

Electronic Supplementary Information

A Computational Mechanistic Study of Ni(0)-catalyzed Annulation of Aromatic Amides with Alkynes: The Effects of Directing Groups

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1. Table of calculated energies and imaginary frequencies.

Table S1. Calculated energies and imaginary frequencies.

stationary point	thermal correction to Gibbs free energy at B3LYP/LANL2DZ/6-31G(d,p) (in a.u.)	single-point energy including solvation energy at M06/SDD/6-311+G(d,p) (in a.u.)	imaginary frequencies
PPh₃	0.197235	-1035.918595	
PhC≡CPh	0.125066	-539.171419	
Ni(PPh₃)₂	0.417133	-2242.848138	
Ni(cod)₂	0.291558	-794.753355	
1	0.156992	-687.053069	
3	0.380996	-1893.979696	
TS1	0.376787	-1893.947048	1133.66 <i>i</i>
4	0.381362	-1893.985142	
4_T	0.376653	-1893.9537031	
5	0.306242	-1397.214328	
TS2	0.311979	-1397.212969	165.29 <i>i</i>
6	0.317375	-1397.243606	
TS3	0.316237	-1397.219959	1289.31 <i>i</i>
7	0.134668	-856.817299	
8	0.294033	-1396.03803	
TS4	0.298905	-1396.003553	218.25 <i>i</i>
9	0.300985	-1396.042439	
TS5	0.301045	-1396.001227	311.02 <i>i</i>
P1	0.304685	-1225.086666	
3'	0.309189	-1169.913821	
TS1'	0.309104	-1169.883843	1082.20 <i>i</i>
4'	0.313504	-1169.905977	
4'_T	0.304495	-1169.8740155	
2	0.170650	-746.208443	
10	0.39248	-1953.113883	
TS6	0.387823	-1953.085539	1059.89 <i>i</i>
11	0.38843	-1953.10964	
2'	0.156213	-745.688325	
12	0.615445	-2988.571834	
TS7	0.610738	-2988.554229	33.68 <i>i</i>
13	0.379192	-1952.62077	
TS8	0.380781	-1952.591814	772.63 <i>i</i>

14	0.381703	-1952.614415	
15	0.309693	-1455.851052	
TS9	0.309844	-1455.85176	340.13 <i>i</i>
16	0.313937	-1455.88927	
17	0.476148	-1995.072294	
TS10	0.47687	-1995.054346	202.29 <i>i</i>
18	0.479588	-1995.106901	
TS11	0.482345	-1995.07792	314.45 <i>i</i>
P2	0.316746	-1284.239528	
15'	0.310868	-1455.840572	
TS9'	0.312149	-1455.824837	216.17 <i>i</i>
16'	0.314035	-1455.838015	
19	0.438464	-1689.49315	
TS12	0.433489	-1689.458793	1149.50 <i>i</i>
20	0.252817	-1149.07727	
21	0.413814	-1688.255217	
TS13	0.416296	-1688.233972	227.87 <i>i</i>
22	0.418575	-1688.29551	
TS14	0.419222	-1688.268636	314.28 <i>i</i>
23	0.150221	-916.652312	
24	0.150321	-916.625551	
26	0.080257	-610.511105	
27	0.079777	-609.017206	

2. On the bonding between Ni and N atom of pyridine.

To elucidate the bonding between Ni and N atom of pyridine, Bader's AIM (Atoms-In-Molecules) method^{1,2} was used. The AIM analysis was performed by Multiwfn.³

In the AIM theory, a bond critical point (BCP) corresponds to the point where the electron density becomes a minimum along the bond path between interacting atoms. The molecular graphs in Fig. S1 show the presence of BCPs and ring critical points (RCPs) in species **4**, **6** and **9**. Particularly, the data show the presence of BCPs between the nickel atom and the nitrogen atom of pyridine in the three species. Furthermore, the magnitude of the electron density $\rho(r)$ and Laplacian of the electron density $\nabla^2\rho(r)$ at the BCP are given in Table S2. All the results indicate that there exists bonding between Ni and N of pyridine in the three complexes. In addition, our results are in consistent with the bonding in the symmetrical pincer palladacycles PdNCN and PdSCS reported by H. Cox.⁴

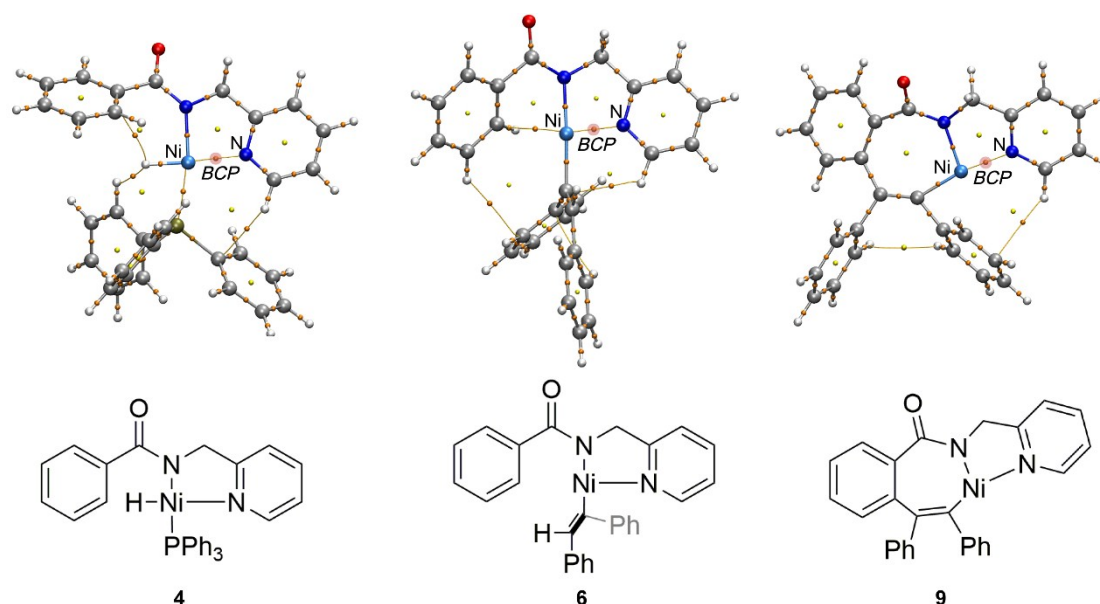


Fig. S1 Molecular graphs with BCPs and RCPs for **4**, **6** and **9**.

Table S2. Electron density $\rho(r)$ and Laplacian of the electron density $\nabla^2\rho(r)$ at the BCP between Ni and N_{pyridine}.

complex	$\rho(r)$	$\nabla^2\rho(r)$
4	0.080	0.493
6	0.094	0.515
9	0.087	0.533

References

- 1 R. F. W. Bader, *Acc. Chem. Res.*, 1985, **18**, 9–15.
- 2 R. F. W. Bader, *Atoms in Molecules: A Quantum Theory*, Oxford University Press, Oxford, UK, 1990.

3 T. Lu and F. Chen, *J. Comput. Chem.*, 2012, **33**, 580–592.

4 S. Boonseng, G. W. Roffe, J. Spencer and H. Cox, *Dalton Trans.*, 2015, **44**, 7570–7577.

3. On the possibility of triplet state.

We have considered the impact of the lowest-lying singlet and triplet electronic states during the optimization of species **4** and **4'**. As seen from **Fig. S2**, for **4** and **4'**, the triplet electronic states are higher in energy than their singlet state counterparts by 16.8 kcal/mol and 12.1 kcal/mol respectively.

Furthermore, we have performed TDDFT calculations on the key steps of the reactions during our study. The TDDFT results reveal that the first triplets are all higher in energy than the ground singlets. Therefore, the triplet potential energy surface (PES) is high-lying and the singlet and triplet surfaces do not cross during the reaction.

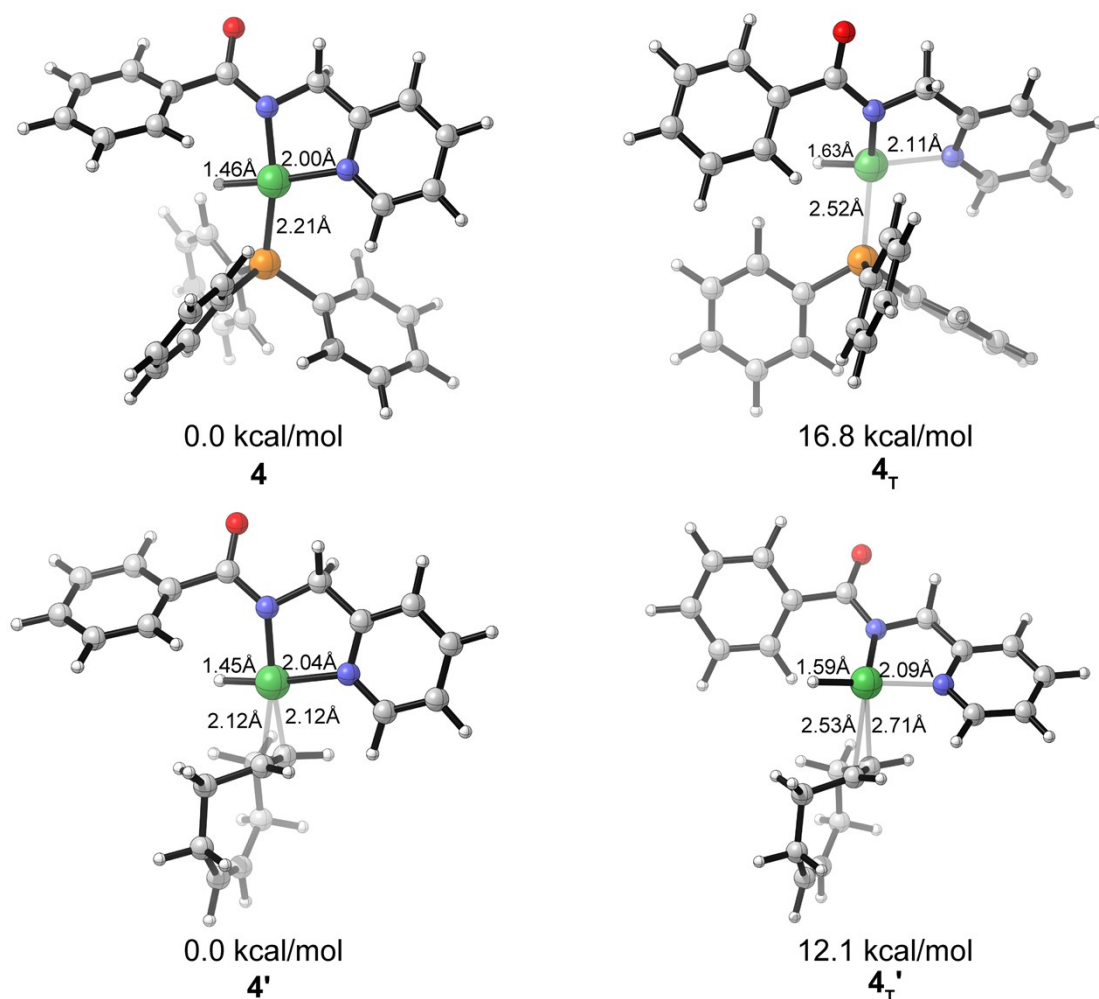


Fig. S2 Optimized structures of the singlet **4**, **4'** and triplet **4_T**, **4'_T** with relative energies.

4. Cartesian coordinates of all optimized structures.

PPh₃

O 1

P	0.00506800	0.00334600	-1.18869300
C	-1.04623200	1.30651600	-0.39251200
C	-1.08031300	2.56461400	-1.01869600
C	-1.82867400	1.10756900	0.75537400
C	-1.85907700	3.60005300	-0.50186600
H	-0.49567500	2.73222200	-1.92071600
C	-2.61757300	2.14095400	1.26625200
H	-1.82649100	0.14184900	1.25159600
C	-2.63225100	3.38949700	0.64219900
H	-1.87001500	4.56733100	-0.99778200
H	-3.21935500	1.96853400	2.15520000
H	-3.24732700	4.19212900	1.04089600
C	1.66002300	0.25710500	-0.39316100
C	2.76578800	-0.32826800	-1.03385400
C	1.88108800	1.01148400	0.76954400
C	4.05287400	-0.18257300	-0.51601200
H	2.61688200	-0.89924700	-1.94773400
C	3.17138000	1.16687600	1.28170700
H	1.04506200	1.48320700	1.27736100
C	4.25913100	0.56807500	0.64364300
H	4.89492500	-0.64668100	-1.02316200
H	3.32513100	1.75593800	2.18251800
H	5.26233600	0.69070800	1.04365400
C	-0.60420600	-1.55908600	-0.39797300
C	-1.68817600	-2.20255200	-1.02032200
C	-0.04028000	-2.14889500	0.74343900
C	-2.20837800	-3.38915900	-0.50389200
H	-2.12586700	-1.77087200	-1.91786400
C	-0.55345200	-3.34381900	1.25364600
H	0.80372900	-1.67643900	1.23670900
C	-1.63977100	-3.96455900	0.63487600
H	-3.05039300	-3.86933100	-0.99598100
H	-0.10300300	-3.78821500	2.13783000
H	-2.03737000	-4.89431800	1.03351000

PhC≡CPh

O 1

C	0.60816900	0.00002000	0.00001200
C	-0.60816800	0.00002600	-0.00000400

C	2.03823700	0.00000800	0.00000400
C	2.75410400	-0.86474100	-0.85136900
C	2.75412500	0.86474500	0.85137200
C	4.14690200	-0.86118600	-0.84794800
H	2.20784500	-1.53341200	-1.50970000
C	4.14692300	0.86116800	0.84793800
H	2.20788200	1.53342400	1.50970800
C	4.84775500	-0.00001400	-0.00000800
H	4.68683500	-1.53318200	-1.50969900
H	4.68687300	1.53315600	1.50968600
H	5.93442200	-0.00002200	-0.00001300
C	-2.03823700	0.00000900	-0.00000100
C	-2.75410500	-0.86473900	0.85137000
C	-2.75412300	0.86474700	-0.85137100
C	-4.14690500	-0.86118600	0.84794400
H	-2.20785100	-1.53340800	1.50970600
C	-4.14692100	0.86116900	-0.84794100
H	-2.20787900	1.53342600	-1.50970500
C	-4.84775500	-0.00001600	0.00000200
H	-4.68683700	-1.53318400	1.50969400
H	-4.68686900	1.53315700	-1.50968900
H	-5.93442200	-0.00002400	0.00000300

Ni(PPh₃)₂

O 1

Ni	0.00193900	0.04599500	-0.11730100
P	-2.14784600	0.01526600	-0.06017800
C	-2.96379500	-1.40317600	-0.93213700
C	-2.35782600	-1.88678400	-2.10400400
C	-4.14323100	-2.01677900	-0.47646200
C	-2.92858200	-2.94534600	-2.81440200
H	-1.43444500	-1.42798000	-2.44958900
C	-4.70880800	-3.08561300	-1.18368400
H	-4.62529800	-1.66628200	0.43368900
C	-4.09656300	-3.54986000	-2.35307800
H	-2.44460300	-3.31193200	-3.71745800
H	-5.61705700	-3.55140700	-0.81689700
H	-4.53803800	-4.38042200	-2.89470800
C	-2.98260000	1.50704200	-0.76670600
C	-2.34288000	2.74846400	-0.58872300
C	-4.19643000	1.47174500	-1.47568300
C	-2.91277900	3.92110900	-1.08300800
H	-1.38940200	2.77891800	-0.06018400
C	-4.75295500	2.64909600	-1.98168000

H	1.67913700	-2.51240900	-1.25478700	C	-5.12402300	2.09658000	0.30753100
H	2.88673200	-0.89110000	-2.44653000	C	-5.24726500	3.33445100	-0.31976400
H	3.55732900	-0.13877100	-1.02153900	H	-4.32930200	4.75827700	-1.65770100
H	3.16133100	2.38966900	0.32334700	H	-2.31299400	3.35140800	-2.04624200
H	1.68079800	2.51235100	1.25453700	H	-5.90429300	1.71976900	0.96039300
Ni	0.00038300	0.00054600	-0.00004700	H	-6.13356400	3.94027400	-0.15012000
1				C	-3.93357100	-0.01666200	0.82661800
O 1				O	-4.94835000	-0.51369800	1.32026800
C	4.62974000	1.31397300	0.09081600	N	-2.70706000	-0.60685000	0.93419600
C	3.44318300	1.85502600	-0.40831900	C	-2.52566100	-1.93328000	1.50376000
C	2.29244400	1.06972600	-0.48386500	H	-3.43275500	-2.17404700	2.05919700
C	2.31941700	-0.26825600	-0.06379400	H	-1.67864800	-1.90476200	2.19983400
C	3.51895100	-0.80805100	0.41941400	C	-2.26008200	-2.98418100	0.44521900
C	4.66547900	-0.02093200	0.50231600	C	-3.15896500	-4.02492900	0.21290900
H	5.52461900	1.92779700	0.15231300	C	-2.88537800	-4.97411900	-0.77126600
H	3.41326000	2.88817700	-0.74407500	H	-4.06887600	-4.07949400	0.80200800
H	1.38438700	1.49825400	-0.89938700	C	-0.85514800	-3.78574600	-1.22748700
H	3.53127300	-1.84947900	0.72432900	C	-1.70667700	-4.84853100	-1.50570700
H	5.58803600	-0.44794400	0.88671000	H	-3.57736400	-5.78961500	-0.96032400
C	1.11900800	-1.17439200	-0.11669500	H	0.07223700	-3.65366300	-1.77359000
O	1.23203000	-2.40261000	-0.11377800	H	-1.44305000	-5.55749500	-2.28397500
N	-0.09352100	-0.56326300	-0.16840300	N	-1.11079200	-2.86196400	-0.27081800
H	-0.20458600	0.42900200	0.00734300	Ni	0.15407800	-1.43677400	-0.08045900
C	-1.32412300	-1.32357800	-0.17195900	P	1.64888100	0.04952300	0.05256500
H	-1.32222000	-2.05622100	0.64772800	C	1.49649700	1.44545000	-1.16405600
H	-1.40796400	-1.90951100	-1.09734300	C	1.03013000	1.13258400	-2.45295100
C	-2.52311200	-0.40192200	-0.03937900	C	1.80469100	2.78143700	-0.86653500
C	-3.82367300	-0.92041200	-0.08854700	C	0.89025300	2.12581100	-3.42281500
C	-4.89894900	-0.04846500	0.04475600	H	0.76926500	0.10322900	-2.68803500
H	-3.98076800	-1.98640800	-0.22917100	C	1.65479800	3.77802100	-1.83521900
C	-3.32279900	1.73759700	0.25797200	H	2.15860200	3.05062100	0.12395400
C	-4.64772200	1.31430700	0.22278800	C	1.20118400	3.45363100	-3.11506800
H	-5.91804600	-0.42381400	0.01022100	H	0.53259200	1.86412100	-4.41543500
H	-3.07841700	2.78940200	0.39374100	H	1.89448700	4.80888400	-1.58682700
H	-5.45672400	2.03017000	0.33019700	H	1.08737200	4.22987200	-3.86739600
N	-2.28021700	0.90379700	0.13048800	C	3.35867400	-0.59986100	-0.27440300
3				C	3.66306400	-1.88680500	0.20164000
O 1				C	4.34607900	0.10901700	-0.97552000
C	-4.23406400	3.79372000	-1.16570000	C	4.92507900	-2.44438300	-0.00467500
C	-3.10107500	3.00674200	-1.38261700	H	2.89884100	-2.45165200	0.73031600
C	-2.97382000	1.76939900	-0.74949500	C	5.60723100	-0.45399600	-1.19044000
C	-3.98332300	1.30589400	0.10784700	H	4.13355100	1.10180500	-1.36038000
				C	5.90067400	-1.72919300	-0.70432100
				H	5.14392500	-3.43998600	0.37291000

