

Supporting information

Deciphering the chain propagation mechanism in regioselective polymerization via alkene difunctionalization

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I. Computational Methodology

All calculations were performed using the Gaussian 16 (Revision C.01) suite of quantum chemical program.¹ The geometries of all stationary points were optimised at the B3LYP² level of theory with Grimme's dispersion correction³ and the Becke–Johnson damping scheme⁴. For geometry optimisations, the Stuttgart–Dresden double- ζ basis set (SDD)⁵ was used for Ni and Br, while the 6-31G(d,p) basis set was employed for all other atoms.⁶ Frequency analysis was performed to verify whether each optimised geometry corresponded to a minimum or a transition state. Additionally, intrinsic reaction coordinate (IRC) calculations were carried out to confirm that each transition state connects to the corresponding minima on both sides of the reaction pathway.⁷ Single-point energy calculations were performed using the M06-L⁸ functional with the larger 6-311++G(d,p)⁹ basis set for all atoms except Ni and Br, for which the SDD basis set was retained. Solvent effects were included during the single-point calculations using the SMD implicit solvation model, with toluene as the continuum dielectric ($\epsilon = 2.37$).¹⁰

Activation strain analysis was performed to understand the effect of the distortion and interaction energy in the transition states.¹¹ The activation strain energy was decomposed into two components: the distortion energy (ΔE_{dist}), which corresponds to the energy required to deform the individual fragments from their equilibrium geometries to the transition state geometry, and the interaction energy (ΔE_{int}), which represents the interaction between the distorted fragments.

$$\Delta E_{act}^{\ddagger} = \Delta E_{dist} + \Delta E_{int}$$

Further partitioning of the interaction energy was carried out using the second-generation Energy Decomposition Analysis (EDA), based on the absolutely localised molecular orbital (ALMO-EDA)¹² method, as implemented in Q-Chem 6.2.¹³ The interaction energy between the reacting fragments can be further dissected as:

$$\Delta E_{int} = \Delta E_{pauli} + \Delta E_{elstat} + \Delta E_{pol} + \Delta E_{ct} + \Delta E_{disp}$$

According to the above equation, the interaction energy ΔE_{int} constitutes of Pauli repulsion (ΔE_{pauli}), electrostatic interaction (ΔE_{elstat}), polarisation (ΔE_{pol}), charge

transfer (ΔE_{ct}) and dispersion (ΔE_{disp}). The ALMO-EDA calculations were performed incorporating the solvent effects, at the M06-L/6-311G(d,p)/SDD level of theory. Natural Bond Orbital (NBO) analysis was conducted on key transition states to characterize donor–acceptor orbital interactions and to obtain the corresponding second-order perturbation stabilisation energies using NBO 7.0.¹⁴ Space-filling models of the key transition states were generated using UCSF Chimera.¹⁵ The transition state geometries were generated using CYL view¹⁶, and NBO plots were generated using Chemcraft software.¹⁷

II. Other possible mechanistic pathways

1. Direct transmetalation in the absence of base

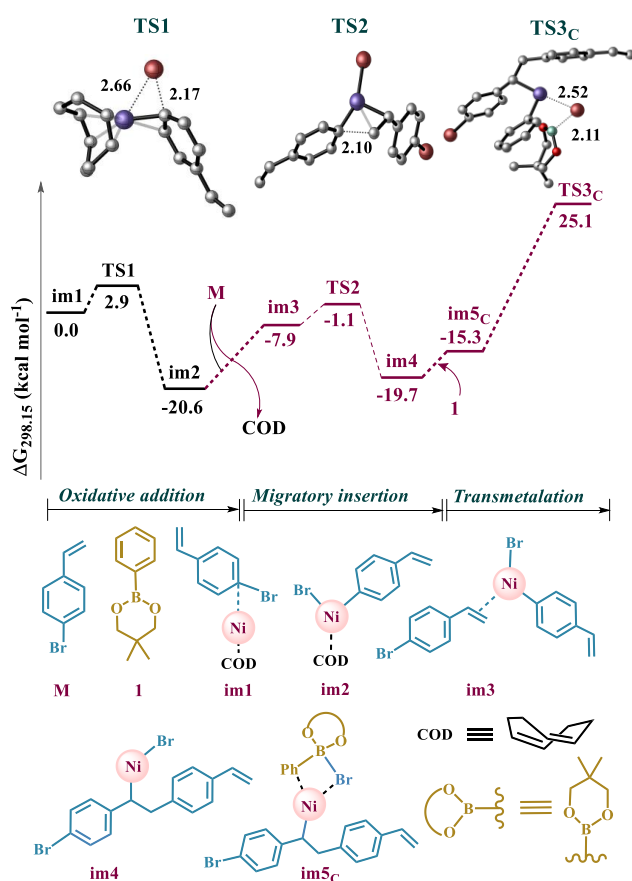


Fig. S1. Computed Gibbs free energy profile diagram for the direct transmetalation in the absence of base KOEt, in kcal/mol, at the SMD/M06L/6-311++G(d,p),SDD(Ni,Br)/B3LYP-D3BJ/6-31G(d),SDD(Ni,Br) level of theory. Key intermediates are provided. The bond length in the transition states is given in Å

A base-free direct transmetalation was evaluated via a transition state of **TS3_C** (Fig. S1). This pathway exhibits a higher activation barrier of 45.7 kcal/mol with respect to the stable intermediate **im2**, rendering it highly unfavourable compared to the base-assisted transmetalation, involving potassium ethoxide (Figure 1a).

2. Competing β -hydride elimination vs transmetalation

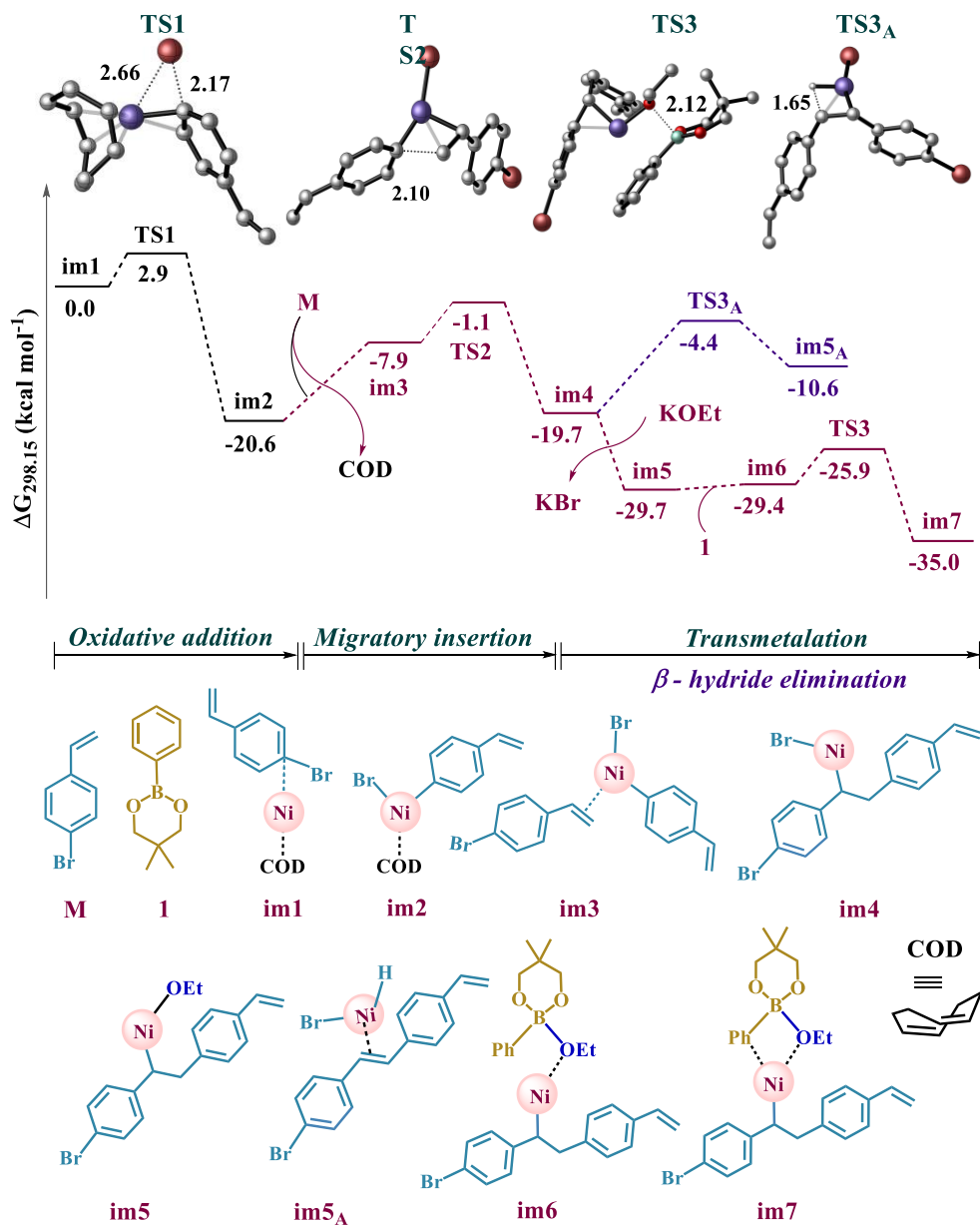


Fig. S2. Computed Gibbs free energy profile diagram of competing β -hydride elimination and transmetalation, in kcal/mol, at the SMD/M06L/6-311++G(d,p),SDD(Ni,Br)//B3LYP-D3BJ/6-31G(d),SDD(Ni,Br) level of theory. Key intermediates are provided. The bond length in the transition states is given in Å

After migratory insertion, there is a possibility of competing β -hydride elimination alongside transmetalation (Fig. S2). The β -hydride elimination occurs via a 4-membered transition state, **TS3_A**, with an energy barrier of 16.2 kcal/mol relative to stable intermediate **im2**, which is higher than that of the competing base-assisted transmetalation. The resulting Ni-alkene π intermediate is unstable when compared to the biaryl precursor obtained from transmetalation, making the β -hydride elimination less favourable.

3. Ligand-free reductive elimination (Absence of COD)

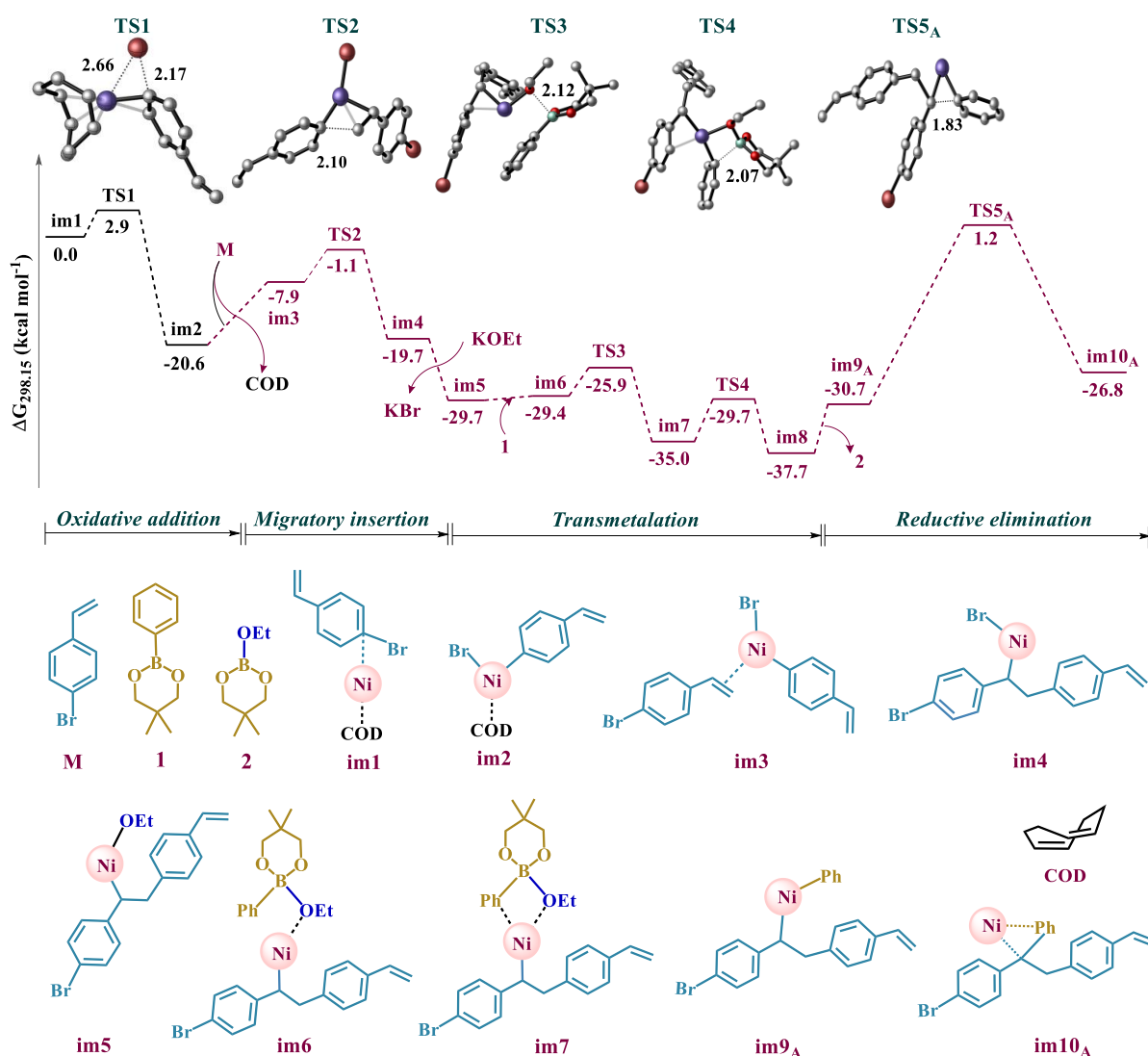


Fig. S3. Computed Gibbs free energy profile diagram for the alkene difunctionalisation of 4-bromostyrene, highlighting reductive elimination in the absence of COD ligand, in kcal/mol at the SMD/M06L/6-311++G(d,p),SDD(Ni,Br)//B3LYP-D3BJ/6-31G(d),SDD(Ni,Br) level of theory. Key intermediates are provided. The bond length in the transition states is given in Å

To investigate the role of ligand in assisting reductive elimination, a ligand-free pathway was examined (Fig. S3). The computed transition state **TS5_A** has an activation energy of 38.9 kcal/mol with respect to the stable intermediate **im8**, which is significantly higher than the ligand-assisted reductive elimination. This highlights the importance of the ligand in the C-C bond formation during reductive elimination.

4. Competing Reductive elimination vs β -hydride elimination

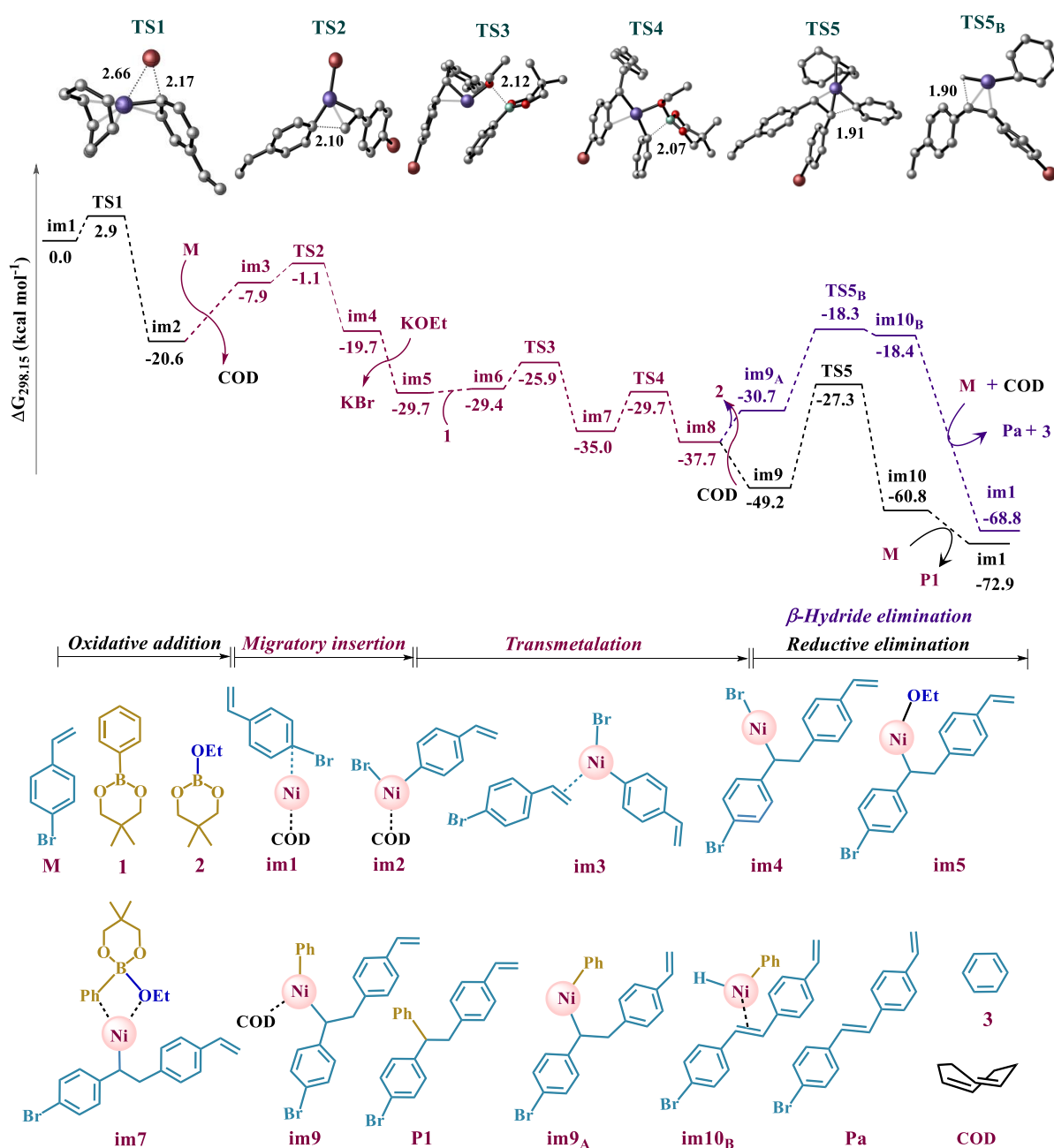


Fig. S4. Computed Gibbs free energy profile diagram for the alkene difunctionalisation of 4-bromostyrene, highlighting reductive elimination and the competing β -hydride elimination, in

kcal/mol at the SMD/M06L/6-311++G(d,p),SDD(Ni,Br)//B3LYP-D3BJ/6-31G(d),SDD(Ni,Br) level of theory. Key intermediates are provided. The bond length in the transition states is given in Å

A competing β -hydride elimination can also occur from the same biaryl intermediate **im8**, via the transition state **TS5_B** (Fig. S4). However, the coordination of COD makes the reductive elimination more feasible (**TS5**) for the formation of difunctionalised product **P1** instead of the Heck product **P_a**.

5. Pathways for the first chain propagation

There are three possible pathways for the first propagation. These pathways follow the same sequence of steps: oxidative addition, migratory insertion, transmetalation and reductive elimination. The only distinction is between species that undergo oxidative addition and those that undergo migratory insertion, while the latter steps remain mechanistically similar.

a. First propagation via the chain-end mechanism and monomer-initiated mechanism

The product formed, **P1** (Figure 1a), can propagate either via a chain-end mechanism (Path A) or via a monomer-initiated mechanism (Path B) (Fig. S5a). In Path A, the bromine end of the product **P1** undergoes oxidative addition, followed by migratory insertion of a molecule of 4-bromostyrene into the Ni-C bond. In contrast, in Path B, the monomer undergoes oxidative addition, followed by migratory insertion of the vinyl end of the product **P1** into the Ni-C bond. In both pathways, the subsequent step involves base-assisted transmetalation with phenylboronic ester, followed by a C-C bond-forming reductive elimination, to give product **P2**. In both these pathways, migratory insertion is identified as the rate-determining step. However, in Path B, the stepwise transmetalation, involving the transfer of the aryl group, occurs via a transition state **TS4_b**, which has a difference in activation free energy of 15.9 kcal/mol relative to Path A.

