Electronic Supplementary Information

Theoretical Mechanistic Study of Metallaphotoredox Catalysis: C–N Cross-Coupling via Ni(II)-Mediated σ-Bond Metathesis

Run-Han Li,[a] Bo Zhu,[a] Shuang Wang,[a] Yun Geng,[a] Li-Kai Yan,[a] Zhong-Min Su,[a] Li-Shuang Yao,[b] Rong-Lin Zhong[c] and Wei Guan*[ab]*

[a]Faculty of Chemistry, National & Local United Engineering Lab for Power Battery, Key Laboratory of Polyoxometalate Science of Ministry of Education, Northeast Normal University, Changchun 130024, People's Republic of China
[b]State Key Laboratory of Applied Optics, Changchun Institute of Optics, Fine Mechanics and Physics, Chinese Academy of Sciences, Changchun 130033, People's Republic of China
[c]Institute of Theoretical Chemistry, Jilin University, Changchun 130023, People's Republic of China

E-mail: guanw580@nenu.edu.cn

Table of contents

1. Computational Models and Details

1.1. Computational Methods

1.1.1. Photophysical Properties of Ir(III)

The ground-state geometry optimization of $Ir^{III}[dF(CF_3)ppy]_2(dtbbpy)PF_6$ (**Ir(III)**) was carried out by using (U)M06 functional with LanL2DZ basis set for iridium atom and 6-31G(d) basis sets for the other atoms in the gas phase. The TD-DFT calculation was performed at the (U)M06/[6-31G(d)/LanL2DZ(Ir)] level in acetonitrile based on the optimized ground-state geometry, where solvent effects of acetonitrile were evaluated with SMD model. The absorption spectra were simulated with the full width at half maximum (FWHM) of 1200 cm^{-1} based on the TD-DFT computational results. As illustrated in Figure S1, the calculated absorption bands of **Ir(III)** at 253, 300 and 395 nm agree well with the experimental values 260, 310 and 380 nm, respectively.[S1] In addition, we have analyzed the transition properties of **Ir(III)**. As shown in Figure S2 and Table S1, the strong absorption bands at 253, 300, 342, and 395 nm are mainly assigned both ligand-to-ligand charge transfer (LLCT) and metal-to-ligand charge transfer MLCT characters.
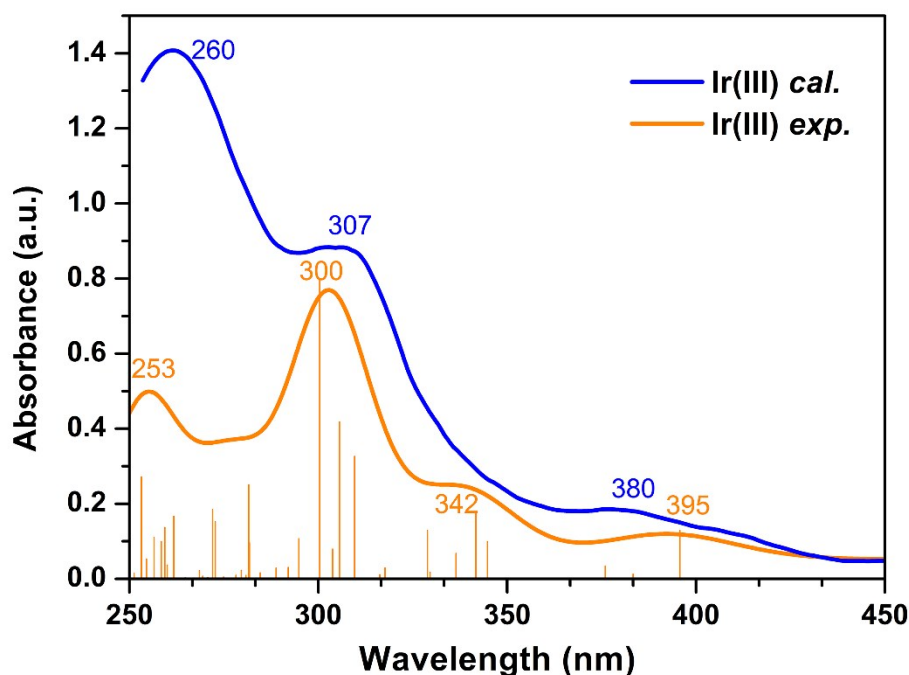
Figure S1. Comparisons of experimental and calculated absorption spectra of **Ir(III)**.
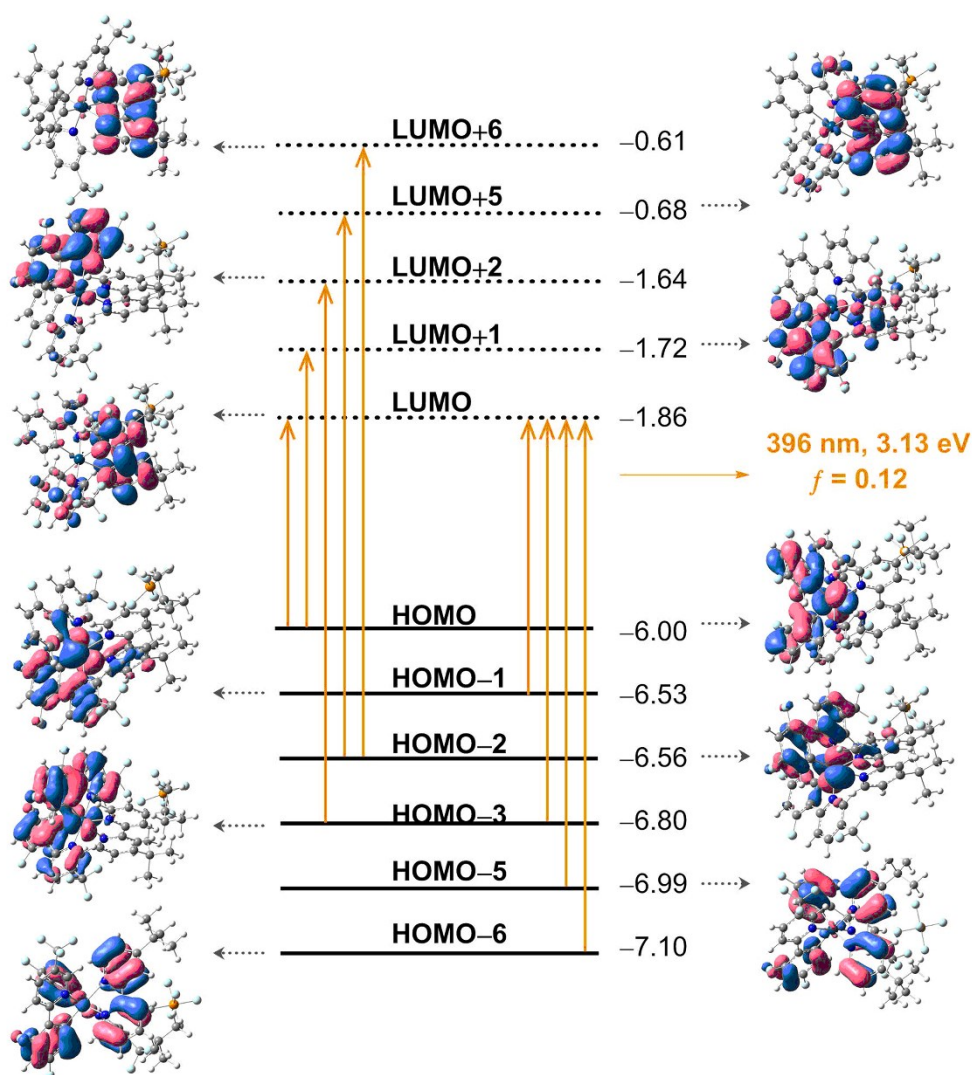
Figure S2. The calculated frontier molecular orbital distributions of **Ir(III)**.

Table S1. Absorption peaks λ_{abs} [in eV (nm)], the oscillator strengths (f), major contributions and assignments (H and L represent HOMO and LUMO, respectively).

λ_{abs}	f	Major Contributions	Assignments
395	0.12	H→L (63%), H→L+1 (31%)	MLCT/LLCT
342	0.16	H-3→L (10%), H→L (58%), H-1→L (21%)	MLCT/LLCT
300	0.75	H-6→L (30%), H-5→L (34%) H-3→L+2 (8%)	MLCT/LLCT
253	0.25	H-2→L+5 (11%), H-2→L+6 (58%)	MLCT/LLCT

1.1.2. Redox Potential

We calculated the standard redox potential ($E_{1/2}^{red}$) according to the equation[S2]:

$$E_{1/2}^{red} = -\frac{\Delta G_r}{nF} - E_{SHE}$$

where F is the Faraday constant and n the number of electrons transferred, $E_{SHE} = 4.28$ eV, and ΔG_r free energy change of the reaction.

Table S2. The experimental and calculated redox potentials of iridium complexes in CH_3CN solvent.

Redox Potential	$E_{1/2}^{red}[*Ir^{III}/Ir^{II}]$	$E_{1/2}^{red}[Ir^{III}/Ir^{II}]$	$E_{1/2}^{red}[Ir^{IV}/Ir^{III}]$	$E_{1/2}^{red}[Ir^{IV}/*Ir^{III}]$
Exp.	1.21	−1.37	1.69	−0.89
Cal.	0.82	−1.60	1.40	−1.05
|Δ|	0.39	0.23	0.29	0.16

Table S3. The calculated redox potentials of Ir, Ni complexes and DABCO in DMA solvent.

Redox Potential	Cal.
$E_{1/2}[*Ir^{III}/Ir^{II}]$	1.04
$E_{1/2}[Ir^{III}/Ir^{II}]$	−1.50
$E_{1/2}[*Ir^{III}/Ir^{IV}]$	−1.41
$E_{1/2}[Ir^{IV}/Ir^{III}]$	1.11
$E_{1/2}[Ni^{III}/Ni^{II}]$ ($E_{1/2}[\mathbf{a5/a4}]$)	0.79
$E_{1/2}[Ni^{I}/Ni^{0}]$ ($E_{1/2}[\mathbf{a6/Ni(0)^S}]$)	−1.75
$E_{1/2}[DABCO^{•+}/DABCO]$	0.53
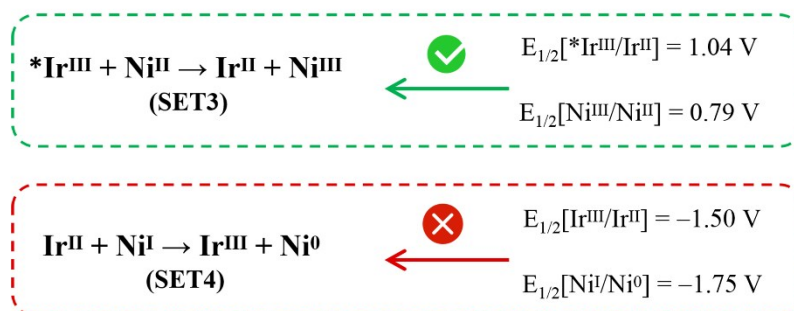
Scheme S1. The single electron transfer processes.

1.1.3. Correction of Translational Entropy in Solution

We evaluated the electronic energy (E_{sol}) with zero-point energy correction in solution. For each species, the E_{sol} is defined through equation:

$$E_{sol} = E_{sol}^{pot} + E_{gas}^{v_0}$$

where E_{sol}^{pot} is the potential energy including non-electrostatic energy in solution and $E_{gas}^{v_0}$ represents the zero-point vibrational energy in the gas phase. In a bimolecular process, such as the coordination of aryl bromide with the nickel center, the entropy change must be taken into consideration because the entropy considerably decreases.

In this case, Gibbs energy (G_{sol}^{o}) is evaluated as follows:

$$G_{sol}^{o} = H_0 - T\left(S_r^o + S_v^o + S_t^o\right)$$
$$= E^T + P\Delta V - T\left(S_r^o + S_v^o + S_t^o\right)$$
$$= E_{sol} + E_{therm} - T\left(S_r^o + S_v^o + S_t^o\right)$$

where ΔV is 0 in solution, E_{therm} is the thermal correction by translational, vibrational, and rotational movement, and S_r^o, S_v^o, and S_t^o are rotational, vibrational, and translational entropies, respectively. In general, the Sackur-Tetrode equation is used to evaluate translational entropy S_t^o. In solution, however, the usual Sackur-Tetrode equation cannot be directly applied to the evaluation of S_t^o, because the translation movement is suppressed very much in solution. In this context, the translational entropy was corrected with the method developed by Whitesides et al.,[19] where the rotational entropy was evaluated in a normal manner. Thermal correction and entropy contributions of vibration movements to the Gibbs energy were evaluated with the frequencies calculated at 298.15 K and 1 atm.

1.2. Model Reaction

Ni(II)$^\text{T}$(**S=3**)   Ni(II)$^\text{S}$(**S=1**)

0.0   14.7
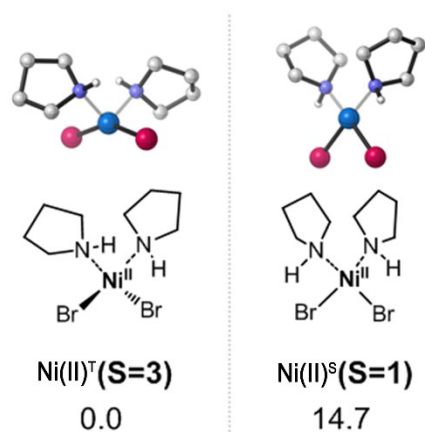
Figure S3. Structures of triplet and singlet Ni(II) complexes. The Gibbs free energies relative to the most stable **Ni(II)$^\text{T}$** conformation are given in kcal/mol. Gray, white, purple, pink and blue spheres represent C, H, N, Br and Ni atoms, respectively.

2. Marcus Theory using in Single Electron Transfer Step

2.1. Recombination Energy and Activation Energy[S3,S4]

According to the Marcus equation, the reorganization energy λ is normally decomposed into internal energy (λ_i) and external energy (λ_o). The internal reorganization energy λ_i can be estimated according to the equation:

$$\lambda_{i1} = \left[E^{D*}(Q_P) + E^A(Q_P)\right] - \left[E^{D*}(Q_R) + E^A(Q_R)\right]$$

$$\lambda_{i2} = \left[E^{D+}(Q_R) + E^{A-}(Q_R)\right] - \left[E^{D+}(Q_P) + E^{A-}(Q_P)\right]$$

$$\lambda_i = (\lambda_{i1} + \lambda_{i2})/2$$

where λ_{i1} represents the difference between the energy of the reactants (R) in the geometry characteristic of the products and that in their equilibrium geometry, λ_{i2} is the difference between the energy of the products (P) in the characteristic of the reactants and that in their equilibrium geometry. Q_R and Q_P are the equilibrium geometries of the reactants and products, respectively.

In addition, the external reorganization energy λ_o was calculated from equation:

$$\lambda_0 = (332\ kcal/mol)(\frac{1}{2a_1} + \frac{1}{2a_2} - \frac{1}{R})(\frac{1}{\varepsilon_{op}} - \frac{1}{\varepsilon})$$

$$\lambda = \lambda_0 + \lambda_i$$

$$\Delta G^{\circ\ddagger} = \frac{(\Delta G + \lambda)^2}{4\lambda}$$

where a_1 is the radii of the oxidant, a_2 is the radii of the reductant, $R = a_1 + a_2$, ε_{op} is the optical dielectric constant ($\varepsilon_{op} = 2.25$), ε is the static dielectric constant for the DMA solvent ($\varepsilon = 35.7$), and ΔG is the free energy change of the reaction.

2.2. Electron Transfer Rate and Electron Coupling Constants[S3,S5,S6]

In the Marcus theory, the electron transfer rate constant is expressed as:

$$k = \sqrt{\frac{4\pi^3}{h^2 \lambda k_B T}} |V_{DA}|^2 exp\left(-\frac{(\Delta G + \lambda)^2}{4\lambda k_B T} \right)$$

where λ is the reorganization energy, V_{DA} is the electronic coupling (charge-transfer integral) between donor and acceptor, ΔG is the free energy change for the electron transfer reaction, k_B is the Boltzmann constant, h is Planck's constant, and T is the temperature ($T = 298.15$ K in our calculations).

The electronic coupling matrix (charge transfer integral) can be calculated with the Generalized Mulliken-Hush (GMH) model:

$$V_{DA} = \frac{\mu_{12} \Delta E_{12}}{\sqrt{(\mu_1 - \mu_2)^2 + 4(\mu_{12})^2}}$$

where μ_{12} is the transition dipole moment, ΔE_{12} is the energy difference, and μ_1 and μ_2 are the permanent dipoles, all of which are calculated between the two eigenstates of the system.

3. References

S1 M. S. Lowry, J. I. Goldsmith, J. D. Slinker, R. Rohl, R. A. Pascal, G. G. Malliaras and S. Bernhard, Single-Layer Electroluminescent Devices and Photoinduced Hydrogen Production from an Ionic Iridium(III) Complex, *Chem. Mater.*, 2005, **17**, 5712.

S2 A. V. Marenich, J. Ho, M. L. Coote, C. J. Cramer and D. G. Truhlar, Computational electrochemistry: prediction of liquid-phase reduction potentials, *Phys. Chem. Chem. Phys.*, 2014, **16**, 15068.

S3 R. A. Marcus, Electron Transfer Reactions in Chemistry: Theory and Experiment (Nobel Lecture), *Angew. Chem. Int. Ed.*, 1993, **32**, 1111.

S4 V. Lemaur, M. Steel, D. Beljonne, J. Bredas and J. Cornil, Photoinduced charge generation and recombination dynamics in model donor/acceptor pairs for organic solar cell applications: A full quantum-chemical treatment, *J. Am. Chem. Soc.*, 2004, **127**, p. 6077.

S5 P. F. Barbara, T. J. Meyer and M. A. Ratner, Contemporary issues in electron transfer research, *J. Phys. Chem.*, 1996, **100**, 13148.

S6 A. Voityuk, Estimation of electronic coupling in pi-stacked donor-bridge-acceptor systems: Correction of the two-state model, J. Chem. Phys., 2006, **124**, 64505.

4. Oxidation State Modulation Mechanism Initiated by Reductive Quenching
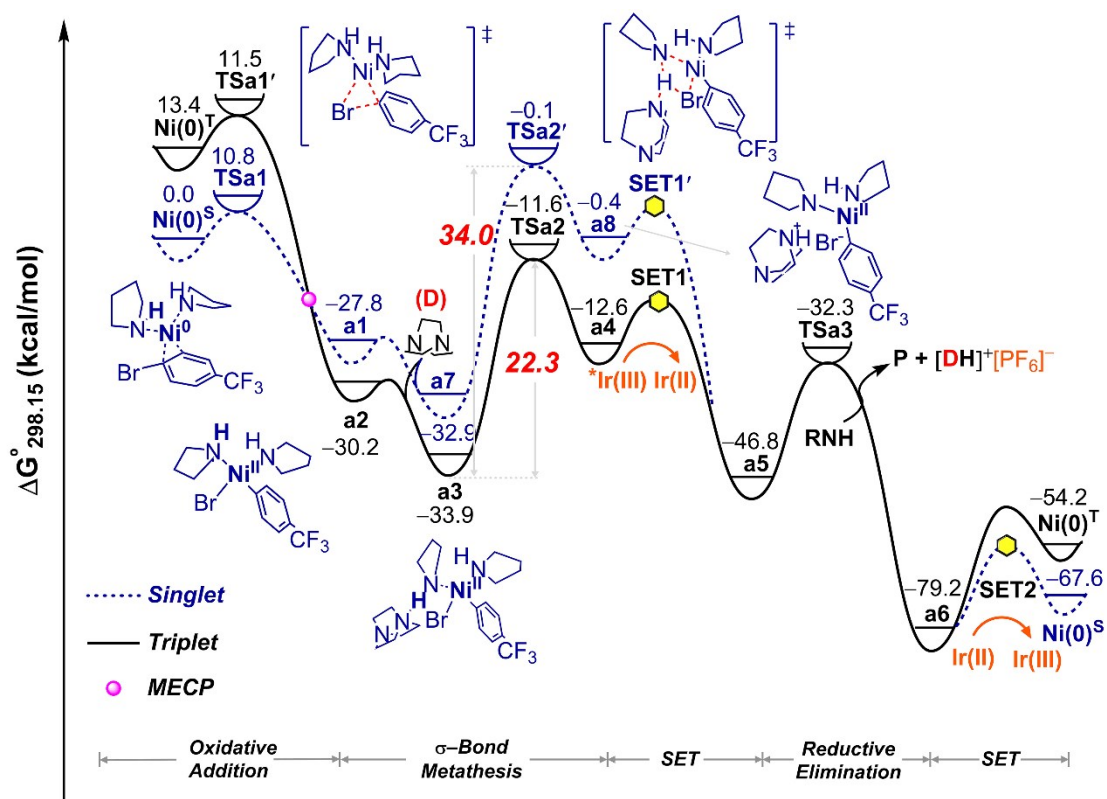
Figure S4. Singlet and triplet Gibbs energy profiles ($\Delta G°_{298.15}$) of the oxidation state modulation mechanism merging Ir^{III}–*Ir^{III}–Ir^{II}–Ir^{III} reductive quenching and Ni^0–Ni^{II}–Ni^{III}–Ni^I–Ni^0 catalytic cycles.

5. Oxidation State Modulation Mechanism Initiated by Oxidative Quenching
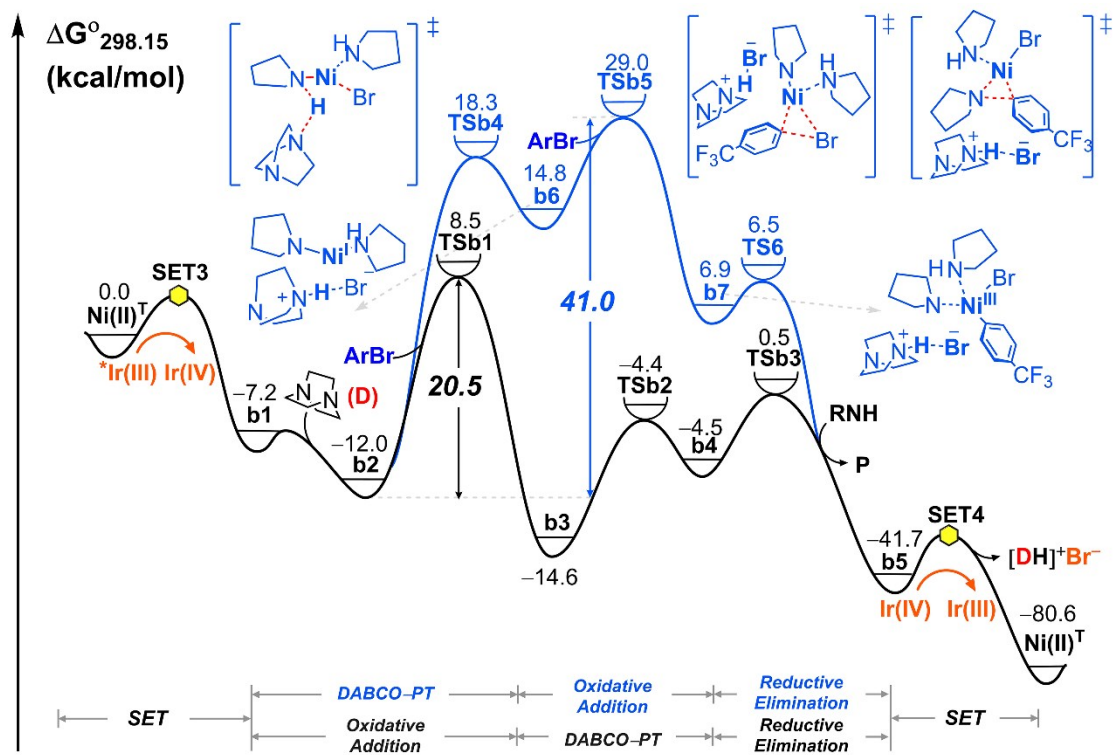
Figure S5. Gibbs energy profiles ($\Delta G^{\circ}_{298.15}$) of the oxidation state modulation mechanism merging Ir^{III}–$*Ir^{III}$–Ir^{IV}–Ir^{III} oxidative quenching and Ni^{II}–Ni^{I}–Ni^{III}–Ni^{I}–Ni^{II} catalytic cycles.

6. Radical Mechanism Initiated by Reductive Quenching
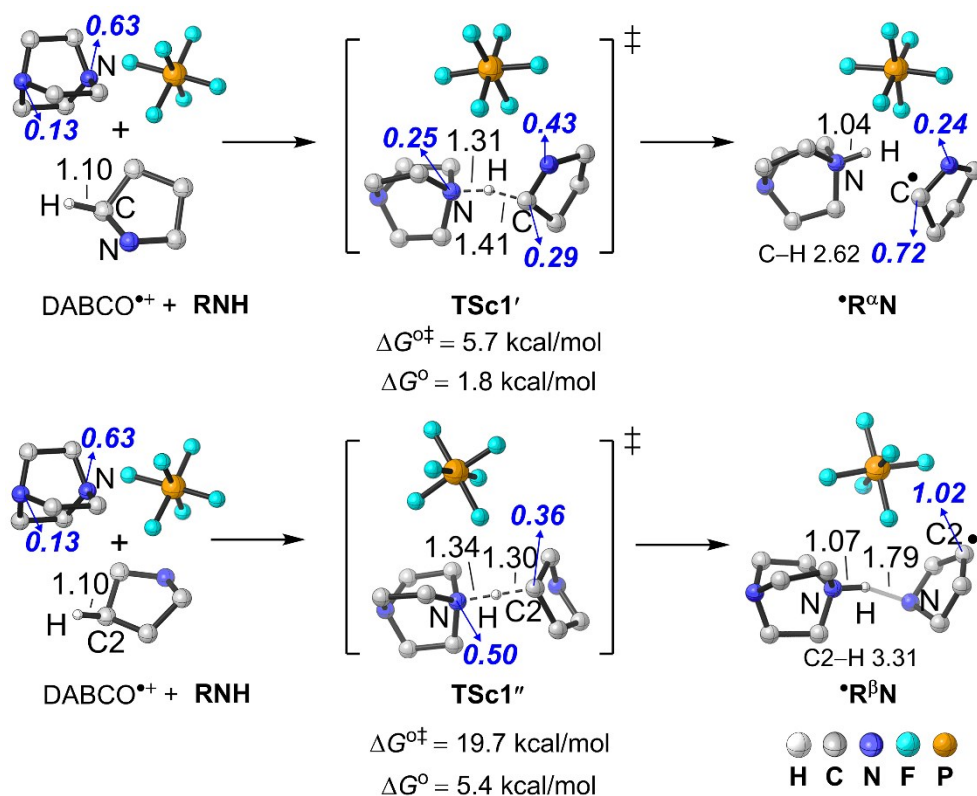
Figure S6. $\Delta G^{\circ\ddagger}$, ΔG°, and optimized structures of α- and β-carbon-centered hydrogen atom transfer processes (selected bond distances are given in angstroms with black non-italic font and spin densities are given in blue italic font).

7. Quenching Mechanism of Photoexcited *Ir(III)

i) Ir(III)/Ni(II) clusters

Cluster 1
0.0

Cluster 2
3.5

Cluster 4
5.2

Cluster 3
4.3

ii) Ir(III)/DABCO clusters

Cluster 1
2.8

Cluster 2
3.0

Cluster 3
6.5
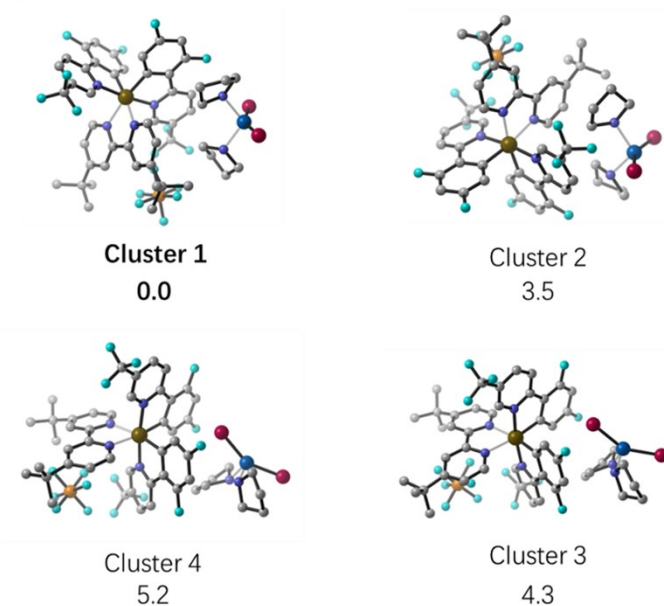
Cluster 4
0.0

Cluster 5
2.7

Cluster 6
0.1
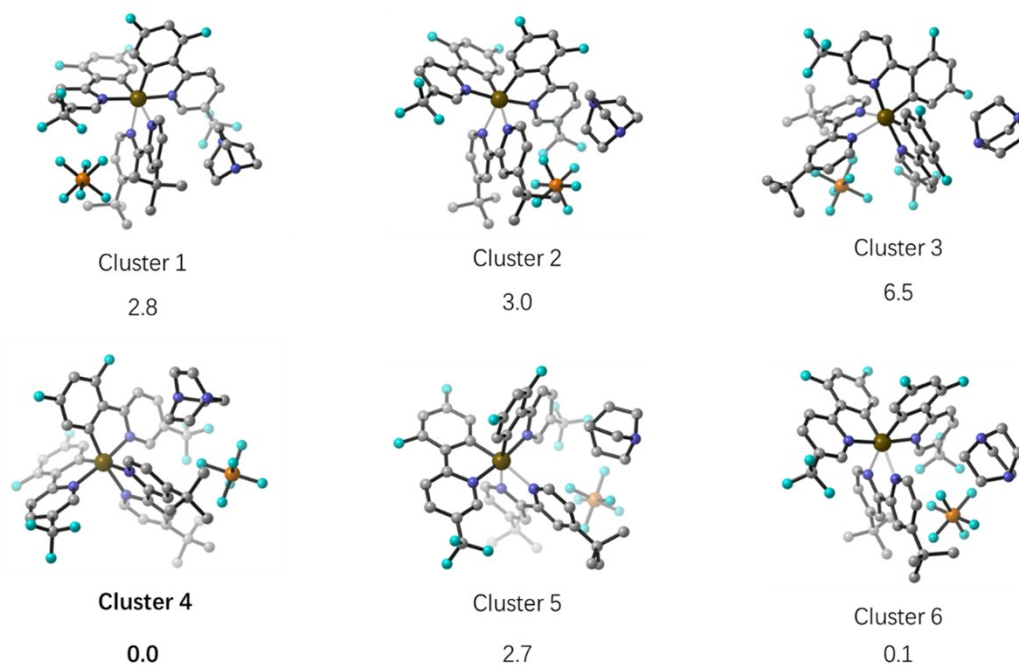
Figure S7. Structure and relative energy of optimized conformers at the (U)M06/[6-31G(d)/LanL2DZ(Ni,Ir)] level. Gray, purple, green, orange, pink, blue, brown spheres represent C, N, F, P, Br, Ni, Ir atoms, respectively. H atoms are omitted for clarity. Electron energies are given in kcal/mol.