H	6.35988300	0.10662700	-1.73920500	N	-0.75524600	2.61767100	-0.42099300
H	6.88136700	-2.16612400	-0.87380600	H	-2.02293600	-0.90585200	-1.10394600
C	1.84334800	0.92691100	1.67771100	P	1.23388400	-0.40145200	0.09270600
C	0.68165700	1.20256600	2.41828300	C	2.27532500	-0.00751500	-1.39431700
C	3.08396600	1.32059100	2.20328000	C	1.62197200	0.08445300	-2.63579900
C	0.75535300	1.86640500	3.64331900	C	3.65866400	0.22149500	-1.34487100
H	-0.28552200	0.88869000	2.03457000	C	2.33442100	0.38160500	-3.79859200
C	3.15857000	1.97755200	3.43420100	H	0.54717300	-0.07355000	-2.68924800
H	3.99759100	1.11146600	1.65516300	C	4.37042100	0.52918500	-2.50789500
C	1.99571400	2.25472600	4.15537900	H	4.18559300	0.16230600	-0.39724200
H	-0.15501000	2.07261500	4.20022400	C	3.71214600	0.60666200	-3.73648700
H	4.12797700	2.27225000	3.82825900	H	1.81289500	0.44328300	-4.75032800
H	2.05581500	2.76469300	5.11336400	H	5.44137700	0.70709700	-2.45138500
H	-2.09019600	1.17007800	-0.95192500	H	4.26784000	0.84486800	-4.63967400
H	-1.88503400	-0.21854200	0.47541400	C	1.26007100	-2.25724500	0.12146500
				C	0.27702600	-2.92164600	0.87221900
TS1				C	2.22065800	-3.02280000	-0.55913100
0 1				C	0.26236900	-4.31461300	0.95390000
Ni	-0.65824500	0.61696300	0.14601200	H	-0.48513400	-2.33942200	1.38265600
C	-4.23881900	-3.49201600	-1.06763100	C	2.19903000	-4.41774600	-0.48518400
C	-3.10170700	-2.75160000	-1.39442700	H	2.98772800	-2.53393100	-1.15171800
C	-2.90481500	-1.48519300	-0.83847300	C	1.22257900	-5.06662700	0.27326600
C	-3.84486700	-0.94502700	0.05035000	H	-0.50705300	-4.81087600	1.53947700
C	-4.99550600	-1.68948000	0.35571100	H	2.94676800	-4.99608400	-1.02207000
C	-5.18708400	-2.95663400	-0.18979200	H	1.20606800	-6.15209200	0.32791300
H	-4.39049100	-4.47791000	-1.50013300	C	2.33297000	0.06086700	1.51307800
H	-2.36623900	-3.15630800	-2.08483900	C	2.30636200	1.39600800	1.95156000
H	-5.73134200	-1.25243900	1.02294200	C	3.17201300	-0.84847500	2.17405500
H	-6.07768900	-3.52620800	0.06355500	C	3.10844000	1.81397300	3.01352900
C	-3.72680500	0.42387000	0.66152000	H	1.64850900	2.10706000	1.45866300
O	-4.75033200	1.03659100	0.99596600	C	3.96838900	-0.43065400	3.24386600
N	-2.46253300	0.93622400	0.82981000	H	3.20398100	-1.88702600	1.86011300
C	-2.36447400	2.29388400	1.37198500	C	3.94087800	0.89980300	3.66451900
H	-3.36337100	2.66011200	1.62252600	H	3.07717500	2.85108400	3.33756200
H	-1.77058800	2.27452000	2.29758100	H	4.60971300	-1.14902600	3.74820100
C	-1.67919200	3.20688700	0.37141500	H	4.55993500	1.22178900	4.49776200
C	-1.95361200	4.57232000	0.28510400	H	-1.56847400	-0.03171700	1.21141700
C	-1.26067600	5.34823000	-0.64359400				
H	-2.70456100	5.01368500	0.93342000	4			
C	-0.08975000	3.36937700	-1.31429700	0 1			
C	-0.31002000	4.73606100	-1.46098600	C	-5.07742100	-2.26734200	0.92237800
H	-1.46503300	6.41168600	-0.73179600	C	-4.14385600	-1.55535300	1.67961500
H	0.64145100	2.84744500	-1.92438300	C	-3.58445100	-0.37849800	1.17835600
H	0.24798100	5.29986100	-2.20177800	C	-3.95738800	0.10887100	-0.08229200

C	-4.91874500	-0.59622800	-0.81993000	H	5.71332400	0.01260900	1.65919500
C	-5.46373900	-1.78342300	-0.33063200	H	6.41904500	1.37541500	-0.29818500
H	-5.50764200	-3.18763200	1.31008700	C	1.02046200	-1.83744500	-1.51118900
H	-3.84994200	-1.91572800	2.66257100	C	-0.16734400	-2.06122800	-2.22524300
H	-5.23515300	-0.19293000	-1.77707400	C	2.18190000	-2.53073600	-1.89736000
H	-6.19707000	-2.32683200	-0.92177600	C	-0.19312500	-2.95935900	-3.29430300
C	-3.45450200	1.41985500	-0.64001900	H	-1.07068500	-1.52954000	-1.94592700
O	-4.24276600	2.11217200	-1.31199400	C	2.15159900	-3.42957400	-2.96412900
N	-2.19086000	1.81462700	-0.33680700	H	3.11601900	-2.36602200	-1.36961000
C	-1.91335900	3.18164300	-0.76751200	C	0.96322300	-3.64677200	-3.66515800
H	-2.71151400	3.86820400	-0.45557200	H	-1.12114000	-3.11649400	-3.83727800
H	-1.87889300	3.26528600	-1.86787400	H	3.05814700	-3.95782500	-3.24767700
C	-0.59860200	3.63272700	-0.19859500	H	0.94127200	-4.34379700	-4.49878900
C	-0.25920500	4.98145400	-0.05662900	H	-2.86076900	0.17467300	1.76761400
C	0.96573600	5.32398100	0.50562100	H	-1.28281100	-0.41053200	-0.28220600
H	0.96284900	5.74385700	-0.37638300				
C	1.42845600	2.98629100	0.73940700	4r			
C	1.82484300	4.30457900	0.92135800	C	-5.25070400	-1.58496900	-0.35359400
H	1.24228000	6.36722400	0.63007000	C	-4.02756900	-1.57895100	0.31918200
H	2.06789000	2.16602700	1.04127800	C	-3.27336800	-0.40456900	0.39447400
H	2.78456700	4.52137100	1.37870500	C	-3.74295000	0.78091000	-0.18325200
N	0.24747900	2.64955000	0.18353200	C	-4.98795200	0.77220900	-0.82962100
Ni	-0.56471700	0.84760100	-0.09695400	C	-5.72833400	-0.40413800	-0.93077400
P	1.04665400	-0.66262200	-0.08198300	H	-5.83421300	-2.50004200	-0.41902900
C	0.95423500	-1.71058300	1.43259100	H	-3.65778900	-2.48782600	0.78722900
C	0.49626600	-1.10582100	2.61465700	H	-5.36708500	1.70248600	-1.24101100
C	1.32214600	-3.06394300	1.45966600	H	-6.68410900	-0.39922800	-1.44902800
C	0.42117800	-1.83491600	3.80209200	C	-3.03116800	2.10059500	-0.03081200
H	0.18897100	-0.06289000	2.60081700	O	-3.72225400	3.11587800	0.16987300
C	1.23863900	-3.79373300	2.64725700	N	-1.66986400	2.11920700	-0.09167800
H	1.66526900	-3.55560700	0.55486000	C	-1.13864200	3.44216500	0.21778500
C	0.79092500	-3.18159900	3.81969000	H	-1.29828500	3.70049300	1.27742000
H	0.06348600	-1.35380100	4.70850800	H	-1.68615900	4.21981400	-0.33650700
H	1.51992900	-4.84349500	2.65316500	C	0.32534300	3.57363000	-0.10183800
H	0.72378300	-3.75299900	4.74166900	C	1.04330800	4.73202300	0.22502300
C	2.80118600	-0.06807300	-0.11600600	C	2.37988500	4.83222600	-0.13927700
C	3.20815300	0.71059400	-1.21467800	H	0.54279200	5.53951100	0.75112100
C	3.71731100	-0.30943400	0.91778800	C	2.21107800	2.65050000	-1.10700400
C	4.50331900	1.22142200	-1.28241100	C	2.97896600	3.77069900	-0.82544700
H	2.50881200	0.91727600	-2.02113300	H	2.94981000	5.72510000	0.10238700
C	5.01414100	0.21084200	0.85104800	H	2.62913800	1.79708300	-1.62987400
H	3.42628500	-0.90629700	1.77640200	H	4.01869000	3.80781600	-1.13295300
C	5.41043700	0.97414800	-0.24726200	N	0.91533700	2.55071900	-0.74708400
H	4.80291900	1.81627000	-2.14117400	Ni	-0.42683600	0.96991300	-1.15147800

P	0.79151800	-0.93295800	-0.02750200	C	5.19965800	0.45629700	1.77493600
C	0.64043600	-0.99348500	1.81071400	H	5.82600800	-1.52838900	2.35016200
C	0.10919100	0.13062700	2.46335900	H	4.31308100	-2.65856800	0.73129600
C	1.02913800	-2.10587400	2.57647800	H	4.41344700	2.29551200	0.95898800
C	-0.01980900	0.14702900	3.85453300	H	5.86953100	0.95699400	2.46966000
H	-0.22742700	0.98175400	1.87855500	C	2.67993200	1.44697900	-0.88047900
C	0.89739600	-2.08654100	3.96479100	O	3.22796000	2.44446100	-1.37849300
H	1.42667700	-2.99190000	2.09166900	N	1.40786000	1.06720700	-1.20139200
C	0.37461000	-0.95983500	4.60637600	C	0.85691900	1.86565800	-2.29752600
H	-0.43939300	1.02101000	4.34523200	H	1.52463800	1.84585900	-3.16970500
H	1.19788700	-2.95440500	4.54591200	H	0.78329500	2.93031200	-2.02088500
H	0.26832700	-0.95039700	5.68787400	C	-0.50637500	1.37060400	-2.68270900
C	2.60264900	-0.78970400	-0.35252400	C	-1.13784400	1.73629300	-3.87653800
C	3.05798500	-0.98729500	-1.66975200	C	-2.41567000	1.25805400	-4.14413500
C	3.52194700	-0.39313500	0.62944200	H	-0.62315600	2.38573900	-4.57803900
C	4.40370200	-0.80556400	-1.98915400	C	-2.35047200	0.10299000	-2.04922100
H	2.36215500	-1.29545800	-2.44602000	C	-3.03796100	0.42295600	-3.21142400
C	4.86895500	-0.20875500	0.30443300	H	-2.92128900	1.52741100	-5.06713800
H	3.19249800	-0.23128300	1.65103600	H	-2.78576300	-0.53762700	-1.28952900
C	5.31362600	-0.41430100	-1.00225300	H	-4.03367000	0.02664600	-3.38094000
H	4.74041300	-0.97093700	-3.00921900	N	-1.11317300	0.56337700	-1.79061400
H	5.56981800	0.09306200	1.07836300	Ni	0.07800100	0.20798300	-0.18328200
H	6.36184900	-0.27340900	-1.25186000	H	2.81577000	-1.30850700	-0.71938200
C	0.39688400	-2.63391300	-0.61673300	H	1.03004500	0.07972100	0.90654500
C	-0.87823900	-2.88141200	-1.14690900	C	-1.16446000	-1.18453900	0.76335400
C	1.32117100	-3.69077500	-0.53748100	C	-1.42454100	-0.04707400	1.19799800
C	-1.22982800	-4.16627500	-1.56727200	C	-1.12354500	-2.59403300	0.49234600
H	-1.58717300	-2.06675700	-1.24776500	C	0.08708200	-3.25129600	0.19967700
C	0.96668300	-4.97164700	-0.96225600	C	-2.31969300	-3.34139300	0.53116700
H	2.32292700	-3.51333600	-0.15758100	C	0.09721300	-4.62317200	-0.04073500
C	-0.31122600	-5.21266000	-1.47363700	H	1.00752400	-2.67742200	0.17971700
H	-2.22076700	-4.34182700	-1.97711000	C	-2.29763000	-4.71190200	0.28657200
H	1.69096300	-5.77953200	-0.89769000	H	-3.25600400	-2.83955200	0.75757300
H	-0.58487100	-6.21055000	-1.80628200	C	-1.09146300	-5.35708900	-0.00110000
H	-2.32920700	-0.40054500	0.92887600	H	1.03743200	-5.12188100	-0.25942500
H	-1.15811400	0.04671200	-2.23949700	H	-3.22471600	-5.27769000	0.32106900
				H	-1.07834700	-6.42643500	-0.19280300
5				C	-1.98970700	1.04267000	1.94597300
0 1				C	-1.29347200	2.25297800	2.12674800
C	5.17545500	-0.93954100	1.70835300	C	-3.26951100	0.89288400	2.52052700
C	4.32106000	-1.57357800	0.80326100	C	-1.86386200	3.28339000	2.87097400
C	3.47695200	-0.81716700	-0.01226500	H	-0.30744000	2.36746400	1.68726100
C	3.48776300	0.58299000	0.05578000	C	-3.83087700	1.93041700	3.25938900
C	4.37555300	1.21053800	0.93999600	H	-3.80997000	-0.03940500	2.38490500

C	-3.13146700	3.12786000	3.43764700	H	-3.05557900	2.96647000	-0.48261800
H	-1.31522300	4.21100800	3.00879900	C	-4.79653900	1.98272600	2.27531400
H	-4.81640900	1.80368900	3.69932700	H	-4.16618800	0.44245600	3.64990900
H	-3.57351000	3.93518000	4.01503100	H	-5.15432500	3.45677200	0.73973000
TS2				H	-5.71731400	2.19774400	2.81062400
0 1				C	0.71605500	2.45787800	-1.11794700
C	4.49892000	0.14840700	2.74453600	C	1.95134300	2.11266200	-1.69118400
C	3.14282700	-0.09329600	2.97523600	C	0.27241100	3.79413900	-1.20422500
C	2.40044700	-0.85140800	2.06700300	C	2.72712700	3.08023400	-2.32750700
C	3.00640000	-1.38520200	0.91972400	H	2.29652500	1.08531600	-1.63235900
C	4.37593900	-1.16270700	0.71527300	C	1.05253900	4.75422400	-1.84160300
C	5.11416700	-0.38985600	1.61047900	H	-0.67960200	4.06898300	-0.75985100
H	5.07526200	0.74351100	3.44849500	C	2.28263300	4.40172400	-2.40595000
H	2.66221400	0.30502900	3.86545600	H	3.68155400	2.79861900	-2.76360500
H	4.84925900	-1.61224700	-0.15206900	H	0.70167800	5.78133100	-1.89530100
H	6.17161900	-0.21375100	1.42921400	H	2.88901000	5.15321400	-2.90417400
C	2.28213000	-2.27863700	-0.05896000	6			
O	2.91102300	-3.21719000	-0.57966100	0 1			
N	0.96068300	-2.05315300	-0.29183200	Ni	1.05225000	-0.14283500	-0.04985600
C	0.34414700	-3.09155500	-1.10418000	C	0.87506400	4.29322400	0.65831400
H	0.60989800	-4.09145600	-0.73556300	C	0.54804500	3.22126700	-0.16972100
H	0.70710600	-3.06809100	-2.14614000	C	1.45972900	2.17020200	-0.33809600
C	-1.14793400	-2.92410600	-1.11321500	C	2.69982700	2.18169100	0.33214500
C	-2.00327200	-3.92514100	-1.58538100	C	3.02210900	3.27088700	1.14677300
C	-3.37448000	-3.70201500	-1.60495400	C	2.11534000	4.31796200	1.30862100
H	-1.58200300	-4.86418900	-1.93102800	H	0.17510100	5.11375700	0.78865300
C	-2.95641700	-1.52632000	-0.69640200	H	-0.39441100	3.20518800	-0.70759500
C	-3.86191400	-2.47363500	-1.15260800	H	3.98281300	3.27077200	1.65217600
H	-4.05314300	-4.46991500	-1.96524000	H	2.37206800	5.15967700	1.94676700
H	-3.29365100	-0.56228200	-0.33893500	C	3.62688400	0.99338500	0.26044200
H	-4.92326000	-2.24838500	-1.15232300	O	4.83084300	1.07859500	0.54393300
N	-1.62561300	-1.74167700	-0.66690000	N	2.95132300	-0.12286400	-0.07168000
Ni	-0.11577200	-0.49476100	-0.17177800	C	3.61881100	-1.39786900	0.01277300
H	1.34950900	-1.04744900	2.25533400	H	4.21839000	-1.61820400	-0.88615100
H	1.10836100	0.26836100	0.02298600	H	4.32713400	-1.42911200	0.85514500
C	-1.16928000	1.17594300	0.20215300	C	2.57048500	-2.46626500	0.18224100
C	-0.13317300	1.49346400	-0.45028500	C	2.89502100	-3.81970800	0.30157500
C	-2.40894500	1.43110100	0.89445000	C	1.88626000	-4.75964900	0.47635800
C	-2.74502500	0.71647900	2.06204600	H	3.93852100	-4.11669200	0.26139600
C	-3.29843300	2.42044400	0.42434000	C	0.29780900	-2.96713400	0.39563400
C	-3.92563700	0.99623500	2.74644800	C	0.56107300	-4.32287000	0.52733300
H	-2.06770800	-0.05080300	2.42524200	H	2.12758300	-5.81411700	0.57450400
C	-4.47958600	2.69078500	1.11247100	H	-0.70942000	-2.57395700	0.43024700

H	-0.26132200	-5.01652900	0.66619100	N	2.84012700	0.76994200	-0.20774500
N	1.27707700	-2.05238800	0.22258000	C	3.16902000	2.16931500	-0.11585400
H	1.28303700	1.45984400	-1.16448600	H	3.93065700	2.37150000	0.65506100
C	-0.87005800	-0.08512800	-0.09151300	H	3.58933200	2.55823300	-1.05723000
C	-1.56260500	-0.13596500	1.06886800	C	1.90329600	2.91306500	0.22448000
C	-1.41942600	0.13700900	-1.44783600	C	1.86670400	4.29485000	0.42575800
C	-1.05273000	-0.69979800	-2.52322300	C	0.65855500	4.91345000	0.72701500
C	-2.23982600	1.24926200	-1.73945500	H	2.78524000	4.86735700	0.34102100
C	-1.50277800	-0.45217900	-3.82054600	C	-0.39292900	2.76487800	0.61052800
H	-0.41253500	-1.55734500	-2.33228600	C	-0.49599000	4.13255700	0.82073900
C	-2.67813300	1.50304300	-3.03835200	H	0.61499500	5.98715700	0.88527700
H	-2.53591300	1.91076900	-0.93043900	H	-1.25780500	2.11556500	0.66467600
C	-2.31369200	0.65347200	-4.08712600	H	-1.46097100	4.57133700	1.05122000
H	-1.21121900	-1.12089700	-4.62684400	N	0.77836100	2.16124100	0.32221000
H	-3.30692400	2.36858800	-3.23301500	H	0.44597700	-1.10826900	-0.42568000
H	-2.65438800	0.85353400	-5.09946000	C	-0.82177500	-0.42533800	-0.01946100
C	-3.01949200	-0.14237700	1.33846400	C	-1.51993400	-0.13851400	-1.14725400
C	-3.46995300	0.28775100	2.60218400	C	-1.35015400	-0.94782000	1.26499900
C	-3.98544300	-0.60622700	0.42373200	C	-0.89003800	-0.43849000	2.49462800
C	-4.82494500	0.28436400	2.93083100	C	-2.25178900	-2.03217700	1.29956700
H	-2.74047400	0.63433000	3.33143100	C	-1.33972600	-0.96357400	3.70724000
C	-5.33974800	-0.61566400	0.75393900	H	-0.17164700	0.37700900	2.49612300
H	-3.67086100	-0.97248700	-0.54743800	C	-2.69262600	-2.56305900	2.51037800
C	-5.76959700	-0.16564200	2.00573500	H	-2.60507300	-2.45733000	0.36466100
H	-5.14238300	0.62907100	3.91200200	C	-2.24194000	-2.02867900	3.72122900
H	-6.06359000	-0.98319600	0.03047300	H	-0.97372100	-0.54622000	4.64184500
H	-6.82645200	-0.17459300	2.25929100	H	-3.38614500	-3.40029300	2.50877200
H	-0.97148300	-0.19327000	1.98706300	H	-2.58474400	-2.44460700	4.66485700
TS3				C	-2.96525400	-0.02380600	-1.42204600
0 1				C	-3.38046000	-0.06121200	-2.76820000
Ni	1.07410000	0.25207300	-0.01013400	C	-3.95145300	0.17560500	-0.43486900
C	2.09172300	-4.09324500	-0.57624800	C	-4.72443600	0.06090200	-3.11618400
C	1.26174000	-2.99694600	-0.31042900	H	-2.63264600	-0.19393400	-3.54679300
C	1.73824500	-1.68250200	-0.42074200	C	-5.29379900	0.30769700	-0.78383600
C	3.09604600	-1.49371400	-0.77440900	H	-3.66559300	0.23407200	0.60923900
C	3.91422500	-2.59020500	-1.04401100	C	-5.68928700	0.24375900	-2.12346000
C	3.41642800	-3.89159700	-0.95761600	H	-5.01676700	0.01871700	-4.16219100
H	1.69295600	-5.10059400	-0.48659100	H	-6.03593400	0.46359900	-0.00501700
H	0.22977800	-3.18160500	-0.02264000	H	-6.73806000	0.34365000	-2.39013100
H	4.95149200	-2.39415100	-1.30205300	H	-0.91491000	0.07712800	-2.03038700
H	4.06166600	-4.73951500	-1.17220600	7			
C	3.70419400	-0.11497400	-0.74523700	0 1			
O	4.85327500	0.13293700	-1.13494600	Ni	-0.05169900	-0.82305900	-0.00004600