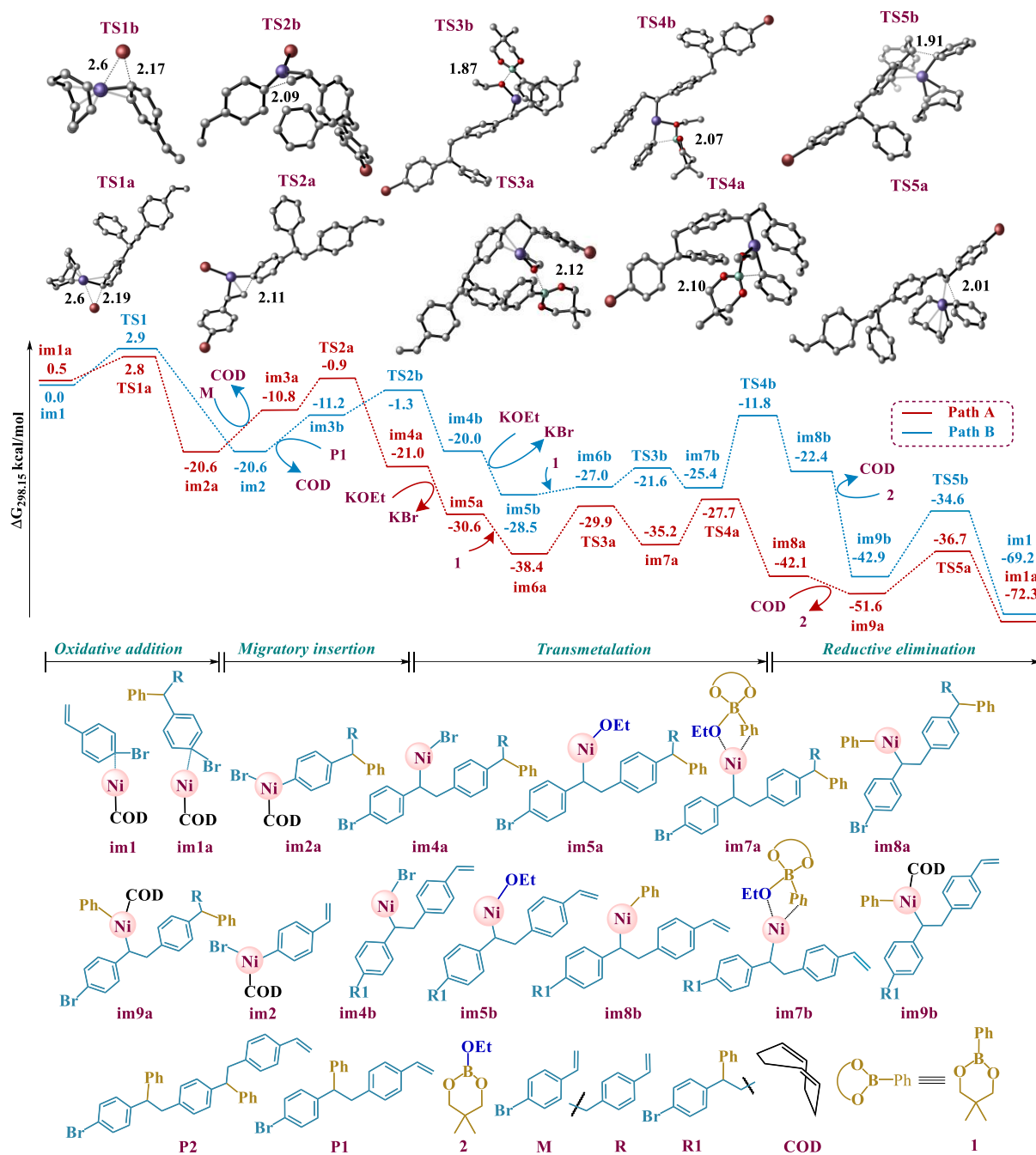


Fig. S5a. Computed Gibbs free energy profile diagram for the first propagation via chain-end mechanism (Path A) and monomer-initiated mechanism (Path B) in kcal/mol at the SMD/M06L/6-311++G(d,p),SDD(Ni,Br)//B3LYP-D3BJ/6-31G(d),SDD(Ni,Br) level of theory. Key intermediates are provided. The bond length in the transition states is given in Å

b. First propagation via the step-growth mechanism

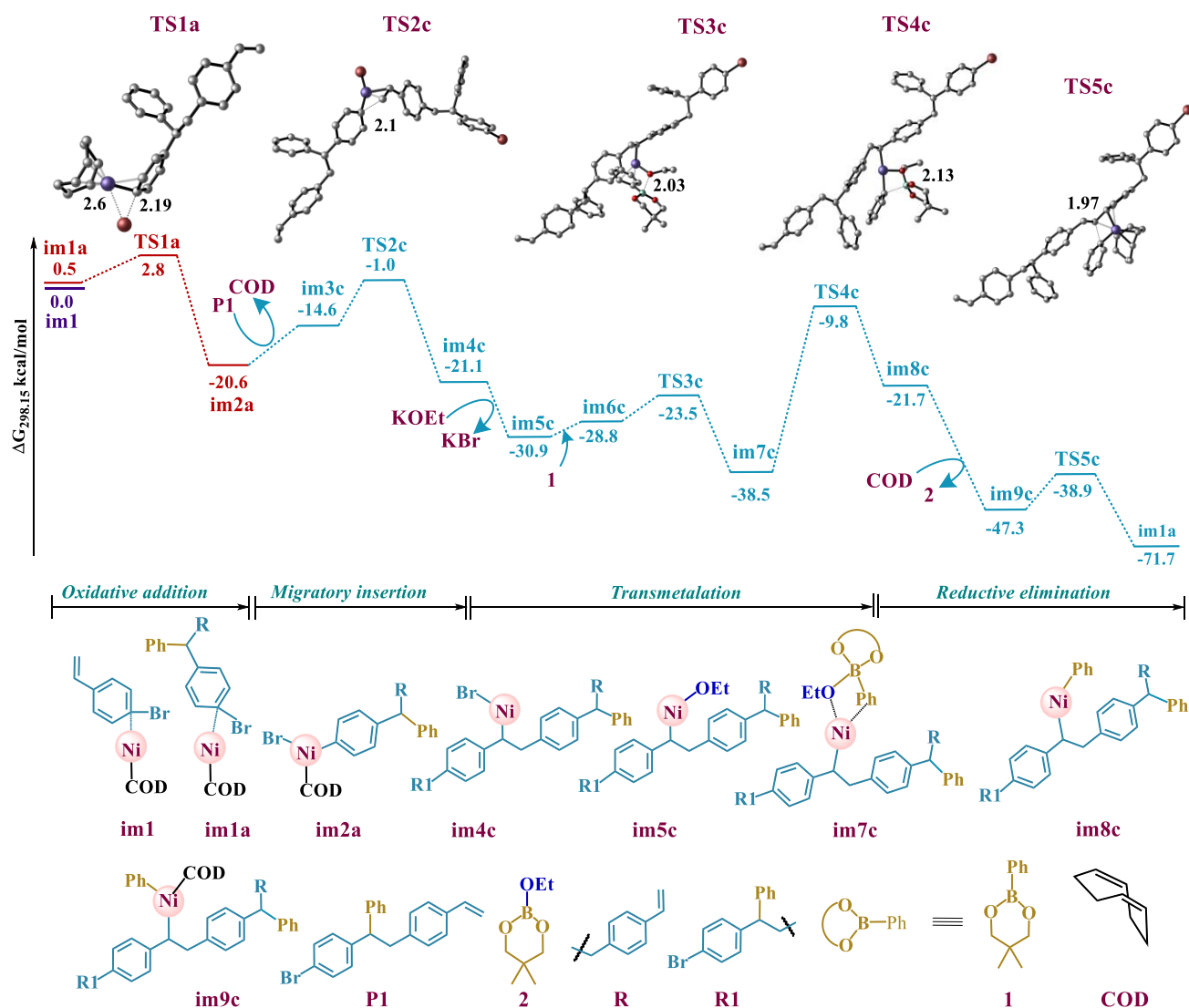


Fig. S5b. Computed Gibbs free energy profile diagram for the first propagation via step-growth mechanism (Path C) in kcal/mol at the SMD/M06L/6-311++G(d,p),SDD(Ni,Br)//B3LYP-D3BJ/6-31G(d),SDD(Ni,Br) level of theory. Key intermediates are provided. The bond length in the transition states is given in Å.

Another possibility of chain propagation is self-coupling of the product **P1** unit via a step-growth polymerisation mechanism (Fig. S5b). The sequence of steps remains the same. The first step involves oxidative addition of bromine to the end of **P1** unit, followed by migratory insertion of the vinyl end of the **P1** unit into the Ni-C bond. The subsequent step involves a base-assisted step-wise transmetalation with phenylboronic ester, followed by a C-C bond-forming reductive elimination resulting in a product with an increased chain length, **P2a**. In this pathway, the transmetalation step possess a very high energy barrier of 28.7 kcal/mol (relative to the stable intermediate **im7c**), making it less favourable pathway compared to Path A.

6. Different possibilities of the second propagation

a. Propagation via the step-growth mechanism and chain-end mechanism

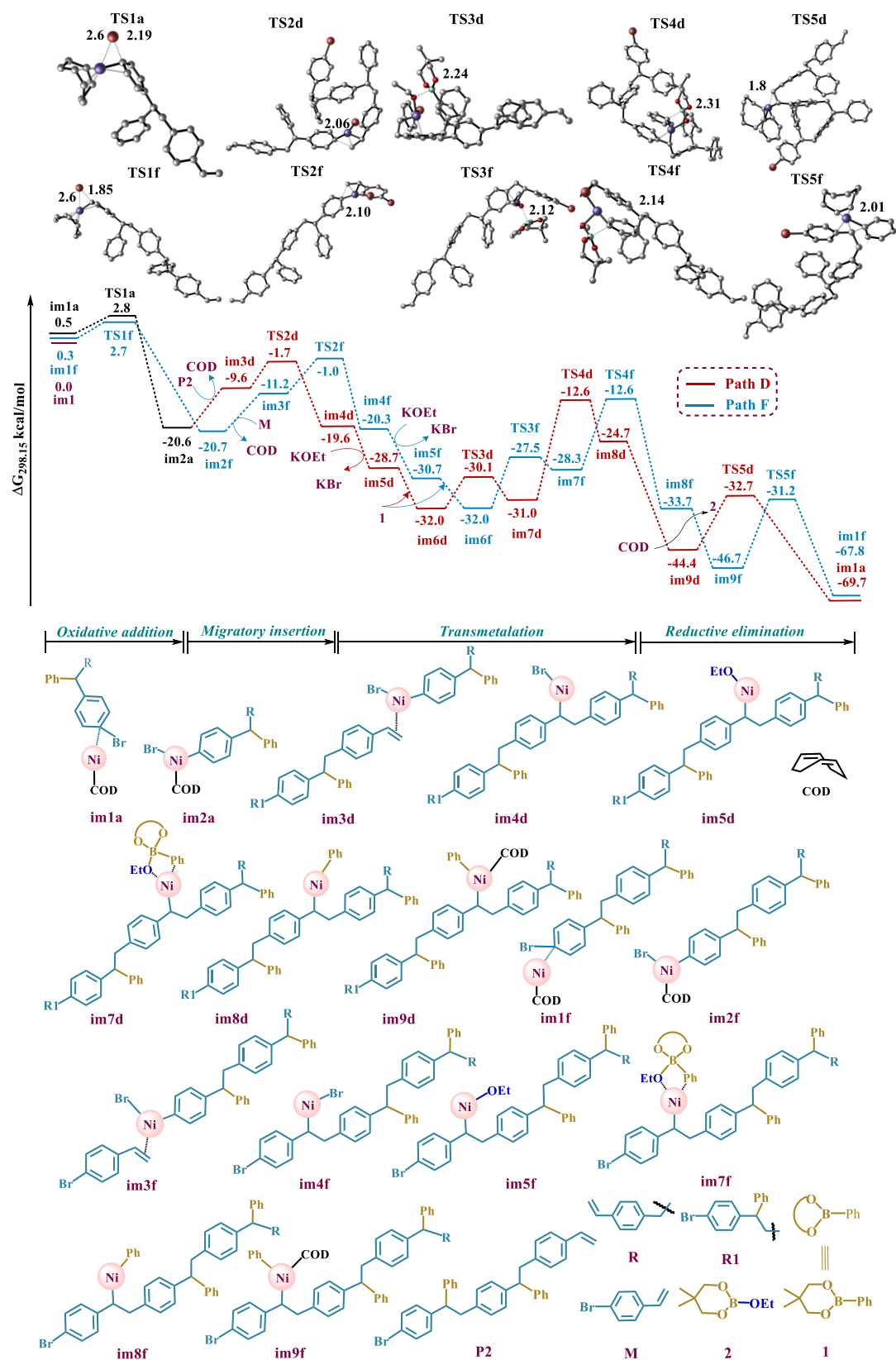


Fig. S6a. Computed Gibbs free energy profile diagram for the second propagation via step-growth and chain-end mechanism (Path D and Path F) in kcal/mol at the SMD/M06L/6-311++G(d,p),SDD(Ni,Br)//B3LYP-D3BJ/6-31G(d),SDD(Ni,Br) level of theory. Key intermediates are provided. The bond length in the transition states is given in Å.

There are four possible pathways for the second propagation. These pathways follow the same sequence of steps: oxidative addition, migratory insertion, transmetalation and reductive elimination. The only distinction is between the species that undergo oxidative addition and migratory insertion, while the latter steps remain mechanistically similar.

For the second propagation, we have considered all the different possibilities; among them, the more favourable pathways are the coupling of **P1** with **P2** via a step-growth mechanism (Path D) and the chain-end mechanism (Path F) (Fig. S6a). In Path D, the product **P1** undergoes oxidative addition to the Ni(COD) species, followed by migratory insertion of **P2** into the Ni-C bond. Subsequent transmetalation and reductive elimination results in the formation of the product **P3** with a greater chain length. In this pathway, migratory insertion is determined as the rate-determining step.

The chain-end type mechanism (Path F) involves the oxidative addition of **P2** with Ni(COD) followed by migratory insertion of the monomer (4-bromostyrene) to the Ni-C bond. The subsequent steps are the same as the previous ones, yielding product **P3a** characterised by a shorter chain compared to **P3**. The energy barriers for the rate-determining migratory insertion step in Paths D and F are nearly identical, suggesting both are equally favourable for the second propagation.

b. Propagation via coupling of the P2 unit with P1 via a step-growth mechanism

In Path E, which involves a coupling mechanism, the **P2** unit undergoes oxidative addition to the catalytically active Ni(COD) species, followed by migratory insertion of the **P1** unit to the Ni-C bond, resulting in the intermediate **im4e** (Fig. S6b). This is followed by the transmetalation and reductive elimination leading to the product **P3**. Here, the migratory insertion and reductive elimination have an activation energy higher compared to Path D and Path F, making it less favourable pathway.

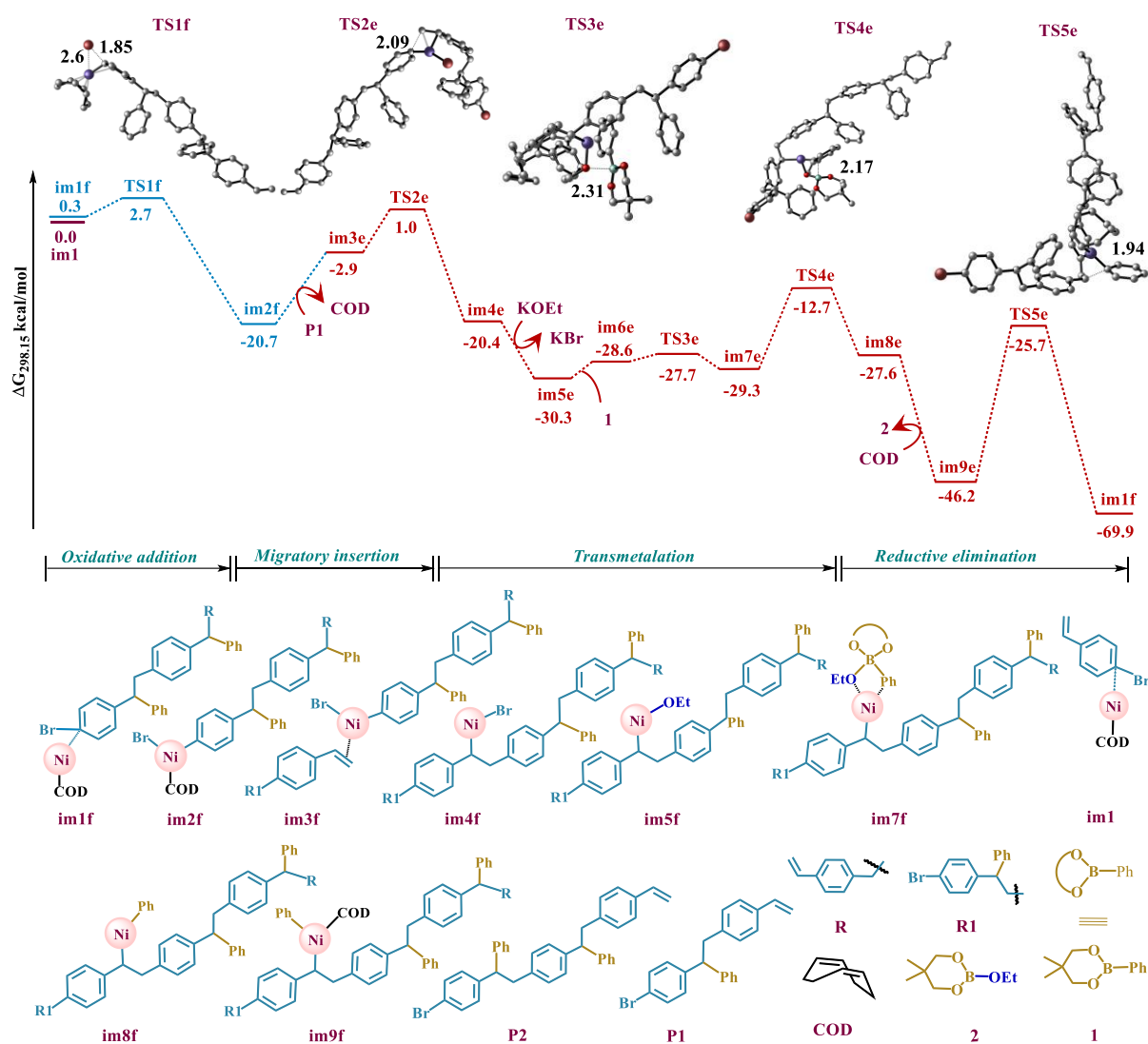


Fig. S6b. Computed Gibbs free energy profile diagram for the second propagation via coupling of P2 unit with P1 unit (Path E) in kcal/mol at the SMD/M06L/6-311++G(d,p),SDD(Ni,Br)//B3LYP-D3BJ/6-31G(d),SDD(Ni,Br) level of theory. Key intermediates are provided. The bond length in the transition states is given in Å.

c. Propagation via a monomer-initiated mechanism

Path G involves a monomer-initiated mechanism; the **P2** undergoes migratory insertion to the Ni-C bond of the oxidative addition product **im2** (Figure 1a). This is followed by the transmetalation and reductive elimination leading to the product **P3a** (Fig. S6c). Here, the reductive elimination traverse through a very high energy barrier compared to Path D and Path F, making it least feasible pathway.

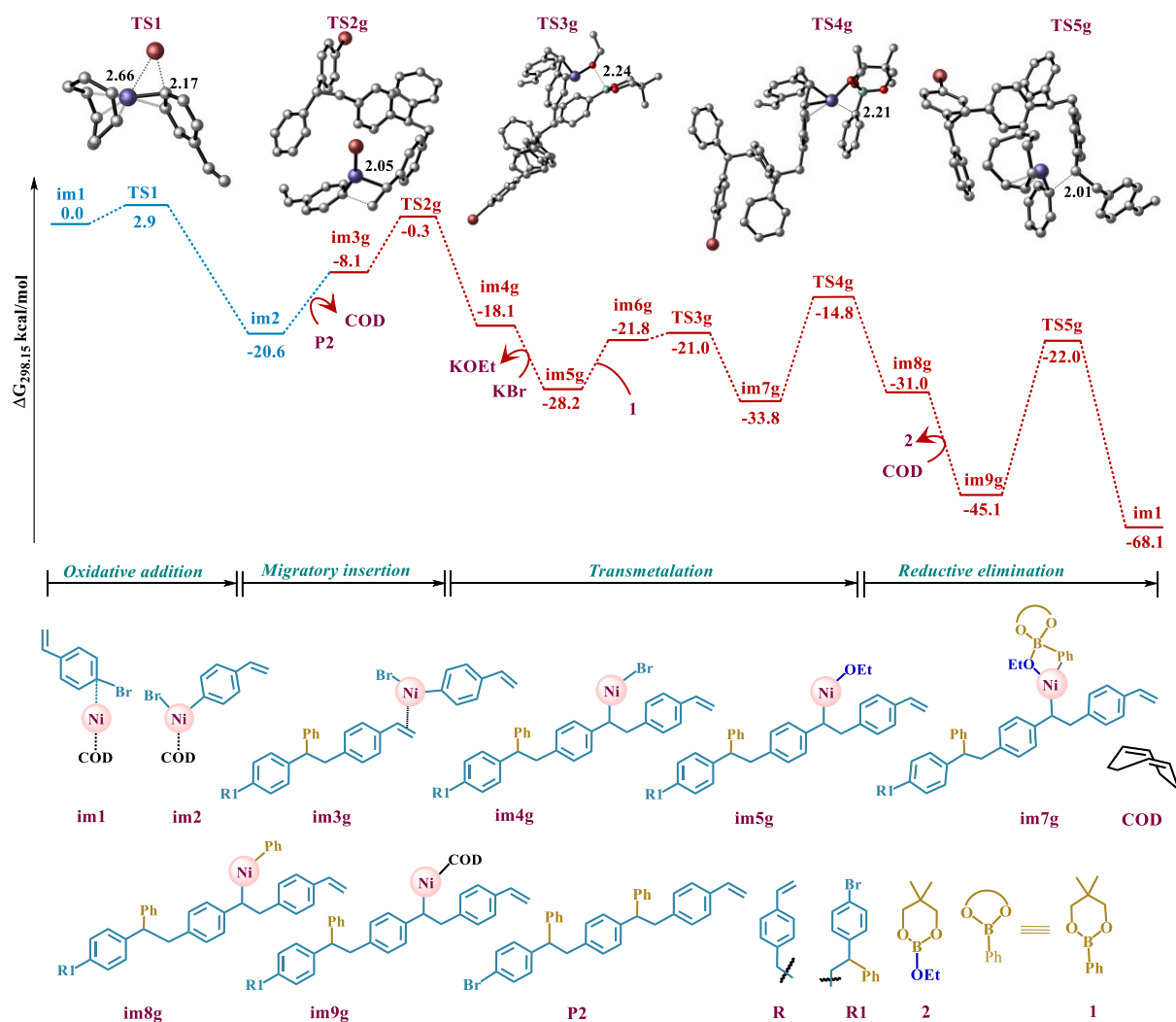


Fig. S6c. Computed Gibbs free energy profile diagram for the second propagation via monomer-initiated mechanism (Path G) in kcal/mol at the SMD/M06L/6-311++G(d,p),SDD (Ni,Br)//B3LYP-D3BJ/6-31G(d),SDD(Ni,Br) level of theory. Key intermediates are provided. The bond length in the transition states is given in Å.

