8197140	C	3.8017650	1.4420780	-0.2708440
H	-0.2640180	5.1300110	1.0022560	C	1.5851300	0.3627010	-3.1935740
C	1.8978470	5.4763710	2.5846990	H	1.6125790	1.2269750	-3.8716340
H	2.7890490	5.2986580	3.1949420	H	0.6057230	0.3719160	-2.7019870
H	2.2255310	5.8578410	1.6102280	H	1.6428290	-0.5370050	-3.8149440
H	1.3192990	6.2772500	3.0626940	C	6.0863700	-1.2700440	-1.6474790
C	4.6940520	1.4453620	-2.4044580	H	7.0381510	-0.7747320	-1.4245780
F	5.6512430	2.0120180	-1.6481870	H	6.1468450	-1.6861640	-2.6586920
F	4.5523190	2.2119660	-3.4940900	H	5.9927830	-2.1141020	-0.9513970
F	5.2082450	0.2707340	-2.8210290	C	3.8176600	2.4793970	0.8108360
Ni	-0.5592780	0.3459050	0.8273160	H	2.8455540	2.5868290	1.3067680
INTa4				H	4.0754730	3.4671220	0.4035920
C	0.5308710	1.5500590	-0.0585550	H	4.5657160	2.2398600	1.5730440
C	0.0050210	3.6462110	-0.7944620	N	1.5127830	2.0431550	-0.8579250
C	1.2157160	3.3276650	-1.3211950	N	-0.3962540	2.5371070	-0.0341260
C	-1.6381380	2.4712280	0.6780250	C	2.1387040	4.0830740	-2.1991090
C	-1.6502080	2.7576000	2.0458490	H	3.1317800	4.1906700	-1.7452650
C	-2.8738260	2.6967440	2.7145350	H	2.2789570	3.5911920	-3.1701550
H	-2.9024770	2.9224060	3.7809270	H	1.7477920	5.0867390	-2.3904390
C	-4.0547170	2.3665210	2.0525470	C	-0.8108540	4.8796470	-0.8874870
C	-3.9975680	2.0851940	0.6860830	H	-1.7939080	4.6977200	-1.3397490
H	-4.9120060	1.8106090	0.1579910	H	-0.9900650	5.3211700	0.1011720
C	-2.8008010	2.1278930	-0.0247610	H	-0.2978400	5.6288260	-1.4979820
C	-0.3917460	3.1063990	2.7793540	C	-0.5541860	-1.6844460	-1.3545480
H	0.1980360	3.8664330	2.2508880	C	-0.7096960	-1.0064790	-0.1361380
H	0.2544040	2.2261210	2.8962950	C	-1.9989520	-0.9541710	0.4106210
				C	-3.0917290	-1.5276490	-0.2329130
				C	-2.9148200	-2.1678090	-1.4561100

C	-1.6378280	-2.2516720	-2.0131430	C	5.3596540	-1.6355190	1.9581670
H	0.4395540	-1.7896290	-1.7926820	H	5.9933800	-1.1087520	1.2363290
H	-2.1631600	-0.4525490	1.3661340	H	5.8311670	-2.6055200	2.1638450
H	-4.0833300	-1.4674850	0.2118510	H	5.3731640	-1.0700690	2.8977370
H	-1.5006310	-2.7694510	-2.9620680	C	2.1052390	-1.4801310	-1.8673040
C	1.9486450	0.1674140	2.0825030	H	1.5971580	-2.3201270	-2.3588050
O	2.6708110	0.2373190	2.9738310	H	3.0304750	-1.2747740	-2.4167690
C	0.9965040	-1.9947860	1.4320670	H	1.4494510	-0.6050130	-1.9760380
C	0.2724400	-2.6314690	2.4416190	C	-3.2308580	-1.0519740	-0.6859380
C	2.0400060	-2.7046500	0.8287460	C	-3.5523090	-0.5463070	-1.9521370
C	0.5683770	-3.9378900	2.8220510	C	-4.7600970	0.1325240	-2.1004000
H	-0.5470210	-2.1077320	2.9368790	H	-5.0208180	0.5387000	-3.0788610
C	2.3290380	-4.0145030	1.2051310	C	-5.6363840	0.3142250	-1.0280800
H	2.6419210	-2.2302180	0.0478590	C	-5.2761140	-0.1945870	0.2183350
C	1.5968370	-4.6552960	2.2065010	H	-5.9431350	-0.0472960	1.0686170
H	-0.0120830	-4.4162740	3.6126110	C	-4.0788870	-0.8848160	0.4139800
H	3.1433130	-4.5516000	0.7155210	C	-2.6054170	-0.6990420	-3.1029250
C	1.8863620	-6.0760830	2.5901710	H	-2.5056640	-1.7458170	-3.4191060
H	1.6946800	-6.2555100	3.6548500	H	-1.5949160	-0.3586090	-2.8388480
H	1.2585030	-6.7819990	2.0294580	H	-2.9452780	-0.1227580	-3.9693060
H	2.9298100	-6.3445770	2.3872240	C	-6.9293190	1.0481410	-1.2176190
C	-4.0464890	-2.8096080	-2.1792740	H	-7.6805770	0.4184090	-1.7116870
F	-5.2400050	-2.5199130	-1.6428560	H	-6.7959400	1.9369580	-1.8457500
F	-3.9432910	-4.1502640	-2.1980450	H	-7.3519770	1.3714570	-0.2600760
F	-4.0948960	-2.4296540	-3.4699200	C	-3.6979140	-1.3900740	1.7707070
Ni	0.7117150	-0.1823400	0.8299390	H	-2.9222430	-0.7494520	2.2151660
INTa5				H	-3.2778570	-2.4035430	1.7353130
C	-0.8660970	-1.1729500	-0.0125460	H	-4.5611610	-1.3973230	2.4441560
C	-0.5284020	-3.3959360	-0.4968910	N	-1.9969520	-1.7515690	-0.5143160
C	-1.8185990	-3.1111910	-0.8079640	N	0.0299770	-2.2038030	-0.0197930
C	1.3690290	-2.0827620	0.4697470	C	-2.9169960	-3.9654770	-1.3170380
C	1.6117250	-2.2928200	1.8342070	H	-3.7781550	-3.9644510	-0.6360170
C	2.9161370	-2.1364160	2.2968900	H	-3.2846780	-3.6343240	-2.2971490
H	3.1194660	-2.2816890	3.3590440	H	-2.5768650	-5.0003250	-1.4219940
C	3.9640530	-1.8005760	1.4380710	C	0.2470780	-4.6567510	-0.5778520
C	3.6847090	-1.6194240	0.0853800	H	1.1479200	-4.5437350	-1.1942890
H	4.4915610	-1.3487290	-0.5956410	H	0.5805430	-4.9976710	0.4108820
C	2.3917770	-1.7473740	-0.4216000	H	-0.3605440	-5.4538020	-1.0174680
C	0.4975830	-2.6542450	2.7665800	C	1.6835420	2.2329540	-1.5991640
H	-0.0190080	-3.5731560	2.4577930	C	1.3044350	2.2765440	-0.2499240
H	-0.2606720	-1.8603540	2.7917510	C	2.2786440	2.0327490	0.7275790
H	0.8718020	-2.8037950	3.7844200	C	3.5860960	1.7341330	0.3700830
				C	3.9412620	1.6837020	-0.9745850
				C	2.9892680	1.9418840	-1.9600480

H	0.9443410	2.4469020	-2.3689060	H	6.0742560	-0.3665620	1.6104070
H	1.9950780	2.0445490	1.7787850	H	6.4250910	-2.0917660	1.6181780
H	4.3259480	1.5219440	1.1378320	H	5.7589320	-1.3258620	3.0693660
H	3.2735970	1.9098040	-3.0107260	C	2.5192530	-1.6890280	-1.8675370
C	-0.5738270	0.8039470	2.6016590	H	2.4619730	-2.6772550	-2.3446270
O	-0.6037690	1.0141430	3.7456850	H	3.3228490	-1.1283300	-2.3570610
C	-0.0913590	2.5865130	0.1329860	H	1.5769820	-1.1685850	-2.0769450
C	-0.3620380	3.5621560	1.1258310	C	-2.9332840	-1.5307990	-0.6730410
C	-1.1777570	2.0621850	-0.6069450	C	-3.2189080	-0.7230980	-1.7789310
C	-1.6528320	3.9362730	1.4202930	C	-4.4928120	-0.1645800	-1.8682770
H	0.4763910	4.0236000	1.6461930	H	-4.7317180	0.4672460	-2.7245870
C	-2.4922550	2.4274130	-0.2531870	C	-5.4637480	-0.3875360	-0.8919670
H	-1.0029000	1.4917910	-1.5168810	C	-5.1418660	-1.2043300	0.1915650
C	-2.7467360	3.3383380	0.7600380	H	-5.8903000	-1.3879700	0.9634900
H	-1.8394130	4.6901480	2.1845040	C	-3.8847380	-1.7920620	0.3206510
H	-3.3266340	1.9963630	-0.8075370	C	-2.1830660	-0.4531960	-2.8261410
C	-4.1479830	3.7118000	1.1351010	H	-1.7968260	-1.3778450	-3.2745750
H	-4.2763240	4.8008720	1.1779050	H	-1.3145440	0.0688460	-2.4023990
H	-4.8767780	3.3136280	0.4195650	H	-2.5914070	0.1668450	-3.6307300
H	-4.4127000	3.3227810	2.1273060	C	-6.8127390	0.2565210	-0.9901270
C	5.3224400	1.3242940	-1.4101410	H	-7.0658980	0.5052990	-2.0264820
F	6.1367080	1.0428130	-0.3862750	H	-6.8462060	1.1903660	-0.4142890
F	5.8986890	2.3055360	-2.1191160	H	-7.6002790	-0.3939610	-0.5935120
F	5.3191730	0.2415390	-2.2152150	C	-3.5707040	-2.6708750	1.4930580
Ni	-0.6479390	0.5328650	0.8808350	H	-2.5510430	-2.5159380	1.8664740
TSa4_5				H	-3.6530730	-3.7355240	1.2343770
C	-0.5875060	-1.3987730	0.0320060	H	-4.2653420	-2.4807630	2.3175910
C	0.0316830	-3.5382460	-0.5028910	N	-1.6207670	-2.0841560	-0.5330770
C	-1.2681240	-3.3951770	-0.8689700	N	0.4272770	-2.3033070	0.0306210
C	1.7508850	-2.0540610	0.5202060	C	-2.2200210	-4.3396780	-1.4994740
C	1.9794160	-2.1025810	1.8992710	H	-3.1037430	-4.5139860	-0.8721860
C	3.2776740	-1.8748350	2.3568760	H	-2.5815570	-3.9702420	-2.4678110
H	3.4701830	-1.9004030	3.4301140	H	-1.7399600	-5.3074480	-1.6731810
C	4.3267400	-1.6099980	1.4786990	C	0.9360140	-4.7109150	-0.5545300
C	4.0565680	-1.5693460	0.1108440	H	1.8035780	-4.5455520	-1.2055230
H	4.8624810	-1.3326750	-0.5852910	H	1.3251570	-4.9606440	0.4410480
C	2.7770290	-1.7856850	-0.3947430	H	0.4003550	-5.5866840	-0.9330410
C	0.8609950	-2.3627600	2.8610330	C	0.9788770	1.5926400	-1.3750140
H	0.2964030	-3.2680450	2.5999520	C	0.6733760	1.3637240	-0.0201360
H	0.1417790	-1.5309100	2.8669390	C	1.7443430	1.3920820	0.8942910
H	1.2426420	-2.4847930	3.8798080	C	3.0573670	1.5424460	0.4728580
C	5.7132260	-1.3369830	1.9753980	C	3.3389610	1.7023890	-0.8817160
				C	2.2867330	1.7465510	-1.8014250
				H	0.1751760	1.6516760	-2.1089600

H	1.5457630	1.2657390	1.9596450	H	7.1621940	-0.0169020	0.3644520
H	3.8672920	1.5226210	1.1990050	H	6.6521170	1.6020430	0.8390470
H	2.5030580	1.8865660	-2.8604620	C	2.4032800	-0.4883530	-2.5323330
C	-2.0807120	0.2990270	2.0082590	H	1.9217810	-1.4716720	-2.6070780
O	-2.7742500	0.3362850	2.9270200	H	3.1059730	-0.3902260	-3.3657180
C	-0.9364490	2.3698120	0.6028490	H	1.6121900	0.2613680	-2.6681780
C	-0.6684220	3.2845990	1.6308490	C	-2.4278100	-0.4988930	-0.0098810
C	-1.8006110	2.7834970	-0.4225400	C	-3.0993200	-0.2840720	-1.2187090
C	-1.2413790	4.5491930	1.6331710	C	-4.4209300	0.1500180	-1.1591890
H	0.0049270	3.0040050	2.4412350	H	-4.9601930	0.3268620	-2.0908640
C	-2.3751680	4.0506500	-0.4117900	C	-5.0671890	0.3750170	0.0577660
H	-2.0346740	2.1031390	-1.2445390	C	-4.3581280	0.1625940	1.2387410
C	-2.1022800	4.9612500	0.6102000	H	-4.8451470	0.3484480	2.1965560
H	-1.0181020	5.2390320	2.4483520	C	-3.0317230	-0.2674730	1.2298020
H	-3.0477150	4.3433740	-1.2193240	C	-2.4035840	-0.4739370	-2.5302970
C	-2.6785570	6.3445620	0.5982630	H	-1.9234380	-1.4575830	-2.6097640
H	-1.9600290	7.0798650	0.2108660	H	-1.6112360	0.2754450	-2.6605750
H	-3.5723070	6.4033900	-0.0335110	H	-3.1048380	-0.3699450	-3.3641910
H	-2.9582310	6.6749950	1.6060240	C	-6.4969590	0.8224930	0.0846330
C	4.7324610	1.7703770	-1.3909200	H	-7.1762940	0.0018900	-0.1805460
F	5.6519780	1.7114320	-0.4171750	H	-6.6773210	1.6298390	-0.6346040
F	4.9737230	2.8887650	-2.0950940	H	-6.7890410	1.1827400	1.0766930
F	5.0054260	0.7492850	-2.2373080	C	-2.2600830	-0.4298910	2.5020990
Ni	-0.8339520	0.4452390	0.7182960	H	-1.4414130	0.3016530	2.5504700
INTa6				H	-1.8005280	-1.4228830	2.5913260
C	-0.0015200	-0.1121870	-0.0583250	H	-2.9027200	-0.2746330	3.3742690
C	0.6799370	-2.2939770	-0.0016370	N	-1.0690440	-0.9525380	-0.0395810
C	-0.6803980	-2.2949020	-0.0020530	N	1.0668010	-0.9512770	-0.0397720
C	2.4254710	-0.4975990	-0.0127880	C	-1.6629640	-3.4034470	0.0211050
C	3.0298070	-0.2590450	1.2275580	H	-2.3717770	-3.3000530	0.8523600
C	4.3547010	0.1687710	1.2347750	H	-2.2556220	-3.4445420	-0.9022150
H	4.8415610	0.3610050	2.1919090	H	-1.1546490	-4.3660960	0.1318710
C	5.0663590	0.3721280	0.0509820	C	1.6650460	-3.4001010	0.0272680
C	4.4214570	0.1408270	-1.1629820	H	2.2653280	-3.4379800	-0.8912170
H	4.9609220	0.3094870	-2.0955900	H	2.3665290	-3.2948790	0.8645620
C	3.0970590	-0.2918740	-1.2206840	H	1.1586590	-4.3642950	0.1331830
C	2.2543260	-0.4098850	2.4988930	C	0.0058880	3.5081930	-0.0443420
H	1.7514430	-1.3830800	2.5707890	O	0.0122870	4.6698010	-0.0154590
H	1.4683300	0.3558230	2.5605300	Ni	-0.0004430	1.8020630	-0.0687630
H	2.9039730	-0.2971510	3.3724330	INTa7			
C	6.4975430	0.8138100	0.0932060	C	-4.0795080	-2.1423770	-0.1963600
H	6.8314330	1.1965720	-0.8770480	C	-3.7997930	-0.9733670	-0.9049110

C	-2.4835700	-0.5711840	-1.0904030
C	-1.4154460	-1.3296190	-0.5837690
C	-1.7176380	-2.5345500	0.0627960
H	-2.2932990	0.3675090	-1.6134420
H	-0.9088380	-3.1826020	0.3990940
C	0.8097850	-1.9934070	-1.7051670
O	0.7353510	-3.1955750	-1.7602560
C	1.9275580	-1.1618700	-2.2933270
C	3.2564650	-1.5374060	-2.0649810
C	1.6610160	0.0456590	-2.9557590
C	4.2938530	-0.7256930	-2.4998150
H	3.4579400	-2.4702030	-1.5392010
C	2.7083110	0.8482950	-3.3916670
H	0.6250610	0.3337940	-3.1420360
C	4.0378050	0.4796870	-3.1618880
H	5.3273420	-1.0219060	-2.3192100
H	2.4959250	1.7814390	-3.9139040
C	5.1571000	1.3756270	-3.5944920
H	5.0483210	2.3808810	-3.1669630
H	6.1314850	0.9833750	-3.2840440
H	5.1777460	1.4972540	-4.6847170
C	0.5795140	0.8214900	0.6754310
C	1.4994300	1.8467320	2.5062040
C	0.3747860	2.5351030	2.1792850
C	2.6500210	-0.1670780	1.5728370
C	3.8776260	0.1463970	0.9753440
C	4.8869440	-0.8116760	1.0228620
H	5.8500370	-0.5853160	0.5622470
C	4.6934810	-2.0554360	1.6264410
C	3.4530450	-2.3333960	2.1976640
H	3.2876740	-3.3018590	2.6706270
C	2.4132360	-1.4029240	2.1852280
C	4.0895100	1.4550350	0.2780710
H	3.9808400	2.3128740	0.9547130
H	3.3598070	1.5939510	-0.5320670
H	5.0913660	1.5037920	-0.1628930
C	5.7912010	-3.0750900	1.6251740
H	5.9298970	-3.5037960	0.6237100
H	5.5748690	-3.9035620	2.3076690
H	6.7511590	-2.6344820	1.9193950
C	1.0834090	-1.7213630	2.7950710
H	0.7401180	-0.9328620	3.4775600
H	1.1238160	-2.6615440	3.3538130
H	0.3104320	-1.8199100	2.0201990

C	-1.3609240	2.3271900	0.4041790
C	-2.5984790	1.9108370	0.9039220
C	-3.7477410	2.3838160	0.2712540
H	-4.7207920	2.0536440	0.6375350
C	-3.6833030	3.2336970	-0.8314950
C	-2.4269280	3.6097480	-1.3116770
H	-2.3608660	4.2653120	-2.1811010
C	-1.2502560	3.1694660	-0.7085230
C	-2.6859210	0.9452150	2.0439100
H	-2.2354370	1.3418290	2.9638340
H	-2.1569080	0.0131550	1.7997040
H	-3.7286540	0.6889970	2.2599410
C	-4.9326990	3.7497270	-1.4779170
H	-4.8353230	3.7924520	-2.5686590
H	-5.1634680	4.7675640	-1.1370570
H	-5.7979860	3.1220270	-1.2391360
C	0.0893730	3.5605070	-1.2521550
H	0.5909610	2.7024850	-1.7208700
H	0.7673040	3.9232460	-0.4686130
H	-0.0085150	4.3455590	-2.0089250
N	-0.1655030	1.8903620	1.0603260
N	1.6047740	0.8122700	1.5700130
Ni	0.3040090	-0.6013700	-0.6685810
C	-0.2626170	3.7249510	2.7902410
H	-0.3641430	4.5474980	2.0707440
H	-1.2704420	3.4995540	3.1626250
H	0.3314820	4.0882160	3.6340850
C	2.4801320	2.0306320	3.6016570
H	2.5179310	1.1562290	4.2640090
H	3.4975920	2.1880410	3.2211820
H	2.2131970	2.8988680	4.2116870
H	-4.6185810	-0.3676090	-1.2945160
H	-3.2515470	-3.8514820	0.8154900
C	-3.0343800	-2.9294690	0.2802210
C	-5.5043950	-2.4874070	0.0572160
F	-6.2197740	-2.5659660	-1.0783080
F	-6.1159450	-1.5481760	0.8082800
F	-5.6551100	-3.6532880	0.6981630

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C	-4.0774690	-1.8978690	-0.9717130
C	-3.8592510	-0.5583350	-1.2985390
C	-2.5650170	-0.0595510	-1.3469820

C	-1.4522770	-0.8666310	-1.0550570	C	-2.5801140	1.6152710	1.3326270
C	-1.6986170	-2.2203320	-0.7885810	C	-3.5668390	2.4955620	0.8830660
H	-2.4228650	0.9934470	-1.5956150	H	-4.6127750	2.2001020	0.9749040
H	-0.8630730	-2.8985950	-0.6128830	C	-3.2515730	3.7230080	0.3061040
C	0.5466580	-0.2197280	-2.7588600	C	-1.9056070	4.0806270	0.1897220
O	0.4712010	-0.4160010	-3.9159340	H	-1.6450160	5.0463500	-0.2462200
C	1.9883120	0.5773290	-2.0811930	C	-0.8859790	3.2421650	0.6317730
C	3.1569010	-0.1902320	-2.0740160	C	-2.9509720	0.2981030	1.9406660
C	2.0871820	1.9597410	-2.2682810	H	-2.8518490	0.3127510	3.0349730
C	4.3961110	0.4180390	-2.2261940	H	-2.3136920	-0.5120560	1.5650870
H	3.0885070	-1.2728330	-1.9548280	H	-3.9902060	0.0417590	1.7081190
C	3.3309300	2.5671670	-2.4013120	C	-4.3235660	4.6474290	-0.1857330
H	1.1777250	2.5607840	-2.3194920	H	-4.2770220	4.7687360	-1.2752580
C	4.5025820	1.8046180	-2.3837750	H	-4.2190010	5.6491680	0.2489300
H	5.3041060	-0.1864860	-2.2191640	H	-5.3228470	4.2760530	0.0638840
H	3.4000210	3.6467370	-2.5351970	C	0.5495510	3.6656530	0.5689530
C	5.8476960	2.4525670	-2.5011230	H	1.1798670	2.9131930	0.0800810
H	6.3243060	2.5517810	-1.5159150	H	0.9652510	3.8123410	1.5757400
H	6.5270840	1.8614260	-3.1260270	H	0.6571040	4.6088380	0.0233600
H	5.7777200	3.4574380	-2.9311650	N	-0.2057290	1.1374800	1.6503500
C	0.5052980	0.2843190	0.8632900	N	1.3758760	-0.2926940	1.7363350
C	1.2154150	0.1869390	3.0416650	Ni	0.2921570	-0.0987270	-1.0516250
C	0.2151510	1.1018520	2.9845530	C	-0.3813140	1.9701490	4.0260740
C	2.3662490	-1.2586480	1.3707750	H	-0.3070690	3.0315530	3.7566450
C	3.6584000	-0.8070530	1.0730800	H	-1.4451580	1.7545670	4.1873100
C	4.6185670	-1.7571010	0.7340840	H	0.1345840	1.8314140	4.9808420
H	5.6315950	-1.4246210	0.5016440	C	2.0456460	-0.2947030	4.1703680
C	4.3161030	-3.1193250	0.6786950	H	1.9679710	-1.3820810	4.2966090
C	3.0228210	-3.5283580	0.9990770	H	3.1092370	-0.0639030	4.0265630
H	2.7784810	-4.5910220	0.9835610	H	1.7254770	0.1723010	5.1065130
C	2.0321270	-2.6159090	1.3675140	H	-4.7100500	0.0917120	-1.5051060
C	3.9842970	0.6535780	1.1076910	H	-3.1575230	-3.7832750	-0.4945280
H	3.7162360	1.1115870	2.0685210	C	-2.9927000	-2.7341360	-0.7298290
H	3.4301790	1.1950440	0.3291000	C	-5.4816520	-2.3710700	-0.8364510
H	5.0533320	0.8205640	0.9374800	F	-6.2201130	-2.0948680	-1.9243550
C	5.3624240	-4.1127090	0.2743060	F	-6.1096890	-1.7663260	0.1934710
H	5.5467530	-4.0775660	-0.8071510	F	-5.5739110	-3.6898450	-0.6228160
H	5.0646540	-5.1370860	0.5218290				
H	6.3206830	-3.9101060	0.7671020				
C	0.6825130	-3.0861960	1.8138830				
H	0.6125190	-3.0875960	2.9107560	INTa8			
H	0.4918730	-4.1101830	1.4757640	C	-4.0272630	-1.9411160	-0.9827240
H	-0.1265070	-2.4461300	1.4444890	C	-3.8531080	-0.5959230	-1.3120800
C	-1.2460290	2.0057880	1.1860450	C	-2.5753450	-0.0540910	-1.3474480
				C	-1.4419470	-0.8213130	-1.0366560