C	4.14689100	-1.49543900	0.00008700	C	1.09650500	0.68681800	-0.94015000
C	2.77196900	-1.78559800	0.00008500	C	0.92689200	-0.52162200	-1.17768000
C	1.83808800	-0.74533200	-0.00000600	C	1.54207900	2.05391900	-0.94494600
C	2.31115300	0.58004700	-0.00005300	C	2.73561000	2.38332800	-1.62281300
C	3.67155700	0.87803400	-0.00006400	C	0.82411000	3.07188200	-0.28830800
C	4.59576700	-0.17248800	0.00000300	C	3.19350200	3.69722400	-1.63816900
H	4.86915200	-2.30951600	0.00015200	H	3.29288300	1.60433800	-2.13325800
H	2.45605700	-2.82903000	0.00015500	C	1.29098300	4.38445800	-0.31291500
H	3.99586100	1.91595600	-0.00010500	H	-0.10034800	2.82196800	0.22302000
H	5.66219000	0.03919700	-0.00002200	C	2.47510600	4.70146300	-0.98290900
C	1.22686200	1.61340600	-0.00001200	H	4.11293900	3.93930400	-2.16413800
O	1.37768800	2.83849300	-0.00005100	H	0.72630300	5.16315000	0.19181200
N	0.01390500	0.98993000	0.00011300	H	2.83571200	5.72619600	-1.00018100
C	-1.23888700	1.70898700	0.00006000	C	0.99044800	-1.86330900	-1.68981700
H	-1.33274300	2.36568600	0.87959900	C	-0.05939800	-2.78164100	-1.49362500
H	-1.33266500	2.36571600	-0.87946300	C	2.12978300	-2.26955900	-2.41519200
C	-2.36932700	0.70874600	0.00002300	C	0.02904400	-4.06967800	-2.01655000
C	-3.71457700	1.08539200	0.00005000	H	-0.93926400	-2.47173400	-0.94004600
C	-4.69963600	0.10345700	0.00002300	C	2.20999500	-3.56106800	-2.92920200
H	-3.97448700	2.13937400	0.00009100	H	2.94453200	-1.56821500	-2.57073800
C	-2.96823700	-1.54748000	-0.00005600	C	1.16077300	-4.46457200	-2.73350200
C	-4.32147000	-1.24224800	-0.00001200	H	-0.79209000	-4.76457200	-1.86564500
H	-5.74975900	0.38063100	0.00006100	H	3.09036600	-3.85981000	-3.49169500
H	-2.62029800	-2.57668400	-0.00009900	H	1.22526400	-5.47029600	-3.13999700
H	-5.05852800	-2.03819200	-0.00001900	H	-1.72023900	-1.40580600	3.41972500
N	-2.01242600	-0.59740700	-0.00003100	C	0.25477200	-0.65513400	3.10061200
8				C	0.94995400	-0.99549600	4.26578300
0 1				C	2.23316900	-0.65909900	1.87699900
Ni	-0.37278100	-0.01115800	0.38721000	C	2.32954000	-1.16355600	4.21452000
C	-3.16504000	0.99662500	-2.70938000	H	0.40288000	-1.12537300	5.19447000
C	-1.93371100	0.72481400	-2.09084500	C	2.98712900	-0.99529000	2.99228200
C	-1.88160300	0.41794400	-0.72792600	H	2.69492500	-0.51735200	0.90594400
C	-3.09035400	0.40730800	-0.00639100	H	2.88657100	-1.42360200	5.10998400
C	-4.31651200	0.66988400	-0.61299200	H	4.06160500	-1.11680500	2.90487600
C	-4.35470700	0.96334600	-1.97895500	N	0.89714600	-0.49013700	1.92214300
H	-3.19019400	1.23083700	-3.77189900	H	-1.53419400	0.29220400	3.80571800
H	-1.03001000	0.75598200	-2.69277700	TS4			
H	-5.22247000	0.64210800	-0.01172800	0 1			
H	-5.30290600	1.17077600	-2.46903700	Ni	0.41806800	0.72256000	-0.29233500
C	-2.95054900	0.09488400	1.44945300	C	-3.11111700	0.60441300	-2.77564500
O	-3.87640600	0.04224000	2.26760100	C	-1.97630000	0.09313300	-2.13151600
N	-1.64019500	-0.12662800	1.72932400	C	-1.43792400	0.74171000	-1.01180400
C	-1.23948700	-0.47577600	3.07139200	C	-2.01622100	1.96998900	-0.59739200

C	-3.15742800	2.45491100	-1.22884100	H	5.54526800	0.53418300	-0.38315400
C	-3.72431000	1.76380100	-2.30468300	N	2.28490800	1.27428600	0.03137500
H	-3.52122100	0.07723100	-3.63325700				
H	-1.54508700	-0.83956600	-2.48009600	9			
H	-3.55634600	3.40881700	-0.89349700	O 1			
H	-4.61840100	2.14736300	-2.78914900	Ni	1.20677300	-0.15079100	-0.00825300
C	-1.22997600	2.87663500	0.32182600	C	-3.55205700	3.35355000	-1.05584600
O	-1.69620400	3.88634400	0.86759400	C	-3.24801200	2.04228100	-0.71651900
N	0.04487000	2.45095700	0.34375500	C	-1.97859100	1.64370100	-0.23312500
C	0.36605100	-1.19932500	-0.35432100	C	-0.99618800	2.65909500	-0.04896100
C	-0.81865800	-0.82429800	0.02650000	C	-1.34169000	3.98571900	-0.38075500
C	1.23283300	-2.36427900	-0.39001600	C	-2.58177500	4.34116000	-0.89563300
C	1.07303200	-3.34905000	-1.38652000	H	-4.54036300	3.59787500	-1.43722200
C	2.25821600	-2.53643700	0.56202600	H	-4.01489900	1.28714000	-0.83972200
C	1.90666100	-4.46600400	-1.42314200	H	-0.59778200	4.75272300	-0.20027900
H	0.29386200	-3.22741400	-2.13392400	H	-2.78971500	5.37714400	-1.15012300
C	3.08236900	-3.66062400	0.52450300	C	0.40205000	2.61008900	0.55618100
H	2.38928000	-1.79031700	1.34035900	O	0.71690700	3.55985600	1.29649100
C	2.91399000	-4.62904500	-0.46853900	N	1.33174300	1.69883200	0.15422800
H	1.76621100	-5.21339400	-2.19982800	C	-0.60536500	-0.42303400	0.04939100
H	3.85801100	-3.78037800	1.27664700	C	-1.79985300	0.18644900	-0.00032300
H	3.56093200	-5.50144500	-0.49865500	C	-0.18249400	-1.82214300	0.01872300
C	-1.96667200	-1.32362800	0.78813300	C	-0.30786400	-2.63219700	-1.14695400
C	-2.28382800	-2.69235000	0.69834200	C	0.65818100	-2.29509700	1.06228500
C	-2.72145200	-0.50733600	1.64622300	C	0.31783400	-3.86495600	-1.22771700
C	-3.32590900	-3.22678100	1.45385100	H	-0.91248100	-2.26905500	-1.97130200
H	-1.70664800	-3.33159000	0.03723500	C	1.29901100	-3.54271400	0.96213700
C	-3.76077200	-1.04882300	2.40100400	H	0.72613800	-1.72804400	1.98697100
H	-2.49140300	0.55001800	1.72374400	C	1.12686600	-4.32534100	-0.17215600
C	-4.06945600	-2.40809900	2.30738700	H	0.18910900	-4.47750200	-2.11615000
H	-3.55915600	-4.28522600	1.37156300	H	1.91484000	-3.89481500	1.78513100
H	-4.33189600	-0.40391300	3.06343100	H	1.61379500	-5.29397500	-0.24668200
H	-4.88404400	-2.82570900	2.89302300	C	-3.03763900	-0.66165100	0.16627800
C	1.09808000	3.15719500	1.02471500	C	-3.59233600	-1.38306300	-0.90225600
H	1.15576000	4.21398900	0.72201800	C	-3.65031800	-0.75636200	1.42579100
H	0.96466000	3.16592000	2.12076900	C	-4.71996600	-2.18640400	-0.71477900
C	2.39499800	2.45889600	0.68453600	H	-3.14637200	-1.30219900	-1.88987000
C	3.64719500	2.99048600	1.00011000	C	-4.77568800	-1.56019300	1.61502600
C	4.79907000	2.30670300	0.62457900	H	-3.23710400	-0.19579100	2.26034000
H	3.70485100	3.93838300	1.52641100	C	-5.31404800	-2.27936200	0.54516100
C	3.40213800	0.61615300	-0.33617500	H	-5.13483900	-2.73677100	-1.55566900
C	4.67530100	1.09798800	-0.06351800	H	-5.23250100	-1.62381000	2.59948500
H	5.77917900	2.71311800	0.85733100	H	-6.19104000	-2.90442000	0.69207900
H	3.25201100	-0.32481200	-0.85199400	C	2.68088100	2.06375600	0.60804500

H	2.72219900	2.16248500	1.70455000	H	-2.53785800	-1.19794800	-2.01553400
H	2.96473400	3.05124300	0.22115600	C	-5.54925800	-0.91788600	-0.45920400
C	3.68013400	1.02917800	0.17989300	H	-5.93473300	0.34177000	1.25074400
C	5.05496400	1.26744000	0.09842700	H	-4.84864400	-2.05610200	-2.15257800
C	3.98694500	-1.19492800	-0.45206100	H	-6.56876500	-1.28937800	-0.52255700
C	5.90381400	0.22821700	-0.26904300	C	0.99695600	1.66889200	1.10497800
H	5.44213000	2.25696500	0.32012300	O	1.86761800	2.12306600	1.86188900
C	5.36157300	-1.02951900	-0.54958300	N	0.99036200	0.31715600	0.75765900
H	3.51075900	-2.14852200	-0.65697600	Ni	1.15770400	-0.05461200	-1.07673300
H	6.97483300	0.39500000	-0.33995600	C	2.09033900	-0.48511200	1.31570800
H	5.98962300	-1.86463000	-0.84141500	C	3.34305500	-0.38247400	0.44938700
N	3.16737300	-0.18737100	-0.09638400	C	4.62543300	-0.53464900	0.97475000
TSS				C	4.21052900	-0.10870700	-1.69533700
O 1				C	5.72609900	-0.47462200	0.12134500
C	-0.86467200	4.78426600	0.19085700	C	5.51641000	-0.25798100	-1.24082300
C	0.08841200	3.89659900	0.65953400	H	3.99619800	0.07007900	-2.74456900
C	-0.07346400	2.50274700	0.52525200	H	6.73208500	-0.58730400	0.51524300
C	-1.25459100	1.97682200	-0.08370100	H	6.34418900	-0.19758700	-1.93986900
C	-2.21997900	2.91565500	-0.53879300	N	3.14376700	-0.17116700	-0.87723300
C	-2.02924600	4.28043200	-0.41542500	H	2.31010800	-0.15630700	2.33460600
H	-0.71489000	5.85586400	0.29066400	H	1.76241500	-1.52992100	1.35011300
H	0.99086900	4.24986600	1.14735500	H	4.75415800	-0.69057100	2.04126800
H	-3.12220800	2.54604100	-1.01406000	P1			
H	-2.78397200	4.96359800	-0.79751000	O 1			
C	-1.49246400	0.54902300	-0.18617100	C	-2.25424800	-2.87111300	-0.35705100
C	-0.42153400	-0.35718000	-0.12683100	C	-1.18951700	-2.02716900	0.03912600
C	-0.60580900	-1.79892000	0.22224600	C	0.04111300	-2.63493100	0.38419100
C	-0.25255500	-2.81589300	-0.68277700	C	0.18924300	-4.03262300	0.34477900
C	-1.08149200	-2.17523600	1.49184800	C	-0.86964300	-4.83838500	-0.03747500
C	-0.38359900	-4.16246700	-0.33911300	C	-2.09487900	-4.24700600	-0.39118000
H	0.11316700	-2.54326100	-1.67047200	H	-3.20498900	-2.43276700	-0.63902900
C	-1.20455000	-3.52043800	1.83972200	H	1.15172300	-4.45183200	0.61842600
H	-1.35437400	-1.40257500	2.20504800	H	-0.75467300	-5.91822400	-0.06782800
C	-0.85769500	-4.51879200	0.92541400	H	-2.92829200	-4.87358600	-0.69876600
H	-0.11498300	-4.93181400	-1.05853700	C	1.19198500	-1.82498100	0.78903000
H	-1.57417600	-3.79016700	2.82577000	O	2.28147400	-2.29594200	1.12573900
H	-0.95684100	-5.56658200	1.19656700	N	0.99971300	-0.43755800	0.79051100
C	-2.89546400	0.04943700	-0.29415900	C	-1.30350400	-0.58033200	0.09170100
C	-3.88600000	0.47826500	0.61232800	C	-0.21467000	0.17121900	0.45653300
C	-3.27586300	-0.86802700	-1.29050200	C	-2.60057600	0.06765400	-0.28594700
C	-5.19344000	0.00035500	0.53230600	C	-2.75034500	0.71046400	-1.52395700
H	-3.62030100	1.18539200	1.39306600	C	-3.70851900	0.01023200	0.57498300
C	-4.58339300	-1.34917700	-1.37022700	C	-3.96669300	1.29201600	-1.88518800

H	-1.90582000	0.75314000	-2.20598800	C	-2.99251800	0.27779600	0.73262000
C	-4.92581700	0.59019300	0.21487000	O	-3.95681200	-0.36636600	1.15010600
H	-3.61244900	-0.49022700	1.53525500	N	-1.70486600	-0.13276900	0.92879900
C	-5.05803700	1.23502500	-1.01663300	C	-1.38639300	-1.41716200	1.53705000
H	-4.06097700	1.78833100	-2.84769700	H	-2.21155300	-1.67978300	2.20145000
H	-5.76956800	0.54021000	0.89855000	H	-0.47077600	-1.30044400	2.12670200
H	-6.00524500	1.68779800	-1.29797700	C	-1.17809900	-2.50722100	0.50527700
C	-0.29856100	1.66468400	0.54651700	C	-2.19899900	-3.39919200	0.17570300
C	0.29665300	2.48554600	-0.42418900	C	-1.98356200	-4.36764600	-0.80313300
C	-1.00415600	2.26141900	1.60200200	H	-3.15411600	-3.31583500	0.68339500
C	0.17925100	3.87326600	-0.34112800	C	0.23234400	-3.49145900	-1.06141600
H	0.86704000	2.02788500	-1.22618600	C	-0.73935000	-4.41275400	-1.43246100
C	-1.11684300	3.64996100	1.68355400	H	-2.76890000	-5.06925000	-1.06839200
H	-1.46848300	1.63494400	2.35800500	H	1.21270500	-3.49569200	-1.52547900
C	-0.52810600	4.45938600	0.71070500	H	-0.51696700	-5.14767900	-2.19933000
H	0.64178000	4.49712100	-1.10162200	N	0.03064000	-2.54830200	-0.11193700
H	-1.66734100	4.09755500	2.50680700	Ni	1.46562300	-1.30653100	0.26134800
H	-0.61890800	5.54070800	0.77220600	H	-1.33567800	1.52589000	-1.14764600
C	2.17860000	0.32658500	1.22244700	H	-0.93062300	0.41820200	0.58263500
H	1.85974200	1.34533800	1.44362600	C	2.50461400	0.15397400	1.07161200
H	2.55065500	-0.12414000	2.14473200	H	2.68401000	-0.13906100	2.11084900
C	3.29757100	0.35203500	0.19283900	C	3.24222100	-0.49672100	0.06703300
C	4.62982100	0.21110000	0.59711000	H	3.95760600	-1.26675600	0.37280800
C	3.92905600	0.62180600	-2.00047400	C	1.96893500	1.56057300	0.90711700
C	5.63763700	0.29662700	-0.35966800	H	1.64736700	1.74188300	-0.12441300
H	4.86540200	0.02603500	1.64093100	H	1.07682900	1.69160700	1.53674800
C	5.28334200	0.50536200	-1.69258700	C	3.55295700	0.14923000	-1.26645500
H	3.60966700	0.77778000	-3.02973700	H	3.68559200	-0.63055000	-2.02962500
H	6.68013200	0.18909800	-0.07209000	H	2.71722400	0.76927300	-1.60840200
H	6.03323700	0.56966800	-2.47525300	C	2.97390200	2.65138400	1.31904500
N	2.95237500	0.55390900	-1.08647600	H	2.45076000	3.62053600	1.30175300
				H	3.23413000	2.49930900	2.37968700
3'				C	4.84064700	0.99423300	-1.25274500
0 1				H	5.68447400	0.33379800	-0.99231100
C	-3.64425800	4.01336200	-1.30849700	H	5.05050600	1.30996300	-2.28711500
C	-2.47463000	3.29529300	-1.56612400	C	4.97751000	2.22924200	-0.38766300
C	-2.23648700	2.08617700	-0.91109400	H	5.92271900	2.72797800	-0.61834800
C	-3.17133400	1.58154200	0.00518700	C	4.27836200	2.85052400	0.57695700
C	-4.35260400	2.29848500	0.24198200	H	4.77903400	3.74352000	0.96040100
C	-4.58403800	3.51118500	-0.40385800				
H	-3.82681800	4.95618800	-1.81740700	TS1'			
H	-1.74936900	3.67202400	-2.28225000	Ni	-0.37590900	0.50224700	0.41524300
H	-5.07827600	1.88742600	0.93616000	N	-1.33857800	-1.18026800	0.67299200
H	-5.49857200	4.06366700	-0.20530200	C	0.82523800	2.08993700	0.41613300

C	1.42963000	1.07000500	1.16920700	H	-4.10674500	3.48386600	-1.76154500
C	-1.19518400	-2.52226800	0.42915800	H	-0.07262400	-0.69509800	1.25991700
C	-2.64303800	-0.74087900	1.17133100				
H	0.28107400	2.86982900	0.95437600	4'			
C	1.35097900	2.49982600	-0.94352300	0 1			
H	1.30320600	1.10519300	2.25254000	C	4.63736000	-2.14285600	-0.71452300
C	2.67928600	0.34445600	0.71943000	C	3.60335300	-1.67247800	-1.52785900
C	0.10304000	-2.98354500	-0.17491200	C	2.86636000	-0.54890700	-1.14789000
O	-2.08219700	-3.35215300	0.67057800	C	3.16278800	0.12704400	0.04418400
H	-3.34427800	-1.57898200	1.14551000	C	4.22433000	-0.33277500	0.83561200
H	-2.56261600	-0.41541400	2.22010900	C	4.94546900	-1.46905600	0.47062900
C	-3.13822500	0.42245800	0.33718600	H	5.20619200	-3.02207900	-1.00681600
H	1.75280600	1.63736000	-1.48583300	H	3.37230000	-2.18013400	-2.46139200
H	0.53072900	2.89050400	-1.56133600	H	4.47720000	0.21841400	1.73603400
C	2.42090100	3.60465900	-0.87920200	H	5.75468200	-1.82310900	1.10463000
H	2.71236200	-0.64922700	1.18184700	C	2.47503100	1.40492500	0.45894100
H	2.67467500	0.17373700	-0.36098600	O	3.16593500	2.30165700	0.97287100
C	3.97227500	1.07771200	1.11832600	N	1.14490700	1.55969000	0.19908600
C	0.83611800	-2.22233300	-1.09552600	C	0.68963000	2.92397100	0.45535100
C	0.54468000	-4.27703400	0.14302000	H	1.33010900	3.65457300	-0.05731700
C	-4.49274600	0.70361500	0.15613600	H	0.76675700	3.18343800	1.52462700
N	-2.17517400	1.20163900	-0.20579200	C	-0.73493700	3.10013800	0.01784200
H	2.65042400	3.91288100	-1.91141700	C	-1.32121300	4.36263300	-0.12922900
H	1.96619200	4.49872600	-0.42126700	C	-2.65193300	4.45762500	-0.51791800
C	3.74743700	3.39099500	-0.18349700	H	-0.72776900	5.25177100	0.06055300
H	3.99664900	1.16521800	2.21731000	C	-2.72666700	2.06749600	-0.58550200
H	4.81745400	0.41321900	0.88018300	C	-3.37294800	3.28343300	-0.75363800
C	4.32902000	2.44179100	0.56817200	H	-3.12217500	5.42919700	-0.64002000
C	1.99646300	-2.74094000	-1.67597300	H	-3.25218800	1.13273100	-0.75399200
H	0.48576000	-1.23168900	-1.37168100	H	-4.41315500	3.30761000	-1.06093000
C	1.71348600	-4.78588500	-0.41898000	N	-1.43640700	1.97014900	-0.20930600
H	-0.04618500	-4.87272700	0.83159100	Ni	-0.27849800	0.32419600	0.11400200
C	-4.86233400	1.81255300	-0.60293700	H	2.06486400	-0.18292900	-1.78155000
H	-5.24133800	0.05626500	0.60253900	H	0.66459300	-0.72307600	0.44118400
C	-2.53565100	2.27075500	-0.93533200	C	-1.83715100	-0.98546000	0.69496300
H	4.38201700	4.26777200	-0.33599000	H	-2.57583200	-0.24344800	0.99754100
H	5.33586900	2.71266100	0.89693800	C	-1.58022900	-1.16519200	-0.64714800
C	2.44236100	-4.01853600	-1.33296600	H	-2.11533800	-0.55671600	-1.37666500
H	2.54846300	-2.14812300	-2.40093900	C	-1.48550200	-2.00938500	1.74331200
H	2.05168100	-5.78398200	-0.15259700	H	-0.56085500	-2.53165000	1.48669400
C	-3.86503300	2.61287300	-1.16112100	H	-1.30347100	-1.50527400	2.70002100
H	-5.91170200	2.04539500	-0.76034500	C	-0.92980300	-2.40616200	-1.20100900
H	-1.72478900	2.86509500	-1.34412600	H	-0.39378100	-2.15913200	-2.12502500
H	3.34801700	-4.41905300	-1.78140200	H	-0.18577200	-2.80318800	-0.50676200