7. Potential formation of a side product

We also looked into the energetics for the formation of potential side-product poly(4-bromostyrene), which occurs by an anionic polymerisation mechanism (Fig. S7). It occurs in the presence of base potassium ethoxide. The reaction proceeds via a transition state, **TSb1**, which has an energy barrier of 50.4 kcal/mol with respect to stable intermediate **im1**.

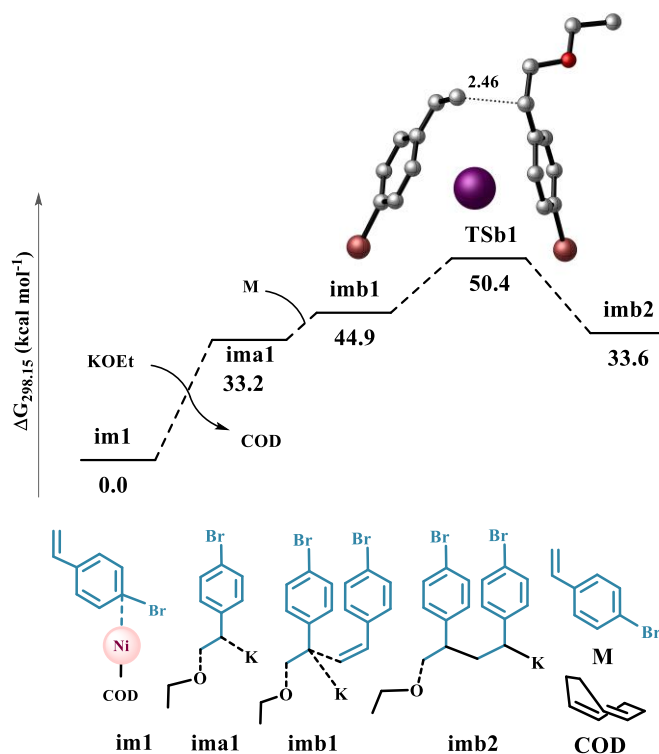


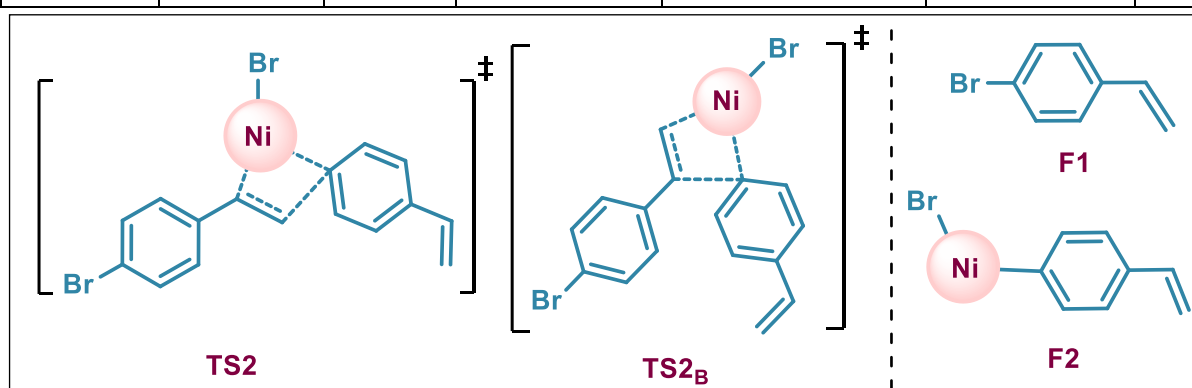
Fig. S7. Computed Gibbs free energy profile diagram for the formation of side-product poly(4-bromostyrene) in kcal/mol at the SMD/M06L/6-311++G(d,p),SDD(Ni,Br)//B3LYP-D3BJ/6-31G(d),SDD(Ni,Br) level of theory. Key intermediates are provided. The bond length in the transition states is given in Å.

III. Distortion-Interaction/Activation-Strain (DI/AS) Analysis

To investigate the selectivity during the migratory insertion step, we have analysed the regioselectivity-controlling transition states **TS2** and **TS2_B** using the distortion–interaction/activation-strain (DI–AS) analysis. The activation strain energy of the transition state (ΔE^\ddagger) is the sum of distortion (ΔE_{dist}) and interaction (ΔE_{int}) energies. As shown in Table S1, the interaction energies are similar for both pathways, and a significant difference of 5.2 kcal/mol is observed for the distortion energy. Lower distortion energy in **TS2** results in a lower activation barrier than in the competing regioselective transition state **TS2_B**. Thus, the observed selectivity is governed by the geometric deformations that are required to reach the transition state.

Table S1. Summary of Distortion-Interaction/Activation-Strain (DI/AS) Analysis for the selectivity-determining Transition States (**TS2** and **TS2_B**). The activation energies (ΔE^\ddagger) are decomposed into distortion (ΔE_{dist}) and interaction energy (ΔE_{int}) contributions. Energies provided are in kcal/mol.

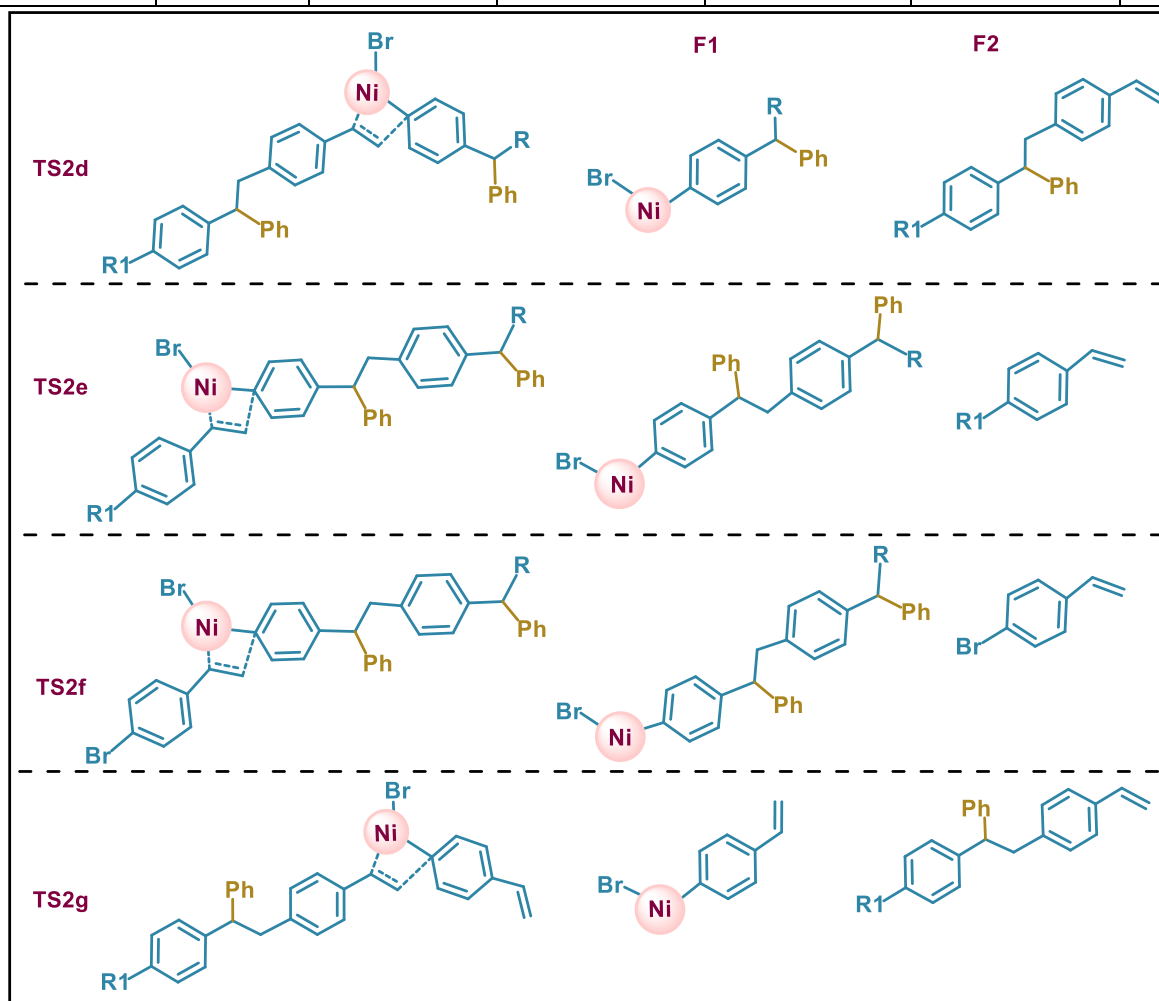
Transition state	Distortion energy (ΔE_{dist})			Interaction energy (ΔE_{int}) (d)	Activation strain ΔE^\ddagger (e) = (c) + (d)	$\Delta\Delta G^\ddagger$
	F1 (a)	F2 (b)	Total (c) = (a) + (b)			
TS2	21.07	12.56	33.62	-61.88	-28.26	0.0
TS2 _B	21.39	17.44	38.83	-63.84	-25.01	2.8



We also performed DI/AS for the migratory insertion step for the second propagation pathways (Path D – Path E) to identify factors influencing the activation barrier, and the results are summarised in Table S2. The DI/AS results highlight that the interaction energy component is the dominant factor accounting for the difference in activation free energies, whereas the distortion energies remain relatively similar. The interaction energy of the competing transition states ($\Delta\Delta E_{\text{int}}$) differs by 14.9 kcal/mol. Thus, the reactivity trends are governed by the difference in the interaction between the reacting fragments.

Table S2. Summary of Distortion-Interaction/Activation-Strain (DI-AS) Analysis for the migratory insertion Transition States (TS2d-TS2g) of second propagation pathways. The activation energies (ΔE^\ddagger) are decomposed into distortion (ΔE_{dist}) and interaction energy (ΔE_{int}) contributions. Energies provided are in kcal/mol.

Transition state	Distortion energy (ΔE_{dist})			Interaction energy (ΔE_{int}) (d)	Activation strain ΔE^\ddagger (e) = (c) + (d)	$\Delta\Delta G^\ddagger$
	F1 (a)	F2 (b)	Total (c) = (a) + (b)			
TS2d	21.36	15.91	37.27	-76.25	-38.98	0.0
TS2e	21.73	15.74	37.47	-66.31	-28.83	2.8
TS2f	20.77	12.26	33.02	-61.39	-28.37	0.8
TS2g	21.18	16.57	37.75	-72.13	-34.39	1.4



IV. Energy Decomposition Analysis

Energy Decomposition Analysis (EDA) was carried out on the selected transition states to obtain further understanding of the factors contributing to the interaction energy. The interaction energy is further decomposed into steric, electronic and dispersion components to identify the factors that control the observed selectivity and reactivity trends.

Although the distortion interaction analysis determines that distortion energy governs the regioselectivity, EDA helps understand the nature of the interactions between the reacting fragments. The EDA results in Table S3 reveal a large variation in the Pauli repulsion component, indicating increased steric congestion in TS2_B compared to TS2. While interaction energy does not account for the observed selectivity, the EDA analysis provides a detailed description of the electronic and steric factors contributing to the interaction energy.

Table S3. Summary of Energy Decomposition Analysis for the selectivity-determining Transition States (TS2 and TS2_B). Energies provided are in kcal/mol

Transition state	Steric effects (ΔE_{steric})		Electronic effects (ΔE_{elec})			Dispersion (ΔE_{disp})
	Distortion (ΔE_{dist})	Paulis (ΔE_{pauli})	Electrostatics (ΔE_{elstat})	Polarisation (ΔE_{pol})	Charge transfer (ΔE_{ct})	
TS2	33.62	252.57	-131.29	-29.32	-90.25	-23.99
TS2 _B	38.83	297.54	-170.01	-66.64	-96.87	-26.74

While DI/AS was performed for the different second propagation pathways, EDA was restricted to the transition states TS2d and TS2e that exhibited a large difference in activation energy. These transition states were evaluated using EDA to identify the steric and electronic factors that determine the difference in reactivity. As shown in Table S4, there are no large differences in the steric and electronic components; however, TS2d exhibits a stronger dispersion interaction ($\Delta\Delta E_{\text{disp}} = 17.38$ kcal/mol). These results indicate that differences in attractive non-covalent interactions account for the variations in interaction energy.

The contribution of electronics, steric and dispersion interactions are shown in the Figure S8.

Table S4. Summary of Energy Decomposition Analysis for the migratory insertion transition states TS2d and TS2e for the second propagation pathways. Energies provided are in kcal/mol.

Transition state	Steric effects (ΔE_{steric})		Electronic effects (ΔE_{elec})			Dispersion (ΔE_{disp})
	Distortion (ΔE_{dist})	Paulis (ΔE_{pauli})	Electrostatics (ΔE_{elstat})	Polarisation (ΔE_{pol})	Charge transfer (ΔE_{ct})	
TS2d	37.37	284.81	-145.18	-36.12	-96.13	-51.34
TS2e	37.47	284.02	-143.31	-43.26	-93.45	-33.96

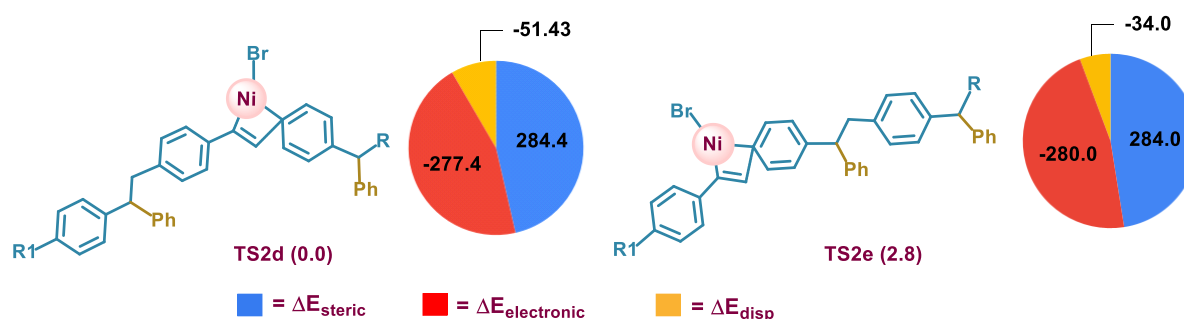


Figure S8. Contributions of different types of interactions (absolute values), as determined by ALMO-EDA analysis for the second propagation migratory insertion transition states TS2d and TS2e. The steric effect (ΔE_{steric}) comprises the sum of distortion energy (ΔE_{dist}) and Pauli repulsion (ΔE_{pauli}), while the electronic effect ($\Delta E_{\text{electronic}}$) corresponds to the sum of electrostatic interaction (ΔE_{elstat}), polarization (ΔE_{pol}) and charge transfer (ΔE_{ct}). Relative Gibbs free energies for the second propagation migratory insertion transition states are provided in kcal mol⁻¹ (values in parentheses)

V. NBO Analysis

1. For first propagation

We have conducted NBO analysis for the transmetalation transition state (TS4a-TS4c) for the different possibilities of chain propagation. Some of the significant donor-acceptor interactions are summarised in the Table S5.

Table S5: Summary of the favourable donor-acceptor interactions for the transmetalation step transition state (TS4a-TS4c) during the first propagation. The donor-acceptor interaction

energies are calculated using second-order perturbation theory (SOPT), and the orbitals involved in the reaction are provided

Interactions	TS4a $\Delta E(\text{SOPT})$ kcal/mol	TS4b $\Delta E(\text{SOPT})$ kcal/mol	TS4c $\Delta E(\text{SOPT})$ kcal/mol
LP(O1) \rightarrow LV(Ni2)	18.94	20.75	14.50
LP(O1) \rightarrow LV(B3)	17.89	17.91	11.16
LP(O1) \rightarrow LV1(B3)	40.93	68.35	105.34
LP(O1) \rightarrow LV2(B3)	121.78	99.74	123.77
LP(O1) \rightarrow LV3(B3)	84.43	70.18	1.35
BD(C4-B3) \rightarrow LV(Ni2)	36.28	23.33	30.17
BD(C4-B3) \rightarrow BD*(Ni2-C5)	34.79	30.81	40.79
Total	355.04	331.07	327.08

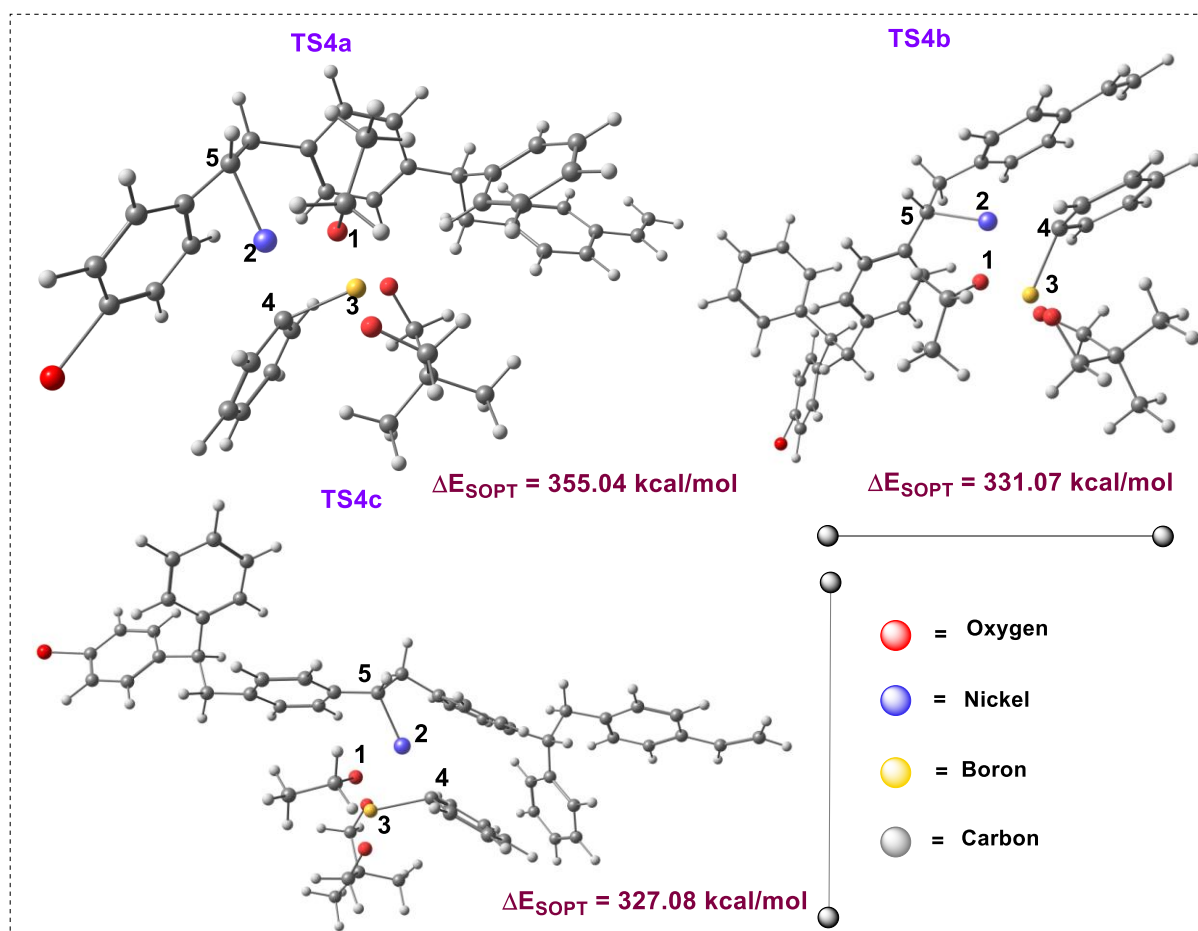


Fig S9. Transition states for the transmetalation steps (TS4a-4c) during the first propagation.

NBO analysis revealed that some of the significant donor-acceptor interactions are from the lone pair orbital of oxygen to the lone vacant orbital of nickel ($LP(O1) \rightarrow LV(Ni2)$) and to the lone vacant orbital of boron ($LP(O1) \rightarrow LV(B3)$) (Fig S9). Another interaction is from the bonding orbital of the B-C bond to the lone vacant orbital of nickel ($BD(C4-B3) \rightarrow LV(Ni2)$) and to the anti-bonding orbital of the Ni-C bond ($BD(C4-B3) \rightarrow BD^*(Ni2-C5)$). The overall SOPT energy is higher for TS4a, which supports a lower activation barrier for the corresponding transition state.