C	-1.6418600	-2.1821400	-0.7774860	C	-3.6431410	2.4200410	0.8755350
H	-2.4632420	1.0012680	-1.6038450	H	-4.6794050	2.0930960	0.9702270
H	-0.7834860	-2.8306230	-0.6014890	C	-3.3680840	3.6676930	0.3210340
C	0.2081790	-0.2342720	-2.8304960	C	-2.0353000	4.0713820	0.2176840
O	0.1259020	-0.3807540	-3.9662050	H	-1.8058360	5.0583560	-0.1868220
C	2.0752100	0.7453560	-1.6337270	C	-0.9871160	3.2571620	0.6412470
C	3.1438650	-0.1288880	-1.8766930	C	-2.9630250	0.2335000	1.9075270
C	2.2907030	2.0993360	-1.9081680	H	-2.8640380	0.2521960	3.0017070
C	4.3847600	0.3357130	-2.3004260	H	-2.3060230	-0.5608100	1.5339910
H	3.0123020	-1.2022140	-1.7200640	H	-3.9961460	-0.0486110	1.6784110
C	3.5357650	2.5696760	-2.3312330	C	-4.4699810	4.5657690	-0.1531310
H	1.4729000	2.8137280	-1.8014040	H	-4.4474450	4.6823680	-1.2439750
C	4.6061340	1.6977620	-2.5275220	H	-4.3790330	5.5717120	0.2744260
H	5.2007750	-0.3712580	-2.4646940	H	-5.4555410	4.1730320	0.1175530
H	3.6757100	3.6340690	-2.5268030	C	0.4216660	3.7661410	0.6388040
C	5.9489510	2.1900360	-2.9786620	H	1.1488590	3.0034940	0.3410340
H	6.7140760	2.0524170	-2.2027150	H	0.7127360	4.1086620	1.6420320
H	6.2994680	1.6488660	-3.8666670	H	0.5284970	4.6216930	-0.0363900
H	5.9238610	3.2567560	-3.2280090	N	-0.2417060	1.1386290	1.5959340
C	0.5022150	0.3102260	0.8112150	N	1.3774810	-0.2551820	1.6887780
C	1.1812070	0.2053050	2.9966950	Ni	0.3317210	0.0027820	-1.1045940
C	0.1641760	1.0989890	2.9351600	C	-0.4601060	1.9464070	3.9780930
C	2.3929370	-1.2130330	1.3640420	H	-0.4010340	3.0118570	3.7217350
C	3.7010110	-0.7592970	1.1438900	H	-1.5215500	1.7122460	4.1280320
C	4.6757400	-1.7090540	0.8486090	H	0.0491970	1.8079020	4.9362480
H	5.6952220	-1.3713920	0.6557470	C	1.9882660	-0.2812410	4.1404690
C	4.3809870	-3.0713010	0.7739470	H	1.9258520	-1.3714220	4.2479080
C	3.0762980	-3.4841120	1.0365290	H	3.0514500	-0.0299330	4.0379420
H	2.8362590	-4.5477690	1.0156640	H	1.6301830	0.1627920	5.0739510
C	2.0668370	-2.5730080	1.3537960	H	-4.7230920	0.0233780	-1.5316580
C	4.0476420	0.6950460	1.2189020	H	-3.0502240	-3.7950850	-0.4958290
H	3.8896110	1.1053580	2.2249610	C	-2.9181020	-2.7409720	-0.7290670
H	3.4358430	1.2865910	0.5262230	C	-5.4171120	-2.4625370	-0.8597300
H	5.0985530	0.8558420	0.9576230	F	-6.1534710	-2.2110510	-1.9540890
C	5.4468510	-4.0592320	0.4105890	F	-6.0710290	-1.8787830	0.1645880
H	5.6573100	-4.0352080	-0.6664420	F	-5.4647710	-3.7832310	-0.6470730
H	5.1532820	-5.0835140	0.6639220				
H	6.3900790	-3.8394240	0.9243070				
C	0.7088460	-3.0554430	1.7614730				
H	0.6309330	-3.1110460	2.8563750				
H	0.5162660	-4.0616740	1.3741550				
H	-0.0949740	-2.3954070	1.4189680				
C	-1.3051720	1.9898380	1.1493860				
C	-2.6283380	1.5614760	1.3019720				
					</		

C	-1.2758120	3.9868690	1.8053150	C	2.8153940	4.4078900	-0.3290170
H	-1.4926500	4.1945090	2.8536000	H	2.1610010	4.9711620	-1.0065560
C	-2.1765550	4.4043410	0.8253940	H	2.6125730	4.7699650	0.6873930
C	-1.8947130	4.1123610	-0.5102600	H	3.8512220	4.6621700	-0.5733870
H	-2.5999140	4.4177630	-1.2845750	C	-2.2063660	-2.0997000	-0.9124980
C	-0.7378080	3.4317380	-0.8829610	C	-1.8899790	-0.8773910	-0.3026560
C	0.8502850	2.8438430	2.5400330	C	-2.9578420	-0.0608050	0.1134510
H	1.8428710	3.3017250	2.4333270	C	-4.2789100	-0.4260390	-0.1117870
H	0.9980990	1.7559720	2.4918120	C	-4.5623180	-1.6364980	-0.7463300
H	0.4747220	3.0906430	3.5380390	C	-3.5254980	-2.4761530	-1.1460320
C	-3.4206660	5.1562320	1.1880990	H	-1.4051990	-2.7769810	-1.2112740
H	-3.3557720	6.2061570	0.8747210	H	-2.7492040	0.8815780	0.6254000
H	-3.6000320	5.1444300	2.2681630	H	-5.0962530	0.2201660	0.2078000
H	-4.3032640	4.7322920	0.6948180	H	-3.7536430	-3.4233690	-1.6299280
C	-0.4829530	3.0703880	-2.3144990	C	0.0881800	-1.2202820	1.1829500
H	0.5640370	3.2220730	-2.6053980	C	0.7833850	-2.4183140	1.0046860
H	-1.1152820	3.6605830	-2.9852030	C	-0.2560900	-0.8391270	2.4866670
H	-0.7112390	2.0101540	-2.5001360	C	1.1539590	-3.1946930	2.1035410
C	3.2011710	-0.5577610	-0.9344760	H	1.0687870	-2.7447500	0.0034600
C	3.1422910	-1.1018840	-2.2199330	C	0.1250410	-1.6175520	3.5768990
C	3.6689890	-2.3799490	-2.4106270	H	-0.8270500	0.0758170	2.6565840
H	3.6323710	-2.8215100	-3.4069450	C	0.8360640	-2.8097370	3.4061210
C	4.2397420	-3.1006360	-1.3631310	H	1.7070310	-4.1220280	1.9422830
C	4.2660040	-2.5250080	-0.0912560	H	-0.1457690	-1.3012930	4.5860220
H	4.6912600	-3.0872880	0.7417010	C	1.2265100	-3.6444480	4.5901990
C	3.7470870	-1.2553260	0.1503380	H	0.3511430	-3.9415960	5.1823260
C	2.5055360	-0.3531470	-3.3496450	H	1.7416310	-4.5615790	4.2826180
H	2.8762440	0.6768960	-3.4267620	H	1.8969980	-3.1022280	5.2702120
H	1.4176450	-0.2871420	-3.2128480	C	-5.9913870	-1.9966160	-0.9685090
H	2.6898310	-0.8536780	-4.3055620	F	-6.6806020	-2.0488380	0.1848030
C	4.8164840	-4.4653700	-1.5863830	F	-6.1432580	-3.1832050	-1.5695540
H	4.4284270	-5.1866240	-0.8571420	F	-6.6242330	-1.0867430	-1.7323800
H	5.9085990	-4.4599960	-1.4776680	Ni	-0.2060600	-0.0948250	-0.2527290
H	4.5850130	-4.8423750	-2.5879490				
C	3.7187020	-0.6759650	1.5297800				
H	2.6799700	-0.5635410	1.8715680				
H	4.1831120	0.3175610	1.5790090	TSa9_10			
H	4.2343570	-1.3299150	2.2401330	C	1.1538990	1.3237060	-0.2413040
N	2.6784730	0.7572590	-0.7116480	C	1.8624720	3.4951050	-0.2693300
N	1.3513830	2.3565670	-0.2259720	C	2.9337700	2.7143230	-0.5799120
C	4.8820160	1.9168940	-1.1132990	C	-0.5174330	3.0085010	0.3654150
H	5.4768460	1.3177960	-0.4125100	C	-0.7643960	3.0970040	1.7387840
H	5.0438410	1.4932440	-2.1128960	C	-2.0426880	3.4776370	2.1472

C	-2.7729640	3.6249770	-0.1341540	H	2.6751460	5.4617690	-0.3146580
H	-3.5611420	3.8170260	-0.8632680	C	-1.7274690	-2.2100400	-1.1520640
C	-1.5096320	3.2561140	-0.5899200	C	-1.4849110	-1.2702810	-0.1398920
C	0.2908770	2.7324360	2.7363440	C	-2.5925950	-0.7063890	0.5231670
H	1.2611650	3.1929000	2.5101690	C	-3.8873890	-1.0258540	0.1442020
H	0.4549330	1.6451570	2.7383600	C	-4.1060420	-1.9436900	-0.8855460
H	-0.0023750	3.0298800	3.7482070	C	-3.0246420	-2.5369350	-1.5313020
C	-4.4163000	4.1793990	1.6821670	H	-0.8892170	-2.6925630	-1.6528030
H	-4.5721740	5.2519450	1.5075040	H	-2.4344880	0.0150270	1.3260650
H	-4.5623010	3.9960330	2.7519090	H	-4.7380040	-0.5642390	0.6448170
H	-5.2074970	3.6510010	1.1375240	H	-3.1983670	-3.2579460	-2.3266050
C	-1.2250980	3.0868700	-2.0495000	C	0.1940900	-1.7921300	0.9590300
H	-0.3234130	3.6305740	-2.3600890	C	1.0807220	-2.7387680	0.4248300
H	-2.0642880	3.4384780	-2.6576540	C	-0.1074660	-1.8718930	2.3274160
H	-1.0533320	2.0288400	-2.2904820	C	1.6881420	-3.6859550	1.2450100
C	3.2630970	0.2302600	-0.8251900	H	1.3387340	-2.7097040	-0.6346250
C	3.4506330	-0.1758020	-2.1503700	C	0.5057950	-2.8220910	3.1366810
C	4.1973450	-1.3316860	-2.3794630	H	-0.8223260	-1.1756660	2.7666240
H	4.3503490	-1.6647820	-3.4065580	C	1.4154880	-3.7460990	2.6130820
C	4.7381100	-2.0742400	-1.3308470	H	2.3994510	-4.3924490	0.8126680
C	4.5193520	-1.6393610	-0.0232390	H	0.2688510	-2.8550270	4.2014250
H	4.9217010	-2.2207270	0.8078790	C	2.0524990	-4.7776580	3.4951490
C	3.7811520	-0.4918230	0.2563830	H	1.3175680	-5.5041370	3.8667510
C	2.8378640	0.5849890	-3.2848920	H	2.8269170	-5.3404560	2.9616850
H	3.2215420	1.6115000	-3.3529550	H	2.5205720	-4.3240870	4.3783340
H	1.7485740	0.6608470	-3.1676670	C	-5.5130840	-2.2586060	-1.2603620
H	3.0397890	0.0912800	-4.2407180	F	-6.2211950	-2.7177560	-0.2137310
C	5.5064840	-3.3340950	-1.5907790	F	-5.6013980	-3.1792560	-2.2282440
H	4.9257690	-4.2177560	-1.2945890	F	-6.1702530	-1.1676820	-1.6948400
H	6.4412060	-3.3620950	-1.0181770	Ni	0.0313820	-0.2249740	-0.0145210
H	5.7558980	-3.4449530	-2.6513500				
C	3.4921480	-0.0913070	1.6686210				
H	2.4401390	-0.3008400	1.9133250				
H	3.6537260	0.9802550	1.8444590				
H	4.1168510	-0.6540730	2.3697710				
N	2.4712180	1.3955090	-0.5619290				
N	0.7917360	2.6205960	-0.0682350				
C	4.3452570	3.0566740	-0.8719600				
H	5.0296930	2.6203140	-0.1328460				
H	4.6602490	2.6890320	-1.8571080				
H	4.4875330	4.1414320	-0.8583110				
C	1.7180640	4.9632980	-0.1336270				
H	0.9888080	5.3677400	-0.8477530				
H	1.3755760	5.2460330	0.8700920				
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H	-0.5238570	4.5871830	-0.1606520	C	3.1178690	-2.6919320	-0.2929100
C	4.4608130	4.5855830	-0.4700600	H	1.0055590	-2.8593200	-0.0161020
H	4.4832760	5.5501670	0.0527830	H	2.4166900	0.8167710	-1.7539030
H	4.2898220	4.8040620	-1.5311800	H	4.7253690	-0.0194350	-1.6387730
H	5.4534310	4.1330950	-0.3759880	H	3.3183230	-3.6831060	0.1079330
C	3.1169900	0.3747370	1.9167480	C	-0.1478370	-0.4895750	-2.7237700
H	3.2260610	0.5413450	2.9976580	O	-0.0617130	-0.6912150	-3.8507770
H	4.0806740	0.0060570	1.5484440	C	-1.9274300	0.7316320	-1.6279830
H	2.3786240	-0.4219990	1.7804320	C	-3.1467320	0.0660690	-1.7823970
C	-2.4594240	-0.9625030	1.5193460	C	-1.8828560	2.0735810	-2.0308820
C	-2.3244270	-2.3506460	1.5761480	C	-4.2872070	0.7293570	-2.2347020
C	-3.4539880	-3.1285350	1.3042620	H	-3.2327570	-0.9903600	-1.5227830
H	-3.3589870	-4.2151680	1.3205350	C	-3.0203880	2.7409860	-2.4788640
C	-4.6922190	-2.5540450	1.0319800	H	-0.9353630	2.6156310	-1.9961230
C	-4.7974300	-1.1603840	1.0442940	C	-4.2487550	2.0810200	-2.5782550
H	-5.7637060	-0.6951140	0.8424530	H	-5.2288580	0.1840190	-2.3233570
C	-3.6979050	-0.3430840	1.2860250	H	-2.9557200	3.7916250	-2.7682050
C	-1.0332210	-3.0035130	1.9599340	C	-5.4759810	2.8082780	-3.0400620
H	-0.9877760	-3.1663460	3.0461350	H	-6.2956290	2.1147320	-3.2592670
H	-0.1616770	-2.4000960	1.6862530	H	-5.8386020	3.5139800	-2.2804530
H	-0.9320810	-3.9864170	1.4854360	H	-5.2821990	3.3934690	-3.9475460
C	-5.8946420	-3.3984960	0.7393990	C	5.5863320	-2.3344600	-0.6029710
H	-5.6537330	-4.4663040	0.7613030	F	6.3103570	-2.0793770	-1.7038430
H	-6.3095840	-3.1699290	-0.2499790	F	5.7098410	-3.6415830	-0.3412490
H	-6.6956270	-3.2202570	1.4677650	F	6.2023680	-1.6797300	0.4034040
C	-3.8274430	1.1483040	1.2773670	Ni	-0.2704500	-0.1375190	-1.0134170
H	-3.2545540	1.5836760	0.4474470	C	-1.3338970	-2.9824630	-1.3194170
H	-3.4496660	1.6016750	2.2035150	O	-1.9407680	-3.3859970	-2.1944840
H	-4.8734510	1.4479040	1.1557630				
N	-1.3274940	-0.1246990	1.7867690				
N	0.3461800	1.1933750	1.5940050	INTa12			
C	-1.9141200	0.0244770	4.2377170	C	-1.6278140	0.7920710	0.2146610
H	-2.9620790	0.3346000	4.1354360	C	-3.8649050	1.2440050	0.1057570
H	-1.9136450	-1.0616360	4.3935760	C	-3.2075810	2.3988060	-0.1744790
H	-1.5154380	0.4897250	5.1439630	C	-3.1586480	-1.0918540	0.6564830
C	0.6238450	2.1311100	3.9230930	C	-3.1119090	-1.4914230	1.9963010
H	1.6751510	1.8582860	4.0771760	C	-3.3777450	-2.8288640	2.2875280
H	0.6080950	3.1819640	3.6076090	H	-3.3400650	-3.1586170	3.3264450
H	0.1189470	2.0679240	4.8915650	C	-3.6943520	-3.7485530	1.2871900
C	1.8117460	-2.2103920	-0.3575940	C	-3.7347760	-3.3065750	-0.0351360
C	1.5179940	-0.9317290	-0.8462190	H	-3.9591520	-4.0185320	-0.8304680
C	2.5973740	-0.1736310	-1.3302940	C	-3.4709900	-1.9815830	-0.3777750
C	3.9047360	-0.6379000	-1.2760360	C	-2.7693780	-0.5213570	3.0847760
C	4.1686600	-1.9015030	-0.7466370	H	-3.3299790	0.4179420	2.9932880

H	-1.7040400	-0.2558400	3.0606760	C	4.7193260	-1.2017120	0.6385590
H	-2.9799470	-0.9483400	4.0703060	C	4.3168570	0.0278540	0.1156620
C	-4.0043800	-5.1741800	1.6291040	H	2.6676150	1.3302930	-0.3085860
H	-3.7611790	-5.8483890	0.8007320	H	1.6885310	-2.4574890	1.4884790
H	-5.0714680	-5.3068140	1.8509640	H	4.0840100	-3.0453390	1.5450280
H	-3.4480660	-5.5069410	2.5122930	H	5.0633040	0.7217660	-0.2701720
C	-3.4799060	-1.5419830	-1.8088360	C	0.5693670	0.8184110	2.1087450
H	-4.2603470	-0.7970070	-2.0115360	O	0.9577120	1.1690480	3.1316020
H	-3.6542160	-2.3934780	-2.4742630	C	0.1459340	-1.0535930	-1.0225630
H	-2.5180740	-1.0912580	-2.0866790	C	0.5796550	-0.6510740	-2.2913700
C	-0.7803110	3.0290750	-0.3208830	C	-0.3153620	-2.3672350	-0.8951290
C	-0.2493820	3.1494420	-1.6147880	C	0.5159850	-1.5079340	-3.3881170
C	0.8365600	4.0010190	-1.7941190	H	0.9912820	0.3510500	-2.4300720
H	1.2721740	4.0979080	-2.7896490	C	-0.3719800	-3.2287340	-1.9907940
C	1.3783120	4.7377010	-0.7365470	H	-0.6446080	-2.7388680	0.0776540
C	0.7932770	4.6236760	0.5215080	C	0.0366380	-2.8141360	-3.2586840
H	1.1931360	5.2046910	1.3534030	H	0.8579520	-1.1619450	-4.3655690
C	-0.2967830	3.7818090	0.7538660	H	-0.7466680	-4.2457500	-1.8578940
C	-0.8638640	2.4266590	-2.7741650	C	-0.0085450	-3.7371150	-4.4406330
H	-1.8090970	2.8982690	-3.0763480	H	-0.4951640	-3.2682210	-5.3055830
H	-1.0847180	1.3778400	-2.5439910	H	0.9982130	-4.0308070	-4.7665870
H	-0.2002380	2.4479310	-3.6448490	H	-0.5570030	-4.6579330	-4.2105840
C	2.5476800	5.6444060	-0.9692430	C	6.1735530	-1.5251410	0.6501640
H	2.9379620	6.0487420	-0.0296310	F	6.4346580	-2.7342290	1.1628120
H	2.2722910	6.4934410	-1.6078580	F	6.8800210	-0.6341380	1.3699810
H	3.3660810	5.1191230	-1.4757500	F	6.7047190	-1.4997240	-0.5852780
C	-0.9326580	3.7392360	2.1110990	Ni	0.1657730	0.0698490	0.5262690
H	-1.4920430	2.8147320	2.2922010				
H	-1.6392540	4.5714590	2.2342780				
H	-0.1820860	3.8462620	2.9013750	TSa12_13			
N	-1.8436620	2.0950500	-0.1030730	C	1.4272900	1.0598370	-0.2119650
N	-2.8753170	0.2746470	0.3301640	C	3.4476710	2.0959060	0.0757620
C	-3.6951840	3.7638090	-0.4802130	C	2.4843890	3.0114430	0.3554070
H	-3.3195740	4.5000440	0.2416260	C	3.4321360	-0.3180790	-0.5881940
H	-3.3786780	4.1010010	-1.4754060	C	3.6501810	-0.6467370	-1.9313950
H	-4.7881150	3.7964030	-0.4513920	C	4.2787690	-1.8579420	-2.2109030
C	-5.3110560	0.9429080	0.2249080	H	4.4573790	-2.1326670	-3.2515840
H	-5.6414560	0.1876620	-0.4993310	C	4.6900240	-2.7237860	-1.1949580
H	-5.5648730	0.5619320	1.2223410	C	4.4631650	-2.3541600	0.1290100
H	-5.9027420	1.8470600	0.0531610	H	4.7703620	-3.0238750	0.9335740
C	2.9693770	0.3611540	0.0950110	C	3.8324960	-1.1541090	0.4579980
C	1.9948370	-0.5239820	0.5785770	C	3.2154100	0.2710970	-3.0315750
C	2.4205160	-1.7451020	1.1069000	H	3.5264900	1.3073800	-2.8481170
C	3.7688420	-2.0877760	1.1370650	H	2.1219130	0.2858870	-3.1294630