C	-2.62046900	-3.02798200	1.95634300	H	-2.40405000	-0.70334200	-1.40249700
H	-2.33004000	-3.67429600	2.79868900	C	-1.04894800	-1.95791500	1.55949600
H	-3.51284700	-2.49185100	2.31859600	H	-0.24230900	-2.54092700	1.10543800
C	-1.96623200	-3.49452200	-1.53797800	H	-0.59949900	-1.36324200	2.36324300
H	-2.64464700	-3.10731700	-2.31588600	C	-1.34295300	-2.65329100	-1.35789100
H	-1.42968800	-4.31986000	-2.03017900	H	-1.10449500	-2.50504500	-2.41613100
C	-2.84038700	-4.11528500	-0.46843400	H	-0.41994000	-2.99601100	-0.88176500
H	-3.43464700	-4.91801100	-0.91166400	C	-2.06796900	-2.92075000	2.19900000
C	-3.08493600	-3.94093900	0.84125600	H	-1.55036200	-3.45979300	3.00656700
H	-3.83500500	-4.63288800	1.23230500	H	-2.83938400	-2.32611700	2.71426500
4r'				C	-2.41696900	-3.75350700	-1.26372300
C	4.72725100	-2.07662800	-0.43258900	H	-3.30404200	-3.42849400	-1.83183800
C	5.27936900	-0.79435000	-0.50854000	H	-2.04109400	-4.62507100	-1.82050800
C	4.50581100	0.31920200	-0.18606300	C	-2.92093800	-4.26965700	0.06770900
C	3.16092900	0.17408700	0.18641500	H	-3.58360000	-5.12116100	-0.10505800
C	2.61936600	-1.11394700	0.26492900	C	-2.79215000	-3.95787200	1.36812200
C	3.39809700	-2.23328600	-0.03547100	H	-3.37164700	-4.60894400	2.02699400
H	5.33182500	-2.94752000	-0.67358900	2			
H	6.31583400	-0.66437600	-0.81010900	0 1			
H	1.58925400	-1.23924600	0.57689900	C	-5.49461300	0.45821900	-0.01274000
H	2.96607900	-3.22824200	0.04054800	C	-4.55664700	1.38479400	0.44601900
C	2.40358200	1.41746300	0.57562500	C	-3.20139200	1.05429900	0.47270600
O	3.03780200	2.34610700	1.10769700	C	-2.77079300	-0.20922700	0.04110800
N	1.05916100	1.47668100	0.34270900	C	-3.72238700	-1.14122100	-0.39702200
C	0.47000600	2.69538700	0.88690000	C	-5.07393600	-0.80670000	-0.43238100
H	1.10064400	3.56561800	0.65406300	H	-6.54973600	0.71748400	-0.03544000
H	0.43864500	2.66619400	1.98909100	H	-4.87925800	2.36282100	0.79271300
C	-0.91969300	2.95847200	0.37335600	H	-2.49003200	1.77551600	0.86667600
C	-1.65893900	4.07361500	0.79179800	H	-3.38312100	-2.12431600	-0.70681300
C	-2.92396600	4.29265300	0.26218700	H	-5.80087700	-1.53373700	-0.78425900
H	-1.22980400	4.75608000	1.51912400	C	-1.33087200	-0.64515600	0.05768500
C	-2.65254500	2.30691000	-1.04146700	O	-1.02407700	-1.83240700	0.15241500
C	-3.43496800	3.39251500	-0.68004800	N	-0.41509500	0.37237500	-0.05465100
H	-3.50723300	5.15511400	0.57204400	H	-0.78879400	1.29122600	-0.25207600
H	-3.00097200	1.57660300	-1.76636700	C	0.99597800	0.29837600	-0.05950600
H	-4.41541100	3.53029900	-1.12360600	C	1.70269500	1.48063200	-0.34351800
N	-1.42713200	2.09138100	-0.52124600	C	1.71944600	-0.86787600	0.21611700
Ni	-0.09666200	0.53575300	-0.96591000	C	3.08898600	1.49840500	-0.35331500
H	4.93170600	1.31720300	-0.21093700	H	1.15614200	2.39694500	-0.55836400
H	0.69468500	-0.44006200	-1.93364000	C	3.11724100	-0.84960800	0.20690800
C	-1.68559300	-1.04490900	0.54982100	H	1.19045800	-1.78589300	0.42903700
H	-2.16618600	-0.14672800	0.93344900	C	3.81356200	0.32930100	-0.07719400
C	-1.80023300	-1.34905300	-0.76156800	H	3.63172100	2.41282600	-0.57254700

H	3.64657100	-1.77053600	0.42372200	C	3.14713600	1.29010000	-1.14880900
O	5.17314200	0.44824800	-0.11146500	C	4.10382600	0.16659000	0.76504900
C	5.95375900	-0.70213100	0.18236700	C	0.79370700	-2.88284700	-1.72391400
H	5.76218700	-1.07412200	1.19753200	C	3.16484900	-2.41391500	-1.75103500
H	5.77566300	-1.51074200	-0.53890600	C	0.87128000	-0.92483300	2.61330800
H	6.99605800	-0.38347000	0.11027600	C	2.26865400	-2.73057800	1.80962200
				C	4.27953000	2.09879800	-1.24323000
10				H	2.32484000	1.42752300	-1.84611100
O 1				C	5.23255300	0.98537900	0.67660800
C	0.86758100	5.43245800	-0.38182600	H	4.04497100	-0.57806900	1.55263500
C	0.43873900	4.62381400	-1.43792000	C	0.98989400	-3.94284800	-2.60888500
C	0.58482300	5.05452300	0.93289500	H	-0.20970500	-2.64507700	-1.37735600
H	1.42005000	6.34647400	-0.58291500	C	3.35869100	-3.46981900	-2.64598900
C	-0.26645000	3.44808100	-1.18361800	H	4.01737100	-1.82467900	-1.42710500
H	0.65858700	4.90488600	-2.46465800	C	0.88506900	-1.48682700	3.89125900
C	-0.12539400	3.88357500	1.18978700	H	0.30194500	-0.01698800	2.42977900
H	0.91455800	5.67637300	1.76124500	C	2.27308000	-3.29389800	3.08772000
C	-0.56464500	3.06321200	0.13733900	H	2.80435000	-3.22734500	1.00592700
H	-0.54797600	2.82092000	-2.02567400	C	5.32538100	1.94913500	-0.32878300
H	-0.36147800	3.58385200	2.20501300	H	4.33932800	2.85440300	-2.02226000
C	-1.33551400	1.83063000	0.52133500	H	6.03850900	0.86821500	1.39660900
O	-1.59335700	1.55240600	1.70393900	C	2.27440300	-4.23793500	-3.07354200
N	-2.06392000	1.18497500	-0.57506900	H	0.13954600	-4.53242800	-2.94164800
C	-3.28903400	0.46775800	-0.33880600	H	4.35994600	-3.69141900	-3.00673800
H	-2.14603400	1.78001400	-1.39615700	C	1.58492100	-2.67145300	4.13151800
C	-3.37172000	-0.55439400	0.61831500	H	0.33888800	-1.00193100	4.69619000
C	-4.41636400	0.78323300	-1.09668200	H	2.81375500	-4.22009500	3.26582600
C	-4.56684900	-1.23628300	0.80422100	H	6.20364500	2.58611200	-0.39462000
H	-2.50322900	-0.80122400	1.21558200	H	2.42744900	-5.05810300	-3.77010100
C	-5.61844700	0.09075600	-0.92334500	H	1.58734500	-3.11219300	5.12514700
H	-4.36666600	1.57786300	-1.83837400				
C	-5.69974100	-0.92480900	0.03545700	TS6			
H	-4.64238700	-2.02623700	1.54527300	O 1			
H	-6.47337400	0.35756400	-1.53375900	Ni	-0.30190100	0.42656300	0.20897100
O	-6.81669200	-1.66443800	0.29210100	C	0.72563700	5.78819200	0.11593400
C	-7.99567100	-1.37711600	-0.44593700	C	1.06131600	4.51887100	0.58993800
H	-8.75584900	-2.07042300	-0.07905500	C	0.10827400	3.49802200	0.59888700
H	-8.33916400	-0.34754900	-0.27898800	C	-1.19255500	3.73433400	0.13269900
H	-7.85127700	-1.54133400	-1.52225800	C	-1.52468500	5.02066900	-0.32232100
Ni	-0.34641700	0.26102200	-0.50656800	C	-0.57268700	6.03721100	-0.33940900
P	1.51474700	-0.72541100	-0.10266700	H	1.46895200	6.58147300	0.10816700
C	3.04929100	0.30775800	-0.14927500	H	2.06491600	4.31998400	0.95671700
C	1.87959600	-2.10978700	-1.27791200	H	-2.54004300	5.20287600	-0.65886000
C	1.57154700	-1.53764500	1.56001100	H	-0.84323300	7.02476900	-0.70398100

C	-2.28976600	2.70576100	0.11465500	C	-4.55280700	-1.11685100	1.02820700
O	-3.46934900	3.05632300	0.13806400	H	-3.14187600	0.13025000	2.07473000
N	-1.92183700	1.36572100	0.04918400	C	-5.05073200	-1.50163500	-0.22241900
H	0.37555000	2.51502000	0.98266300	H	-4.90862100	-1.23639700	-2.34951100
P	1.51298000	-0.74090900	-0.00130100	H	-4.95034600	-1.54008900	1.94364500
C	1.95548600	-1.63948800	1.55185600	O	-6.04422300	-2.41626600	-0.41576700
C	1.66262200	-1.00440800	2.77085000	C	-6.63852400	-3.01511200	0.72695400
C	2.54333700	-2.91336600	1.57550800	H	-7.11653300	-2.26862800	1.37495300
C	1.96267900	-1.62183400	3.98550700	H	-7.40158300	-3.69742700	0.34568100
H	1.19369300	-0.02257700	2.76546000	H	-5.90738800	-3.58847300	1.31268300
C	2.83704700	-3.53320300	2.79236200				
H	2.76722600	-3.42721600	0.64545300	11			
C	2.55092400	-2.88879500	3.99780000	0 1			
H	1.73120400	-1.11665700	4.91945700	C	6.22214100	-1.31026200	-0.23063200
H	3.28909100	-4.52158600	2.79687100	C	5.12795200	-1.33147000	-1.09958400
H	2.77850800	-3.37525300	4.94259200	C	4.14457700	-0.34513500	-1.01444100
C	3.03496600	0.21713400	-0.42759600	C	4.24812600	0.68229800	-0.06537400
C	2.91536700	1.25393600	-1.36880900	C	5.36100900	0.70736500	0.78728900
C	4.28909200	-0.03624500	0.14823300	C	6.33647100	-0.28650900	0.71341900
C	4.02879700	2.01040100	-1.73466300	H	6.98469800	-2.08267300	-0.29419500
H	1.94532300	1.47198500	-1.80773100	H	5.04074600	-2.11663200	-1.84661500
C	5.40091100	0.72890100	-0.21352400	H	5.44813700	1.52133100	1.49979000
H	4.40082000	-0.82703800	0.88363800	H	7.18810200	-0.26053400	1.38880800
C	5.27383500	1.75098700	-1.15578600	C	3.25701200	1.81480400	0.04131300
H	3.92107600	2.80816700	-2.46469600	O	3.62451300	2.89230900	0.52907500
H	6.36547600	0.52490000	0.24409500	N	2.01252100	1.58519000	-0.48351600
H	6.13927900	2.34647200	-1.43437800	Ni	0.67655000	0.27592600	-0.28137100
C	1.43605200	-2.06344100	-1.28804300	P	-0.96440000	-1.16629700	0.05056200
C	0.20195700	-2.69874300	-1.50315100	C	-0.65691000	-2.77011000	-0.79893200
C	2.54640100	-2.45810700	-2.04972700	C	0.06005800	-2.75037400	-2.00581200
C	0.08439300	-3.71746800	-2.44909100	C	-1.11745300	-3.99664200	-0.29757200
H	-0.66949000	-2.38706200	-0.93308900	C	0.29885900	-3.93327500	-2.70614900
C	2.42406800	-3.47211200	-3.00276000	H	0.44104600	-1.80760500	-2.38983000
H	3.50600500	-1.97081500	-1.90665800	C	-0.86933200	-5.18001200	-0.99593600
C	1.19539600	-4.10448700	-3.20261000	H	-1.66075600	-4.03399400	0.64166400
H	-0.87668900	-4.20040600	-2.60412700	C	-0.16566500	-5.15015000	-2.20174900
H	3.29022100	-3.76489700	-3.59051100	H	0.85468800	-3.90457000	-3.63940100
H	1.10242800	-4.89100500	-3.94685700	H	-1.22531200	-6.12531200	-0.59513400
H	-0.93200000	1.16241600	-0.96240800	H	0.02738800	-6.07291600	-2.74233500
C	-2.98897600	0.40394700	-0.04977200	C	-2.63742400	-0.63796100	-0.51958200
C	-3.49864000	0.01571700	-1.29848500	C	-3.12421300	0.59971900	-0.06511200
C	-3.52375600	-0.17363400	1.10418400	C	-3.41995600	-1.39498400	-1.40339400
C	-4.51209200	-0.92926900	-1.38643100	C	-4.37276900	1.06320600	-0.47762800
H	-3.09204700	0.46126400	-2.20219000	H	-2.52500300	1.20341600	0.61086800

C	-4.66844400	-0.92453100	-1.81956700	H	-4.84132100	2.50365000	0.00000400
H	-3.06072800	-2.35175500	-1.76821200	H	-2.41141200	1.91681500	-0.00056600
C	-5.14724300	0.30211200	-1.35778200	H	-3.37372900	-2.23199900	0.00028500
H	-4.73331900	2.02441500	-0.12170100	H	-5.81983500	-1.68775000	0.00095500
H	-5.26469200	-1.52055500	-2.50539000	C	-1.27173700	-0.59030400	-0.00049200
H	-6.11734600	0.66671400	-1.68479300	O	-1.01639600	-1.82451500	-0.00079600
C	-1.21063200	-1.57820700	1.83004300	N	-0.44874100	0.46363500	-0.00028200
C	-0.11403300	-1.51092900	2.70489800	C	0.92864700	0.32058600	-0.00023100
C	-2.46397700	-1.96527400	2.33321400	C	1.68481600	1.52429800	-0.00021400
C	-0.26780100	-1.83642100	4.05359400	C	1.68504200	-0.87960700	-0.00008400
H	0.85543500	-1.19896000	2.32854500	C	3.07168800	1.53899100	-0.00005000
C	-2.61292000	-2.28872100	3.68284500	H	1.13096700	2.46070900	-0.00032400
H	-3.32571300	-2.00789500	1.67403700	C	3.08505500	-0.86957100	0.00011500
C	-1.51549300	-2.22630800	4.54451600	H	1.14568300	-1.81726600	-0.00012300
H	0.58804200	-1.77833000	4.72047000	C	3.79123100	0.33562000	0.00013400
H	-3.58769900	-2.58648500	4.05994400	H	3.62157000	2.47751600	-0.00004100
H	-1.63382700	-2.47515600	5.59573900	H	3.61203700	-1.81973300	0.00026700
H	3.29688800	-0.36043700	-1.69009500	O	5.16915300	0.45124800	0.00038900
H	1.54325100	-0.79299600	0.19598200	C	5.92340900	-0.74199700	0.00033300
C	0.99412300	2.55282000	-0.45973300	H	5.72981300	-1.35452600	0.89344800
C	-0.01536700	2.39750600	-1.44592500	H	5.72986100	-1.35442800	-0.89285900
C	0.80061700	3.55447800	0.52366700	H	6.97545900	-0.44102500	0.00038500
C	-1.16152500	3.19880200	-1.44873800				
H	0.15807100	1.70530400	-2.26835600	12			
C	-0.32909400	4.36031800	0.50514300	-1 1			
H	1.56364200	3.70106900	1.27602700	Ni	-0.04799500	-0.09976300	-0.28458000
C	-1.32641500	4.18607000	-0.47675000	P	-0.40918900	2.02347600	0.03996400
H	-1.92069700	3.08061200	-2.21528900	P	1.49290100	-1.23159600	0.74264800
H	-0.43458500	5.12625700	1.26586900	C	1.89371500	-3.00042400	0.24783300
O	-2.46544100	4.93181200	-0.55925600	C	1.15268000	-3.57265700	-0.79347300
C	-2.67076300	5.96526800	0.39545600	C	2.86036000	-3.78813100	0.89712500
H	-3.62033200	6.43365800	0.12721800	C	1.37453800	-4.89692800	-1.18608500
H	-2.74334900	5.56752900	1.41638700	H	0.39365600	-2.97380800	-1.28669500
H	-1.87550400	6.72078400	0.35596900	C	3.08484100	-5.10805200	0.50667700
				H	3.44091900	-3.36875500	1.71470900
2'				C	2.34102800	-5.66630700	-0.53862000
-1 1				H	0.78791200	-5.32123200	-1.99720100
C	-5.49196500	0.44495900	0.00052300	H	3.83635700	-5.70396600	1.02019000
C	-4.53006200	1.46040300	0.00006600	H	2.51402600	-6.69675600	-0.84084700
C	-3.17163000	1.14260100	-0.00026500	C	3.19605600	-0.47330300	0.69474100
C	-2.74481900	-0.19418300	-0.00018900	C	3.47806000	0.68295500	1.44871500
C	-3.71873400	-1.20252700	0.00024500	C	4.18419200	-0.93275400	-0.19284100
C	-5.07899600	-0.88992400	0.00060900	C	4.71248000	1.32720000	1.34858600
H	-6.55162900	0.69264800	0.00080000	H	2.72462400	1.08779500	2.11850200