2. For the second propagation

We have also conducted NBO analysis of the reductive elimination transition state (TS5d-TS5g) for different possibilities of second propagation, due to the large variation in energy across the transition states. Some of the significant donor-acceptor interactions are summarised in the Table S6.

Table S6: Summary of the favourable donor-acceptor interactions for the reductive elimination transition state (TS5d-TS5g) during the first propagation. The donor-acceptor interaction

energies are calculated using second-order perturbation theory (SOPT), and the orbitals involved in the reaction are provided.

Interactions	TS5d $\Delta E(\text{SOPT})$ kcal/mol	TS5e $\Delta E(\text{SOPT})$ kcal/mol	TS5f $\Delta E(\text{SOPT})$ kcal/mol	TS5g $\Delta E(\text{SOPT})$ kcal/mol
BD(C1-C2) \rightarrow LV(Ni3)	67.58	31.14	36.17	26.02
BD(C4-C5) \rightarrow LV(Ni3)	34.41	12.73	31.32	15.74
LP(Ni3) \rightarrow BD*(C1-C2)	37.18	21.03	27.60	16.47
BD(C1-C2) \rightarrow RY(Ni3)	24.96	16.08	15.86	7.16
LP(C5) \rightarrow BD*(C4-C5)	32.38	-	-	-
Total	196.51	80.98	110.95	65.39

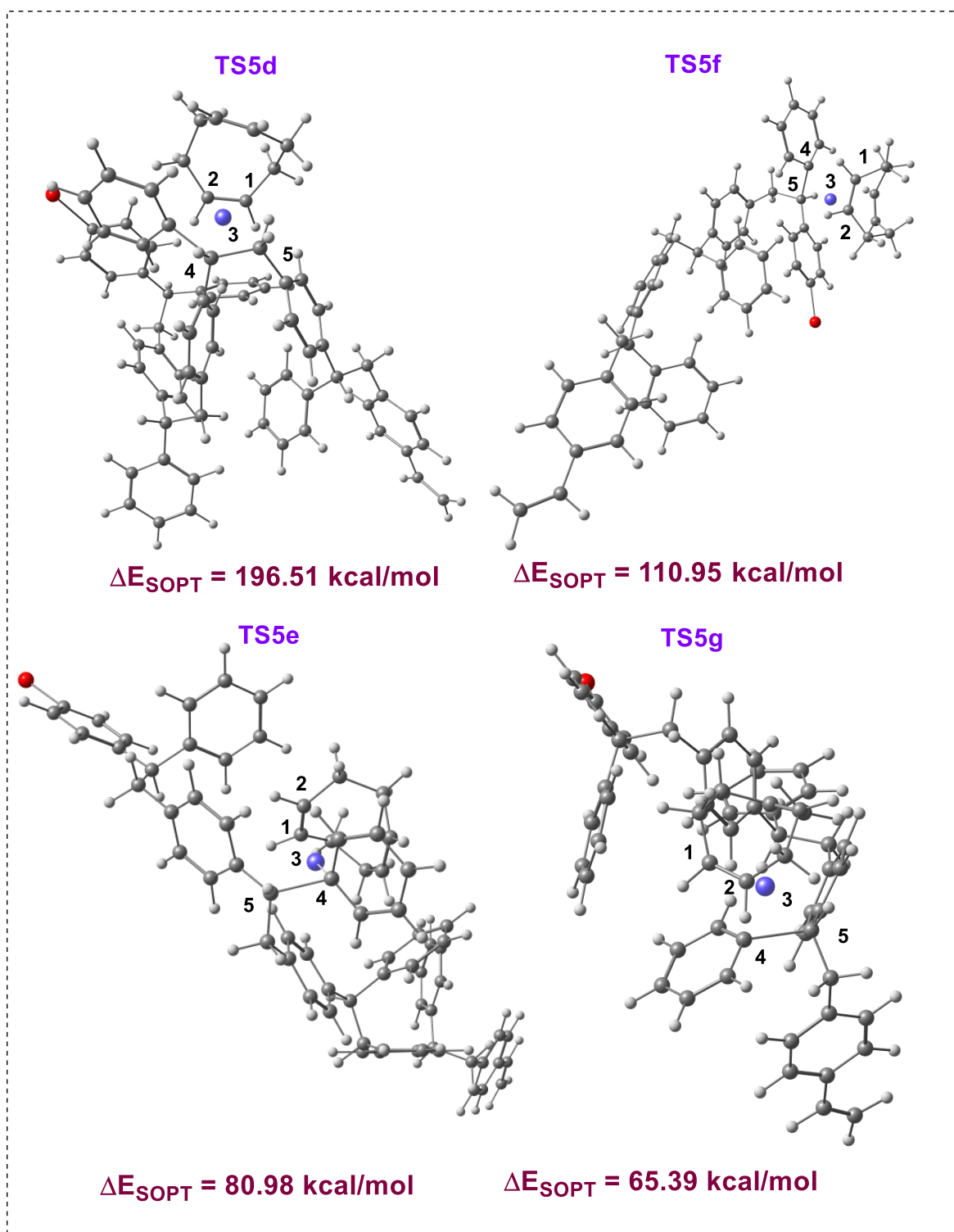


Fig S10. Transition states for the reductive elimination step (TS5d-TS5g) during the second propagation.

NBO analysis revealed that some of the significant donor-acceptor interactions are from the bonding orbital of the C-C bond to the lone vacant orbital of nickel ($\text{BD}(\text{C1-C2}) \rightarrow \text{LV}(\text{Ni3})$),

BD(C4-C5) \rightarrow LV(Ni3)) and to the Rydberg state of nickel (BD(C1-C2) \rightarrow RY(Ni3)), for the transition states TS5d-TS5g (Figure S10). Another interaction is from the lone pair orbital of nickel to the anti-bonding orbital of the C-C bond (LP(Ni3) \rightarrow BD*(C1-C2)). An additional interaction was observed from the lone pair orbital of the carbon atom to the lone vacant orbital of nickel (BD(C4-B3) \rightarrow LV(Ni2)) and to the anti-bonding orbital of the C-C bond (LP(C5) \rightarrow BD*(C4-C5)). The overall SOPT energy is lowest for TS5g, which supports a higher activation barrier for the corresponding transition state, as supported by the SOPT values and space-filling model (Figure S10). The key donor-acceptor orbital interactions (BD (C1-C2) \rightarrow LV Ni) in transition states **TS5g** and space-filling model is provided in Fig S11.

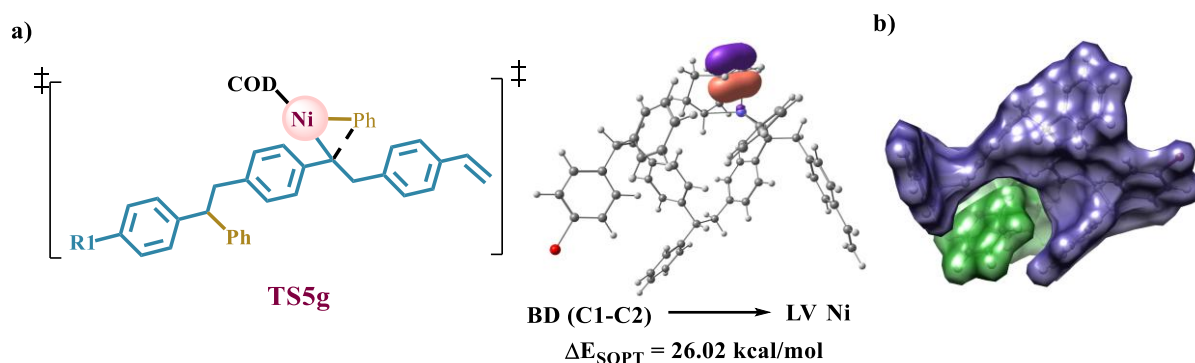


Fig S11. Natural Bond Orbital (NBO) analysis illustrating the key donor-acceptor orbital interactions (BD (C1-C2) \rightarrow LV Ni) in transition states **TS5g**. The interacting orbitals are visualised using isosurface plots (0.05 au), with the corresponding second-order perturbation theory (SOPT) stabilisation energy in kcal mol⁻¹ indicating the strength of the donor-acceptor interaction. BD stands for Bonding Orbital, whereas LV denotes Lone Vacant Orbital. Space-filling models of the **TS5g** is also provided. The blue surface represents the Ni-center with the aryl backbone; the green surface represents the COD ligand.

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VI. Cartesian coordinates of the optimized geometries

M

SCF Energy (a.u.) = -322.454657

Thermal correction to Gibbs free energy (a.u.) = 0.088666

Charge = 0, Multiplicity = 1

C	2.13306400	0.22546700	0.00009700
C	1.32899800	1.37635100	0.00007400
C	-0.06308800	1.29722700	0.00001100
C	-0.65644600	0.04086300	0.00002900
C	0.10391500	-1.12675400	0.00014600
C	1.49126300	-1.02564300	0.00019100
H	1.80203700	2.35492900	0.00006700
H	-0.66886000	2.19610100	-0.00000900
H	-0.37835200	-2.09760600	0.00022300
H	2.07994200	-1.93739700	0.00036900
C	3.59495200	0.37793200	0.00001100
C	4.51151900	-0.59743900	-0.00026000
H	3.94163600	1.41083800	0.00022400
H	5.57171300	-0.36546700	-0.00023500
H	4.25062500	-1.65208300	-0.00050000
Br	-2.60753700	-0.09478100	-0.00005500

COD

SCF Energy (a.u.) = -312.072495

Thermal correction to Gibbs free energy (a.u.) = 0.149898

Charge = 0, Multiplicity = 1

C	0.03791400	1.69046600	-0.22985600
C	-1.19091500	1.24033600	-0.50570700
C	-1.92102200	0.01840800	-0.00960800
C	-1.09048300	-1.08809400	0.67172300
C	-0.03791300	-1.69046600	-0.22985800
C	1.19091500	-1.24033600	-0.50570800
C	1.92102200	-0.01840800	-0.00960700
C	1.09048300	1.08809300	0.67172500
H	0.34664800	2.60144200	-0.74292800

H	-1.78131300	1.84073700	-1.19934100
H	-2.44545700	-0.42443400	-0.86877500
H	-2.71958300	0.33657100	0.67942900
H	-0.65545300	-0.71179900	1.59972500
H	-1.78489500	-1.88198300	0.97258100
H	-0.34664800	-2.60144100	-0.74293200
H	1.78131400	-1.84073600	-1.19934300
H	2.44545700	0.42443500	-0.86877400
H	2.71958200	-0.33657200	0.67943000
H	0.65545200	0.71179700	1.59972700
H	1.78489500	1.88198200	0.97258400

KBr

SCF Energy (a.u.) = -613.387919

Thermal correction to Gibbs free energy (a.u.) = -0.024226

Charge = 0, Multiplicity = 1

K	0.00000000	0.00000000	-1.89524100
Br	0.00000000	0.00000000	1.02884500

KOEt

SCF Energy (a.u.) = -754.412228

Thermal correction to Gibbs free energy (a.u.) = 0.038043

Charge = 0, Multiplicity = 1

K	-1.95120600	-0.13916700	-0.00007400
O	0.22345200	0.42109800	0.00049000
C	1.56802400	0.63937000	-0.00025800
C	2.38535800	-0.66808100	-0.00001500
H	1.91541000	1.23245500	0.88322300
H	1.91457400	1.23205400	-0.88432200
H	3.47025400	-0.48741800	-0.00040200
H	2.13263300	-1.26434200	0.88755900
H	2.13213200	-1.26510100	-0.88693500

1

SCF Energy (a.u.) = -603.699862

Thermal correction to Gibbs free energy (a.u.) = 0.207918

Charge = 0, Multiplicity = 1

C	-4.35311300	0.00006800	0.18177800
C	-3.65791700	1.20949400	0.10700100
C	-2.27171500	1.20554200	-0.04186700
C	-1.55377100	-0.00007900	-0.11866000
C	-2.27183800	-1.20559400	-0.04180100
C	-3.65806700	-1.20941400	0.10706900
H	-5.43391000	0.00014300	0.29784500
H	-4.19773700	2.15108600	0.16481100
H	-1.72944800	2.14509300	-0.10003100
H	-1.72971300	-2.14522800	-0.09993100
H	-4.19795000	-2.15096200	0.16501100
C	2.07147000	1.23350000	-0.48614000
C	2.07152400	-1.23348200	-0.48621900
C	2.75430800	0.00000900	0.12319100
H	2.31297800	1.30662500	-1.55578800
H	2.42704300	-2.14908900	-0.00025900
B	-0.00399300	-0.00003900	-0.28132700
O	0.65387500	1.20108800	-0.34056900
O	0.65393200	-1.20112900	-0.34071600
H	2.42697200	2.14910100	-0.00016000
H	2.31308100	-1.30656000	-1.55585900
C	4.24003900	0.00005600	-0.25495000
H	4.37869300	0.00013500	-1.34263500
H	4.74495600	0.88459900	0.15027200
H	4.74497400	-0.88453500	0.15014400
C	2.59703400	-0.00004900	1.65263700
H	3.07189200	-0.88678100	2.08782300
H	3.07178700	0.88670700	2.08788600
H	1.54616700	-0.00012500	1.95556300

2

SCF Energy (a.u.) = -526.524648

Thermal correction to Gibbs free energy (a.u.) = 0.190408

Charge = 0, Multiplicity = 1

C	1.54268800	1.27611300	0.22679900
C	0.96832900	-0.73677000	-1.07946000
C	1.86746900	-0.21561300	0.05098600
H	1.87986900	1.83642200	-0.65738700
H	1.06625000	-1.82374900	-1.17964200
B	-0.76277900	0.66365200	-0.13080800
O	0.15448600	1.51682200	0.42474500
O	-0.40964300	-0.45556900	-0.85069700
H	2.07034700	1.68166500	1.09762300
H	1.26888200	-0.28423000	-2.03517300
C	3.33771700	-0.37430900	-0.35318600
H	3.56026900	0.16410000	-1.28211400
H	4.00028600	0.01367000	0.42904800
H	3.58839600	-1.43043500	-0.50617500
C	1.59035100	-0.98319600	1.35395800
H	1.80312100	-2.05068100	1.22480200
H	2.22483500	-0.60643800	2.16421400
H	0.54882000	-0.88434300	1.67255100
O	-2.07702500	0.95437900	0.07420300
C	-3.09543400	0.07647900	-0.40429300
C	-3.31116200	-1.09145900	0.54945300
H	-2.83903200	-0.29090300	-1.40463200
H	-4.00495500	0.68101000	-0.48467700
H	-4.14385900	-1.71803400	0.20879300
H	-2.41113100	-1.71272600	0.59926000
H	-3.54049200	-0.72610200	1.55600700

im1

SCF Energy (a.u.) = -805.560571

Thermal correction to Gibbs free energy (a.u.) = 0.258240

Charge = 0, Multiplicity = 1

Ni	-0.59468300	-0.20919000	-0.25209600
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C	-1.77722300	-0.51714600	1.52118800
C	-2.48465900	0.22311100	0.60424000
C	-3.48098400	-0.29299600	-0.41227900
C	-3.10538400	-1.65180400	-1.06036100
C	-1.62586000	-1.76757600	-1.36698000
C	-0.67221200	-2.29973300	-0.53504700
C	-0.88310100	-2.83086400	0.86684000
C	-1.88568600	-2.01519300	1.72965700
H	-1.20708400	0.03227500	2.26723400
H	-2.44392900	1.30606800	0.70230000
H	-3.56104000	0.46296400	-1.20245400
H	-4.48297700	-0.36888700	0.03683000
H	-3.41964900	-2.47814700	-0.41769500
H	-3.67405800	-1.75873000	-1.99076600
H	-1.32616500	-1.53989200	-2.38909200
H	0.31590500	-2.48448200	-0.95293400
H	0.09317700	-2.82668700	1.36411800
H	-1.20671400	-3.88228500	0.83496000
H	-2.90867300	-2.34592600	1.53236400
H	-1.69124300	-2.24309400	2.78332300
C	0.69312900	1.16748200	0.01795400
C	0.98437400	0.56884600	-1.26114500
C	2.13598600	-0.26309700	-1.38932300
C	2.91407400	-0.61296900	-0.30058900
C	2.57554300	-0.05088700	0.97427300
C	1.54329500	0.83981900	1.12586800
H	0.54797100	0.99229700	-2.16319500
H	2.40521800	-0.62794300	-2.37853300
H	3.17091500	-0.31105900	1.84396000
H	1.34577400	1.29489400	2.09149200
C	4.05477000	-1.51312200	-0.48486100
C	4.89678300	-1.96864900	0.45356300
H	4.21080900	-1.83680000	-1.51431000
H	5.71078800	-2.63825600	0.19472700

H	4.81353300	-1.69633300	1.50193500
Br	-0.09538600	3.04902900	0.05761200

TS1

SCF Energy (a.u.) = -805.557090

Thermal correction to Gibbs free energy (a.u.) = 0.259425

Charge = 0, Multiplicity = 1

Ni	-0.70523600	-0.06141900	-0.26876900
C	-0.59298600	-1.52269600	1.27835900
C	-1.50176100	-0.54546700	1.63310100
C	-3.00082400	-0.58375000	1.42249800
C	-3.43867000	-1.20146900	0.06831000
C	-2.51636300	-0.84278800	-1.08370500
C	-1.44787400	-1.59211200	-1.52283700
C	-0.91074900	-2.85891100	-0.88925200
C	-0.94104900	-2.86684800	0.66266700
H	0.42774200	-1.41392800	1.63740000
H	-1.14605800	0.26024000	2.27246300
H	-3.36046800	0.45024600	1.46783400
H	-3.50137600	-1.11992800	2.24369000
H	-3.51446900	-2.28867900	0.15416400
H	-4.44867400	-0.84609300	-0.16411500
H	-2.84521900	-0.02506900	-1.72430300
H	-1.02984100	-1.34825900	-2.49815700
H	0.12884000	-2.96981000	-1.21825000
H	-1.44965400	-3.74047700	-1.26923400
H	-1.92013900	-3.19822400	1.01887600
H	-0.22210700	-3.61494400	1.01458400
C	0.74558600	1.05871300	0.02411100
C	1.17871200	0.60621600	-1.25090900
C	2.41649100	-0.06888300	-1.31467900
C	3.23740900	-0.20970100	-0.19768700
C	2.82439000	0.40327700	1.02267000
C	1.62198400	1.06197500	1.13656300

H	0.67445500	0.90604900	-2.16197600
H	2.76089300	-0.44339700	-2.27629100
H	3.47018600	0.34172900	1.89338000
H	1.30937100	1.50682500	2.07513500
C	4.50702900	-0.92945600	-0.32670100
C	5.41467100	-1.16602800	0.63103500
H	4.70788400	-1.31163800	-1.32769700
H	6.32248100	-1.71958200	0.41359000
H	5.29449700	-0.82402600	1.65515800
Br	-0.78536300	2.59046500	-0.09834200

im2

SCF Energy (a.u.) = -805.594980

Thermal correction to Gibbs free energy (a.u.) = 0.259842

Charge = 0, Multiplicity = 1

Ni	-0.79873800	0.10660400	-0.00686100
C	-1.10782500	-1.94611000	-0.46420500
C	-1.00499700	-1.75682400	0.90191200
C	-2.12257900	-1.65470600	1.91408900
C	-3.43004800	-1.01751400	1.39051700
C	-3.16554700	0.21626400	0.56139400
C	-3.02438700	0.27009600	-0.78686100
C	-3.04374800	-0.87979200	-1.76706200
C	-2.38688900	-2.18040900	-1.24958300
H	-0.18343800	-2.17915100	-0.98573600
H	-0.01819000	-1.89024400	1.33788700
H	-1.74936700	-1.05849000	2.75552400
H	-2.33384600	-2.65442000	2.32320400
H	-4.01062800	-1.74620000	0.82088000
H	-4.04602800	-0.73953100	2.25242300
H	-3.12878500	1.16192000	1.09748900
H	-2.92707000	1.25824900	-1.22872300
H	-2.50995200	-0.55103100	-2.66586400
H	-4.07462400	-1.08931200	-2.08754100

H	-3.09479600	-2.75139700	-0.64357900
H	-2.14954700	-2.81136600	-2.11248500
C	1.07431300	-0.05831500	-0.07995300
C	1.69126600	-0.28692000	-1.31209800
C	3.07457600	-0.46495300	-1.38336000
C	3.87832400	-0.42433900	-0.23372400
C	3.24404200	-0.18119700	0.99790100
C	1.86615400	0.00249100	1.07371100
H	1.10560100	-0.30959700	-2.22819100
H	3.54163100	-0.63784000	-2.35077800
H	3.83469900	-0.12135800	1.90762200
H	1.41089500	0.21889200	2.03685500
C	5.32700000	-0.62944200	-0.36643200
C	6.23796100	-0.67491800	0.61405000
H	5.67151600	-0.75913000	-1.39259900
H	7.28909900	-0.83119000	0.39279700
H	5.97890800	-0.55857000	1.66283100
Br	-0.53963200	2.43041100	0.01252300

im3

SCF Energy (a.u.) = -815.953499

Thermal correction to Gibbs free energy (a.u.) = 0.195257

Charge = 0, Multiplicity = 1

Ni	2.34479500	-0.21646300	0.21030700
C	1.25957900	1.27453000	0.28325500
C	1.62839400	2.41620100	1.00035700
C	0.94385500	3.61512000	0.79084200
C	-0.13341900	3.69481900	-0.10646200
C	-0.50534100	2.52734800	-0.79943700
C	0.17063800	1.32810300	-0.59848200
H	2.45228600	2.38697600	1.70932400
H	1.24519100	4.50545200	1.33795900
H	-1.33677300	2.55220800	-1.49730700
H	-0.15417200	0.43805100	-1.13127400
C	-0.82811500	4.97931200	-0.27102500