8. Tolerance of σ-Bond Metathesis
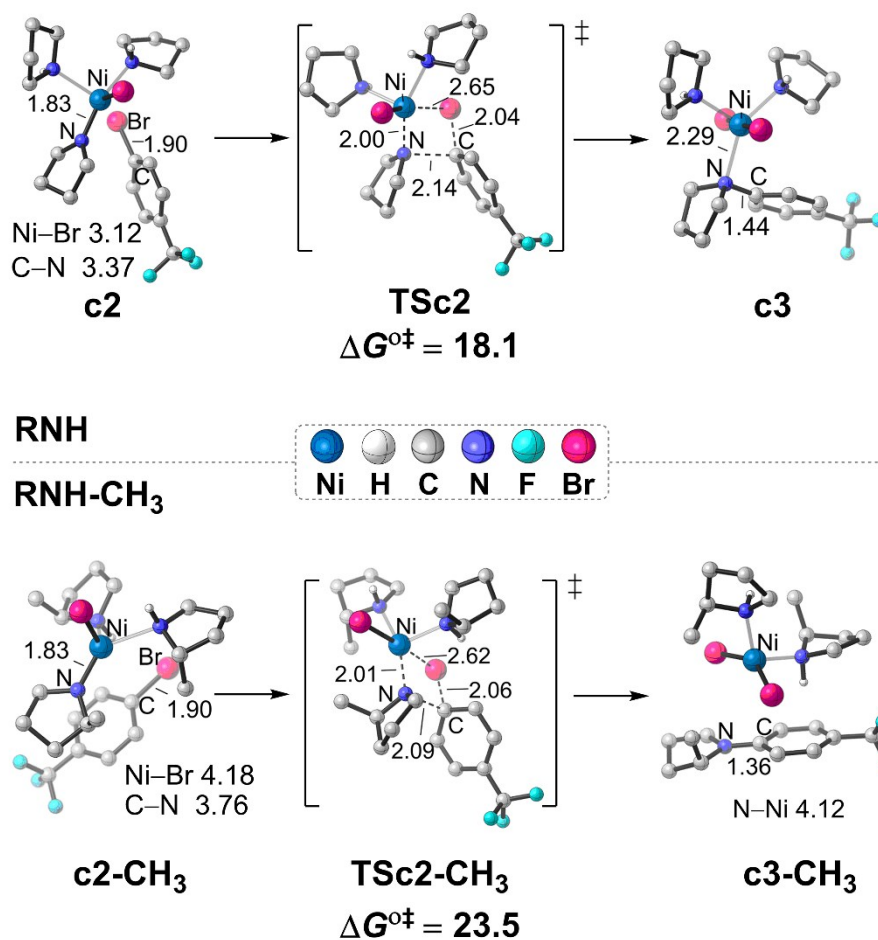
Figure S8. Comparisons of σ-bond metathesis involving pyrrolidine (**RNH**) and 2-methylpyrrolidine (**RNH–CH₃**). Gibbs activation energies and selected bond lengths are given in kcal/mol and angstroms, respectively.

8.1. Buried Volume Calculations

The complexes of **c2** and **c2-CH$_3$** were used as models to comparison the percentage buried volume, %V$_{Bur}$, for the ligand backbones of the pyrrolidine and 2-methylpyrrolidine. The radius (R) of the sphere around the metal center was set to 3.5 Å and a mesh of 0.1 Å was used to scan the sphere. ArBr groups and Br atom remaining on the Ni of **c2** and **c2-CH$_3$** were removed in order to analyze the influence of the ancillary ligand only. We selected different z-axis directions to conduct steric maps scanning on these two compounds (Figures 6 and S9). %V$_{Bur}$ of **c2** and **c2-CH$_3$** are 68.7% and 74.5%.
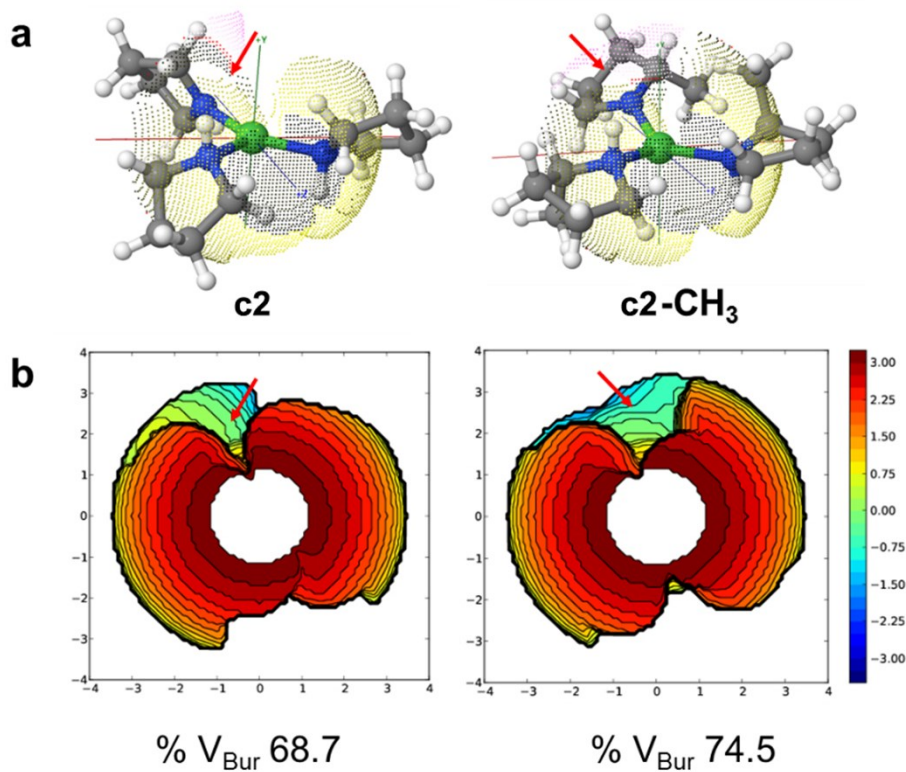
Figure S9. a) Ball-and-stick representations of complexes **c2** and c**2-CH$_3$**. b) Steric crowding maps along the ligand direction with nickel as the center and buried volume calculations for **c2** and **c2-CH$_3$.** The red arrow is the attacking direction of **ArBr**.

8.2. Strain Distortion/Interaction Model
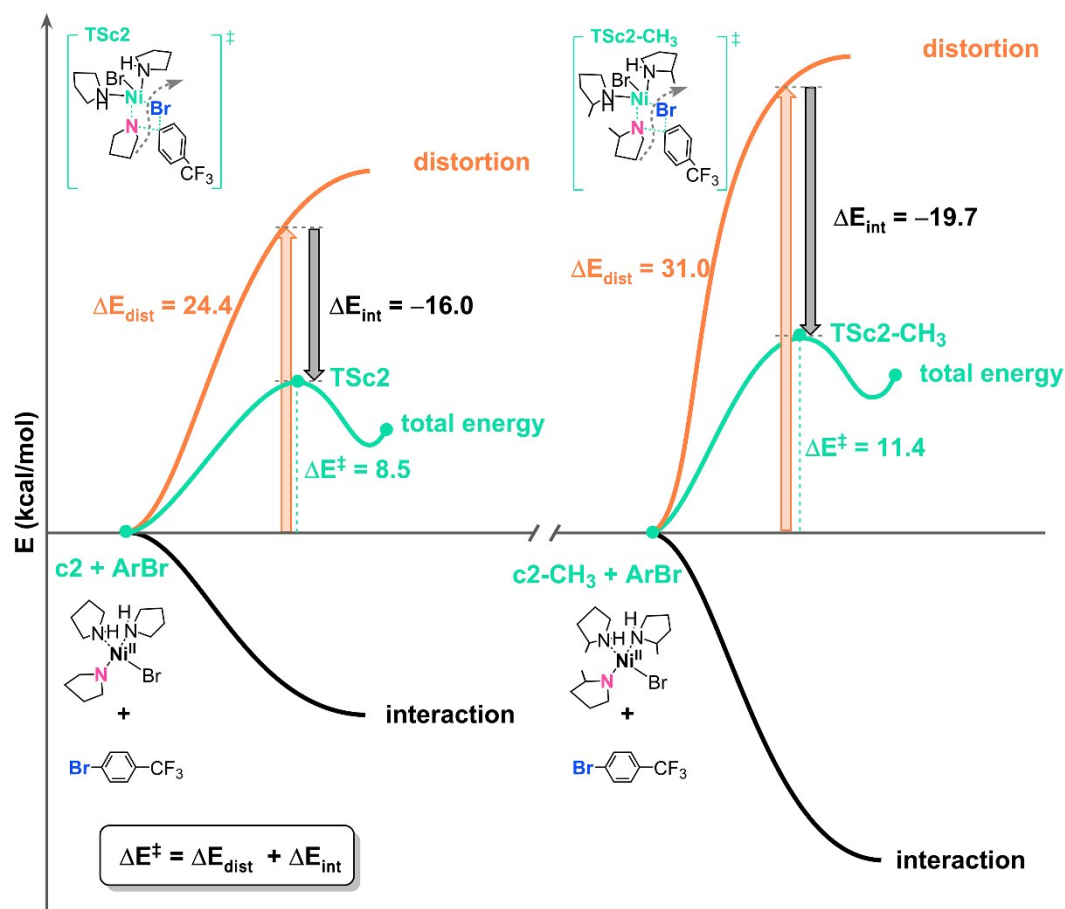
Figure S10. Strain distortion/interaction analysis of σ-bond metathesis with different substrates. Energies are given in kcal/mol.

9. Cartesian Coordinates of Optimized Structures

RNH

N	-0.0003289	-1.2469337	-0.4274706
H	-0.0006219	-2.2314617	-0.1808586
C	1.1514561	-0.5294727	0.1056184
H	2.0740411	-0.8264057	-0.4062846
H	1.2917591	-0.7098727	1.1906094
C	0.7731001	0.9353703	-0.1286316
H	1.1561971	1.2762373	-1.0966616
H	1.1972441	1.5910763	0.6393284
C	-0.7725189	0.9358533	-0.1284576
H	-1.1556419	1.2773063	-1.0962696
H	-1.1960529	1.5915783	0.6398234
C	-1.1517789	-0.5288287	0.1054854

| H | -2.0744399 | -0.8251347 | -0.4066466 |
| H | -1.2924149 | -0.7093117 | 1.1904154 |

ArBr

C	-0.7363617	0.0271676	-0.0000252
C	-0.0546627	-1.1882864	-0.0000082
C	1.3314833	-1.2085374	0.0000038
C	2.0228493	-0.0010564	0.0000028
C	1.3553563	1.2161416	-0.0000012
C	-0.0349457	1.2264786	-0.0000122
H	-0.6161907	-2.1212544	-0.0000092
H	1.8781493	-2.1483324	0.0000168
H	1.9190513	2.1458746	0.0000008
H	-0.5727367	2.1711276	-0.0000072
C	-2.2330147	-0.0060134	-0.0000012
F	-2.7019427	-0.6548144	1.0739168
F	-2.7019827	-0.6550234	-1.0737782
F	-2.7697357	1.2166696	-0.0001012
Br	3.9146833	-0.0201414	0.0000028

aniline product (P)

N	1.2198537	0.0008220	0.0028014
C	2.0358317	-1.2017590	0.0288344
H	1.9968737	-1.7329650	-0.9396196
H	1.6815627	-1.9012210	0.8006584
C	3.4339627	-0.6711600	0.3217624
H	4.2241537	-1.3291070	-0.0561136
H	3.5717217	-0.5692610	1.4075024
C	3.4210597	0.7060340	-0.3332936
H	3.5517737	0.6059640	-1.4200666
H	4.2042037	1.3758570	0.0383354
C	2.0173857	1.2158050	-0.0296306
H	1.6472717	1.9097920	-0.7988926
H	1.9783537	1.7465310	0.9390344
C	-0.1485583	-0.0111320	0.0034844
C	-0.8836343	1.1888070	0.1039744
C	-0.8641143	-1.2198620	-0.0946016
C	-2.2650733	1.1677780	0.1040564
H	-0.3634423	2.1393590	0.1969264
C	-2.2491933	-1.2247920	-0.0916626
H	-0.3295363	-2.1624220	-0.1867976
C	-2.9632693	-0.0356210	0.0079094

H	-2.8191043	2.1024110	0.1869994
H	-2.7831713	-2.1690920	-0.1708646
C	-4.4517833	-0.0012600	-0.0024006
F	-4.9929233	-1.2253350	-0.0165296
F	-4.9416503	0.6401450	1.0716244
F	-4.9285553	0.6556830	-1.0734296

DABCO

C	0.7754671	-1.3740704	-0.0193040
C	-0.7754259	-1.3741034	-0.0185240
H	1.1817520	-1.8722674	-0.9116980
H	1.1826610	-1.8973774	0.8581820
H	-1.1826080	-1.8731204	-0.9100500
H	-1.1816930	-1.8966394	0.8598520
C	0.7753311	0.7037046	-1.1802981
H	1.1816630	1.7256396	-1.1655590
H	1.1823640	0.2054696	-2.0723261
C	-0.7755309	0.7031036	-1.1805260
H	-1.1826850	1.7247246	-1.1668431
H	-1.1818880	0.2037276	-2.0722241
C	-0.7753649	0.6709236	1.1992190
H	-1.1817110	1.6928776	1.2125700
H	-1.1824010	0.1483486	2.0772050
C	0.7755230	0.6703596	1.1994320
H	1.1826360	1.6919926	1.2138360
H	1.1819100	0.1466736	2.0770579
N	-1.2791150	-0.0000034	0.0000940
N	1.2791150	0.0000366	-0.0000950

DABCO·+

C	1.9368565	1.1222850	-0.7797998
C	0.3314425	1.1298510	-0.7868738
H	2.3077255	2.0561230	-0.3429448
H	2.3093065	1.0404910	-1.8069028
H	-0.0771425	2.0363700	-0.3330698
H	-0.0758305	1.0170770	-1.7948518
C	1.9381395	0.1139210	1.3609922
H	2.3094935	-0.7314720	1.9507972
H	2.3113005	1.0441900	1.8034142
C	0.3325845	0.1167200	1.3727742
H	-0.0758275	-0.7293330	1.9313432
H	-0.0741145	1.0461940	1.7792872

C	0.3317645	-1.2470620	-0.5845528
H	-0.0743975	-2.0639950	0.0174732
H	-0.0778545	-1.3075220	-1.5961098
C	1.9374175	-1.2358300	-0.5826158
H	2.3108515	-2.0842650	0.0014572
H	2.3076935	-1.3239480	-1.6100178
N	-0.0352445	-0.0002510	0.0007092
N	2.4040975	0.0002310	-0.0006948
P	-3.2631825	-0.0000080	0.0000672
F	-4.1561675	1.0906440	-0.7654798
F	-2.2826385	-0.1173420	-1.3225338
F	-2.2819305	1.2041220	0.5593842
F	-4.1554725	0.1180040	1.3276332
F	-4.1564775	-1.2081880	-0.5617888
F	-2.2823925	-1.0870070	0.7629042

Ir(III)

N	-3.2891190	0.3071409	0.6506368
N	-0.4336470	-1.9396401	-1.3143092
C	-2.8800130	-2.2707641	0.4345848
C	-2.6105690	-3.6334721	0.2943898
C	-3.4478280	-4.5630591	0.8887538
C	-4.5647430	-4.2058301	1.6346538
C	-4.8272950	-2.8590731	1.7650248
C	-4.0204140	-1.8700291	1.1872658
C	-4.2427250	-0.4395861	1.2826278
C	-5.3102550	0.2090929	1.9218878
C	-5.3921910	1.5853309	1.9024188
C	-4.4048150	2.3229899	1.2482018
C	-3.3699340	1.6449619	0.6379838
C	-2.7535850	-0.9416791	-2.0494182
C	-3.9956020	-0.3982891	-2.3801622
C	-4.4868110	-0.5438241	-3.6684232
C	-3.7930060	-1.2153921	-4.6639002
C	-2.5687720	-1.7569421	-4.3235792
C	-2.0193380	-1.6461381	-3.0420412
C	-0.7437060	-2.2084821	-2.6174222
C	0.1302480	-2.9854071	-3.3827072
C	1.2737980	-3.5116791	-2.8076992
C	1.5473040	-3.2538361	-1.4704992
C	0.6744290	-2.4493921	-0.7635342
H	-1.7592180	-3.9973591	-0.2790862

H	-5.2072320	-4.9510131	2.0924288
H	-6.0693090	-0.3802521	2.4206378
H	-6.2202950	2.0983689	2.3889088
H	-2.5764510	2.1702369	0.1113618
H	-4.6028980	0.1425829	-1.6550532
H	-4.1911490	-1.3188361	-5.6681532
H	-0.1007170	-3.1832591	-4.4216532
H	1.9554410	-4.1235521	-3.3943292
H	0.8735840	-2.1977951	0.2745728
C	0.5918470	0.4108409	1.1498888
C	1.7126740	0.4318699	1.9760768
C	1.8042960	-0.4180981	3.0743848
C	0.6968280	-1.2382871	3.3295248
C	-0.3845230	-1.2239801	2.4722528
N	-0.4323020	-0.4378911	1.3858608
H	2.5614800	1.0452209	1.6960818
H	0.6862080	-1.9233311	4.1745248
H	-1.2388180	-1.8844681	2.6186368
C	0.4773500	1.2407939	-0.0683992
C	1.3853710	2.2431499	-0.3957362
C	-0.7298260	1.6685959	-1.9993882
C	1.2443560	2.9787119	-1.5699102
H	2.2401170	2.4118479	0.2477808
H	-1.5911490	1.4005189	-2.6114712
C	0.1374200	2.6751959	-2.3709132
H	-0.0474780	3.2094259	-3.3002582
N	-0.5682510	0.9588199	-0.8738792
Ir	-1.7918880	-0.7508111	-0.2962612
C	-4.4889920	3.8156529	1.2240578
F	-5.9033800	-2.5144981	2.4857318
F	-3.1808840	-5.8583811	0.7477668
F	-1.9048470	-2.4043271	-5.2893982
F	-5.6714760	-0.0159791	-3.9723412
C	2.6873720	-3.9233391	-0.7637552
P	4.2995150	-0.0912881	-0.7819882
F	2.7328390	-0.4959341	-0.4738512
F	3.7795360	0.8372919	-2.0111652
F	4.1257970	1.2145199	0.2225068
F	4.7486120	-0.9680371	0.5068068
F	4.4147710	-1.3709181	-1.7504812
F	5.8174290	0.3306879	-1.0676802
F	-5.6425360	4.2178419	0.6805858

F	-4.4473940	4.3173249	2.4629648
F	-3.4920410	4.3623879	0.5258088
F	2.2923010	-5.1387561	-0.3347642
F	3.7241720	-4.1157371	-1.5699442
F	3.0800510	-3.2423861	0.3069448
C	3.0599550	-0.5240541	3.9241558
C	4.0954940	0.5363039	3.5570808
H	4.4457410	0.4268399	2.5229728
H	3.7033410	1.5545849	3.6937238
H	4.9679420	0.4287389	4.2146298
C	3.6764790	-1.9060611	3.6658448
H	4.5897130	-2.0199651	4.2661028
H	2.9918380	-2.7213721	3.9376568
H	3.9475090	-2.0128501	2.6081498
C	2.7013050	-0.3760721	5.4061498
H	2.2421080	0.6012379	5.6101168
H	2.0118700	-1.1557601	5.7562968
H	3.6132570	-0.4526101	6.0132388
C	2.2228120	4.0626029	-1.9933912
C	1.4767110	5.4006299	-2.0614052
H	0.6494500	5.3823349	-2.7837882
H	1.0647830	5.6766839	-1.0806622
H	2.1700000	6.1943269	-2.3716642
C	2.7847670	3.7075599	-3.3756002
H	3.5072920	4.4749729	-3.6852322
H	3.2991980	2.7403759	-3.3432532
H	2.0023500	3.6624979	-4.1450052
C	3.3912480	4.1958649	-1.0208542
H	3.0561200	4.4978089	-0.0179002
H	3.9563400	3.2598889	-0.9357602
H	4.0746500	4.9751129	-1.3825692

*Ir(III)

N	-3.2520095	0.3074351	0.6210907
N	-0.4257435	-1.9664199	-1.3309953
C	-2.8188065	-2.2842889	0.4701587
C	-2.5278185	-3.6448959	0.3590997
C	-3.3449265	-4.5744669	0.9693877
C	-4.4903315	-4.1996199	1.7062867
C	-4.7985505	-2.8760739	1.8160897
C	-4.0029775	-1.8503239	1.2249797
C	-4.2452675	-0.4697409	1.2860947

C	-5.3373165	0.2103891	1.9027537
C	-5.4256125	1.5690971	1.8739807
C	-4.3965755	2.3125101	1.2153797
C	-3.3498165	1.6340681	0.6164007
C	-2.7635355	-0.9594629	-2.0458063
C	-3.9989405	-0.3951989	-2.3634353
C	-4.5061345	-0.5481039	-3.6444023
C	-3.8323065	-1.2457889	-4.6362933
C	-2.6115395	-1.8030389	-4.3065223
C	-2.0427275	-1.6828979	-3.0348373
C	-0.7608955	-2.2470139	-2.6243343
C	0.1005625	-3.0245409	-3.4013043
C	1.2628505	-3.5320859	-2.8456343
C	1.5686905	-3.2534969	-1.5200903
C	0.7020675	-2.4512959	-0.7998963
H	-1.6679035	-3.9988639	-0.2074303
H	-5.1171285	-4.9532649	2.1746907
H	-6.1036625	-0.3791679	2.3929027
H	-6.2587195	2.0924791	2.3368617
H	-2.5611605	2.1759351	0.0971627
H	-4.5819735	0.1636471	-1.6326273
H	-4.2432575	-1.3553669	-5.6349053
H	-0.1509475	-3.2375149	-4.4324463
H	1.9355035	-4.1455699	-3.4406213
H	0.9192535	-2.1829349	0.2313007
C	0.5837895	0.4243861	1.1578867
C	1.7015205	0.4561431	1.9877797
C	1.7918525	-0.3863289	3.0922167
C	0.6834635	-1.2029109	3.3545817
C	-0.3939045	-1.1995729	2.4932217
N	-0.4371425	-0.4254919	1.3986137
H	2.5496175	1.0697111	1.7060697
H	0.6707275	-1.8782729	4.2071827
H	-1.2472465	-1.8606649	2.6425077
C	0.4712735	1.2427021	-0.0689563
C	1.3723005	2.2510191	-0.3970103
C	-0.7202185	1.6408421	-2.0164193
C	1.2369775	2.9728911	-1.5803543
H	2.2186015	2.4347861	0.2536437
H	-1.5755125	1.3635681	-2.6325553
C	0.1412215	2.6511411	-2.3896203
H	-0.0405265	3.1758001	-3.3249143

N	-0.5621405	0.9434701	-0.8827373
Ir	-1.7953295	-0.7743599	-0.3004713
C	-4.4783505	3.7959331	1.1842837
F	-5.8899325	-2.5370689	2.5170457
F	-3.0728805	-5.8746839	0.8788077
F	-1.9728605	-2.4730499	-5.2725143
F	-5.6830635	-0.0062139	-3.9449943
C	2.7365915	-3.9040329	-0.8379623
P	4.2785665	-0.0814789	-0.7648563
F	2.7070975	-0.4595229	-0.4435283
F	3.7629575	0.8319521	-2.0063753
F	4.1262175	1.2407451	0.2192067
F	4.7218615	-0.9440129	0.5353357
F	4.3678275	-1.3825299	-1.7095573
F	5.7998645	0.3119721	-1.0673593
F	-5.6210345	4.2058411	0.6144397
F	-4.4677845	4.3119821	2.4219977
F	-3.4664555	4.3493181	0.5066457
F	2.3487565	-5.0935539	-0.3363083
F	3.7270395	-4.1457459	-1.6891823
F	3.1923895	-3.1815309	0.1759057
C	3.0511355	-0.4979109	3.9350767
C	4.0894095	0.5576281	3.5626397
H	4.4332275	0.4476951	2.5267317
H	3.7021445	1.5773221	3.7024817
H	4.9650615	0.4459991	4.2151257
C	3.6542665	-1.8850179	3.6683007
H	4.5848195	-1.9986269	4.2412837
H	2.9739115	-2.6937409	3.9691877
H	3.8918915	-2.0045679	2.6034207
C	2.7049045	-0.3510019	5.4199567
H	2.2573085	0.6302671	5.6301387
H	2.0104485	-1.1245309	5.7736327
H	3.6206805	-0.4384359	6.0197217
C	2.2081115	4.0629811	-2.0044033
C	1.4503795	5.3942621	-2.0777723
H	0.6256545	5.3668711	-2.8027533
H	1.0326345	5.6689111	-1.0992203
H	2.1379135	6.1930661	-2.3876603
C	2.7769285	3.7099371	-3.3843753
H	3.4942245	4.4827041	-3.6926203
H	3.2991355	2.7469541	-3.3501153

H	1.9976915	3.6582481	-4.1565633
C	3.3725125	4.2075681	-1.0288203
H	3.0327045	4.5142651	-0.0289563
H	3.9407765	3.2742091	-0.9363393
H	4.0536515	4.9876471	-1.3928363

Ir(II)

N	-1.8157945	-1.8819866	-0.8328342
N	-1.8170515	1.8811014	0.8329228
C	-3.1669625	0.2961494	-1.3790782
C	-3.8550765	1.4844494	-1.6378132
C	-4.7937425	1.5301504	-2.6542602
C	-5.0979145	0.4326874	-3.4502262
C	-4.4197195	-0.7387736	-3.1870452
C	-3.4595935	-0.8486366	-2.1739992
C	-2.7083045	-2.0489716	-1.8527292
C	-2.8254045	-3.3066326	-2.4639042
C	-2.0413625	-4.3564846	-2.0347212
C	-1.1330935	-4.1549436	-0.9949292
C	-1.0499815	-2.9021296	-0.4214182
C	-3.1670265	-0.2978476	1.3788818
C	-3.8545255	-1.4865366	1.6374508
C	-4.7935685	-1.5327266	2.6535258
C	-5.0987065	-0.4353926	3.4492998
C	-4.4210885	0.7364474	3.1863138
C	-3.4606035	0.8468064	2.1736618
C	-2.7099105	2.0475624	1.8526008
C	-2.8278065	3.3051384	2.4637998
C	-2.0442155	4.3554234	2.0348588
C	-1.1355735	4.1544044	0.9952868
C	-1.0516585	2.9016574	0.4217578
H	-3.6765505	2.3900364	-1.0587442
H	-5.8373205	0.4884944	-4.2425432
H	-3.5361915	-3.4429486	-3.2695082
H	-2.1260065	-5.3375556	-2.4995692
H	-0.3622645	-2.6859526	0.3936498
H	-3.6752595	-2.3920556	1.0585038
H	-5.8384325	-0.4915696	4.2412908
H	-3.5388575	3.4410744	3.2692308
H	-2.1295065	5.3364294	2.4997268
H	-0.3636185	2.6858804	-0.3931442
C	1.2011865	0.2324784	-0.6717332

C	2.3684125	0.5252534	-1.4230332
C	2.3135015	0.9764054	-2.7219322
C	1.0253455	1.1399594	-3.2978692
C	-0.0873775	0.8546334	-2.5371322
N	-0.0375045	0.4237064	-1.2692762
H	3.3367035	0.3948954	-0.9424602
H	0.8903865	1.4863784	-4.3174102
H	-1.0903695	0.9828434	-2.9481462
C	1.2012925	-0.2318116	0.6717838
C	2.3686435	-0.5241536	1.4230658
C	-0.0869995	-0.8542536	2.5372848
C	2.3139205	-0.9751676	2.7220198
H	3.3368785	-0.3935736	0.9424428
H	-1.0899365	-0.9828036	2.9483228
C	1.0258435	-1.1390726	3.2980348
H	0.8910595	-1.4854206	4.3176238
N	-0.0373035	-0.4234586	1.2693738
Ir	-1.7303835	-0.0004106	0.0000328
C	-0.2791965	-5.2896986	-0.5301382
F	-4.7145605	-1.7968566	-3.9576352
F	-5.4398345	2.6716124	-2.8917652
F	-4.7168825	1.7944084	3.9567078
F	-5.4390785	-2.6745566	2.8908378
C	-0.2821155	5.2896144	0.5308028
C	3.5988405	-1.2895006	3.4834408
C	3.3211385	-1.7589456	4.9101398
H	4.2704965	-1.9702166	5.4205448
H	2.7930695	-0.9944356	5.4965128
H	2.7241055	-2.6809906	4.9281758
C	4.4729145	-0.0329856	3.5578488
H	5.3988095	-0.2453326	4.1117878
H	4.7564405	0.3307974	2.5619468
H	3.9460775	0.7812054	4.0739728
C	4.3622585	-2.4019346	2.7561388
H	5.2851375	-2.6502236	3.3002308
H	3.7528305	-3.3132306	2.6845598
H	4.6440145	-2.1076006	1.7369648
C	3.5982985	1.2912914	-3.4833382
C	4.3613355	2.4038654	-2.7558542
H	4.6431625	2.1094624	-1.7367202
H	5.2841395	2.6525444	-3.2998962
H	3.7516015	3.3149474	-2.6841412