C	5.41246200	-0.27627900	-0.30823400	C	2.82220300	3.81419300	-1.81248100
H	3.99602600	-1.81049700	-0.80256300	H	2.43641200	2.19722300	-0.45154200
C	5.68760800	0.85106100	0.46717400	C	2.26966300	4.83027900	-2.59759600
H	4.90625100	2.21013700	1.95342400	H	0.44382100	5.80506700	-3.20537500
H	6.15641200	-0.65382900	-1.00616600	H	3.89717100	3.64935500	-1.80432400
H	6.64664900	1.35655200	0.38305800	H	2.91000700	5.46257200	-3.20805700
C	1.23574400	-1.55773100	2.57102700	C	2.42940500	-0.59749100	-4.88698400
C	2.20885000	-1.41176300	3.57225400	C	2.08345700	0.12483900	-3.74364400
C	-0.03702800	-2.02052000	2.95162100	C	0.90044200	-0.16513300	-3.05728400
C	1.91545400	-1.70162600	4.90848700	C	0.03796600	-1.17558000	-3.50165500
H	3.20554600	-1.06669700	3.31741400	C	0.39069000	-1.88054100	-4.66524100
C	-0.32808600	-2.32059100	4.28279200	C	1.57486500	-1.60481400	-5.34618100
H	-0.80757100	-2.14699600	2.19661400	H	3.35181100	-0.37460000	-5.41935900
C	0.64696600	-2.15642200	5.27054600	H	2.72767000	0.92235300	-3.38235100
H	2.68638500	-1.57510500	5.66561200	H	0.63495800	0.41892400	-2.17405900
H	-1.32039600	-2.67858700	4.54682700	H	-0.29371900	-2.64502400	-5.01768000
H	0.42001100	-2.38310400	6.30957900	H	1.83043000	-2.17245200	-6.23884200
C	-2.13563800	2.66732000	-0.29380900	C	-1.27460100	-1.55480200	-2.83322900
C	-2.78352200	3.66466700	0.45272100	O	-2.06290900	-2.23093100	-3.53856600
C	-2.82593600	2.08409900	-1.37007700	N	-1.45067600	-1.15622100	-1.54934000
C	-4.07945400	4.07370000	0.12605200	C	-2.63555000	-1.50286600	-0.86854000
H	-2.27890200	4.12684500	1.29579900	C	-2.72786000	-1.11074400	0.49078500
C	-4.11448400	2.50228000	-1.70541500	C	-3.76126500	-2.19065700	-1.38145700
H	-2.35116700	1.28424800	-1.93128300	C	-3.83722900	-1.37954900	1.28081900
C	-4.74699100	3.49770300	-0.95679600	H	-1.88216300	-0.56866700	0.91447800
H	-4.56669000	4.84391600	0.72027600	C	-4.88384800	-2.46557200	-0.58961200
H	-4.62905000	2.03482100	-2.54129500	H	-3.74443100	-2.50969400	-2.41202900
H	-5.75617500	3.81477700	-1.20941200	C	-4.93538000	-2.06563900	0.74680800
C	-0.10158200	2.75595600	1.73452500	H	-3.87116000	-1.05963200	2.31948400
C	0.36679400	4.06223600	1.95487700	O	-5.99049400	-2.29061300	1.60453500
C	-0.35039700	1.94473700	2.85389400	H	-5.71516300	-2.99698400	-1.04327700
C	0.57959700	4.53943000	3.25148100	C	-7.12158200	-2.96221800	1.08895600
H	0.56807600	4.71439000	1.11030300	H	-7.84132400	-3.02458500	1.91052700
C	-0.14883100	2.42206500	4.15019500	H	-7.58313400	-2.41367700	0.25502500
H	-0.68546400	0.92259800	2.70544200	H	-6.87941300	-3.98056900	0.75136400
C	0.31981100	3.72252200	4.35377200				
H	0.94706700	5.55284700	3.39798700	TS7			
H	-0.34525100	1.77084100	4.99840400	-1 1			
H	0.48764200	4.09296500	5.36232900	Ni	0.53618500	0.93719500	-0.25968200
C	0.60320200	3.18614500	-1.01677000	P	2.28848300	0.35279300	0.66357200
C	0.06215900	4.21116900	-1.80883200	P	-1.38055200	-1.60201500	-0.27415700
C	1.99668700	2.99585300	-1.04075900	C	-2.74272700	-1.43933600	-1.52221100
C	0.88740200	5.02113600	-2.59550000	C	-2.48203500	-0.62663000	-2.63714600
H	-1.00920700	4.38333000	-1.81640600	C	-4.00319700	-2.04938600	-1.41262500

C	-3.45006200	-0.44030100	-3.62706000	C	3.11199800	-2.78141100	3.34576800
H	-1.52318400	-0.12444700	-2.71772500	H	4.09247300	-1.93766200	1.62910000
C	-4.97300000	-1.85825000	-2.39846800	C	1.03998600	-1.73547500	4.00795700
H	-4.23122900	-2.67120100	-0.55169800	H	0.38330400	-0.09371500	2.77731900
C	-4.69750200	-1.05583500	-3.50948400	C	2.01679500	-2.71532500	4.20959700
H	-3.22974100	0.19966000	-4.47724100	H	3.87675800	-3.54144100	3.49173100
H	-5.94520900	-2.33564700	-2.29827600	H	0.17507100	-1.68077700	4.66451100
H	-5.45608500	-0.90353900	-4.27359300	H	1.92097600	-3.42494100	5.02803400
C	-0.63247600	-3.24179200	-0.71781700	C	3.62223900	-0.39280800	-0.42207400
C	0.36440900	-3.75689600	0.13341200	C	4.97875800	-0.03228000	-0.38413100
C	-0.91991600	-3.94132900	-1.90091400	C	3.21906800	-1.35451200	-1.36612700
C	1.03315300	-4.93999800	-0.17794900	C	5.90190600	-0.61264500	-1.25996900
H	0.61782500	-3.22752200	1.04743000	H	5.32145800	0.70896000	0.33140200
C	-0.23990500	-5.12089300	-2.21840400	C	4.14094500	-1.94592100	-2.23066000
H	-1.67794700	-3.56573800	-2.58093900	H	2.17028100	-1.63339900	-1.42370000
C	0.73517400	-5.62767900	-1.35818600	C	5.48782700	-1.57328400	-2.18388300
H	1.79622200	-5.31676600	0.49867700	H	6.94667500	-0.31222300	-1.21674500
H	-0.47858700	-5.64511700	-3.14108200	H	3.80454700	-2.69175800	-2.94707700
H	1.26285200	-6.54554800	-1.60584800	H	6.20561800	-2.02485600	-2.86480900
C	-2.32155800	-2.01286600	1.27447100	C	1.35583000	1.75709100	-5.58421000
C	-2.64250200	-3.31260800	1.69951800	C	1.77137400	1.35202800	-4.31326400
C	-2.71603600	-0.92877700	2.07833500	C	1.00045700	1.65670600	-3.18842400
C	-3.34031700	-3.52196200	2.89171200	C	-0.19907000	2.37192200	-3.31042400
H	-2.34261500	-4.16787800	1.10140000	C	-0.59864800	2.78333600	-4.59294600
C	-3.42125300	-1.13785000	3.26481400	C	0.16426900	2.47577100	-5.71922500
H	-2.46450200	0.08342700	1.77567700	H	1.95535400	1.51820800	-6.46026000
C	-3.73307200	-2.43576500	3.67724100	H	2.69881900	0.79693500	-4.19159000
H	-3.57826200	-4.53619400	3.20469800	H	1.33117700	1.34264800	-2.19333700
H	-3.71551600	-0.28316900	3.86880600	H	-1.51986700	3.35104300	-4.67336900
H	-4.27505500	-2.60016600	4.60560100	H	-0.16791500	2.80018700	-6.70345100
C	3.23917000	1.75189000	1.48244200	C	-1.10728100	2.75447600	-2.14843000
C	3.99583700	1.61982500	2.65818800	O	-2.04103300	3.54633700	-2.40679200
C	3.15972600	3.02174800	0.88486500	N	-0.83434800	2.21599900	-0.93561500
C	4.64889500	2.72142500	3.21976700	C	-1.71324000	2.56171200	0.12297800
H	4.07411400	0.65300100	3.14677900	C	-1.17857700	2.94299000	1.37239100
C	3.82286600	4.11970400	1.43516600	C	-3.11527600	2.48789700	0.02837800
H	2.55155000	3.14167300	-0.00867600	C	-1.99377900	3.22380100	2.46566800
C	4.56757600	3.97402100	2.60894200	H	-0.09902700	3.01242900	1.46890500
H	5.22181300	2.59751500	4.13638100	C	-3.94338700	2.76636600	1.12132500
H	3.74638700	5.09175300	0.95339200	H	-3.56472100	2.21010500	-0.91696700
H	5.07300200	4.83132500	3.04758800	C	-3.38713100	3.13468800	2.35076300
C	2.25950400	-0.88338400	2.07397300	H	-1.56368700	3.51796400	3.41968200
C	3.23327800	-1.87198600	2.29015400	O	-4.11111300	3.42418300	3.48719500
C	1.15924300	-0.83530300	2.94791100	H	-5.01864200	2.68734600	0.99693400

C	-5.52063700	3.35611500	3.40201000	C	-0.12612000	3.04862700	-1.14264700
H	-5.89976300	3.62340200	4.39264300	C	0.75969600	3.41000600	-0.11220600
H	-5.92417900	4.06545300	2.66507500	C	0.45792200	4.53964700	0.66204300
H	-5.87129400	2.34521600	3.14827500	C	1.96016900	3.49315200	-2.17938200
13				H	0.11575100	2.20155600	-1.77876800
-1 1				H	1.16318600	4.83436700	1.43313100
Ni	0.30135300	0.46598000	-0.16166600	H	-0.94027200	6.12829000	1.07064800
P	-1.39744700	-0.67801600	0.03559400	C	2.06217700	2.67753300	0.15434500
C	-2.35298600	-0.49308900	1.63462100	O	3.00271800	3.34739500	0.63262000
C	-2.36719400	0.77994600	2.23015800	N	2.04746600	1.35934800	-0.17147200
C	-3.02518700	-1.53947800	2.28604500	C	3.22368100	0.58434600	-0.14954800
C	-3.04649900	1.00477000	3.42814800	C	3.15070100	-0.70856200	-0.72469600
H	-1.82997300	1.59305600	1.74913100	C	4.47735600	0.96646400	0.37371500
C	-3.69694600	-1.31859600	3.49221700	C	4.24237000	-1.56361000	-0.76813300
H	-3.02294700	-2.53606300	1.85426800	H	2.19353900	-1.02317800	-1.13522300
C	-3.71225800	-0.04586900	4.06574200	C	5.58340100	0.10686800	0.33003200
H	-3.04459700	1.99845900	3.86996000	H	4.57353200	1.94737500	0.81577300
H	-4.20667500	-2.14456400	3.98363900	C	5.47803700	-1.16301800	-0.23975700
H	-4.23307500	0.12492400	5.00507700	H	4.15949100	-2.55031000	-1.21711600
C	-2.76099000	-0.45011000	-1.23189600	O	6.50342400	-2.07946400	-0.33038700
C	-2.36802100	-0.27426900	-2.57067100	H	6.52288500	0.45095700	0.75209300
C	-4.13164100	-0.40632000	-0.93408100	C	7.77220000	-1.69053900	0.15494000
C	-3.31210300	-0.08025400	-3.57942100	H	8.44345800	-2.53396600	-0.03118200
H	-1.30750700	-0.28099800	-2.81318800	H	8.16031500	-0.80528700	-0.36950300
C	-5.07959800	-0.19878700	-1.94142600	H	7.75565000	-1.48229400	1.23474800
H	-4.46709600	-0.53138600	0.09100400	TS8			
C	-4.67433800	-0.03872000	-3.26714400	-1 1			
H	-2.98423600	0.04866400	-4.60847300	Ni	-0.35259900	1.30297400	-0.06070600
H	-6.13648300	-0.16237100	-1.68597900	P	-1.30950500	-0.64398800	-0.07807000
H	-5.41150100	0.12335400	-4.05007300	C	-0.35526200	-2.22783800	-0.33349400
C	-1.16715900	-2.53439200	-0.03267900	C	-0.55312700	-3.41177500	0.39364300
C	-2.07424800	-3.42787700	-0.62466000	C	0.64070000	-2.21042000	-1.32396700
C	0.00935100	-3.05701300	0.53142900	C	0.21399500	-4.54976800	0.12767900
C	-1.81379400	-4.80154900	-0.65008800	H	-1.30860500	-3.45176800	1.17263700
H	-2.98943000	-3.05334200	-1.07384400	C	1.39709400	-3.34956500	-1.60050200
C	0.26476700	-4.42857600	0.51825000	H	0.83244500	-1.28995900	-1.86942000
H	0.73301500	-2.37100200	0.96481200	C	1.18617700	-4.52395400	-0.87379100
C	-0.64578100	-5.30683900	-0.07676000	H	0.05012300	-5.45655700	0.70583000
H	-2.52627000	-5.47568000	-1.12074500	H	2.16477700	-3.31215700	-2.36920400
H	1.18197400	-4.80992300	0.96087500	H	1.78475000	-5.40857500	-1.07775900
H	-0.44205200	-6.37485800	-0.09959100	C	-2.16796000	-0.95651100	1.54426600
C	-1.59580900	4.88983400	-0.57231400	C	-3.34496400	-1.71083800	1.67414400
C	-1.29079000	3.78698400	-1.37417100	C	-1.60915700	-0.38347600	2.69931500

C	-3.94151100	-1.89456100	2.92441800	C	6.86208000	-2.16482600	-0.13011500
H	-3.80186500	-2.15488400	0.79460600	H	7.43628000	-1.23868500	0.01836500
C	-2.20067900	-0.57229000	3.94947900	H	7.46381800	-3.01122300	0.21379900
H	-0.71480200	0.22771900	2.60794300	H	6.66041500	-2.28602700	-1.20464600
C	-3.36969300	-1.32841200	4.06575100				
H	-4.85522800	-2.47902800	3.00489300	14			
H	-1.75249700	-0.11953100	4.83050300	-1 1			
H	-3.83623900	-1.46926800	5.03779500	Ni	-1.02657100	1.20996500	0.38504400
C	-2.71133600	-0.90259000	-1.29238700	P	-0.91228200	-1.03886200	0.01920000
C	-2.90062400	-2.08117000	-2.03082000	C	0.60811700	-2.05521800	-0.32665100
C	-3.62208300	0.15076700	-1.48238300	C	1.00501200	-3.15692400	0.44435100
C	-3.96367100	-2.20103900	-2.93168300	C	1.41935900	-1.66573300	-1.40702000
H	-2.21525500	-2.91355300	-1.91095400	C	2.17375300	-3.85993400	0.13613500
C	-4.69072600	0.02791600	-2.36984400	H	0.40192800	-3.47608500	1.28802500
H	-3.47796400	1.07777400	-0.93450700	C	2.57990100	-2.37183900	-1.71887500
C	-4.86492300	-1.14997400	-3.10176200	H	1.14281100	-0.80150000	-2.00481200
H	-4.08426100	-3.12121900	-3.49901500	C	2.96139300	-3.47356100	-0.94766400
H	-5.38231800	0.85745500	-2.49710200	H	2.46460300	-4.71129000	0.74722000
H	-5.69056800	-1.24343100	-3.80319300	H	3.19392800	-2.05208100	-2.55679200
C	-1.45057200	5.53235600	0.41714400	H	3.87115300	-4.01947600	-1.18519100
C	-1.66116400	4.15070800	0.35155500	C	-1.71060300	-1.98037400	1.40376500
C	-0.64110300	3.25586700	-0.02805300	C	-2.41925700	-3.17881900	1.23196200
C	0.62959000	3.81782700	-0.31923200	C	-1.58948600	-1.44917700	2.69758900
C	0.82596200	5.20191100	-0.29847600	C	-2.98704400	-3.83284800	2.32810100
C	-0.20900300	6.06612700	0.06650900	H	-2.53947500	-3.60209100	0.23931100
H	-2.26291700	6.19032000	0.72195400	C	-2.14755700	-2.10752900	3.79471100
H	-2.65118900	3.75873400	0.58378600	H	-1.07223500	-0.50366100	2.83748400
H	1.81878500	5.57599100	-0.53569200	C	-2.84891100	-3.30141700	3.61210800
H	-0.04472200	7.14164000	0.08947600	H	-3.54004600	-4.75683200	2.17625900
C	1.83946300	2.92974600	-0.49859600	H	-2.04455100	-1.67990300	4.78882900
O	2.90081700	3.41847000	-0.93762100	H	-3.29297800	-3.81015200	4.46432200
N	1.62191400	1.65943400	-0.04947700	C	-1.94063200	-1.47934000	-1.47151500
C	2.68630000	0.74802700	0.03852400	C	-1.76584700	-2.68411700	-2.17458100
C	2.56112900	-0.31951100	0.95841900	C	-2.91338700	-0.57459700	-1.92789300
C	3.88541100	0.79215300	-0.70600900	C	-2.54905400	-2.98197000	-3.29157500
C	3.55769300	-1.26962200	1.13525000	H	-1.00554800	-3.39085300	-1.85724400
H	1.64819700	-0.38178900	1.54321900	C	-3.69385900	-0.87248000	-3.04725000
C	4.89198300	-0.16672700	-0.53797800	H	-3.04791400	0.36541400	-1.40279800
H	4.03062700	1.60126300	-1.40738200	C	-3.51652100	-2.07625100	-3.73145700
C	4.74040800	-1.20247800	0.38684300	H	-2.39642100	-3.91977600	-3.82062200
H	3.43552800	-2.07858400	1.85092100	H	-4.43733500	-0.15549700	-3.38675200
H	5.79344800	-0.08312700	-1.13767500	H	-4.12199400	-2.30434300	-4.60545300
O	5.67608100	-2.18411700	0.63672100	C	-3.33838300	4.83613900	0.45015100
H	-1.45655100	2.17780300	-0.54792500	C	-3.03391400	3.47771300	0.61862600

C	-1.73710800	2.98280600	0.39537400	C	0.55527600	1.19997000	-1.20220900
C	-0.76102400	3.91776500	-0.00699000	C	1.08667000	2.50893200	-1.16068800
C	-1.05592200	5.27126300	-0.19461100	C	1.41966200	0.17830100	-1.62300400
C	-2.35227700	5.73702800	0.03623500	C	2.40615100	2.76732200	-1.51134000
H	-4.35142500	5.19115700	0.63905600	H	0.44302100	3.32672900	-0.85825100
H	-3.82577900	2.79858600	0.92965000	C	2.75238000	0.42502800	-1.97313900
H	-0.25828700	5.93964900	-0.51167200	H	1.03354600	-0.83397700	-1.69044400
H	-2.59244900	6.79011800	-0.10003500	C	3.25423900	1.72749300	-1.91805100
C	0.63917400	3.40878300	-0.18512600	H	2.80403900	3.77841600	-1.47646000
O	1.56846400	4.17093400	-0.50886100	H	3.37618100	-0.40404800	-2.29084700
N	0.73040300	2.07514000	0.10807600	O	4.54377900	2.08846000	-2.23892300
C	2.01266500	1.49919000	0.18319000	C	5.41690400	1.07126200	-2.68679500
C	2.31926900	0.63408300	1.25460600	H	6.37277600	1.55915000	-2.89800800
C	3.03718000	1.73547700	-0.75279300	H	5.57693300	0.29682300	-1.92241300
C	3.56883600	0.03865100	1.38693400	H	5.05265400	0.59044700	-3.60612800
H	1.54988800	0.44523400	1.99901600	C	0.29523600	-1.68831400	0.87803300
C	4.29840200	1.14376800	-0.62792400	C	0.44350200	-0.65651800	1.54959600
H	2.84578300	2.40555200	-1.58122000	C	0.47942500	-2.97799800	0.27738600
C	4.57394200	0.29020200	0.44512400	C	-0.42631400	-3.48431800	-0.67480900
H	3.78571500	-0.62489900	2.21989300	C	1.59756800	-3.76172000	0.63647300
H	5.05480000	1.36177400	-1.37538200	C	-0.21814400	-4.73737600	-1.24814200
O	5.78236800	-0.33434300	0.66333500	H	-1.28694200	-2.88269600	-0.94860900
H	-2.43149900	0.76395900	0.64622200	C	1.79652300	-5.01258700	0.05853500
C	6.80814300	-0.12434900	-0.28538200	H	2.30234500	-3.37716500	1.36787300
H	7.10035100	0.93378900	-0.34989900	C	0.89085800	-5.50605800	-0.88621600
H	7.66797000	-0.70623300	0.05915400	H	-0.92626400	-5.11303900	-1.98224700
H	6.52158700	-0.47371300	-1.28803000	H	2.66216400	-5.60479500	0.34510900
15				H	1.05007200	-6.48236600	-1.33703200
-1 1				C	0.87631700	0.35237500	2.47079400
Ni	-1.41823400	-0.47720500	0.49400100	C	0.31342300	1.64355400	2.47494300
C	-5.61338900	0.22296500	-0.12736700	C	1.88437800	0.04474200	3.41021200
C	-4.44361500	-0.36772600	0.37167100	C	0.74857900	2.59491100	3.39515300
C	-3.17175400	0.08741600	-0.01651600	H	-0.45292000	1.88216600	1.74513500
C	-3.12664400	1.16835000	-0.92027600	C	2.31134800	1.00283300	4.32535900
C	-4.28653300	1.76880500	-1.41765000	H	2.32165100	-0.94947800	3.41463400
C	-5.53888300	1.29470900	-1.02170300	C	1.74457700	2.28116200	4.32335600
H	-6.58629300	-0.15368800	0.18666500	H	0.30585400	3.58749200	3.38534200
H	-4.53201500	-1.19612900	1.07071900	H	3.08776100	0.75034700	5.04342200
H	-4.18429600	2.60080900	-2.11045700	H	2.07861300	3.02710800	5.04007900
H	-6.44787500	1.75342400	-1.40690400	H	-2.11652200	-1.41312800	1.41928700
C	-1.77386100	1.65033500	-1.36098700	TS9			
O	-1.65364300	2.60674600	-2.14780900	-1 1			
N	-0.76975600	0.89579700	-0.82347900	Ni	-0.98231400	0.59120900	-0.24326200