C	-1.87718200	5.23806400	-1.06164300
H	-0.42273200	5.79315000	0.32955500
H	-2.31127500	6.23188100	-1.10391200
H	-2.34007500	4.48413400	-1.69214800
Br	3.90131400	-1.44249900	-1.00714600
C	1.22183500	-1.57217700	1.28068400
C	1.93113900	-0.69113200	2.10583200
H	2.90510700	-0.99002500	2.48715900
H	1.43060900	0.10746000	2.64245200
H	1.72651300	-2.48377900	0.96657100
C	-0.20700200	-1.51432300	0.95488400
C	-1.10276400	-0.65477800	1.61111300
C	-0.68781000	-2.32430400	-0.08703400
C	-2.43796200	-0.59002100	1.23035900
H	-0.75523600	-0.02033300	2.41886200
C	-2.02077800	-2.26553800	-0.48694200
H	-0.00161600	-2.98882300	-0.60489400
C	-2.87697300	-1.39262200	0.17848300
H	-3.12386200	0.07899900	1.73652600
H	-2.38277300	-2.88422200	-1.29970700
Br	-4.74285700	-1.28783800	-0.37389500

im3_A

SCF Energy (a.u.) = -1128.041760

Thermal correction to Gibbs free energy (a.u.) = 0.372335

Charge = 0, Multiplicity = 1

Ni	-1.59128800	-0.27664800	-0.61018900
C	-2.09968900	-1.30988900	1.80649300
C	-1.04817400	-0.47869900	1.97828800
C	-1.01103800	0.82157400	2.74304600
C	-2.29850300	1.68479800	2.73764000
C	-2.91392100	1.82646200	1.37276400
C	-3.84094800	0.99365000	0.87146200
C	-4.45830600	-0.17666500	1.59676500

C	-3.48706600	-1.11889800	2.37446400
H	-1.91542500	-2.25473300	1.30413100
H	-0.07951900	-0.82896600	1.62704000
H	-0.18921600	1.42289300	2.34626900
H	-0.74583100	0.60095900	3.78825400
H	-3.03046400	1.27106900	3.43621600
H	-2.03092000	2.67518400	3.12339000
H	-2.56276600	2.65207300	0.76286200
H	-4.23441600	1.19429100	-0.12337400
H	-5.00199800	-0.77380300	0.86538100
H	-5.20153600	0.19620700	2.31677400
H	-3.38647200	-0.76506300	3.40543900
H	-3.96727800	-2.10044300	2.43333800
C	-0.48752900	1.26318400	-0.55342400
C	-1.01769500	2.35300300	-1.26080500
C	-0.34502500	3.57339500	-1.31441500
C	0.89572700	3.75035700	-0.67860000
C	1.43435700	2.64959100	0.00723300
C	0.75829100	1.43190700	0.06154800
H	-1.97296700	2.25821200	-1.77528000
H	-0.78372700	4.40402700	-1.86332000
H	2.39597000	2.73822200	0.50501300
H	1.22193600	0.61196000	0.59926700
C	1.56643900	5.05458100	-0.76602800
C	2.73303200	5.40784700	-0.21159900
H	1.03006600	5.79986100	-1.35336200
H	3.13443700	6.40742400	-0.34488100
H	3.32790300	4.72682600	0.39088000
Br	-3.42565000	-1.84363300	-1.15757800
C	-0.20438200	-1.54025600	-1.65981000
C	-0.78215300	-0.61587300	-2.51962300
H	-1.67838800	-0.88187400	-3.06819700
H	-0.22713900	0.24711100	-2.86794300
H	-0.74568100	-2.46727800	-1.48752700

C	1.16368800	-1.50473500	-1.13208200
C	2.16305100	-0.68002000	-1.67166900
C	1.48808600	-2.32445500	-0.03814500
C	3.44196500	-0.65061600	-1.12320500
H	1.94152200	-0.04947000	-2.52522800
C	2.75745500	-2.29733500	0.53379600
H	0.72726000	-2.97907000	0.37900300
C	3.71706000	-1.45191200	-0.01825000
H	4.20680500	-0.00799400	-1.54330900
H	2.99543800	-2.92252000	1.38649800
Br	5.49936800	-1.39622200	0.77337500

TS2

SCF Energy (a.u.) = -815.945221

Thermal correction to Gibbs free energy (a.u.) = 0.197789

Charge = 0, Multiplicity = 1

Ni	-1.25501400	1.29350600	0.21055300
C	-2.39155100	-0.13512800	0.61860700
C	-3.72256100	0.18810600	0.91943600
C	-4.74744800	-0.65508400	0.49260500
C	-4.47649400	-1.84776900	-0.19928400
C	-3.12958800	-2.17898400	-0.44799800
C	-2.09698300	-1.35042900	-0.02793800
H	-3.96053900	1.09842900	1.46256600
H	-5.77991500	-0.38739200	0.70276800
H	-2.88674900	-3.09773900	-0.97259600
H	-1.06560700	-1.62810200	-0.22606900
C	-5.59937900	-2.69688200	-0.61738100
C	-5.53343300	-3.84543000	-1.30249300
H	-6.58138900	-2.32436600	-0.32816900
H	-6.43464400	-4.39195600	-1.56092600
H	-4.59547100	-4.28168500	-1.63417600
Br	-0.50277800	3.01544200	-1.10209800
C	0.09263800	1.14052200	1.61697100

C	-1.06244000	0.47309300	2.12297200
H	-1.73171300	1.03350100	2.76957100
H	-1.00580600	-0.58086100	2.36866000
H	0.23863700	2.18149600	1.89837500
C	1.30139500	0.44632400	1.13445700
C	1.42760400	-0.95276900	1.12799500
C	2.37431800	1.21478900	0.65104200
C	2.58261800	-1.56997800	0.65315000
H	0.62640800	-1.57931100	1.50605300
C	3.53489300	0.61515500	0.17361400
H	2.27949500	2.29567200	0.62128300
C	3.62234200	-0.77480500	0.18072000
H	2.67181500	-2.65019500	0.65744800
H	4.35187300	1.21868600	-0.20420000
Br	5.24444600	-1.63111900	-0.48461400

TS2_A

SCF Energy (a.u.) = -1128.030010

Thermal correction to Gibbs free energy (a.u.) = 0.371060

Charge = 0, Multiplicity = 1

Ni	0.92229200	1.09127700	-0.87740300
C	-0.62881300	0.91029700	2.10384500
C	-0.50792700	-0.37088700	1.73100500
C	0.38696400	-1.43080300	2.32869600
C	1.75709800	-0.96663200	2.89268800
C	2.50893400	-0.00553300	2.00627600
C	2.38364500	1.32934800	1.99801100
C	1.47806700	2.18642000	2.84799300
C	0.10232900	1.58305200	3.23819800
H	-1.31213000	1.53629300	1.53664600
H	-1.13544200	-0.71093500	0.90983600
H	0.57417400	-2.18403700	1.55647300
H	-0.15031500	-1.96294800	3.12881100
H	1.61843700	-0.52930100	3.88438200

H	2.37040100	-1.86370200	3.04291600
H	3.21955600	-0.45053400	1.31566100
H	3.02297100	1.88639400	1.31306600
H	1.30168300	3.11585600	2.30083400
H	2.00378000	2.47026500	3.77281800
H	0.22094200	0.88402300	4.07038300
H	-0.51604100	2.40353700	3.62100300
C	1.95901200	-0.43548500	-1.30125300
C	3.30396200	-0.08969600	-1.50468800
C	4.31344000	-0.98478400	-1.15111500
C	4.01448500	-2.25752800	-0.63520300
C	2.65719000	-2.61674300	-0.50721900
C	1.64729400	-1.72974800	-0.85112700
H	3.56486600	0.88454400	-1.91083000
H	5.35375400	-0.69599600	-1.27916800
H	2.39206100	-3.60048400	-0.13205200
H	0.60924600	-2.02664700	-0.74203100
C	5.11668700	-3.15358900	-0.26463400
C	5.01934100	-4.35244000	0.32413700
H	6.11025400	-2.77078000	-0.49518800
H	5.90637300	-4.93204800	0.55841800
H	4.06739200	-4.79814600	0.59874100
Br	0.46182700	3.34680700	-0.38533100
C	-0.42928300	0.95265300	-2.30555100
C	0.68458800	0.24146100	-2.82379400
H	1.37495600	0.77957500	-3.46655000
H	0.59418100	-0.81007100	-3.06566200
H	-0.55555300	1.98750300	-2.60699200
C	-1.61799300	0.30250700	-1.72123100
C	-1.84356500	-1.08245100	-1.78831000
C	-2.54989400	1.09747600	-1.03014500
C	-2.94560600	-1.66495100	-1.16531900
H	-1.16294600	-1.72284100	-2.33949900
C	-3.65290000	0.53127700	-0.39898400

H	-2.37394500	2.16597500	-0.95305300
C	-3.83118500	-0.84823500	-0.46872400
H	-3.11037400	-2.73475300	-1.22327800
H	-4.35335800	1.15168100	0.14789400
Br	-5.35937800	-1.65818100	0.43397000

TS2_B

SCF Energy (a.u.) = -815.940063

Thermal correction to Gibbs free energy (a.u.) = 0.197036

Charge = 0, Multiplicity = 1

Ni	-1.86077500	-1.11938600	0.17149100
C	-1.57414400	0.70057600	0.58959400
C	-0.89967200	1.40984300	-0.41858400
C	-1.33970400	2.67749800	-0.78353100
C	-2.42451300	3.28865200	-0.12673300
C	-3.05139300	2.58338700	0.91758700
C	-2.62465000	1.31235400	1.29127300
H	-0.04103700	0.97001100	-0.91643500
H	-0.82333900	3.20306600	-1.58046500
H	-3.88421800	3.04437800	1.44258000
H	-3.11780000	0.79142300	2.10779500
C	-2.91566000	4.62943500	-0.47000800
C	-2.45640200	5.43509600	-1.43590000
H	-3.74667300	4.97864300	0.14163800
H	-2.89982900	6.41119500	-1.60400400
H	-1.63566000	5.16078200	-2.09251300
Br	-2.67532000	-2.93186800	-0.94630800
C	-0.41347600	-0.59307900	1.68308800
C	-1.06186300	-1.88002800	1.70648500
H	-1.83248200	-2.05062200	2.45720600
H	-0.50160900	-2.76811000	1.42687000
H	-0.62565400	0.06187300	2.52326600
C	0.96020400	-0.43347700	1.14072100
C	1.44716000	-1.24255900	0.10299200

C	1.78880800	0.56801100	1.66144600
C	2.73703900	-1.06650300	-0.39324900
H	0.81150900	-2.00537800	-0.33747300
C	3.08333100	0.75536100	1.17985900
H	1.41736700	1.21416800	2.45232800
C	3.53860100	-0.06845700	0.15538100
H	3.10674000	-1.69282300	-1.19681400
H	3.72008300	1.52970700	1.59164500
Br	5.34367100	0.19009200	-0.53997600

im4

SCF Energy (a.u.) = -815.977055

Thermal correction to Gibbs free energy (a.u.) = 0.199992

Charge = 0, Multiplicity = 1

Ni	0.03350100	-1.52054800	-0.14885000
C	2.44953900	0.23147400	1.24025100
C	3.00396900	-0.01143600	-0.02217200
C	3.46309700	1.04331800	-0.80666000
C	3.39538500	2.37401900	-0.35855500
C	2.86137800	2.60638100	0.92124300
C	2.40042700	1.55272000	1.70362800
H	3.05395100	-1.02895000	-0.39892800
H	3.88375000	0.83550300	-1.78728100
H	2.80485400	3.61877000	1.30884300
H	1.97977800	1.75796000	2.68530700
C	3.88463500	3.44843400	-1.23439900
C	3.88390200	4.76321700	-0.98263100
H	4.28448900	3.10645600	-2.18856200
H	4.27265100	5.47017800	-1.70857300
H	3.50304900	5.18554500	-0.05681500
Br	1.02926400	-3.34003200	-1.04017000
C	0.42899600	-1.31153300	1.70629500
C	1.85580800	-0.89677500	2.04790600
H	2.47578700	-1.79411900	1.94667200

H	1.87012200	-0.62842800	3.11570600
H	0.13645000	-2.20241500	2.26583800
C	-0.69340300	-0.43749000	1.39430500
C	-0.54019000	0.50848900	0.33171300
C	-2.02089300	-0.75830400	1.81538900
C	-1.67956000	1.10327900	-0.26197500
H	0.43308900	0.91087700	0.07983800
C	-3.12063600	-0.15851900	1.24429800
H	-2.15353400	-1.49159500	2.60535800
C	-2.93352200	0.76351100	0.19374500
H	-1.55216500	1.83456900	-1.05176500
H	-4.12173100	-0.40133000	1.58175000
Br	-4.50475400	1.58225000	-0.61194100

im5

SCF Energy (a.u.) = -957.020830

Thermal correction to Gibbs free energy (a.u.) = 0.265688

Charge = 0, Multiplicity = 1

Ni	-0.13245900	1.53069300	-0.12573700
C	-2.45425200	-0.16123400	1.29839500
C	-2.98119700	0.19917800	0.05083100
C	-3.51353700	-0.76957400	-0.79509400
C	-3.54755400	-2.12690800	-0.42913500
C	-3.03548200	-2.47611700	0.83214400
C	-2.50222500	-1.50813700	1.67808900
H	-2.94372400	1.23720200	-0.26881800
H	-3.91062900	-0.47268500	-1.76271400
H	-3.05095700	-3.51245000	1.15529500
H	-2.10030500	-1.80362600	2.64446200
C	-4.11233200	-3.10600700	-1.36877000
C	-4.22769500	-4.42813900	-1.19260300
H	-4.46801200	-2.67855700	-2.30598000
H	-4.66363600	-5.05754300	-1.96192300
H	-3.89903800	-4.93240600	-0.28800700

C	-0.40037200	1.33710600	1.75200100
C	-1.79241800	0.87456800	2.17685600
H	-2.42083300	1.77221800	2.21635500
H	-1.73295600	0.49367700	3.20789200
H	-0.09314300	2.21960000	2.31826200
C	0.72565400	0.47923500	1.39668500
C	0.55782700	-0.48907900	0.36050500
C	2.06266100	0.82512300	1.76518400
C	1.68561700	-1.08308700	-0.25626800
H	-0.41720000	-0.90927800	0.14485600
C	3.15345000	0.23580500	1.16658800
H	2.21086600	1.56997100	2.54179400
C	2.94805700	-0.71186500	0.14376700
H	1.54179800	-1.83545900	-1.02328600
H	4.16076700	0.50113100	1.46717900
Br	4.50824800	-1.52144900	-0.70250400
O	-1.04258700	2.80450200	-0.90481000
C	-0.75882900	4.18337100	-0.83405000
H	-1.08978500	4.58206500	0.13999900
H	0.32185400	4.38546300	-0.91560900
C	-1.49651900	4.91269900	-1.95399800
H	-2.57492300	4.73852500	-1.87262900
H	-1.31010200	5.99271800	-1.90688200
H	-1.16430800	4.54311500	-2.93025000

im6

SCF Energy (a.u.) = -1560.749058

Thermal correction to Gibbs free energy (a.u.) = 0.502484

Charge = 0, Multiplicity = 1

Ni	-0.07632100	-0.64553900	1.02709800
C	0.16478200	2.49504200	1.80732400
C	1.17877900	2.16199300	0.90102200
C	1.41263600	2.94783900	-0.22285100
C	0.65267200	4.10087100	-0.48187200

C	-0.34306400	4.44849500	0.44797200
C	-0.57852800	3.65876200	1.56968600
H	1.77006300	1.26588300	1.04698300
H	2.19007700	2.64486400	-0.91867100
H	-0.94152500	5.34113400	0.29273000
H	-1.36761100	3.93681300	2.26458300
C	0.92723000	4.87861600	-1.69813600
C	0.26573200	5.95436700	-2.14316500
H	1.76679400	4.51022200	-2.28774200
H	0.56027900	6.45075100	-3.06245000
H	-0.58539700	6.37936500	-1.61814500
C	-0.71654200	0.20468400	2.61965100
C	-0.15183400	1.58279800	2.97116600
H	0.76220500	1.40919500	3.55162900
H	-0.84973000	2.09361900	3.65133000
H	-0.66785400	-0.46376300	3.48242200
C	-1.93377700	0.00562200	1.83413300
C	-2.14119800	0.69914600	0.61319300
C	-2.82640800	-1.06433900	2.14167600
C	-3.22303800	0.37468200	-0.22381200
H	-1.52407200	1.54760200	0.35189100
C	-3.88398300	-1.38808900	1.31627700
H	-2.66625500	-1.62625900	3.05753100
C	-4.06952700	-0.65223800	0.13545700
H	-3.37956500	0.92980600	-1.13993200
H	-4.55922000	-2.19742100	1.57008400
Br	-5.55197800	-1.13114700	-1.04389300
C	-1.82200400	-1.35769900	-2.35090100
C	-1.38560700	-2.33375000	-1.46134900
C	-0.11649500	-2.22722500	-0.87067700
C	0.72708300	-1.12540200	-1.15110800
C	0.23128200	-0.12142600	-2.01837800
C	-1.01289600	-0.24524700	-2.62360500
H	-2.79623400	-1.45052600	-2.82164700

H	-2.01749100	-3.18788200	-1.23613300
H	0.26679500	-3.03620700	-0.25579100
H	0.85888700	0.73789700	-2.23210900
H	-1.36228100	0.52243700	-3.30926300
C	4.29219000	-2.43854100	-0.62247000
C	4.33573200	0.03118700	-0.48353300
C	5.02079800	-1.18247400	-1.12913300
H	4.51066100	-2.59923200	0.43949100
H	4.74754200	0.96447300	-0.88373600
B	2.25080200	-1.14393700	-0.73764700
O	2.88199200	-2.35917300	-0.79157000
O	2.93389900	0.05141600	-0.73090100
H	4.63456300	-3.32232500	-1.17294100
H	4.50336100	0.02839100	0.60206300
C	6.48823100	-1.23381100	-0.68919700
H	6.57844200	-1.28742000	0.40230600
H	6.99137400	-2.11099700	-1.11254400
H	7.03001300	-0.34375500	-1.03020600
C	4.92536900	-1.08971000	-2.66026100
H	5.42322700	-0.18331200	-3.02450500
H	5.40936200	-1.95393400	-3.12953200
H	3.88534400	-1.06222500	-2.99719700
O	1.55545800	-1.26686600	1.53074700
C	2.14461400	-1.02152800	2.77571700
C	3.42971100	-1.83075000	2.94077000
H	1.45961400	-1.29251700	3.59648900
H	2.38546500	0.04947100	2.90820900
H	3.82518500	-1.71887700	3.95805900
H	3.23605300	-2.89231500	2.75274500
H	4.20166400	-1.49231500	2.24198400

TS3

SCF Energy (a.u.) = -1560.742981

Thermal correction to Gibbs free energy (a.u.) = 0.502071

Charge = 0, Multiplicity = 1

Ni	-0.03378400	-0.77714600	0.97547100
C	0.59126000	2.51269300	1.64785800
C	1.24632500	2.11912500	0.47553600
C	1.34211600	2.98796600	-0.60687800
C	0.81040000	4.28775000	-0.55753900
C	0.18678000	4.69014600	0.63639800
C	0.08196900	3.81716800	1.71540500
H	1.67726300	1.12940800	0.40038800
H	1.83503700	2.64495900	-1.51317600
H	-0.22425600	5.69155900	0.72252600
H	-0.42039500	4.14680200	2.62250200
C	0.93142200	5.15616000	-1.73672700
C	0.48090700	6.40942600	-1.87561800
H	1.45040000	4.70002200	-2.57978500
H	0.62931500	6.95702800	-2.80100700
H	-0.04643500	6.93568000	-1.08462300
C	-0.42007100	0.29395900	2.51326300
C	0.40608100	1.54191700	2.79408400
H	1.38911000	1.18316300	3.12399900
H	-0.02878300	2.07880300	3.65076300
H	-0.39192000	-0.38918700	3.36804800
C	-1.70405900	0.26197400	1.80899100
C	-2.22706600	1.29116300	0.97436400
C	-2.36064400	-1.00125600	1.76655300
C	-3.34309300	1.07571300	0.18343900
H	-1.74934300	2.26132600	0.95929400
C	-3.48809500	-1.22161400	0.96711600
H	-2.02434100	-1.79544300	2.42835800
C	-3.95861700	-0.18130000	0.18752800
H	-3.72961500	1.87193600	-0.44275400
H	-3.97084500	-2.19097200	0.95653300
Br	-5.49498300	-0.48355700	-0.97708800
C	-2.16486900	-2.76272800	-1.55973600