C	4.4728065	0.0350914	-3.5579462
H	3.9462315	-0.7792036	-4.0741752
H	5.3986125	0.2478364	-4.1118802
H	4.7564835	-0.3287416	-2.5621062
C	3.3204395	1.7608714	-4.9099622
H	2.7925515	0.9963144	-5.4964362
H	2.7231715	2.6827654	-4.9278422
H	4.2697295	1.9724644	-5.4203602
F	0.4769975	-5.7615556	-1.5289992
F	0.5327745	-4.9354926	0.4663738
F	-1.0319805	-6.3115106	-0.1029792
F	-1.0353095	6.3112024	0.1038198
F	0.4738215	5.7615784	1.5298098
F	0.5300635	4.9359624	-0.4657312

Ir(IV)

N	3.2381711	-0.0234901	-0.2571658
N	-0.0155989	-2.4656861	0.4603802
C	2.5643401	-2.3996871	-1.1143308
C	2.1908061	-3.6893501	-1.5023488
C	2.9773771	-4.3904681	-2.3981528
C	4.1471221	-3.8722081	-2.9508918
C	4.5177201	-2.6067091	-2.5615818
C	3.7668541	-1.8431791	-1.6518488
C	4.1130481	-0.5233411	-1.1816628
C	5.2248451	0.2497439	-1.5672628
C	5.4242851	1.4970479	-1.0214448
C	4.5180531	1.9830609	-0.0750708
C	3.4415051	1.1791219	0.2872292
C	2.2706581	-2.1389971	1.7195472
C	3.5182041	-1.9579311	2.3171162
C	3.8086811	-2.6101941	3.5056102
C	2.9028741	-3.4466341	4.1405152
C	1.6757711	-3.6292281	3.5316712
C	1.3252371	-3.0060141	2.3303392
C	0.0685471	-3.1903701	1.6139032
C	-0.9761239	-4.0489651	1.9621782
C	-2.0428229	-4.2190591	1.0991022
C	-2.0696589	-3.5263231	-0.1046828
C	-1.0505259	-2.6322781	-0.3736608
H	1.2945221	-4.1699341	-1.1134558
H	4.7459681	-4.4437031	-3.6526368

H	5.9141281	-0.1431371	-2.3037728
H	6.2742621	2.1067669	-1.3207288
H	2.7240821	1.5027299	1.0390172
H	4.2806431	-1.3155701	1.8782952
H	3.1440761	-3.9471511	5.0728362
H	-0.9313699	-4.5968221	2.8951422
H	-2.8545369	-4.8972171	1.3521262
H	-1.0574549	-2.0279661	-1.2765338
C	-0.3539069	0.9204569	-0.9069648
C	-1.2833619	1.5430869	-1.7240978
C	-1.3869429	1.2129239	-3.0736238
C	-0.4519769	0.3011879	-3.5688508
C	0.4534051	-0.2905351	-2.7044348
N	0.4817861	-0.0221061	-1.3948918
H	-2.0216539	2.1979339	-1.2726378
H	-0.4428949	0.0095559	-4.6153388
H	1.1636151	-1.0397901	-3.0541888
C	-0.2839899	1.1729239	0.5416302
C	-1.0080949	2.1825039	1.1607402
C	0.5263251	0.4651529	2.5897292
C	-1.0483709	2.2848399	2.5464452
H	-1.6027639	2.8527219	0.5542632
H	1.1759471	-0.2287541	3.1227192
C	-0.2293559	1.4051629	3.2610842
H	-0.1938079	1.4252029	4.3479902
N	0.4940221	0.3345569	1.2561022
Ir	1.5637101	-1.1743831	0.1070722
C	4.7835561	3.2865609	0.6186252
F	5.6438351	-2.1091861	-3.0875978
F	2.6143351	-5.6156071	-2.7601698
F	0.8090691	-4.4404321	4.1499652
F	5.0011741	-2.4269581	4.0704482
C	-3.1053649	-3.8499881	-1.1401598
P	-3.8924919	-0.1562441	0.6016192
F	-2.8567429	-0.4690671	-0.6349788
F	-2.6221119	-0.2471511	1.6267552
F	-3.5899679	1.4508149	0.3930422
F	-5.1063929	-0.0491691	-0.4487108
F	-4.1510309	-1.7415951	0.7887002
F	-4.8658229	0.1931039	1.8363862
F	5.7946941	3.1453999	1.4853832
F	5.1405711	4.2294389	-0.2514618

F	3.7224061	3.7157489	1.2987332
F	-4.2680819	-4.1875481	-0.5933058
F	-3.3021319	-2.8603591	-2.0036868
F	-2.6876689	-4.9154401	-1.8551318
C	-2.5374949	1.7705379	-3.8923618
C	-2.4514719	1.3557379	-5.3583258
H	-3.2964399	1.7872509	-5.9101138
H	-1.5275059	1.7133829	-5.8353288
H	-2.5090689	0.2653969	-5.4796138
C	-2.5390509	3.3010519	-3.8196758
H	-3.3738169	3.6975479	-4.4132358
H	-2.6662019	3.6690929	-2.7940818
H	-1.6064169	3.7217969	-4.2208088
C	-3.8391329	1.2162789	-3.2924268
H	-4.6974669	1.5972569	-3.8632498
H	-3.8573669	0.1188829	-3.3299158
H	-3.9754699	1.4921779	-2.2398608
C	-2.0092579	3.2142969	3.2663972
C	-2.7212639	4.1631229	2.3050362
H	-3.3365089	3.6108659	1.5829582
H	-3.3907819	4.8205309	2.8746432
H	-2.0133569	4.8048479	1.7603462
C	-1.2707079	4.0405269	4.3223502
H	-1.9839979	4.6900409	4.8474292
H	-0.7826759	3.4153079	5.0814322
H	-0.5037989	4.6812149	3.8651112
C	-3.0680269	2.3216039	3.9330482
H	-2.6233979	1.6625459	4.6910482
H	-3.8172809	2.9512339	4.4332602
H	-3.5781939	1.6904989	3.1933752
Br	2.2889451	2.9651479	-1.7524158

Ni(II)^T

Ni	-0.00745700	0.01219500	-0.43160100
Br	1.32645700	-1.82379700	-1.00572100
C	3.58773200	0.77336600	0.44944200
C	3.30419300	0.61456800	1.93943200
C	1.81203400	0.30966000	1.95082400
C	2.38629300	1.56768800	-0.03397600
H	4.53477200	1.27908400	0.23239300
H	3.59330900	-0.20945500	-0.04191500
H	3.51070100	1.55498900	2.47179300

H	3.89323900	-0.17794100	2.41416900
H	1.64495200	-0.76273700	1.78542400
H	1.29907300	0.60594200	2.87380600
H	2.17212800	1.43336600	-1.10220200
H	2.51165800	2.64363000	0.15218400
N	1.24569500	1.05508900	0.79066700
H	0.67358400	1.84047400	1.09759400
C	-3.56133100	-1.44040000	0.83709300
C	-3.31190100	-0.08322100	1.48595300
C	-1.86401800	-0.19461800	1.93489900
C	-2.26973500	-1.67986200	0.06817700
H	-3.70076400	-2.21339400	1.60761700
H	-4.44051700	-1.45530100	0.18387300
H	-3.99030800	0.14082300	2.31645300
H	-3.39397700	0.71783600	0.73832000
H	-1.37009000	0.77920000	2.03397600
H	-1.78640000	-0.72457000	2.89625600
H	-2.31555800	-1.20875800	-0.92425700
H	-2.00564500	-2.73243200	-0.07730300
N	-1.20207300	-0.99893100	0.87093100
H	-0.58156900	-1.69898600	1.27413300
Br	-1.35059200	1.83095600	-1.03055700

Ni(II)^S

N	-0.8750509	1.4407462	-0.1956553
H	-1.5409839	2.0987692	-0.6125343
C	-0.4927269	2.0404482	1.1058017
H	-0.0673089	1.2591212	1.7511477
H	-1.3946849	2.4308462	1.5891797
C	0.5525071	3.0778722	0.7299097
H	1.1603581	3.4078712	1.5795467
H	0.0553951	3.9644622	0.3100907
C	1.3652851	2.3530632	-0.3445733
H	2.1545091	1.7504552	0.1271727
H	1.8589871	3.0366292	-1.0437963
C	0.3471741	1.4348942	-1.0452243
H	0.7298101	0.4143212	-1.1553603
H	0.0703241	1.7833062	-2.0468003
Ni	-2.1372989	-0.0596578	-0.0033923
Br	-3.7981479	1.5223022	-0.2421693
Br	-3.6852099	-1.7525248	0.2357027
N	-0.7788019	-1.4688008	0.1921427
H	-1.3863059	-2.1571838	0.6481367

C	-0.3837029	-2.0728928	-1.1159563
H	-0.3686619	-1.2945188	-1.8882733
H	-1.1635879	-2.7876928	-1.3999103
C	1.0037891	-2.7020518	-0.8961153
H	1.7740621	-2.1144878	-1.4150403
H	1.0640241	-3.7238328	-1.2856433
C	1.2241161	-2.6311828	0.6172547
H	2.2820101	-2.5908778	0.8997817
H	0.7780841	-3.5037088	1.1160007
C	0.4516591	-1.3778588	1.0021957
H	1.0135921	-0.4757418	0.7233097
H	0.1867861	-1.3020928	2.0630707

Ni(0)^S

Ni	0.80690400	-0.26573100	-0.31732000
Br	1.77579900	2.67751700	-0.99086800
C	-1.54638500	1.60825300	1.25118600
C	-2.36042100	0.89571800	0.32208200
C	-1.87162400	0.56834000	-0.91581200
C	-0.51747500	0.82551200	-1.26906800
C	0.32070600	1.52974600	-0.31022900
C	-0.26854000	1.96605100	0.92734700
H	-1.96842700	1.89523900	2.21365900
H	-2.52958600	0.09861900	-1.64713100
H	-0.24846900	0.83065500	-2.32885000
H	0.32251700	2.58030000	1.60714100
C	-3.71717200	0.47509100	0.75331200
F	-4.42651600	1.48475900	1.27995000
F	-4.44466800	-0.04633700	-0.24531200
F	-3.65407300	-0.47150400	1.71554800
C	0.51229500	-2.77902800	-1.92833000
C	-0.83534000	-2.64311100	0.03035900
C	-1.75062600	-2.89470400	-1.17781100
C	-0.90660200	-2.52940900	-2.40276900
H	1.27663300	-2.24832900	-2.50956300
H	0.73750200	-3.86012900	-1.95591900
H	-0.75246200	-3.53981200	0.66255300
H	-1.19721300	-1.82033000	0.66058900
H	-2.04290300	-3.95206600	-1.21966200
H	-2.67435200	-2.30696200	-1.11289900
H	-1.16058900	-3.12150500	-3.28909400
H	-1.02626400	-1.46915500	-2.65670200

N	0.49719500	-2.27903000	-0.53626600
H	1.22712900	-2.74443500	-0.00224000
C	3.51511500	-1.34127300	0.56552000
C	2.44128100	0.00200900	2.13557300
C	2.20226300	-1.41647600	2.62428300
C	3.14340800	-2.26002400	1.74480900
H	3.40379000	-1.81117900	-0.42052200
H	4.56270000	-1.01101800	0.65676100
H	3.36499300	0.41627400	2.57817500
H	1.61220100	0.68923300	2.34071900
H	2.39761800	-1.53539900	3.69548200
H	1.15108500	-1.68462200	2.44572200
H	4.04487500	-2.55722200	2.29361400
H	2.66798000	-3.19559300	1.41790400
N	2.59729600	-0.19368700	0.68460500
H	2.98553600	0.64141800	0.24284300

Ni(0)^T

Ni	0.6284945	-0.5382290	-0.2903391
Br	1.3497545	-3.6392080	-0.4212871
C	-2.4429445	-2.0642760	-1.1632331
C	-2.9617235	-1.8265940	0.1355179
C	-2.1159055	-2.0156290	1.2551659
C	-0.7867945	-2.3176370	1.0881439
C	-0.1939435	-2.3358190	-0.2339431
C	-1.1172735	-2.3611500	-1.3476131
H	-3.1072065	-1.9870060	-2.0235371
H	-2.5259705	-1.9048510	2.2580909
H	-0.1447345	-2.4801330	1.9536329
H	-0.7258095	-2.5484170	-2.3467131
C	-4.2869795	-1.2009320	0.2906799
F	-5.1702815	-1.5973090	-0.6355881
F	-4.8329485	-1.4110320	1.4949889
F	-4.2155025	0.1621400	0.1560089
C	3.4551715	0.0337090	-0.7463701
C	2.6367785	0.9598860	1.2214789
C	3.2625375	-0.3612000	1.6527429
C	3.8874135	-0.9313370	0.3610169
H	3.2024325	-0.4665040	-1.6886661
H	4.2393105	0.7837760	-0.9450511
H	3.3782245	1.7770340	1.2671499
H	1.7603795	1.2525990	1.8124509

H	3.9915905	-0.2193690	2.4581269
H	2.4837255	-1.0398500	2.0276909
H	4.9795505	-0.9989970	0.4165939
H	3.4981245	-1.9369190	0.1623229
N	2.2544935	0.6987720	-0.1837731
H	2.0591525	1.5691580	-0.6762041
C	-1.2925785	1.4281480	-1.5472831
C	-1.0541655	1.8399440	0.7218959
C	-0.3318595	3.0024610	0.0359019
C	-0.4531195	2.7014240	-1.4749111
H	-1.0385975	0.7719900	-2.3882061
H	-2.3678645	1.6686470	-1.6118841
H	-2.1029595	2.1071360	0.9357409
H	-0.5934935	1.5152190	1.6641219
H	-0.7804595	3.9642710	0.3077339
H	0.7208195	3.0521290	0.3485319
H	-0.9129935	3.5233670	-2.0341721
H	0.5346905	2.5308580	-1.9266031
N	-1.0084575	0.7534410	-0.2695021
H	-1.7580755	0.0862900	-0.0708501

TSa1

C	0.6836228	2.0340607	-0.7001671
C	-0.8480372	2.1550467	1.1055379
C	-0.3778122	3.5770037	0.8408009
C	0.9263848	3.3398397	0.0788969
H	1.5136748	1.3298387	-0.5717881
H	0.5503758	2.1965177	-1.7768361
H	-1.9081952	2.0487487	1.3643689
H	-0.2663532	1.6959647	1.9163139
H	-1.1095492	4.1051827	0.2096899
H	-0.2420622	4.1667907	1.7549669
H	1.2033648	4.1763657	-0.5725081
H	1.7513468	3.1949217	0.7905849
N	-0.5610962	1.4236557	-0.1463851
H	-1.3190062	1.6495497	-0.7882171
C	-2.8875792	-0.5328873	-1.7749091
C	-2.4690182	-2.6161813	-0.8753431
C	-3.6002462	-2.0304203	-0.0226571
C	-3.7652682	-0.5829713	-0.5315171
H	-2.5205902	0.4677467	-2.0365931
H	-3.4339532	-0.9295663	-2.6500651

H	-2.8791552	-3.2161633	-1.7063931
H	-1.7721152	-3.2425963	-0.3072431
H	-4.5187662	-2.6174513	-0.1357791
H	-3.3233262	-2.0393423	1.0372789
H	-4.8052702	-0.3144393	-0.7476711
H	-3.3828042	0.1216517	0.2198019
N	-1.7745682	-1.4216713	-1.4071791
H	-1.2102392	-1.6630093	-2.2188091
Ni	-0.4572492	-0.6594193	-0.0104141
C	3.5313838	-1.0467353	0.3236959
C	2.6202298	-1.9804813	-0.1380701
C	1.2977018	-1.9715953	0.3294569
C	0.8866888	-0.9033933	1.1817889
C	1.8549598	-0.0481663	1.7636299
C	3.1484458	-0.1038073	1.3025199
H	2.9486238	-2.7593503	-0.8242111
H	0.6593668	-2.8376263	0.1581829
H	1.5655768	0.6778967	2.5222349
H	3.8960368	0.5890577	1.6897049
C	4.9426278	-1.0291963	-0.1444511
F	5.2106318	-2.0045833	-1.0210041
F	5.8129728	-1.1566923	0.8716699
F	5.2507198	0.1364067	-0.7454801
Br	-0.8224752	-1.3784983	2.3925669

TSa1'

Ni	0.5476396	-0.5175047	-0.2492512
Br	0.7962096	-3.5812527	-0.5643862
C	-2.9320244	-1.5685527	-1.2273192
C	-3.4709994	-1.4547257	0.0661827
C	-2.6558154	-1.7228317	1.1812248
C	-1.3229354	-2.0375477	1.0129598
C	-0.7234484	-2.0047167	-0.2844452
C	-1.5992544	-1.8773997	-1.4051333
H	-3.5720224	-1.3901677	-2.0906212
H	-3.0830184	-1.6668807	2.1820148
H	-0.6973524	-2.2507177	1.8805858
H	-1.1859584	-1.9631117	-2.4102982
C	-4.8396794	-0.9187137	0.2627897
F	-5.6492304	-1.1737677	-0.7726852
F	-5.4288684	-1.3958397	1.3671868
F	-4.8265554	0.4313433	0.4035488

C	3.4511886	-0.6884727	-0.7001473
C	2.8705986	0.4536323	1.2490408
C	3.1674906	-0.9642867	1.7093858
C	3.7530616	-1.6475147	0.4589018
H	3.0512536	-1.1929777	-1.5867793
H	4.3530216	-0.1260147	-0.9921452
H	3.7846186	1.0730543	1.2777968
H	2.0887006	0.9598433	1.8282818
H	3.8440826	-0.9847617	2.5707608
H	2.2323186	-1.4601317	2.0072067
H	4.8326156	-1.8134257	0.5494208
H	3.2712836	-2.6162367	0.2887407
N	2.4354106	0.2504263	-0.1509922
H	2.4567566	1.1299983	-0.6645032
C	-1.0385224	1.7406003	-1.4061373
C	-0.4142234	2.2826343	0.7587908
C	0.4734726	3.1520753	-0.1369672
C	0.1082796	2.7315283	-1.5781512
H	-1.0842714	0.9670703	-2.1811513
H	-2.0099054	2.2642303	-1.3840933
H	-1.3263324	2.8336233	1.0440628
H	0.0740146	1.9456013	1.6814308
H	0.2932656	4.2172583	0.0451338
H	1.5380926	2.9789743	0.0739998
H	-0.1770924	3.5807973	-2.2080942
H	0.9563326	2.2391413	-2.0739363
N	-0.7563464	1.1328363	-0.0933272
H	-1.5858514	0.6528853	0.2611188

a1

C	0.3603938	1.8001495	-1.5547503
C	0.0858008	1.9182465	0.8375127
C	0.9723938	3.0606935	0.3698897
C	1.5586188	2.4850585	-0.9132543
H	0.6399698	0.9563885	-2.1911243
H	-0.2225492	2.5109985	-2.1574663
H	-0.7244222	2.2140085	1.5149647
H	0.6879168	1.1509865	1.3358057
H	0.3742758	3.9592595	0.1521797
H	1.7294168	3.3323015	1.1137987
H	2.0070308	3.2372295	-1.5715413
H	2.3300338	1.7381425	-0.6753663

N	-0.4937132	1.3240955	-0.4100703
H	-1.4063472	1.7570225	-0.5316613
C	-3.4114302	0.4270275	0.7157437
C	-3.8811952	-1.3117595	-0.7480523
C	-4.1898002	-1.8490975	0.6531357
C	-3.6709232	-0.7681765	1.6182667
H	-2.6812712	1.1353915	1.1285287
H	-4.3488752	0.9743845	0.5142227
H	-4.7873132	-0.8983275	-1.2199563
H	-3.4372412	-2.0645955	-1.4050393
H	-5.2651862	-2.0242055	0.7739207
H	-3.6650312	-2.7960915	0.8148307
H	-4.3731672	-0.5288675	2.4244237
H	-2.7264532	-1.0898265	2.0776057
N	-2.9075812	-0.2106575	-0.5207673
H	-2.9654822	0.4319815	-1.3098883
Ni	-0.8477562	-0.6494505	-0.3730193
C	3.7672548	-1.2948955	0.0447227
C	3.1806698	-1.2728895	-1.2196673
C	1.8020178	-1.1439995	-1.3425113
C	0.9865078	-1.0031915	-0.2152213
C	1.5865838	-1.0816485	1.0458127
C	2.9649848	-1.2119175	1.1799877
H	3.8057378	-1.3761265	-2.1055843
H	1.3524638	-1.1779815	-2.3369023
H	0.9637968	-1.0614835	1.9430187
H	3.4197318	-1.2664505	2.1677357
C	5.2524038	-1.3496155	0.1739357
F	5.8199958	-2.0599015	-0.8101713
F	5.6419918	-1.8901175	1.3357517
F	5.8015528	-0.1213155	0.1205907
Br	-1.0858072	-2.9107775	-0.4443683

a2

Ni	1.0707772	-0.6348991	0.9186186
Br	2.6586942	-2.0258131	2.0092076
C	-3.0274898	0.6532789	0.3076976
C	-3.6991848	-0.4214151	0.8883236
C	-2.9770018	-1.4566821	1.4687056
C	-1.5836388	-1.4132971	1.4546686
C	-0.8745708	-0.3560341	0.8642686
C	-1.6389598	0.6766109	0.3027526

H	-3.6019368	1.4635829	-0.1421274
H	-3.5014408	-2.2923261	1.9281176
H	-1.0391578	-2.2413881	1.9188726
H	-1.1479698	1.5309969	-0.1722204
C	-5.1925628	-0.4105881	0.8787606
F	-5.6742118	-0.2876571	-0.3688074
F	-5.7201128	-1.5218911	1.4018266
F	-5.6817508	0.6289089	1.5731526
C	0.6857142	-0.3772801	-2.0820194
C	1.8330542	-2.2931781	-1.4163984
C	0.3955632	-2.7501691	-1.5899814
C	-0.3070168	-1.5397281	-2.2355684
H	0.2142132	0.5515399	-1.7405614
H	1.2046912	-0.1745861	-3.0330174
H	2.3930562	-2.3820121	-2.3630504
H	2.3830842	-2.8010251	-0.6176184
H	0.3197612	-3.6629781	-2.1902484
H	-0.0371308	-2.9673801	-0.6027954
H	-0.5298018	-1.7139381	-3.2946124
H	-1.2543868	-1.3173091	-1.7300924
N	1.6583592	-0.8596361	-1.0770074
H	2.5494242	-0.3706251	-1.1458084
C	1.1401182	2.4307739	1.4532256
C	3.2079732	1.5035429	0.9094056
C	2.8187392	2.3535569	-0.3034054
C	1.4187982	2.9102479	0.0325216
H	0.0821142	2.2380559	1.6615326
H	1.5165082	3.1618029	2.1879466
H	3.8300552	2.0912069	1.6033076
H	3.7526052	0.5799739	0.6798126
H	3.5552042	3.1457269	-0.4769914
H	2.7850022	1.7564129	-1.2252514
H	1.3646572	4.0014509	-0.0437244
H	0.6692842	2.5039459	-0.6598194
N	1.9156662	1.1817879	1.5483596
H	2.0652092	0.9084309	2.5200416

a3

Ni	1.1107324	0.9264822	-0.4483686
Br	2.0296674	-0.0036038	-2.4182846
C	-2.9079756	1.8614762	-1.3870976
C	-3.5758466	1.9049112	-0.1633806

C	-2.8757596	1.6763472	1.0152814
C	-1.5098966	1.4009162	0.9595514
C	-0.8131096	1.3392682	-0.2507756
C	-1.5472026	1.5818182	-1.4229026
H	-3.4646276	2.0404912	-2.3075866
H	-3.3975026	1.7132242	1.9699644
H	-0.9917806	1.2218962	1.9059064
H	-1.0497706	1.5274922	-2.3950126
C	-5.0377586	2.2079102	-0.1623196
F	-5.7232156	1.3314092	-0.9132536
F	-5.5693056	2.1794882	1.0656364
F	-5.2912366	3.4215172	-0.6767046
C	1.1882324	3.8780702	-0.0113546
C	3.2922584	2.8832032	-0.0856216
C	3.0841964	3.5132712	-1.4690276
C	1.6256864	4.0153812	-1.4613276
H	0.1099394	3.7425462	0.1224134
H	1.5217404	4.7445192	0.5850994
H	3.8320824	3.5690712	0.5878974
H	3.8389124	1.9329622	-0.1239966
H	3.8017424	4.3245902	-1.6356526
H	3.2314884	2.7654012	-2.2566566
H	1.5193764	5.0420402	-1.8273866
H	0.9984124	3.3729452	-2.0953736
N	1.9154004	2.6633332	0.4175134
H	1.8988964	2.5670792	1.4310964
C	1.5086634	-0.0914938	2.4093244
C	2.5331484	-1.4221948	0.8206254
C	3.6821794	-0.6659278	1.4697944
C	3.0141414	0.1404342	2.6024034
H	0.8947594	0.7959232	2.6081924
H	1.1539884	-0.8925138	3.0807624
H	2.3411224	-2.3726438	1.3516444
H	2.6811734	-1.6303078	-0.2442246
H	4.4686364	-1.3370758	1.8315554
H	4.1449964	0.0004762	0.7294994
H	3.3363194	-0.1865148	3.5975484
H	3.2714024	1.2068122	2.5291594
N	1.3792424	-0.5200798	1.0092014
H	0.5112434	-1.0573128	0.8229174
C	-1.7882256	-1.8663968	-0.7052936
C	-2.6617186	-3.0062758	-1.2797866

H	-2.3456586	-1.2288988	-0.0035996
H	-1.3944616	-1.2058428	-1.4904986
H	-3.6328976	-3.0671508	-0.7676256
H	-2.8675386	-2.8565168	-2.3488206
C	-1.1125096	-3.3913208	1.0106224
H	-0.2492416	-3.7341988	1.6028464
H	-1.7825196	-2.8455348	1.6918024
C	-1.8390576	-4.5692748	0.3132974
H	-1.2765476	-5.5082058	0.4206554
H	-2.8376066	-4.7364988	0.7416854
C	-0.6573596	-4.2070178	-1.7203256
H	-0.1951806	-5.2042928	-1.6933056
H	-0.7864176	-3.9361838	-2.7776566
C	0.2032994	-3.1596388	-0.9743896
H	1.0261374	-3.6381458	-0.4210266
H	0.6501884	-2.4184888	-1.6542386
N	-1.9866476	-4.2949108	-1.1144946
N	-0.6308286	-2.4382458	0.0034704

TSa2

C	-3.2442073	-2.4821957	-1.2255406
C	-1.2544303	-3.6759757	-1.3695576
C	-1.7772433	-3.9714747	0.0317144
C	-3.1379823	-3.2420597	0.0997924
H	-3.7023713	-1.4883097	-1.1404356
H	-3.8198893	-3.0630957	-1.9659376
H	-1.6235283	-4.4233477	-2.0937366
H	-0.1615213	-3.6294467	-1.4306686
H	-1.8594813	-5.0481887	0.2170214
H	-1.0804253	-3.5595877	0.7735914
H	-3.9798763	-3.9323027	0.2265104
H	-3.1587013	-2.5417207	0.9447904
N	-1.8395883	-2.3577107	-1.6583136
H	-1.7737213	-2.0988467	-2.6439196
C	-1.4743333	-0.3559557	2.2121724
C	-2.7492823	0.9928943	0.8447074
C	-3.7759833	0.2530283	1.6995864
C	-2.9087043	-0.3772337	2.7986294
H	-0.9911693	-1.3437377	2.2287174
H	-0.8356733	0.3111353	2.8314204
H	-2.5232063	1.9737963	1.3292594
H	-3.0764633	1.2052223	-0.1824676