C	-3.86018800	3.74220000	0.28251100	C	2.54565300	-2.50604900	2.07305900
C	-3.35466800	2.48797000	-0.08455700	H	1.50723900	-0.62203800	1.91601300
C	-1.97406400	2.23602800	-0.09083300	C	1.65432900	-4.31381100	0.74278400
C	-1.11592500	3.28461100	0.29283400	H	-0.09749000	-3.84798900	-0.42233800
C	-1.61642800	4.53717000	0.66035200	C	2.60819400	-3.83499000	1.64595500
C	-2.99185000	4.77305800	0.65214100	H	3.28820600	-2.12152000	2.76771900
H	-4.93561200	3.91397700	0.27369500	H	1.69584700	-5.34583900	0.40141800
H	-4.05501100	1.70276300	-0.36172800	H	3.39625300	-4.49057500	2.00867400
H	-0.90749600	5.30699300	0.95526000	H	-2.09895100	0.55982400	-1.16638300
H	-3.38418000	5.74835700	0.93329800				
C	0.36003400	3.01767900	0.32057500	16			
O	1.17344400	3.92579000	0.57283200	-1 1			
N	0.63423000	1.71676400	0.01698900	Ni	0.09637400	0.64870500	-0.17106300
C	1.97137400	1.32010400	-0.17916200	C	-1.33172900	4.55730900	-0.98882300
C	3.05712000	1.77752200	0.60360400	C	-1.37365500	3.18014800	-0.72721700
C	2.26827800	0.39719200	-1.19595200	C	-0.19151800	2.46395800	-0.50941900
C	4.35212800	1.32276400	0.37611700	C	1.03335800	3.15875600	-0.56101100
H	2.87148900	2.50504900	1.38249200	C	1.07576000	4.53170900	-0.81846200
C	3.56612500	-0.06438600	-1.43184800	C	-0.11034500	5.23594900	-1.03418900
H	1.45366100	0.03414800	-1.81685000	H	-2.26037500	5.10133500	-1.15543500
C	4.62177400	0.39800800	-0.64114800	H	-2.33687700	2.67934300	-0.68639900
H	5.17852700	1.67994200	0.98599600	H	2.04490200	5.02404800	-0.84623300
H	3.73390300	-0.77979800	-2.22983200	H	-0.08482900	6.30486000	-1.23645300
O	5.93675700	0.01525200	-0.78345700	C	2.29334200	2.37346500	-0.33876500
C	6.24261900	-0.90347900	-1.81400600	O	3.41150500	2.91988200	-0.37299000
H	7.32258700	-1.06991300	-1.76587700	N	2.00469300	1.06120200	-0.10979500
H	5.72842600	-1.86531400	-1.67473300	C	2.97808900	0.08324900	0.11524400
H	5.98871200	-0.50733200	-2.80789200	C	2.53811700	-1.19353200	0.54235900
C	-1.71476900	-1.19542800	-0.15562500	C	4.37009900	0.24094100	-0.06278700
C	-0.48889900	-1.25906700	0.22404700	C	3.41742500	-2.24542100	0.76105500
C	-2.97416400	-1.89726400	-0.33459500	H	1.47490200	-1.35757100	0.71534400
C	-4.00271500	-1.41816600	-1.16537700	C	5.25950300	-0.81574900	0.16043800
C	-3.18751900	-3.11576000	0.34673700	H	4.74342200	1.20701800	-0.37206500
C	-5.19207900	-2.12942700	-1.31950200	C	4.79441800	-2.06765800	0.57165100
H	-3.85324300	-0.48330100	-1.69805000	H	3.05374100	-3.21565000	1.08894000
C	-4.38023500	-3.81959800	0.19817600	H	6.31989000	-0.64017500	0.00823000
H	-2.40745300	-3.49779200	0.99878200	O	5.58762900	-3.16594800	0.81726400
C	-5.38980700	-3.33249400	-0.63786400	C	6.98484200	-3.01267100	0.66456700
H	-5.96867300	-1.73896400	-1.97288500	H	7.39155300	-2.24587400	1.33960800
H	-4.52280200	-4.75262100	0.73857500	H	7.42787600	-3.97925400	0.92031600
H	-6.31947000	-3.88371100	-0.75498800	H	7.26186000	-2.75800300	-0.36872900
C	0.56935600	-2.12878400	0.70004000	C	-1.63224000	-0.10561600	-0.14658600
C	1.54439600	-1.65895300	1.60039900	C	-1.55827900	-1.27241800	-0.84732300
C	0.64344900	-3.47396400	0.27897800	C	-2.79317700	0.32473300	0.65516300

C	-4.08624000	0.40221800	0.09558400	C	4.00889200	-2.03985400	0.92422000
C	-2.63600600	0.75134300	1.98990600	H	2.47192800	-1.26954400	2.21646300
C	-5.17139600	0.86408400	0.84131300	C	4.28732000	-2.73429900	-0.25735100
H	-4.23035300	0.09646700	-0.93724400	H	3.45277200	-3.73402900	-1.96402800
C	-3.72406900	1.19209600	2.74193100	H	4.80772200	-1.67974600	1.56347400
H	-1.64216400	0.73460400	2.42984100	O	5.54973500	-3.02306700	-0.71594200
C	-4.99966600	1.25366400	2.17203000	C	6.64872000	-2.59938600	0.06949100
H	-6.15561400	0.91680100	0.38056700	H	6.63797200	-3.05445400	1.06993600
H	-3.57324900	1.50246400	3.77356300	H	7.54652100	-2.92957200	-0.46028300
H	-5.84545600	1.61091600	2.75456000	H	6.68011600	-1.50600500	0.17596800
C	-2.41596400	-2.47903800	-0.83654900	C	0.60214700	0.69265600	-0.18598000
C	-2.38867700	-3.34018200	-1.95268500	C	1.36933800	1.25869700	0.77389200
C	-3.23353100	-2.85175800	0.25013300	C	0.67944900	1.04876100	-1.61784500
C	-3.16179800	-4.49952800	-1.99902200	C	0.23586100	2.30875100	-2.07707200
H	-1.75132800	-3.08427200	-2.79670600	C	1.12738600	0.12999400	-2.59039100
C	-4.00356200	-4.01261600	0.20630100	C	0.24500800	2.63379200	-3.43392800
H	-3.25351500	-2.23044200	1.13844200	H	-0.10931600	3.03865200	-1.34982100
C	-3.97839800	-4.84263700	-0.91874700	C	1.14822700	0.46130300	-3.94536400
H	-3.12260200	-5.13830300	-2.87853700	H	1.47615200	-0.84597400	-2.26763900
H	-4.62193400	-4.27521500	1.06180500	C	0.70353300	1.71342300	-4.37988200
H	-4.57952400	-5.74804200	-0.94858300	H	-0.10190900	3.61515800	-3.75245600
H	-0.71293100	-1.37746100	-1.53724100	H	1.51096800	-0.26753100	-4.66755700
17				H	0.71297300	1.96650100	-5.43753200
-1 1				C	2.49128900	2.22084200	0.69589300
Ni	-0.88819500	-0.49655600	0.45459000	C	2.82543100	2.95317700	1.85526900
C	-4.42854400	-2.21234300	2.35107300	C	3.28580900	2.43704300	-0.44969800
C	-3.63943200	-1.31750800	1.61292600	C	3.87850000	3.86630200	1.87012300
C	-2.28517500	-1.57875800	1.35269700	H	2.23622800	2.79879000	2.75730100
C	-1.76464100	-2.77606100	1.86914600	C	4.34029600	3.34918500	-0.43568500
C	-2.53364700	-3.68098300	2.60442200	H	3.08591400	1.86989000	-1.35095100
C	-3.87923500	-3.39774400	2.84904600	C	4.64319400	4.07574000	0.71971800
H	-5.47767400	-1.98298100	2.53608300	H	4.10161100	4.41648000	2.78209600
H	-4.10578100	-0.40696600	1.23891800	H	4.93550200	3.48777400	-1.33601600
H	-2.06551400	-4.59117500	2.97327600	H	5.46673900	4.78601500	0.72544300
H	-4.49385400	-4.09119600	3.42005900	H	1.15123100	0.97790100	1.80752000
C	-0.32270000	-3.03871500	1.57776800	C	-2.10727100	1.22297800	0.30222100
O	0.24853600	-4.08278800	1.92721700	C	-2.34532000	0.48068200	-0.66853600
N	0.25591700	-2.00305700	0.88912200	C	-2.15389800	2.30651500	1.24176800
C	1.60883700	-2.22966100	0.50491100	C	-1.75538000	2.13773400	2.58209800
C	1.91093300	-2.93632600	-0.67219300	C	-2.62416800	3.57010800	0.82494400
C	2.68110800	-1.80182700	1.29349700	C	-1.83243800	3.20197000	3.47746100
C	3.22604300	-3.18558500	-1.05350100	H	-1.39737800	1.16629000	2.90596400
H	1.09152600	-3.29705400	-1.28882000	C	-2.69399400	4.62890500	1.72692700
				H	-2.92712000	3.70942400	-0.20854700

C	-2.29858400	4.45027200	3.05563100	H	5.75516900	-4.39324300	-0.94248600
H	-1.52542400	3.05552500	4.50977500	H	6.16473000	-4.46851600	-2.67701400
H	-3.05541900	5.59737800	1.39049400	H	5.81297700	-2.89397400	-1.91629700
H	-2.35227300	5.27873300	3.75716500	C	1.05702700	0.83278500	0.42259000
C	-2.91761200	-0.07401100	-1.86311900	C	1.72508000	1.02799400	1.58797300
C	-3.59617800	0.77796300	-2.76087600	C	1.53243300	1.30058400	-0.89945400
C	-2.83147400	-1.44741800	-2.16196400	C	1.91976000	2.64216200	-1.10981900
C	-4.17763300	0.26352000	-3.91613000	C	1.53838800	0.44661600	-2.02227800
H	-3.65526900	1.84008900	-2.54372400	C	2.31076800	3.09941400	-2.36778700
C	-3.41891600	-1.95216200	-3.31994200	H	1.90620800	3.32968700	-0.27005200
H	-2.30718600	-2.10243600	-1.47520500	C	1.94646700	0.89957900	-3.27700800
C	-4.09295400	-1.10272100	-4.20084700	H	1.22971300	-0.58612900	-1.89937100
H	-4.69626200	0.93219000	-4.59866900	C	2.33411900	2.22964200	-3.46119800
H	-3.34645300	-3.01504200	-3.53507200	H	2.59717700	4.14173700	-2.49344900
H	-4.54593400	-1.50097400	-5.10521400	H	1.95340400	0.20793300	-4.11686400
				H	2.64046000	2.58441700	-4.44259200
TS10				C	3.09257800	1.52652300	1.86608000
-1 1				C	3.36650000	2.06693000	3.14032400
Ni	-0.68161500	-0.08242700	0.58348100	C	4.17283200	1.43402100	0.96268400
C	-3.72198800	-0.63516100	3.54387600	C	4.63768400	2.52263200	3.48756100
C	-3.04721900	-0.00674200	2.49013300	H	2.55770900	2.12889800	3.86627000
C	-2.21451300	-0.74392800	1.63588100	C	5.44499200	1.88641500	1.30981100
C	-2.03852000	-2.11732100	1.88555300	H	4.01355800	0.98841300	-0.01273300
C	-2.73486500	-2.74513900	2.91932700	C	5.68851800	2.43939800	2.57087000
C	-3.58722500	-2.01032000	3.74640800	H	4.80879900	2.93856400	4.47838100
H	-4.36735000	-0.04738100	4.19352900	H	6.25639600	1.79705600	0.59037400
H	-3.19376100	1.05609900	2.32188200	H	6.68306300	2.78878000	2.83775000
H	-2.56152800	-3.80678200	3.07706500	H	1.20486800	0.74616800	2.50732200
H	-4.12769900	-2.50190900	4.55208900	C	-1.77468200	1.36442100	-0.05538400
C	-0.96758300	-2.85742000	1.13863000	C	-2.49712900	0.28374700	-0.12832700
O	-0.94172100	-4.10004800	1.10324300	C	-1.75578400	2.75264500	-0.48676400
N	-0.05917600	-1.99028800	0.62039800	C	-1.11869600	3.73064900	0.30149000
C	1.02668200	-2.55243600	-0.09541100	C	-2.38846200	3.16913500	-1.67729300
C	0.82768400	-3.32518000	-1.25787300	C	-1.13605700	5.07464700	-0.07037300
C	2.34768000	-2.33951200	0.31832200	H	-0.60869900	3.41789100	1.20718900
C	1.89928600	-3.84603800	-1.97336400	C	-2.39058300	4.51072800	-2.05390800
H	-0.18608100	-3.51649800	-1.59543300	H	-2.86953500	2.42831000	-2.30902200
C	3.43619100	-2.85429000	-0.39548700	C	-1.77105000	5.47188900	-1.24941700
H	2.52532400	-1.75272100	1.21295300	H	-0.64361700	5.81220500	0.55903700
C	3.21538500	-3.61225000	-1.54895900	H	-2.87776900	4.80730600	-2.97993800
H	1.73836200	-4.43971200	-2.86950200	H	-1.77802500	6.51879200	-1.54292800
H	4.44122800	-2.65588500	-0.03829800	C	-3.69869600	-0.29650000	-0.72209500
O	4.20384700	-4.16547500	-2.32652600	C	-4.81795500	0.51961000	-0.98042800
C	5.54718000	-3.96029900	-1.93125500	C	-3.76228100	-1.65450700	-1.08285200

C	-5.95774100	-0.00688100	-1.58669200	H	-0.71329300	-7.46263200	0.56640000
H	-4.78698900	1.56794300	-0.69840800	C	-1.80485800	-0.14497500	-2.26023800
C	-4.90288900	-2.17550600	-1.69081300	O	-2.81102900	-0.24100500	-2.98933700
H	-2.91121300	-2.29643100	-0.88108500	N	-1.67236800	0.59949100	-1.13375900
C	-6.00600400	-1.35631100	-1.94632800	Ni	0.05181800	0.54678700	-0.25120300
H	-6.81263900	0.63886100	-1.77346700	C	-2.73469400	1.36264000	-0.60302100
H	-4.92964700	-3.22746000	-1.96385000	C	-3.99840300	1.55880800	-1.19839000
H	-6.89599600	-1.76680000	-2.41671600	C	-2.51270400	2.01912300	0.63171000
18				C	-4.97125100	2.36927700	-0.60101000
-1 1				H	-4.21003000	1.06813900	-2.13667100
C	0.82895100	-1.36032100	-4.68756700	C	-3.47570800	2.82034100	1.22877800
C	-0.21793500	-0.67691200	-4.07539200	H	-1.55690300	1.87717000	1.13241300
C	-0.56319300	-0.89522000	-2.73045100	C	-4.72131300	3.00886000	0.61467000
C	0.14737900	-1.87271500	-1.98855000	H	-5.92439900	2.48733900	-1.10699200
C	1.16971500	-2.58908000	-2.64299700	H	-3.27912400	3.30862300	2.17961500
C	1.52580000	-2.33136400	-3.96430900	O	-5.60949700	3.82325100	1.27812500
H	1.08615600	-1.15075100	-5.72323900	C	-6.87371500	4.03802800	0.68104900
H	-0.80523400	0.03890500	-4.64317200	H	-7.42371400	4.69773700	1.35795600
H	1.69777100	-3.35973500	-2.08775700	H	-6.78720700	4.52744000	-0.29984100
H	2.33729200	-2.88873300	-4.42685700	H	-7.43728400	3.10180000	0.56188500
C	-0.14339600	-2.19472900	-0.55373800	H	0.78443200	2.68333400	-0.39448900
C	-0.19825800	-1.19956900	0.36632500	C	1.77916800	2.29361600	-0.10629800
C	-0.65087000	-1.35276300	1.76706600	C	1.81780500	0.99107400	0.26852300
C	0.14986600	-0.96928200	2.86127100	C	2.97063600	0.27498200	0.83226800
C	-1.94613500	-1.83868500	2.04187100	C	3.46016000	-0.90431000	0.23566600
C	-0.31248400	-1.09582500	4.17065100	C	3.58011900	0.70418100	2.03112600
H	1.14544700	-0.58048400	2.67570000	C	4.52771800	-1.60505100	0.79760400
C	-2.41227300	-1.95048900	3.35192000	H	2.99545000	-1.25945400	-0.67915800
H	-2.58844900	-2.11975300	1.21272800	C	4.63386400	-0.00940300	2.60208700
C	-1.59713800	-1.58472700	4.42560900	H	3.21251800	1.60668000	2.51234100
H	0.33346200	-0.80509600	4.99642900	C	5.11865800	-1.16639500	1.98618800
H	-3.41832200	-2.32273000	3.53269000	H	4.89315800	-2.50609300	0.30978000
H	-1.95931100	-1.67317800	5.44717700	H	5.07986400	0.34305900	3.52974900
C	-0.30098500	-3.64788600	-0.22922200	H	5.94151900	-1.72206800	2.42940000
C	-1.09655300	-4.48065000	-1.04039800	C	2.81965800	3.33196200	-0.25668900
C	0.35598300	-4.23867300	0.86609000	C	2.42964100	4.68521200	-0.32231900
C	-1.24815600	-5.83744600	-0.75522700	C	4.19548500	3.04489400	-0.37273800
H	-1.60583500	-4.05159300	-1.89898700	C	3.36718600	5.70687200	-0.46711200
C	0.20615400	-5.59630300	1.15162900	H	1.37194100	4.93167200	-0.25276400
H	0.99778300	-3.62435900	1.48962100	C	5.13195300	4.06654600	-0.51931600
C	-0.59852800	-6.40423000	0.34464700	H	4.52807400	2.01324300	-0.35994300
H	-1.87707400	-6.45309300	-1.39464700	C	4.72774200	5.40427200	-0.56194400
H	0.72832100	-6.02526800	2.00406200	H	3.03389900	6.74152900	-0.50810300
				H	6.18630800	3.81398600	-0.60839300

H	5.46213800	6.19780600	-0.67615600	C	1.90037200	-2.73818000	0.18618200
				C	4.61790300	-2.49186900	-0.39135600
TS11				H	4.05385900	-0.76802400	-1.53930900
-1 1				C	2.80676200	-3.65292200	0.71232600
C	-0.29710500	1.86970300	-4.89703200	H	0.84138000	-2.83084200	0.41059900
C	0.29113600	0.75197700	-4.32988600	C	4.17304400	-3.53850600	0.42660800
C	0.64595800	0.71496500	-2.96642800	H	5.66906600	-2.37825600	-0.63238700
C	0.43748000	1.86265100	-2.13727500	H	2.47097900	-4.46661400	1.34846200
C	-0.14753500	3.00122500	-2.75861800	O	4.98615000	-4.48813500	0.98568200
C	-0.51555300	3.00363900	-4.09283000	C	6.37759100	-4.40738700	0.72783800
H	-0.58466000	1.87092200	-5.94538000	H	6.83427200	-5.24121700	1.26721000
H	0.50201200	-0.13082600	-4.92524300	H	6.60154400	-4.50952900	-0.34299000
H	-0.33249600	3.88392600	-2.15531300	H	6.80805000	-3.46605400	1.09626400
H	-0.98421300	3.88953400	-4.51674000	H	-2.35995800	-2.47107600	-1.01403000
C	0.81507300	1.86370000	-0.73913800	C	-2.92622900	-1.76755900	-0.39404200
C	0.88502900	0.63712100	-0.04979500	C	-2.23736300	-0.70625600	0.11517200
C	1.56982200	0.52689700	1.27525700	C	-2.83688400	0.26818700	1.05131800
C	0.92902200	-0.05547700	2.38086200	C	-3.06995400	1.60701900	0.67223800
C	2.88873900	0.98829400	1.44207200	C	-3.13442200	-0.08605700	2.38557400
C	1.57150900	-0.14970500	3.61640400	C	-3.59417800	2.53498200	1.57307900
H	-0.08559500	-0.42152200	2.26086900	H	-2.83142500	1.91217700	-0.34324700
C	3.53708000	0.88301100	2.67173500	C	-3.64252200	0.84687200	3.29016900
H	3.40134900	1.43803000	0.59729500	H	-2.96459600	-1.11164700	2.70545700
C	2.87941200	0.31591800	3.76647000	C	-3.88201700	2.16436600	2.89043900
H	1.04896800	-0.59196200	4.46138900	H	-3.76989200	3.55765900	1.24536200
H	4.55784800	1.24392900	2.77564200	H	-3.85911500	0.54007800	4.31179200
H	3.38371500	0.23556200	4.72672400	H	-4.28007400	2.89171800	3.59396900
C	1.04586100	3.16304700	-0.04897000	C	-4.34260800	-2.18184200	-0.28389500
C	1.88699700	4.14536200	-0.61501500	C	-4.67954900	-3.50525700	-0.64337500
C	0.43404200	3.47343300	1.18270200	C	-5.40254000	-1.33977800	0.11761300
C	2.11577700	5.36519000	0.02142900	C	-5.99044900	-3.97438100	-0.58368600
H	2.37428200	3.93830400	-1.56421100	H	-3.88639600	-4.17378200	-0.97319700
C	0.66929500	4.68942400	1.82477200	C	-6.71464100	-1.80769200	0.17497500
H	-0.24420800	2.75441500	1.62975800	H	-5.19758300	-0.30741600	0.37312500
C	1.51131100	5.64464400	1.25043100	C	-7.02156100	-3.12743300	-0.16907800
H	2.77657200	6.09589100	-0.44057500	H	-6.20781000	-5.00276000	-0.86505400
H	0.17866800	4.89475800	2.77373400	H	-7.50713700	-1.12978900	0.48547700
H	1.69031400	6.59392000	1.74992100	H	-8.04711200	-3.48593600	-0.12325500
C	1.38911100	-0.48179000	-2.51388100				
O	1.96505800	-1.23500100	-3.30840400	P2			
N	1.40308500	-0.71338300	-1.12752000	0 1			
Ni	-0.40499500	-0.67110400	-0.48571600	C	3.60956200	-1.98648200	-0.10913700
C	2.33247900	-1.68250400	-0.62939300	C	2.24178500	-1.63539000	-0.03317500
C	3.70064100	-1.57434600	-0.90491300	C	1.29107700	-2.68075300	0.04359100