C	-1.27660100	-3.65123200	-0.94358300
C	0.02656300	-3.24891100	-0.65480100
C	0.48132000	-1.94764500	-0.97110600
C	-0.44938800	-1.05929600	-1.56402700
C	-1.75415600	-1.46598400	-1.86323500
H	-3.17738600	-3.07841600	-1.79611300
H	-1.59743500	-4.66237400	-0.70693600
H	0.72825200	-3.95394500	-0.21912500
H	-0.11068900	-0.06537600	-1.84080600
H	-2.44475500	-0.77375600	-2.33427600
C	3.58013800	-0.03377200	-1.92518600
C	4.33085000	-2.22507400	-1.05369800
C	4.69414200	-0.72790900	-1.13538100
H	3.57986500	-0.38859900	-2.96730700
H	4.94597700	-2.71599800	-0.28926700
B	2.00783300	-1.50854800	-0.82258700
O	2.29707900	-0.25771600	-1.36019800
O	2.96405200	-2.50265400	-0.76049600
H	3.74749100	1.04970500	-1.94270000
H	4.56184100	-2.70391600	-2.01552800
C	6.02321300	-0.58906800	-1.88983000
H	5.95792100	-0.99836000	-2.90518700
H	6.31735100	0.46417000	-1.96627300
H	6.82625000	-1.11862200	-1.36336800
C	4.81307000	-0.07966200	0.25260600
H	5.58237400	-0.58060800	0.85164900
H	5.10048600	0.97395700	0.14903100
H	3.86789000	-0.12507900	0.79585800
O	1.78543500	-1.03654500	1.23244300
C	2.00021000	-2.09409500	2.15474200
C	3.45914000	-2.19993900	2.58670800
H	1.68456500	-3.05766900	1.72303300
H	1.38517600	-1.92975100	3.05334700
H	3.56410400	-2.98324100	3.34786900

H	4.10165700	-2.45548800	1.74215000
H	3.80706200	-1.25311700	3.01325200

im7

SCF Energy (a.u.) = -1560.758545

Thermal correction to Gibbs free energy (a.u.) = 0.503081

Charge = 0, Multiplicity = 1

Ni	0.04770500	0.40335100	-1.38663300
C	-0.29593400	-3.04995200	-1.15455300
C	0.49763500	-2.59707300	-0.09262300
C	0.42767800	-3.21050700	1.15507200
C	-0.42672200	-4.29860500	1.39628100
C	-1.19944000	-4.76751800	0.31972200
C	-1.12923900	-4.15548900	-0.92746700
H	1.17914900	-1.76713500	-0.22568800
H	1.05684700	-2.83336700	1.95773700
H	-1.85901900	-5.61925000	0.45563200
H	-1.74235300	-4.53560300	-1.74214400
C	-0.46879400	-4.89345200	2.73937500
C	-1.25131100	-5.89502500	3.16012500
H	0.22284800	-4.44537100	3.45243100
H	-1.19603900	-6.25509900	4.18258300
H	-1.97002200	-6.39137400	2.51372300
C	-0.70793900	-0.92175600	-2.58843200
C	-0.27724900	-2.37910400	-2.51485400
H	0.73538600	-2.43076500	-2.93369500
H	-0.90657100	-2.96403900	-3.20252500
H	-0.54873300	-0.49579700	-3.58351700
C	-1.81655700	-0.34646400	-1.85851200
C	-2.62525100	-0.99820000	-0.87613800
C	-1.90975400	1.07893300	-1.95068800
C	-3.49125600	-0.27979300	-0.08465700
H	-2.56780200	-2.07224300	-0.76462500
C	-2.80972800	1.80585700	-1.13677800

H	-1.45878100	1.59545700	-2.79723000
C	-3.57061300	1.12110900	-0.22278000
H	-4.11219300	-0.78673100	0.64543900
H	-2.89270400	2.87924600	-1.24659300
Br	-4.81912700	2.09354000	0.91880700
C	-1.21103800	3.07327100	1.34920300
C	-0.40435500	3.64940600	0.36519500
C	0.64283600	2.91267800	-0.19022300
C	0.93405700	1.59593200	0.23592300
C	0.08009500	1.03533500	1.21602800
C	-0.97964300	1.75946100	1.76371400
H	-2.02976600	3.63987000	1.78341900
H	-0.58894600	4.67057300	0.04058000
H	1.29502300	3.36252500	-0.93484300
H	0.29169600	0.03001800	1.57047200
H	-1.62148900	1.30865700	2.51555800
C	3.49645000	0.51761300	1.82620400
C	4.02832500	2.42724900	0.33515200
C	4.64154700	1.42915700	1.33868900
H	2.79827700	1.12157000	2.43470300
H	4.81865500	3.03959900	-0.11905300
B	2.33440600	0.83313500	-0.25089500
O	2.81119500	-0.09831200	0.75777400
O	3.32627800	1.78085000	-0.70535100
H	3.89535500	-0.27290500	2.47609900
H	3.35545800	3.11245800	0.88219900
C	5.23017800	2.19268700	2.52930500
H	4.46493200	2.79031200	3.03994200
H	5.66274600	1.50195200	3.26357300
H	6.02725600	2.87288700	2.20482200
C	5.72925300	0.59663300	0.64732800
H	6.56285700	1.23513000	0.32910300
H	6.12887600	-0.16762700	1.32530800
H	5.32906200	0.09619400	-0.23697800

O	1.87821000	0.01351500	-1.43490300
C	2.77883900	-0.41897400	-2.45972800
C	3.50093700	-1.69868200	-2.05859600
H	3.49002300	0.39302000	-2.63453800
H	2.18654000	-0.56661700	-3.36887000
H	4.22876100	-1.97618300	-2.83077100
H	4.02333000	-1.55087400	-1.11074300
H	2.79951900	-2.52867900	-1.92747000

TS4

SCF Energy (a.u.) = -1560.748334

Thermal correction to Gibbs free energy (a.u.) = 0.501300

Charge = 0, Multiplicity = 1

Ni	0.21248800	0.05127200	-1.43433500
C	-1.18069100	-3.15100900	-1.04047000
C	-0.30483300	-2.88207900	0.01870600
C	-0.58521000	-3.33792700	1.30342100
C	-1.73832100	-4.08978400	1.58348900
C	-2.59654500	-4.38603300	0.51058200
C	-2.31827900	-3.92610200	-0.77260000
H	0.59969100	-2.31220500	-0.15267400
H	0.10763800	-3.10178200	2.10748600
H	-3.49050800	-4.97898800	0.67888800
H	-3.00617500	-4.15813900	-1.58293000
C	-1.98881300	-4.53073100	2.96266600
C	-3.03854000	-5.22716200	3.41630000
H	-1.21691500	-4.24066500	3.67534400
H	-3.11819600	-5.49812300	4.46435800
H	-3.85145900	-5.55182600	2.77252500
C	-0.91126900	-1.09011100	-2.58948400
C	-0.93570600	-2.60500700	-2.43283400
H	0.03199000	-2.97713000	-2.79846800
H	-1.68831700	-3.03117000	-3.11321300
H	-0.64201400	-0.78932500	-3.60667500

C	-1.77848600	-0.15805900	-1.90786700
C	-2.70454000	-0.45234800	-0.85360900
C	-1.44035100	1.22146000	-2.10336500
C	-3.26620300	0.55163400	-0.10056700
H	-2.97891200	-1.47917300	-0.65578600
C	-2.04310800	2.24961800	-1.33540600
H	-0.88018000	1.51489900	-2.99033000
C	-2.92625700	1.89920100	-0.35002800
H	-3.97319400	0.31098400	0.68569000
H	-1.78357200	3.28437200	-1.52022000
Br	-3.75990300	3.28372900	0.74652400
C	0.22005900	3.81102000	1.22050100
C	0.95463700	3.86419000	0.03261100
C	1.30184200	2.68013300	-0.62164100
C	0.93048000	1.41529000	-0.12295700
C	0.21410200	1.39867200	1.09234000
C	-0.14332800	2.57290000	1.75580400
H	-0.06159600	4.72858800	1.73012400
H	1.25218700	4.82564500	-0.37970700
H	1.88457900	2.73465300	-1.53931800
H	-0.06721700	0.43978000	1.52207800
H	-0.71022500	2.52771300	2.68196400
C	3.01133200	-0.00231300	2.01340000
C	4.21378000	1.38032500	0.33847600
C	4.39929400	0.52306300	1.60386500
H	2.38601600	0.83396300	2.35918100
H	5.18774100	1.68035600	-0.06485000
B	2.39579100	-0.03894500	-0.30330000
O	2.35661600	-0.67289200	0.94614900
O	3.52801100	0.68327900	-0.69332800
H	3.10367200	-0.71825400	2.83822600
H	3.65404400	2.29365200	0.58823700
C	4.96150900	1.40292200	2.72610700
H	4.30101300	2.25230700	2.93726400

H	5.07859400	0.82729600	3.65199100
H	5.94745900	1.79985500	2.45603000
C	5.34391200	-0.65459700	1.32291700
H	6.31633000	-0.29923400	0.96134300
H	5.51536000	-1.23757700	2.23577400
H	4.92223000	-1.32646800	0.57129200
O	1.85833300	-0.90210200	-1.35077300
C	2.60042100	-1.13932500	-2.56492400
C	3.74326400	-2.10575300	-2.30697800
H	2.96849200	-0.18598400	-2.95534500
H	1.88126100	-1.55918400	-3.27254200
H	4.24834900	-2.34464900	-3.25027500
H	4.47327400	-1.65981600	-1.62743900
H	3.36796600	-3.03459000	-1.86560500

im8

SCF Energy (a.u.) = -1560.759068

Thermal correction to Gibbs free energy (a.u.) = 0.499303

Charge = 0, Multiplicity = 1

Ni	-0.12681200	-0.36863100	-1.46771400
C	1.97289700	2.69196600	-1.15523100
C	1.08350900	2.62693600	-0.07700400
C	1.44110200	3.12830700	1.16999600
C	2.69439600	3.72322800	1.39209400
C	3.57697700	3.80373500	0.30138800
C	3.21891600	3.29899700	-0.94484600
H	0.11367500	2.16604100	-0.20309500
H	0.73375100	3.05188700	1.99246000
H	4.55409500	4.26025100	0.42748900
H	3.92553000	3.36240900	-1.76937000
C	3.02094800	4.22682200	2.73332300
C	4.15241600	4.82594900	3.12525400
H	2.23346500	4.08158500	3.47286000
H	4.28270500	5.15737600	4.15063200

H	4.98471900	5.00896500	2.45118300
C	1.30637200	0.62103700	-2.56765200
C	1.61891700	2.10750700	-2.50600900
H	0.73803200	2.63592900	-2.90021000
H	2.43333000	2.33996400	-3.20886200
H	0.97869000	0.31542200	-3.56590300
C	1.90004000	-0.41758000	-1.79765200
C	2.78482000	-0.26090200	-0.66764600
C	1.31052400	-1.72613100	-1.98091100
C	3.07429300	-1.31423700	0.15793800
H	3.24865000	0.69848900	-0.48520100
C	1.65951900	-2.81656200	-1.12801400
H	0.85469500	-1.97439700	-2.93929400
C	2.49840400	-2.59070700	-0.07853500
H	3.75267000	-1.17953000	0.99341200
H	1.23450600	-3.79559900	-1.31349100
Br	2.93659700	-4.04502800	1.15526600
C	-2.83471300	-3.46095900	0.96217100
C	-3.19460200	-3.08668800	-0.33353800
C	-2.39290600	-2.19126800	-1.05348200
C	-1.21508600	-1.64286500	-0.51470400
C	-0.87159600	-2.05242000	0.78859700
C	-1.66420900	-2.93954800	1.52230800
H	-3.45103600	-4.15752400	1.52494500
H	-4.09772800	-3.49143400	-0.78615000
H	-2.71064800	-1.90926500	-2.05695100
H	0.04126100	-1.67237800	1.24357500
H	-1.36526000	-3.23090300	2.52711200
C	-2.50967700	0.74258100	2.02014000
C	-4.46246400	0.25358300	0.57104100
C	-4.02130700	0.96345500	1.85957600
H	-2.29252400	-0.31104800	2.22502900
H	-5.50449500	0.49301200	0.33686900
B	-2.36065100	0.90658000	-0.36363900

O	-1.77980500	1.11749000	0.84590400
O	-3.67957700	0.64995400	-0.56450400
H	-2.11746100	1.34821700	2.84307100
H	-4.36634800	-0.83280800	0.67458200
C	-4.74596800	0.32294400	3.04991900
H	-4.53018100	-0.74962300	3.11457900
H	-4.43582200	0.79044100	3.99158100
H	-5.83122400	0.44798700	2.95925200
C	-4.33761500	2.46539100	1.77943400
H	-5.41346700	2.62828200	1.64752600
H	-4.02828700	2.97457500	2.69929600
H	-3.81912400	2.94315700	0.94267300
O	-1.52974400	1.08906700	-1.48013100
C	-2.13445400	1.32770700	-2.77543800
C	-2.73027600	2.72346600	-2.83498200
H	-2.88812800	0.55735200	-2.95964000
H	-1.32344900	1.21481100	-3.49649700
H	-3.12928900	2.91493700	-3.83743000
H	-3.54830700	2.82763000	-2.11622400
H	-1.96595600	3.47600100	-2.61529500

im9

SCF Energy (a.u.) = -1346.326601

Thermal correction to Gibbs free energy (a.u.) = 0.460056

Charge = 0, Multiplicity = 1

Ni	1.97836700	-0.25644700	0.12929600
C	-1.79162600	-2.15766300	0.94527700
C	-2.76142800	-1.88469300	1.91312500
C	-4.07430100	-2.32753500	1.76155800
C	-4.46777000	-3.06407300	0.63468600
C	-3.48606900	-3.34751500	-0.33335200
C	-2.18022700	-2.90338900	-0.17931100
H	-2.48658900	-1.32105000	2.80220200
H	-4.81092800	-2.09846100	2.52820700

H	-3.74861900	-3.92533600	-1.21443800
H	-1.44095600	-3.14003300	-0.94064600
C	-5.86455200	-3.50400900	0.51853600
C	-6.42061200	-4.19367200	-0.48557600
H	-6.49798500	-3.22114100	1.35944500
H	-7.47145300	-4.46470600	-0.46200800
H	-5.86122300	-4.51107300	-1.36121900
C	0.07532400	-0.73949700	-0.06122800
C	-0.36359300	-1.66743200	1.08013400
H	-0.24114300	-1.18670300	2.05924200
H	0.31115000	-2.53113100	1.07864300
H	0.00217900	-1.29020300	-1.00053700
C	-0.66214900	0.54486800	-0.22013500
C	-1.40232400	1.15714500	0.80518900
C	-0.56683900	1.23580900	-1.44529800
C	-1.97935900	2.41865800	0.64170300
H	-1.53903900	0.64745600	1.75161100
C	-1.13167700	2.49333800	-1.63085600
H	-0.01685500	0.77503700	-2.26256500
C	-1.82486100	3.07650800	-0.57163200
H	-2.54257000	2.87434900	1.44856500
H	-1.03760700	3.00933000	-2.57998100
Br	-2.61085800	4.85686900	-0.80715600
C	3.02464000	-4.19972900	-2.22331800
C	3.02633400	-4.18397900	-0.82802600
C	2.68440600	-3.01690300	-0.13649200
C	2.33164600	-1.84116900	-0.81876000
C	2.32459200	-1.88070800	-2.22286300
C	2.67370900	-3.04105000	-2.91940200
H	3.28949600	-5.10503900	-2.76264400
H	3.29262800	-5.08103700	-0.27345500
H	2.69381000	-3.03197800	0.95236100
H	2.03573200	-0.99507400	-2.78732900
H	2.66372700	-3.04168600	-4.00712400

C	1.79052100	1.09559100	2.02554500
C	1.85456600	2.03846900	1.04961500
C	3.07621800	2.79383300	0.57879700
C	3.81017500	2.08145200	-0.57822900
C	4.05054100	0.60437000	-0.37799200
C	4.24342400	-0.07573800	0.78732700
C	4.29808000	0.49008100	2.18994000
C	2.91261500	0.54488800	2.87528800
H	0.79553500	0.76840400	2.31681700
H	0.91446900	2.35110300	0.60818500
H	3.76129200	2.97788000	1.40882000
H	2.75607600	3.77912700	0.22316600
H	3.21593500	2.19706900	-1.49310200
H	4.76612700	2.58979000	-0.77503100
H	4.18251600	0.03677800	-1.29653400
H	4.47181800	-1.13465400	0.69520800
H	4.76024300	1.47932100	2.18810400
H	4.95067100	-0.14787800	2.79585400
H	2.62938900	-0.47075600	3.17773900
H	2.99151800	1.12486400	3.80713400

TS5

SCF Energy (a.u.) = -1346.290628

Thermal correction to Gibbs free energy (a.u.) = 0.459060

Charge = 0, Multiplicity = 1

Ni	2.17858200	-0.78879800	-0.27610400
C	-0.98642700	-2.16685700	-0.89620300
C	-1.53982800	-2.14987000	0.38713200
C	-2.89421400	-2.40414700	0.57879100
C	-3.74460800	-2.69036800	-0.50131700
C	-3.17776200	-2.71936900	-1.78809500
C	-1.82642300	-2.46196800	-1.97908900
H	-0.90928000	-1.91329500	1.23784800
H	-3.30672800	-2.37782200	1.58431800

H	-3.80160600	-2.94012600	-2.64869400
H	-1.41293100	-2.47988000	-2.98499400
C	-5.16842000	-2.94344300	-0.24263000
C	-6.11223400	-3.26409600	-1.13650400
H	-5.46025700	-2.85227000	0.80336400
H	-7.14028000	-3.42593100	-0.82844800
H	-5.90451000	-3.37746000	-2.19694000
C	0.62181100	-0.24866500	-1.44105500
C	0.45104800	-1.79459200	-1.14364800
H	1.02999100	-2.16799200	-0.24611500
H	0.84632200	-2.34752100	-2.00034200
H	0.53570200	-0.16799100	-2.52166700
C	-0.42146500	0.62674800	-0.81179500
C	-0.41320400	0.92532200	0.55514700
C	-1.46854400	1.12584200	-1.59404700
C	-1.42575300	1.68435300	1.13820800
H	0.39705500	0.55282800	1.17143300
C	-2.49660200	1.88373100	-1.03278600
H	-1.49599700	0.90458400	-2.65744100
C	-2.45964200	2.14727600	0.33146900
H	-1.40890100	1.90653300	2.19944800
H	-3.30942400	2.25458000	-1.64650400
Br	-3.90149200	3.19838300	1.13983300
C	3.86159100	2.67062600	-2.79131100
C	3.84399200	1.36208100	-3.28805200
C	3.05424100	0.38967300	-2.68200300
C	2.28578300	0.68914500	-1.53564200
C	2.27537100	2.01698000	-1.07691900
C	3.06774600	2.99018100	-1.68996000
H	4.47277200	3.43090000	-3.26877400
H	4.44538300	1.10093100	-4.15543800
H	3.04335300	-0.62007600	-3.08703600
H	1.65612000	2.29043800	-0.22952700
H	3.05929500	4.00561300	-1.30132600

C	1.34236100	-1.08409600	2.92725300
C	1.99919900	0.06599400	3.12291600
C	3.48388700	0.31165000	3.07424900
C	4.03211600	0.63707500	1.67087300
C	3.94131200	-0.43365600	0.60157600
C	3.59428600	-1.78993600	0.71987400
C	3.27764000	-2.58463400	1.98765400
C	1.87072600	-2.45606400	2.60082200
H	0.25633000	-1.04455100	3.02227800
H	1.39276700	0.94862900	3.32917100
H	4.03328100	-0.53312900	3.49548800
H	3.71083300	1.16843000	3.72039400
H	3.55046500	1.54853800	1.29252700
H	5.09554500	0.89699900	1.78535400
H	4.55157600	-0.17974100	-0.26467000
H	3.98886900	-2.42313500	-0.07900900
H	4.03169900	-2.37515800	2.75363700
H	3.40616700	-3.64586600	1.74303000
H	1.15447200	-2.92870000	1.91427100
H	1.83593000	-3.07491900	3.51167100

im10

SCF Energy (a.u.) = -1346.344997

Thermal correction to Gibbs free energy (a.u.) = 0.460069

Charge = 0, Multiplicity = 1

Ni	2.70887800	0.19249300	-0.00983100
C	-1.35935700	2.23198700	0.16516100
C	-2.05655000	1.78004800	-0.95931000
C	-3.36531500	2.18814900	-1.19918500
C	-4.02787600	3.06487400	-0.32500800
C	-3.32003500	3.52465500	0.79987900
C	-2.01268300	3.11629600	1.03540000
H	-1.57648400	1.08077800	-1.63846500
H	-3.89059700	1.81781000	-2.07611100

H	-3.79678800	4.20748800	1.49652800
H	-1.48706300	3.48274700	1.91476400
C	-5.41283200	3.45731600	-0.62063500
C	-6.18925800	4.29203100	0.08151700
H	-5.82893400	3.00097500	-1.51863000
H	-7.20531200	4.50721100	-0.23382600
H	-5.85089800	4.78977700	0.98614000
C	0.01540100	0.52544800	1.48619000
C	0.02148200	1.72019800	0.48141800
H	0.52599000	1.38781000	-0.43416200
H	0.62342800	2.53167900	0.90342000
H	-0.37381300	0.92507400	2.43478500
C	-0.97594400	-0.52739500	1.01998800
C	-0.64494600	-1.48537100	0.05424500
C	-2.29456600	-0.48770100	1.48560200
C	-1.60063500	-2.36692100	-0.45173400
H	0.37752600	-1.55178800	-0.29669700
C	-3.26940300	-1.35574700	0.99349300
H	-2.57772400	0.25577500	2.22488300
C	-2.90456300	-2.28119400	0.02341700
H	-1.33077600	-3.10403900	-1.19959700
H	-4.28987100	-1.30329100	1.35488300
Br	-4.26239200	-3.50029200	-0.69201400
C	3.85394600	-0.87632700	2.99335500
C	3.74229100	0.41615100	2.52445500
C	2.54388700	0.87841600	1.89981300
C	1.42091800	-0.01313000	1.77364700
C	1.56050700	-1.32087900	2.33617300
C	2.73868100	-1.74549000	2.91068100
H	4.77502500	-1.21300800	3.46025800
H	4.56789400	1.11309800	2.64139500
H	2.41788600	1.95269100	1.77738900
H	0.70504200	-1.98750700	2.31705900
H	2.80671800	-2.75002200	3.31905800