H	-4.5691853	0.9010793	2.0934904
H	-4.2577153	-0.5249857	1.0888054
H	-2.9600783	0.2087723	3.7260444
H	-3.2361403	-1.3942017	3.0514434
N	-1.5783703	0.1358103	0.8501014
Ni	-0.9712563	-0.7515647	-0.6611086
C	3.7514937	-1.6496157	-0.3051036
C	3.0430747	-1.4076717	0.8729104
C	1.6641437	-1.2254967	0.8258684
C	0.9373577	-1.2644777	-0.3764006
C	1.6874017	-1.5373407	-1.5349356
C	3.0685467	-1.7259617	-1.5146626
H	3.5797187	-1.3647917	1.8223724
H	1.1415117	-1.0315257	1.7669264
H	1.1811677	-1.5746227	-2.5060816
H	3.6179447	-1.9207187	-2.4344016
C	5.2336687	-1.7849757	-0.2285336
F	5.8153707	-0.6293567	0.1492274
F	5.7848447	-2.1347797	-1.3952146
F	5.6069737	-2.7003817	0.6803214
Br	-1.5131563	0.8200383	-2.6435846
H	-0.2453293	1.4709933	-0.6451456
C	1.6121017	2.0895643	-1.3449476
C	2.6218207	3.1827123	-0.9461026
H	1.9760357	1.0653703	-1.1986996
H	1.2398857	2.1677913	-2.3728786
H	3.4853187	2.7469943	-0.4262886
H	3.0024207	3.7016233	-1.8346976
C	0.8280127	2.2421263	0.9740484
H	-0.0902073	2.1857913	1.5694414
H	1.3833837	1.3084913	1.1258244
C	1.6697867	3.5123273	1.2129124
H	1.1263867	4.2363113	1.8345504
H	2.6005417	3.2638213	1.7379564
C	0.7741577	4.6626743	-0.6710746
H	0.3891937	5.4987703	-0.0736306
H	1.0289087	5.0595723	-1.6623106
C	-0.2791223	3.5420553	-0.7817696
H	-1.1009513	3.6396253	-0.0612826
H	-0.7183483	3.4140803	-1.7774396
N	2.0006707	4.1622503	-0.0539566
N	0.4157987	2.2589353	-0.4593276

a4

Ni	-1.1829815	-0.7990127	0.2069404
Br	-1.5137835	0.6725963	-2.0209326
C	2.6516905	-2.4071197	-0.8664316
C	3.4506165	-2.0702767	0.2238234
C	2.8719285	-1.4711697	1.3432184
C	1.5087335	-1.1927027	1.3489084
C	0.6758215	-1.4683067	0.2474914
C	1.2913355	-2.1084937	-0.8426136
H	3.1004815	-2.8863347	-1.7356466
H	3.4947805	-1.2289007	2.2051294
H	1.0783255	-0.7200217	2.2369554
H	0.7012255	-2.3467967	-1.7328086
C	4.9294415	-2.2487127	0.1742104
F	5.5516085	-1.0953437	-0.1576636
F	5.4390495	-2.6167427	1.3571864
F	5.3098935	-3.1589017	-0.7290306
C	-2.2337745	-3.4462297	-0.8213366
C	-3.9282395	-1.8241447	-0.7014596
C	-3.6975485	-2.1080717	-2.1937926
C	-2.4173375	-2.9599367	-2.2496816
H	-1.1976555	-3.6950967	-0.5588026
H	-2.8698725	-4.3275967	-0.6239556
H	-4.7967355	-2.3883447	-0.3232626
H	-4.0876365	-0.7606887	-0.4832226
H	-4.5574315	-2.6395017	-2.6191386
H	-3.5637005	-1.1758787	-2.7532236
H	-2.4790775	-3.7874547	-2.9651976
H	-1.5684235	-2.3241677	-2.5375606
N	-2.6907355	-2.2869797	-0.0340196
H	-2.8728545	-2.5463817	0.9328744
C	-2.1875045	-0.1731227	2.8205504
C	-2.3589175	1.6092653	1.4068504
C	-3.8029375	1.3746353	1.8839174
C	-3.6884975	0.1720963	2.8450804
H	-1.9737755	-1.2478107	2.9299794
H	-1.6766725	0.3359353	3.6647504
H	-1.8772665	2.3703413	2.0606474
H	-2.2967125	1.9601593	0.3680374
H	-4.2369635	2.2609223	2.3642204
H	-4.4413555	1.1294623	1.0239614

H	-4.0499205	0.3981423	3.8565084
H	-4.2829945	-0.6764037	2.4765324
N	-1.7007915	0.3294773	1.5556134
H	0.1722645	1.5855923	-1.3203266
C	2.2291265	1.2026763	-1.3308036
C	3.5042045	1.9843233	-0.9671206
H	2.1141745	0.2760403	-0.7622526
H	2.1344895	0.9603793	-2.3967856
H	4.1991295	1.3358493	-0.4187886
H	4.0271105	2.3440813	-1.8632946
C	0.9680905	2.2342383	0.5107894
H	0.1760885	2.9739533	0.6861044
H	0.6266865	1.2803183	0.9339084
C	2.3525285	2.7023393	0.9911814
H	2.2582305	3.5251203	1.7113864
H	2.8859385	1.8821133	1.4906044
C	2.4008695	4.0944633	-0.9469576
H	2.0658985	4.9075273	-0.2894206
H	3.0606945	4.5366833	-1.7039726
C	1.1955335	3.3957583	-1.6175646
H	0.2434665	3.9244213	-1.4848436
H	1.3349485	3.2190373	-2.6915166
N	3.1668725	3.1454663	-0.1426686
N	1.0608175	2.0632293	-0.9712636

a5

C	-1.2797520	2.7991488	1.7840756
C	0.1634290	4.0224598	0.3051546
C	-0.7226440	4.9787858	1.0899636
C	-1.9349830	4.1040328	1.3830286
H	-1.9370580	1.9288148	1.7424036
H	-0.8729450	2.8699088	2.8020226
H	1.2395480	4.2240968	0.3830796
H	-0.1073550	4.0568238	-0.7585674
H	-0.2395380	5.2774168	2.0317956
H	-0.9508720	5.8891708	0.5238536
H	-2.5920110	4.5009038	2.1645166
H	-2.5353920	3.9589798	0.4712386
N	-0.1396410	2.6480428	0.8256046
H	0.6597250	2.2888998	1.3524736
C	2.9302570	1.4432208	-0.6560814
C	1.9909700	2.6977798	-2.4137814

C	3.5123300	2.7340498	-2.5505784
C	3.9250240	1.4660618	-1.8103254
H	3.2596940	2.1109178	0.1646806
H	2.7519370	0.4692338	-0.1866034
H	1.5187530	2.1363658	-3.2387364
H	1.5082510	3.6872178	-2.3953714
H	3.8422200	2.7645028	-3.5946594
H	3.9235290	3.6192208	-2.0432734
H	3.7619500	0.5844008	-2.4483834
H	4.9695080	1.4637688	-1.4800054
N	1.6953930	1.9747338	-1.1918114
Ni	-0.0814740	1.3759258	-0.7022124
C	-4.4399980	-0.1999432	0.0165676
C	-3.4043900	-0.6720102	0.8152416
C	-2.1046100	-0.2141042	0.6084916
C	-1.8170690	0.7162378	-0.3958354
C	-2.8725060	1.1745038	-1.1937714
C	-4.1721170	0.7309008	-0.9873794
H	-3.6171920	-1.3858852	1.6096746
H	-1.3135310	-0.5490742	1.2817066
H	-2.6715850	1.8770398	-2.0046534
H	-4.9889880	1.0974648	-1.6097864
C	-5.8442650	-0.6704472	0.1916066
F	-6.2890910	-1.3222912	-0.8961784
F	-6.6906450	0.3539848	0.3831656
F	-5.9847300	-1.5014962	1.2321916
Br	0.0654300	-0.1370832	-2.4651674
H	0.5124640	-2.0304302	0.9009426
C	-0.5675340	-3.1142712	-0.5287504
C	-0.1993100	-4.2534722	-1.4975694
H	-1.3936500	-3.3629942	0.1484626
H	-0.7938670	-2.1695572	-1.0390704
H	-1.0025450	-4.9991382	-1.5446804
H	-0.0554630	-3.8559052	-2.5112154
C	0.8683120	-4.0526362	1.2280956
H	1.7915280	-3.8461752	1.7811906
H	0.0453880	-4.0810402	1.9501056
C	0.9426610	-5.2972072	0.3190156
H	1.8107600	-5.9141932	0.5826586
H	0.0486660	-5.9231642	0.4377456
C	2.1535380	-3.9734672	-1.2460934
H	3.0601680	-4.4494212	-0.8495764

H	2.3161260	-3.7957832	-2.3164824
C	1.8537200	-2.6474572	-0.5246294
H	2.6448900	-2.3048082	0.1504676
H	1.5865930	-1.8310902	-1.2086234
N	1.0417900	-4.9094192	-1.0852644
N	0.6394180	-2.8807142	0.3308296
P	1.5286480	-0.2297772	2.6717216
F	0.7255520	-1.6419242	2.9037416
F	0.9811890	-0.2809472	1.0889916
F	0.1930260	0.5841158	3.0671926
F	2.0594730	-0.2178732	4.1683426
F	2.8241760	-1.0671622	2.1651816
F	2.2707140	1.1732328	2.3178966

TSa3

C	0.9841558	3.0236152	-1.4167242
C	0.3032668	3.0640282	0.8833398
C	0.3429958	4.4958382	0.3753428
C	1.3171868	4.3842232	-0.7953452
H	1.8696168	2.4708952	-1.7546342
H	0.3054648	3.1129792	-2.2736682
H	-0.5759342	2.8164312	1.4882738
H	1.2084188	2.8289912	1.4647068
H	-0.6590462	4.7776262	0.0226708
H	0.6550518	5.2191472	1.1375988
H	1.2260308	5.2028562	-1.5176512
H	2.3527688	4.3922572	-0.4225072
N	0.2786968	2.2485312	-0.3502882
H	-0.7030672	2.2129252	-0.6317762
C	1.1417508	-1.8611948	1.5231238
C	1.4728138	0.2496592	2.5428888
C	1.8945948	-0.8650578	3.5093958
C	2.2238548	-2.0260198	2.5776718
H	0.1828928	-2.2664468	1.9053538
H	1.3412798	-2.3787118	0.5750498
H	2.3285138	0.9078782	2.3301228
H	0.6757258	0.8874022	2.9526448
H	2.7301748	-0.5650678	4.1515668
H	1.0552818	-1.1400578	4.1642678
H	3.2143698	-1.8869608	2.1186958
H	2.2066008	-3.0041378	3.0724298
N	1.0043118	-0.4187978	1.3283568

Ni	0.6067898	0.2558662	-0.3649502
C	5.2154578	-0.0787298	-0.8502532
C	4.3804088	-1.1411418	-1.1972312
C	3.0339598	-1.1090478	-0.8613802
C	2.5209798	-0.0071168	-0.1770662
C	3.3489408	1.0555742	0.1596408
C	4.6987868	1.0231832	-0.1816162
H	4.7856898	-1.9914058	-1.7451812
H	2.3854838	-1.9268348	-1.1742082
H	2.9540388	1.9307512	0.6748538
H	5.3468728	1.8586372	0.0732948
C	6.6624458	-0.1710318	-1.2099622
F	7.2534898	-1.2034148	-0.5873952
F	7.3427428	0.9318592	-0.8864362
F	6.8284968	-0.3771938	-2.5241382
Br	-0.2227672	-0.3225668	-2.4877472
H	-2.8119792	-0.3750458	-0.9845332
C	-3.3959542	-2.0172318	-2.1206582
C	-3.7227132	-3.4904298	-1.8044452
H	-4.2224272	-1.4742328	-2.5934882
H	-2.4935422	-1.8718348	-2.7254522
H	-4.6203022	-3.8132588	-2.3463312
H	-2.9000332	-4.1480848	-2.1138172
C	-4.4035102	-1.2766358	-0.0095222
H	-4.1390792	-0.8274268	0.9532598
H	-5.0724692	-0.5784628	-0.5183212
C	-4.9389472	-2.7173958	0.0934658
H	-5.2097942	-2.9562488	1.1294598
H	-5.8426572	-2.8453978	-0.5164412
C	-2.6872932	-3.4451188	0.3430908
H	-2.8937362	-3.4988948	1.4202588
H	-1.9823492	-4.2518968	0.1045078
C	-2.0906742	-2.0792738	-0.0436252
H	-1.8175222	-1.4429028	0.8073348
H	-1.2232332	-2.1433668	-0.7114232
N	-3.9408042	-3.6796928	-0.3707722
N	-3.1400082	-1.3405758	-0.8118242
P	-3.4531882	2.2770042	-0.3967802
F	-3.9407422	1.1872562	-1.5324912
F	-2.3587112	1.1131842	0.1283938
F	-2.3194162	2.8002192	-1.4433602
F	-4.4975642	3.3539132	-0.9260932

| F | -4.5268252 | 1.6617042 | 0.6385508 |
| F | -2.8741132 | 3.2699102 | 0.7299258 |

a6(b1)

Ni	-0.0803406	1.0554085	0.0249876
C	3.1169364	0.6309595	-0.7085144
C	2.5958474	-0.8083755	-0.9242474
C	1.9384254	-1.1782175	0.4052896
C	2.7190154	0.9778385	0.7243096
H	4.1991304	0.7149215	-0.8573614
H	2.6304754	1.3256215	-1.4041714
H	3.3891474	-1.5169005	-1.1882364
H	1.8577014	-0.8283935	-1.7368074
H	1.0760184	-1.8509245	0.3100156
H	2.6696474	-1.6638705	1.0751866
H	2.4533114	2.0312775	0.8637196
H	3.5188854	0.7014305	1.4335606
N	1.5280594	0.1274145	0.9436196
H	1.2999264	0.0737745	1.9361226
C	-3.2690926	0.6859695	-0.3082674
C	-2.9680856	-0.0061285	1.0403536
C	-1.9413386	-1.0848805	0.6998456
C	-2.3723166	-0.0269775	-1.3203054
H	-4.3241396	0.6135565	-0.5948934
H	-3.0072116	1.7496695	-0.2576754
H	-3.8600996	-0.4386895	1.5074676
H	-2.5383946	0.7154325	1.7463806
H	-1.2197656	-1.2795085	1.5031636
H	-2.4424346	-2.0353015	0.4442126
H	-1.9850706	0.6323005	-2.1055864
H	-2.9032456	-0.8716305	-1.7929944
N	-1.2565706	-0.5303875	-0.4855754
H	-0.7325816	-1.2506365	-0.9825504
Br	-0.0918386	3.3352465	0.0089506

a7

C	2.7370454	2.3375790	-0.8255943
C	2.2602974	2.0059260	1.5148267
C	3.3840134	3.0183000	1.3611877
C	3.9747884	2.6163870	0.0144837
H	2.9146094	1.6124940	-1.6249053
H	2.3504314	3.2636980	-1.2756573

H	1.4515974	2.3098420	2.1905367
H	2.6594204	1.0487960	1.8681437
H	2.9858214	4.0439160	1.3161067
H	4.1032654	2.9722260	2.1863487
H	4.6164684	3.3827810	-0.4339403
H	4.5669054	1.6957430	0.1200587
N	1.7126014	1.8067060	0.1370427
H	0.8910134	2.4013370	0.0532157
C	-1.1131716	1.3156280	-1.7263643
C	-1.4965646	1.7364150	0.5831617
C	-2.2652006	2.7705140	-0.2562513
C	-2.4098156	2.1027360	-1.6222653
H	-0.2729336	1.9818040	-1.9891113
H	-1.1189106	0.4907760	-2.4487183
H	-2.1575016	1.1782800	1.2577367
H	-0.7235076	2.2030850	1.2113247
H	-3.2253286	3.0446230	0.1965687
H	-1.6788796	3.6970690	-0.3553113
H	-3.2601766	1.4051370	-1.6193843
H	-2.5555036	2.8165370	-2.4412883
N	-0.8978276	0.7660160	-0.3700523
Ni	1.0003984	-0.0038880	-0.2164703
C	5.3640914	-1.7017660	-0.0913053
C	4.8009164	-1.3013770	-1.3017823
C	3.4874894	-0.8474040	-1.3379453
C	2.7187654	-0.7550630	-0.1722103
C	3.2862674	-1.2077790	1.0234327
C	4.5990484	-1.6656580	1.0717717
H	5.3891804	-1.3620920	-2.2164983
H	3.0471884	-0.5778440	-2.3006163
H	2.6869054	-1.2242620	1.9364597
H	5.0288644	-2.0103030	2.0109957
C	6.7994734	-2.1033080	-0.0369373
F	7.0587274	-2.9300750	0.9845497
F	7.6074144	-1.0375470	0.1195937
F	7.1976914	-2.7161100	-1.1602223
Br	0.1762744	-2.0995180	-0.6252913
H	-1.5004796	-0.0631920	-0.3090983
C	-3.0477756	-1.7819220	1.2338787
C	-4.1611626	-2.8269740	1.4866177
H	-2.0834136	-2.2431030	0.9789917
H	-2.8822556	-1.1416640	2.1145667

H	-3.7608726	-3.8503130	1.4746797
H	-4.6455946	-2.6779430	2.4627417
C	-3.5493486	-1.7431330	-1.1064303
H	-3.8729676	-1.0853430	-1.9285133
H	-2.5456166	-2.1172140	-1.3540613
C	-4.5652336	-2.8843020	-0.8584783
H	-5.3570236	-2.8979470	-1.6213073
H	-4.0744226	-3.8673930	-0.8800793
C	-5.8076026	-1.4014510	0.5277227
H	-6.5542366	-1.3293250	-0.2764753
H	-6.3478956	-1.3218700	1.4820657
C	-4.7237076	-0.3007080	0.3945827
H	-4.9625466	0.4103470	-0.4123223
H	-4.6216556	0.2826090	1.3233407
N	-5.1936386	-2.7251100	0.4539027
N	-3.4242056	-0.9144080	0.1042517

TSa2'

C	-1.7764273	1.9760008	1.5987773
C	-1.9181723	2.9531928	-0.6000787
C	-2.8438753	3.7006798	0.3475123
C	-3.1367573	2.6305258	1.3938053
H	-1.8524993	0.9290608	1.9058193
H	-1.1824113	2.5178358	2.3499423
H	-1.2614323	3.5865978	-1.2086997
H	-2.5006243	2.3161528	-1.2748637
H	-2.3255553	4.5561948	0.8076643
H	-3.7412303	4.0796888	-0.1543967
H	-3.5546783	3.0254018	2.3266413
H	-3.8450983	1.8926818	0.9889183
N	-1.0820863	2.0818088	0.2778893
H	-0.1970053	2.5599078	0.4262933
C	1.9947627	1.7520958	0.6062833
C	1.8707437	1.7830758	-1.7446467
C	2.4675987	3.1050998	-1.2682137
C	3.0688977	2.7024358	0.0691573
H	1.2787017	2.3542358	1.2282523
H	2.4289977	1.0451738	1.3501143
H	2.6445857	1.2061058	-2.3013667
H	1.0522197	1.9369018	-2.4662897
H	3.1868447	3.5497338	-1.9683867
H	1.6633957	3.8431098	-1.1029017

H	4.0122347	2.1565058	-0.0989097
H	3.2885097	3.5403918	0.7434453
N	1.4179257	1.0784828	-0.5398877
Ni	-0.4582023	0.4859308	-0.6573427
C	-4.7681933	-1.4144002	-0.2669907
C	-3.7853973	-1.6412702	0.6897023
C	-2.5204843	-1.0814092	0.5212483
C	-2.2004033	-0.2794042	-0.5815267
C	-3.2029033	-0.1022162	-1.5474807
C	-4.4696343	-0.6480862	-1.3948067
H	-4.0110293	-2.2527742	1.5618453
H	-1.7640913	-1.2779222	1.2890533
H	-2.9805073	0.4649008	-2.4548567
H	-5.2379053	-0.4925112	-2.1532747
C	-6.1391103	-1.9831292	-0.1358927
F	-6.4379673	-2.8110832	-1.1505687
F	-7.0804063	-1.0225412	-0.1533287
F	-6.3062153	-2.6751902	0.9989453
Br	0.0250907	-1.0866982	-2.3620227
H	1.5948667	-1.4544242	-1.1071227
C	2.4405257	-3.3491762	-0.8457027
C	3.4915247	-3.9633432	0.1075743
H	1.4539817	-3.8239792	-0.7822547
H	2.7430777	-3.3523872	-1.8997547
H	3.1185387	-4.8967492	0.5474183
H	4.4172737	-4.2035542	-0.4312517
C	1.6571577	-1.8699192	0.9221313
H	1.5352747	-0.8065402	1.1527333
H	0.6541777	-2.3071872	0.8331383
C	2.5941917	-2.6389252	1.8754363
H	2.8629437	-2.0190372	2.7403253
H	2.1112657	-3.5464292	2.2608873
C	4.4605117	-1.8439502	0.6240423
H	4.6289887	-1.1308822	1.4422103
H	5.4444967	-2.1246152	0.2270033
C	3.5770317	-1.2213082	-0.4742447
H	3.3288507	-0.1613962	-0.3491747
H	3.9760767	-1.3630412	-1.4870237
N	3.8217807	-3.0342582	1.1860813
N	2.2672587	-1.9301702	-0.4370297

a8

C	1.7300336	1.9764979	-1.6107064
C	1.8870686	2.9929129	0.5696326
C	2.8005866	3.7274629	-0.3998494
C	3.0891216	2.6402609	-1.4296234
H	1.8078616	0.9249519	-1.9014214
H	1.1258356	2.5034779	-2.3642424
H	1.2322436	3.6342339	1.1719346
H	2.4790416	2.3716549	1.2508996
H	2.2740026	4.5721949	-0.8703024
H	3.7005946	4.1194999	0.0870786
H	3.4967946	3.0204749	-2.3730214
H	3.8044866	1.9128059	-1.0183064
N	1.0482916	2.1009319	-0.2848534
H	0.1578886	2.5697979	-0.4327144
C	-2.0225344	1.7304349	-0.5883114
C	-1.8555554	1.8798829	1.7566836
C	-2.6239224	3.0932479	1.2309926
C	-3.1986174	2.5600959	-0.0731504
H	-1.3648604	2.4181059	-1.1924164
H	-2.3486044	0.9715109	-1.3328144
H	-2.5130534	1.2675099	2.4120666
H	-1.0092554	2.1800379	2.4001786
H	-3.3767874	3.4793679	1.9301276
H	-1.9246114	3.9174179	1.0087596
H	-4.0605694	1.9048439	0.1375956
H	-3.5318054	3.3366079	-0.7739834
N	-1.4185834	1.1261979	0.5771996
Ni	0.4453276	0.5184949	0.6840476
C	4.7616186	-1.3680791	0.2819596
C	3.7711866	-1.6156571	-0.6615874
C	2.5050506	-1.0593171	-0.4906164
C	2.1907806	-0.2408391	0.6016826
C	3.2016196	-0.0422701	1.5547736
C	4.4696726	-0.5843551	1.3995136
H	3.9921216	-2.2399981	-1.5258324
H	1.7430416	-1.2714791	-1.2487324
H	2.9853816	0.5391669	2.4546336
H	5.2443156	-0.4115621	2.1476766
C	6.1327316	-1.9361881	0.1497366
F	6.4330346	-2.7634711	1.1645936
F	7.0734606	-0.9752611	0.1654096
F	6.2985936	-2.6293451	-0.9846734

Br	-0.0171334	-1.0403861	2.4114206
H	-1.4376624	-1.8403441	1.2252926
C	-2.4565244	-3.6101981	0.6837096
C	-3.5040644	-3.9810891	-0.3942324
H	-1.5136604	-4.1630611	0.5889376
H	-2.8203424	-3.7383781	1.7104156
H	-3.1388374	-4.8008491	-1.0258534
H	-4.4392464	-4.3183491	0.0705756
C	-1.5347104	-1.9385061	-0.8390124
H	-1.2683304	-0.8733831	-0.8608714
H	-0.6029544	-2.5185641	-0.8658124
C	-2.5738134	-2.3748141	-1.8923994
H	-2.8251874	-1.5411931	-2.5608104
H	-2.1855484	-3.1896161	-2.5174124
C	-4.3601044	-1.7522361	-0.4364394
H	-4.5842134	-0.9070251	-1.1005894
H	-5.3130594	-2.0944011	-0.0121164
C	-3.3721364	-1.3353141	0.6711936
H	-2.9947244	-0.2985411	0.6245496
H	-3.7425204	-1.5290551	1.6859876
N	-3.8027484	-2.8355741	-1.2481144
N	-2.1455054	-2.1713801	0.5015616

b2

Ni	-0.9801505	-0.7837230	-0.5907739
Br	-0.6363925	-2.7503470	-1.7589259
N	-0.5445315	1.1970840	-0.7779759
H	0.4122345	1.2845870	-0.3992089
C	-0.5541925	1.4597240	-2.2351099
H	-0.0778695	0.6364630	-2.7823779
H	-0.0026275	2.3915730	-2.4544509
C	-2.0400835	1.6168280	-2.5400829
H	-2.4753165	0.6309350	-2.7531699
H	-2.2145375	2.2528620	-3.4150739
C	-2.6332805	2.2027000	-1.2395409
H	-3.4437105	1.5645760	-0.8632429
H	-3.0522155	3.2059260	-1.3795509
C	-1.4579035	2.2266500	-0.2582769
H	-1.7390635	2.0119660	0.7796051
H	-0.9643145	3.2145330	-0.2773689
N	-1.7612505	-1.4491300	1.2126521
H	-1.0207255	-2.0621980	1.5546181

C	-2.1573685	-0.4485130	2.2169171
H	-1.4267195	0.3714620	2.2390601
H	-2.1898505	-0.8981660	3.2241021
C	-3.5699085	-0.0243950	1.7780741
H	-3.5735255	0.9729360	1.3203911
H	-4.2402365	0.0245110	2.6443631
C	-4.0140445	-1.1063580	0.7716161
H	-3.9375455	-0.7379560	-0.2620699
H	-5.0444005	-1.4422590	0.9318161
C	-2.9969905	-2.2180550	0.9640831
H	-2.8572695	-2.8678470	0.0938841
H	-3.2519365	-2.8331180	1.8452571
C	3.5661285	1.1446590	0.3673991
C	4.6519075	0.0640810	0.6086391
H	3.8451865	1.8257340	-0.4497219
H	3.3956755	1.7600090	1.2628351
H	5.5567835	0.2632590	0.0168881
H	4.9552675	0.0300220	1.6652811
C	2.4912155	-0.2252440	-1.2689819
H	1.5550445	-0.7585890	-1.4967489
H	2.6613965	0.5170550	-2.0636509
C	3.6703775	-1.2176380	-1.1396989
H	3.3646305	-2.2313590	-1.4341069
H	4.5183245	-0.9293840	-1.7777859
C	3.0151795	-1.5873460	1.1149861
H	2.5985345	-2.5478580	0.7779391
H	3.3923125	-1.7288210	2.1383631
C	1.9482435	-0.4695640	1.0471341
H	0.9530625	-0.8777890	0.8006851
H	1.8633555	0.0814870	1.9968271
N	4.1437965	-1.2573610	0.2449751
N	2.2993045	0.5013950	-0.0004939

TSb1
Ni	1.3728611	0.5077186	0.2885060
C	0.9080371	-1.5131154	3.3281360
C	-0.5869929	-1.1919414	3.1577820
C	-0.6334709	0.2554406	2.6423940
C	1.5869361	-0.1542334	3.2676030
H	1.1300991	-2.0471554	4.2584590
H	1.2428891	-2.1403594	2.4915950
H	-1.1310169	-1.2781744	4.1060920

H	-1.0578259	-1.8867144	2.4518910
H	-1.2812249	0.3830466	1.7638850
H	-0.9970989	0.9353816	3.4295610
H	2.6316671	-0.1664954	2.9354540
H	1.5488781	0.3391926	4.2541480
N	0.7622101	0.5867976	2.2961120
H	0.9514621	1.5859386	2.3858750
C	0.6551981	3.0057836	-2.0743750
C	0.2154011	3.8472136	-0.8619990
C	-0.6336949	2.8947476	-0.0056200
C	-0.2145209	1.7625416	-1.9836660
H	0.5338311	3.5270386	-3.0307420
H	1.7126221	2.7283126	-1.9670520
H	-0.3688319	4.7262396	-1.1594860
H	1.0925171	4.1892476	-0.3027770
H	-0.3887969	2.9484316	1.0632620
H	-1.7097239	3.1241016	-0.1136780
H	0.2043201	0.8707396	-2.4716140
H	-1.2068789	1.9554946	-2.4375380
N	-0.3487089	1.5484056	-0.5329180
H	-1.1304159	0.9038066	-0.3570910
Br	2.9466661	2.2646876	0.7123370
C	5.3889781	-1.0329624	-0.7934370
C	4.9059211	-1.5504094	0.4112150
C	3.5514941	-1.5337614	0.6881790
C	2.6885871	-0.9363394	-0.2333660
C	3.1439881	-0.5081584	-1.4837020
C	4.5090111	-0.5207064	-1.7393120
H	5.6047391	-1.9688744	1.1345220
H	3.1697331	-1.9440174	1.6202950
H	2.4520561	-0.0883724	-2.2132920
H	4.8883261	-0.1342744	-2.6821910
C	6.8578301	-1.1049914	-1.0540920
F	7.2683151	-2.3772764	-1.1868250
F	7.5624061	-0.5859564	-0.0401970
F	7.2111091	-0.4564204	-2.1676370
Br	0.6502931	-1.7163074	-0.2850960
C	-3.0578219	-1.4198744	0.3676770
C	-4.3428389	-2.1724224	-0.0576300
H	-2.1638789	-2.0613824	0.3344970
H	-3.1382889	-1.0249934	1.3922000
H	-4.1277969	-3.2150074	-0.3310260

H	-5.0846099	-2.1946524	0.7532930
C	-2.6906229	-0.7988744	-1.9076300
H	-2.4771309	0.0542706	-2.5686940
H	-1.8086349	-1.4556714	-1.9328450
C	-3.9921469	-1.5301764	-2.3197890
H	-4.4662729	-1.0512824	-3.1882320
H	-3.7985449	-2.5773624	-2.5913500
C	-5.2599919	-0.1294914	-0.8672140
H	-5.7511599	0.3387576	-1.7318270
H	-5.9890139	-0.1392694	-0.0445920
C	-3.9645949	0.6255456	-0.4710500
H	-3.7606779	1.4701586	-1.1473200
H	-4.0178659	1.0312416	0.5511360
N	-2.8176249	-0.2871444	-0.5349180
N	-4.9496649	-1.5156614	-1.2142830

b3

Ni	0.4623893	0.9356829	-0.1771836
Br	-0.4937167	0.9395879	2.1017354
C	4.2075903	-0.4841551	-1.0242856
C	4.7094593	-0.9542041	0.1824934
C	3.9459853	-0.8630791	1.3468974
C	2.6734693	-0.3069231	1.3093034
C	2.1671183	0.1510939	0.0969804
C	2.9283663	0.0729839	-1.0633636
H	4.8067673	-0.5543471	-1.9295266
H	4.3582223	-1.2286601	2.2873074
H	2.0754853	-0.2215801	2.2167274
H	2.5358393	0.4403099	-2.0161776
C	6.0714123	-1.5640781	0.2800634
F	6.8471943	-0.8889581	1.1399884
F	6.0083963	-2.8240131	0.7334454
F	6.7056133	-1.5917461	-0.8961406
C	2.5121443	4.6904699	-0.4814296
C	2.4855313	4.5137449	1.0516194
C	2.1368833	3.0439379	1.2546714
C	1.9117143	3.3904269	-1.0395336
H	1.9238573	5.5623849	-0.7901186
H	3.5295133	4.8410869	-0.8603396
H	1.7083693	5.1476879	1.4993624
H	3.4340013	4.7804779	1.5305464
H	3.0240193	2.4037059	1.1641554