H	3.6301370	-0.0451450	-3.9938710	C	-4.0475360	-0.4955400	0.0872510
C	5.3638560	-4.0183510	-1.5342410	H	-2.3921200	0.7300510	0.6743530
H	5.5916380	-4.6022420	-0.6364230	H	-1.4282650	-2.9580030	-1.3431140
H	6.3060490	-3.8506790	-2.0711320	H	-3.8268270	-3.4887660	-1.5047180
H	4.7344170	-4.6376200	-2.1851850	H	-4.7906110	0.1945450	0.4864850
C	3.5397920	-0.7972210	1.8810710	C	-0.4927600	0.2838620	-2.3887760
H	3.9159360	0.1987870	2.1489010	O	-0.7940930	0.3907650	-3.4957540
H	3.9849940	-1.5247540	2.5682130	C	-0.1385410	-1.3341670	0.8107340
H	2.4551680	-0.7895150	2.0571260	C	-0.4361380	-1.0964690	2.1595720
C	-0.0315380	2.9236870	0.3869190	C	0.6390330	-2.4695330	0.5181760
C	-0.5756200	2.8769680	1.6783790	C	0.0490230	-1.9269910	3.1656730
C	-1.8648220	3.3707390	1.8606540	H	-1.0766810	-0.2564620	2.4306380
H	-2.3063310	3.3370840	2.8575130	C	1.1255700	-3.2918770	1.5260080
C	-2.6028440	3.9065340	0.8021880	H	0.8758020	-2.7106540	-0.5207360
C	-2.0152180	3.9600460	-0.4598720	C	0.8406510	-3.0392840	2.8716190
H	-2.5753260	4.3864790	-1.2928430	H	-0.1971920	-1.7095040	4.2059260
C	-0.7253280	3.4793040	-0.6927940	H	1.7428080	-4.1531460	1.2645030
C	0.2150750	2.3326810	2.8280170	C	1.3634970	-3.9401190	3.9494950
H	1.0674870	2.9812340	3.0729600	H	1.2399810	-3.4933360	4.9425710
H	0.6274300	1.3400110	2.6080460	H	0.8455880	-4.9085380	3.9617080
H	-0.4066420	2.2501630	3.7257620	H	2.4314250	-4.1550060	3.8104870
C	-4.0054980	4.3863640	1.0189000	C	-5.9198260	-1.9625140	-0.6112150
H	-4.3125880	5.0993740	0.2463920	F	-6.1890200	-3.1626460	-1.1406940
H	-4.1210390	4.8703990	1.9953850	F	-6.5583710	-1.0492130	-1.3677940
H	-4.7169970	3.5505300	0.9897810	F	-6.5218230	-1.9197940	0.5918460
C	-0.1059910	3.5909340	-2.0530180	Ni	-0.1008760	-0.0989260	-0.6830280
H	0.6227170	2.7947580	-2.2434600				
H	0.4207440	4.5480610	-2.1692990				
H	-0.8710740	3.5484540	-2.8355900	INTa13			
N	1.2631510	2.3533280	0.1734550	C	0.0540160	1.3985250	0.0245990
N	2.7752680	0.9132030	-0.2670970	C	0.8252170	3.5326890	0.3716930
C	2.5656210	4.4302080	0.7744060	C	-0.5301570	3.5785390	0.4417850
H	2.1367680	5.1096330	0.0262720	C	2.4848430	1.7117090	-0.0948950
H	2.0265330	4.6067830	1.7143850	C	3.0024880	1.7270010	-1.3973620
H	3.6085510	4.7225730	0.9303620	C	4.2940270	1.2457800	-1.5894970
C	4.9260110	2.1913410	0.0801760	H	4.7110990	1.2423880	-2.5976440
H	5.3792900	1.5049250	0.8071050	C	5.0747300	0.7874840	-0.5265300
H	5.3524690	1.9462020	-0.9009940	C	4.5283260	0.7981720	0.7542500
H	5.2403030	3.2078280	0.3360810	H	5.1257140	0.4493120	1.5980270
C	-2.6993500	-0.1959950	0.1826260	C	3.2283060	1.2467720	0.9928830
C	-1.7192610	-1.0652320	-0.3428220	C	2.1946380	2.2535950	-2.5428240
C	-2.1589260	-2.2552910	-0.9443860	H	2.0031990	3.3309280	-2.4460670
C	-3.5087420	-2.5629260	-1.0311160	H	1.2141340	1.7651640	-2.5998500
C	-4.4616260	-1.6843390	-0.5181320	H	2.7121390	2.0924380	-3.4938790

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H	-2.8351100	-0.5566160	-2.1635710	C	4.2060240	1.5896290	-0.4938060
H	-4.5198280	-0.8416220	-2.6497120	C	4.2419000	1.4158060	0.8887850
C	-7.0300430	0.9544950	1.2585120	C	3.0635460	1.2428920	1.6110690
H	-7.8871730	0.4802790	0.7647430	H	0.9159040	1.0678750	1.4852090
H	-6.9536250	1.9715150	0.8541360	H	2.9306680	1.6703680	-2.2367000
H	-7.2606770	1.0381380	2.3255690	H	5.1332230	1.7220620	-1.0477960
C	-2.9390190	-1.3703180	3.0454140	H	3.1029490	1.1010430	2.6885190
H	-2.8024030	-2.4581230	3.0995340	C	0.5139870	1.2509370	-1.2229540
H	-3.3791160	-1.0417360	3.9922470	O	0.5433740	1.1949410	-2.4475600
H	-1.9353930	-0.9309650	2.9713790	C	-0.9448100	2.3819770	-0.5752680
C	1.1719700	-2.2387710	-0.5861160	C	-0.7592480	3.3046880	0.4609090
C	2.1698880	-2.1713310	0.3923490	C	-1.7921030	2.7492070	-1.6335030
C	3.4811510	-1.9551010	-0.0264420	C	-1.4378000	4.5221690	0.4652710
H	4.2679900	-1.8642700	0.7237870	H	-0.0815350	3.0800310	1.2831630
C	3.8057660	-1.8223190	-1.3762250	C	-2.4812740	3.9519190	-1.6176540
C	2.7829870	-1.9017700	-2.3210870	H	-1.8735110	2.0809790	-2.4911380
H	3.0191700	-1.7769750	-3.3787460	C	-2.3123000	4.8624280	-0.5660950
C	1.4542680	-2.1021290	-1.9498100	H	-1.2831150	5.2257650	1.2837610
C	1.8346110	-2.2752550	1.8480190	H	-3.1477570	4.2104640	-2.4416690
H	1.3567930	-3.2321810	2.0968090	C	-3.0254940	6.1796690	-0.5816840
H	1.1346280	-1.4848870	2.1520670	H	-4.0926710	6.0562180	-0.8040350
H	2.7357590	-2.1831770	2.4629600	H	-2.9389700	6.6975620	0.3798950
C	5.2243550	-1.5895300	-1.7982980	H	-2.6165350	6.8470370	-1.3518790
H	5.7092760	-2.5245620	-2.1088650	C	5.5649580	1.2768480	1.5679690
H	5.8196420	-1.1714470	-0.9786010	F	6.4997840	2.0717600	1.0345380
H	5.2809740	-0.9029200	-2.6515050	F	6.0341190	0.0158500	1.4598640
C	0.3635690	-2.0867410	-2.9745600	F	5.5037340	1.5498030	2.8757680
H	-0.1332200	-1.1055180	-2.9719700				
H	-0.4045360	-2.8476940	-2.7876290				
H	0.7702420	-2.2483920	-3.9782650				
N	-0.1904120	-2.4147520	-0.1774670	INTb2			
N	-2.2236510	-1.9925580	0.3322150	C	-0.8550340	-1.4795440	0.0439250
Ni	-0.8635540	0.4870640	-0.2724080	C	-1.8154120	-3.4949940	0.5328970
C	-0.0737870	-4.9327250	-0.1133390	C	-0.4983650	-3.7201460	0.2768320
H	0.3313040	-5.0590360	-1.1254690	C	-3.2370540	-1.4032230	0.5242070
H	0.7748040	-4.9962100	0.5803710	C	-3.9731140	-1.1049700	-0.6313570
H	-0.7360440	-5.7794290	0.0905590	C	-5.1524740	-0.3810490	-0.4793680
C	-3.2452160	-4.2753950	0.6614580	H	-5.7372570	-0.1360930	-1.3669120
H	-3.6606910	-4.0795190	1.6585260	C	-5.5965280	0.0493200	0.7718150
H	-4.0639940	-4.1467320	-0.0585120	C	-4.8327780	-0.2628270	1.8954990
H	-2.9350880	-5.3242760	0.6294020	H	-5.1653610	0.0733660	2.8779850
C	1.8467870	1.2383980	0.9415310	C	-3.6413890	-0.9795020	1.7953540
C	1.7981210	1.3923130	-0.4444640	C	-3.4853770	-1.5021820	-1.9898050
C	2.9874350	1.5715070	-1.1550060	H	-3.0408950	-2.5054150	-1.9987550
				H	-2.7058530	-0.8069190	-2.3357570

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C	-1.7910640	-6.0235400	-0.9722610
H	-2.8181820	-5.6379230	-0.9449140
H	-1.7395000	-6.8397620	-0.2418470
H	-1.6254640	-6.4489390	-1.9677370
C	0.3122250	-2.9099240	2.3629390
H	1.3101790	-3.0613670	2.7957580
H	-0.4156610	-3.4038410	3.0147620
H	0.1038740	-1.8322370	2.3870330
C	2.9130230	1.5223490	0.4219830
C	2.4847940	2.2402180	1.5435940
C	2.5281880	3.6336970	1.4792640
H	2.1923710	4.2110660	2.3413390
C	3.0002520	4.3010400	0.3500720
C	3.4610500	3.5444050	-0.7301230
H	3.8580740	4.0542000	-1.6090320
C	3.4328490	2.1515860	-0.7174590
C	2.0329370	1.5382470	2.7871150
H	2.8747560	1.0557880	3.3022150
H	1.2950120	0.7558730	2.5731150
H	1.5830180	2.2445030	3.4927190
C	3.0225480	5.7980470	0.2890970
H	4.0022010	6.1712180	-0.0326960
H	2.7939260	6.2455940	1.2619950
H	2.2875220	6.1791540	-0.4313600
C	3.9643840	1.3531440	-1.8669550
H	3.2203770	0.6542850	-2.2684960
H	4.8377390	0.7581270	-1.5668500
H	4.2769640	2.0105740	-2.6844810
N	2.7887920	0.0965530	0.4309500
N	1.9216740	-1.8542050	0.2283350
Ni	0.1351130	0.3337970	-0.5940950
C	5.1017420	-0.3685980	1.3223830
H	5.6769630	0.1108660	0.5192200
H	5.0290010	0.3572710	2.1418260
H	5.6839950	-1.2219200	1.6826540
C	3.7645810	-3.3989250	0.9847420
H	3.1778860	-3.9410180	1.7377190
H	3.7673780	-4.0135680	0.0752030
H	4.7947350	-3.3324760	1.3470950
C	-1.0205420	2.2238470	-1.2531820
C	-0.8431700	1.2337800	-2.2403920
C	-1.9655850	0.4744420	-2.6570200
C	-3.2140770	0.7454440	-2.1482040
C	-3.3779090	1.7594650	-1.1858150

C	-2.3021150	2.5058550	-0.7563260
H	-0.1657270	2.8203110	-0.9263000
H	-1.8210010	-0.3263650	-3.3805850
H	-4.0780370	0.1673560	-2.4711770
H	-2.4340980	3.2712430	0.0029590
C	0.5356140	0.6656050	-2.3965120
O	1.1904220	0.4563870	-3.3893360
C	-1.0492790	0.0820020	0.9249580
C	-1.3179800	0.9330660	2.0052650
C	-1.9483950	-0.9824750	0.7433450
C	-2.4209200	0.7474400	2.8397270
H	-0.6754770	1.7993780	2.1869790
C	-3.0488010	-1.1794600	1.5748810
H	-1.7924450	-1.6895690	-0.0765300
C	-3.3099710	-0.3091370	2.6354890
H	-2.6057440	1.4434640	3.6604000
H	-3.7234400	-2.0196480	1.3950200
C	-4.5352120	-0.4731020	3.4842880
H	-4.7564690	-1.5287580	3.6844670
H	-4.4328640	0.0370070	4.4492800
H	-5.4193110	-0.0510850	2.9861440
C	-4.7422400	1.9561490	-0.6033460
F	-5.2028000	0.8285630	-0.0433010
F	-5.6301680	2.2976810	-1.5513140
F	-4.7710160	2.9081720	0.3326650

TSb3_4

C	1.7250100	0.5594240	-0.0804640
C	3.9745200	0.5125230	0.2825880
C	3.5525660	1.7780140	0.5324700
C	2.8423430	-1.6041430	-0.4455130
C	2.8803530	-1.9404710	-1.8026570
C	2.8745930	-3.2954620	-2.1354900
H	2.9064920	-3.5793280	-3.1880390
C	2.8311360	-4.2905730	-1.1599600
C	2.8038220	-3.9101740	0.1827520
H	2.7572940	-4.6781240	0.9563730
C	2.8072660	-2.5711560	0.5669330
C	2.9259770	-0.8848040	-2.8649510
H	3.6963350	-0.1290140	-2.6637560
H	1.9739390	-0.3424480	-2.9389790
H	3.1332110	-1.3273930	-3.8444420
C	2.7961100	-5.7397630	-1.5389610

H	1.7908360	-6.1597030	-1.4051910	H	-2.1731540	2.1222590	-0.4207230
H	3.4738720	-6.3361100	-0.9169640	H	-1.8040010	-1.5770700	-2.5838570
H	3.0763410	-5.8902890	-2.5869550	H	-4.1594860	-2.1496440	-2.0030480
C	2.7341290	-2.1808980	2.0101870	H	-4.5308530	1.5472710	0.1631260
H	3.6156490	-1.6115720	2.3333480	C	-0.3981050	0.8365770	-2.1120220
H	2.6560430	-3.0664570	2.6489180	O	-0.2670140	1.1996730	-3.2414720
H	1.8528200	-1.5529040	2.1975550	C	-0.5082210	-1.0134800	0.9759260
C	1.3157750	2.9242620	0.4324360	C	-1.0517030	-0.6181090	2.2074880
C	0.6805310	3.1519560	1.6569890	C	-0.4067960	-2.4007410	0.7742890
C	-0.1961190	4.2353160	1.7430250	C	-1.4425880	-1.5384500	3.1815540
H	-0.7084820	4.4228270	2.6872750	H	-1.1806940	0.4464840	2.4251080
C	-0.4245450	5.0823260	0.6602150	C	-0.7930740	-3.3278540	1.7396910
C	0.2563600	4.8377420	-0.5353810	H	0.0067610	-2.7820440	-0.1649640
H	0.0964880	5.5016790	-1.3860400	C	-1.3145910	-2.9117600	2.9675120
C	1.1365610	3.7676520	-0.6734020	H	-1.8557670	-1.1859730	4.1290520
C	0.9664090	2.2957510	2.8520600	H	-0.6824390	-4.3971530	1.5428910
H	1.9437040	2.5410190	3.2903350	C	-1.7608370	-3.9056490	3.9989880
H	0.9848480	1.2282330	2.6040270	H	-1.1486150	-4.8156410	3.9788760
H	0.2143250	2.4504050	3.6328360	H	-1.7079190	-3.4898800	5.0123310
C	-1.3691770	6.2403900	0.7673700	H	-2.8011970	-4.2194400	3.8358290
H	-0.8445860	7.1967190	0.6471680	C	-5.8733290	-0.7243800	-0.5498940
H	-1.8770750	6.2590830	1.7370730	F	-5.9025110	-1.8876770	0.1128670
H	-2.1378350	6.2018800	-0.0140480	F	-6.6110770	-0.8966240	-1.6572390
C	1.8675840	3.5272890	-1.9583020	F	-6.4981070	0.1825690	0.2060980
H	1.5793990	2.5733820	-2.4176740				
H	2.9549730	3.4967650	-1.8083290				
H	1.6519510	4.3213970	-2.6799540				
N	2.1714000	1.7846550	0.2994060	INTb7			
N	2.8344030	-0.2188220	-0.0828080	C	-0.7082590	-1.5060420	-0.0229920
Ni	-0.0440770	0.1505240	-0.5093350	C	-1.5071860	-3.5339210	-0.7131420
C	4.2860340	2.9972860	0.9437560	C	-0.1949140	-3.6972820	-0.3918670
H	4.2130370	3.7905100	0.1884090	C	-3.0493020	-1.5175980	-0.6509820
H	3.8980210	3.4115960	1.8826730	C	-3.3183000	-0.8835920	-1.8714710
H	5.3465690	2.7741610	1.0927740	C	-4.5094910	-0.1712900	-1.9865060
C	5.3226860	-0.1001320	0.3276700	H	-4.7302020	0.3371270	-2.9259450
H	5.3946900	-0.8877630	1.0888770	C	-5.4131500	-0.0756160	-0.9274950
H	5.5916160	-0.5575490	-0.6328220	C	-5.1163260	-0.7339590	0.2649680
H	6.0779610	0.6566120	0.5595420	H	-5.8142090	-0.6691500	1.1001120
C	-2.6206920	1.1932400	-0.7749170	C	-3.9325630	-1.4504400	0.4332900
C	-1.8591460	0.3131680	-1.5449710	C	-2.3375970	-0.9270370	-3.0022710
C	-2.4122270	-0.8905460	-1.9958290	H	-1.9328800	-1.9331310	-3.1666280
C	-3.7187520	-1.2117420	-1.6703510	H	-1.4777190	-0.2727510	-2.7999570
C	-4.4698790	-0.3280160	-0.8913710	H	-2.8001610	-0.5868730	-3.9341940
C	-3.9333450	0.8747070	-0.4456600	C	-6.6552060	0.7504450	-1.0581910
				H	-6.4375280	1.8066450	-0.8519410

H	-5.4415390	-4.8686220	1.0603570	H	4.6468620	0.1007700	-1.4582100
C	-3.9746370	0.6567520	1.3430990	H	2.9497930	-3.7799350	-0.7269880
H	-3.7098170	1.0684570	2.3256380	C	0.0313320	-0.4488780	-2.6389440
H	-5.0457060	0.8166630	1.1835820	O	0.0519960	-0.7098270	-3.7900350
H	-3.4331370	1.2419200	0.5867880	C	-2.0996880	0.7731640	-1.6286100
C	1.3029270	1.9931690	1.1738250	C	-2.3018540	2.1441150	-1.8387560
C	0.9567350	3.2689480	0.7145440	C	-3.1849180	-0.0739130	-1.8825790
C	1.9763140	4.0793600	0.2145890	C	-3.5432460	2.6458530	-2.2282850
H	1.7246210	5.0749210	-0.1527180	H	-1.4780070	2.8451950	-1.6952160
C	3.3057270	3.6578190	0.1908080	C	-4.4270720	0.4277850	-2.2686150
C	3.6136190	2.3941440	0.6958710	H	-3.0746310	-1.1530700	-1.7596390
H	4.6517410	2.0584120	0.7023030	C	-4.6311520	1.7973170	-2.4454130
C	2.6280170	1.5416300	1.1903910	H	-3.6711830	3.7204250	-2.3734260
C	-0.4475320	3.7786820	0.8223160	H	-5.2571510	-0.2610960	-2.4384740
H	-0.6951640	4.0339920	1.8623730	C	-5.9570670	2.3411630	-2.8888440
H	-1.1871670	3.0404180	0.4922980	H	-6.7569320	1.6020390	-2.7643710
H	-0.5807730	4.6860620	0.2242740	H	-6.2398870	3.2378050	-2.3230800
C	4.3786480	4.5341110	-0.3795240	H	-5.9442730	2.6278620	-3.9491890
H	4.0994750	5.5925530	-0.3410720	C	5.2912030	-2.3672290	-0.7062490
H	4.5711480	4.2892270	-1.4323420	F	5.7614710	-1.7299680	0.3821690
H	5.3270690	4.4118560	0.1556870	F	6.1697530	-2.1273220	-1.6887140
C	2.9780320	0.1937560	1.7391050	F	5.3306220	-3.6761180	-0.4438310
H	2.3481200	-0.5945720	1.3095510				
H	2.8346730	0.1520630	2.8272710				
H	4.0229190	-0.0574610	1.5333150	Prl			
N	0.2743590	1.1334490	1.6756990	C	-0.3801050	-1.1316020	0.3479910
N	-1.3129960	-0.2895260	1.7873560	C	0.3483150	0.0119350	-0.0097600
Ni	-0.4322280	0.0560660	-1.0477430	C	-0.3618460	1.1624390	-0.3702250
C	0.5981500	1.8556640	4.0711930	C	-1.7496080	1.1781000	-0.3731720
H	1.6664850	1.6183570	4.1577090	C	-2.4529080	0.0333000	-0.0175500
H	0.5268970	2.9293550	3.8545150	C	-1.7643780	-1.1239240	0.3433100
H	0.1363200	1.6817490	5.0476840	H	0.1498230	-2.0294060	0.6586090
C	-1.8463280	-0.3934860	4.2501620	H	0.1814380	2.0531880	-0.6780910
H	-2.9132690	-0.1453870	4.1797690	H	-2.2849180	2.0783040	-0.6613500
H	-1.7748760	-1.4866110	4.3154910	H	-2.3191580	-2.0153620	0.6299140
H	-1.4669390	0.0228350	5.1881540	C	1.8246210	0.0021080	-0.0051490
C	1.5569580	-2.2354270	-1.3078180	C	2.5524080	1.1420840	0.3600850
C	1.3930500	-0.8896790	-1.6447490	C	2.5406320	-1.1439400	-0.3640860
C	2.5091660	-0.0490350	-1.7028290	C	3.9381600	1.1310170	0.3650290
C	3.7715800	-0.5461300	-1.4144020	H	2.0223680	2.0401690	0.6725630
C	3.9198700	-1.8872300	-1.0593250	C	3.9295400	-1.1491610	-0.3588020
C	2.8179260	-2.7366120	-1.0018130	H	2.0033760	-2.0371320	-0.6782790
H	0.6888980	-2.8950440	-1.2954690	C	4.6539750	-0.0142800	0.0048070
H	2.3835320	0.9974750	-1.9825160	H	4.4834220	2.0265730	0.6621720