C	2.20613900	-0.26523600	-1.92075900
C	3.06192500	-1.24688000	-1.40724900
C	4.54149000	-1.40624100	-1.73785100
C	5.50392300	-0.56979400	-0.85612100
C	5.09801700	0.86127200	-0.58716700
C	4.43249800	1.71193400	-1.39781200
C	3.97242000	1.42919100	-2.80522600
C	2.53760400	0.85671800	-2.88486800
H	1.13857300	-0.48697300	-1.89591200
H	2.58857300	-2.13928000	-0.99626900
H	4.71463100	-1.18548600	-2.79551900
H	4.81559400	-2.45931000	-1.60743800
H	5.58726800	-1.06284900	0.12025200
H	6.51176000	-0.60066100	-1.29829600
H	5.41413800	1.24785100	0.37894700
H	4.22527600	2.71071100	-1.01461200
H	4.67210000	0.75022800	-3.29754300
H	3.99826100	2.36109600	-3.38239700
H	1.82608200	1.67309900	-2.69746000
H	2.34865200	0.53046500	-3.92012500

P1

SCF Energy (a.u.) = -863.257443

Thermal correction to Gibbs free energy (a.u.) = 0.289566

Charge = 0, Multiplicity = 1

C	2.46909100	-1.04643000	0.64814600
C	3.06249900	-1.95368200	-0.24142600
C	4.42617800	-1.91676300	-0.50570900
C	5.25517300	-0.96483500	0.11420200
C	4.65625700	-0.06005600	1.00515900
C	3.28954600	-0.09850600	1.26705000
H	2.44189600	-2.70016100	-0.73264000
H	4.85233300	-2.63625000	-1.19816100
H	5.27504800	0.68738900	1.49563500

H	2.84936500	0.62676500	1.94551800
C	6.70216600	-0.87808700	-0.12738600
C	7.44087900	-1.65399600	-0.93039300
H	7.20433700	-0.08233000	0.42263100
H	8.50980100	-1.49481300	-1.03141000
H	7.01907800	-2.46917000	-1.51184100
C	0.23053600	-0.23104500	-0.21963300
C	0.97714500	-1.05224500	0.86596900
H	0.59986100	-2.08188200	0.84722300
H	0.74505100	-0.63645100	1.85299900
H	0.54104200	-0.64191300	-1.18912700
C	-1.28511900	-0.35027600	-0.14624000
C	-1.96278600	-0.88576700	0.95236500
C	-2.04492300	0.12414800	-1.22554300
C	-3.35963800	-0.95312200	0.98172300
H	-1.41110200	-1.26268600	1.80659200
C	-3.43564100	0.06520100	-1.22048100
H	-1.53533800	0.55803500	-2.08196800
C	-4.07445400	-0.47635800	-0.10775400
H	-3.87269300	-1.37113200	1.84032800
H	-4.00961000	0.43376300	-2.06300000
Br	-6.03052000	-0.56606500	-0.08211200
C	1.61318800	3.86827500	-0.02789600
C	2.12974700	2.99644800	-0.98662200
C	1.66351000	1.68335900	-1.06124900
C	0.67681900	1.22389200	-0.18345200
C	0.16109700	2.10710700	0.77292000
C	0.62628100	3.41902600	0.85270400
H	1.97389500	4.89123100	0.03202100
H	2.89872900	3.33524900	-1.67524000
H	2.08308100	1.00013600	-1.79474900
H	-0.61629900	1.76598800	1.45130700
H	0.21442800	4.09277700	1.59907700

im5c

SCF Energy (a.u.) = -1419.695707

Thermal correction to Gibbs free energy (a.u.) = 0.433666

Charge = 0, Multiplicity = 1

Ni	-0.80531700	-0.48161300	0.14411400
C	-1.98012100	-2.25721500	0.89751400
C	-2.85085800	-1.21904300	1.30892600
C	-4.05099500	-0.99296300	0.63032900
C	-4.41725300	-1.76851700	-0.47339400
C	-3.54748400	-2.80369300	-0.88183800
C	-2.35946100	-3.03896000	-0.21849800
H	-2.61890700	-0.62813500	2.19013600
H	-4.69566600	-0.18357400	0.95729400
H	-3.80818600	-3.41853700	-1.73642200
H	-1.70191600	-3.83873800	-0.54857000
C	-5.67591400	-1.46848700	-1.16527200
C	-6.10779300	-2.00539300	-2.31306000
H	-6.29371400	-0.71468900	-0.67902700
H	-7.05641300	-1.70520900	-2.74653200
H	-5.53563800	-2.74215400	-2.86910300
Br	-1.80238800	0.15034000	-2.00026700
C	0.10861600	-1.26577700	1.66779600
C	-0.71865600	-2.55091800	1.70385600
H	-0.97322800	-2.85005100	2.72944800
H	-0.18588900	-3.39105500	1.24994300
H	-0.07375100	-0.62842600	2.53497400
C	1.53933700	-1.32137300	1.31893000
C	2.04080700	-2.18021000	0.32083700
C	2.44235300	-0.41463700	1.90742000
C	3.37257000	-2.12730200	-0.08736300
H	1.37475800	-2.88376000	-0.16985100
C	3.77637800	-0.34670700	1.51456500
H	2.08320000	0.26056200	2.67886900
C	4.22329500	-1.20309900	0.51135600

H	3.73556500	-2.78694700	-0.86744000
H	4.45343600	0.36241900	1.97761700
Br	6.08469600	-1.09020500	-0.08029900
C	-3.44412100	2.16389900	3.16364300
C	-3.79106300	2.48567200	1.84871600
C	-2.81110600	2.53126800	0.85739500
C	-1.47003400	2.24276000	1.15727100
C	-1.13719300	1.93369400	2.48672400
C	-2.11077800	1.89666100	3.48523300
H	-4.20766700	2.12935700	3.93611900
H	-4.82622300	2.70107600	1.59730900
H	-3.08581900	2.75793800	-0.16788500
H	-0.10314600	1.71514100	2.73999800
H	-1.83325300	1.66124800	4.50931100
C	0.74659900	3.24094500	-1.84452700
C	1.47799100	1.02619700	-1.05196200
C	1.97765600	2.41377400	-1.45195300
H	0.26106100	2.80898100	-2.72685800
H	2.28117400	0.41567600	-0.64414800
B	-0.38817000	2.23070300	0.03062100
O	-0.22152500	3.28991300	-0.78879400
O	0.46082000	1.11110300	-0.01324700
H	1.02477000	4.27617300	-2.06459400
H	1.01901900	0.51645000	-1.90249800
C	2.89867400	2.25759000	-2.66924800
H	2.37457100	1.78931700	-3.51006300
H	3.27022600	3.23406000	-3.00008400
H	3.76678500	1.63664100	-2.42011800
C	2.74033200	3.07263000	-0.29098100
H	3.59428100	2.45257000	0.00289100
H	3.11725500	4.05765100	-0.58812800
H	2.10721900	3.21005700	0.59071200

TS3_c

SCF Energy (a.u.) = -1419.629569

Thermal correction to Gibbs free energy (a.u.) = 0.431952

Charge = 0, Multiplicity = 1

Ni	-1.27782800	-0.59058100	0.51377300
C	-2.44142200	-2.48167100	-0.36706900
C	-3.22721000	-2.28836400	0.78790800
C	-4.50878000	-1.74210300	0.69416700
C	-5.04419600	-1.35429600	-0.54155700
C	-4.26146100	-1.55836000	-1.69517400
C	-2.98929900	-2.10191700	-1.60772600
H	-2.84758500	-2.60555200	1.75528000
H	-5.09696000	-1.60043400	1.59679900
H	-4.65126900	-1.27631900	-2.66759500
H	-2.39587600	-2.23583000	-2.50826200
C	-6.38126000	-0.74603900	-0.58015700
C	-6.97572300	-0.17881900	-1.63722000
H	-6.91480200	-0.75922800	0.36957300
H	-7.96992300	0.24846500	-1.55491300
H	-6.50022200	-0.10896600	-2.61138100
Br	-2.68314600	1.34118500	-0.29821900
C	-0.18468900	-2.17487100	0.68888900
C	-1.03681100	-3.05666800	-0.25288300
H	-1.07756800	-4.09209300	0.11532300
H	-0.58851400	-3.09268800	-1.24953100
H	-0.28071900	-2.50681200	1.72807300
C	1.24599500	-2.05360000	0.31459200
C	1.63211900	-1.60646000	-0.96135800
C	2.26010600	-2.31336900	1.24951100
C	2.96996800	-1.39584000	-1.28554800
H	0.87033000	-1.35951900	-1.69290700
C	3.60671500	-2.10961300	0.94751700
H	1.98772400	-2.65275300	2.24509800
C	3.94059500	-1.64339600	-0.31866800
H	3.24966100	-1.02799000	-2.26631400

H	4.37552900	-2.30222600	1.68727400
Br	5.82240700	-1.30890300	-0.75305600
C	1.02363900	1.62127000	3.96086800
C	-0.37113700	1.56385600	3.87780400
C	-0.98218600	1.05074100	2.73525300
C	-0.22222100	0.56168500	1.64688300
C	1.17752200	0.64189100	1.75457400
C	1.79581100	1.16712700	2.89163200
H	1.50173900	2.02600600	4.84892700
H	-0.98107300	1.92479100	4.70208400
H	-2.06760700	1.04497100	2.67809500
H	1.79424500	0.29870600	0.93555500
H	2.88093800	1.21889300	2.93732600
C	0.97567100	3.47009600	0.06054900
C	0.75313400	2.13187200	-2.07107200
C	1.66485300	3.09725400	-1.29068100
H	0.93202000	4.55466300	0.18695500
H	1.33234700	1.58338500	-2.81922200
B	-0.60328600	1.72457100	-0.21867400
O	-0.37961100	3.01027500	0.17227900
O	0.14243800	1.14896000	-1.22025300
H	1.53831300	3.04985100	0.89963700
H	-0.03803500	2.68900100	-2.58919600
C	1.87430500	4.35685300	-2.14596800
H	0.92820400	4.88755000	-2.30415300
H	2.57265600	5.04562400	-1.65692600
H	2.29169800	4.10420700	-3.12829700
C	3.01854700	2.42442500	-1.00961500
H	3.56805300	2.25175600	-1.94256500
H	3.64450700	3.05347500	-0.36587700
H	2.88550300	1.45862400	-0.51542000

TS3_A

SCF Energy (a.u.) = -815.946558

Thermal correction to Gibbs free energy (a.u.) = 0.193747

Charge = 0, Multiplicity = 1

Ni	-0.75990900	2.15529400	0.49771300
C	-2.37463200	-0.33468100	0.91889600
C	-3.03926000	-0.14398800	-0.29574900
C	-3.60700000	-1.22693200	-0.96361300
C	-3.53493900	-2.52900000	-0.44458900
C	-2.86972700	-2.70825200	0.78211100
C	-2.30123600	-1.63259500	1.45047700
H	-3.08912500	0.84816100	-0.73388500
H	-4.11133200	-1.06088600	-1.91179500
H	-2.79065600	-3.69980700	1.21610200
H	-1.78128900	-1.79566200	2.39036200
C	-4.14494600	-3.63363600	-1.19816400
C	-4.17110400	-4.92752800	-0.85656100
H	-4.62011900	-3.33605100	-2.13220800
H	-4.65326300	-5.66223300	-1.49334300
H	-3.72122400	-5.30541600	0.05731500
Br	-0.49840200	3.60686100	-1.21251200
C	-0.35458200	0.89439100	1.96134000
C	-1.74611500	0.78233600	1.69609200
H	-2.16069500	2.16037100	0.88086200
H	-2.37412300	1.17603100	2.49666900
H	-0.08527200	1.45173100	2.85864000
C	0.76336600	0.18785200	1.32952200
C	0.65658100	-0.55653700	0.13272700
C	2.04275700	0.33692400	1.90636000
C	1.78028300	-1.13375100	-0.45109200
H	-0.30389700	-0.68564200	-0.34794800
C	3.16951900	-0.24164500	1.33554800
H	2.14839900	0.91675700	2.81911300
C	3.02109500	-0.97461900	0.15955200
H	1.68678300	-1.69754500	-1.37180100
H	4.14475100	-0.12119800	1.79259400

Br 4.59120600 -1.79220000 -0.65130900

im5_A

SCF Energy (a.u.) = -815.957048

Thermal correction to Gibbs free energy (a.u.) = 0.194504

Charge = 0, Multiplicity = 1

Ni	-0.88060600	2.01373800	0.50673400
C	-2.27868600	-0.42128100	1.10262100
C	-3.42331500	-0.14933600	0.33726400
C	-4.06455800	-1.16612600	-0.36139000
C	-3.60345000	-2.49236500	-0.30873900
C	-2.47074800	-2.76241000	0.48249500
C	-1.82029300	-1.74937000	1.17138400
H	-3.79315400	0.87020200	0.27413600
H	-4.93934000	-0.93229900	-0.96206800
H	-2.09679400	-3.77799800	0.56304100
H	-0.95093100	-1.98291800	1.77738900
C	-4.31849000	-3.52674600	-1.06727200
C	-4.01752000	-4.82953300	-1.13775000
H	-5.18163300	-3.16488900	-1.62463100
H	-4.61846600	-5.50855600	-1.73399200
H	-3.17296500	-5.26886000	-0.61435100
Br	-0.84228800	3.21231900	-1.40769200
C	-0.25330000	0.87563800	2.07116200
C	-1.62125300	0.66893100	1.85934700
H	-1.39611600	3.11366700	1.25030600
H	-2.28431900	1.23625800	2.50952200
H	0.01313000	1.52400400	2.90313200
C	0.89694900	0.23200900	1.41164700
C	0.82086200	-0.37401800	0.13939100
C	2.16159800	0.34029600	2.01905900
C	1.96219000	-0.86023600	-0.49353000
H	-0.13137400	-0.47953500	-0.36818500
C	3.30564800	-0.16138400	1.40782200

H	2.24609800	0.82503500	2.98764900
C	3.18931700	-0.75757200	0.15399400
H	1.89035500	-1.31247300	-1.47561900
H	4.27125100	-0.08102600	1.89343000
Br	4.78547500	-1.45929800	-0.71497400

im9_A

SCF Energy (a.u.) = -1346.326601

Thermal correction to Gibbs free energy (a.u.) = 0.460056

Charge = 0, Multiplicity = 1

Ni	1.97836700	-0.25644700	0.12929600
C	-1.79162600	-2.15766300	0.94527700
C	-2.76142800	-1.88469300	1.91312500
C	-4.07430100	-2.32753500	1.76155800
C	-4.46777000	-3.06407300	0.63468600
C	-3.48606900	-3.34751500	-0.33335200
C	-2.18022700	-2.90338900	-0.17931100
H	-2.48658900	-1.32105000	2.80220200
H	-4.81092800	-2.09846100	2.52820700
H	-3.74861900	-3.92533600	-1.21443800
H	-1.44095600	-3.14003300	-0.94064600
C	-5.86455200	-3.50400900	0.51853600
C	-6.42061200	-4.19367200	-0.48557600
H	-6.49798500	-3.22114100	1.35944500
H	-7.47145300	-4.46470600	-0.46200800
H	-5.86122300	-4.51107300	-1.36121900
C	0.07532400	-0.73949700	-0.06122800
C	-0.36359300	-1.66743200	1.08013400
H	-0.24114300	-1.18670300	2.05924200
H	0.31115000	-2.53113100	1.07864300
H	0.00217900	-1.29020300	-1.00053700
C	-0.66214900	0.54486800	-0.22013500
C	-1.40232400	1.15714500	0.80518900
C	-0.56683900	1.23580900	-1.44529800

C	-1.97935900	2.41865800	0.64170300
H	-1.53903900	0.64745600	1.75161100
C	-1.13167700	2.49333800	-1.63085600
H	-0.01685500	0.77503700	-2.26256500
C	-1.82486100	3.07650800	-0.57163200
H	-2.54257000	2.87434900	1.44856500
H	-1.03760700	3.00933000	-2.57998100
Br	-2.61085800	4.85686900	-0.80715600
C	3.02464000	-4.19972900	-2.22331800
C	3.02633400	-4.18397900	-0.82802600
C	2.68440600	-3.01690300	-0.13649200
C	2.33164600	-1.84116900	-0.81876000
C	2.32459200	-1.88070800	-2.22286300
C	2.67370900	-3.04105000	-2.91940200
H	3.28949600	-5.10503900	-2.76264400
H	3.29262800	-5.08103700	-0.27345500
H	2.69381000	-3.03197800	0.95236100
H	2.03573200	-0.99507400	-2.78732900
H	2.66372700	-3.04168600	-4.00712400
C	1.79052100	1.09559100	2.02554500
C	1.85456600	2.03846900	1.04961500
C	3.07621800	2.79383300	0.57879700
C	3.81017500	2.08145200	-0.57822900
C	4.05054100	0.60437000	-0.37799200
C	4.24342400	-0.07573800	0.78732700
C	4.29808000	0.49008100	2.18994000
C	2.91261500	0.54488800	2.87528800
H	0.79553500	0.76840400	2.31681700
H	0.91446900	2.35110300	0.60818500
H	3.76129200	2.97788000	1.40882000
H	2.75607600	3.77912700	0.22316600
H	3.21593500	2.19706900	-1.49310200
H	4.76612700	2.58979000	-0.77503100
H	4.18251600	0.03677800	-1.29653400

H	4.47181800	-1.13465400	0.69520800
H	4.76024300	1.47932100	2.18810400
H	4.95067100	-0.14787800	2.79585400
H	2.62938900	-0.47075600	3.17773900
H	2.99151800	1.12486400	3.80713400

TS5_A

SCF Energy (a.u.) = -1346.290628

Thermal correction to Gibbs free energy (a.u.) = 0.459060

Charge = 0, Multiplicity = 1

Ni	2.17858200	-0.78879800	-0.27610400
C	-0.98642700	-2.16685700	-0.89620300
C	-1.53982800	-2.14987000	0.38713200
C	-2.89421400	-2.40414700	0.57879100
C	-3.74460800	-2.69036800	-0.50131700
C	-3.17776200	-2.71936900	-1.78809500
C	-1.82642300	-2.46196800	-1.97908900
H	-0.90928000	-1.91329500	1.23784800
H	-3.30672800	-2.37782200	1.58431800
H	-3.80160600	-2.94012600	-2.64869400
H	-1.41293100	-2.47988000	-2.98499400
C	-5.16842000	-2.94344300	-0.24263000
C	-6.11223400	-3.26409600	-1.13650400
H	-5.46025700	-2.85227000	0.80336400
H	-7.14028000	-3.42593100	-0.82844800
H	-5.90451000	-3.37746000	-2.19694000
C	0.62181100	-0.24866500	-1.44105500
C	0.45104800	-1.79459200	-1.14364800
H	1.02999100	-2.16799200	-0.24611500
H	0.84632200	-2.34752100	-2.00034200
H	0.53570200	-0.16799100	-2.52166700
C	-0.42146500	0.62674800	-0.81179500
C	-0.41320400	0.92532200	0.55514700
C	-1.46854400	1.12584200	-1.59404700

C	-1.42575300	1.68435300	1.13820800
H	0.39705500	0.55282800	1.17143300
C	-2.49660200	1.88373100	-1.03278600
H	-1.49599700	0.90458400	-2.65744100
C	-2.45964200	2.14727600	0.33146900
H	-1.40890100	1.90653300	2.19944800
H	-3.30942400	2.25458000	-1.64650400
Br	-3.90149200	3.19838300	1.13983300
C	3.86159100	2.67062600	-2.79131100
C	3.84399200	1.36208100	-3.28805200
C	3.05424100	0.38967300	-2.68200300
C	2.28578300	0.68914500	-1.53564200
C	2.27537100	2.01698000	-1.07691900
C	3.06774600	2.99018100	-1.68996000
H	4.47277200	3.43090000	-3.26877400
H	4.44538300	1.10093100	-4.15543800
H	3.04335300	-0.62007600	-3.08703600
H	1.65612000	2.29043800	-0.22952700
H	3.05929500	4.00561300	-1.30132600
C	1.34236100	-1.08409600	2.92725300
C	1.99919900	0.06599400	3.12291600
C	3.48388700	0.31165000	3.07424900
C	4.03211600	0.63707500	1.67087300
C	3.94131200	-0.43365600	0.60157600
C	3.59428600	-1.78993600	0.71987400
C	3.27764000	-2.58463400	1.98765400
C	1.87072600	-2.45606400	2.60082200
H	0.25633000	-1.04455100	3.02227800
H	1.39276700	0.94862900	3.32917100
H	4.03328100	-0.53312900	3.49548800
H	3.71083300	1.16843000	3.72039400
H	3.55046500	1.54853800	1.29252700
H	5.09554500	0.89699900	1.78535400
H	4.55157600	-0.17974100	-0.26467000