H	1.6231873	2.8005349	2.1893404
H	2.6995193	2.7077579	-1.3853786
H	1.1834633	3.5197099	-1.8452046
N	1.2464193	2.7361019	0.1121024
H	0.3526213	3.2124229	0.2735374
C	-0.2354717	-1.2279181	-1.9869626
C	-0.0050727	-2.7333701	-1.9750146
C	0.7666543	-2.9414171	-0.6771926
C	0.0351103	-2.0122521	0.2719704
H	0.6124403	-0.7087151	-2.4531126
H	-1.1393887	-0.9022771	-2.5116046
H	-0.9671677	-3.2664511	-1.9272456
H	0.5242473	-3.0800521	-2.8697796
H	0.7676423	-3.9794821	-0.3263146
H	1.8129813	-2.6210771	-0.7935656
H	-0.9030657	-2.4739451	0.6141694
H	0.6003373	-1.7205571	1.1591474
N	-0.3295607	-0.8196861	-0.5508696
C	-4.8513207	-1.5833171	1.7755204
C	-3.3610427	-1.5482131	1.3612114
H	-5.0231687	-1.0152921	2.7008124
H	-5.1960137	-2.6119821	1.9553274
H	-2.7116377	-1.1087831	2.1317934
H	-2.9895997	-2.5631621	1.1475034
C	-5.3254667	0.4262509	0.6023554
H	-5.9050207	0.8439969	-0.2338176
H	-5.6514827	0.9462909	1.5142704
C	-3.8060297	0.5818479	0.3707724
H	-3.5701487	1.2130429	-0.4946686
H	-3.2822767	1.0206869	1.2311424
C	-3.9207567	-1.4051001	-0.9580526
H	-3.8531517	-0.7489041	-1.8387976
H	-3.3959657	-2.3437141	-1.2026006
C	-5.3916467	-1.6596511	-0.5407516
H	-6.0945297	-1.2880231	-1.2998046
H	-5.5918837	-2.7330791	-0.4083326
N	-5.6801517	-0.9901151	0.7266784
N	-3.2019637	-0.7448771	0.1382164
H	-1.3235077	-0.5947671	-0.3281856
Br	-1.1937567	1.9857019	-1.5858096

TSb2

Ni	0.2972480	0.7156549	-0.0434358
Br	-0.6868820	1.0113049	2.2325502
C	4.0917700	-0.5141281	-1.1495728
C	4.7203090	-0.7733471	0.0676092
C	4.0355140	-0.5890601	1.2636792
C	2.7097950	-0.1577621	1.2450682
C	2.0806030	0.0761469	0.0293532
C	2.7690280	-0.0850431	-1.1695228
H	4.6418910	-0.6503231	-2.0805508
H	4.5347370	-0.7821321	2.2108202
H	2.1721650	-0.0035091	2.1816242
H	2.2805240	0.1282489	-2.1225898
C	6.1457050	-1.2224671	0.0421132
F	6.9446930	-0.2830811	-0.4865618
F	6.6170480	-1.5068641	1.2600552
F	6.2997040	-2.3189561	-0.7148978
C	2.0881760	4.5948239	-0.7200238
C	2.2062870	4.5410489	0.8165102
C	1.6889180	3.1475679	1.2037412
C	1.7543600	3.1623129	-1.1190818
H	1.2716760	5.2651889	-1.0219478
H	2.9990330	4.9575169	-1.2095708
H	1.6104490	5.3322769	1.2875232
H	3.2398270	4.6780429	1.1554362
H	2.5157690	2.4493299	1.3880172
H	1.0268890	3.1181179	2.0721912
H	2.6607330	2.5443829	-1.1866778
H	1.1853360	3.0533669	-2.0463508
N	0.9602730	2.6393119	0.0161582
H	0.0389300	3.0862699	-0.0149058
C	-0.1037240	-1.8168461	-1.3942268
C	0.0299540	-3.2852441	-1.0131558
C	0.7673180	-3.1870851	0.3137222
C	0.0535830	-2.0168061	0.9703842
H	0.8259180	-1.4850631	-1.8806448
H	-0.9103740	-1.6020911	-2.1055718
H	-0.9625060	-3.7426231	-0.8570888
H	0.5500820	-3.8731571	-1.7786708
H	0.7338060	-4.1024201	0.9168602
H	1.8240470	-2.9321121	0.1375972
H	-0.8636210	-2.3716181	1.4744312
H	0.6418680	-1.5167861	1.7441472

N	-0.3316330	-1.0895701	-0.1232938
C	-4.9400730	-1.2929391	1.3705782
C	-3.4070630	-1.4258541	1.2567992
H	-5.2162620	-0.6656401	2.2282842
H	-5.4067150	-2.2755151	1.5200252
H	-2.8583340	-1.0227021	2.1173882
H	-3.0898490	-2.4657631	1.0965872
C	-5.0173230	0.6982079	0.0740312
H	-5.3624990	1.1113079	-0.8834718
H	-5.4859920	1.2895419	0.8714532
C	-3.4826200	0.7540129	0.1845152
H	-3.0001890	1.3339569	-0.6097258
H	-3.1180580	1.1353939	1.1442752
C	-3.5045580	-1.2682331	-1.1705068
H	-3.2074430	-0.6066611	-1.9946808
H	-2.9951620	-2.2318291	-1.3062988
C	-5.0310170	-1.4179211	-1.0052788
H	-5.5557640	-1.0418331	-1.8928848
H	-5.3145510	-2.4719751	-0.8802578
N	-5.4970500	-0.6813571	0.1665762
N	-2.9606470	-0.6458781	0.0686742
H	-1.8063180	-0.7142381	0.0076872
Br	-0.8977410	1.3131009	-2.1550158

b4

Ni	0.3188140	0.6764360	-0.0648112
Br	-0.6873570	0.9170670	2.2131958
C	4.1479100	-0.4515160	-1.1239532
C	4.7681980	-0.7276980	0.0936058
C	4.0643900	-0.5929220	1.2855128
C	2.7290670	-0.1937730	1.2619878
C	2.1066440	0.0588690	0.0461328
C	2.8152650	-0.0548640	-1.1470402
H	4.7119700	-0.5501790	-2.0513742
H	4.5576600	-0.7990340	2.2330848
H	2.1771840	-0.0774380	2.1958338
H	2.3331500	0.1687170	-2.1020132
C	6.2022800	-1.1472380	0.0727848
F	6.9845520	-0.1912630	-0.4517692
F	6.6752590	-1.4243580	1.2918568
F	6.3820650	-2.2393570	-0.6854432
C	2.0183250	4.6045760	-0.6950132

C	2.1835220	4.5221610	0.8355808
C	1.6727810	3.1222680	1.2135678
C	1.7000310	3.1733200	-1.1106682
H	1.1784030	5.2623310	-0.9584242
H	2.9062680	4.9968590	-1.2036142
H	1.6084550	5.3081520	1.3398758
H	3.2286880	4.6477320	1.1421288
H	2.5032890	2.4258680	1.3883618
H	1.0171190	3.0836340	2.0869488
H	2.6162850	2.5729640	-1.2052642
H	1.1147880	3.0703460	-2.0291382
N	0.9362780	2.6212920	0.0292628
H	0.0052540	3.0476940	0.0177318
C	-0.0503730	-1.7851100	-1.5032332
C	0.1050430	-3.2705070	-1.1966962
C	0.8452370	-3.2318510	0.1325208
C	0.1242690	-2.0971030	0.8430788
H	0.8675090	-1.4228630	-1.9949952
H	-0.8714680	-1.5470820	-2.1928332
H	-0.8814800	-3.7465790	-1.0608782
H	0.6291020	-3.8136440	-1.9921412
H	0.8185180	-4.1764760	0.6894408
H	1.9001330	-2.9618600	-0.0323902
H	-0.7909280	-2.4850090	1.3305708
H	0.7081290	-1.6333400	1.6433728
N	-0.2652340	-1.1258370	-0.2004152
C	-4.9102270	-1.4016610	1.4148648
C	-3.3763700	-1.4517690	1.2643038
H	-5.1973750	-0.8355610	2.3104558
H	-5.3227010	-2.4132890	1.5209938
H	-2.8187300	-1.0662420	2.1267778
H	-3.0069830	-2.4598030	1.0329568
C	-5.1222870	0.6500960	0.2296648
H	-5.5124400	1.0948080	-0.6954942
H	-5.6010950	1.1710670	1.0686618
C	-3.5914270	0.7860060	0.3087908
H	-3.1525530	1.4226520	-0.4670922
H	-3.2163120	1.1311250	1.2780928
C	-3.5397250	-1.1740640	-1.1564302
H	-3.2821270	-0.4611050	-1.9497462
H	-2.9787450	-2.1000520	-1.3381102
C	-5.0520820	-1.4053540	-0.9643462

H	-5.6147760	-1.0070310	-1.8179812
H	-5.2825180	-2.4768550	-0.8924292
N	-5.5241310	-0.7568030	0.2566068
N	-3.0091750	-0.5828450	0.1075548
H	-1.9351960	-0.5754150	0.0284518
Br	-1.0680180	1.3787110	-2.0508722

TSb3

Ni	0.3281836	0.5361212	-0.1267351
Br	-0.7520544	0.8001012	2.2017929
C	4.1590766	-0.4567088	-1.1631741
C	4.7894806	-0.6412658	0.0667409
C	4.0419796	-0.6436308	1.2405559
C	2.6625346	-0.4668768	1.1881279
C	2.0345956	-0.2943088	-0.0427021
C	2.7807286	-0.2927658	-1.2217961
H	4.7537586	-0.4421238	-2.0764691
H	4.5387926	-0.7738038	2.1996539
H	2.0857026	-0.4251098	2.1122529
H	2.2893406	-0.1346958	-2.1833681
C	6.2718656	-0.8176358	0.0813669
F	6.8993566	0.2507252	-0.4363411
F	6.7544016	-1.0030818	1.3144699
F	6.6511316	-1.8704608	-0.6594631
C	2.3246556	4.3550192	-0.6631821
C	2.2478786	4.2798922	0.8739809
C	1.8622936	2.8318652	1.1487419
C	1.6673316	3.0533132	-1.1531781
H	1.8019496	5.2396872	-1.0466531
H	3.3609196	4.4212512	-1.0155851
H	1.4653906	4.9514432	1.2551099
H	3.1846426	4.5644092	1.3667689
H	2.7403676	2.1701662	1.1044189
H	1.3433056	2.6534712	2.0954819
H	2.4226826	2.3237082	-1.4776901
H	0.9478736	3.1693472	-1.9676371
N	0.9845736	2.4608172	0.0201219
H	0.0859406	2.9326222	0.1487169
C	0.1903916	-2.0817118	-1.4793421
C	0.1267766	-3.5557628	-1.0748611
C	0.7296026	-3.5378478	0.3234579
C	0.1345316	-2.2575058	0.8873849

H	1.1389746	-1.8823628	-2.0056441
H	-0.6076514	-1.7774358	-2.1714961
H	-0.9183734	-3.9015918	-1.0253261
H	0.6543966	-4.2071368	-1.7814101
H	0.4994786	-4.4283658	0.9210449
H	1.8245396	-3.4352768	0.2632159
H	-0.9013974	-2.4433188	1.2449419
H	0.6703606	-1.8546338	1.7527049
N	0.1053046	-1.3217988	-0.2309391
C	-5.4698014	-0.7808318	1.1669259
C	-4.0063374	-0.7027858	1.6519309
H	-6.0877454	-0.0215788	1.6639949
H	-5.9040464	-1.7606498	1.4025679
H	-3.8520274	-0.0300848	2.5036269
H	-3.5788434	-1.6782828	1.9160129
C	-5.1452494	0.8148692	-0.5743541
H	-5.1061174	0.9259392	-1.6658601
H	-5.9146424	1.5023862	-0.2006391
C	-3.7741534	1.1318552	0.0518099
H	-3.0472724	1.5538352	-0.6549041
H	-3.8312694	1.7795702	0.9351989
C	-3.1743324	-1.1526968	-0.6111731
H	-2.6239794	-0.6559078	-1.4212541
H	-2.5860184	-2.0147668	-0.2742131
C	-4.6402234	-1.4836028	-0.9515541
H	-4.8060154	-1.4149888	-2.0338641
H	-4.9035354	-2.5044798	-0.6436421
N	-5.5494524	-0.5593898	-0.2740291
N	-3.2005144	-0.1716338	0.5166519
H	-2.2273184	0.0205522	0.8743739
Br	-0.9467204	1.1559292	-2.1856651

b5

Ni	1.1687542	0.2822145	0.1708963
C	3.9040253	1.1458295	-1.4997677
C	3.9079553	1.9231285	-0.1618657
C	2.6603993	2.7962645	-0.2373547
C	2.5911103	1.5506285	-2.1752707
H	4.7696203	1.3862555	-2.1283037
H	3.9184013	0.0615135	-1.3274377
H	4.8202413	2.5108375	-0.0072697
H	3.8071373	1.2328945	0.6891953

H	2.2076013	3.0252345	0.7326343
H	2.8775653	3.7382365	-0.7737427
H	2.1125803	0.7393325	-2.7328077
H	2.7530833	2.4100925	-2.8505667
N	1.7557743	1.9445675	-1.0291007
H	0.9153582	2.4424785	-1.3140467
H	-1.1673158	-0.3439285	-0.7466127
Br	0.2119242	1.6895455	1.9775823
C	-2.2235667	1.4571255	-0.6743447
C	-3.6987998	1.8601325	-0.4782987
H	-1.5414678	1.8820715	0.0772833
H	-1.8338218	1.6747125	-1.6776017
H	-3.7752747	2.6924075	0.2322973
H	-4.1542587	2.1891445	-1.4219547
C	-2.4606137	-0.3944375	0.9154643
H	-2.4396368	-1.4912475	0.9652513
H	-1.6500388	0.0207495	1.5303433
C	-3.8373517	0.2158415	1.2416823
H	-4.4989678	-0.5268095	1.7054553
H	-3.7245397	1.0479855	1.9494113
C	-4.5205867	-0.3200075	-0.9785067
H	-5.0447757	-1.1840995	-0.5495907
H	-5.1133418	0.0299345	-1.8332397
C	-3.0941337	-0.7057115	-1.4260567
H	-2.8838187	-1.7808815	-1.3738467
H	-2.8442227	-0.3689445	-2.4395977
N	-4.4787397	0.7328255	0.0322023
N	-2.1487837	-0.0260745	-0.4985757
Br	0.4764832	-1.1725875	-1.7549327
C	1.9334152	-3.3203245	0.6349063
C	0.5568083	-3.1023475	1.2935583
C	0.7868963	-1.9578755	2.2702663
C	2.7884993	-2.1353625	1.1037163
H	2.3909003	-4.2717265	0.9314193
H	1.8315822	-3.3163995	-0.4558037
H	0.1699493	-3.9985275	1.7927083
H	-0.1625808	-2.7965335	0.5212893
H	-0.0947248	-1.3418875	2.4837523
H	1.1716383	-2.3449885	3.2320173
H	3.3962423	-1.6959465	0.3021213
H	3.4664113	-2.4448635	1.9183573
N	1.8102573	-1.1479235	1.5927143

| H | 2.2307483 | -0.4925485 | 2.2499703 |

TSb4

Ni	-1.2201848	-0.2802087	0.6111307
C	-3.7768688	-2.3476177	-0.6377083
C	-3.6993278	-1.0297317	-1.4391853
C	-3.9062078	0.0572463	-0.3905923
C	-3.8474358	-1.9112857	0.8281767
H	-4.6477108	-2.9539847	-0.9132583
H	-2.8772418	-2.9534967	-0.7972643
H	-4.4380378	-0.9691297	-2.2469853
H	-2.7015938	-0.9165987	-1.8864503
H	-3.4163948	1.0099533	-0.6299223
H	-4.9846888	0.2400193	-0.2279243
H	-3.2540708	-2.5468037	1.4932937
H	-4.8935928	-1.8891307	1.1813067
N	-3.2903728	-0.5461107	0.8025737
H	-3.5286838	-0.0322707	1.6478907
C	-1.3364328	3.3666963	0.6486707
C	-1.3111768	3.1768043	-0.8799883
C	-0.3824538	1.9549723	-1.0801473
C	-0.2474008	2.4009883	1.1305367
H	-1.1697018	4.4082263	0.9562437
H	-2.3053018	3.0470263	1.0606127
H	-0.9333518	4.0665373	-1.4025063
H	-2.3176768	2.9803553	-1.2752523
H	-0.7385858	1.2713493	-1.8665573
H	0.6189072	2.3335533	-1.4147553
H	-0.3840608	2.0699613	2.1699767
H	0.7365372	2.9369053	1.0843887
N	-0.2961668	1.2921983	0.2036727
H	1.0537262	-0.8082387	0.8488927
Br	-0.5323508	-2.5814557	1.0548197
C	2.8501112	-1.8317217	1.1907287
C	4.2256252	-1.8675937	0.4937557
H	2.9065802	-1.5580757	2.2513937
H	2.2674782	-2.7559407	1.1129917
H	5.0362582	-1.8648347	1.2334377
H	4.3355262	-2.7796967	-0.1073473
C	2.6405642	0.5760983	0.7850257
H	2.0234602	1.2844303	0.2223877
H	2.4950572	0.7888033	1.8512397

C	4.1207502	0.5075773	0.3585237
H	4.3806832	1.3714813	-0.2660623
H	4.7884222	0.5230503	1.2303577
C	3.4300762	-0.8217037	-1.4938283
H	3.5028882	0.0946783	-2.0943433
H	3.7204432	-1.6600077	-2.1397883
C	2.0008392	-1.0180947	-0.9554843
H	1.2598452	-0.3170277	-1.3561693
H	1.6046022	-2.0330437	-1.0751993
N	4.3893372	-0.7176607	-0.3935333
N	2.0493542	-0.7674487	0.5182247

b6

Ni	-1.05282800	0.26482100	0.31709700
C	-3.60211500	-1.80046900	-0.93797500
C	-3.52486800	-0.48291000	-1.74043800
C	-3.73408400	0.60513600	-0.69314100
C	-3.68375300	-1.36242100	0.52656500
H	-4.46789500	-2.41165900	-1.21858200
H	-2.69804500	-2.40174100	-1.09004900
H	-4.26280800	-0.42369700	-2.54905600
H	-2.52681800	-0.36932400	-2.18680900
H	-3.24175400	1.55695100	-0.93094000
H	-4.81289000	0.78980700	-0.53477900
H	-3.09713600	-1.99815200	1.19724500
H	-4.73266300	-1.33803600	0.87140500
N	-3.12405500	0.00150800	0.50293100
H	-3.36496300	0.51623200	1.34695100
C	-1.16447200	3.92096500	0.34642500
C	-1.13468400	3.73021100	-1.18200500
C	-0.21507300	2.50052800	-1.37791200
C	-0.08236300	2.94956700	0.83234700
H	-0.99342400	4.96173500	0.65420300
H	-2.13642600	3.60639500	0.75494900
H	-0.74717200	4.61653400	-1.70316200
H	-2.14117400	3.54237400	-1.58130700
H	-0.57492000	1.81794700	-2.16355900
H	0.78988600	2.87047400	-1.71179700
H	-0.22294100	2.62102100	1.87205000
H	0.90479900	3.47978700	0.78733400
N	-0.13618000	1.83992100	-0.09283900
H	1.27841863	-1.20079678	0.65835922

Br	-0.36534800	-2.03641400	0.76452800
C	3.30056155	-1.73984004	0.62478262
C	4.55141926	-1.21363928	-0.10846258
H	3.40622832	-1.74638003	1.71650489
H	2.96650239	-2.73569384	0.31404899
H	5.41261406	-1.17519573	0.57060316
H	4.82277419	-1.87428997	-0.94227845
C	2.44288182	0.53802194	0.91680597
H	1.60390960	1.16736193	0.60170773
H	2.37408502	0.42011518	2.00521800
C	3.83142163	0.99314248	0.42428919
H	3.78778654	2.02439918	0.05195394
H	4.57032111	0.97071411	1.23652682
C	3.29249478	0.04402480	-1.69360719
H	3.06225015	1.06667933	-2.02057588
H	3.70954090	-0.48963492	-2.55702905
C	2.03015160	-0.66654843	-1.17066102
H	1.09591558	-0.11521892	-1.32716511
H	1.88984401	-1.68440145	-1.55260683
N	4.31359184	0.12362520	-0.64821495
N	2.18487348	-0.80061383	0.31056994

TSb5

Ni	-1.4968103	-1.1706218	-0.2673798
C	-4.6698993	0.4789012	-0.9281728
C	-4.9662873	0.6225922	0.5660412
C	-4.1907373	-0.5276398	1.2297132
C	-4.4376503	-1.0106938	-1.0836128
H	-5.4820253	0.8471192	-1.5653608
H	-3.7481213	1.0050382	-1.2132098
H	-6.0432353	0.5092012	0.7515192
H	-4.6741113	1.6026562	0.9635282
H	-3.3609633	-0.1767448	1.8522982
H	-4.8535423	-1.1382618	1.8605132
H	-3.8857753	-1.2711418	-1.9943728
H	-5.3969963	-1.5584138	-1.0776318
N	-3.6357783	-1.3376218	0.1161292
H	-3.7162423	-2.3270518	0.3334052
C	-0.5311973	1.0184002	3.1805112
C	-1.5702013	1.8995122	2.4979932
C	-1.4383233	1.4787752	1.0303082
C	-0.6689113	-0.2851068	2.3929142

H	0.4766207	1.4428752	3.0339452
H	-0.6851113	0.9009182	4.2608472
H	-1.4191513	2.9753102	2.6583532
H	-2.5732573	1.6499682	2.8795612
H	-2.3839183	1.6054742	0.4752952
H	-0.7276793	2.1708362	0.5171172
H	-1.4658653	-0.9173578	2.8548892
H	0.2530407	-0.8988148	2.4413572
N	-0.9681023	0.1056222	1.0327082
H	0.4730537	0.8841502	-1.5585698
Br	-1.2594373	0.2531272	-2.4875148
C	2.3705687	0.8233262	-2.4094558
C	3.7962587	1.1937972	-1.9551498
H	2.2129047	-0.2508158	-2.5515878
H	2.0542187	1.3330212	-3.3282808
H	4.3370757	0.3053852	-1.6023138
H	4.3685587	1.6234602	-2.7872298
C	1.9170067	0.7379272	-0.0064538
H	1.0766217	0.8300282	0.6947632
H	2.0798497	-0.3369348	-0.1465068
C	3.2105737	1.4919112	0.3374732
H	3.0368677	2.2602682	1.1035802
H	3.9622197	0.7968602	0.7295562
C	2.8522867	3.2525422	-1.2248808
H	2.9406057	4.0557392	-0.4824258
H	3.1894197	3.6594062	-2.1877998
C	1.3948237	2.7540392	-1.3098338
H	0.7898967	3.0410242	-0.4413538
H	0.8620247	3.0749272	-2.2134428
N	3.7460247	2.1577352	-0.8550478
N	1.4439497	1.2635982	-1.3265818
C	2.5325427	-2.8473978	0.0364262
C	1.5560547	-3.0835568	1.0012302
C	0.2117477	-3.0803088	0.6510532
C	-0.1628603	-2.7167168	-0.6559138
C	0.8275657	-2.5220328	-1.6463008
C	2.1576737	-2.5881258	-1.2912918
H	1.8464657	-3.3009058	2.0269792
H	-0.5532233	-3.3230858	1.3868122
H	0.5208847	-2.3121528	-2.6690418
H	2.9334267	-2.4453838	-2.0460368
C	3.9806227	-2.8174038	0.3731202

F	4.2280317	-3.1497258	1.6404192
F	4.4988407	-1.5756148	0.1855752
F	4.7015247	-3.6282408	-0.4115218
Br	-1.8744403	-3.5075988	-1.3716578

b7

Ni	-1.6945186	-1.6278293	-0.0840827
C	-4.6792326	0.4816847	-1.2889167
C	-5.2716746	0.4724697	0.1221943
C	-4.5600376	-0.6831983	0.8437313
C	-4.2848696	-0.9620653	-1.5201447
H	-5.3877266	0.8434907	-2.0425647
H	-3.7769396	1.1041207	-1.3652627
H	-6.3515356	0.2770737	0.0762993
H	-5.1444896	1.4290747	0.6465003
H	-3.8784536	-0.3391403	1.6319623
H	-5.2815766	-1.3598763	1.3217543
H	-3.5026876	-1.0801083	-2.2765057
H	-5.1536666	-1.5741583	-1.8113297
N	-3.7800926	-1.4134403	-0.1904187
H	-3.9576976	-2.4142553	-0.1134417
C	-0.8959866	0.9475307	3.1164403
C	-1.9264276	1.7322647	2.3147223
C	-1.7817566	1.1227937	0.9251493
C	-0.9938246	-0.4473263	2.4999433
H	0.1097114	1.3664547	2.9501623
H	-1.0731156	0.9501047	4.1976963
H	-1.7648066	2.8166487	2.3241473
H	-2.9380046	1.5451367	2.7071953
H	-2.6666826	1.2128277	0.2873043
H	-0.9800946	1.6137127	0.3426423
H	-1.7374896	-1.0724163	3.0298013
H	-0.0480326	-1.0067373	2.5311023
N	-1.4308196	-0.2723953	1.1258783
H	0.6105434	0.9105767	-1.3226687
Br	-1.1242996	0.5885867	-2.3549617
C	2.5083464	0.9953477	-2.1610377
C	3.9140704	1.4299017	-1.7107747
H	2.4215554	-0.0759393	-2.3630897
H	2.1263674	1.5353127	-3.0357327
H	4.5190454	0.5555287	-1.4347437
H	4.4380954	1.9573847	-2.5176137

C	2.0846984	0.7383447	0.2438143
H	1.2787634	0.8266917	0.9837913
H	2.2727604	-0.3259763	0.0718753
C	3.3669584	1.5161817	0.6044883
H	3.2010954	2.2011847	1.4470663
H	4.1596954	0.8155977	0.8948703
C	2.8546394	3.3670497	-0.8085707
H	2.9059934	4.1134297	-0.0072227
H	3.1478834	3.8682727	-1.7400207
C	1.4301504	2.7842247	-0.9178657
H	0.8211114	2.9719597	-0.0233977
H	0.8558594	3.1178817	-1.7906847
N	3.8235684	2.3053747	-0.5398157
N	1.5732004	1.3062187	-1.0377637
C	2.8521114	-2.8503043	-0.1000127
C	2.0886214	-3.0622413	1.0417883
C	0.7234794	-2.7746233	1.0226623
C	0.1210614	-2.2021843	-0.0983747
C	0.8844094	-2.0757203	-1.2682527
C	2.2321244	-2.4043693	-1.2707457
H	2.5566224	-3.4560723	1.9423633
H	0.1272404	-3.0103983	1.9048863
H	0.4117374	-1.6926383	-2.1731087
H	2.8235754	-2.3077203	-2.1833877
C	4.3357994	-2.9440093	-0.0739017
F	4.8038334	-3.6035203	0.9876223
F	4.8865554	-1.6997563	-0.0272277
F	4.8384214	-3.5220043	-1.1698877
Br	-2.0431676	-3.5600153	-1.3163227

TSb6

Ni	-1.3602719	-0.2298885	-0.5492716
C	-4.4680249	1.9139545	0.4425404
C	-4.6534929	0.4695625	0.9304934
C	-4.4494419	-0.3715265	-0.3187696
C	-3.7397479	1.7985425	-0.9049356
H	-5.4329819	2.4201945	0.3127984
H	-3.8793449	2.4956375	1.1602844
H	-5.6303199	0.2918715	1.3951934
H	-3.8756889	0.2255525	1.6652964
H	-4.1051569	-1.3915815	-0.1016116
H	-5.3784969	-0.4228405	-0.9139026

H	-2.8220399	2.3939375	-0.9616266
H	-4.3957929	2.1129815	-1.7319476
N	-3.4019039	0.3617385	-1.0459816
H	-3.3898119	0.1069545	-2.0320766
C	-1.7877149	-4.3319495	-0.3034746
C	-2.3700759	-3.9981665	1.0650444
C	-1.8398989	-2.5844235	1.3089064
C	-1.9688289	-3.0105985	-1.0393396
H	-0.7121129	-4.5507125	-0.2105356
H	-2.2718509	-5.1809325	-0.8006556
H	-2.0786309	-4.6988055	1.8565014
H	-3.4698179	-3.9881375	1.0103654
H	-2.4825149	-1.9936365	1.9800924
H	-0.8437259	-2.6380875	1.7863524
H	-2.9866129	-2.9385135	-1.4768486
H	-1.2667429	-2.8890505	-1.8772356
N	-1.7888579	-1.9912535	-0.0154896
H	0.7586611	1.4942185	0.3662274
Br	-1.1846719	1.1869455	1.4912784
C	1.1963401	3.4234035	-0.2089776
C	2.4769331	4.2396775	-0.4670606
H	0.5674051	3.2574235	-1.0919826
H	0.5656931	3.8309785	0.5899174
H	2.6169101	4.4192115	-1.5407036
H	2.4181321	5.2195345	0.0236884
C	2.5632481	1.4519875	-0.7516236
H	2.7402331	0.4172475	-0.4375796
H	2.0147991	1.4337125	-1.7005786
C	3.8438221	2.3091755	-0.7519966
H	4.6849311	1.7491855	-0.3224976
H	4.1237111	2.5855695	-1.7760796
C	3.4486271	3.1774735	1.4316604
H	4.3812561	2.7639185	1.8351224
H	3.2305261	4.0984325	1.9881064
C	2.2969341	2.1607015	1.5780514
H	2.6368151	1.1483005	1.8288864
H	1.5278031	2.4497655	2.3033424
N	3.6551881	3.5308035	0.0301314
N	1.6285161	2.0634455	0.2471604
C	2.9409651	-2.1402335	-0.1906276
C	2.2388931	-2.1681005	-1.3943076
C	0.9101561	-1.7640255	-1.4363506