H	4.4655060	-2.0518460	-0.6495130	C	-0.6201300	-1.1946520	0.4753660
C	6.1511180	-0.0086930	0.0098510	C	-1.7526900	-2.9785630	1.3422970
H	6.5466240	0.2862480	0.9894700	C	-0.5651730	-3.4452140	0.8679680
H	6.5593460	-0.9949700	-0.2334670	C	-2.8328720	-0.6997990	1.3783340
H	6.5515580	0.7062000	-0.7201210	C	-3.8756720	-0.5806790	0.4540620
C	-3.9462100	0.0016930	0.0024850	C	-4.8860180	0.3423980	0.7265050
F	-4.4946090	1.1541150	-0.3955930	H	-5.7044310	0.4515230	0.0133260
F	-4.4150000	-0.2572460	1.2334210	C	-4.8667880	1.1345220	1.8734430
F	-4.4305760	-0.9644710	-0.7934710	C	-3.8045700	0.9879990	2.7671990
INTq1				H	-3.7723540	1.6075470	3.6645420
C	-2.5440710	1.1774950	-4.6499470	C	-2.7734650	0.0797510	2.5400400
C	-1.1834210	1.3152330	-4.4587780	C	-3.8786890	-1.3799470	-0.8122220
C	-0.6663650	1.6511940	-3.1949550	H	-3.8821710	-2.4615190	-0.6231350
C	-1.5625830	1.8434950	-2.1099480	H	-2.9855250	-1.1637540	-1.4158960
C	-2.9465120	1.7156830	-2.3317360	H	-4.7579530	-1.1452380	-1.4214750
C	-3.4316800	1.3824430	-3.5808950	C	-5.9560500	2.1257720	2.1491170
H	-2.9310810	0.9148610	-5.6322170	H	-5.5539970	3.1411300	2.2515950
H	-0.4739620	1.1714090	-5.2713010	H	-6.4790350	1.8960780	3.0861110
C	-1.0133000	2.1500210	-0.8171720	H	-6.7012130	2.1400580	1.3469180
H	-3.6243710	1.8705950	-1.4916000	C	-1.6124410	-0.0152090	3.4798850
H	-4.5034900	1.2779820	-3.7377760	H	-1.3071890	-1.0529560	3.6640080
C	0.3966510	2.3277350	-0.7048150	H	-1.8473940	0.4516580	4.4417590
C	1.1798290	2.0823690	-1.8890460	H	-0.7369830	0.5032970	3.0632080
H	-1.6760490	2.5254240	-0.0341350	C	1.3886730	-2.3498410	-0.2905830
H	2.2658080	2.1885950	-1.8217930	C	2.5495980	-2.3196300	0.4932870
N	0.7020820	1.7721120	-3.0614690	C	3.7768520	-2.3061250	-0.1664370
C	0.9479230	2.8433310	0.5698890	H	4.6931790	-2.2925090	0.4267880
O	0.2555590	3.5086910	1.3357440	C	3.8640750	-2.2917470	-1.5605190
C	2.3648570	2.5354870	0.9344030	C	2.6851430	-2.3055850	-2.3025270
C	3.0201850	1.3575580	0.5631070	H	2.7373050	-2.2844410	-3.3912360
C	3.0449550	3.4546270	1.7414600	C	1.4321490	-2.3391210	-1.6889540
C	4.3271180	1.1202160	0.9745730	C	2.4747700	-2.2517110	1.9875000
H	2.4979890	0.6014880	-0.0280350	H	1.9979730	-3.1385140	2.4250190
C	4.3527980	3.2202810	2.1324860	H	1.8867810	-1.3841690	2.3162360
H	2.5213470	4.3561000	2.0516200	H	3.4747140	-2.1609670	2.4243960
C	5.0192050	2.0497210	1.7512200	C	5.2036450	-2.2519150	-2.2300020
H	4.8172220	0.1898900	0.6853510	H	5.1094880	-2.2375770	-3.3206040
H	4.8750470	3.9522560	2.7483300	H	5.8152320	-3.1212320	-1.9569600
C	6.4404720	1.8169970	2.1615010	H	5.7696790	-1.3592830	-1.9336360
H	6.7476560	0.7804050	1.9860200	C	0.1753810	-2.3172090	-2.5015000
H	7.1259760	2.4624380	1.5969290	H	-0.3163790	-1.3365920	-2.4225760
H	6.5951590	2.0423990	3.2234160	H	-0.5532070	-3.0623480	-2.1556870
				H	0.3870880	-2.5036590	-3.5588650
				N	0.1092030	-2.3350520	0.3510680

N	-1.7595780	-1.6028890	1.0908310	H	4.8380770	-0.1428650	5.3881830
Ni	-0.1355710	0.5397550	-0.1042470	C	-0.3641050	-1.5073750	-0.6047800
C	0.0011680	-4.8128770	0.8081140	C	-1.1950590	-3.5248760	-1.2848710
H	0.2326480	-5.1035540	-0.2248760	C	0.0840420	-3.4396270	-1.7430580
H	0.9317320	-4.9033910	1.3831770	C	-2.6657740	-2.0066870	0.0733510
H	-0.7113710	-5.5402070	1.2087910	C	-3.6236620	-1.2460210	-0.6031150
C	-2.8784090	-3.6649600	2.0180180	C	-4.8100540	-0.9473960	0.0667640
H	-3.0467620	-3.2684230	3.0279270	H	-5.5712690	-0.3587520	-0.4464370
H	-3.8203420	-3.5479130	1.4668410	C	-5.0430230	-1.3769250	1.3718820
H	-2.6744910	-4.7360290	2.1110250	C	-4.0527010	-2.1179000	2.0180670
TSq1_2				H	-4.2151830	-2.4456740	3.0457460
C	-1.4246960	6.5411820	-1.8705340	C	-2.8506420	-2.4373360	1.3926030
C	-0.2386530	5.8640500	-1.7260560	C	-3.3645330	-0.7209920	-1.9809710
C	-0.2004500	4.6204660	-1.0530570	H	-2.9639170	-1.4875080	-2.6560960
C	-1.4112340	4.0865690	-0.5224080	H	-2.6184080	0.0866030	-1.9473660
C	-2.6189140	4.8082460	-0.6852910	H	-4.2792500	-0.3163890	-2.4261800
C	-2.6254810	6.0102570	-1.3472850	C	-6.3174690	-1.0370670	2.0831090
H	-1.4445390	7.4966100	-2.3904570	H	-6.1445240	-0.2926320	2.8706090
H	0.6981970	6.2544820	-2.1178100	H	-6.7538190	-1.9181520	2.5689170
C	-1.3367060	2.8481460	0.1496120	H	-7.0653290	-0.6242750	1.3976670
H	-3.5369680	4.3906390	-0.2734110	C	-1.7675970	-3.1598660	2.1322700
H	-3.5551710	6.5612330	-1.4706090	H	-1.2729680	-3.9262360	1.5230350
C	-0.1328750	2.1791490	0.2500900	H	-2.1613760	-3.6399350	3.0340030
C	1.0137470	2.8260730	-0.2986910	H	-0.9866460	-2.4537670	2.4475020
H	-2.2266770	2.4185830	0.6146660	C	1.8900750	-1.6980550	-1.5354160
H	1.9909640	2.3448180	-0.2135330	C	2.9237770	-2.1105850	-0.6831760
N	0.9963880	3.9806490	-0.9274080	C	4.1941170	-1.5819660	-0.8961700
C	-0.1346760	1.0020650	1.6922730	H	5.0109370	-1.8944820	-0.2434160
O	-1.1630050	1.0615640	2.3609840	C	4.4451610	-0.6517440	-1.9075560
C	1.2012470	0.8343730	2.3519890	C	3.3882310	-0.2591630	-2.7256140
C	2.3523410	0.4792370	1.6447680	H	3.5656330	0.4715940	-3.5152410
C	1.2854430	0.9897670	3.7391370	C	2.1007530	-0.7737770	-2.5631740
C	3.5597290	0.2985640	2.3087370	C	2.6584190	-3.0320200	0.4665300
H	2.2876000	0.3126260	0.5669330	H	2.2101480	-3.9828700	0.1516830
C	2.4931990	0.8117800	4.3966240	H	1.9611650	-2.5717430	1.1805190
H	0.3808630	1.2506580	4.2845080	H	3.5836830	-3.2579590	1.0065540
C	3.6526230	0.4700360	3.6918030	C	5.8242150	-0.0992610	-2.0999130
H	4.4506780	0.0213140	1.7439200	H	5.8363810	0.7063350	-2.8410670
H	2.5476850	0.9390740	5.4779020	H	6.5212500	-0.8756280	-2.4405880
C	4.9629940	0.3175040	4.4011700	H	6.2275870	0.3005900	-1.1612940
H	5.6641670	-0.2967400	3.8254210	C	0.9782870	-0.3080210	-3.4379370
H	5.4418740	1.2926400	4.5616210	H	0.3439380	0.4171050	-2.9064840
				H	0.3231970	-1.1309930	-3.7500510
				H	1.3618340	0.1860950	-4.3362540

N	0.5692470	-2.2029540	-1.3094440	H	2.8467610	4.2392340	4.8045560
N	-1.4408340	-2.3349940	-0.5929500	H	3.8732890	2.8285670	5.0525700
Ni	-0.2460820	0.2851930	-0.0273910	C	0.8685710	-1.2870960	-0.6023850
C	0.8961660	-4.3629920	-2.5695010	C	1.7238210	-3.3552520	-1.0376330
H	1.2110950	-3.8904620	-3.5089770	C	2.6660640	-2.4427800	-1.4016910
H	1.8082450	-4.6850560	-2.0512610	C	-0.5817880	-3.1784420	-0.0415660
H	0.3215400	-5.2588870	-2.8231840	C	-1.7090250	-3.2146400	-0.8661340
C	-2.2220910	-4.5827070	-1.4345940	C	-2.8871660	-3.7391510	-0.3330890
H	-2.5641350	-4.9600230	-0.4625030	H	-3.7768960	-3.7780760	-0.9624400
H	-3.1105770	-4.2180390	-1.9659030	C	-2.9540570	-4.2110780	0.9760270
H	-1.8202940	-5.4293960	-1.9992660	C	-1.8079180	-4.1462310	1.7690270
INTq2				H	-1.8522380	-4.4946590	2.8017200
C	-6.0401300	4.0444640	-0.9506690	C	-0.6141460	-3.6195110	1.2865350
C	-4.7216160	4.3116750	-1.2251260	C	-1.6741880	-2.6748720	-2.2624940
C	-3.7208780	3.3446000	-0.9647150	H	-0.7736730	-2.9840770	-2.8084930
C	-4.0994070	2.0911360	-0.4036770	H	-1.6803770	-1.5742480	-2.2532430
C	-5.4675190	1.8438190	-0.1332640	H	-2.5494630	-3.0033910	-2.8321100
C	-6.4177540	2.7978460	-0.4013830	C	-4.2294750	-4.7637360	1.5351910
H	-6.8023650	4.7940490	-1.1534700	H	-4.6430510	-4.1016580	2.3063020
H	-4.4024350	5.2624310	-1.6478600	H	-4.0717330	-5.7411720	2.0072480
C	-3.0690440	1.1593490	-0.1332490	H	-4.9930010	-4.8831680	0.7593940
H	-5.7473630	0.8816860	0.2956390	C	0.5728940	-3.4589940	2.1833830
H	-7.4662330	2.5993570	-0.1884600	H	1.5098740	-3.7864130	1.7159920
C	-1.7494370	1.4450600	-0.4283350	H	0.4405670	-4.0186910	3.1146950
C	-1.5141710	2.7352520	-0.9923290	H	0.6998930	-2.3998990	2.4501170
H	-3.3318930	0.2039110	0.3320330	C	2.7682010	0.0731960	-1.3154590
H	-0.4859530	3.0189300	-1.2491740	C	3.6661490	0.5289250	-0.3414610
N	-2.4257990	3.6488920	-1.2550110	C	4.2576190	1.7739930	-0.5353290
C	-0.5414960	0.1578530	1.4584140	H	4.9527410	2.1501150	0.2176100
O	-1.3217470	-0.5634980	2.0417980	C	3.9617110	2.5639970	-1.6486480
C	0.4484230	1.0262170	2.1648690	C	3.0499620	2.0813150	-2.5852320
C	1.2133630	1.9755990	1.4875240	H	2.7997260	2.6921060	-3.4532090
C	0.6433320	0.8494530	3.5397100	C	2.4373250	0.8353690	-2.4396920
C	2.1488220	2.7405900	2.1724780	C	3.9214250	-0.2620050	0.9034420
H	1.0767570	2.0987690	0.4120970	H	4.3033870	-1.2694810	0.6953900
C	1.5884370	1.6058760	4.2151210	H	2.9921860	-0.3838780	1.4789550
H	0.0397330	0.1082990	4.0598930	H	4.6460850	0.2468270	1.5468030
C	2.3524700	2.5681180	3.5436820	C	4.6059640	3.9067170	-1.8129920
H	2.7399770	3.4803900	1.6317950	H	4.2675840	4.4078090	-2.7255000
H	1.7402710	1.4583430	5.2843110	H	5.6988690	3.8237260	-1.8605540
C	3.3442870	3.4082290	4.2872410	H	4.3745600	4.5648920	-0.9657570
H	4.0893400	3.8453370	3.6135690	C	1.4151860	0.3631670	-3.4274140
				H	0.3960050	0.4923180	-3.0288200
				H	1.5266070	-0.7012330	-3.6696180

H	1.4732720	0.9362270	-4.3582000	H	-6.2340420	-1.0713140	-2.6069160
N	2.1210030	-1.1883460	-1.1143150	H	-5.9285420	-2.4516610	-3.6723270
N	0.6390060	-2.6216640	-0.5485180	H	-5.9601060	-2.6868460	-1.9289320
Ni	-0.4005140	0.1267750	-0.3545690	C	-0.4382240	-0.2205420	1.1303090
C	4.0022710	-2.5971010	-2.0224610	C	-1.2868470	-0.1000960	3.2491570
H	4.0642110	-2.0529660	-2.9738620	C	-0.1145330	-0.7880600	3.3204120
H	4.8026820	-2.2099140	-1.3786580	C	-2.5674490	0.9687580	1.3781610
H	4.2133440	-3.6515740	-2.2241640	C	-3.6957260	0.2636270	0.9405590
C	1.7035930	-4.8340810	-1.1176780	C	-4.7668950	0.9974890	0.4394780
H	1.5801750	-5.2947910	-0.1290480	H	-5.6568240	0.4648910	0.0983120
H	0.8757770	-5.1910710	-1.7438760	C	-4.7239270	2.3902200	0.3444640
H	2.6378500	-5.2079030	-1.5469600	C	-3.5784380	3.0525160	0.7802100
INTq3				H	-3.5294310	4.1395230	0.7108150
C	5.9980810	2.9678400	-1.3953390	C	-2.4866020	2.3631260	1.3119010
C	4.7306030	3.4413030	-1.1604970	C	-3.7287080	-1.2329130	0.9634360
C	3.6186640	2.5651080	-1.1773180	H	-3.4908970	-1.6422990	1.9536320
C	3.8304750	1.1826960	-1.4462400	H	-2.9909140	-1.6520030	0.2645920
C	5.1489890	0.7233610	-1.6860880	H	-4.7144690	-1.6064430	0.6664580
C	6.2095690	1.5953200	-1.6594730	C	-5.8862840	3.1424990	-0.2287340
H	6.8464650	3.6488480	-1.3801180	H	-6.8093690	2.9392190	0.3281450
H	4.5387130	4.4928360	-0.9552140	H	-6.0748700	2.8520480	-1.2704920
C	2.7008080	0.3296980	-1.4485580	H	-5.7161720	4.2238390	-0.2122750
H	5.3002350	-0.3377640	-1.8881150	C	-1.2833980	3.1016870	1.8130890
H	7.2188000	1.2331750	-1.8452940	H	-1.2840130	3.1736990	2.9093770
C	1.4528760	0.8263590	-1.1527950	H	-1.2606610	4.1234620	1.4210160
C	1.3644340	2.2299550	-0.9231240	H	-0.3457680	2.6095630	1.5285980
H	2.8319390	-0.7263940	-1.6947030	C	1.6061470	-1.4832670	1.6315480
H	0.3831670	2.6727180	-0.7162230	C	2.8066040	-0.7804710	1.7685450
N	2.3779780	3.0722200	-0.9348410	C	3.9832110	-1.4192460	1.3775550
C	0.0755330	-0.9890850	-2.4150870	H	4.9278850	-0.8827640	1.4714140
O	0.9121460	-1.5779230	-3.0579620	C	3.9778180	-2.7084320	0.8491290
C	-1.4126220	-1.2288320	-2.5305430	C	2.7553250	-3.3697250	0.7134820
C	-2.3222400	-0.1713010	-2.4295870	H	2.7353310	-4.3748490	0.2897030
C	-1.8957160	-2.5383090	-2.6797990	C	1.5551530	-2.7767540	1.0971220
C	-3.6893210	-0.4182660	-2.5118430	C	2.8226140	0.6362050	2.2488390
H	-1.9508270	0.8476910	-2.3059830	H	2.3611470	0.7527730	3.2380980
C	-3.2582660	-2.7744990	-2.7367550	H	2.2628620	1.2811460	1.5563220
H	-1.1795360	-3.3546770	-2.7617050	H	3.8464980	1.0196760	2.3041560
C	-4.1769210	-1.7169450	-2.6551450	C	5.2495840	-3.3763950	0.4236600
H	-4.3912180	0.4129550	-2.4549900	H	5.1723280	-3.7629970	-0.5999570
H	-3.6319690	-3.7918570	-2.8537160	H	5.4893390	-4.2312980	1.0691560
C	-5.6478800	-1.9898630	-2.7172310	H	6.0985980	-2.6855570	0.4586980
				C	0.2491080	-3.4816230	0.8945130
				H	-0.3024740	-3.0439200	0.0486250

H	-0.4072940	-3.4054390	1.7710480	C	-5.8130820	-2.2873940	-2.5996140
H	0.4068070	-4.5424260	0.6751560	H	-6.4489580	-2.0113730	-1.7476460
N	0.3822490	-0.8428190	2.0162600	H	-6.2901370	-1.8716840	-3.4960190
N	-1.4584760	0.2319620	1.9021620	H	-5.8296440	-3.3785370	-2.6888470
Ni	-0.0587740	-0.2096170	-0.7963020	C	-0.3519390	-0.2721760	0.8951160
C	0.5893720	-1.4152850	4.4629350	C	-1.0729380	-0.2738960	3.0702060
H	0.7636560	-2.4847650	4.2887670	C	0.0767530	-0.9937080	3.0288120
H	1.5699220	-0.9551390	4.6424180	C	-2.4584550	0.9287880	1.3927240
H	0.0011070	-1.3145820	5.3798640	C	-3.6522200	0.2601650	1.0953740
C	-2.2700130	0.2775280	4.2911690	C	-4.7628030	1.0303430	0.7634490
H	-2.3727090	1.3662790	4.3828440	H	-5.6990680	0.5247670	0.5184100
H	-3.2685400	-0.1212230	4.0716960	C	-4.7005270	2.4239550	0.7050450
H	-1.9602490	-0.1099120	5.2664160	C	-3.4957380	3.0509880	1.0173100
TSq3_4				H	-3.4351790	4.1393120	0.9886670
C	6.0744500	3.0729800	-1.0877300	C	-2.3616260	2.3234290	1.3846960
C	4.8129310	3.5750150	-0.8838650	C	-3.7187840	-1.2345700	1.1141840
C	3.6791550	2.7305190	-0.9635970	H	-3.4304260	-1.6462090	2.0904400
C	3.8613850	1.3507460	-1.2637420	H	-3.0342920	-1.6680170	0.3720910
C	5.1744540	0.8621880	-1.4742850	H	-4.7304070	-1.5849940	0.8839460
C	6.2568990	1.7031900	-1.3857810	C	-5.9141740	3.2183630	0.3285680
H	6.9403990	3.7284710	-1.0235350	H	-6.6801260	3.1739600	1.1135040
H	4.6418640	4.6254440	-0.6560070	H	-6.3764980	2.8309410	-0.5878540
C	2.7081250	0.5300860	-1.3125800	H	-5.6715800	4.2729330	0.1618990
H	5.3060610	-0.1950690	-1.7079190	C	-1.1088210	3.0220540	1.8158860
H	7.2615570	1.3178110	-1.5481650	H	-1.0321530	3.0469860	2.9119270
C	1.4581670	1.0468250	-1.0478510	H	-1.0954090	4.0594480	1.4663280
C	1.4108290	2.4513100	-0.8125010	H	-0.2030560	2.5271870	1.4482440
H	2.8434590	-0.5286150	-1.5480890	C	1.7002420	-1.6106620	1.2430020
H	0.4341020	2.9244260	-0.6639470	C	2.9295160	-0.9779830	1.4536230
N	2.4448690	3.2663580	-0.7591320	C	4.0809590	-1.6390610	1.0253700
C	-0.3115800	-0.0521110	-2.7556110	H	5.0473830	-1.1546310	1.1699800
O	-0.1549640	-0.0474920	-3.9190890	C	4.0254050	-2.8828850	0.3989250
C	-1.8141840	-0.7588570	-2.0504780	C	2.7764520	-3.4750800	0.1981400
C	-2.9173990	0.1022970	-2.0644560	H	2.7174020	-4.4480670	-0.2919750
C	-2.0270980	-2.1246240	-2.2648130	C	1.5998630	-2.8607450	0.6210040
C	-4.1999920	-0.3956830	-2.2474360	C	3.0127400	0.3745990	2.0895630
H	-2.7652140	1.1754710	-1.9372490	H	2.7559030	0.3488580	3.1568730
C	-3.3149210	-2.6210440	-2.4369310	H	2.3194690	1.0784180	1.6112220
H	-1.1752480	-2.8039570	-2.3149940	H	4.0240130	0.7854250	2.0030630
C	-4.4200830	-1.7649970	-2.4261920	C	5.2760970	-3.5849150	-0.0348420
H	-5.0518080	0.2861040	-2.2469900	H	5.1614100	-4.0336920	-1.0285020
H	-3.4713770	-3.6886390	-2.5914900	H	5.5331580	-4.3992970	0.6551850
				H	6.1314490	-2.9015540	-0.0679660
				C	0.2653350	-3.5107740	0.4221620

H	-0.3898140	-2.8944010	-0.2075630	H	-3.0445270	4.4164730	0.7019680
H	-0.2678040	-3.6470730	1.3730790	C	-2.1614380	2.5204340	1.1844070
H	0.3717770	-4.4928560	-0.0495090	C	-3.9365940	-0.8653370	1.2650020
N	0.5027430	-0.9684850	1.6948870	H	-3.7810590	-1.1721410	2.3081320
N	-1.3139170	0.1503350	1.7587810	H	-3.2697040	-1.4780850	0.6448250
Ni	-0.1554500	0.0268710	-1.0362660	H	-4.9688270	-1.1147090	0.9989320
C	0.7991980	-1.7363510	4.0891230	C	-5.6041260	3.7271470	0.0859650
H	0.8677910	-2.8074130	3.8593980	H	-6.5496390	3.4637270	0.5740920
H	1.8248100	-1.3740260	4.2327540	H	-5.7706180	3.6466300	-0.9959930
H	0.2760810	-1.6352260	5.0449140	H	-5.3898170	4.7786520	0.3049100
C	-1.9850970	0.0599100	4.1886810	C	-0.8471540	3.1179700	1.5872160
H	-2.1024170	1.1443910	4.3093980	H	-0.8548410	3.3745350	2.6560980
H	-2.9895960	-0.3566290	4.0373800	H	-0.6432050	4.0446970	1.0402180
H	-1.5963940	-0.3397340	5.1300300	H	-0.0044050	2.4375420	1.4272230
INTq4				C	1.6582750	-1.5800800	1.3013610
C	5.9659100	3.0497500	-1.2619910	C	2.8719210	-0.8971530	1.4549160
C	4.6942820	3.5398240	-1.0946600	C	4.0423530	-1.5663910	1.0994020
C	3.5762900	2.6719990	-1.1381280	H	4.9953330	-1.0441770	1.1942650
C	3.7881650	1.2819060	-1.3582880	C	4.0244050	-2.8707850	0.6068050
C	5.1101270	0.8058900	-1.5354880	C	2.7970420	-3.5255670	0.4979900
C	6.1765570	1.6698970	-1.4851930	H	2.7688560	-4.5548010	0.1372660
H	6.8191000	3.7237810	-1.2261000	C	1.6008280	-2.9062590	0.8586980
H	4.5033660	4.5978630	-0.9260140	C	2.9234530	0.5083240	1.9687870
C	2.6514440	0.4371290	-1.3600730	H	2.5991970	0.5791800	3.0155060
H	5.2612690	-0.2607620	-1.7062240	H	2.2718740	1.1705540	1.3845270
H	7.1893350	1.2954480	-1.6191510	H	3.9423610	0.9051660	1.9131780
C	1.3925920	0.9433940	-1.1243950	C	5.2956080	-3.5680790	0.2281820
C	1.3125510	2.3575370	-0.9895480	H	5.1826190	-4.1298680	-0.7061840
H	2.8070250	-0.6311930	-1.5358960	H	5.6005850	-4.2879910	0.9987840
H	0.3241880	2.8174050	-0.8883250	H	6.1200450	-2.8584290	0.0991510
N	2.3295790	3.1954740	-0.9774790	C	0.3115210	-3.6673340	0.8489100
C	-0.0987550	-0.1175460	-2.8489330	H	-0.5352820	-3.0594780	0.5138120
O	0.0041060	-0.1270180	-3.9923230	H	0.0630200	-4.0202790	1.8599490
C	-0.3918670	-0.2454420	0.8304730	H	0.3800000	-4.5507790	0.2054360
C	-1.0830510	-0.0464700	3.0048620	N	0.4460410	-0.9120450	1.6738770
C	0.0304980	-0.8196170	3.0077250	N	-1.3298970	0.2800410	1.6659310
C	-2.4045980	1.1453820	1.2769050	Ni	-0.2421070	-0.1266630	-1.1073010
C	-3.6779820	0.5968470	1.0725790	C	0.7416060	-1.5096640	4.1096050
C	-4.7016230	1.4614410	0.6940820	H	0.8120360	-2.5894130	3.9261890
H	-5.6952420	1.0489870	0.5120420	H	1.7660080	-1.1409410	4.2455040
C	-4.4880930	2.8319300	0.5309480	H	0.2079820	-1.3671810	5.0539210
C	-3.2181750	3.3433240	0.7896860	C	-1.9414660	0.4383170	4.1109590
				H	-1.9734140	1.5346140	4.1469550
				H	-2.9781110	0.0913370	4.0178860