C	1.70328700	-4.02436900	0.04659300	H	-0.23632900	1.59270500	-2.06467800
C	3.04879100	-4.34551400	-0.02676100	C	-1.04368500	4.04641700	0.14946900
C	4.00173100	-3.31596600	-0.10688900	H	-0.89517000	3.87030400	2.29442500
H	4.35712800	-1.20303100	-0.16873500	H	-1.07419700	3.92032200	-2.00349500
H	0.93890200	-4.79192800	0.10675600	H	-1.41012500	5.06916000	0.17649400
H	3.36528100	-5.38479200	-0.02400500				
H	5.05908500	-3.56157500	-0.16589800	15'			
C	-0.14862000	-2.39830200	0.11305100	-1 1			
O	-1.01435200	-3.26848400	0.17266900	Ni	0.26732500	0.00943700	0.03102500
N	-0.50023100	-1.03433800	0.09928200	C	2.65331600	2.51975200	2.69864300
C	-1.92066800	-0.75350700	0.12304500	C	2.36525500	1.54830200	1.72897600
C	-2.64041400	-0.71228000	-1.06736800	C	1.05791700	1.33882000	1.26548400
C	-2.58416800	-0.56781700	1.33923800	C	0.05168800	2.13769800	1.83582900
C	-4.01524200	-0.46799100	-1.06044600	C	0.31745500	3.10867000	2.80541600
H	-2.12821700	-0.87843500	-2.01048900	C	1.63047800	3.30675800	3.23771000
C	-3.95016000	-0.32092400	1.35854700	H	3.67994000	2.66467800	3.03454700
H	-2.02776600	-0.62262300	2.26993100	H	3.18780100	0.94998400	1.33670400
C	-4.67614200	-0.26808100	0.15813300	H	-0.50859500	3.69001200	3.20919700
H	-4.55304600	-0.43904000	-2.00097800	H	1.85579800	4.06019300	3.99037300
H	-4.47884200	-0.17212200	2.29489100	C	-1.34710500	1.88105800	1.36852000
O	-6.00921400	-0.02108000	0.28414700	O	-2.31346400	2.53772200	1.78617500
C	-6.80585700	0.00513400	-0.89394900	N	-1.39556800	0.86579400	0.44126400
H	-7.82794200	0.19567600	-0.55977300	C	-2.65853200	0.52488900	-0.10394000
H	-6.49633500	0.80869400	-1.57515300	C	-2.81825100	0.38447200	-1.49555000
H	-6.77465500	-0.95490100	-1.42506800	C	-3.79030200	0.30130300	0.69517900
C	1.78326500	-0.25687300	-0.02192700	C	-4.04004300	0.03343800	-2.05862200
C	0.44148600	0.00561400	0.04620200	H	-1.95621100	0.54967700	-2.13424300
C	2.79079600	0.85215700	-0.07555000	C	-5.02501200	-0.05451500	0.14145800
C	3.32548500	1.39375600	1.10330700	H	-3.70524300	0.41127500	1.76987500
C	3.25378000	1.34172200	-1.30635900	C	-5.15751600	-0.18989400	-1.24370400
C	4.28277400	2.40835200	1.05365100	H	-4.14802700	-0.07263900	-3.13490500
H	2.98606300	1.01704400	2.06449700	H	-5.86839300	-0.22314800	0.80321800
C	4.21162300	2.35591000	-1.35808100	O	-6.32191000	-0.53230800	-1.89339300
H	2.85752200	0.92482400	-2.22858100	C	-7.46343600	-0.79541400	-1.10163700
C	4.72830700	2.89290700	-0.17751600	H	-7.77170600	0.08321100	-0.51651100
H	4.68116500	2.81891400	1.97796900	H	-8.26600400	-1.05322700	-1.79852300
H	4.55406800	2.72534900	-2.32131900	H	-7.30273000	-1.64010900	-0.41642700
H	5.47394100	3.68279100	-0.21657700	C	2.11995400	-0.40151700	-0.75348900
C	-0.09153100	1.40571500	0.07863500	C	1.69977200	-1.40911900	-0.13965900
C	-0.28136000	2.06197000	1.30283800	C	2.93665000	0.44365100	-1.57716600
C	-0.38317300	2.08903700	-1.10971900	C	4.18982600	-0.02566300	-2.02985600
C	-0.75503800	3.37359900	1.33798000	C	2.51332700	1.72751500	-1.97339200
H	-0.05313000	1.54343700	2.22972000	C	4.98771800	0.76645200	-2.85048700
C	-0.85556800	3.40130700	-1.07397600	H	4.52486800	-1.01520500	-1.73256300

C	3.32058700	2.51431500	-2.79236600	H	-5.28320400	3.86405000	-1.03941200
H	1.55377900	2.09379600	-1.62476700	H	-4.27692600	5.89372300	-0.00150300
C	4.55793600	2.04040900	-3.23560700	C	-2.28078500	-0.87692900	-1.22049900
H	5.94936900	0.38910400	-3.18986000	C	-1.41270700	-1.53451300	-2.11208300
H	2.97923300	3.50361800	-3.08594600	C	-3.66810500	-1.01983700	-1.40971500
H	5.18322300	2.65734200	-3.87594200	C	-1.91741000	-2.29027300	-3.16810900
C	1.68774100	-2.74259900	0.39797800	H	-0.34058600	-1.43945300	-1.97050900
C	0.52726000	-3.29958600	0.96814600	C	-4.16994400	-1.77862600	-2.46766900
C	2.86628500	-3.51920700	0.36199300	H	-4.35156100	-0.54762100	-0.71022200
C	0.54496700	-4.59813200	1.47364800	C	-3.29766500	-2.41501400	-3.35315100
H	-0.37649000	-2.70021900	0.99451200	H	-1.22911700	-2.78526900	-3.84870100
C	2.87595600	-4.81376600	0.87365300	H	-5.24553500	-1.87728100	-2.59430500
H	3.76908900	-3.09450900	-0.06781500	H	-3.68866300	-3.00773900	-4.17640200
C	1.71509900	-5.36032600	1.43054600	N	1.55763900	-0.64904200	0.63383300
H	-0.36100200	-5.01505400	1.90619700	C	2.81586700	-0.11883600	0.27825700
H	3.79184900	-5.39859400	0.83705600	C	3.65037000	-0.66619300	-0.71538100
H	1.72479700	-6.37117300	1.83030000	C	3.28712800	1.03781400	0.93656200
H	-0.48241200	-1.04371900	-0.80049000	C	4.88110200	-0.08644900	-1.04381800
				H	3.33692700	-1.56582800	-1.22733900
TS9'				C	4.50991400	1.61534600	0.62016800
-1 1				H	2.66154500	1.48120200	1.70325300
C	-1.40479300	-3.87740800	2.37819400	C	5.32150500	1.06007400	-0.37802100
C	-0.23171600	-3.60200500	1.67201700	H	5.48224700	-0.54494200	-1.82256800
C	-0.01965900	-2.34173600	1.10880200	H	4.85477600	2.50509400	1.14064200
C	-1.00798200	-1.34019600	1.21208600	O	6.51232100	1.70649800	-0.62299500
C	-2.16217700	-1.61381700	1.96061500	C	7.34851400	1.17833200	-1.63293300
C	-2.35807200	-2.87081100	2.54465400	H	7.67569100	0.15391500	-1.40334200
H	-1.56281900	-4.86096300	2.81504400	H	6.85764300	1.18081100	-2.61679200
H	0.56119900	-4.33963200	1.57740400	H	8.22714700	1.82825900	-1.67545100
H	-2.92685000	-0.85007000	2.07065300	Ni	-0.10511700	0.38982900	0.87574800
H	-3.26357100	-3.06296200	3.11673000	H	0.51386600	1.74724000	1.18202800
C	1.34397600	-1.99341600	0.57669500				
O	2.13862400	-2.88813900	0.23316200	16'			
C	-1.74765800	-0.04013300	-0.14494100	-1 1			
C	-1.76789500	1.16176100	0.36632800	Ni	-0.37287400	-1.21908500	-0.11289600
C	-2.45651000	2.43532400	0.26045500	C	1.93520900	4.07248800	-1.45901400
C	-1.90564200	3.59531400	0.84179300	C	2.42173200	2.84073900	-1.03793800
C	-3.69000800	2.56290800	-0.41718200	C	1.60284100	1.87370800	-0.41183300
C	-2.55013200	4.82675600	0.74166800	C	0.24049500	2.19369900	-0.19739800
H	-0.96078500	3.50174100	1.36702000	C	-0.22681000	3.45673000	-0.61074900
C	-4.33535900	3.79381300	-0.51030300	C	0.59100700	4.38475800	-1.24724900
H	-4.13357000	1.68773500	-0.88058400	H	2.59997700	4.77992900	-1.94972700
C	-3.77011000	4.93425000	0.06866300	H	3.46690700	2.60148600	-1.20849000
H	-2.09988700	5.70619100	1.19633500	H	-1.26436000	3.70967600	-0.41115100

H	0.18537000	5.34357500	-1.56151300	19			
C	-0.84283200	1.42157800	0.55380500	-1 1			
O	-1.24142500	1.95638700	1.59872900	Ni	-0.03580300	0.64643000	0.00388000
N	-1.44445700	0.37266200	-0.10595600	C	-1.87094200	4.44788900	0.79875900
C	-2.85214400	0.21581900	0.00225300	C	-1.75213100	3.05526700	0.68387600
C	-3.50701300	-0.38457600	-1.09805800	C	-0.52215700	2.44576600	0.38581300
C	-3.66767800	0.65443600	1.06003200	C	0.58864100	3.30437000	0.22725200
C	-4.88453100	-0.52961500	-1.14607400	C	0.47476500	4.69454600	0.31962400
H	-2.89720900	-0.73905500	-1.92330300	C	-0.76174400	5.27546400	0.60535600
C	-5.06331700	0.51634500	1.01555800	H	-2.83968800	4.88619300	1.03708400
H	-3.20405100	1.11068100	1.92231700	H	-2.63939700	2.44520100	0.82277800
C	-5.68259100	-0.07460300	-0.08505100	H	1.36994900	5.29565700	0.17779000
H	-5.36732300	-0.99002400	-2.00426200	H	-0.85870000	6.35665700	0.68633500
H	-5.64590500	0.87134400	1.85997300	C	1.93247900	2.67098700	0.02774300
O	-7.04022000	-0.25649400	-0.22727800	O	2.96227500	3.35888600	-0.10742100
C	-7.87323200	0.18744200	0.82468300	N	1.83860100	1.31248300	0.09149100
H	-8.89863400	-0.04432400	0.52252600	C	2.99930100	0.52787600	0.18224000
H	-7.65658200	-0.33206600	1.76933600	C	2.96394100	-0.64754200	0.96722600
H	-7.78763100	1.27139800	0.98985500	C	4.21881800	0.81872400	-0.46325700
C	2.20615200	0.55166100	-0.09396000	C	4.06682200	-1.48277400	1.09394300
C	1.43889500	-0.55113900	-0.11237600	H	2.04388000	-0.89114500	1.48983200
C	3.66305600	0.51822900	0.26542200	C	5.33482700	-0.01819700	-0.33972500
C	4.58442100	-0.34196300	-0.35523000	H	4.29559000	1.72527900	-1.04840800
C	4.14021700	1.35036500	1.29764400	C	5.26803800	-1.17637500	0.43867000
C	5.92146800	-0.38224800	0.04728700	H	4.02027800	-2.37790800	1.70924800
H	4.25392200	-0.98210500	-1.16562900	H	6.25037900	0.25456500	-0.85508500
C	5.47354400	1.30963100	1.70298400	O	6.30743900	-2.05965700	0.63192500
H	3.44834600	2.02845700	1.78983400	C	7.53376800	-1.77921900	-0.01272000
C	6.37397700	0.44124900	1.07928900	H	7.96541500	-0.82390400	0.31901800
H	6.61171700	-1.05657600	-0.45484500	H	8.21601100	-2.58919200	0.26096400
H	5.80929000	1.95639100	2.51047800	H	7.42952900	-1.75842500	-1.10742000
H	7.41487300	0.40995200	1.39209500	C	-1.83530200	-0.05236500	0.14035700
C	1.62958600	-1.97686700	-0.11437000	C	-2.90928300	0.28125400	-0.61585700
C	0.94794900	-2.73602700	0.88749500	C	-1.82532400	-1.15274700	1.13445800
C	2.11375200	-2.69583600	-1.25854100	C	-1.46067200	-0.91375700	2.47886000
C	0.87202500	-4.14804600	0.79265100	C	-2.05063600	-2.49653000	0.75559500
H	0.66436900	-2.25574600	1.82047200	C	-1.35532800	-1.95737200	3.39699800
C	2.02356600	-4.06905100	-1.32894000	H	-1.25970000	0.10794600	2.78896100
H	2.55518600	-2.13272100	-2.07556100	C	-1.92647200	-3.54292200	1.67400500
C	1.40913600	-4.80993500	-0.29126300	H	-2.35719400	-2.70930600	-0.26566600
H	0.38875100	-4.70138500	1.59364100	C	-1.58070700	-3.28059900	3.00080800
H	2.42354200	-4.58958700	-2.19625300	H	-1.08231400	-1.73785400	4.42682400
H	1.34926600	-5.89299500	-0.36157300	H	-2.10864400	-4.56573300	1.35031500
H	-1.57828100	-2.17354300	-0.01342500	H	-1.48372500	-4.09325900	3.71639900

C	-4.30943900	-0.19639400	-0.58756500	C	3.08528600	0.60418400	0.17135100
C	-5.10020400	-0.02815300	-1.74438900	C	3.19998500	-0.46110000	1.08770500
C	-4.93681300	-0.76784600	0.53993400	C	4.22985500	0.94409100	-0.56915700
C	-6.43293500	-0.43436300	-1.78891800	C	4.39413200	-1.15199900	1.25297900
H	-4.64923600	0.42971600	-2.62277700	H	2.32826700	-0.74107000	1.67065000
C	-6.27051700	-1.17215100	0.49764000	C	5.43917200	0.25958500	-0.40342100
H	-4.37738500	-0.87980500	1.46193200	H	4.17734400	1.76877900	-1.26951500
C	-7.02879300	-1.01477700	-0.66636600	C	5.52727100	-0.79738100	0.50801800
H	-7.00888800	-0.29225300	-2.70105000	H	4.47006600	-1.97298500	1.96089000
H	-6.72422100	-1.60510700	1.38674300	H	6.29849200	0.56246500	-0.99276800
H	-8.06937100	-1.32902500	-0.69390300	O	6.66213300	-1.53767500	0.74387200
H	-2.74990400	1.04929100	-1.37550200	C	7.82648300	-1.20841600	0.01184100
C	1.72401500	-2.77289500	-2.29456000	H	8.16525100	-0.18258800	0.21602600
C	0.76266600	-1.57842100	-2.25162400	H	8.60063100	-1.90796800	0.33939100
H	2.67143800	-2.52123100	-1.80839100	H	7.67852600	-1.32465100	-1.07134200
H	1.29456500	-3.64087400	-1.77739800	C	-1.69226800	-0.78635800	-0.00429700
H	1.92964500	-3.07038600	-3.33013800	C	-2.56090100	-0.49888300	-1.00916400
C	-0.58663000	-1.93258600	-2.88746200	C	-2.08686000	-1.29077100	1.33943700
C	1.37742000	-0.35241900	-2.92283300	C	-1.76319100	-0.59409300	2.51878800
H	-1.29775300	-1.10973800	-2.77091100	C	-2.72628600	-2.54015500	1.47068900
H	-0.46369300	-2.14179100	-3.95682600	C	-2.09677700	-1.10841300	3.77316900
H	-1.02087000	-2.82889400	-2.42580400	H	-1.24898400	0.35907700	2.43921300
H	1.55587800	-0.56189800	-3.98411300	C	-3.04664800	-3.06019400	2.72470200
H	0.70814400	0.51046200	-2.84515200	H	-2.96888500	-3.10403100	0.57363000
H	2.32884200	-0.08838800	-2.45453600	C	-2.73970200	-2.34369400	3.88461100
O	0.56209600	-1.22960800	-0.84572600	H	-1.84437700	-0.54252600	4.66702600
H	0.01212200	-1.91968700	-0.43371000	H	-3.53731100	-4.02862200	2.79527200
TS12				H	-2.98958200	-2.74746400	4.86283700
-1 1				C	-4.03359300	-0.42382600	-1.05529400
Ni	0.15684800	0.38410300	-0.09132700	C	-4.65653900	-0.43129200	-2.32013500
C	-2.22790900	3.90820100	0.49879800	C	-4.86059400	-0.30033900	0.08004600
C	-1.90867000	2.54451600	0.41504300	C	-6.04150800	-0.34908000	-2.44988300
C	-0.58304300	2.11892100	0.23556300	H	-4.03604500	-0.50604000	-3.21052900
C	0.40355300	3.12090500	0.15507000	C	-6.24498900	-0.20818300	-0.04995500
C	0.09724500	4.48151200	0.22421800	H	-4.41393800	-0.26287000	1.06620800
C	-1.22975500	4.88122600	0.39568100	C	-6.84478000	-0.23898600	-1.31239700
H	-3.26527100	4.20898100	0.64083400	H	-6.49333900	-0.36359500	-3.43877600
H	-2.71493400	1.82010600	0.48805600	H	-6.85899100	-0.10637100	0.84159700
H	0.90602600	5.20511900	0.15115400	H	-7.92542800	-0.16851400	-1.40802200
H	-1.48447200	5.93770200	0.45382000	H	-2.10872900	-0.26968300	-1.97586300
C	1.81570800	2.64258200	0.04565500	C	2.51074000	-2.46315100	-1.90193400
O	2.78623200	3.41639000	0.02116400	C	1.06419000	-1.94101000	-1.95001200
N	1.85304600	1.27558600	0.04048800	H	3.20732000	-1.65511800	-1.66306800
				H	2.60657600	-3.23286800	-1.12820000

H	2.80780600	-2.90260600	-2.86431800	C	-2.20805300	2.89030500	0.31908900
C	0.12271100	-3.09744000	-2.34413100	H	-0.98383200	4.48785100	-0.51673600
C	0.96470600	-0.80582900	-2.98686400	H	-2.60540400	4.37567300	-1.22319700
H	-0.91904200	-2.75864600	-2.39011800	H	-2.38993200	5.08782600	0.39372500
H	0.38509400	-3.51761900	-3.32411100	C	-3.70063400	2.64178300	0.62144200
H	0.18111200	-3.90077500	-1.59997100	C	-1.39837500	2.79938000	1.63101000
H	1.26730800	-1.14839700	-3.98589100	H	-3.83930800	1.64815400	1.06136800
H	-0.06173000	-0.42635700	-3.06241100	H	-4.10913800	3.38438100	1.32071700
H	1.61102600	0.02955200	-2.69812200	H	-4.28458600	2.68909200	-0.30581400
O	0.71972600	-1.49577200	-0.63991600	H	-1.72393100	3.54326400	2.37210500
H	-0.54972600	-1.29872500	-0.43113900	H	-1.50535300	1.80394600	2.07886500
20				H	-0.33222200	2.96469900	1.43012800
-1 1				O	-1.75168200	1.97900300	-0.64713000
Ni	-0.93881100	0.39770600	-0.38896400	21			
C	-4.31471500	-2.14539900	-0.21145900	-1 1			
C	-3.56593400	-0.96977300	-0.37407500	Ni	-0.36175800	-0.17123100	0.22608300
C	-2.17357500	-0.99835000	-0.23473600	C	-3.00538000	-2.56273700	2.68967000
C	-1.55173600	-2.22779500	0.04541700	C	-2.56509200	-1.50157800	1.88469400
C	-2.29350200	-3.39791000	0.21865900	C	-1.24514500	-1.44667400	1.40972800
C	-3.68415400	-3.35688200	0.09042800	C	-0.39076000	-2.49519700	1.79096000
H	-5.39778900	-2.11283200	-0.32174300	C	-0.81592100	-3.56355000	2.58264800
H	-4.07465500	-0.03984700	-0.61069100	C	-2.13656400	-3.60166500	3.03534300
H	-1.76812700	-4.32346300	0.44291500	H	-4.03500400	-2.57712300	3.04556600
H	-4.27387400	-4.26217800	0.22010900	H	-3.27619800	-0.71763800	1.63200600
C	-0.05767400	-2.20469200	0.12956200	H	-0.09966100	-4.34115600	2.83829200
O	0.60982900	-3.21134900	0.42361400	H	-2.48411800	-4.42515300	3.65624200
N	0.40077400	-0.95510700	-0.17756300	C	1.02886300	-2.37497100	1.34167000
C	1.75550700	-0.60256300	-0.16592000	O	1.89251100	-3.21664500	1.63635200
C	2.13357400	0.59181200	-0.82452600	N	1.21952500	-1.21894200	0.63516200
C	2.78177600	-1.32351900	0.47972100	C	2.54786900	-0.89839400	0.26585100
C	3.44492800	1.04963700	-0.82246100	C	3.33525200	-1.76226900	-0.51879500
H	1.37575100	1.16194000	-1.35917800	C	3.13737000	0.29255600	0.70518100
C	4.10387600	-0.86785800	0.47860500	C	4.65153900	-1.44786200	-0.84213800
H	2.53117700	-2.25276100	0.97220700	H	2.90602300	-2.69743500	-0.86301500
C	4.44807400	0.32269600	-0.16824600	C	4.45926100	0.62146700	0.38928500
H	3.71257400	1.96958500	-1.33536100	H	2.54291100	0.97756000	1.29948400
H	4.85604300	-1.45960500	0.99050300	C	5.22546500	-0.25230400	-0.38952300
O	5.71756700	0.85097400	-0.22677500	H	5.25570500	-2.12212100	-1.44370600
C	6.74880900	0.15915600	0.45011200	H	4.87122200	1.55783600	0.75059600
H	6.89865700	-0.85422100	0.05063000	O	6.53283500	-0.03315300	-0.75762100
H	7.66162700	0.73978000	0.29036100	C	7.14307600	1.17066700	-0.33411200
H	6.55684900	0.08977300	1.53054600	H	8.16055800	1.15452000	-0.73501400
C	-2.03968200	4.29995400	-0.28682300	H	6.62068200	2.05638200	-0.72269700