C	0.2650791	-1.3032055	-0.2828026
C	0.9673981	-1.3125285	0.9281154
C	2.2946881	-1.7229575	0.9721304
H	2.7390431	-2.4864615	-2.3071876
H	0.4000791	-1.7500215	-2.3988526
H	0.4891951	-0.9490575	1.8361684
H	2.8384811	-1.7087215	1.9173304
C	4.4104231	-2.3756855	-0.1547176
F	4.8487451	-3.0876045	-1.1963756
F	4.8018371	-3.0028635	0.9613474
F	5.0813871	-1.2000395	-0.1784706
Br	-0.5682779	1.1795705	-2.3700556

TSc1

C	-2.9348721	-1.1273626	1.3860082
C	-1.5309691	-0.4783196	1.3601422
H	-3.6179571	-0.5805476	2.0508792
H	-2.8837931	-2.1625796	1.7490862
H	-1.5144711	0.4837094	1.8966112
H	-0.7523321	-1.1193676	1.7876782
C	-3.5392681	0.2107064	-0.4841798
H	-4.0541561	0.2006434	-1.4545878
H	-4.1375811	0.8309914	0.1979722
C	-2.0980811	0.7600904	-0.6227468
H	-1.8116821	0.9103384	-1.6746408
H	-1.9662921	1.7217164	-0.1006388
C	-1.2086341	-1.4711396	-0.8134708
H	-0.8256751	-1.2647816	-1.8209118
H	-0.5065931	-2.1711446	-0.3502308
C	-2.6685381	-1.9785756	-0.8220128
H	-3.0984751	-1.9542536	-1.8332808
H	-2.7281501	-3.0167706	-0.4692928
N	-1.1506791	-0.2081336	-0.0424338
N	-3.5102931	-1.1484626	0.0429552
P	2.4811859	-1.9892486	0.0145562
F	1.5010379	-3.2649476	-0.1360378
F	1.3901719	-1.3080656	1.0602342
F	3.2404099	-2.6556056	1.2577262
F	3.5269629	-2.5991146	-1.0321148
F	1.6764339	-1.2481026	-1.2198458
F	3.3919069	-0.6310266	0.1684182
C	2.6638129	2.7501074	0.7178912

C	3.0091319	2.3288144	-0.7109468
C	1.7122259	1.6900304	-1.2006758
C	1.7425029	1.6245724	1.1792172
H	2.1260829	3.7093844	0.7244822
H	3.7947459	1.5652464	-0.7011708
H	3.3336149	3.1609984	-1.3434898
H	1.8291619	0.8624754	-1.9114918
H	0.1635349	0.4734534	-0.0341578
H	2.3089619	0.7477784	1.5383332
H	1.0076189	1.8801574	1.9554552
H	3.5435239	2.8530814	1.3606632
N	1.0714139	1.1847814	-0.0141198
H	1.0240529	2.4284714	-1.6558298

RN·

C	-3.1417897	0.1923711	1.1911632
C	-1.6072557	0.3444011	1.1513972
H	-3.6258297	1.1738371	1.2748912
H	-3.4583787	-0.4029249	2.0575602
H	-1.2662397	1.3678151	0.9607202
H	-1.0950547	-0.0233759	2.0485212
C	-3.1156217	0.2301971	-1.1915118
H	-3.5930877	-0.1835439	-2.0886698
H	-3.4190407	1.2829651	-1.1163528
C	-1.5810997	0.1000451	-1.2811678
H	-1.2421247	-0.5848999	-2.0665568
H	-1.0534687	1.0525791	-1.4033688
C	-1.6017597	-1.8865389	0.1494722
H	-1.0622157	-2.4880399	-0.5864038
H	-1.2800227	-2.2298079	1.1378092
C	-3.1306547	-1.8510829	-0.0334708
H	-3.4253037	-2.3048719	-0.9888638
H	-3.6300427	-2.4178099	0.7624382
N	-1.1155397	-0.4784019	0.0108072
N	-3.6249377	-0.4738289	-0.0164678
P	2.0522443	-2.2246109	0.0260292
F	0.9631073	-3.4242179	0.0643002
F	1.1406153	-1.4176779	1.1676122
F	2.9049273	-2.9048309	1.1940092
F	2.8843803	-2.9586209	-1.1239418
F	1.1170643	-1.4747649	-1.1338188
F	3.0492853	-0.9471769	-0.0125278

C	3.0683993	2.5883011	0.6929572
C	3.3734893	2.0219481	-0.6908828
C	1.9836393	1.6166661	-1.1864778
C	1.9087663	1.6995311	1.1419312
H	2.7359453	3.6349351	0.6199242
H	4.0029923	1.1285581	-0.6047848
H	3.8749433	2.7353551	-1.3549578
H	1.9773543	0.7347281	-1.8433748
H	-0.0769007	-0.4634109	0.0184722
H	2.2831293	0.7487451	1.5622132
H	1.2517533	2.1454301	1.9052832
H	3.9226333	2.5557071	1.3786262
N	1.1478013	1.3500811	-0.0353858
H	1.5038993	2.4362391	-1.7571538

TSc1'

P	2.9219846	-1.5697600	0.0196870
F	3.6486996	-2.0323180	1.3673090
F	2.0626616	-0.4437420	0.8703750
F	4.0524126	-0.4392240	-0.2618070
F	3.7118926	-2.6473140	-0.8575180
F	1.6987486	-2.6224810	0.2754770
F	2.1317486	-1.0468270	-1.3471570
C	1.3621706	2.7959790	1.0445270
C	0.2473816	2.9621960	0.0077450
C	0.5611156	1.8274060	-0.9480660
C	2.5564186	2.3511640	0.2038440
H	1.1019696	1.9885670	1.7441440
H	0.3201076	3.9383810	-0.4993840
H	-0.7586694	2.8984360	0.4438060
H	0.1081566	1.8178970	-1.9521750
H	2.3750696	0.8626890	-1.3385560
H	3.1356946	3.2143690	-0.1645150
H	3.2410386	1.6668190	0.7133030
H	1.5603686	3.7033300	1.6244490
N	1.9329706	1.6840250	-0.9278930
C	-0.8806094	-0.7492000	1.2150940
C	-1.8694184	-1.9304070	1.3438860
H	0.1599676	-1.0431610	1.3711710
H	-1.1201334	0.0792150	1.8973080
H	-1.3210894	-2.8818700	1.3511170
H	-2.4402854	-1.8667540	2.2796880

C	-0.8394764	-1.3270670	-1.1450720
H	-0.7522274	-0.8778260	-2.1441840
H	0.1055306	-1.8221120	-0.9128060
C	-2.0561424	-2.2669320	-1.0036290
H	-2.7439674	-2.1731920	-1.8555480
H	-1.7255144	-3.3122990	-0.9608420
C	-3.4028974	-0.6349700	0.0657720
H	-4.1997694	-0.6859680	-0.6879770
H	-3.8708984	-0.3598520	1.0208140
C	-2.3296024	0.4046050	-0.3406160
H	-2.4145024	0.7098750	-1.3933260
H	-2.3691074	1.3104460	0.2786160
N	-0.9987194	-0.2184340	-0.1664880
N	-2.8008834	-1.9533990	0.2152970
H	-0.1021954	0.6897090	-0.4458690

˙RᵅN

P	2.6867263	-1.7786095	-0.0160582
F	3.4084683	-2.3552005	1.2862618
F	1.8372953	-0.7079785	0.9398458
F	3.8313563	-0.6519225	-0.2112442
F	3.4450603	-2.7918715	-0.9883092
F	1.4546883	-2.8478285	0.1716878
F	1.8671513	-1.1371865	-1.3007262
C	1.2545413	2.8957025	1.0096798
C	0.5166953	3.1663675	-0.3065152
C	0.9830263	2.0074535	-1.1357652
C	2.5948353	2.3213975	0.5428468
H	0.7126743	2.1269595	1.5866788
H	0.8454803	4.1356075	-0.7283422
H	-0.5748347	3.2319655	-0.1893932
H	0.7315033	1.8909315	-2.1922342
H	2.7255363	0.8648075	-1.0013242
H	3.3513613	3.1171015	0.4426268
H	2.9961443	1.5598325	1.2216758
H	1.3631823	3.7793835	1.6488938
N	2.2919993	1.7500885	-0.7626832
C	-0.9618377	-1.3694735	1.2393118
C	-2.3674717	-1.9961735	1.1584038
H	-0.1493917	-2.0962345	1.3004448
H	-0.8483247	-0.6507645	2.0602078
H	-2.3001927	-3.0832795	1.0229358

H	-2.9270067	-1.8166865	2.0852128
C	-0.9893457	-1.4837065	-1.2172862
H	-0.6631917	-0.9209515	-2.0993672
H	-0.3164217	-2.3364195	-1.0932272
C	-2.4858887	-1.8491005	-1.2185402
H	-3.0157367	-1.3538075	-2.0430452
H	-2.6152857	-2.9304345	-1.3508452
C	-3.1170387	0.0099435	0.1247708
H	-3.7955787	0.4190445	-0.6345712
H	-3.5171687	0.2937915	1.1070638
C	-1.6914857	0.5662745	-0.0719912
H	-1.5363677	1.0591565	-1.0382862
H	-1.3810497	1.2671755	0.7118338
N	-0.7535077	-0.5958245	-0.0302902
N	-3.1222147	-1.4455185	0.0343758
H	0.2316163	-0.2640105	-0.0647122

TSc1"

C	-0.2764834	-2.8869300	0.7684808
C	-0.2648354	-1.4135080	1.2683078
H	-1.3026014	-3.1690280	0.5070238
H	0.0826646	-3.5639420	1.5542118
H	-1.2691854	-0.9920190	1.3372958
H	0.2532726	-1.2984610	2.2294408
C	0.0088306	-2.2390290	-1.4960832
H	0.6341326	-2.3717070	-2.3885122
H	-0.9997644	-2.6035610	-1.7219962
C	-0.0677194	-0.7372540	-1.0914702
H	0.5346996	-0.0803300	-1.7310302
H	-1.0977854	-0.3804630	-1.0693772
C	1.9009946	-1.0476550	0.2637548
H	2.4343036	-0.4284900	-0.4686462
H	2.3279556	-0.8685150	1.2592018
C	1.9079546	-2.5705420	-0.1118842
H	2.5500386	-2.7368850	-0.9861252
H	2.3115256	-3.1627060	0.7195358
N	0.4944146	-0.6265740	0.2730388
N	0.5670446	-3.0339860	-0.4103622
P	-3.6310704	0.2110590	-0.0175802
F	-4.2642224	-0.3033860	1.3660758
F	-2.2886514	0.7269760	0.8168608
F	-2.8820024	-1.2538850	-0.1972972

F	-4.8795934	-0.3205290	-0.8650682
F	-4.2832664	1.6652350	0.1592608
F	-2.8805764	0.7050920	-1.3938102
N	1.1146196	2.4396740	-1.2047612
H	1.0471596	2.9596620	-2.0756202
C	2.1270786	2.9957920	-0.3085182
H	2.0630636	4.0985220	-0.2325492
H	3.1391726	2.7438190	-0.6496072
C	1.7724626	2.3777110	1.0555858
H	1.8747106	3.0998550	1.8775228
H	2.4404956	1.5391990	1.3108448
C	0.3331246	1.9365100	0.8845168
H	-0.3579214	1.9683570	1.7309468
H	0.3956836	0.6625800	0.6254558
C	-0.1251444	2.4929550	-0.4321362
H	-0.4932204	3.5300450	-0.2628182
H	-0.9513594	1.9363410	-0.8921082

•R$^\beta$N

C	2.0800909	-1.8304049	1.3897261
C	0.8662459	-0.8891069	1.2727321
H	1.7569509	-2.8152339	1.7483341
H	2.8252479	-1.4486329	2.1012571
H	-0.0876931	-1.4173109	1.2662931
H	0.8326639	-0.1115249	2.0464471
C	1.7230099	-2.3453449	-0.9095789
H	2.2234879	-2.6695249	-1.8308289
H	1.1433489	-3.1941549	-0.5254389
C	0.7899309	-1.1555639	-1.1810419
H	1.0504739	-0.6050269	-2.0952859
H	-0.2678111	-1.4227369	-1.2195419
C	2.3279379	0.4313181	-0.1654979
H	2.3172789	1.0937671	-1.0401439
H	2.4812509	1.0478481	0.7299061
C	3.3508709	-0.7205929	-0.2807869
H	3.7280869	-0.8089879	-1.3083389
H	4.2143249	-0.5323059	0.3701841
N	0.9775299	-0.1876009	-0.0490459
N	2.7332659	-1.9875199	0.0904771
P	-2.7948861	-1.6324339	0.0284881
F	-3.1402541	-1.8524849	1.5813931
F	-1.7821631	-0.3853949	0.4592701

F	-1.5038721	-2.6477049	0.1779991
F	-3.7257991	-2.8516369	-0.4205179
F	-3.9944211	-0.5699329	-0.1375699
F	-2.3490591	-1.3685809	-1.5299689
N	-0.4504741	2.1098501	-0.7850019
H	0.0799969	2.4845301	-1.5698209
C	-0.4024841	3.0393021	0.3598411
H	-0.4928611	4.0905511	0.0349831
H	0.5502599	2.9352091	0.9019201
C	-1.6234041	2.6368001	1.1810361
H	-1.9648381	3.4451531	1.8427641
H	-1.3896101	1.7703631	1.8287591
C	-2.5982221	2.2510561	0.1250321
H	-3.5952101	1.8744931	0.3232101
H	0.2479979	0.5794121	-0.1767319
C	-1.8879061	1.9803721	-1.1521359
H	-2.1539561	2.7074011	-1.9445889
H	-2.0953281	0.9723151	-1.5381869
A			
C	-1.7952526	1.4211484	-0.2268984
C	-0.2456366	1.3571394	-0.2179284
H	-2.2266676	1.7462344	-1.1816584
H	-2.2251626	2.0281134	0.5793996
H	0.1814134	1.7011154	-1.1670444
H	0.1830734	1.9800734	0.5755576
C	-1.7988506	-0.9062006	-1.1157984
H	-2.2311586	-1.8950096	-0.9190024
H	-2.2301856	-0.5108746	-2.0437154
C	-0.2490326	-0.8684716	-1.0681734
H	0.1772864	-1.8629246	-0.8924204
H	0.1778914	-0.4931356	-2.0053564
C	-0.2469346	-0.4922436	1.2842976
H	0.1789524	-1.4921926	1.4266036
H	0.1820474	0.1561854	2.0569296
C	-1.7966616	-0.5122456	1.3441466
H	-2.2293656	-1.5127666	1.4669456
H	-2.2262226	0.1534684	2.1028756
N	0.1604764	-0.0016456	-0.0008774
N	-2.2802226	0.0014684	0.0007896
P	3.4248864	-0.0000296	-0.0000354
F	4.3356294	1.3142904	-0.2133134

F	2.4686704	0.8462324	1.0360606
F	2.4694534	0.4743094	-1.2513024
F	4.3366484	-0.8418036	-1.0308264
F	4.3354634	-0.4719506	1.2451996
F	2.4696454	-1.3209686	0.2140786
H	-3.3001826	0.0026854	0.0014676

B

C	1.0401602	0.4665153	1.3216596
C	-0.5010738	0.3470473	1.3352996
H	1.4921922	-0.1512577	2.1085986
H	1.3596902	1.5025543	1.4962406
H	-0.8740248	-0.4274067	2.0179926
H	-1.0180108	1.2815913	1.5889316
C	1.1246652	-1.3248997	-0.2500164
H	1.6048092	-1.6691837	-1.1753344
H	1.4789152	-1.9733047	0.5624056
C	-0.4169528	-1.3724967	-0.3711774
H	-0.7666568	-1.6005147	-1.3863454
H	-0.8914788	-2.0911867	0.3093876
C	-0.4693488	0.9661573	-1.0080094
H	-0.9220348	0.7078713	-1.9739614
H	-0.8861988	1.9339033	-0.7001574
C	1.0765692	0.9330443	-1.0161944
H	1.4607692	0.5768183	-1.9813224
H	1.4948992	1.9339853	-0.8479104
N	-0.9345658	-0.0337427	-0.0251034
N	1.5736782	0.0385763	0.0287246
H	-2.1439108	-0.0471377	-0.0359814
Br	-3.8820908	0.0030673	0.0022736

c1

Ni	-0.1565816	0.3438015	-0.4478461
Br	-1.0957166	1.8861825	1.1595589
C	-4.0073276	1.1647145	-1.0209641
C	-4.4089916	-0.1352695	-0.3321541
C	-3.0717956	-0.6353435	0.1968309
C	-2.7058816	0.7930935	-1.7174281
H	-4.7604956	1.5455715	-1.7196631
H	-3.8061976	1.9385825	-0.2681491
H	-4.8266556	-0.8446555	-1.0625851
H	-5.1483166	0.0030665	0.4650649

H	-2.8172846	-0.1145625	1.1277079
H	-3.0263096	-1.7183315	0.3633519
H	-2.0215196	1.6402735	-1.8395941
H	-2.8813026	0.3564235	-2.7104841
N	-2.0799606	-0.2541635	-0.8432991
H	-1.8767586	-1.0661145	-1.4274961
C	1.8226984	-2.3206865	2.2413319
C	1.1307434	-3.2114555	1.2160409
C	-0.1895456	-2.4897545	0.9785529
C	1.4972894	-0.9368445	1.7012339
H	1.3758374	-2.4624515	3.2370629
H	2.9006984	-2.5003405	2.3254499
H	0.9903344	-4.2469785	1.5454529
H	1.7076204	-3.2261375	0.2795479
H	-0.5842666	-2.6717945	-0.0272801
H	-0.9447116	-2.7917345	1.7197619
H	2.1852084	-0.6844675	0.8813109
H	1.5398164	-0.1249055	2.4365889
N	0.1178734	-1.0426995	1.1556719
H	-0.5264706	-0.6228445	1.8249309
Br	0.3887714	-1.2690945	-2.1920011
N	1.3168474	1.3674135	-0.7888291
C	1.7166034	2.5241315	0.0126539
H	0.9111674	3.2641015	0.0368889
C	3.0149524	3.0061565	-0.6156001
H	3.5772924	3.6773045	0.0440679
H	2.8031114	3.5422115	-1.5520431
C	3.7084944	1.6854805	-0.9026371
H	4.1419214	1.2846415	0.0270999
H	4.5131124	1.7473665	-1.6444011
C	2.5502194	0.8080145	-1.3665381
H	2.6827454	-0.2489045	-1.0977361
H	2.4366454	0.8112675	-2.4625321
H	1.9060874	2.2297365	1.0630989

c2

Ni	-0.5762015	0.1600154	-0.7031251
C	1.9545515	2.3791334	-0.1693561
C	1.3567585	2.3119584	1.2529169
C	-0.1115755	2.6863304	1.0686059
C	0.7669405	2.7114304	-1.0763691
H	2.7441585	3.1336464	-0.2583981

H	2.3869955	1.4089914	-0.4445821
H	1.8581415	2.9795374	1.9625679
H	1.4411455	1.2917864	1.6512949
H	-0.7874555	2.2027734	1.7856729
H	-0.2483555	3.7782934	1.1593499
H	0.7939435	2.2137824	-2.0547181
H	0.6986225	3.7989054	-1.2495611
N	-0.3980165	2.2438774	-0.3010101
H	-1.2697455	2.6223734	-0.6746831
C	-3.1108845	-1.9831546	0.1545199
C	-3.8058505	-0.7065156	0.6590279
C	-2.7213645	0.0714854	1.4160839
C	-1.7899795	-2.0201426	0.9057149
H	-3.7010225	-2.8905906	0.3240059
H	-2.9195705	-1.8917266	-0.9220251
H	-4.6508035	-0.9275386	1.3219209
H	-4.1787825	-0.1222946	-0.1891441
H	-2.6878825	1.1320914	1.1361339
H	-2.8756155	0.0083064	2.5057709
H	-0.9922925	-2.5418716	0.3654669
H	-1.9126975	-2.4797756	1.9020209
N	-1.4459165	-0.5870076	1.0470089
H	-0.7456665	-0.4598756	1.7777059
Br	-2.2975475	0.6013874	-2.3229621
N	0.9406435	-0.8829776	-0.7410901
C	1.7080805	-0.9589586	-1.9772751
H	1.0390705	-1.0711946	-2.8430971
C	2.6619755	-2.1316656	-1.7784331
H	3.5280485	-2.1103436	-2.4510171
H	2.1266485	-3.0789396	-1.9392651
C	3.0243555	-1.9724206	-0.3065311
H	3.7691175	-1.1689406	-0.1956671
H	3.4418335	-2.8766066	0.1527539
C	1.6917375	-1.5405296	0.3141689
H	1.8478725	-0.8760446	1.1860969
H	1.1454635	-2.4233776	0.7017739
H	2.3011235	-0.0336116	-2.1522721

TSc2

Ni	-0.8597719	0.1082457	0.2552444
Br	-1.4504979	-0.5139603	2.5132254
C	1.0406261	-3.3611173	-1.0277446

C	1.9737511	-3.0819033	0.1431994
C	1.2282491	-1.9608593	0.8551104
C	0.5977441	-1.9518373	-1.4186226
H	1.5091681	-3.9050753	-1.8576036
H	0.1787381	-3.9539773	-0.6824706
H	2.9460061	-2.7192883	-0.2219646
H	2.1541461	-3.9541273	0.7828544
H	0.4462971	-2.3685613	1.5174424
H	1.8694081	-1.3332793	1.4955824
H	-0.3922549	-1.9376403	-1.9005116
H	1.2993181	-1.5529503	-2.1758486
N	0.6401291	-1.1365773	-0.2020256
C	-1.8664209	4.2390687	-0.3323656
C	-1.3588929	4.3403327	1.1026024
C	-0.7648119	2.9573077	1.3051064
C	-2.4115549	2.8097737	-0.4180786
H	-2.6212249	4.9902207	-0.5904746
H	-1.0247009	4.3583087	-1.0289396
H	-2.1922589	4.5057607	1.8019624
H	-0.6297489	5.1451507	1.2486374
H	0.1945651	2.8853797	0.7740104
H	-0.6132499	2.6485027	2.3454964
H	-2.2186339	2.3501277	-1.3972466
H	-3.4957419	2.7795607	-0.2468726
N	-1.7289859	2.0302777	0.6543824
H	-2.4060919	1.7635417	1.3703064
C	-4.7458869	-1.3869313	-0.3736896
C	-3.8501889	-2.4199973	0.2973034
C	-2.5293959	-2.2385093	-0.4313676
C	-3.8050049	-0.1978253	-0.4824126
H	-5.0540049	-1.7320713	-1.3722596
H	-5.6514259	-1.1509063	0.1965514
H	-4.2257189	-3.4465653	0.2254714
H	-3.7120119	-2.1716543	1.3589854
H	-1.6618599	-2.5296173	0.1684344
H	-2.5149639	-2.8110573	-1.3706426
H	-3.7722789	0.3308897	0.4791574
H	-4.0671479	0.5225407	-1.2660816
N	-2.4538949	-0.7713543	-0.7473476
H	-2.2317309	-0.6556963	-1.7360516
C	4.6905721	0.3252437	0.3245704
C	4.3857971	-0.0718333	-0.9768766

C	3.0914141	0.0090177	-1.4626466
C	2.0559581	0.4175147	-0.6043956
C	2.3707531	0.9047007	0.6766434
C	3.6735591	0.8254557	1.1372544
H	5.1839651	-0.4193473	-1.6329156
H	2.8793151	-0.2376243	-2.5005236
H	1.5853641	1.2599767	1.3440564
H	3.9014401	1.1563877	2.1483614
C	6.1050151	0.2586157	0.7806094
F	6.9016071	1.0777337	0.0711414
F	6.6199331	-0.9736373	0.6299904
F	6.2436251	0.5937827	2.0690584
Br	0.5438921	1.3523627	-1.6147736

c3

Ni	-0.7520710	0.2767633	0.0538776
Br	-1.3297640	-0.1644747	2.3965996
C	0.4090460	-3.8849717	-1.3323944
C	0.5150300	-4.1282937	0.1853446
C	-0.0852470	-2.8699167	0.8105476
C	-0.1096070	-2.4469567	-1.4421264
H	1.3864150	-3.9948287	-1.8186684
H	-0.2736460	-4.5860347	-1.8264954
H	1.5658530	-4.2273417	0.4885326
H	-0.0049060	-5.0342257	0.5167246
H	-1.1778910	-2.9372137	0.8826586
H	0.2864590	-2.6343387	1.8083906
H	-1.2072190	-2.4360437	-1.4986294
H	0.2425050	-1.8601497	-2.2917214
N	0.2295050	-1.7834707	-0.1599594
C	0.3373470	4.2301803	-0.5590604
C	1.2194810	3.9540493	0.6528476
C	0.9543450	2.4774863	0.8938766
C	-0.9269580	3.4253093	-0.2687714
H	0.1282530	5.2936693	-0.7211524
H	0.8147780	3.8320623	-1.4650534
H	0.8885320	4.5484813	1.5181956
H	2.2799360	4.1697313	0.4796856
H	1.5350760	1.8652853	0.1868866
H	1.1692800	2.1223163	1.9086906
H	-1.3764260	3.0336393	-1.1872174
H	-1.6757050	4.0229933	0.2703336

N	-0.4981060	2.2930113	0.6051136
H	-0.9987410	2.3268453	1.4933246
C	-4.9524150	0.6422483	0.0124266
C	-4.6018430	-0.7337877	0.5657076
C	-3.4254250	-1.1512277	-0.3046504
C	-3.5731120	1.2467143	-0.2010594
H	-5.4874420	0.5482393	-0.9446624
H	-5.5723310	1.2414493	0.6888956
H	-5.4274320	-1.4530737	0.5273676
H	-4.2613820	-0.6455487	1.6069326
H	-2.7545780	-1.8490627	0.2078466
H	-3.7673730	-1.6169047	-1.2410204
H	-3.1884220	1.6427873	0.7483266
H	-3.5333480	2.0433523	-0.9527324
N	-2.7042430	0.1139213	-0.6232494
H	-2.5233990	0.1767873	-1.6263104
C	4.1569200	-0.2521577	0.3071856
C	3.7431530	-0.7142597	-0.9394724
C	2.4770720	-1.2498257	-1.1092114
C	1.5909850	-1.3227297	-0.0289574
C	2.0138200	-0.8528487	1.2207126
C	3.2878630	-0.3278367	1.3874666
H	4.4219840	-0.6529067	-1.7888094
H	2.1827260	-1.5901297	-2.0967344
H	1.3176570	-0.8481647	2.0582416
H	3.5959140	0.0393133	2.3637386
C	5.5302290	0.3215513	0.4352606
F	5.6973000	1.3736893	-0.3793054
F	6.4692330	-0.5732597	0.0950636
F	5.7982490	0.7313753	1.6791006
Br	-0.0559130	0.8287313	-2.2484784

TSc3

Ni	-0.0535827	-0.1318237	0.1340704
Br	-0.6624577	-0.0879067	-2.2327756
C	1.0307153	-4.3621357	0.5613844
C	-0.1338137	-4.5117947	-0.4102916
C	-0.2874137	-3.0868247	-0.9318496
C	0.7234903	-3.0037307	1.1836894
H	1.1102223	-5.1671497	1.3001984
H	1.9819023	-4.3169597	0.0082354
H	-1.0416387	-4.8142657	0.1345164

H	0.0378193	-5.2449507	-1.2056836
H	0.3952713	-2.8844887	-1.7792806
H	-1.2812557	-2.8057857	-1.3046636
H	1.5838783	-2.4676347	1.6111744
H	0.0041503	-3.1067957	2.0188794
N	0.0972043	-2.2036957	0.1500774
C	0.2976163	4.3979993	0.8898574
C	0.4153673	4.3257983	-0.6315546
C	-0.1461297	2.9470243	-0.9350076
C	0.4645533	2.9381043	1.3518164
H	1.0281663	5.0726873	1.3512204
H	-0.6998947	4.7661743	1.1689044
H	1.4718093	4.3704133	-0.9420286
H	-0.1138607	5.1360073	-1.1466736
H	-1.2437937	2.9324563	-0.8641696
H	0.1095273	2.5288233	-1.9123956
H	-0.3204447	2.6404963	2.0565184
H	1.4164513	2.7539993	1.8671584
N	0.4008433	2.0815663	0.1351334
H	1.3634033	1.8823783	-0.1326006
C	4.6220183	0.1212573	-0.0413976
C	4.2843433	-0.0131757	-1.5343206
C	2.7950393	0.3042133	-1.5841366
C	3.2621833	-0.0404237	0.6771094
H	5.3558933	-0.6248357	0.2851114
H	5.0549323	1.1063103	0.1753034
H	4.4489373	-1.0451627	-1.8775796
H	4.8900423	0.6409943	-2.1721966
H	2.6357403	1.3967493	-1.5457416
H	2.2405943	-0.0627647	-2.4540566
H	2.9834483	0.8819643	1.2111424
H	3.2494433	-0.8419177	1.4260524
N	2.2452173	-0.2993117	-0.3579036
H	2.1931383	-1.3048517	-0.5297976
C	-4.5520667	-0.0629067	0.1242994
C	-3.8807417	1.1358373	0.3653384
C	-2.5842037	1.1281773	0.8479914
C	-1.9275307	-0.0952787	1.0191094
C	-2.6304947	-1.2971217	0.8890214
C	-3.9300147	-1.2753077	0.4064224
H	-4.3835187	2.0829643	0.1723944
H	-2.0669127	2.0640763	1.0400054