H	-1.5566550	0.0862070	5.0725990	H	-4.9936860	-0.8873180	-2.4355220
C	-1.9138740	-1.0664420	-1.5471490	H	-2.2947540	-4.2183840	-2.4524820
C	-3.0290570	-0.2844280	-1.8701530	C	-4.9067150	-3.5670770	-2.9047220
C	-2.0541910	-2.4536670	-1.6777480	H	-5.5521870	-3.8443530	-2.0600200
C	-4.2457720	-0.8600140	-2.2314520	H	-5.5492680	-3.0812790	-3.6488880
H	-2.9584660	0.8052370	-1.8267520	H	-4.5308470	-4.4985260	-3.3431500
C	-3.2704740	-3.0328800	-2.0362840	C	-0.3352690	-0.1802120	0.9242500
H	-1.1973120	-3.1066180	-1.5064950	C	-1.0625720	-0.1802280	3.0964910
C	-4.3917850	-2.2461700	-2.3104820	C	0.1124580	-0.8548160	3.0681690
H	-5.1005170	-0.2202930	-2.4599110	C	-2.5432920	0.8702780	1.4165460
H	-3.3507310	-4.1184540	-2.1180290	C	-3.6824110	0.0786470	1.1986390
C	-5.7040980	-2.8767180	-2.6693770	C	-4.8685500	0.7247900	0.8652130
H	-5.5828260	-3.6678550	-3.4196360	H	-5.7597470	0.1243320	0.6753470
H	-6.1823030	-3.3403120	-1.7956840	C	-4.9423210	2.1153500	0.7452310
H	-6.4081450	-2.1402290	-3.0730110	C	-3.7976130	2.8652720	0.9994500
INTq5				H	-3.8414900	3.9528800	0.9269690
C	6.3268400	2.6402100	-0.8681360	C	-2.5882640	2.2649100	1.3616590
C	5.1413740	3.2589490	-0.5573460	C	-3.6190160	-1.4138650	1.3003850
C	3.9112040	2.5727720	-0.7076160	H	-3.2307730	-1.7459990	2.2726060
C	3.9200710	1.2346820	-1.1907040	H	-2.9553970	-1.8289990	0.5297990
C	5.1570430	0.6270830	-1.5181170	H	-4.6103790	-1.8575020	1.1611890
C	6.3353550	1.3124880	-1.3545220	C	-6.2336970	2.7744070	0.3682590
H	7.2684550	3.1708250	-0.7430120	H	-7.0092310	2.5932240	1.1231670
H	5.1058230	4.2800950	-0.1829980	H	-6.6196760	2.3850450	-0.5818300
C	2.6779910	0.5621830	-1.2778690	H	-6.1182330	3.8581990	0.2635130
H	5.1530530	-0.3988490	-1.8880970	C	-1.4037770	3.1107020	1.7108020
H	7.2825720	0.8364190	-1.5998910	H	-1.4128180	3.3776960	2.7768740
C	1.5048110	1.1703570	-0.8834360	H	-1.4127800	4.0492530	1.1444770
C	1.6301900	2.5266510	-0.4713810	H	-0.4554770	2.6017120	1.5106400
H	2.6813740	-0.4685080	-1.6471950	C	1.7140410	-1.5376620	1.2991340
H	0.7259900	3.0822130	-0.2060410	C	2.9721680	-0.9411300	1.4329050
N	2.7558110	3.2074610	-0.3710270	C	4.0814020	-1.6574790	0.9795050
C	-0.0263460	0.3573020	-2.7235600	H	5.0668750	-1.1959300	1.0537470
O	0.0832240	0.4672750	-3.8612020	C	3.9612050	-2.9252460	0.4148730
C	-1.6892630	-0.9686150	-1.5633390	C	2.6941890	-3.5083450	0.3528430
C	-2.9719060	-0.4726940	-1.8243040	H	2.5874310	-4.5181290	-0.0458510
C	-1.4684290	-2.3241930	-1.8358790	C	1.5589640	-2.8432530	0.8113880
C	-4.0006210	-1.3054620	-2.2583640	C	3.1507950	0.4073740	2.0578930
H	-3.1941920	0.5842160	-1.6699350	H	3.0801020	0.3532730	3.1531790
C	-2.4976880	-3.1629950	-2.2630480	H	2.3911440	1.1222830	1.7217060
H	-0.4673980	-2.7443420	-1.7194220	H	4.1369240	0.8184870	1.8163160
C	-3.7862650	-2.6694700	-2.4718300	C	5.1586420	-3.6471550	-0.1231890
				H	5.1598920	-3.6452490	-1.2210770
				H	5.1726240	-4.6975140	0.1911420

H	6.0927750	-3.1806180	0.2073010	C	0.4443010	4.5924840	-1.6649110
C	0.2351780	-3.5427830	0.8687720	H	0.4420400	2.5985140	-2.4591860
H	-0.5976480	-2.9020670	0.5611800	C	0.1541460	5.4318900	-0.5863440
H	0.0204710	-3.8802540	1.8928090	H	-0.6128290	5.4854060	1.4210280
H	0.2311310	-4.4328140	0.2302070	H	0.8473970	5.0256030	-2.5822180
N	0.5439820	-0.8339240	1.7366200	C	0.4186710	6.9058420	-0.6685090
N	-1.3218350	0.2116230	1.7774320	H	0.0622280	7.3289420	-1.6161330
Ni	-0.1713620	0.1499950	-0.9924550	H	-0.0745650	7.4493160	0.1454020
C	0.8716570	-1.5393610	4.1407980	H	1.4922150	7.1294080	-0.6057860
H	1.0203470	-2.6033150	3.9167710	C	-0.8934890	-1.1948960	-0.0732280
H	1.8660800	-1.1011120	4.2929640	C	-2.0051030	-3.1463630	0.3591860
H	0.3309270	-1.4717990	5.0895170	C	-0.7416170	-3.4744560	-0.0146780
C	-1.9696520	0.1627350	4.2163260	C	-3.3031220	-1.0241700	0.4540740
H	-2.1115540	1.2474450	4.3013560	C	-4.2035320	-1.0165300	-0.6219280
H	-2.9650680	-0.2838000	4.0970830	C	-5.3889970	-0.3036200	-0.4758340
H	-1.5547610	-0.1952030	5.1632130	H	-6.0922470	-0.2746010	-1.3091750
C	-1.5356380	2.7716040	-1.5283180	C	-5.6882430	0.3932310	0.6966710
O	-2.1209550	3.0262310	-2.4717020	C	-4.7684990	0.3607320	1.7417430
INTq6				H	-4.9869470	0.9018450	2.6628540
C	5.9119360	0.5871320	2.0345230	C	-3.5643420	-0.3384300	1.6432630
C	4.7175270	0.3850350	2.6806380	C	-3.8831770	-1.7087680	-1.9117180
C	3.4901850	0.5389280	1.9897310	H	-3.9617750	-2.8012220	-1.8323500
C	3.5088580	0.9015930	0.6142400	H	-2.8595030	-1.4894080	-2.2435280
C	4.7560980	1.1121820	-0.0236390	H	-4.5684980	-1.3869460	-2.7021640
C	5.9313780	0.9568270	0.6693550	C	-6.9709990	1.1574090	0.8131800
H	6.8509470	0.4656970	2.5707600	H	-7.0849360	1.6093260	1.8039050
H	4.6718850	0.1023660	3.7309020	H	-7.8385760	0.5099890	0.6361970
C	2.2679710	1.0118840	-0.0533300	H	-7.0205020	1.9636060	0.0710020
H	4.7605830	1.3869050	-1.0792470	C	-2.5789390	-0.3136510	2.7682130
H	6.8850990	1.1183890	0.1698990	H	-2.0758630	-1.2785530	2.9068750
C	1.0823910	0.7331050	0.5919960	H	-3.0667360	-0.0407520	3.7094440
C	1.2025310	0.4002710	1.9702690	H	-1.7943620	0.4320410	2.5767230
H	2.2788740	1.3086510	-1.1054900	C	1.2885720	-2.1921140	-0.6925180
H	0.2959170	0.1773190	2.5433250	C	2.3235150	-2.4870000	0.2047830
N	2.3262870	0.3071650	2.6545060	C	3.6336800	-2.3887820	-0.2614970
C	-2.0455230	1.1547050	-1.3010320	H	4.4530520	-2.5807060	0.4344460
O	-2.8702710	1.5666290	-1.9858650	C	3.9263930	-2.0286820	-1.5756070
C	-0.2940450	2.6338040	-0.4264290	C	2.8672110	-1.7558900	-2.4402890
C	-0.5955330	3.4759490	0.6460700	H	3.0780140	-1.4749960	-3.4728720
C	0.2171120	3.2211390	-1.5891140	C	1.5398210	-1.8319400	-2.0218780
C	-0.3755560	4.8500250	0.5664080	C	2.0803740	-2.8693650	1.6342950
H	-0.9947090	3.0575260	1.5723170	H	2.3710030	-3.9120880	1.8194060
				H	1.0344550	-2.7502590	1.9348390
				H	2.6824670	-2.2433640	2.3028440

C	5.3497140	-1.9167130	-2.0277640	C	-1.3374540	4.2997490	-1.9232720
H	5.8892710	-2.8630810	-1.8974140	H	0.3935300	3.0592750	-2.1711730
H	5.8840160	-1.1604880	-1.4369330	C	-2.5807280	4.4876280	-1.3066730
H	5.4191320	-1.6325630	-3.0830540	H	-4.0034670	3.6062310	0.0410350
C	0.4267840	-1.5075670	-2.9704970	H	-0.9621040	5.0655730	-2.6036320
H	-0.0182120	-0.5268350	-2.7413700	C	-3.3727470	5.7372980	-1.5439900
H	-0.3841200	-2.2466020	-2.9200120	H	-2.9505340	6.5945670	-1.0021360
H	0.7917970	-1.4750760	-4.0021220	H	-3.3868930	6.0114420	-2.6062360
N	-0.0748440	-2.2649950	-0.2518740	H	-4.4113090	5.6252070	-1.2127280
N	-2.0778410	-1.7512870	0.3022250	C	-0.2021660	-1.4863940	-0.0830500
Ni	-0.6036220	0.7313300	-0.3152320	C	-0.6345510	-3.5009620	0.9143740
C	-0.0998470	-4.7970580	-0.2013600	C	0.6693000	-3.5097470	0.5324130
H	0.4032820	-4.8585700	-1.1743890	C	-2.4815070	-1.7959520	0.7345780
H	0.6500610	-5.0178970	0.5680960	C	-3.4300280	-2.0027170	-0.2745840
H	-0.8540380	-5.5890450	-0.1658480	C	-4.7062260	-1.4731510	-0.0900730
C	-3.1372020	-3.9844180	0.8193570	H	-5.4536040	-1.6168380	-0.8712220
H	-3.4518050	-3.7004720	1.8321670	C	-5.0471420	-0.7631650	1.0607330
H	-4.0200720	-3.8984880	0.1741330	C	-4.0821020	-0.6048420	2.0564560
H	-2.8434890	-5.0378130	0.8468040	H	-4.3386260	-0.0646410	2.9687180
TSq6_7				C	-2.7920180	-1.1160610	1.9189610
C	4.4946260	2.9115440	2.8594470	C	-3.0993800	-2.7962000	-1.5014810
C	3.1808660	2.6993170	3.2062010	H	-3.1109390	-3.8748160	-1.2923680
C	2.2373220	2.2966210	2.2354770	H	-2.1015540	-2.5612720	-1.8887340
C	2.6562570	2.1109470	0.8873290	H	-3.8276420	-2.6096040	-2.2973880
C	4.0134040	2.3481030	0.5565520	C	-6.4091120	-0.1580490	1.2152130
C	4.9119130	2.7363710	1.5212860	H	-7.1624860	-0.7038110	0.6367900
H	5.2163200	3.2204200	3.6125460	H	-6.4198290	0.8810380	0.8608780
H	2.8276750	2.8308320	4.2272710	H	-6.7279110	-0.1440280	2.2633980
C	1.6979280	1.6666440	-0.0505730	C	-1.7866050	-0.9661540	3.0199280
H	4.3284920	2.2100890	-0.4783040	H	-1.6933080	-1.8925670	3.6035610
H	5.9521410	2.9149970	1.2554840	H	-2.0826720	-0.1748490	3.7163640
C	0.3857300	1.4337560	0.3316590	H	-0.7855150	-0.7276580	2.6418670
C	0.0877930	1.6947080	1.7064750	C	2.1668390	-1.8541180	-0.6149250
H	2.0212830	1.5020490	-1.0823440	C	3.1293560	-1.3063410	0.2427140
H	-0.9455740	1.5711440	2.0441460	C	4.3365090	-0.8931730	-0.3162450
N	0.9442310	2.0823430	2.6193780	H	5.0895570	-0.4467640	0.3344850
C	-1.3589620	0.0028620	-2.4568410	C	4.5922290	-1.0059720	-1.6835300
O	-1.8282660	-0.0177430	-3.5087590	C	3.6097710	-1.5607690	-2.5019840
C	-1.0303780	2.1583340	-0.8194120	H	3.7962210	-1.6593050	-3.5721490
C	-2.2763060	2.3470190	-0.1997420	C	2.3880930	-1.9982760	-1.9881370
C	-0.5772690	3.1645630	-1.6859920	C	2.8576880	-1.1288870	1.7040280
C	-3.0355010	3.4869790	-0.4477880	H	2.6597860	-2.0827500	2.2108360
H	-2.6646300	1.5852090	0.4812290	H	1.9782840	-0.4904530	1.8642020
				H	3.7081180	-0.6534480	2.2044800

C	5.9059520	-0.5554010	-2.2462860	H	-1.2800000	-1.2638220	-1.5844630
H	5.8384000	-0.3518970	-3.3203860	C	-1.5998860	-4.0129940	1.1273530
H	6.6824210	-1.3191770	-2.1071000	H	0.5349080	-4.1497770	1.0670550
H	6.2619030	0.3548260	-1.7489600	C	-2.7570950	-3.3522230	0.6633850
C	1.3467210	-2.5874450	-2.8897340	H	-3.4962000	-1.8573560	-0.6816800
H	0.5357440	-1.8730170	-3.0839020	H	-1.7042990	-4.8339670	1.8362750
H	0.8802000	-3.4807620	-2.4555530	C	-4.1106140	-3.7662930	1.1526480
H	1.7797150	-2.8646060	-3.8563010	H	-4.2885000	-4.8368980	0.9868850
N	0.9078040	-2.2657600	-0.0695090	H	-4.2180520	-3.5915970	2.2311150
N	-1.1417120	-2.2555490	0.5286380	H	-4.9086580	-3.2109280	0.6456860
Ni	-0.5816530	0.2819930	-0.8625260	C	-0.6844540	1.1855120	0.0772470
C	1.7228120	-4.5449810	0.6521540	C	-1.6373340	3.2115490	-0.4577330
H	2.0979710	-4.8636870	-0.3290810	C	-0.3168250	3.4343670	-0.2372550
H	2.5878780	-4.1856130	1.2238340	C	-3.0950960	1.1852240	-0.4370160
H	1.3324390	-5.4311490	1.1616180	C	-3.8742520	0.8997330	0.6881960
C	-1.4701180	-4.5172820	1.5948090	C	-5.0945580	0.2507190	0.4914540
H	-1.8909370	-4.1359290	2.5336380	H	-5.7078000	0.0095230	1.3607260
H	-2.3151720	-4.8380480	0.9724560	C	-5.5402810	-0.1059020	-0.7794630
H	-0.8780650	-5.4057400	1.8332680	C	-4.7330080	0.1956500	-1.8790870
INTq7				H	-5.0632530	-0.0904310	-2.8789650
C	6.0281180	-1.3861900	-1.6602740	C	-3.5060340	0.8384780	-1.7318070
C	4.8868820	-1.3448310	-2.4235190	C	-3.3957720	1.2292290	2.0669360
C	3.6274310	-1.6297250	-1.8450720	H	-2.9271820	2.2203360	2.1196380
C	3.5560250	-1.9556120	-0.4607110	H	-2.6326170	0.5044280	2.3864110
C	4.7466390	-1.9743210	0.3049600	H	-4.2191990	1.1964900	2.7877870
C	5.9570330	-1.7043750	-0.2841980	C	-6.8416910	-0.8239130	-0.9723190
H	6.9947940	-1.1757850	-2.1128980	H	-7.3250190	-1.0468510	-0.0150890
H	4.9101650	-1.1011790	-3.4838800	H	-6.6963520	-1.7729310	-1.5040420
C	2.2861620	-2.2395370	0.0841780	C	-2.6426310	1.1310990	-2.9210410
H	4.6824530	-2.2115580	1.3666060	H	-2.6798680	2.1918160	-3.2046750
H	6.8686320	-1.7285310	0.3095070	H	-2.9662420	0.5505940	-3.7910390
C	1.1640810	-2.2119240	-0.7207220	H	-1.5868210	0.9001190	-2.7259660
C	1.3617550	-1.8576780	-2.0862300	C	1.6148020	1.9884420	0.4164180
H	2.2004910	-2.4733590	1.1456990	C	2.5341580	1.7607410	-0.6106880
H	0.4922160	-1.8310060	-2.7486460	C	3.8694730	1.5558750	-0.2599500
N	2.5191730	-1.5785890	-2.6342000	H	4.5982820	1.3619560	-1.0482450
C	-0.1283570	-1.0077840	2.4624810	C	4.2867110	1.5743630	1.0692840
O	-0.0052680	-1.2790390	3.5873590	C	3.3377040	1.8137950	2.0659680
C	-0.1799000	-2.5572580	-0.2129610	H	3.6532830	1.8368430	3.1103180
C	-1.3420760	-1.9504310	-0.7443060	C	1.9969480	2.0361070	1.7631490
C	-0.3495570	-3.6276990	0.7038530	C	2.0933030	1.7241240	-2.0414630
C	-2.6094890	-2.3457380	-0.2765240	H	1.7268790	2.7034090	-2.3793870
				H	1.2726770	1.0099820	-2.1889050

H	2.9153910	1.4258010	-2.7001150	C	0.9054070	3.2173600	-2.0808870
C	5.7243310	1.3576940	1.4339000	H	-1.1758590	2.9384240	-1.7159840
H	5.8309890	0.5740580	2.1948170	C	2.4233970	2.8066730	-0.2608280
H	6.1717700	2.2688930	1.8523270	H	1.4965950	2.3158410	1.6409060
H	6.3194450	1.0615880	0.5629920	C	2.2286050	3.1834660	-1.5754310
C	0.9913570	2.3299760	2.8323510	H	0.7418380	3.5300900	-3.1120340
H	0.1407910	1.6385890	2.7739130	H	3.4345740	2.7831430	0.1472600
H	0.5806470	3.3442240	2.7317750	C	3.3812500	3.5154960	-2.4697060
H	1.4386330	2.2454060	3.8279240	H	4.3127870	3.6208550	-1.9022080
N	0.2395880	2.1911600	0.0817010	H	3.5411120	2.7266480	-3.2187540
N	-1.8350810	1.8369300	-0.2688020	H	3.2131850	4.4476530	-3.0237750
Ni	-0.4190200	-0.5950160	0.7932150	C	1.2476310	-1.1521840	-0.0041180
C	0.4940590	4.6738050	-0.2829270	C	1.3562260	-3.4279200	0.2251750
H	0.9871950	4.8739830	0.6769840	C	2.6237390	-2.9515070	0.3435320
H	1.2854680	4.6141400	-1.0418200	C	-0.8797880	-2.3659840	-0.1735770
H	-0.1349560	5.5366420	-0.5232840	C	-1.3790680	-2.6532710	-1.4508920
C	-2.7476230	4.1332090	-0.7950160	C	-2.7590950	-2.7135200	-1.6136710
H	-3.2106450	3.8922740	-1.7613150	H	-3.1674890	-2.9268910	-2.6023840
H	-3.5443400	4.0969660	-0.0405010	C	-3.6329950	-2.4860250	-0.5486240
H	-2.3841570	5.1639930	-0.8487530	C	-3.0983610	-2.1796030	0.7005730
INTq8				H	-3.7706720	-1.9702130	1.5341430
C	-7.3597200	1.0823600	-0.1738690	C	-1.7202650	-2.1135490	0.9148280
C	-6.2478890	0.7810950	-0.9210580	C	-0.4499580	-2.8301430	-2.6120160
C	-4.9532980	1.0855000	-0.4355010	H	0.3281430	-3.5788360	-2.4150810
C	-4.8274140	1.7213010	0.8324450	H	0.0732750	-1.8900170	-2.8368580
C	-5.9914440	2.0166160	1.5833450	H	-0.9973060	-3.1338590	-3.5100660
C	-7.2322610	1.7015730	1.0906590	C	-5.1130300	-2.5719850	-0.7598260
H	-8.3506650	0.8458000	-0.5551600	H	-5.6681180	-2.0831520	0.0483710
H	-6.3233930	0.3088570	-1.8983870	H	-5.4496200	-3.6162780	-0.8072180
C	-3.5275280	2.0406250	1.2722080	H	-5.4024150	-2.0966590	-1.7048360
H	-5.8789810	2.5002270	2.5527700	C	-1.1710400	-1.7183140	2.2506350
H	-8.1242330	1.9314200	1.6687790	H	-0.2876580	-2.3064800	2.5311360
C	-2.4383160	1.7561700	0.4800120	H	-1.9266600	-1.8366270	3.0343910
C	-2.6805260	1.0761720	-0.7463940	H	-0.8601530	-0.6619440	2.2440980
H	-3.3740010	2.5233340	2.2366520	C	3.6199610	-0.6457290	0.3280750
H	-1.8286910	0.7635360	-1.3573500	C	3.9010000	-0.1224180	1.5934770
N	-3.8717180	0.7491440	-1.1916440	C	4.9649650	0.7734810	1.7086890
C	-1.0845130	2.1340570	1.0009490	H	5.1996330	1.1904490	2.6888200
O	-0.9151240	2.1636750	2.2217130	C	5.7280740	1.1492380	0.6040410
C	0.0028840	2.4801650	0.0632020	C	5.3999070	0.6208770	-0.6468700
C	-0.1726650	2.8667080	-1.2999870	H	5.9789750	0.9201850	-1.5224430
C	1.3418600	2.4310040	0.5687540	C	4.3480960	-0.2774580	-0.8089260
				C	3.0460200	-0.4730170	2.7707270
				H	2.9214120	-1.5576360	2.8857730