H	7.19468800	1.24212000	0.76183700	C	2.37466900	1.13120600	2.06538400
C	-1.89872800	1.26152300	0.29669100	C	1.09367100	1.07367100	1.49087800
C	-2.24528400	0.40865200	-0.53684000	C	0.03071400	1.75521900	2.12027000
C	-1.82667200	2.39453800	1.17227000	C	0.27080000	2.51179000	3.27115900
C	-0.99809200	2.39843200	2.31110700	C	1.54787900	2.57836100	3.82737500
C	-2.61238000	3.53367400	0.89639800	H	3.59489100	1.90650300	3.65905700
C	-0.96542700	3.50858400	3.15157200	H	3.20353100	0.60833000	1.60046800
H	-0.38777200	1.52654500	2.52148600	H	-0.57727700	3.01874400	3.72366900
C	-2.57228900	4.63851400	1.74297700	H	1.72456100	3.16670900	4.72476200
H	-3.24572800	3.54187200	0.01428300	C	-1.37230500	1.59092300	1.60898500
C	-1.74879200	4.63179700	2.87256100	O	-2.25884400	2.39401900	1.96678300
H	-0.32121300	3.49668900	4.02682300	N	-1.46643500	0.51061800	0.79764100
H	-3.18228700	5.50962700	1.51727700	C	-2.64609800	0.19700800	0.09688600
H	-1.71731200	5.49693600	3.52990300	C	-2.67852500	-1.00857400	-0.64620900
C	-3.00168400	-0.33601300	-1.50343200	C	-3.80181600	1.00682900	0.04905200
C	-2.72113600	-1.68554100	-1.79398900	C	-3.79000700	-1.36980400	-1.39694800
C	-4.06208500	0.30011300	-2.18505700	H	-1.81608800	-1.66743000	-0.58448200
C	-3.48315200	-2.37505000	-2.73489600	C	-4.91889700	0.64203000	-0.71127300
H	-1.91085700	-2.17902900	-1.26888900	H	-3.81721300	1.92499300	0.61808900
C	-4.81518800	-0.39746900	-3.12596000	C	-4.92374200	-0.54738300	-1.44238600
H	-4.28366300	1.34116700	-1.96941500	H	-3.79931900	-2.30201000	-1.95688400
C	-4.52997800	-1.73707900	-3.40537200	H	-5.78029400	1.30256000	-0.71493800
H	-3.25386400	-3.41614400	-2.94619100	O	-5.97245200	-0.99494300	-2.21567400
H	-5.62686900	0.10758900	-3.64360500	C	-7.13782800	-0.19668000	-2.26283000
H	-5.11852500	-2.27868600	-4.14139700	H	-7.84122600	-0.71962100	-2.91721400
C	-0.35052500	2.26786300	-2.69993000	H	-7.59766400	-0.07834200	-1.27079300
C	0.75527100	1.32618600	-2.14883400	H	-6.93941600	0.80080200	-2.68147800
H	-1.33962100	1.80430800	-2.63124900	C	1.94109600	-0.39103800	-0.56166300
H	-0.37152800	3.19821400	-2.11815000	C	1.54501600	0.85114500	-0.48599200
H	-0.17951400	2.53036100	-3.75453800	C	2.87292000	-1.32835700	-1.13707000
C	2.12009800	2.02038800	-2.38552600	C	4.18678200	-0.94464600	-1.48791400
C	0.73527400	0.00764100	-2.95871200	C	2.48356200	-2.67041100	-1.34124500
H	2.93992600	1.36597900	-2.07431800	C	5.07257200	-1.86780300	-2.04024700
H	2.27248900	2.28733600	-3.44164500	H	4.50737600	0.07859000	-1.31234200
H	2.17926800	2.93961500	-1.78906300	C	3.37346600	-3.58208800	-1.90479000
H	0.90055300	0.17826400	-4.03281000	H	1.48545000	-2.95343200	-1.01760800
H	1.51849800	-0.66676300	-2.59575800	C	4.66831000	-3.18831700	-2.25866100
H	-0.22907100	-0.50220900	-2.84723000	H	6.08088700	-1.55557600	-2.30248400
O	0.62446100	1.10881700	-0.77929600	H	3.05839100	-4.61113000	-2.06251500
				H	5.35911200	-3.90535800	-2.69569100
				C	1.60116300	2.12681100	-1.19445000
				C	2.44628700	2.23074600	-2.32106400
				C	0.83196300	3.24970500	-0.83968700
				C	2.52343100	3.41294300	-3.05214100
TS13							
-1 1							
Ni	0.33615500	-0.37187100	0.46370800				
C	2.59616400	1.87312600	3.22920500				

H	3.03440400	1.37035500	-2.62404600	H	-0.46634200	-2.16413100	4.56491900
C	0.91241100	4.43094200	-1.57650300	H	-0.75528400	-4.77271400	1.15410800
H	0.16898500	3.19893000	0.01467000	H	-1.00302100	-4.40065100	3.60545200
C	1.75930500	4.52358800	-2.68242500	C	2.61708100	-1.67538000	-0.70113800
H	3.18278200	3.46575700	-3.91532600	C	2.87194100	-2.21026500	-1.97888800
H	0.30484000	5.28260500	-1.28106700	C	3.26751100	-2.26805600	0.39675700
H	1.82148600	5.44726400	-3.25218700	C	3.72196100	-3.30337700	-2.14853700
C	-1.40916200	-2.51317200	2.47546800	H	2.39094500	-1.76435700	-2.84523400
C	-0.22871100	-3.01368000	1.61166400	C	4.11869200	-3.36080400	0.22847000
H	-1.24583100	-1.47708600	2.78990400	H	3.10209200	-1.86111600	1.38945000
H	-2.34311200	-2.53996500	1.90296900	C	4.34953300	-3.88706900	-1.04482900
H	-1.54245700	-3.12892800	3.37655600	H	3.89318100	-3.70066000	-3.14667200
C	-0.52131000	-4.46621200	1.16922200	H	4.60800600	-3.79759100	1.09617700
C	1.05807000	-3.00658400	2.47094400	H	5.01395500	-4.73774900	-1.17647200
H	0.31384500	-4.85841900	0.57543600	C	-0.53469600	0.96101700	-2.16610000
H	-0.67789000	-5.13784500	2.02502600	O	-1.05533400	0.82414900	-3.28914200
H	-1.42084300	-4.49480400	0.54284000	N	-1.16357300	0.87540000	-0.96639800
H	0.96325800	-3.63437100	3.36865800	Ni	0.20201200	1.18080300	0.64521200
H	1.90873100	-3.37507800	1.88436600	C	-2.52362100	0.50285700	-0.86467100
H	1.29203900	-1.98550500	2.79595200	C	-3.26456300	-0.16652300	-1.85829800
O	-0.05924700	-2.25619500	0.44406200	C	-3.19874100	0.79070200	0.34415700
22				C	-4.59977300	-0.53120400	-1.65339800
-1 1				H	-2.79061000	-0.38918100	-2.80297800
C	2.59709600	2.82657900	-3.15932300	C	-4.52205200	0.42772100	0.55393100
C	1.27960200	2.40575700	-3.00197500	H	-2.66314700	1.30846000	1.13722200
C	0.93504100	1.34948500	-2.14205000	C	-5.24097000	-0.23857900	-0.44721200
C	1.96205300	0.65835900	-1.45172900	H	-5.12364500	-1.04613500	-2.45235600
C	3.29365300	1.07427800	-1.65809400	H	-5.01847300	0.65728400	1.49289200
C	3.61429500	2.15054200	-2.48071600	O	-6.54711900	-0.54884000	-0.15117400
H	2.82928600	3.66200500	-3.81567700	C	-7.30031800	-1.22943900	-1.13642100
H	0.48214100	2.88594500	-3.56117400	H	-8.29467900	-1.38325000	-0.70813500
H	4.08926500	0.53812700	-1.14815900	H	-7.39789700	-0.63928800	-2.05893800
H	4.65232700	2.45460500	-2.59523000	H	-6.86441600	-2.20735500	-1.38510600
C	1.70597500	-0.49675700	-0.53410000	C	2.63382100	2.00379600	2.68103800
C	0.74396500	-0.41405700	0.41919000	C	1.28355000	2.74771100	2.61526000
C	0.28379500	-1.51515000	1.29152200	H	2.58203100	1.17831800	3.40133300
C	0.09948900	-1.30990600	2.67474100	H	2.88406000	1.58273100	1.70176300
C	-0.04562500	-2.78107200	0.76270900	H	3.45246100	2.67035400	2.98650600
C	-0.34335200	-2.34402000	3.49887300	C	1.39366300	3.92174400	1.61880200
H	0.29148800	-0.31716600	3.07266200	C	0.93817100	3.30208000	4.01400600
C	-0.50433900	-3.80715800	1.58807100	H	0.43169700	4.44511900	1.54654200
H	0.05811300	-2.95177700	-0.30442800	H	2.15742900	4.65212100	1.92119500
C	-0.64587300	-3.59917700	2.96276900	H	1.65314000	3.55423800	0.61967400
				H	1.69747700	4.00621800	4.38066300

H	-0.02690500	3.82224700	3.98434400	C	2.12493100	0.68488900	0.71689200
H	0.85357700	2.48008800	4.73502200	C	2.88381300	-0.05848400	1.62913200
O	0.24761700	1.86683700	2.26189300	C	2.79049200	1.31824200	-0.34198700
TS14				C	4.26873700	-0.16549500	1.50138800
-1 1				H	2.38559300	-0.55161200	2.45768000
C	-3.10360900	1.23050400	3.87811000	C	4.17000100	1.20965200	-0.48523300
C	-1.82735900	1.53487600	3.43844400	H	2.21249800	1.89659400	-1.05705100
C	-1.23150900	0.85297900	2.35690600	C	4.92097300	0.46918300	0.43599000
C	-1.93581900	-0.20879400	1.70073100	H	4.82273900	-0.74500600	2.23157800
C	-3.23843600	-0.50850300	2.19448500	H	4.68423300	1.69737600	-1.30823700
C	-3.81030500	0.19200100	3.24041100	O	6.27234800	0.42576000	0.21387500
H	-3.55201200	1.78181000	4.70084400	C	7.07368200	-0.30811200	1.12344200
H	-1.24035400	2.30962000	3.92138500	H	8.10245400	-0.21027000	0.76699900
H	-3.80824700	-1.29408300	1.70911400	H	7.00976700	0.09533900	2.14352700
H	-4.81943900	-0.05823800	3.56232100	H	6.80319400	-1.37302600	1.14090200
C	-1.35037300	-0.93494500	0.59943800	C	-2.82646500	3.71725900	-0.94179100
C	-0.32188100	-0.32034000	-0.15241000	C	-2.36193400	2.89385100	-2.16259000
C	0.50290500	-1.10746900	-1.12559600	H	-2.89410800	3.07434800	-0.05657600
C	0.56621300	-0.72086700	-2.47628400	H	-2.09654900	4.50809100	-0.72656200
C	1.24084100	-2.23335800	-0.72063500	H	-3.80701000	4.18931800	-1.10067800
C	1.32516300	-1.45004300	-3.39327000	C	-2.28895800	3.81857500	-3.39845400
H	0.00602600	0.15549500	-2.79363200	C	-3.37851100	1.76293100	-2.43320300
C	2.01407600	-2.95104400	-1.63336200	H	-1.93776300	3.25155100	-4.26932900
H	1.20193000	-2.54574900	0.31858900	H	-3.26126200	4.26635900	-3.64699500
C	2.05709600	-2.56409100	-2.97505700	H	-1.57359300	4.63086100	-3.21851100
H	1.35047700	-1.14094800	-4.43585300	H	-4.38550600	2.14895100	-2.64668500
H	2.58263100	-3.81494000	-1.29647500	H	-3.05399300	1.16197000	-3.29232800
H	2.65832500	-3.12443600	-3.68745200	H	-3.44413300	1.09871300	-1.56400900
C	-1.87353800	-2.28356700	0.25033900	O	-1.08526700	2.35970800	-1.96469100
C	-2.03444900	-3.27837600	1.23979400	23			
C	-2.23945100	-2.62851900	-1.06738800	-1 1			
C	-2.52133300	-4.54744900	0.92900200	Ni	-1.23431700	-1.59719300	-0.03802300
H	-1.75920200	-3.04805100	2.26559300	C	-5.11701300	0.04848000	0.05138400
C	-2.71682700	-3.90101200	-1.38241100	C	-4.11245600	-0.93029200	0.03011700
H	-2.15202500	-1.88161900	-1.84985400	C	-2.76477500	-0.55424200	0.00013900
C	-2.86273700	-4.87083600	-0.38755300	C	-2.44241100	0.81799200	-0.00408400
H	-2.62284600	-5.29092800	1.71711900	C	-3.44394200	1.79183000	0.01454300
H	-2.98796800	-4.13063800	-2.41072800	C	-4.78659300	1.40744400	0.04185400
H	-3.23810500	-5.86149400	-0.63315100	H	-6.16317100	-0.25361500	0.07421000
C	0.18195700	1.17701100	2.08181300	H	-4.38259900	-1.98267700	0.03480000
O	0.89246100	1.77617400	2.89875400	H	-3.15085600	2.83899700	0.00918400
N	0.69851200	0.74761900	0.83888800	H	-5.57165900	2.16097600	0.05632900
Ni	-0.35342800	1.50551000	-0.55113700	C	-0.98640800	1.18816500	-0.02036700

O	-0.61595400	2.37676500	-0.03361000	H	3.83635100	1.55855300	-1.26728100
N	-0.21528800	0.06492600	-0.01184600	O	5.34830300	-0.11503700	0.30358000
C	1.17880000	0.07129000	-0.00455400	H	-0.06877200	-2.72083500	-0.53600200
C	1.82934800	-1.18672800	0.03506200	C	6.12575300	0.75742800	-0.49456300
C	2.01224500	1.21059000	-0.03216100	H	5.92899800	1.81360400	-0.26188500
C	3.21185000	-1.30691900	0.04490200	H	7.17052500	0.53259700	-0.26278700
H	1.22907200	-2.09776400	0.06726200	H	5.95543700	0.59180800	-1.56777900
C	3.40639200	1.09318100	-0.02157100				
H	1.54810500	2.18664800	-0.06029300	25			
C	4.01997500	-0.16186400	0.01633100	O 1			
H	3.68568200	-2.28449300	0.07762500	Ni	-0.97546500	-1.40406500	-0.00017200
H	4.00097800	2.00112000	-0.04436200	C	3.12107400	-0.55182300	0.00094600
O	5.38031800	-0.37783200	0.03109300	C	1.94111100	-1.31697400	0.00134000
H	-1.98877900	-2.92351100	-0.07235600	C	0.72007300	-0.64874700	0.00024200
C	6.22102200	0.75889600	0.01417600	C	0.66244700	0.74888100	-0.00095900
H	6.05711500	1.40457800	0.88876600	C	1.83284700	1.50363700	-0.00098900
H	7.24719100	0.38154600	0.04048900	C	3.06744100	0.84409900	-0.00018800
H	6.08569500	1.35670900	-0.89857400	H	4.08425700	-1.05688800	0.00156000
				H	2.00518700	-2.40346900	0.00241800
24				H	1.76849900	2.58865000	-0.00147600
-1 1				H	3.98995000	1.41864800	-0.00034000
Ni	-1.22816500	-1.64794800	-0.29808800	C	-0.72517700	1.31191700	-0.00103900
C	-5.13118400	0.15257900	-0.03248800	O	-1.01207500	2.51073300	0.00189900
C	-4.15289100	-0.84472700	-0.17302200	N	-1.63553700	0.29546600	-0.00460900
C	-2.78872600	-0.52636900	-0.10558600	C	-3.06046800	0.56526300	0.00214400
C	-2.44767400	0.81823200	0.10458700	H	-3.60795900	-0.38588300	-0.00073300
C	-3.40527000	1.82422100	0.24076100	H	-3.36583600	1.12656700	0.89562000
C	-4.76028600	1.48590800	0.17229400	H	-3.37178900	1.13454800	-0.88414700
H	-6.18708900	-0.11128600	-0.08297200				
H	-4.47755700	-1.87478000	-0.33375700	26			
H	-3.08404400	2.85167900	0.39749700	-1 1			
H	-5.52397900	2.25409300	0.27739800	Ni	0.96169700	-1.44861200	0.00131400
C	-0.97894600	1.08581800	0.18029200	C	-3.14611900	-0.46948700	-0.00236800
O	-0.50009100	2.21481200	0.35125400	C	-1.98776200	-1.26376800	-0.00029200
N	-0.25906500	-0.08198400	0.06310100	C	-0.72551300	-0.66302200	0.00112000
C	1.15244400	-0.05481300	0.09622000	C	-0.64201700	0.74444400	0.00145000
C	1.85920500	-0.94091600	0.93083800	C	-1.79233000	1.53324200	-0.00018800
C	1.90130700	0.83471000	-0.68903800	C	-3.05229600	0.92471900	-0.00231800
C	3.24759100	-0.94027300	0.97509600	H	-4.12550300	-0.94651600	-0.00414100
H	1.29507000	-1.64352500	1.53546400	H	-2.07534700	-2.34700600	0.00004400
C	3.29831200	0.85079200	-0.64536600	H	-1.68300200	2.61566000	0.00001200
H	1.38139200	1.53413400	-1.33377700	H	-3.95487200	1.53291800	-0.00434600
C	3.98100400	-0.04202600	0.18731400	C	0.74464000	1.32968300	0.00116700
H	3.78622000	-1.63120800	1.61794400	O	0.96503000	2.55730300	0.00604200

N	1.66447900	0.34407000	-0.00411000
H	0.45576600	-2.90194000	0.00842000
C	3.05771500	0.73572200	-0.00533900
H	3.69034500	-0.15901800	0.07214800
H	3.34789200	1.27100800	-0.92516700
H	3.30771300	1.39991300	0.83728700

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Ni	1.09226100	-1.38406200	-0.00513500
C	-3.16099700	-0.64743600	0.00243000
C	-1.95310400	-1.36550300	0.00257900
C	-0.71986800	-0.69864700	0.00299700
C	-0.74693300	0.70622600	0.00308000
C	-1.93460100	1.43620400	0.00017000
C	-3.15465200	0.75059200	0.00053700
H	-4.11065300	-1.18178100	0.00335500
H	-1.99748700	-2.45662900	0.00258100
H	-1.89451000	2.52373800	-0.00323500
H	-4.09422800	1.30003100	-0.00124500
C	0.60762500	1.34338900	0.00094700
O	0.80424100	2.57059200	-0.01598300
N	1.59031200	0.40358800	0.02066600
C	2.96672800	0.86440700	0.00889000
H	3.62531100	0.01866300	0.20971200
H	3.24813700	1.30217300	-0.96289700
H	3.13016800	1.63868400	0.77197400
H	2.51864700	-2.11638000	-0.02303500