H	-2.1467607	-2.2459157	1.1125654
H	-4.4669017	-2.2084387	0.2510214
C	-5.9600097	-0.0021317	-0.3659386
F	-6.0718767	0.7758823	-1.4509046
F	-6.7800997	0.5238363	0.5597144
F	-6.4442707	-1.2082337	-0.6819636
Br	-0.3836767	-0.1124707	2.5394754

c4

Ni	0.5605569	-0.1222835	-0.0420652
Br	0.7971999	-0.7908515	2.4925888
C	-0.0905421	4.1000555	0.2554988
C	-0.8397081	3.5675765	1.4685508
C	-0.1028451	2.2631845	1.7311198
C	0.1415359	2.8255715	-0.5467172
H	-0.6360331	4.8597375	-0.3142932
H	0.8722529	4.5351395	0.5638678
H	-1.8861271	3.3459335	1.2057058
H	-0.8383101	4.2396475	2.3331848
H	0.8401659	2.4344175	2.2849138
H	-0.6436811	1.5056235	2.3046668
H	1.0020959	2.8230085	-1.2262292
H	-0.7313561	2.5876535	-1.1793312
N	0.2677189	1.7504135	0.4236088
C	-1.4432171	-3.3410015	-0.5186202
C	-0.5195151	-3.6568105	0.6748138
C	0.8625479	-3.2086695	0.2215128
C	-0.5485511	-2.6182685	-1.5233752
H	-1.8742241	-4.2441905	-0.9656292
H	-2.2795081	-2.7015175	-0.2104802
H	-0.5265181	-4.7158195	0.9556438
H	-0.8026481	-3.0753095	1.5610758
H	1.4941319	-2.8723565	1.0485958
H	1.3783759	-4.0093255	-0.3359482
H	-1.0352531	-1.8122675	-2.0770432
H	-0.1373551	-3.3277555	-2.2594912
N	0.5811939	-2.0944225	-0.7143032
H	1.3665469	-1.9424815	-1.3487362
C	4.7752419	0.9847665	0.2458648
C	4.9862719	-0.3436775	-0.4946332
C	3.5808989	-0.9771125	-0.5728512
C	3.2913029	1.2545635	0.0485708

H	4.9885149	0.8680015	1.3180578
H	5.4116219	1.7930365	-0.1319912
H	5.7050209	-0.9904515	0.0209718
H	5.3753929	-0.1701895	-1.5053242
H	3.2373709	-1.0155285	-1.6147032
H	3.5287189	-1.9826645	-0.1374962
H	3.0782989	1.6254765	-0.9640142
H	2.8482069	1.9398915	0.7831528
N	2.6666589	-0.0767495	0.1659048
H	2.6851289	-0.3385965	1.1575538
C	-4.2048371	0.0674195	-0.1833702
C	-3.5562621	-0.2464885	1.0080688
C	-2.1670381	-0.2806305	1.0657828
C	-1.4267381	-0.0035595	-0.0821032
C	-2.0680231	0.3321975	-1.2693592
C	-3.4612451	0.3569635	-1.3197482
H	-4.1406041	-0.4739685	1.8994288
H	-1.6689921	-0.5406265	1.9972768
H	-1.4894041	0.5584155	-2.1636482
H	-3.9626451	0.6087665	-2.2517552
C	-5.6999841	0.0888195	-0.1939712
F	-6.1805881	0.9711785	0.6943108
F	-6.2071131	-1.1050085	0.1440758
F	-6.1986051	0.4125995	-1.3905632
Br	1.0444989	0.3785245	-2.5365722

TSc4

Ni	0.6338806	0.0827027	0.0465756
Br	0.8371746	1.2994237	-2.2551534
C	-1.0495964	-3.7164253	-0.8766114
C	-1.4933214	-2.8038893	-2.0254804
C	-0.3427164	-1.8162183	-2.1493684
C	-0.0197774	-2.8798413	-0.1021474
H	-1.8882614	-4.0108163	-0.2354594
H	-0.5916034	-4.6382103	-1.2563044
H	-2.4092964	-2.2577773	-1.7597414
H	-1.6854524	-3.3422653	-2.9598014
H	0.5110536	-2.2631863	-2.6964374
H	-0.5564084	-0.8652803	-2.6420114
H	0.9829466	-3.3431563	-0.0998544
H	-0.2473734	-2.7076873	0.9537716
N	0.1341846	-1.6093463	-0.7928974

C	-1.0098274	3.4568917	0.6081836
C	0.2994636	3.9602267	-0.0254544
C	1.3936576	3.0571877	0.5483536
C	-0.5599014	2.4707627	1.6736596
H	-1.6197264	4.2603737	1.0361306
H	-1.6233454	2.9425517	-0.1418494
H	0.4992816	5.0115437	0.2124726
H	0.2676036	3.8568907	-1.1154234
H	2.1075276	2.7372417	-0.2161674
H	1.9432606	3.5615247	1.3600586
H	-1.2883414	1.6884617	1.9097386
H	-0.3119464	2.9988627	2.6096816
N	0.6828706	1.8858937	1.1173176
H	1.2119436	1.4750687	1.8903656
C	4.7251536	-1.2669963	-0.3752524
C	4.8674166	-0.4122033	0.8807136
C	3.7104506	0.5894537	0.7785986
C	3.2143056	-1.3581273	-0.4983864
H	5.1471486	-0.7513533	-1.2511254
H	5.2108366	-2.2461433	-0.2914244
H	5.8420746	0.0806127	0.9692836
H	4.7269116	-1.0409973	1.7708556
H	3.2308306	0.7352427	1.7523016
H	4.0385396	1.5651687	0.3976146
H	2.8115256	-2.0391143	0.2639646
H	2.8391356	-1.6567353	-1.4860474
N	2.7334436	0.0069037	-0.1872844
H	2.7732546	0.5441697	-1.0575684
C	-4.1554974	-0.0055673	0.2962766
C	-3.5180554	0.5840357	-0.7930214
C	-2.1343984	0.5253387	-0.9143654
C	-1.3926564	-0.1035683	0.0836776
C	-2.0199904	-0.7105813	1.1663216
C	-3.4081274	-0.6511373	1.2735766
H	-4.1067474	1.0935677	-1.5553374
H	-1.6370254	0.9983547	-1.7591114
H	-1.4346944	-1.1842753	1.9518346
H	-3.9031284	-1.1092113	2.1269136
C	-5.6492804	0.0527467	0.3618546
F	-6.2046634	-0.6381793	-0.6441594
F	-6.0927834	1.3118527	0.2510546
F	-6.1302144	-0.4463433	1.5037376

| Br | 1.1082806 | -0.9584203 | 2.3683576 |

c2-CH₃

Ni	-1.5161201	-0.6306840	0.3003404
Br	-3.2659791	-1.5505250	1.6927254
C	0.3708349	-1.5747640	-3.3617866
C	0.7058789	-2.6923930	-2.3666666
C	-0.4639701	-2.6488820	-1.3808296
C	-0.5566471	-0.6223060	-2.5726966
H	1.2705979	-1.0650510	-3.7287276
H	-0.1455991	-1.9782980	-4.2424826
H	1.6436769	-2.4661560	-1.8366526
H	0.8296069	-3.6724770	-2.8462316
H	-0.1763231	-3.0356810	-0.3861696
H	-1.5108321	-0.4775870	-3.1168676
H	-0.1154811	0.3856070	-2.4664586
N	-0.7632881	-1.2240350	-1.2682736
C	1.7090759	0.5151580	2.9752844
C	1.6187779	-0.9857110	3.2429684
C	0.6390739	-1.4372650	2.1709234
C	0.2873089	0.9117060	2.5323314
H	2.0372179	1.0920860	3.8494734
H	2.4284669	0.7066130	2.1665314
H	1.1989089	-1.1807010	4.2413184
H	2.5899759	-1.4922040	3.1828804
H	1.1447639	-1.5186680	1.1957704
H	0.1348689	-2.3918220	2.3673984
H	0.3351209	1.5945360	1.6693564
N	-0.3685271	-0.3566890	2.0961434
H	-1.1182191	-0.5858610	2.7550284
C	-3.4291481	3.2014420	-0.0217226
C	-4.2715071	2.3726160	-0.9831206
C	-3.3490901	1.2242620	-1.4295296
C	-2.6365711	2.1129330	0.6811054
H	-2.7434171	3.8668250	-0.5715896
H	-4.0235721	3.8201010	0.6605644
H	-4.6648571	2.9414290	-1.8338106
H	-5.1323861	1.9495440	-0.4427646
H	-2.8685961	1.4790480	-2.3875116
H	-3.2652621	1.5616890	1.3970844
H	-1.7374851	2.4606250	1.2073614
N	-2.2486801	1.1811780	-0.3985706

H	-1.4120821	1.5668440	-0.8358666
C	4.5905909	0.0873870	-0.0939736
C	4.6984219	1.4773130	-0.0907676
C	3.5811999	2.2601130	-0.3394926
C	2.3657839	1.6305460	-0.5874756
C	2.2349679	0.2499070	-0.5942096
C	3.3676109	-0.5217720	-0.3446416
H	5.6616329	1.9446980	0.1074614
H	3.6471159	3.3454300	-0.3406926
H	1.2627859	-0.2261270	-0.7610796
H	3.2897989	-1.6077810	-0.3399086
C	5.8195489	-0.7157660	0.2039054
F	6.2591119	-0.4753000	1.4464294
F	6.8192319	-0.3955230	-0.6264386
F	5.6064059	-2.0287540	0.0977604
Br	0.8420999	2.7236830	-0.9022696
C	-4.0820961	-0.0915550	-1.5705516
H	-4.8985681	0.0164950	-2.2979726
H	-3.4106801	-0.8924290	-1.9039736
H	-4.5053051	-0.4029180	-0.6063916
C	-0.5202021	1.5480200	3.6483604
H	-0.1400471	2.5482430	3.8905234
H	-1.5803051	1.6415170	3.3750654
H	-0.4653021	0.9345450	4.5600424
C	-1.6688661	-3.4499820	-1.8661326
H	-1.4311221	-4.5206610	-1.9363026
H	-2.5102351	-3.3244820	-1.1723716
H	-1.9940911	-3.1113270	-2.8611636

TSc2-CH$_3$

Ni	-0.7854787	0.0273039	0.4011564
Br	-1.7401227	-0.2830911	2.5879034
C	2.1434433	-3.0184781	-0.6638596
C	2.7337403	-2.5260651	0.6643894
C	1.5626183	-1.7843661	1.3216734
C	0.8765163	-2.1605431	-0.8675176
H	2.8548013	-2.8979841	-1.4898616
H	1.8845093	-4.0843821	-0.6185756
H	3.5804523	-1.8523111	0.4924204
H	3.0951263	-3.3485761	1.2950854
H	1.9048653	-0.9813441	1.9956984
H	-0.0195397	-2.8031411	-0.8193606

H	0.8511823	-1.6653241	-1.8539376
N	0.8634553	-1.1565131	0.1903464
C	-1.2717097	4.3913129	-0.1473486
C	-0.8727597	4.3383709	1.3223514
C	-0.5598917	2.8613639	1.4798744
C	-2.1042217	3.1144049	-0.3361886
H	-1.8351887	5.2906279	-0.4265576
H	-0.3698337	4.3508809	-0.7744616
H	-1.7110957	4.6305929	1.9723234
H	-0.0203287	4.9833189	1.5644074
H	0.4206743	2.6576679	1.0262964
H	-0.5559767	2.4763989	2.5052164
H	-1.9269847	2.6918589	-1.3380176
N	-1.5953757	2.1477419	0.6868454
H	-2.3520507	1.9000679	1.3285984
C	-4.2158357	-0.8228761	-2.0828596
C	-4.0702757	-2.2231691	-1.5014286
C	-2.6351897	-2.2861041	-0.9361686
C	-3.3311467	-0.0196981	-1.1476636
H	-3.8166487	-0.7727681	-3.1074096
H	-5.2524927	-0.4682481	-2.1112346
H	-4.2613697	-3.0219931	-2.2271166
H	-4.7859467	-2.3550881	-0.6762756
H	-1.9828407	-2.8502391	-1.6178376
H	-3.8096547	0.1081809	-0.1644686
H	-3.0395957	0.9662129	-1.5253416
N	-2.1284647	-0.8589341	-0.9546356
H	-1.5757917	-0.7668191	-1.8101106
C	4.9433023	0.5556369	-0.0165746
C	4.4964993	0.0010609	-1.2157926
C	3.1444833	-0.0733401	-1.5045146
C	2.2070453	0.3553829	-0.5488876
C	2.6531183	0.9847199	0.6248234
C	4.0086133	1.0488329	0.8947624
H	5.2217743	-0.3531851	-1.9480616
H	2.8072583	-0.4604521	-2.4640286
H	1.9329153	1.3513269	1.3554794
H	4.3465453	1.4947309	1.8278934
C	6.4043053	0.5796539	0.2639994
F	7.1022873	1.0988009	-0.7599116
F	6.8952873	-0.6572901	0.4555894
F	6.7042163	1.2946119	1.3552424

Br	0.5678593	1.1860809	-1.4786856
C	-2.5995527	-2.9212221	0.4337204
H	-3.0712367	-3.9120551	0.3825284
H	-1.5778207	-3.0409101	0.8067154
H	-3.1439537	-2.3118471	1.1659084
C	-3.5874517	3.3780739	-0.1421986
H	-3.9819737	3.9995529	-0.9559296
H	-4.1728597	2.4498939	-0.1141656
H	-3.7652227	3.9104209	0.8032614
C	0.7273183	-2.7747601	2.1278084
H	1.3242093	-3.1510641	2.9700874
H	-0.1802057	-2.3149371	2.5287994
H	0.4476633	-3.6459671	1.5157844

c3-CH$_3$

Ni	-0.3863219	-0.8389480	0.0651014
Br	0.1030361	0.0335710	-2.0599786
C	-0.7958239	4.5887220	1.9248934
C	-1.1896859	4.8016170	0.4726874
C	-0.0708709	4.1291700	-0.3244986
C	-0.2163999	3.1811260	1.9109454
H	-0.0153439	5.3067340	2.2152424
H	-1.6302769	4.6980210	2.6269084
H	-1.3204749	5.8537140	0.1928954
H	-2.1384319	4.2816720	0.2623834
H	0.7549731	4.8513190	-0.4810596
H	-0.9875899	2.4066850	2.0691774
H	0.5433931	3.0381350	2.6910074
N	0.3847211	3.0670450	0.5810944
C	1.6152401	-3.6793800	1.5058564
C	2.6729061	-3.3965810	0.4435024
C	1.9726781	-2.4144430	-0.4859686
C	0.3142471	-3.7298410	0.7108184
H	1.7897131	-4.6042370	2.0692164
H	1.5546201	-2.8460100	2.2209204
H	2.9505601	-4.3174630	-0.0883486
H	3.5961431	-2.9686870	0.8520564
H	2.1947301	-1.3780970	-0.2054936
H	2.2454631	-2.5132320	-1.5414876
H	-0.5367399	-3.4625560	1.3527064
N	0.5007951	-2.6485560	-0.3026226
H	0.0839021	-2.9148000	-1.1953276

C	-4.1644159	-1.5707260	-1.7555826
C	-4.6343869	-1.0022210	-0.4159356
C	-3.3557819	-0.4467380	0.2063054
C	-2.7249599	-2.0385220	-1.4889046
H	-4.8065819	-2.3809130	-2.1183816
H	-4.1665129	-0.7902820	-2.5272656
H	-5.0387579	-1.8026850	0.2212084
H	-5.4154869	-0.2394910	-0.5233756
H	-3.3919809	-0.4149170	1.3027314
H	-2.0262929	-1.6698380	-2.2485916
H	-2.6361629	-3.1322080	-1.4389946
N	-2.3309039	-1.4718140	-0.1656396
H	-2.3906499	-2.2089380	0.5380144
C	3.8382741	0.7570200	-0.0204366
C	3.0282181	0.5592240	1.0950504
C	1.9018001	1.3364270	1.2970674
C	1.5319441	2.3378130	0.3768904
C	2.3778491	2.5493670	-0.7305256
C	3.5000091	1.7643170	-0.9242576
H	3.2660161	-0.2218560	1.8178704
H	1.2664521	1.1186360	2.1496274
H	2.1496201	3.3255880	-1.4557526
H	4.1296711	1.9368090	-1.7957826
C	4.9689461	-0.1612960	-0.3147786
F	4.6198041	-1.1286950	-1.1931386
F	5.4078751	-0.8000690	0.7816954
F	6.0159261	0.4717840	-0.8592266
Br	-0.5864259	-0.7957930	2.4277534
C	-2.9804409	0.9259740	-0.3184676
H	-3.7624429	1.6502020	-0.0531836
H	-2.0337859	1.2771290	0.1193954
H	-2.8540709	0.9322400	-1.4092526
C	0.0592941	-5.0683080	0.0405514
H	-0.0906289	-5.8535420	0.7920774
H	-0.8439539	-5.0355480	-0.5862766
H	0.9005551	-5.3685990	-0.5993226
C	-0.5703889	3.6289180	-1.6695956
H	-0.8787799	4.4837780	-2.2871626
H	0.1734711	3.0474110	-2.2238796
H	-1.4410939	2.9756620	-1.5251556

c2-L

Ni	-0.4905414	-0.7905666	0.0117782
Br	-1.5757804	-2.9511786	-0.0387598
C	-4.2516094	0.8144734	-0.6880018
C	-4.3499004	0.1249684	0.6685342
C	-2.9243684	0.2678624	1.1934342
C	-2.8722534	0.3631124	-1.1701378
H	-5.0562594	0.5429264	-1.3812108
H	-4.2759214	1.9076784	-0.5582648
H	-4.5745874	-0.9426806	0.5323902
H	-5.1064064	0.5575664	1.3341682
H	-2.7854904	1.2632624	1.6646442
H	-2.6496224	-0.4863666	1.9445102
H	-2.3820264	1.0870294	-1.8433148
H	-2.9405594	-0.5894696	-1.7269868
N	-2.0741084	0.1414614	0.0245542
C	2.5242856	-0.8050556	-0.0012648
C	3.8479806	-1.2369706	-0.0058578
C	4.1090586	-2.6008666	-0.0098328
C	3.0443836	-3.4898826	-0.0096718
C	1.7502046	-2.9804226	-0.0052788
N	1.4960706	-1.6710126	-0.0004628
H	5.1361686	-2.9605726	-0.0130338
H	4.6690766	-0.5245306	-0.0053518
H	3.2028676	-4.5651426	-0.0131688
H	0.8610006	-3.6142496	-0.0073918
C	2.1398246	0.6220434	0.0038142
C	3.0553806	1.6730404	-0.0079008
C	0.3658416	2.1048774	0.0291932
C	2.5839976	2.9780234	-0.0006318
H	4.1250476	1.4808614	-0.0233738
H	-0.7203484	2.2022224	0.0467762
H	3.2839316	3.8111234	-0.0098628
C	1.2132406	3.2045474	0.0188082
H	0.8040916	4.2113594	0.0259862
N	0.8173316	0.8505284	0.0211682

TSc2-L

Ni	0.8179252	-0.2966428	0.3958357
Br	1.0003252	-0.1758858	2.7678367
C	-0.9600388	3.1854222	-0.6878573
C	-2.0248368	2.8294182	0.3414287
C	-1.3955938	1.6179382	1.0173877

C	-0.5266678	1.8047162	-1.1754763
H	-1.3137238	3.8327592	-1.5003813
H	-0.1248718	3.7056292	-0.1890893
H	-2.9573988	2.5410502	-0.1653083
H	-2.2547008	3.6421152	1.0407777
H	-0.6871888	1.9291472	1.8029477
H	-2.1204868	0.9468202	1.5055267
H	0.4989472	1.7784562	-1.5757393
H	-1.1808108	1.5009142	-2.0145163
N	-0.6950798	0.8868352	-0.0419133
C	-4.6212378	-0.8370588	0.1898917
C	-4.3039458	-0.2309058	-1.0257683
C	-2.9970918	-0.1775628	-1.4800553
C	-1.9610938	-0.6586828	-0.6592013
C	-2.2852498	-1.3610958	0.5179207
C	-3.6000238	-1.4147808	0.9447147
H	-5.1028308	0.1767922	-1.6455923
H	-2.7734208	0.2375782	-2.4604163
H	-1.4992108	-1.8075368	1.1281237
H	-3.8354158	-1.9190758	1.8796547
C	-6.0470428	-0.9067368	0.6039267
F	-6.7822628	-1.6581018	-0.2364213
F	-6.6262748	0.3069522	0.6077257
F	-6.2011968	-1.4247038	1.8289827
Br	-0.3706978	-1.4082428	-1.7061283
C	3.4402772	-1.5527288	-0.0188593
C	4.4428252	-2.5095958	-0.1608903
C	4.1273352	-3.8457558	0.0450107
C	2.8279852	-4.1950578	0.3913567
C	1.8828152	-3.1838548	0.5006237
N	2.1851382	-1.9057198	0.2934167
H	4.8952902	-4.6090578	-0.0604013
H	5.4563842	-2.2225678	-0.4291723
H	2.5465552	-5.2290098	0.5707597
H	0.8468052	-3.3909778	0.7693737
C	3.6651022	-0.0973928	-0.1508143
C	4.9227632	0.4777902	-0.3160463
C	2.6769282	1.9958612	-0.0185343
C	5.0348022	1.8610462	-0.3372993
H	5.8099522	-0.1435678	-0.4052113
H	1.7496022	2.5452872	0.1443647
H	6.0101132	2.3265462	-0.4618083

C	3.8964652	2.6397602	-0.1732533
H	3.9470902	3.7247362	-0.1548563
N	2.5669692	0.6687292	-0.0365743

c3-L

Ni	-1.1532331	-0.0963154	-0.0978678
Br	-1.1119481	-0.6712994	2.1506472
C	-0.4773391	-4.2010984	-0.6646178
C	0.1157789	-4.7014834	0.6489272
C	0.9024999	-3.4987264	1.1668432
C	0.6471449	-3.3522764	-1.2333058
H	-0.7921281	-5.0045614	-1.3400988
H	-1.3494521	-3.5553034	-0.4696938
H	0.7937539	-5.5442884	0.4510072
H	-0.6377221	-5.0424324	1.3676082
H	0.3074199	-2.8947614	1.8680722
H	1.8355039	-3.7933924	1.6738352
H	0.2815549	-2.5975624	-1.9400488
H	1.4095279	-3.9740804	-1.7395518
N	1.1881339	-2.7201184	-0.0371908
C	3.7098739	0.6175156	-0.0270368
C	3.2587559	0.0744276	-1.2335258
C	2.4352739	-1.0335934	-1.2489618
C	2.0211919	-1.6388974	-0.0407188
C	2.4836089	-1.0815404	1.1710722
C	3.3098679	0.0283186	1.1711882
H	3.5628219	0.5297786	-2.1755618
H	2.0976849	-1.4366754	-2.1998798
H	2.1654979	-1.5095004	2.1177662
H	3.6456689	0.4452766	2.1183242
C	4.5259979	1.8562826	-0.0561188
F	3.7900539	2.9273586	-0.4557158
F	5.5441469	1.7824096	-0.9235448
F	5.0346639	2.1736586	1.1389362
Br	-0.9663471	-0.3281414	-2.4023278
C	-1.7421401	2.6880346	0.1046592
C	-1.5614271	4.0619626	0.2227552
C	-0.2679571	4.5663866	0.2814452
C	0.8117639	3.6964566	0.2161362
C	0.5572099	2.3352506	0.0985532
N	-0.6841841	1.8610496	0.0501092
H	-0.1071971	5.6383196	0.3745442

H	-2.4150801	4.7334796	0.2685292
H	1.8383729	4.0476166	0.2507092
H	1.3615299	1.6001156	0.0383752
C	-3.0603911	2.0269336	0.0260902
C	-4.2820401	2.6945626	0.0599752
C	-4.1364101	-0.0253804	-0.1706468
C	-5.4540511	1.9552646	-0.0260398
H	-4.3223661	3.7768136	0.1523162
H	-4.0011881	-1.1036244	-0.2597438
H	-6.4171641	2.4604476	-0.0008858
C	-5.3886181	0.5718276	-0.1440668
H	-6.2867261	-0.0353154	-0.2135078
N	-3.0201951	0.6908206	-0.0877648

TSc3-L

Ni	-0.1478627	-0.0691473	-0.1492096
Br	0.6751383	-0.3856583	-2.4118296
C	-0.9340097	4.2661557	0.0082394
C	0.0748653	4.2042577	-1.1323456
C	0.0411573	2.7257817	-1.5045666
C	-0.6684067	2.9449997	0.7243694
H	-0.8213667	5.1378477	0.6624664
H	-1.9596277	4.2807047	-0.3927826
H	1.0769243	4.4745937	-0.7651406
H	-0.1599337	4.8654107	-1.9735046
H	-0.7678327	2.4961597	-2.2249086
H	0.9455543	2.3113777	-1.9712576
H	-1.5123467	2.5400087	1.3004344
H	0.1558763	3.0493087	1.4554124
N	-0.2498157	1.9948717	-0.2894336
C	4.3964753	-0.4098273	0.4296944
C	3.6378763	-1.5132063	0.8196554
C	2.2858583	-1.3742963	1.0801654
C	1.6678113	-0.1343323	0.8783324
C	2.4442293	0.9939237	0.5995054
C	3.7984573	0.8429767	0.3399534
H	4.1198413	-2.4836253	0.9364884
H	1.7031063	-2.2229133	1.4294444
H	1.9881343	1.9771147	0.5127894
H	4.3944563	1.7085917	0.0598244
C	5.8534963	-0.6053603	0.1756924
F	6.0704993	-1.5463823	-0.7544676

F	6.4939173	-1.0186533	1.2823594
F	6.4567843	0.5144417	-0.2361206
Br	-0.0356447	0.0626967	2.2735584
C	-2.8817177	-1.3309623	0.1571104
C	-4.1804147	-1.4584383	0.6501824
C	-5.0053517	-0.3429423	0.6681104
C	-4.5198217	0.8640297	0.1809774
C	-3.2040087	0.9069687	-0.2626296
N	-2.3986827	-0.1509943	-0.2592696
H	-6.0201017	-0.4182393	1.0536624
H	-4.5366117	-2.4132823	1.0298774
H	-5.1393867	1.7567907	0.1536534
H	-2.7679847	1.8314577	-0.6445416
C	-1.9678297	-2.4814923	-0.0102106
C	-2.4442077	-3.7881703	-0.1125176
C	0.1750593	-3.1656943	-0.5003856
C	-1.5517047	-4.8093893	-0.4032236
H	-3.5060477	-3.9983893	-0.0095816
H	1.2013903	-2.8574303	-0.6936726
H	-1.9023067	-5.8356243	-0.4925766
C	-0.2170517	-4.4933903	-0.6155816
H	0.5117563	-5.2538493	-0.8832156
N	-0.6685887	-2.1887813	-0.1689866

c4-L
Ni	0.2716140	0.1041842	-0.0250946
Br	-0.1500960	0.2794442	-2.3731276
C	0.5911550	-4.3023658	0.5258264
C	0.0820680	-4.2517298	-0.9086136
C	0.4327930	-2.8229678	-1.3170666
C	0.2353960	-2.9066988	1.0261834
H	0.1588290	-5.1005088	1.1283124
H	1.6885020	-4.4375668	0.5467144
H	-1.0091330	-4.3723598	-0.9138576
H	0.5104560	-5.0153948	-1.5713696
H	1.4759200	-2.7421288	-1.6960276
H	-0.1843330	-2.3669388	-2.1050996
H	0.8330250	-2.5106318	1.8588274
H	-0.8115260	-2.8514008	1.3785074
N	0.3362450	-2.0207178	-0.1123456
C	-4.4307970	0.2336972	0.4867624
C	-3.6369910	1.2278752	1.0480454

C	-2.2517230	1.1570832	0.9525674
C	-1.6573080	0.1049282	0.2657974
C	-2.4453330	-0.9145008	-0.2536726
C	-3.8310650	-0.8473938	-0.1496976
H	-4.1047760	2.0565092	1.5768424
H	-1.6413380	1.9106482	1.4403134
H	-2.0022810	-1.7522798	-0.7898526
H	-4.4421130	-1.6385528	-0.5815796
C	-5.9158510	0.3904402	0.5055024
F	-6.3244220	1.2761942	-0.4178006
F	-6.3578140	0.8452522	1.6868894
F	-6.5539490	-0.7587898	0.2534494
Br	0.5249010	0.1499502	2.3435814
C	2.8997440	1.4638512	-0.0406466
C	4.2583210	1.6500472	0.2103904
C	5.0853350	0.5464022	0.3432164
C	4.5343870	-0.7216998	0.2290914
C	3.1680060	-0.8259878	0.0081104
N	2.3706320	0.2314832	-0.1292356
H	6.1432220	0.6739682	0.5511954
H	4.6612750	2.6497412	0.3303634
H	5.1394620	-1.6190328	0.3321284
H	2.6783700	-1.8033648	-0.0333116
C	1.9629000	2.5896532	-0.2218906
C	2.3994810	3.8908662	-0.4704886
C	-0.2358290	3.2264332	-0.4643626
C	1.4606650	4.8838692	-0.7050446
H	3.4603050	4.1230822	-0.5126936
H	-1.2748360	2.9027892	-0.4980606
H	1.7806880	5.9042232	-0.9042946
C	0.1147730	4.5468622	-0.7131346
H	-0.6561640	5.2837832	-0.9240956
N	0.6592060	2.2797502	-0.1961516

c2-O
Ni	1.4395284	0.4470132	-1.0464522
Br	3.6807834	1.2217752	-0.7550902
C	-1.3378276	2.8204582	1.2008278
C	-0.5931996	3.8717642	0.3720888
C	0.1962604	3.0188232	-0.6077622
C	-0.4366466	1.5703322	1.1506458
H	-1.5369066	3.1529792	2.2258088