H	2.0344780	-0.0567440	2.6466390	C	2.1488190	2.6099110	0.4330950
H	3.4670630	-0.0757990	3.6997930	C	1.1920480	4.3797650	-1.4716410
C	6.8596990	2.1224820	0.7395330	H	-0.4720820	3.0466680	-1.6869680
H	7.7888820	1.7207270	0.3170690	C	2.8775370	3.7451250	0.1135590
H	7.0501780	2.3774450	1.7872110	H	2.5068260	1.9343290	1.2118210
H	6.6471820	3.0575790	0.2046250	C	2.4083070	4.6518060	-0.8464170
C	3.9649710	-0.7901740	-2.1614380	H	0.8053260	5.0822910	-2.2106650
H	2.9743480	-0.4106800	-2.4479090	H	3.8220700	3.9480600	0.6215070
H	3.9020270	-1.8854150	-2.1912150	C	3.1853550	5.8930520	-1.1631130
H	4.6840820	-0.4686300	-2.9217870	H	4.2496510	5.6733020	-1.3130450
N	2.5313810	-1.5632880	0.1937390	H	2.8122220	6.3822130	-2.0694240
N	0.5380970	-2.3125390	0.0077470	H	3.1255140	6.6251500	-0.3468880
Ni	0.6740530	0.6308620	-0.0477820	C	0.9074930	-1.4840540	-0.2493940
C	3.9158150	-3.6332340	0.5901610	C	0.6701990	-3.7387810	0.0246980
H	4.6344470	-3.4471080	-0.2186210	C	1.9928210	-3.4523410	0.1686190
H	4.3851340	-3.2888320	1.5207850	C	-1.3858090	-2.3398850	-0.3455790
H	3.7709860	-4.7151600	0.6668530	C	-1.9885300	-2.4087510	-1.6073760
C	0.8078360	-4.8012410	0.3131970	C	-3.3624450	-2.1967590	-1.6837320
H	0.0684220	-4.8866410	1.1202930	H	-3.8488280	-2.2337900	-2.6591030
H	0.3046500	-5.1040310	-0.6146660	C	-4.1268330	-1.9197830	-0.5491060
H	1.6066730	-5.5221970	0.5120810	C	-3.4852480	-1.8394010	0.6852930
TSq8_9				H	-4.0684880	-1.6003070	1.5759610
C	-6.6910620	1.9726800	0.1407310	C	-2.1125890	-2.0498280	0.8141640
C	-5.6891330	1.7493390	-0.7720550	C	-1.1702720	-2.6491620	-2.8381190
C	-4.3471490	1.6139400	-0.3455980	H	-0.5886950	-3.5780190	-2.7764480
C	-4.0484250	1.7370090	1.0425130	H	-0.4484180	-1.8360100	-2.9963000
C	-5.1032080	1.9526830	1.9617930	H	-1.8072350	-2.7087350	-3.7262990
C	-6.3983110	2.0662160	1.5202140	C	-5.6073450	-1.7231110	-0.6601600
H	-7.7205480	2.0746690	-0.1957170	H	-6.0079220	-1.1781730	0.2024450
H	-5.8892790	1.6657270	-1.8383530	H	-6.1317860	-2.6868150	-0.7140540
C	-2.6953540	1.6342860	1.4311150	H	-5.8692530	-1.1632430	-1.5657060
H	-4.8639000	2.0349590	3.0212050	C	-1.4396570	-1.9253040	2.1464000
H	-7.2038690	2.2355670	2.2309810	H	-0.7885670	-2.7823840	2.3625880
C	-1.7267210	1.4181070	0.4801500	H	-2.1812200	-1.8532620	2.9489860
C	-2.1481620	1.2545440	-0.8658890	H	-0.8079330	-1.0258780	2.1954180
H	-2.4056920	1.7278900	2.4779880	C	3.2987820	-1.2939280	0.1794920
H	-1.3879910	1.0165590	-1.6186820	C	3.5779790	-0.7980900	1.4574030
N	-3.3883870	1.3519500	-1.2793170	C	4.7090630	0.0054710	1.6093150
C	-0.2908930	1.2696700	0.8914250	H	4.9410220	0.4028020	2.5982400
O	0.0189860	1.3044550	2.0807540	C	5.5273780	0.3337330	0.5302210
C	0.9517820	2.3021700	-0.2359380	C	5.2051710	-0.1713700	-0.7312070
C	0.4705320	3.2251610	-1.1704920	H	5.8326440	0.0844240	-1.5862490
				C	4.0940980	-0.9865590	-0.9312530
				C	2.6547470	-1.0463290	2.6103660

H	2.3034030	-2.0850940	2.6527750	C	0.9948370	3.1281500	-1.4509570
H	1.7625900	-0.4048270	2.5328640	C	2.3737290	2.6603600	0.4474630
H	3.1474100	-0.8150240	3.5606200	C	1.7164410	4.2998960	-1.6814320
C	6.7102760	1.2366330	0.7034720	H	0.1697170	2.8876960	-2.1240480
H	7.6171240	0.8047500	0.2629680	C	3.0986860	3.8236050	0.2149320
H	6.9123600	1.4390950	1.7605290	H	2.6376400	2.0337480	1.3033860
H	6.5443380	2.2014370	0.2068140	C	2.7817820	4.6637750	-0.8578680
C	3.7334820	-1.4887090	-2.2951020	H	1.4474470	4.9466830	-2.5182770
H	2.7834140	-1.0558350	-2.6377080	H	3.9229800	4.0966470	0.8771570
H	3.6067170	-2.5788000	-2.3140750	C	3.5546350	5.9266440	-1.0948920
H	4.5045610	-1.2250650	-3.0256160	H	4.6347670	5.7376970	-1.1424900
N	2.1100560	-2.0720070	-0.0074110	H	3.2589400	6.4084920	-2.0335260
N	0.0308730	-2.5208130	-0.2342200	H	3.3977470	6.6551320	-0.2882550
Ni	0.7376730	0.3976200	-0.3495500	C	0.7725870	-1.4629980	-0.1447620
C	3.1625550	-4.3115810	0.4654010	C	0.4462050	-3.7185350	-0.0307630
H	3.9039270	-4.2903280	-0.3440190	C	1.7761730	-3.4939380	0.1514410
H	3.6764250	-3.9886740	1.3799600	C	-1.5374840	-2.2354320	-0.4349320
H	2.8500470	-5.3509450	0.6044500	C	-2.0064610	-2.1832780	-1.7525650
C	-0.0733110	-5.0169350	0.1157820	C	-3.3595360	-1.9209000	-1.9511130
H	-0.8520930	-4.9748560	0.8879440	H	-3.7419310	-1.8618660	-2.9707650
H	-0.5713720	-5.2728020	-0.8282510	C	-4.2301260	-1.7083270	-0.8816810
H	0.6052740	-5.8377880	0.3671930	C	-3.7220360	-1.7673060	0.4151290
INTq9				H	-4.3901600	-1.5836690	1.2580390
C	-6.6299510	2.2347880	0.2835590	C	-2.3766340	-2.0348550	0.6660900
C	-5.6148960	2.0795960	-0.6286790	C	-1.0760820	-2.3397390	-2.9160640
C	-4.2962950	1.8061540	-0.1953490	H	-0.3389050	-3.1375290	-2.7622090
C	-4.0356290	1.7165990	1.2030720	H	-0.5082930	-1.4153020	-3.0914420
C	-5.1031660	1.8722370	2.1202100	H	-1.6317920	-2.5604660	-3.8330860
C	-6.3753750	2.1225930	1.6691990	C	-5.6792390	-1.4219480	-1.1266070
H	-7.6408990	2.4452010	-0.0585260	H	-6.1411390	-0.9198020	-0.2683600
H	-5.7863080	2.1582770	-1.7000800	H	-6.2429700	-2.3464180	-1.3105200
C	-2.7060260	1.4687380	1.6045340	H	-5.8127530	-0.7825010	-2.0070670
H	-4.8916410	1.7966170	3.1859810	C	-1.8443350	-2.0559990	2.0662780
H	-7.1910260	2.2443800	2.3780730	H	-1.3342970	-2.9985700	2.3046190
C	-1.7273930	1.3139480	0.6506110	H	-2.6550460	-1.9241690	2.7906910
C	-2.1057400	1.3978100	-0.7132680	H	-1.1140510	-1.2519960	2.2341540
H	-2.4454310	1.3982250	2.6609510	C	3.1813680	-1.4054150	0.2468520
H	-1.3270530	1.2553830	-1.4697540	C	3.5519210	-0.9923180	1.5300190
N	-3.3234350	1.6354510	-1.1356290	C	4.7491290	-0.2888540	1.6625060
C	-0.3190430	1.0174480	1.0585790	H	5.0572630	0.0414820	2.6550250
O	0.0149980	1.0302700	2.2307410	C	5.5462140	0.0194820	0.5612860
C	1.3211360	2.2640070	-0.3958100	C	5.1308390	-0.3983800	-0.7046400
				H	5.7400050	-0.1545450	-1.5760610
				C	3.9470190	-1.1075190	-0.8871650

C	2.6596920	-1.2321280	2.7077930	C	-0.4761400	1.5676830	0.3973200
H	2.2439180	-2.2475700	2.7196630	C	0.2332980	2.0858670	1.4883550
H	1.8064680	-0.5365490	2.6871550	C	-1.6982910	2.1900960	0.1003460
H	3.1988040	-1.0716310	3.6470640	C	-0.2620690	3.1376320	2.2620600
C	6.8148900	0.8001130	0.7189770	H	1.2181580	1.6806080	1.7373610
H	7.6514000	0.3171810	0.1994920	C	-2.1935820	3.2468070	0.8610590
H	7.0909380	0.9146810	1.7723820	H	-2.2957490	1.8393220	-0.7462400
H	6.7125890	1.8059430	0.2919230	C	-1.4863410	3.7353280	1.9639510
C	3.4780990	-1.4996480	-2.2542690	H	0.3179340	3.5092770	3.1089040
H	2.6289470	-0.8754580	-2.5687960	H	-3.1536480	3.7003450	0.6019730
H	3.1328450	-2.5405920	-2.2939260	C	-2.0246490	4.8729500	2.7809200
H	4.2733040	-1.3723080	-2.9953930	H	-1.3847400	5.0846520	3.6452110
N	1.9447850	-2.1101550	0.0797900	H	-2.0973320	5.7982790	2.1935480
N	-0.1419870	-2.4612920	-0.2081130	H	-3.0332570	4.6620760	3.1600740
Ni	0.7996400	0.4601700	-0.2531390	C	-0.5075550	-1.3490240	0.1241540
C	2.9129360	-4.4136740	0.3852330	C	-1.8348890	-2.9554260	1.0573640
H	3.6815280	-4.3115380	-0.3918620	C	-0.5487600	-3.2889900	1.3320890
H	3.4017250	-4.2179980	1.3483230	C	-2.9548670	-1.0791170	-0.1419550
H	2.5720810	-5.4532080	0.3867230	C	-3.3862560	-1.3103540	-1.4545960
C	-0.3419700	-4.9721090	-0.0810840	C	-4.5296990	-0.6431120	-1.8881920
H	-1.1402510	-4.9835890	0.6714680	H	-4.8818110	-0.8075890	-2.9076380
H	-0.8212130	-5.1101500	-1.0590090	C	-5.2429630	0.2152360	-1.0480930
H	0.3032690	-5.8368680	0.1016410	C	-4.7885060	0.4016600	0.2557440
INTq10				H	-5.3296810	1.0769740	0.9196130
C	3.2731210	4.8432360	-0.1707540	C	-3.6438520	-0.2362200	0.7354550
C	3.8155070	3.5807340	-0.3051330	C	-2.6564150	-2.2632420	-2.3500020
C	3.0783610	2.5518040	-0.9132810	H	-2.5774180	-3.2603870	-1.8953500
C	1.7696010	2.8148970	-1.3816000	H	-1.6295070	-1.9372970	-2.5613310
C	1.2396860	4.1071880	-1.2459890	H	-3.1763340	-2.3730090	-3.3070120
C	1.9810120	5.1079990	-0.6487170	C	-6.4801840	0.9011940	-1.5422420
H	3.8477370	5.6354710	0.3035880	H	-6.8425760	1.6458060	-0.8257020
H	4.8172610	3.3450470	0.0479430	H	-7.2926730	0.1831450	-1.7124240
C	1.0188120	1.7307300	-1.9552950	H	-6.3035330	1.4102850	-2.4972940
H	0.2261270	4.3000390	-1.5955590	C	-3.1552590	0.0044480	2.1301290
H	1.5568140	6.1036370	-0.5408950	H	-3.2080730	-0.9007590	2.7497350
C	1.6775990	0.4957730	-2.1622740	H	-3.7503610	0.7813240	2.6210540
C	3.0002830	0.3466560	-1.5795800	H	-2.1100150	0.3416310	2.1243270
H	0.0875340	1.9598100	-2.4782070	C	1.6746450	-2.2931730	0.7472540
H	3.4686830	-0.6412090	-1.6258220	C	2.3464580	-1.5502690	1.7276590
N	3.6670770	1.3033720	-1.0208410	C	3.7358400	-1.4895880	1.6567070
C	0.8634050	-0.6910920	-2.3348040	H	4.2762200	-0.8980620	2.3965870
O	0.6761130	-1.5735250	-3.1249550	C	4.4510300	-2.1620270	0.6639830
				C	3.7481300	-2.9438860	-0.2514000
				H	4.2966860	-3.4956620	-1.0159050

C	2.3543480	-3.0306050	-0.2284730	O	-0.3314820	1.3379950	-3.2268840
C	1.6009380	-0.8939610	2.8485970	C	-0.7311140	-0.8495890	1.0198930
H	1.2347750	-1.6410980	3.5669700	C	-1.4145600	-0.3233890	2.1255030
H	0.7261110	-0.3332670	2.5004390	C	-0.6060090	-2.2501060	0.9911420
H	2.2494230	-0.2038200	3.3980880	C	-1.9046610	-1.1322680	3.1534040
C	5.9386720	-2.0162990	0.5746820	H	-1.5769880	0.7566450	2.1989500
H	6.2059880	-1.0187680	0.2020960	C	-1.0909330	-3.0653570	2.0105640
H	6.3785400	-2.7530900	-0.1056810	H	-0.0921470	-2.7293010	0.1520320
H	6.4164520	-2.1292020	1.5551340	C	-1.7434410	-2.5171330	3.1190700
C	1.6247410	-3.9074170	-1.1995830	H	-2.4242280	-0.6806880	4.0009470
H	0.7067920	-3.4432720	-1.5754830	H	-0.9555070	-4.1485720	1.9538050
H	1.3430560	-4.8625320	-0.7343880	C	-2.2657720	-3.3965330	4.2166000
H	2.2553960	-4.1408160	-2.0636550	H	-2.5876490	-2.8089590	5.0843000
N	0.2440570	-2.2979830	0.7453420	H	-3.1291970	-3.9905970	3.8873190
N	-1.7851710	-1.7595460	0.3271490	H	-1.5065680	-4.1098860	4.5627740
Ni	0.2170130	0.1652990	-0.7642330	C	1.6325510	0.4898060	-0.1011980
C	0.0360180	-4.4213800	2.0872550	C	3.8854530	0.3812890	0.2246890
H	0.6585020	-5.0656090	1.4527300	C	3.5058230	1.6635020	0.4573180
H	0.6716860	-4.0704830	2.9102090	C	2.6689330	-1.7230360	-0.4001260
H	-0.7557140	-5.0409760	2.5185480	C	2.6573450	-2.1332800	-1.7387460
C	-3.1137190	-3.6353050	1.3677000	C	2.5874510	-3.5004810	-1.9976370
H	-3.7682810	-3.0222720	2.0000110	H	2.5759170	-3.8406040	-3.0341840
H	-3.6750350	-3.8674430	0.4533000	C	2.5365490	-4.4420650	-0.9675120
H	-2.9262110	-4.5767580	1.8928510	C	2.5541350	-3.9904620	0.3507960
TSq10_11				H	2.4969750	-4.7139890	1.1648750
C	-6.5680100	-1.1597030	-0.5839130	C	2.6188160	-2.6317090	0.6622310
C	-5.9095930	0.0218920	-0.3468550	C	2.7056560	-1.1355200	-2.8548490
C	-4.5657880	0.1847390	-0.7531020	H	3.5074040	-0.3990370	-2.7139080
C	-3.9122510	-0.8966500	-1.4157450	H	1.7702250	-0.5639900	-2.9247220
C	-4.6157020	-2.1034570	-1.6442480	H	2.8660110	-1.6322560	-3.8170310
C	-5.9184430	-2.2321590	-1.2350240	C	2.4821890	-5.9054250	-1.2852250
H	-7.6016200	-1.2763400	-0.2656630	H	2.2355730	-6.5022040	-0.4008470
H	-6.3904230	0.8576370	0.1559150	H	3.4461290	-6.2653810	-1.6678310
C	-2.5683500	-0.7085710	-1.7998230	H	1.7337990	-6.1200600	-2.0571750
H	-4.1019480	-2.9220390	-2.1461930	C	2.5798060	-2.1669360	2.0848790
H	-6.4572060	-3.1604280	-1.4097500	H	3.4799130	-1.6061800	2.3686210
C	-1.9488340	0.4894140	-1.5226070	H	2.4869180	-3.0179400	2.7675510
C	-2.6955480	1.4998790	-0.8567400	H	1.7162130	-1.5096980	2.2560870
H	-2.0237190	-1.5203240	-2.2861480	C	1.2828310	2.8581970	0.3883020
H	-2.2001220	2.4494680	-0.6285210	C	0.6478970	3.0824890	1.6173700
N	-3.9459660	1.3720630	-0.4885700	C	-0.2414600	4.1500530	1.7021630
C	-0.4643140	0.8906060	-2.1296710	H	-0.7530010	4.3361620	2.6475700
				C	-0.4978300	4.9816270	0.6089180
				C	0.1805960	4.7432690	-0.5854000

H	0.0003170	5.3934880	-1.4418770	C	-0.8033870	0.8309360	-2.0346180
C	1.0859160	3.6887480	-0.7192240	O	-1.2317200	1.1453680	-3.0532340
C	0.9301900	2.2065860	2.7982700	C	-0.2262230	-1.0548770	1.0616390
H	1.9923040	2.2336390	3.0759690	C	-0.6315040	-0.7147390	2.3554210
H	0.6797530	1.1574630	2.5944540	C	0.2719740	-2.3506830	0.8709090
H	0.3478440	2.5254420	3.6688770	C	-0.5078220	-1.6117040	3.4175470
C	-1.4871330	6.1005770	0.7287960	H	-1.0725090	0.2647360	2.5493640
H	-2.5064020	5.7145860	0.8565100	C	0.3838830	-3.2500920	1.9278490
H	-1.4842920	6.7402240	-0.1598780	H	0.5839960	-2.6739480	-0.1246610
H	-1.2746200	6.7312630	1.6004750	C	0.0034910	-2.8947430	3.2249110
C	1.8239100	3.4601570	-2.0021240	H	-0.8271960	-1.3116070	4.4169960
H	1.7980440	2.4077150	-2.3076040	H	0.7836450	-4.2502320	1.7457700
H	2.8799720	3.7517080	-1.9133190	C	0.1202420	-3.8714690	4.3574720
H	1.3869100	4.0515680	-2.8127680	H	0.0150610	-3.3752080	5.3291610
N	2.1214430	1.7056980	0.2538500	H	-0.6533890	-4.6495590	4.3059080
N	2.7172810	-0.3223170	-0.1079240	H	1.0884570	-4.3882270	4.3500840
Ni	-0.1576930	0.1713650	-0.5305850	C	1.4402980	0.8777720	-0.2009790
C	4.2806930	2.8679900	0.8350150	C	3.6512690	1.4404700	-0.1170230
H	4.1797630	3.6643940	0.0863750	C	2.9397580	2.5656260	0.1530130
H	3.9496260	3.2841610	1.7949820	C	3.0564810	-0.9333720	-0.6401370
H	5.3440060	2.6269240	0.9253360	C	3.0232540	-1.3422140	-1.9789020
C	5.2161630	-0.2688860	0.2556230	C	3.3593300	-2.6638750	-2.2645990
H	5.2705820	-1.0654120	1.0087060	H	3.3365070	-3.0014570	-3.3016610
H	5.4685770	-0.7233560	-0.7109780	C	3.7287610	-3.5608300	-1.2604310
H	5.9918600	0.4658370	0.4912660	C	3.7497010	-3.1117730	0.0587960
INTq11				H	4.0161320	-3.8062670	0.8564480
C	-6.8143070	-2.3843670	-0.8059400	C	3.4165950	-1.8002500	0.3964910
C	-6.2793670	-1.2503010	-0.2464990	C	2.6233560	-0.3981480	-3.0710240
C	-4.8885130	-0.9992260	-0.3173340	H	3.1270170	0.5731230	-2.9827200
C	-4.0462250	-1.9393900	-0.9761860	H	1.5434320	-0.1980860	-3.0500560
C	-4.6261400	-3.0992940	-1.5441760	H	2.8613570	-0.8153200	-4.0545350
C	-5.9794020	-3.3171620	-1.4613630	C	4.1046910	-4.9696440	-1.6046590
H	-7.8846840	-2.5700570	-0.7472460	H	4.1167810	-5.6122810	-0.7181570
H	-6.8967890	-0.5139550	0.2641520	H	5.1034100	-5.0159130	-2.0579200
C	-2.6593620	-1.6556420	-1.0305620	H	3.4062610	-5.4052780	-2.3285980
H	-3.9765990	-3.8156680	-2.0469680	C	3.4039360	-1.3547180	1.8255800
H	-6.4150600	-4.2123600	-1.9006620	H	4.1423690	-0.5669230	2.0237860
C	-2.1584320	-0.5125300	-0.4561550	H	3.6257050	-2.1929370	2.4939100
C	-3.1040520	0.3533610	0.1633810	H	2.4187230	-0.9564430	2.1026120
H	-2.0029620	-2.3718150	-1.5313030	C	0.4717200	3.0636550	0.2894660
H	-2.7449510	1.2855450	0.6175040	C	-0.0877190	3.1681260	1.5690340
N	-4.3993780	0.1413010	0.2444560	C	-1.2537450	3.9191150	1.7095080
				H	-1.7127120	3.9995920	2.6955510
				C	-1.8500450	4.5610070	0.6227270