H	-2.3075266	2.5899052	0.7394968
H	0.1001064	4.4481212	1.0021458
H	-1.2641896	4.5851022	-0.1196922
H	-0.4503426	2.6132532	-1.3998482
H	1.0547504	3.5090982	-1.0811132
H	-0.9911946	0.7012932	0.7714448
H	-0.0109436	1.3040092	2.1252798
N	0.6704384	1.8789192	0.2102068
H	1.4908814	2.1944892	0.7321448
C	2.9347944	-2.1736338	1.7023908
C	3.4586954	-2.3756768	0.2850438
C	2.1864654	-2.3134868	-0.5414282
C	1.8893824	-1.0802118	1.5133808
H	2.4661034	-3.0981528	2.0717178
H	3.7127604	-1.8820758	2.4167018
H	4.0018094	-3.3167478	0.1450268
H	4.1153574	-1.5411128	0.0021708
H	2.3596174	-2.0535678	-1.5941352
H	1.6447594	-3.2721318	-0.5064872
H	2.3558484	-0.0891738	1.5905118
H	1.0602324	-1.1341448	2.2297818
N	1.3740354	-1.2498888	0.1220188
H	0.3893824	-1.5170998	0.1384448
C	-3.0432536	-1.7978968	0.3757108
C	-2.0031356	-1.9518278	-0.5412502
C	-1.7117076	-0.9536088	-1.4706482
C	-2.4905896	0.2073072	-1.4687592
C	-3.5386136	0.3587972	-0.5700342
C	-3.8132536	-0.6412488	0.3632908
H	-3.2555486	-2.5880758	1.0945958
H	-1.4176746	-2.8756168	-0.5503692
H	-2.2618276	0.9880102	-2.1952482
H	-4.1515516	1.2597502	-0.5961382
H	-4.6315936	-0.5201798	1.0709758
C	-0.5691866	-1.0811868	-2.4542632
H	-0.9958946	-1.1642858	-3.4737542
H	-0.0645556	-2.0578238	-2.2719662
O	0.2951734	-0.0123438	-2.4074142

TSc2-O

Ni	0.4170118	0.9163209	0.1495511
Br	0.1496548	2.6804869	1.7976311

C	2.8993368	-1.9525031	2.4251911
C	1.9066528	-1.4570371	3.4799311
C	0.8211668	-0.8236961	2.6259121
C	2.7467868	-0.9564391	1.2580461
H	3.9285338	-2.0093171	2.7967881
H	2.6191908	-2.9596651	2.0866661
H	2.3671408	-0.6933551	4.1244211
H	1.5348608	-2.2579771	4.1288381
H	0.2125988	-1.5952411	2.1395891
H	0.1504798	-0.1226371	3.1334521
H	2.5563838	-1.4831371	0.3135021
H	3.6327238	-0.3216061	1.1246561
N	1.5786308	-0.0954901	1.5821881
H	1.9147628	0.7541879	2.0438771
C	2.5717008	3.8355809	-0.5668879
C	1.8246918	3.6086849	-1.8957719
C	2.0332078	2.1321189	-2.2081229
C	3.0798148	2.4542459	-0.1582059
H	3.4012358	4.5447649	-0.6626399
H	1.8837098	4.2111729	0.1983401
H	2.1908848	4.2419929	-2.7111079
H	0.7554438	3.8203069	-1.7697119
H	1.2060718	1.6694839	-2.7584549
H	2.9618638	1.9817839	-2.7842129
H	3.0358718	2.2915789	0.9244931
H	4.1171798	2.2950749	-0.4969559
N	2.1834118	1.5090539	-0.8703549
H	2.6432298	0.6023139	-0.9751269
C	1.4615308	-1.8280381	-2.5833489
C	0.3559138	-1.3867621	-1.8611519
C	-0.0962302	-2.0965411	-0.7429069
C	0.5768328	-3.2625281	-0.3766079
C	1.6778108	-3.7106161	-1.1015549
C	2.1297038	-2.9899121	-2.2036319
H	1.7907478	-1.2687981	-3.4592469
H	-0.1835152	-0.4894451	-2.1702669
H	0.2325928	-3.8249401	0.4935451
H	2.1904208	-4.6228491	-0.7991849
H	2.9916198	-3.3376931	-2.7703079
C	-1.2785982	-1.5998091	0.0510801
H	-1.3390722	-2.1533701	1.0063231
H	-2.2147362	-1.8494971	-0.4881529

O	-1.2501962	-0.2248371	0.2650691
C	-5.3884712	0.3364749	0.0540091
C	-4.6080542	1.1379729	0.9010281
C	-3.2680122	1.3402229	0.6583121
C	-2.6792242	0.6924749	-0.4413489
C	-3.4459242	-0.0719631	-1.3240749
C	-4.8006132	-0.2535841	-1.0542829
H	-5.0716382	1.6115069	1.7662781
H	-2.6451492	1.9543659	1.3072571
H	-2.9987632	-0.4895931	-2.2247259
H	-5.4035322	-0.8480061	-1.7375909
C	-6.8315202	0.1653669	0.3669611
F	-7.4628572	-0.6102401	-0.5245939
F	-7.4821432	1.3411279	0.4003091
F	-7.0192532	-0.3907521	1.5774451
Br	-1.2639032	1.9093109	-1.4601589

c3-O

Ni	-0.3308707	-1.1601014	-0.1740811
Br	0.4174323	-3.0325334	1.1327379
C	-2.0461297	1.4442026	2.9645029
C	-0.7057997	1.0349956	3.5825659
C	0.0659483	0.5134476	2.3821829
C	-2.1949367	0.5341596	1.7281649
H	-2.8835647	1.3416166	3.6636799
H	-2.0153257	2.4955576	2.6479099
H	-0.8440947	0.2245916	4.3134399
H	-0.1990467	1.8598956	4.0956999
H	0.4235013	1.3287716	1.7402929
H	0.9165053	-0.1342154	2.6232969
H	-2.3106737	1.1342866	0.8162379
H	-3.0510097	-0.1485664	1.7979029
N	-0.9449937	-0.2628704	1.6239599
H	-1.0659627	-1.1367764	2.1448799
C	-2.6718527	-3.9390354	-0.3820221
C	-2.1704287	-3.6656144	-1.8121001
C	-2.4957837	-2.2022054	-2.0525581
C	-2.9970377	-2.5567914	0.1932389
H	-3.5616227	-4.5791164	-0.3661931
H	-1.8911697	-4.4222504	0.2147449
H	-2.6343047	-4.3136374	-2.5634701
H	-1.0833587	-3.8034584	-1.8723471

H	-1.8378707	-1.7214874	-2.7825491
H	-3.5492907	-2.0716704	-2.3559641
H	-2.6554207	-2.4345774	1.2272589
H	-4.0810877	-2.3585964	0.1617409
N	-2.3038447	-1.6012074	-0.7084901
H	-2.7516047	-0.6823564	-0.6744941
C	-2.6918547	1.7837716	-1.9731511
C	-1.3251257	1.5238876	-2.0411481
C	-0.4278417	2.2547116	-1.2582921
C	-0.9211627	3.2418526	-0.4034271
C	-2.2859937	3.5043396	-0.3346801
C	-3.1742937	2.7759166	-1.1223221
H	-3.3795287	1.2243466	-2.6080201
H	-0.9319887	0.7494596	-2.7012351
H	-0.2209167	3.8209556	0.2012379
H	-2.6569427	4.2865276	0.3259919
H	-4.2410847	2.9895196	-1.0805311
C	1.0493893	2.0174756	-1.3646521
H	1.5821753	2.9770926	-1.2650881
H	1.3068983	1.5682096	-2.3356771
O	1.4653063	1.1367586	-0.3260821
C	5.4080563	-0.1376714	-0.1796841
C	4.3998643	-0.8069744	0.5173829
C	3.0922303	-0.3707854	0.4445269
C	2.7752983	0.7469576	-0.3332831
C	3.7719033	1.4045586	-1.0501651
C	5.0880553	0.9590446	-0.9642511
H	4.6428463	-1.6896904	1.1068999
H	2.3007633	-0.9311934	0.9408519
H	3.5446833	2.2594986	-1.6804091
H	5.8674403	1.4741666	-1.5203441
C	6.8104823	-0.6334074	-0.0550371
F	7.6667033	0.0554256	-0.8185841
F	6.9113253	-1.9236864	-0.4012371
F	7.2490543	-0.5474904	1.2112539
Br	0.7779583	-1.3980354	-2.2410141

TSc3-O

Ni	0.3469963	0.1343452	-0.2221354
Br	1.4708993	0.9291222	-2.1638394
C	-3.8132527	0.9301282	-0.5378184
C	-3.4427597	1.5011492	-1.9035094

C	-1.9885717	1.0801302	-2.0309574
C	-2.5381717	1.1119362	0.2950906
H	-4.6846787	1.4116512	-0.0794884
H	-4.0378367	-0.1414158	-0.6348984
H	-3.5276017	2.5992992	-1.9060724
H	-4.0705357	1.1163892	-2.7158304
H	-1.9024467	0.0102642	-2.2547744
H	-1.3928637	1.6313862	-2.7648894
H	-2.3333137	0.2396022	0.9277656
H	-2.5965167	1.9918732	0.9519906
N	-1.4198897	1.2998802	-0.6760484
H	-1.1156037	2.2716942	-0.6494504
C	2.5759703	3.6246122	0.1526276
C	2.8765433	3.3690422	1.6362926
C	1.6237783	2.6505022	2.1700326
C	1.0632293	3.5187912	0.0777466
H	2.9505013	4.5898772	-0.2047954
H	3.0023623	2.8364572	-0.4829404
H	3.0297453	4.3098002	2.1793556
H	3.7924023	2.7795422	1.7726716
H	1.8233333	1.7102092	2.6986806
H	1.0872973	3.3046762	2.8773526
H	0.7195223	3.3029182	-0.9418534
H	0.5856403	4.4486442	0.4403516
N	0.7892013	2.3858212	0.9774976
H	-0.1856277	2.3634312	1.2728426
C	-4.3191877	-2.5879238	1.4827766
C	-2.9551457	-2.5302528	1.2120096
C	-2.4903667	-2.6647278	-0.0960684
C	-3.4079677	-2.8425238	-1.1316894
C	-4.7706587	-2.9041308	-0.8635994
C	-5.2279157	-2.7773298	0.4463506
H	-4.6728807	-2.4874978	2.5076476
H	-2.2345207	-2.3710488	2.0151546
H	-3.0420877	-2.9363598	-2.1554924
H	-5.4790177	-3.0553138	-1.6766234
H	-6.2945917	-2.8282898	0.6583756
C	-1.0167207	-2.5479468	-0.3949614
H	-0.7465897	-3.2490808	-1.2106154
H	-0.4275417	-2.8327368	0.4941906
O	-0.7396667	-1.2636598	-0.8326584
C	4.6329003	-1.7536988	-0.1359464

C	4.4368353	-0.5463488	0.5240296
C	3.1480013	-0.0994078	0.7858336
C	2.0752933	-0.8507968	0.3360976
C	2.2440583	-2.0857998	-0.2748484
C	3.5386963	-2.5205338	-0.5273434
H	5.2900143	0.0497622	0.8402196
H	2.9925003	0.8408732	1.2991756
H	1.4033513	-2.6790728	-0.6150834
H	3.6981123	-3.4651348	-1.0460384
C	6.0043263	-2.2802128	-0.4140184
F	6.9618913	-1.4154018	-0.0659494
F	6.1658203	-2.5619948	-1.7132304
F	6.2326283	-3.4210898	0.2538796
Br	0.3126773	-0.6440798	2.0374266

c4-O

Ni	0.3309146	0.3768031	-0.1558475
Br	0.7947876	0.9647381	-2.3868515
C	-4.0802994	1.1240531	0.1026415
C	-3.8710054	0.9186441	-1.4034545
C	-2.4908794	0.2869671	-1.4700265
C	-2.6566154	1.1456241	0.6951565
H	-4.6415324	2.0389021	0.3258715
H	-4.6449474	0.2847911	0.5302095
H	-3.8694694	1.8822561	-1.9348065
H	-4.6458874	0.2928791	-1.8617065
H	-2.5337174	-0.7672219	-1.1718355
H	-1.9751204	0.3537611	-2.4325935
H	-2.4777904	0.3009361	1.3700125
H	-2.4344494	2.0573831	1.2648595
N	-1.7086854	1.0157911	-0.4418935
H	-1.5513304	1.9471091	-0.8364955
C	2.2671266	3.7845741	-0.3646905
C	2.6511526	3.6643731	1.1164405
C	1.4592646	2.9428511	1.7695805
C	0.7571936	3.6424471	-0.3417705
H	2.5986096	4.7219381	-0.8242425
H	2.6828526	2.9522621	-0.9490595
H	2.7852416	4.6536651	1.5715265
H	3.5970066	3.1256091	1.2494685
H	1.7090106	2.0531571	2.3579605
H	0.9239186	3.6298461	2.4444315

H	0.3397126	3.3625491	-1.3146225
H	0.2817626	4.5762571	0.0106705
N	0.5689636	2.5599431	0.6447815
H	-0.3853704	2.5501151	1.0006765
C	-3.9679074	-2.5482239	1.3094205
C	-2.5819484	-2.4750999	1.2193365
C	-1.9375514	-2.9545989	0.0785535
C	-2.6846534	-3.4691089	-0.9837125
C	-4.0685794	-3.5317269	-0.8943455
C	-4.7112554	-3.0683009	0.2526915
H	-4.4696054	-2.1893869	2.2069235
H	-1.9852864	-2.0298959	2.0150535
H	-2.1698704	-3.8111109	-1.8816265
H	-4.6492834	-3.9409269	-1.7188475
H	-5.7967664	-3.1145809	0.3224445
C	-0.4333274	-2.8106399	-0.0718635
H	-0.0268864	-3.6705169	-0.6295765
H	0.0636136	-2.6986899	0.9022045
O	-0.3361704	-1.6657959	-0.8474505
C	4.6951806	-1.4792249	-0.1071035
C	4.4227666	-0.3473929	0.6488295
C	3.1524016	0.2236381	0.6167205
C	2.1597016	-0.3389879	-0.1667335
C	2.4342956	-1.4603859	-0.9462945
C	3.6981926	-2.0349479	-0.9044925
H	5.1968936	0.0877971	1.2772375
H	2.9499896	1.0849111	1.2415605
H	1.6882526	-1.8675689	-1.6262895
H	3.9197676	-2.9102879	-1.5146405
C	6.0453336	-2.1178679	-0.1107005
F	6.8956366	-1.5249139	0.7339605
F	6.6027896	-2.0812909	-1.3303575
F	5.9764016	-3.4131349	0.2330225
Br	0.1374556	-0.2847449	2.1116845

c2-S

Ni	-2.1724749	0.2343883	-0.7905704
Br	-3.9765969	1.6516563	-0.1663804
C	-1.6180629	-3.3175657	0.6803276
C	-3.1346159	-3.3975657	0.8187806
C	-3.5738959	-2.0274517	0.3248466
C	-1.3133969	-1.9106027	1.1733176

H	-1.0809909	-4.0854947	1.2485506
H	-1.3326659	-3.4014817	-0.3785494
H	-3.4160179	-3.5342727	1.8738626
H	-3.5837409	-4.2134677	0.2419996
H	-3.6527579	-2.0160857	-0.7726874
H	-4.5293059	-1.6720087	0.7239536
H	-0.3874009	-1.4994547	0.7513846
H	-1.2393369	-1.8843357	2.2711536
N	-2.4789049	-1.0944297	0.7360956
H	-2.8126009	-0.4998277	1.4928696
C	-0.0921109	3.1104993	1.3900126
C	-0.8112929	3.7261833	0.1947606
C	-0.6162179	2.6725573	-0.8854564
C	-0.5466459	1.6621873	1.3017596
H	0.9991121	3.1733063	1.2553596
H	-0.3482669	3.5777673	2.3476126
H	-0.4197139	4.7051263	-0.1027444
H	-1.8842919	3.8285703	0.4097896
H	-1.4135559	2.6775523	-1.6401844
H	0.3489821	2.7969373	-1.3969494
H	-1.5582399	1.5596013	1.7179026
H	0.1176561	0.9436153	1.7982556
N	-0.6019409	1.3646403	-0.1547634
H	0.2382221	0.8524863	-0.4271184
C	3.3995111	0.2108793	-0.1839704
C	2.6616321	-0.9750347	-0.1755804
C	1.6598451	-1.1716757	-1.1237454
C	1.3608581	-0.2095587	-2.0887994
C	2.1385531	0.9555773	-2.0994914
C	3.1345891	1.1748943	-1.1595294
H	2.8570961	-1.7514087	0.5606146
H	1.0683991	-2.0876477	-1.1015244
H	1.9444771	1.7164903	-2.8576234
H	3.7286061	2.0868813	-1.1604094
O	4.3807371	0.5163633	0.7010246
C	4.6998581	-0.4384947	1.6816616
H	5.0438181	-1.3823927	1.2325676
H	5.5096361	-0.0102797	2.2777316
H	3.8420381	-0.6481887	2.3392486
C	0.2310661	-0.3790887	-3.0700224
H	0.5370981	-1.0375097	-3.8952594
H	-0.0065609	0.5937753	-3.5226244

| S | -1.3001869 | -1.1466117 | -2.3914614 |

TSc2-S

Ni	0.2084731	-0.8455915	0.1194938
Br	1.1738181	-2.6968875	1.3621338
C	-3.3240839	0.1588325	2.6507418
C	-2.2069829	0.0860395	3.6913088
C	-0.9619609	0.1682405	2.8245638
C	-2.7261289	-0.5268945	1.4085188
H	-4.2576059	-0.3101235	2.9817458
H	-3.5483069	1.2102705	2.4181498
H	-2.2287879	-0.8779235	4.2213448
H	-2.2645769	0.8811645	4.4432798
H	-0.8043699	1.1911385	2.4542648
H	-0.0321369	-0.1668255	3.2959948
H	-2.8652059	0.0978815	0.5156228
H	-3.1766609	-1.5077095	1.2102218
N	-1.2712789	-0.7037375	1.6682728
H	-1.1107149	-1.6610335	1.9950408
C	-0.7547919	-4.1928845	-1.2430812
C	-0.1781529	-3.4673075	-2.4728942
C	-0.9319449	-2.1453905	-2.5242792
C	-1.7010399	-3.1826885	-0.5951662
H	-1.2882089	-5.1132695	-1.5059422
H	0.0454341	-4.4477305	-0.5398732
H	-0.2986089	-4.0309665	-3.4044722
H	0.8936021	-3.2790005	-2.3347222
H	-0.3581949	-1.3229495	-2.9671462
H	-1.8738889	-2.2531425	-3.0892712
H	-1.6599309	-3.2146405	0.4991828
H	-2.7432209	-3.3535915	-0.9138662
N	-1.2439219	-1.8642665	-1.1027142
H	-2.0089009	-1.1876845	-1.0597892
C	6.1516221	0.5650895	-0.0061362
C	5.4990501	-0.5241135	0.5845218
C	4.1462621	-0.7278735	0.4100498
C	3.4182521	0.2017235	-0.3482262
C	4.0630641	1.2495725	-1.0072002
C	5.4258171	1.4386475	-0.8042002
H	6.0685821	-1.2238605	1.1959968
H	3.6301101	-1.5660615	0.8764898
H	3.5191301	1.9027085	-1.6867252

H	5.9278791	2.2665235	-1.3004792
C	7.6137411	0.7260705	0.2135578
F	7.9137551	0.8407195	1.5187288
F	8.1092671	1.8073025	-0.4027202
F	8.3075821	-0.3360225	-0.2305492
Br	1.9925501	-0.7812555	-1.7063402
C	-3.0732549	2.0822995	-1.1598582
C	-2.7107319	2.7837965	-0.0086512
C	-1.3684829	2.8537505	0.3595598
C	-0.3660839	2.2467335	-0.3945092
C	-0.7478239	1.5710235	-1.5630132
C	-2.0792799	1.4815925	-1.9398432
H	-3.4587769	3.2815285	0.6041458
H	-1.0944159	3.4080915	1.2588938
H	0.0249401	1.1201215	-2.1862112
H	-2.3761919	0.9703445	-2.8552762
O	-4.3462599	1.9227305	-1.5965962
C	-5.3810309	2.4510845	-0.8036402
H	-5.3109059	3.5456415	-0.7191302
H	-6.3170819	2.1910605	-1.3037092
H	-5.3769869	2.0124475	0.2072368
C	1.0707631	2.3200275	0.0209898
H	1.2433971	3.1971555	0.6565628
H	1.7246391	2.4285235	-0.8571722
S	1.6551831	0.8515515	0.9667898

c3-S

Ni	-0.2700860	1.0252808	-0.0217290
Br	-1.2856230	2.5907738	1.5240210
C	3.2232020	-0.2981592	2.4931370
C	2.0802610	-0.3706772	3.5041820
C	0.8650010	-0.4032272	2.5938580
C	2.6317200	0.5010538	1.3172920
H	4.1342780	0.1577008	2.8965460
H	3.4828310	-1.3121912	2.1542560
H	2.0519080	0.5335188	4.1305890
H	2.1462770	-1.2376992	4.1712140
H	0.7743840	-1.3863232	2.1097070
H	-0.0904740	-0.1647252	3.0736470
H	2.8078970	-0.0172222	0.3652250
H	3.0572830	1.5098448	1.2412250
N	1.1654270	0.6091818	1.5557320

H	0.9766740	1.5121778	2.0019690
C	0.6506070	4.5275908	-0.8011320
C	0.2528820	3.9652488	-2.1793890
C	1.0738480	2.6929478	-2.3291060
C	1.6002940	3.4866108	-0.2114130
H	1.1378530	5.5073018	-0.8639900
H	-0.2295870	4.6246118	-0.1560310
H	0.4446500	4.6636918	-3.0015090
H	-0.8118710	3.7041808	-2.1946760
H	0.5712600	1.9226058	-2.9215970
H	2.0640060	2.9075368	-2.7674010
H	1.4738700	3.3669128	0.8705970
H	2.6525840	3.7475108	-0.4177020
N	1.2591060	2.2333358	-0.9298690
H	2.0478630	1.5855318	-0.8974110
C	-6.0967150	-0.7264322	0.0771500
C	-5.3290800	0.3287128	0.5664360
C	-3.9618430	0.1818678	0.7331200
C	-3.3621490	-1.0390632	0.4182640
C	-4.1290100	-2.0993112	-0.0597260
C	-5.4978800	-1.9388302	-0.2388680
H	-5.8048480	1.2793228	0.8024310
H	-3.3546620	1.0132708	1.0904630
H	-3.6703360	-3.0588492	-0.2904540
H	-6.0995750	-2.7616932	-0.6166000
C	-7.5663940	-0.5121332	-0.0989210
F	-8.1467840	-0.1500692	1.0542330
F	-8.1940470	-1.6099162	-0.5348940
F	-7.8168980	0.4686248	-0.9756840
Br	-1.7594180	1.0428168	-1.9049390
C	3.1778530	-2.0368422	-1.2048830
C	2.6033940	-2.9057682	-0.2749190
C	1.2163390	-2.9568782	-0.1522150
C	0.3831760	-2.1595302	-0.9341290
C	0.9762960	-1.2942232	-1.8648370
C	2.3537870	-1.2346122	-2.0023470
H	3.2199980	-3.5498132	0.3475840
H	0.7715950	-3.6442852	0.5699840
H	0.3329750	-0.6674612	-2.4839610
H	2.8212690	-0.5791572	-2.7365420
O	4.5097190	-1.8879212	-1.3981920
C	5.3810750	-2.6613432	-0.6094150

H	5.2241980	-3.7383842	-0.7686300
H	6.3946010	-2.3975162	-0.9207390
H	5.2634150	-2.4360192	0.4621940
C	-1.1049730	-2.2158092	-0.7806710
H	-1.4477150	-3.2483722	-0.6415200
H	-1.6175540	-1.7616182	-1.6379000
S	-1.6081320	-1.2276892	0.6988820

TSc3-S

Ni	-0.8538008	0.4104193	-0.7117634
Br	-1.1688648	2.7626453	-1.6420254
C	-1.4539888	1.2023023	3.5344336
C	-2.8352798	1.6007253	3.0279326
C	-2.8067348	1.0366663	1.6185586
C	-0.5552378	1.4176103	2.3144706
H	-1.1173828	1.7721543	4.4079566
H	-1.4558538	0.1378183	3.8121756
H	-2.9351428	2.6961673	2.9957776
H	-3.6565968	1.2023123	3.6344416
H	-2.9483118	-0.0543057	1.6396526
H	-3.5480168	1.4587163	0.9308656
H	0.2396742	0.6639703	2.2548396
H	-0.0762998	2.4056243	2.3289386
N	-1.4438788	1.3362873	1.1176926
H	-1.4763918	2.2591833	0.6722606
C	3.1969002	2.1701303	-0.5111804
C	2.7473362	2.3625823	-1.9544444
C	1.7579632	1.2196903	-2.1835984
C	1.8956782	1.7385893	0.1443066
H	3.9422822	1.3596933	-0.4426964
H	3.6294992	3.0712693	-0.0597694
H	3.5712452	2.3535303	-2.6771604
H	2.2212122	3.3227563	-2.0522164
H	0.9155482	1.5238743	-2.8098874
H	2.2400012	0.3486723	-2.6464134
H	1.2325342	2.6058753	0.2765346
H	2.0186832	1.2317403	1.1099186
N	1.2610532	0.8165433	-0.8239664
H	1.6427962	-0.1119577	-0.6415674
C	-5.3933848	-0.8722967	-0.7915024
C	-4.4533908	-1.8052047	-0.3792744
C	-3.1016148	-1.5724477	-0.6271284

C	-2.6948288	-0.3623467	-1.1888384
C	-3.6447758	0.5277223	-1.7040724
C	-4.9870158	0.2816523	-1.4713214
H	-4.7711518	-2.7303877	0.0958186
H	-2.3791418	-2.3529137	-0.3898924
H	-3.3208578	1.4332523	-2.2113844
H	-5.7370708	0.9916003	-1.8191774
C	-6.8557838	-1.0794297	-0.5632244
F	-7.5393298	-1.0632677	-1.7150414
F	-7.3695288	-0.1012317	0.1980386
F	-7.1199058	-2.2398977	0.0456256
Br	-0.8700118	-0.8719027	-2.7217704
C	4.5514312	-1.4870217	-0.4938774
C	4.0296332	-1.6729057	0.7883666
C	2.7364272	-2.1642727	0.9356576
C	1.9407792	-2.4703977	-0.1717534
C	2.4828002	-2.2828287	-1.4495424
C	3.7719762	-1.8068667	-1.6120284
H	4.6178542	-1.4411597	1.6724726
H	2.3307022	-2.3052707	1.9384256
H	1.8674262	-2.4882697	-2.3259774
H	4.2018952	-1.6565537	-2.6004754
O	5.7831692	-0.9981717	-0.7579334
C	6.6041012	-0.6486227	0.3317016
H	6.8185192	-1.5182797	0.9701586
H	7.5387442	-0.2777807	-0.0951974
H	6.1466862	0.1441683	0.9426176
C	0.5202642	-2.9223797	0.0059676
H	0.4451132	-3.8369847	0.6064396
H	0.0467642	-3.0902667	-0.9712524
S	-0.3771188	-1.5803227	0.8653096

c4-S

Ni	-0.8932894	0.3435857	-0.7225919
Br	-1.2019144	2.6372817	-1.7918559
C	-1.2415154	1.6535097	3.4662631
C	-2.6745394	1.9133857	3.0197551
C	-2.7275694	1.1264477	1.7234041
C	-0.4517034	1.6824487	2.1544281
H	-0.8631844	2.3769857	4.1972601
H	-1.1724254	0.6547547	3.9221531
H	-2.8306274	2.9838167	2.8180861

H	-3.4272374	1.5917257	3.7484621
H	-2.7967904	0.0481157	1.9306381
H	-3.5507354	1.3898287	1.0508491
H	0.3502446	0.9349867	2.1473221
H	0.0077876	2.6627517	1.9744351
N	-1.4303404	1.4085587	1.0598211
H	-1.5464144	2.2696587	0.5131891
C	3.1938726	2.0847057	-0.7688239
C	2.6624706	2.2446767	-2.1873579
C	1.6782646	1.0872647	-2.3348319
C	1.9278936	1.6805977	-0.0323219
H	3.9390856	1.2720827	-0.7228999
H	3.6550446	2.9932577	-0.3627949
H	3.4429456	2.2277477	-2.9566079
H	2.1206866	3.1972707	-2.2742679
H	0.8151496	1.3466777	-2.9510809
H	2.1589766	0.2015807	-2.7696119
H	1.2838216	2.5589567	0.1144211
H	2.1004486	1.1959497	0.9373951
N	1.2260976	0.7423107	-0.9394969
H	1.6024766	-0.1865553	-0.7453239
C	-5.4693594	-0.9443883	-0.7307089
C	-4.5256894	-1.7723773	-0.1372429
C	-3.1713544	-1.4702813	-0.2527649
C	-2.7674464	-0.3117153	-0.9073079
C	-3.7042194	0.4782487	-1.5698409
C	-5.0542434	0.1695617	-1.4583569
H	-4.8415474	-2.6642323	0.3996151
H	-2.4456454	-2.1577133	0.1822451
H	-3.3851494	1.3484037	-2.1373019
H	-5.7948634	0.8002867	-1.9494659
C	-6.9335314	-1.2118063	-0.6038799
F	-7.5431094	-1.2061423	-1.7967809
F	-7.5390434	-0.2685193	0.1355871
F	-7.1907644	-2.3912203	-0.0268419
Br	-0.7879954	-1.1161693	-2.5745669
C	4.5109616	-1.5761933	-0.4706879
C	4.0747526	-1.7679633	0.8426481
C	2.7944396	-2.2589743	1.0699201
C	1.9270306	-2.5589583	0.0113131
C	2.3854246	-2.3668523	-1.3019029
C	3.6622396	-1.8968333	-1.5407109

H	4.7192296	-1.5416293	1.6877841
H	2.4546306	-2.4099483	2.0948881
H	1.7072996	-2.5526813	-2.1342539
H	4.0318766	-1.7466113	-2.5533039
O	5.7169006	-1.0811443	-0.8131069
C	6.5888136	-0.6793023	0.2196341
H	6.8689656	-1.5263173	0.8622571
H	7.4834006	-0.2888303	-0.2702599
H	6.1375796	0.1122047	0.8362951
C	0.5109836	-2.9747793	0.2828091
H	0.4346376	-3.8279423	0.9659561
H	-0.0295304	-3.1806413	-0.6500739
S	-0.1826514	-1.4829013	1.0703911