C	-1.2271120	4.4796870	-0.6229130	N	-4.1778500	-0.0076760	0.1211260
H	-1.6656150	5.0005550	-1.4747440	C	-0.6581830	0.2021790	-2.3998280
C	-0.0573410	3.7456520	-0.8129410	O	-0.9761850	0.2466200	-3.5066890
C	0.5675640	2.5278010	2.7541970	C	-0.4085480	-1.1108750	0.9518300
H	1.4702490	3.0785600	3.0524790	C	-0.7060000	-0.6906410	2.2566030
H	0.8731360	1.4941950	2.5529240	C	0.3127280	-2.3143980	0.8176970
H	-0.1060920	2.5196450	3.6171890	C	-0.2926290	-1.4229740	3.3662080
C	-3.1437080	5.2972360	0.7862650	H	-1.2893660	0.2176720	2.4104880
H	-3.9955290	4.6199080	0.6423090	C	0.7245180	-3.0371110	1.9282860
H	-3.2457600	6.1057790	0.0542230	H	0.5667190	-2.6855850	-0.1779830
H	-3.2409030	5.7283300	1.7887920	C	0.4271450	-2.6105980	3.2279280
C	0.6296850	3.7364110	-2.1448720	H	-0.5411610	-1.0652340	4.3664090
H	1.0558610	2.7587140	-2.3973400	H	1.2990660	-3.9548170	1.7871980
H	1.4600900	4.4562870	-2.1583920	C	0.8610540	-3.4134320	4.4168890
H	-0.0595180	4.0240690	-2.9453010	H	0.6926350	-2.8698860	5.3534550
N	1.5935050	2.1946740	0.0963060	H	0.3151090	-4.3638390	4.4883490
N	2.7092430	0.4198350	-0.3203870	H	1.9284810	-3.6671430	4.3663820
Ni	-0.3344770	0.0979950	-0.4623310	C	1.3520430	1.0172580	-0.3208700
C	3.3605430	3.9561310	0.4406750	C	3.4594770	1.8870480	-0.1320670
H	2.9596020	4.6613650	-0.2988010	C	2.5837210	2.9028400	0.0849650
H	3.0164690	4.2932180	1.4267690	C	3.1990830	-0.5656720	-0.6185300
H	4.4511110	4.0392310	0.4239360	C	3.3431700	-1.0153260	-1.9333460
C	5.1092410	1.2095160	-0.2458960	C	3.8185970	-2.3136570	-2.1293150
H	5.4805870	0.4705130	0.4749930	H	3.9365120	-2.6824060	-3.1488620
H	5.3746280	0.8423450	-1.2456070	C	4.1519810	-3.1418490	-1.0600340
H	5.6569990	2.1416050	-0.0777000	C	4.0053550	-2.6487560	0.2385340
TSq11_12				H	4.2616900	-3.2870090	1.0858740
C	-6.6731190	-2.5039950	-0.8161640	C	3.5269430	-1.3649380	0.4843830
C	-6.1066880	-1.3308670	-0.3779120	C	2.9867770	-0.1484820	-3.1012470
C	-4.7026340	-1.1867340	-0.3229360	H	3.3123410	0.8897430	-2.9626870
C	-3.8722390	-2.2717880	-0.7279360	H	1.9005040	-0.1186430	-3.2588440
C	-4.4847720	-3.4697350	-1.1726890	H	3.4396380	-0.5292210	-4.0224140
C	-5.8527790	-3.5820840	-1.2159810	C	4.6529330	-4.5358550	-1.2853620
H	-7.7552360	-2.6070160	-0.8566160	H	5.6096210	-4.7049250	-0.7761200
H	-6.7120470	-0.4829910	-0.0631450	H	4.7975900	-4.7465550	-2.3500950
C	-2.4729500	-2.0936700	-0.6774950	H	3.9486780	-5.2796750	-0.8916870
H	-3.8480090	-4.2991670	-1.4795880	C	3.3307470	-0.8596400	1.8791810
H	-6.3109700	-4.5067930	-1.5610300	H	3.8751260	0.0766610	2.0610280
C	-1.9320070	-0.9036100	-0.2286760	H	3.6711530	-1.5970990	2.6138160
C	-2.8730580	0.1019040	0.1725550	H	2.2677460	-0.6587900	2.0733980
H	-1.8287010	-2.9196020	-0.9853660	C	0.0621770	3.0056860	0.2136670
H	-2.4860980	1.0553630	0.5514640	C	-0.4114830	3.0405580	1.5323580
				C	-1.6855430	3.5585260	1.7532660
				H	-2.0793640	3.5744790	2.7703160

C	-2.4758620	4.0350140	0.7048700	H	-1.7247370	-0.4023270	2.1250220
C	-1.9472180	4.0285630	-0.5846440	N	-3.3304260	-0.8704540	0.9475970
H	-2.5480750	4.4119640	-1.4099690	C	-0.5488290	-1.3539100	-2.3236780
C	-0.6755390	3.5224580	-0.8565750	O	-0.8403920	-1.9965470	-3.2497640
C	0.4281440	2.5385180	2.6671310	C	0.0656430	-2.3671460	1.5108030
H	1.2945080	3.1906300	2.8441630	C	0.3645870	-2.0915280	2.8519470
H	0.8204270	1.5317030	2.4726240	C	1.1002810	-2.8286750	0.6877440
H	-0.1514640	2.5014160	3.5956680	C	1.6454810	-2.2905730	3.3502180
C	-3.8787580	4.4946040	0.9553710	H	-0.4246060	-1.7457960	3.5187580
H	-4.5711030	3.6424930	0.9284270	C	2.3801430	-3.0236280	1.1925540
H	-4.2136130	5.2089920	0.1954790	H	0.9014540	-3.0174290	-0.3657180
H	-3.9838770	4.9661220	1.9389760	C	2.6754240	-2.7655210	2.5313110
C	-0.1248060	3.5542530	-2.2494550	H	1.8544170	-2.0816720	4.3997320
H	0.5177170	2.6929000	-2.4630630	H	3.1672890	-3.3849930	0.5308700
H	0.4806110	4.4561130	-2.4144590	C	4.0530540	-2.9747670	3.0816490
H	-0.9325390	3.5684910	-2.9889040	H	4.4674810	-2.0458000	3.4958420
N	1.3073430	2.3455130	-0.0367460	H	4.0529050	-3.7085460	3.8978440
N	2.6797600	0.7468130	-0.3789840	H	4.7442470	-3.3385100	2.3124800
Ni	-0.2660710	-0.0574820	-0.6728710	C	0.6586210	1.3377700	-0.3663470
C	2.7913290	4.3404070	0.3750870	C	2.0744240	3.1316070	-0.2086210
H	2.4388540	4.9786490	-0.4455890	C	0.8255480	3.5749890	0.0952660
H	2.2519640	4.6524520	1.2784040	C	3.0436350	0.8843720	-0.7353760
H	3.8537300	4.5531750	0.5287760	C	3.4064590	0.6045950	-2.0554880
C	4.9405260	1.8611260	-0.1533860	C	4.4674120	-0.2773370	-2.2654950
H	5.3485740	1.1413140	0.5675020	H	4.7588420	-0.5166810	-3.2888000
H	5.3360130	1.5864320	-1.1398540	C	5.1545780	-0.8626720	-1.2036100
H	5.3395150	2.8480830	0.1000310	C	4.7694100	-0.5441660	0.0998140
INTq12				H	5.3009860	-0.9951200	0.9402730
C	-5.6739790	-2.2532340	-1.4802800	C	3.7106330	0.3216270	0.3590920
C	-5.1304280	-1.4361830	-0.5200150	C	2.6510610	1.2044560	-3.1988720
C	-3.8405460	-1.7007440	-0.0023270	H	2.5767350	2.2963270	-3.1132190
C	-3.1160890	-2.8233480	-0.4917690	H	1.6202790	0.8204620	-3.2213230
C	-3.7009940	-3.6483290	-1.4821650	H	3.1280400	0.9675040	-4.1551330
C	-4.9541820	-3.3686190	-1.9659530	C	6.2854700	-1.8171920	-1.4388570
H	-6.6648740	-2.0431170	-1.8769570	H	7.2367520	-1.4122960	-1.0704020
H	-5.6595480	-0.5657700	-0.1361660	H	6.4100580	-2.0437030	-2.5029100
C	-1.8273190	-3.0514690	0.0326330	H	6.1195730	-2.7655750	-0.9110930
H	-3.1319630	-4.4978200	-1.8579980	C	3.2623990	0.5923570	1.7612310
H	-5.3969940	-4.0025310	-2.7306850	H	3.0148330	1.6474220	1.9326370
C	-1.2953740	-2.1935480	0.9713530	H	4.0358310	0.3049540	2.4821550
C	-2.1209910	-1.1111110	1.3906680	H	2.3596740	0.0083200	1.9935990
H	-1.2547950	-3.9096800	-0.3214040	C	-1.4009560	2.4569360	0.3603080
				C	-1.7278680	2.3496280	1.7198880
				C	-3.0743260	2.3313770	2.0672650

H	-3.3496730	2.2291950	3.1182680	H	-0.8527030	-2.5438670	-0.3504050
C	-4.0792790	2.3923230	1.1003680	H	2.6433740	-1.1929670	1.8302550
C	-3.7140760	2.4979440	-0.2384940	N	0.9024470	-1.2228710	2.8745020
H	-4.4907360	2.5356240	-1.0034100	C	1.8600390	-2.4910970	-0.5445250
C	-2.3766170	2.5306190	-0.6367400	O	1.3834410	-3.3143910	-1.3194350
C	-0.6590510	2.1985110	2.7599690	C	3.3150150	-2.1363560	-0.6504490
H	-0.0090610	3.0809200	2.8299660	C	3.8523890	-0.8823960	-0.3371840
H	-0.0023970	1.3461690	2.5322860	C	4.1770990	-3.1208150	-1.1428980
H	-1.0998040	2.0324080	3.7487460	C	5.2075600	-0.6295560	-0.5077250
C	-5.5162220	2.2826360	1.5060010	H	3.2029060	-0.0759360	0.0022800
H	-5.7272280	1.2745950	1.8880400	C	5.5326450	-2.8702040	-1.2920610
H	-6.1921250	2.4710090	0.6647970	H	3.7570460	-4.0876830	-1.4106630
H	-5.7691830	2.9864490	2.3084500	C	6.0730920	-1.6195350	-0.9772770
C	-2.0017040	2.5925410	-2.0840690	H	5.6000020	0.3632000	-0.2819350
H	-1.5660610	1.6343680	-2.4075910	H	6.1905200	-3.6531940	-1.6687150
H	-1.2472880	3.3640720	-2.2858310	C	7.5398360	-1.3608930	-1.1322070
H	-2.8774250	2.7981620	-2.7079330	H	7.7671490	-0.2898370	-1.1039810
N	-0.0154310	2.4615370	0.0015780	H	8.1137430	-1.8397330	-0.3279860
N	1.9460850	1.7655460	-0.4780680	H	7.9219920	-1.7634280	-2.0777700
Ni	-0.0552210	-0.2987860	-1.0681440	C	-1.1330860	1.1045900	-0.3967150
C	0.3193130	4.9250760	0.4365370	C	-1.7406020	3.3101270	-0.2939150
H	-0.4448200	5.2629330	-0.2753590	C	-2.8156340	2.6128080	-0.7462250
H	-0.1376460	4.9552280	1.4341600	C	0.6015110	2.6148590	0.3819230
H	1.1341860	5.6554450	0.4212940	C	1.5877070	3.0472150	-0.5101580
C	3.3752410	3.8356410	-0.2967210	C	2.9052660	3.1018790	-0.0478070
H	4.1052630	3.4419980	0.4223680	H	3.6906680	3.4121180	-0.7384520
H	3.8220500	3.7347040	-1.2942460	C	3.2407960	2.7539160	1.2585150
H	3.2478840	4.9032470	-0.0934760	C	2.2183970	2.3746120	2.1328930
INTq13				H	2.4622250	2.1056920	3.1616680
C	-2.4582510	-1.8627030	4.1951230	C	0.8918570	2.3016710	1.7187230
C	-1.1310710	-1.4853740	4.1173180	C	1.2667030	3.4388730	-1.9202220
C	-0.4382700	-1.5598800	2.8965100	H	1.0457820	4.5128860	-1.9883230
C	-1.1224880	-1.9856390	1.7337900	H	0.3968700	2.9024020	-2.3160370
C	-2.4669270	-2.3801890	1.8359530	H	2.1162800	3.2443660	-2.5827730
C	-3.1247060	-2.3259680	3.0496190	C	4.6665310	2.7536310	1.7200920
H	-2.9836060	-1.8128460	5.1463930	H	5.3357550	3.1901160	0.9706200
H	-0.5805440	-1.1403690	4.9907920	H	5.0126680	1.7306280	1.9221430
C	-0.3942380	-2.0258700	0.4965370	H	4.7894070	3.3176250	2.6525690
H	-2.9827480	-2.7161470	0.9361880	C	-0.1941470	1.8958970	2.6664080
H	-4.1675040	-2.6330880	3.1139750	H	-0.9886620	2.6529320	2.7173710
C	1.0249640	-1.8806290	0.5192670	H	0.2030940	1.7478720	3.6756110
C	1.5722260	-1.3992380	1.7744140	H	-0.6688710	0.9573170	2.3549020
				C	-3.3066820	0.1737560	-1.0568910
				C	-4.1959390	-0.2267600	-0.0512790

C	-5.0613970	-1.2827600	-0.3305290	H	5.2745140	-3.8716230	-1.9979830
H	-5.7581940	-1.6101810	0.4431080	C	0.2684130	-1.6188710	-0.0528010
C	-5.0412920	-1.9443570	-1.5597280	C	-0.3356650	-1.8168730	-1.3272600
C	-4.1312230	-1.5214390	-2.5280820	H	2.0647000	-2.0051390	1.0550060
H	-4.1038090	-2.0280910	-3.4934300	H	-1.3823370	-1.5310180	-1.4682780
C	-3.2529150	-0.4621510	-2.3005260	N	0.2647770	-2.3176750	-2.3853170
C	-4.1859090	0.4324040	1.2940490	C	-0.6951050	-1.9306590	1.5424550
H	-4.4113660	1.5048240	1.2412110	O	-0.0634660	-2.5906010	2.3575150
H	-3.1987350	0.3358510	1.7691870	C	-2.1487650	-2.1999800	1.2938700
H	-4.9196450	-0.0297320	1.9620550	C	-2.9637410	-1.3001800	0.6046920
C	-5.9559220	-3.1026850	-1.8181010	C	-2.7265080	-3.3546160	1.8311060
H	-6.9224660	-2.9736250	-1.3179440	C	-4.3230100	-1.5467130	0.4586380
H	-5.5229350	-4.0394440	-1.4434420	H	-2.5343720	-0.3879080	0.1839300
H	-6.1428220	-3.2394500	-2.8887820	C	-4.0812640	-3.6021840	1.6734990
C	-2.2728940	-0.0359720	-3.3486040	H	-2.0870860	-4.0431960	2.3794790
H	-1.2518820	-0.3356510	-3.0753540	C	-4.9036780	-2.7007840	0.9869250
H	-2.2576880	1.0534860	-3.4825660	H	-4.9431200	-0.8281280	-0.0774680
H	-2.5068190	-0.4956150	-4.3139750	H	-4.5212370	-4.5072610	2.0932000
N	-2.4230180	1.2659210	-0.7827250	C	-6.3680790	-2.9742940	0.8297820
N	-0.7271130	2.3696700	-0.0927110	H	-6.8747800	-2.1637270	0.2940730
Ni	0.2175600	-0.3062650	-0.4381590	H	-6.5450810	-3.9037170	0.2738160
C	-4.1439630	3.0673600	-1.2209430	H	-6.8602900	-3.0903760	1.8037720
H	-4.2936350	2.8199400	-2.2803600	C	0.3580850	1.4869550	0.0587060
H	-4.9733880	2.6107510	-0.6673890	C	0.3448260	3.4451630	-1.1304700
H	-4.2327680	4.1531920	-1.1184300	C	1.6157900	3.2457270	-0.6951830
C	-1.5415690	4.7560920	-0.0405130	C	-1.7878520	2.1306730	-0.9352570
H	-1.1366440	4.9336280	0.9638410	C	-2.7539870	2.6142740	-0.0433230
H	-0.8425720	5.2085420	-0.7561050	C	-4.0914050	2.3323250	-0.3142810
H	-2.4909040	5.2943810	-0.1181530	H	-4.8552630	2.6934240	0.3755630
C	1.2809450	0.1600700	-1.8054830	C	-4.4744510	1.5972930	-1.4379730
O	1.7854090	0.3508590	-2.8259060	C	-3.4835260	1.1431490	-2.3072170
TSq13_14				H	-3.7663680	0.5628010	-3.1862160
C	3.5521770	-3.6167290	-3.2908990	C	-2.1315480	1.4097630	-2.0854080
C	2.2422010	-3.2156320	-3.3863790	C	-2.3618980	3.4066100	1.1649880
C	1.5637860	-2.7057150	-2.2544120	H	-1.7980950	4.3096080	0.8976070
C	2.2611410	-2.6122640	-1.0148120	H	-1.7172750	2.8259690	1.8359590
C	3.6068840	-3.0514380	-0.9420660	H	-3.2439470	3.7170390	1.7334970
C	4.2405050	-3.5387960	-2.0575370	C	-5.9215930	1.3177810	-1.7115550
H	4.0670240	-4.0052410	-4.1670530	H	-6.3951710	2.1554630	-2.2403380
H	1.6900410	-3.2745440	-4.3219420	H	-6.4866090	1.1669700	-0.7838560
C	1.5707490	-2.0604110	0.0824050	H	-6.0479140	0.4271930	-2.3374070
H	4.1242010	-2.9862590	0.0153250	C	-1.0939220	0.9512880	-3.0638840
				H	-0.7796190	1.7713220	-3.7243650
				H	-1.4804920	0.1495750	-3.7016240

H	-0.1911860	0.5756040	-2.5697160	H	-1.2704770	-3.9474540	4.0927080
C	2.7480700	1.4081280	0.5875190	C	-1.5683620	-1.9263280	-0.0015640
C	3.5614090	0.6388180	-0.2594980	H	-3.9330850	-3.2731550	-0.0596110
C	4.6677700	0.0071070	0.2984870	H	-4.8220480	-4.6984120	1.7638470
H	5.3072050	-0.6003590	-0.3441660	C	-0.3517070	-1.3079770	0.1858770
C	4.9610770	0.1046990	1.6619050	C	0.3323570	-1.6392140	1.3883060
C	4.1288570	0.8751410	2.4676170	H	-2.1438180	-1.7626050	-0.9165570
H	4.3455760	0.9635570	3.5331050	H	1.3296120	-1.2186680	1.5572010
C	3.0182540	1.5487630	1.9507490	N	-0.1224810	-2.4161080	2.3508150
C	3.2300280	0.4786210	-1.7114010	C	0.8419910	-1.5909980	-1.8867660
H	3.2701320	1.4309340	-2.2568300	O	0.1311950	-2.1595040	-2.6912160
H	2.2149750	0.0800900	-1.8412200	C	2.2213270	-2.0664550	-1.5763700
H	3.9218800	-0.2181180	-2.1965950	C	3.0701980	-1.3229850	-0.7567470
C	6.1389340	-0.6256120	2.2311270	C	2.6850220	-3.2649710	-2.1277480
H	7.0537370	-0.4139090	1.6644600	C	4.3592780	-1.7673880	-0.4893620
H	5.9873490	-1.7123900	2.1952360	H	2.7103860	-0.3851420	-0.3257430
H	6.3185430	-0.3535910	3.2764080	C	3.9690260	-3.7069850	-1.8566330
C	2.1867750	2.4175000	2.8452320	H	2.0135710	-3.8317390	-2.7696070
H	1.1917270	2.6132490	2.4333400	C	4.8263660	-2.9657900	-1.0325160
H	2.6728200	3.3896330	3.0061990	H	5.0127560	-1.1784700	0.1549530
H	2.0596390	1.9563360	3.8311470	H	4.3271920	-4.6430760	-2.2855140
N	1.5968250	2.0417680	0.0196160	C	6.2091580	-3.4630200	-0.7447920
N	-0.4031130	2.3608480	-0.6536390	H	6.7810620	-2.7468790	-0.1454640
Ni	-0.2344130	-0.0846720	1.1098110	H	6.1842610	-4.4125580	-0.1953070
C	2.8409940	4.0678790	-0.8284060	H	6.7673120	-3.6490380	-1.6708300
H	3.2160860	4.3907400	0.1516940	C	-0.4344020	1.5687860	-0.0152130
H	3.6559190	3.5232500	-1.3218550	C	-0.5054950	3.5085500	1.1900650
H	2.6352990	4.9668550	-1.4173440	C	-1.7681550	3.2511780	0.7600330
C	-0.2572890	4.5361440	-1.9324540	C	1.6834170	2.2787380	0.9774000
H	-0.7626810	4.1528050	-2.8276650	C	2.6362060	2.8047340	0.0960510
H	-1.0036770	5.1079810	-1.3659260	C	3.9778920	2.5127660	0.3376370
H	0.5150790	5.2372180	-2.2627830	H	4.7312310	2.8991660	-0.3501750
C	-0.7928540	0.5173800	2.6753490	C	4.3776460	1.7420400	1.4301550
O	-1.1139340	0.8716700	3.7253640	C	3.4004740	1.2703690	2.3067890
INTq14				H	3.6969910	0.6730240	3.1696320
C	-3.1016270	-4.4062810	3.0512050	C	2.0455020	1.5368620	2.1095630
C	-1.8736430	-3.8090830	3.1974110	C	2.2476350	3.6905130	-1.0486230
C	-1.3463450	-2.9855840	2.1735510	H	2.1840660	4.7383500	-0.7241490
C	-2.1068520	-2.7840580	0.9867310	H	1.2727320	3.4294100	-1.4736620
C	-3.3655840	-3.4213840	0.8596690	H	2.9928700	3.6473170	-1.8496290
C	-3.8542400	-4.2123520	1.8702850	C	5.8285270	1.4502290	1.6665680
H	-3.4993660	-5.0376190	3.8431180	H	6.3301200	2.2990720	2.1496890
				H	6.3595490	1.2605330	0.7263910
				H	5.9639530	0.5805180	2.3187430

C	1.0247200	1.0685300	3.1012300	C	4.8241400	0.9208820	0.0268620
H	0.7387120	1.8816820	3.7829580	C	6.0155910	0.8492450	0.7067210
H	1.4153670	0.2498750	3.7144530	H	6.9756600	0.6379440	2.6392830
H	0.1054730	0.7146760	2.6222750	H	4.8224910	0.4799220	3.8890280
C	-2.8278830	1.3769340	-0.5296880	C	2.3301290	0.8557080	0.0733600
C	-3.6170350	0.5848270	0.3212920	H	4.8049410	1.0367460	-1.0578650
C	-4.7005820	-0.0851030	-0.2341410	H	6.9584790	0.9157850	0.1668550
H	-5.3184400	-0.7120130	0.4105510	C	1.1417980	0.7044080	0.7683550
C	-5.0014710	0.0021660	-1.5970390	C	1.3140720	0.5554140	2.1761570
C	-4.1982510	0.7997470	-2.4039970	H	2.3317290	0.9673820	-1.0165360
H	-4.4225140	0.8848510	-3.4682650	H	0.4257040	0.4207000	2.8041360
C	-3.1053260	1.5062320	-1.8913850	N	2.4515170	0.5381260	2.8464960
C	-3.2887630	0.4420040	1.7751210	C	-1.6094900	1.2140040	-1.6893320
H	-3.3822030	1.3899840	2.3216500	O	-2.3532640	0.9239950	-2.5923280
H	-2.2570550	0.0933620	1.9103020	C	-0.7721250	2.4511850	-1.5058980
H	-3.9509090	-0.2868940	2.2535830	C	-0.7907900	3.1208930	-0.2711810
C	-6.1589210	-0.7632760	-2.1615040	C	0.2584360	2.7451020	-2.4252900
H	-7.0786550	-0.5750700	-1.5945430	C	0.1501480	4.1183580	0.0005910
H	-5.9757160	-1.8446700	-2.1194230	H	-1.5905730	2.9119750	0.4406880
H	-6.3471180	-0.5014340	-3.2078310	C	1.1805340	3.7288310	-2.1405910
C	-2.2962510	2.3757160	-2.8059630	H	0.2984880	2.1928940	-3.3641090
H	-1.4978550	2.9141710	-2.2848890	C	1.1424150	4.4303350	-0.9189120
H	-2.9365400	3.1192870	-3.2968470	H	0.1158270	4.6473590	0.9514460
H	-1.8352260	1.7814410	-3.6046850	H	1.9584820	3.9725600	-2.8638290
N	-1.6984390	2.0529760	0.0369550	C	2.1788280	5.4679430	-0.6244920
N	0.2902770	2.4660830	0.7017860	H	2.2770720	6.1811660	-1.4517960
Ni	0.2743270	0.0417840	-1.0425860	H	1.9428560	6.0297660	0.2848500
C	-3.0243130	4.0265230	0.8856720	H	3.1639260	5.0050180	-0.4825020
H	-3.4055900	4.3280150	-0.0991310	C	-1.1043400	-1.0434150	-0.0271040
H	-3.8212660	3.4567950	1.3796050	C	-2.4243410	-2.7973240	0.5937070
H	-2.8524770	4.9365990	1.4680770	C	-1.2363050	-3.3092040	0.1826210
C	0.0561170	4.6283420	1.9810140	C	-3.4243080	-0.4993360	0.6110610
H	0.6292720	4.2704580	2.8452630	C	-4.3939530	-0.4267610	-0.4013620
H	0.7306970	5.2555370	1.3836560	C	-5.4253390	0.4948680	-0.2489950
H	-0.7456590	5.2708730	2.3569150	H	-6.1783520	0.5767180	-1.0339850
C	0.9857030	0.8982610	-2.4350680	C	-5.5118180	1.3270230	0.8693950
O	1.4378130	1.3758030	-3.3784360	C	-4.5381310	1.2138760	1.8581300
INTq15				H	-4.5919080	1.8527780	2.7405920
C	6.0251880	0.6912850	2.1120110	C	-3.4813910	0.3076500	1.7496730
C	4.8446600	0.6045910	2.8079360	C	-4.3100560	-1.2887740	-1.6224010
C	3.6018010	0.6648100	2.1304950	H	-4.5873290	-2.3308800	-1.4126620
C	3.5905710	0.8308220	0.7179310	H	-3.2956150	-1.2854370	-2.0359310
				H	-4.9841280	-0.9170860	-2.4002610
				C	-6.6376490	2.3068740	0.9992510

H	-6.4853590	2.9861620	1.8442630	C	3.6005780	0.8328500	0.6150470
H	-7.5967800	1.7956860	1.1526450	C	4.8202030	1.1163960	-0.0465150
H	-6.7444060	2.9145180	0.0927100	C	6.0207660	0.9876920	0.6092110
C	-2.4182830	0.2608580	2.8010140	H	7.0106450	0.4627340	2.4656160
H	-2.0348940	-0.7531380	2.9692460	H	4.8817200	-0.0476350	3.6615290
H	-2.7897660	0.6513980	3.7541800	C	2.3347670	0.9183520	-0.0126670
H	-1.5597840	0.8779050	2.5004430	H	4.7845860	1.4251490	-1.0923860
C	0.9209440	-2.3223320	-0.6213970	H	6.9527710	1.2064830	0.0911080
C	1.9318290	-2.5332940	0.3250020	C	1.1654500	0.5797300	0.6430480
C	3.2482890	-2.5745100	-0.1301350	C	1.3561090	0.1860910	2.0006430
H	4.0524100	-2.6928720	0.5992000	H	2.3180400	1.2351740	-1.0619600
C	3.5673610	-2.4246350	-1.4791480	H	0.4769820	-0.1026620	2.5904950
C	2.5299950	-2.2386300	-2.3920230	N	2.4989700	0.0992120	2.6554010
H	2.7631330	-2.1280790	-3.4518810	C	-1.7147690	1.3883330	-1.4034500
C	1.1967340	-2.1849370	-1.9870320	O	-2.5481380	1.5520650	-2.2358800
C	1.6429790	-2.7083990	1.7850670	C	-0.6453670	2.5853250	-0.9767650
H	1.6106670	-3.7731390	2.0564860	C	-0.8707200	3.3590530	0.1647030
H	0.6870580	-2.2639000	2.0820690	C	0.2877050	3.0154570	-1.9291370
H	2.4265200	-2.2444230	2.3939040	C	-0.1564870	4.5344760	0.3618500
C	4.9978040	-2.4552660	-1.9221030	H	-1.6036000	3.0288200	0.9015680
H	5.4282890	-3.4600820	-1.8228470	C	0.9865100	4.1942780	-1.7329920
H	5.6116680	-1.7843750	-1.3075130	H	0.4596390	2.4137430	-2.8227090
H	5.1044500	-2.1513730	-2.9689520	C	0.7793350	4.9660040	-0.5807080
C	0.1013110	-1.9788470	-2.9878230	H	-0.3208860	5.1280510	1.2601580
H	-0.3618960	-0.9880350	-2.8878940	H	1.7119150	4.5324760	-2.4729730
H	-0.7057150	-2.7138610	-2.8680310	C	1.5508870	6.2322270	-0.3782260
H	0.4870830	-2.0666250	-4.0086900	H	1.3687080	6.9436440	-1.1934740
N	-0.4387200	-2.2170340	-0.1820330	H	1.2834060	6.7232140	0.5627460
N	-2.3294110	-1.4076780	0.4386230	H	2.6304150	6.0386920	-0.3615820
Ni	-0.4901540	0.6904010	-0.3218920	C	-1.0688830	-1.1602060	-0.1154290
C	-0.7570260	-4.7063360	0.0714680	C	-2.3677620	-2.9943100	0.2712800
H	-0.3902060	-4.9195280	-0.9407570	C	-1.1440370	-3.4382150	-0.1176070
H	0.0653480	-4.9239270	0.7647070	C	-3.4100300	-0.7228230	0.4951280
H	-1.5711390	-5.4050250	0.2863060	C	-4.3365540	-0.5119970	-0.5363870
C	-3.6147420	-3.4521260	1.1847480	C	-5.3841600	0.3708350	-0.2959940
H	-3.8106600	-3.0739810	2.1967580	H	-6.1061860	0.5602630	-1.0914850
H	-4.5267580	-3.2891930	0.5979650	C	-5.5236600	1.0347280	0.9246520
H	-3.4530960	-4.5315470	1.2602300	C	-4.5830960	0.7964810	1.9234900
				H	-4.6785280	1.3068350	2.8827140
				C	-3.5152320	-0.0826050	1.7321210
				C	-4.1840880	-1.1799590	-1.8675660
				H	-4.4001750	-2.2558100	-1.8181050
				H	-3.1639290	-1.0702570	-2.2548560
				H	-4.8672600	-0.7393460	-2.6001010
TSq15_6							
C	6.0534520	0.5639950	1.9578630				
C	4.8860570	0.2812040	2.6238360				
C	3.6348210	0.4082680	1.9724900				

C	-6.6591400	1.9889000	1.1377230	C	-3.6559980	2.1021890	-1.4956760
H	-6.6185580	2.4505290	2.1297180	C	-2.3281170	2.5790280	-1.6929760
H	-7.6291970	1.4852760	1.0413090	C	-2.0479850	3.9534810	-1.5092500
H	-6.6447010	2.7931990	0.3920910	C	-3.0430360	4.8184690	-1.1262550
C	-2.4934290	-0.2849220	2.8076690	H	-5.1331490	5.0390630	-0.6068060
H	-2.1335600	-1.3207050	2.8537770	H	-5.6626830	2.6264400	-0.9451840
H	-2.8975850	-0.0165700	3.7892200	C	-1.3389910	1.6335960	-2.0527390
H	-1.6119690	0.3474430	2.6291820	H	-1.0313840	4.3068220	-1.6784140
C	1.0290040	-2.3204490	-0.6919650	H	-2.8243820	5.8744590	-0.9865490
C	1.9807460	-2.6591420	0.2794690	C	-1.6983670	0.3159630	-2.2461220
C	3.3258110	-2.5971480	-0.0797890	C	-3.0605290	-0.0465180	-2.0291460
H	4.0813450	-2.8185120	0.6771220	H	-0.3055130	1.9539530	-2.2068780
C	3.7326840	-2.2207130	-1.3583880	H	-3.3443750	-1.0930400	-2.1664290
C	2.7539590	-1.9097920	-2.3013520	N	-3.9988820	0.7905150	-1.6654390
H	3.0544980	-1.6172370	-3.3083560	C	-0.6711330	-0.7618230	-2.5477260
C	1.3952060	-1.9524410	-1.9913300	O	-0.7801390	-1.5764450	-3.4298930
C	1.6166680	-3.0528200	1.6800880	C	1.6303170	-1.3142010	-1.4974570
H	1.8007650	-4.1226920	1.8493440	C	1.6854520	-2.7005690	-1.6771430
H	0.5672690	-2.8518350	1.9216240	C	2.8165520	-0.5894490	-1.6677950
H	2.2309490	-2.4991970	2.3999290	C	2.8911200	-3.3439300	-1.9508320
C	5.1906780	-2.1342720	-1.6892720	H	0.7703520	-3.2915550	-1.6147270
H	5.6888560	-3.1051260	-1.5726340	C	4.0168190	-1.2353690	-1.9629470
H	5.6977120	-1.4294730	-1.0163420	H	2.8206490	0.4962380	-1.5523070
H	5.3533460	-1.7952440	-2.7180910	C	4.0794720	-2.6242780	-2.0953520
C	0.3688270	-1.5762200	-3.0154870	H	2.9091090	-4.4284680	-2.0717290
H	-0.0670770	-0.5890190	-2.7992470	H	4.9277410	-0.6463360	-2.0920890
H	-0.4668800	-2.2878400	-3.0425260	C	5.3802950	-3.3179650	-2.3741830
H	0.8119610	-1.5348600	-4.0156930	H	6.0331240	-2.7105760	-3.0128040
N	-0.3587820	-2.2982250	-0.3318130	H	5.9404880	-3.5248950	-1.4515720
N	-2.3019820	-1.5963590	0.2503550	H	5.2252110	-4.2802270	-2.8762860
Ni	-0.5317100	0.6256700	-0.3246550	C	0.2056610	-0.0996770	1.0031090
C	-0.6270020	-4.8097710	-0.3312870	C	0.7448720	0.4902210	3.1476030
H	-0.1743240	-4.9119390	-1.3256090	C	-0.3233210	-0.3472680	3.2170350
H	0.1366870	-5.0907210	0.4047660	C	2.1607870	1.3664700	1.2826340
H	-1.4412450	-5.5371010	-0.2599840	C	1.9603020	2.6801840	0.8515770
C	-3.5794960	-3.7230250	0.7133710	C	3.0588060	3.3742310	0.3415430
H	-3.8295210	-3.4815980	1.7551520	H	2.9212070	4.3996610	-0.0035260
H	-4.4608060	-3.4796140	0.1072960	C	4.3244600	2.7936050	0.2734850
H	-3.4185250	-4.8034880	0.6532070	C	4.4836930	1.4834890	0.7291200
				H	5.4666860	1.0133330	0.6721000
				C	3.4153140	0.7459680	1.2323700
				C	0.6086050	3.3190870	0.9365490
				H	0.1862980	3.2462980	1.9475230
				H	-0.1126590	2.8319030	0.2665590
INTq18							
C	-4.3557660	4.3430780	-0.9137160				
C	-4.6578190	3.0151550	-1.0957340				

H	0.6567270	4.3795530	0.6680060	C	-5.1664850	2.6465900	-0.8802960
C	5.4966670	3.5488800	-0.2746980	C	-3.9514510	1.9877880	-1.1797560
H	5.2056800	4.5411630	-0.6347720	C	-2.7501390	2.7524440	-1.2316300
H	5.9607380	3.0111560	-1.1107410	C	-2.7989370	4.1461080	-0.9916020
H	6.2760190	3.6846720	0.4856920	C	-3.9934320	4.7582620	-0.7051410
C	3.5851810	-0.6794160	1.6556190	H	-6.1241080	4.4993230	-0.4211030
H	3.2008760	-0.8624160	2.6677560	H	-6.0717110	2.0441710	-0.8454300
H	4.6395080	-0.9726410	1.6295630	C	-1.5508320	2.0610190	-1.5169710
H	3.0356040	-1.3463140	0.9759690	H	-1.8733790	4.7187600	-1.0421530
C	-1.6736150	-1.5879140	1.5013420	H	-4.0288800	5.8293750	-0.5208750
C	-1.3534650	-2.9381500	1.3033220	C	-1.5741090	0.6991230	-1.7087200
C	-2.3688030	-3.7868080	0.8709230	C	-2.8341840	0.0430300	-1.6552940
H	-2.1408760	-4.8406750	0.7052080	H	-0.6120670	2.6178510	-1.5819970
C	-3.6677450	-3.3251410	0.6450660	H	-2.8696890	-1.0365950	-1.8327240
C	-3.9485950	-1.9795860	0.8736440	N	-3.9742410	0.6403460	-1.3990180
H	-4.9573480	-1.6040120	0.6986500	C	-0.3322170	-0.0246070	-2.7101190
C	-2.9642340	-1.0890450	1.3058710	O	-0.4841000	-0.0607630	-3.8791300
C	0.0319660	-3.4502060	1.5494490	C	1.9020640	-0.9768710	-1.5752310
H	0.4169560	-3.1368240	2.5289680	C	2.1360640	-2.3456830	-1.7566310
H	0.7409450	-3.0754680	0.7984180	C	2.9808240	-0.1134780	-1.8103180
H	0.0538240	-4.5439900	1.5119920	C	3.4011810	-2.8316270	-2.0888440
C	-4.7306560	-4.2702200	0.1732790	H	1.3177220	-3.0585020	-1.6418920
H	-4.4522960	-4.7383000	-0.7788360	C	4.2434420	-0.5980120	-2.1446690
H	-5.6889800	-3.7611030	0.0277970	H	2.8452950	0.9662030	-1.7207790
H	-4.8894940	-5.0840100	0.8919470	C	4.4812470	-1.9679410	-2.2780340
C	-3.2745420	0.3588910	1.5307240	H	3.5520280	-3.9056860	-2.2131850
H	-2.6441110	1.0083780	0.9075770	H	5.0640170	0.1043120	-2.3066900
H	-3.0979530	0.6579130	2.5726660	C	5.8506800	-2.4917900	-2.5948370
H	-4.3193860	0.5769780	1.2879600	H	6.4255260	-1.7815110	-3.2010210
N	-0.6324020	-0.6877810	1.8973340	H	6.4353990	-2.6803520	-1.6835050
N	1.0484260	0.6207550	1.7873620	H	5.8044700	-3.4390520	-3.1450200
Ni	0.0790220	-0.4195630	-0.9400550	C	0.2547780	-0.3627220	0.8791860
C	-1.0877040	-0.8799830	4.3686240	C	0.7908080	-0.0977380	3.0904260
H	-2.1386990	-0.5635030	4.3470830	C	-0.2254940	-0.9952680	3.0286180
H	-1.0829040	-1.9774010	4.3793150	C	2.0894720	1.2076390	1.4112180
H	-0.6535630	-0.5334660	5.3112570	C	1.7434820	2.5531150	1.2494170
C	1.5144540	1.1956190	4.1983930	C	2.7531820	3.4484670	0.8960110
H	2.5650440	0.8785540	4.2205190	H	2.5011800	4.5009710	0.7606880
H	1.5103160	2.2816730	4.0388620	C	4.0745370	3.0344950	0.7296660
H	1.0828980	1.0013740	5.1849520	C	4.3796440	1.6859880	0.9184740
				H	5.4072470	1.3456320	0.7822810
				C	3.4040200	0.7509090	1.2589760
				C	0.3393140	3.0208640	1.4792290
				H	0.0257340	2.8546010	2.5188670
TSq18_19							
C	-5.1845580	4.0005770	-0.6488210				

H	-0.3807760	2.4809720	0.8521570	C	-5.6542500	3.7226040	-0.9831880
H	0.2415590	4.0908170	1.2683380	C	-5.4552280	2.3820580	-1.2053620
C	5.1525190	4.0166020	0.3852570	C	-4.1477720	1.8399620	-1.2121530
H	4.7382800	4.9464840	-0.0188090	C	-3.0396310	2.7030830	-0.9823990
H	5.8494550	3.6064480	-0.3547230	C	-3.2743350	4.0816510	-0.7649010
H	5.7465330	4.2803460	1.2701980	C	-4.5538250	4.5810910	-0.7628700
C	3.7419530	-0.6982460	1.4211790	H	-6.6624230	4.1314140	-0.9789860
H	3.4928970	-1.0714270	2.4234950	H	-6.2839070	1.6996340	-1.3837920
H	4.8100400	-0.8698540	1.2527680	C	-1.7475310	2.1179140	-0.9690300
H	3.1864010	-1.3091230	0.6956870	H	-2.4199390	4.7366660	-0.5915710
C	-1.5716380	-1.9903760	1.1771250	H	-4.7255560	5.6415880	-0.5908830
C	-1.2370150	-3.2843360	0.7614010	C	-1.5793940	0.7620250	-1.1344910
C	-2.2577710	-4.0879450	0.2550160	C	-2.7649940	0.0235610	-1.4186760
H	-2.0145890	-5.0955050	-0.0845890	H	-0.8881460	2.7755710	-0.8185190
C	-3.5781090	-3.6412680	0.1833950	H	-2.6781020	-1.0494820	-1.6245290
C	-3.8740260	-2.3556410	0.6364090	N	-3.9891930	0.5071400	-1.4474900
H	-4.8980640	-1.9858140	0.5734210	C	0.0850360	0.0094410	-2.8770530
C	-2.8860730	-1.5108560	1.1409750	O	0.0334410	0.0977820	-4.0204530
C	0.1585610	-3.8072230	0.9094310	C	1.9134400	-0.9067010	-1.5716060
H	0.3927400	-4.0138680	1.9634610	C	2.1277690	-2.2775370	-1.7530950
H	0.9104050	-3.0944350	0.5510460	C	2.9969280	-0.0561410	-1.8243600
H	0.2854720	-4.7441610	0.3571570	C	3.3861410	-2.7811550	-2.0830840
C	-4.6606210	-4.5369940	-0.3371030	H	1.2969870	-2.9761640	-1.6446990
H	-4.2699250	-5.2672360	-1.0541300	C	4.2533800	-0.5554280	-2.1588030
H	-5.4527990	-3.9652530	-0.8327550	H	2.8663340	1.0260690	-1.7521830
H	-5.1322350	-5.1022880	0.4776120	C	4.4748370	-1.9295680	-2.2791740
C	-3.2232960	-0.1359850	1.6290480	H	3.5246990	-3.8569350	-2.2038130
H	-2.5314250	0.6187170	1.2335570	H	5.0804620	0.1354930	-2.3335950
H	-3.1661310	-0.0729010	2.7245180	C	5.8368920	-2.4717850	-2.5944280
H	-4.2377340	0.1462440	1.3299370	H	6.4194090	-1.7736490	-3.2069420
N	-0.5372540	-1.1337670	1.6724460	H	6.4186980	-2.6585250	-1.6810950
N	1.0681000	0.2693220	1.7680050	H	5.7780270	-3.4236970	-3.1349220
Ni	0.2079730	-0.2539870	-1.0800580	C	0.2834920	-0.3272520	0.7970350
C	-0.9355210	-1.7555890	4.0833930	C	0.8770910	-0.1073730	2.9981460
H	-2.0020620	-1.4998950	4.1296070	C	-0.1264020	-1.0166560	2.9424170
H	-0.8741070	-2.8376630	3.9101450	C	2.1360940	1.2438660	1.3439020
H	-0.4982240	-1.5496690	5.0648830	C	1.8074030	2.6008360	1.2605740
C	1.5346330	0.4688920	4.2393750	C	2.8238510	3.4982000	0.9254860
H	2.6044070	0.2274250	4.1955920	H	2.5813830	4.5584630	0.8426240
H	1.4545400	1.5630390	4.2740680	C	4.1369450	3.0788680	0.7240030
H	1.1409140	0.0752560	5.1812990	C	4.4320290	1.7217780	0.8685670
				H	5.4569450	1.3783190	0.7205310
				C	3.4511410	0.7845330	1.1814130
				C	0.4401300	3.1064020	1.6071630

INTq19

H	0.3707460	3.3194440	2.6833320	C	1.6342030	0.4470070	4.1447520
H	-0.3523570	2.3889590	1.3715430	H	2.7048400	0.2127880	4.0899080
H	0.2207670	4.0448930	1.0855160	H	1.5480110	1.5395910	4.1968550
C	5.2206410	4.0620800	0.4017200	H	1.2516010	0.0395970	5.0852410
H	4.8121800	5.0009870	0.0131610				
H	5.9191250	3.6623840	-0.3424470				
H	5.8116900	4.3068250	1.2940570	Pr2			
C	3.7938220	-0.6650630	1.3336290	C	-4.9715540	-0.0535350	-0.0201720
H	3.6108080	-1.0249660	2.3548320	C	-4.0871670	0.9775190	0.1744300
H	4.8503980	-0.8388840	1.1054760	C	-2.6936020	0.7412350	0.1327190
H	3.1971510	-1.2892350	0.6557430	C	-2.2208120	-0.5784130	-0.1129170
C	-1.5190120	-2.0035560	1.1401620	C	-3.1564900	-1.6219340	-0.3115360
C	-1.1766840	-3.2866550	0.6978100	C	-4.5027810	-1.3640310	-0.2652110
C	-2.2027830	-4.1115650	0.2362030	H	-6.0420910	0.1344790	0.0130970
H	-1.9522900	-5.1091440	-0.1268080	H	-4.4202210	1.9948600	0.3662520
C	-3.5354160	-3.7006970	0.2434180	C	-0.8251780	-0.7784040	-0.1539010
C	-3.8398140	-2.4360900	0.7467740	H	-2.7869110	-2.6290250	-0.4996540
H	-4.8767810	-2.0987820	0.7569460	H	-5.2179300	-2.1689920	-0.4167650
C	-2.8500630	-1.5710130	1.2099730	C	0.0353240	0.2780590	0.0461540
C	0.2265130	-3.8007640	0.8016360	C	-0.5563490	1.5496800	0.2933840
H	0.4488070	-4.1102090	1.8327980	H	-0.4387050	-1.7751040	-0.3681080
H	0.9764270	-3.0512990	0.5276370	H	0.1005110	2.4012780	0.4867150
H	0.3715880	-4.6788610	0.1636960	N	-1.8439560	1.7860240	0.3354230
C	-4.6228120	-4.6088460	-0.2438850	C	1.4998230	0.1194960	0.0232890
H	-4.2348330	-5.3723300	-0.9266190	C	2.3306840	1.1210640	-0.4882100
H	-5.4052900	-4.0503850	-0.7696440	C	2.1023300	-1.0470280	0.5120240
H	-5.1076750	-5.1323460	0.5906240	C	3.7103850	0.9586500	-0.5145180
C	-3.2133250	-0.2297310	1.7682530	H	1.8924780	2.0291690	-0.8985220
H	-2.5562850	0.5628100	1.3911330	C	3.4787460	-1.2041530	0.4813550
H	-3.1389530	-0.2169220	2.8644580	H	1.4799690	-1.8293810	0.9433900
H	-4.2438300	0.0310880	1.5082490	C	4.3099280	-0.2041430	-0.0323320
N	-0.4791600	-1.1271240	1.5926180	H	4.3364870	1.7491570	-0.9261760
N	1.1166240	0.2935530	1.6776450	H	3.9261410	-2.1175870	0.8728240
Ni	0.1635700	-0.1250760	-1.1362530	C	5.7959380	-0.3879360	-0.0553910
C	-0.7845870	-1.8178560	4.0008780	H	6.2004110	-0.5104310	0.9571680
H	-1.8498240	-1.5760480	4.1061300	H	6.0800970	-1.2852070	-0.6190990
H	-0.7209450	-2.8929430	3.7899280	H	6.3021040	0.4678570	-0.5140810
H	-0.3048250	-1.6400490	4.9678120				