H	3.98886900	-2.42313500	-0.07900900
H	4.03169900	-2.37515800	2.75363700
H	3.40616700	-3.64586600	1.74303000
H	1.15447200	-2.92870000	1.91427100
H	1.83593000	-3.07491900	3.51167100

im10_A

SCF Energy (a.u.) = -1346.344997

Thermal correction to Gibbs free energy (a.u.) = 0.460069

Charge = 0, Multiplicity = 1

Ni	2.70887800	0.19249300	-0.00983100
C	-1.35935700	2.23198700	0.16516100
C	-2.05655000	1.78004800	-0.95931000
C	-3.36531500	2.18814900	-1.19918500
C	-4.02787600	3.06487400	-0.32500800
C	-3.32003500	3.52465500	0.79987900
C	-2.01268300	3.11629600	1.03540000
H	-1.57648400	1.08077800	-1.63846500
H	-3.89059700	1.81781000	-2.07611100
H	-3.79678800	4.20748800	1.49652800
H	-1.48706300	3.48274700	1.91476400
C	-5.41283200	3.45731600	-0.62063500
C	-6.18925800	4.29203100	0.08151700
H	-5.82893400	3.00097500	-1.51863000
H	-7.20531200	4.50721100	-0.23382600
H	-5.85089800	4.78977700	0.98614000
C	0.01540100	0.52544800	1.48619000
C	0.02148200	1.72019800	0.48141800
H	0.52599000	1.38781000	-0.43416200
H	0.62342800	2.53167900	0.90342000
H	-0.37381300	0.92507400	2.43478500
C	-0.97594400	-0.52739500	1.01998800
C	-0.64494600	-1.48537100	0.05424500
C	-2.29456600	-0.48770100	1.48560200

C	-1.60063500	-2.36692100	-0.45173400
H	0.37752600	-1.55178800	-0.29669700
C	-3.26940300	-1.35574700	0.99349300
H	-2.57772400	0.25577500	2.22488300
C	-2.90456300	-2.28119400	0.02341700
H	-1.33077600	-3.10403900	-1.19959700
H	-4.28987100	-1.30329100	1.35488300
Br	-4.26239200	-3.50029200	-0.69201400
C	3.85394600	-0.87632700	2.99335500
C	3.74229100	0.41615100	2.52445500
C	2.54388700	0.87841600	1.89981300
C	1.42091800	-0.01313000	1.77364700
C	1.56050700	-1.32087900	2.33617300
C	2.73868100	-1.74549000	2.91068100
H	4.77502500	-1.21300800	3.46025800
H	4.56789400	1.11309800	2.64139500
H	2.41788600	1.95269100	1.77738900
H	0.70504200	-1.98750700	2.31705900
H	2.80671800	-2.75002200	3.31905800
C	2.20613900	-0.26523600	-1.92075900
C	3.06192500	-1.24688000	-1.40724900
C	4.54149000	-1.40624100	-1.73785100
C	5.50392300	-0.56979400	-0.85612100
C	5.09801700	0.86127200	-0.58716700
C	4.43249800	1.71193400	-1.39781200
C	3.97242000	1.42919100	-2.80522600
C	2.53760400	0.85671800	-2.88486800
H	1.13857300	-0.48697300	-1.89591200
H	2.58857300	-2.13928000	-0.99626900
H	4.71463100	-1.18548600	-2.79551900
H	4.81559400	-2.45931000	-1.60743800
H	5.58726800	-1.06284900	0.12025200
H	6.51176000	-0.60066100	-1.29829600
H	5.41413800	1.24785100	0.37894700

H	4.22527600	2.71071100	-1.01461200
H	4.67210000	0.75022800	-3.29754300
H	3.99826100	2.36109600	-3.38239700
H	1.82608200	1.67309900	-2.69746000
H	2.34865200	0.53046500	-3.92012500

TS5_B

SCF Energy (a.u.) = -1034.174338

Thermal correction to Gibbs free energy (a.u.) = 0.279767

Charge = 0, Multiplicity = 1

Ni	-1.18044600	-2.43882300	0.37868800
C	1.80713500	-1.90999700	0.66869200
C	2.18134700	-2.56419200	-0.50762300
C	3.41341100	-2.30359900	-1.10440400
C	4.31574600	-1.38211900	-0.55230000
C	3.93592200	-0.73024100	0.63487800
C	2.70865500	-0.98759300	1.22903500
H	1.49365000	-3.26818100	-0.96424100
H	3.67988400	-2.81972800	-2.02345000
H	4.60424200	-0.00955700	1.09545200
H	2.43106300	-0.45957200	2.13662300
C	5.59567200	-1.13782500	-1.23159700
C	6.55481900	-0.27765500	-0.86797300
H	5.75275700	-1.73605300	-2.12882200
H	7.46602000	-0.17976300	-1.44947800
H	6.47405900	0.35734200	0.00984300
C	-0.43475000	-1.09151400	1.61024500
C	0.51311400	-2.13753000	1.39027500
H	-0.17883400	-3.55292300	0.32100100
H	0.57406100	-2.87101900	2.19288800
H	-1.02389600	-1.17244500	2.52163800
C	-0.35585400	0.28825700	1.08175600
C	0.19104400	0.61621200	-0.17114300
C	-0.87010100	1.32889000	1.86913300

C	0.23357700	1.93364500	-0.61537800
H	0.57478500	-0.16612700	-0.81492400
C	-0.83728600	2.65693100	1.44008600
H	-1.30537500	1.09862700	2.83817500
C	-0.28099600	2.93923200	0.19962300
H	0.65470500	2.17129600	-1.58547900
H	-1.23879900	3.44868700	2.06215700
Br	-0.22753600	4.79346300	-0.42470700
C	-5.04054300	-1.53465200	-1.46647900
C	-4.20573900	-2.65468000	-1.47505800
C	-3.04620400	-2.59975100	-0.69640300
C	-2.71490300	-1.47891800	0.04946200
C	-3.54022400	-0.36202400	0.05434400
C	-4.71116000	-0.40180100	-0.71109500
H	-5.95305300	-1.54230000	-2.05566900
H	-4.45496200	-3.53473600	-2.06086700
H	-2.36184800	-3.49371700	-0.69003700
H	-3.27700100	0.52976200	0.61726700
H	-5.37129000	0.46181200	-0.72906700

im10_B

SCF Energy (a.u.) = -1034.174362

Thermal correction to Gibbs free energy (a.u.) = 0.279565

Charge = 0, Multiplicity = 1

Ni	-1.12769600	-2.48765500	0.35450900
C	1.82851100	-1.86929700	0.67304900
C	2.24501000	-2.56628300	-0.46455400
C	3.47795900	-2.29283100	-1.05328900
C	4.33985400	-1.31565300	-0.53280500
C	3.91874000	-0.62162200	0.61571000
C	2.69067100	-0.89209200	1.20255700
H	1.58838100	-3.31379400	-0.89611100
H	3.77723400	-2.84302900	-1.94202700
H	4.55549200	0.14127300	1.05249600

H	2.38241100	-0.33338800	2.08124400
C	5.62218200	-1.06076900	-1.20351000
C	6.54493400	-0.15035800	-0.86903200
H	5.81515200	-1.69715400	-2.06686000
H	7.46228300	-0.04991000	-1.44036400
H	6.42718700	0.52460200	-0.02589100
C	-0.43143600	-1.09835200	1.60426200
C	0.53652000	-2.11678900	1.38934500
H	-0.17781800	-3.64314000	0.24747000
H	0.59247600	-2.87270200	2.17067000
H	-1.03825800	-1.19796800	2.50189000
C	-0.37793400	0.28313600	1.07627400
C	0.14639000	0.61550200	-0.18467800
C	-0.88824900	1.31752600	1.87331900
C	0.17106400	1.93330800	-0.62848400
H	0.52564000	-0.16465500	-0.83407300
C	-0.87200200	2.64653800	1.44532400
H	-1.30633300	1.08258400	2.84878000
C	-0.33815000	2.93402100	0.19631300
H	0.57413100	2.17538700	-1.60510500
H	-1.26971100	3.43464500	2.07440100
Br	-0.30983100	4.78870000	-0.42703400
C	-5.00384400	-1.59162400	-1.44443400
C	-4.15470800	-2.70071900	-1.46875000
C	-2.98764700	-2.63331300	-0.70293900
C	-2.66420600	-1.51418500	0.04513400
C	-3.50251800	-0.40776400	0.06755400
C	-4.68113200	-0.45917800	-0.68590300
H	-5.92240800	-1.60772800	-2.02388400
H	-4.39784500	-3.58063900	-2.05712600
H	-2.28936400	-3.51919200	-0.71097700
H	-3.24641700	0.48380300	0.63358200
H	-5.35274100	0.39563200	-0.69095000

P

SCF Energy (a.u.) = -630.950078

Thermal correction to Gibbs free energy (a.u.) = 0.192888

Charge = 0, Multiplicity = 1

C	2.49668300	1.42546900	-0.01293200
C	3.70538000	1.37302500	0.69875100
C	4.47902900	0.21703000	0.71498500
C	4.09036600	-0.93006700	0.00492600
C	2.89470600	-0.86411100	-0.73669600
C	2.11856800	0.28389900	-0.74746100
H	4.03331600	2.24813800	1.25413000
H	5.40466200	0.19865000	1.28499200
H	2.57569400	-1.72027900	-1.32290700
H	1.21096700	0.31068600	-1.34013200
C	4.94090700	-2.12542100	0.05512300
C	4.70558800	-3.31267500	-0.51835400
H	5.85653600	-2.00559900	0.63388300
H	5.40945100	-4.13216600	-0.41338600
H	3.81449800	-3.51605500	-1.10555900
C	0.38076800	2.84476000	-0.09513600
C	1.71592600	2.67123200	-0.02181100
H	2.31747900	3.57857100	0.02502600
H	0.02914200	3.87149600	-0.18955400
C	-0.69237100	1.83820300	-0.04239000
C	-0.61394800	0.69324800	0.76999600
C	-1.87181000	2.04903500	-0.77496700
C	-1.65744800	-0.22626400	0.82401000
H	0.27243300	0.52461600	1.37084600
C	-2.92543700	1.13640000	-0.73895400
H	-1.96286300	2.93845400	-1.39291200
C	-2.79833000	0.00582900	0.05991100
H	-1.58604300	-1.10356000	1.45676100
H	-3.82548500	1.30657300	-1.31858300
Br	-4.26746400	-1.28505900	0.12638300

3

SCF Energy (a.u.) = -232.2775

Thermal correction to Gibbs free energy (a.u.) = 0.073396

Charge = 0, Multiplicity = 1

C	-1.33846600	-0.39754200	0.00000400
C	-0.32483700	-1.35790600	0.00006600
C	1.01349800	-0.96036500	-0.00005400
C	1.33843100	0.39765300	0.00000700
C	0.32495000	1.35787600	0.00006000
C	-1.01357700	0.96028600	-0.00005600
H	-2.37973500	-0.70694700	-0.00006500
H	-0.57774600	-2.41433100	0.00008000
H	1.80212100	-1.70738400	-0.00015000
H	2.37977200	0.70679300	0.00000900
H	0.57761100	2.41435300	0.00001600
H	-1.80202000	1.70750500	-0.00006000

im1a

SCF Energy (a.u.) = -1346.363384

Thermal correction to Gibbs free energy (a.u.) = 0.459968

Charge = 0, Multiplicity = 1

C	-4.01025300	-0.74736900	-0.98645400
C	-4.86700800	-1.80192700	-0.63811800
C	-6.23244700	-1.59941700	-0.47972400
C	-6.79932400	-0.32584900	-0.66690100
C	-5.93832700	0.72542200	-1.01935000
C	-4.57020500	0.51952900	-1.17493400
H	-4.45206700	-2.79636200	-0.48820100
H	-6.86606300	-2.43920000	-0.21115600
H	-6.35137200	1.72023100	-1.16781400
H	-3.92383200	1.35551200	-1.42757300
C	-8.23484300	-0.05274600	-0.51162400
C	-9.19820200	-0.92296500	-0.18396300

H	-8.51817900	0.98477600	-0.68857100
H	-10.23215800	-0.60434000	-0.09686900
H	-9.00111100	-1.97407600	0.00790500
C	-1.83014200	-0.92094100	0.30942600
C	-2.52224400	-0.96765200	-1.07899000
H	-2.31627700	-1.94343300	-1.53512400
H	-2.07315600	-0.20377400	-1.72404000
H	-2.33204000	-1.66971000	0.93792200
C	-0.34966900	-1.25827900	0.26783700
C	0.31536700	-1.42826300	1.52534000
C	0.38054100	-1.36880200	-0.89246400
C	1.66562200	-1.63721200	1.60249800
H	-0.27419000	-1.37825400	2.43707400
C	1.80607100	-1.55999800	-0.88663500
H	-0.11188200	-1.32308400	-1.85879900
C	2.44438500	-1.59756700	0.40354000
H	2.15912600	-1.78759100	2.55704900
H	2.28206300	-1.99100100	-1.76375300
Br	4.25070600	-2.49710700	0.49371900
C	-2.49941000	2.98425500	2.07192900
C	-3.37114400	1.93060400	2.35031300
C	-3.14487800	0.66787300	1.80032800
C	-2.04656200	0.43862400	0.96532800
C	-1.17453000	1.50060800	0.69787300
C	-1.39745700	2.76431200	1.24227200
H	-2.67403400	3.96677400	2.50143500
H	-4.23072800	2.09031000	2.99535000
H	-3.83605600	-0.14449400	2.00714100
H	-0.30748400	1.32056500	0.07130600
H	-0.70832100	3.57635200	1.02317800
Ni	2.75504100	0.13614200	-0.42876800
C	2.92390900	1.78279200	0.91278500
C	4.13788600	1.14209100	0.82425700
C	5.27641100	1.48360300	-0.11204500

C	4.83050200	1.94496400	-1.52650800
C	3.62972700	1.18379100	-2.05787000
C	2.32279200	1.59202200	-1.94000000
C	1.85179400	2.82348300	-1.19849700
C	2.54409900	3.05532900	0.17676400
H	2.24962800	1.47058900	1.70898400
H	4.36895400	0.39042500	1.57511600
H	5.89006600	0.58119800	-0.21291100
H	5.93035900	2.25213800	0.32760800
H	4.61314700	3.01671900	-1.52225100
H	5.67220700	1.80824500	-2.21449800
H	3.84379200	0.35676700	-2.73425600
H	1.57233900	1.08684400	-2.54458500
H	0.77273700	2.72896600	-1.04562500
H	1.98771000	3.72171400	-1.81961200
H	3.43346200	3.67753600	0.04270100
H	1.86272300	3.63450800	0.80974400

TS1a

SCF Energy (a.u.) = -1346.360421

Thermal correction to Gibbs free energy (a.u.) = 0.460622

Charge = 0, Multiplicity = 1

C	-4.24073800	-0.88973500	-0.85582400
C	-5.07341800	-1.86708500	-0.29162400
C	-6.42720700	-1.63027000	-0.08682700
C	-7.00527600	-0.39796200	-0.44035900
C	-6.16783900	0.57663300	-1.00602600
C	-4.81165400	0.33679800	-1.20941200
H	-4.64920800	-2.82859000	-0.01035300
H	-7.04268800	-2.41123600	0.34916400
H	-6.59003800	1.53864600	-1.28629200
H	-4.18337300	1.11589600	-1.63191600
C	-8.42921700	-0.09113300	-0.24590900
C	-9.37043300	-0.88987400	0.27252500

H	-8.72353300	0.90745100	-0.56874000
H	-10.39764900	-0.55263000	0.36875300
H	-9.16121300	-1.89877700	0.61725300
C	-1.98768800	-0.79774700	0.30180200
C	-2.76030600	-1.13529000	-1.00151300
H	-2.57297100	-2.18592200	-1.25360800
H	-2.36441000	-0.52705500	-1.82238400
H	-2.46702400	-1.36861600	1.10746600
C	-0.51921200	-1.18089100	0.26693800
C	0.15799100	-1.32985000	1.50706600
C	0.20099300	-1.34497000	-0.90616600
C	1.51811400	-1.54163400	1.57947600
H	-0.41413400	-1.23702300	2.42754000
C	1.59910800	-1.56686500	-0.88717500
H	-0.30538400	-1.33864600	-1.86646700
C	2.24959900	-1.52298100	0.37128800
H	2.03077600	-1.61936800	2.53197900
H	2.11350000	-1.89594700	-1.78196000
Br	4.25470700	-2.39562400	0.32765200
C	-2.51772500	3.41632700	1.17596300
C	-3.26399200	2.45752500	1.86102200
C	-3.07765500	1.10043100	1.59161300
C	-2.14232900	0.68085600	0.64135100
C	-1.39321800	1.65093500	-0.03734300
C	-1.58206900	3.00768700	0.22212500
H	-2.66246400	4.47299600	1.38226800
H	-3.99652600	2.76384900	2.60259200
H	-3.67748800	0.35776100	2.11079500
H	-0.65291200	1.33631500	-0.76724600
H	-0.99919400	3.74713800	-0.32089900
Ni	3.18691600	-0.08920200	-0.34259200
C	2.51737500	1.58235000	0.80475700
C	3.72881000	1.14028600	1.29833100
C	5.09907900	1.67659500	0.93986800

C	5.27196200	2.02488100	-0.56237400
C	4.55761000	1.05936500	-1.49241900
C	3.28506400	1.22247000	-1.99485000
C	2.31446400	2.33105000	-1.64184500
C	2.32872700	2.75002500	-0.14692700
H	1.61079600	1.20397500	1.27078100
H	3.70616300	0.45739800	2.14556500
H	5.82990900	0.90491300	1.20616700
H	5.34999800	2.56042500	1.54685500
H	4.92798100	3.04437300	-0.75664400
H	6.34171700	2.01730200	-0.79923600
H	5.17420800	0.28329800	-1.94455900
H	2.99275900	0.59862000	-2.83807500
H	1.30947500	1.97492600	-1.89641000
H	2.49280400	3.21700700	-2.27076800
H	3.10329200	3.50250700	0.02435800
H	1.37488000	3.23595000	0.08357900

im2a

SCF Energy (a.u.) = -1346.397459

Thermal correction to Gibbs free energy (a.u.) = 0.460400

Charge = 0, Multiplicity = 1

C	4.68949700	-0.83407200	0.85809000
C	5.25990100	-1.91895100	0.17615600
C	6.62540000	-1.97605900	-0.07442700
C	7.48034900	-0.94330700	0.35025800
C	6.90492000	0.14003300	1.03311300
C	5.53621700	0.19494900	1.28181300
H	4.61854900	-2.73001200	-0.16190900
H	7.03275300	-2.83260800	-0.60291800
H	7.54409000	0.95289400	1.36947700
H	5.11487900	1.05452600	1.79541200
C	8.93053400	-0.94981200	0.11319400
C	9.65027000	-1.89330600	-0.50703000

H	9.45389800	-0.07388500	0.49663800
H	10.72419900	-1.78865600	-0.62525800
H	9.20706100	-2.79691000	-0.91636500
C	2.47817800	-0.14275100	-0.17739500
C	3.19742500	-0.75338400	1.05684200
H	2.78550400	-1.75332400	1.23741200
H	2.97512000	-0.14431700	1.94008600
H	2.79793600	-0.73212800	-1.04626700
C	0.96127000	-0.23062700	-0.10434100
C	0.22352300	-0.10385600	-1.28989800
C	0.25712700	-0.40041200	1.09037400
C	-1.16939600	-0.14332500	-1.28538400
H	0.75310900	0.02693600	-2.23131900
C	-1.14336500	-0.43263300	1.10403300
H	0.79028300	-0.51647200	2.02907000
C	-1.86589000	-0.29962700	-0.08183500
H	-1.70905500	-0.07556400	-2.22663100
H	-1.65755000	-0.58488600	2.05036200
Br	-3.73239900	-2.54972100	-0.61380900
C	3.92495900	3.90324800	-0.73814900
C	4.44390100	2.85818100	-1.50272500
C	3.95829100	1.56064400	-1.33519800
C	2.94870300	1.28702700	-0.40690200
C	2.43087600	2.34361200	0.35247800
C	2.91565900	3.64099200	0.19143000
H	4.30121900	4.91445400	-0.86609000
H	5.23030600	3.04996500	-2.22758800
H	4.37914700	0.74534000	-1.91746000
H	1.63632100	2.14525100	1.06679600
H	2.50235800	4.44957500	0.78868500
Ni	-3.74722800	-0.28686400	-0.01945400
C	-3.81375200	1.60455300	0.94332400
C	-3.82061600	1.75317200	-0.43176600
C	-5.00669800	1.99931800	-1.33530000

C	-6.33590900	1.36422300	-0.86678200
C	-6.14678800	-0.05424100	-0.38532700
C	-5.92475200	-0.45221400	0.89243100
C	-5.76089300	0.41623300	2.11809900
C	-5.00769100	1.74396900	1.87234800
H	-2.83798800	1.62267000	1.42123900
H	-2.85616800	1.90839800	-0.90854100
H	-4.75268000	1.60127300	-2.32515900
H	-5.14014800	3.08332200	-1.47159700
H	-6.80010700	1.97516900	-0.08970600
H	-7.03207100	1.36121300	-1.71234500
H	-6.24205800	-0.83721500	-1.13427900
H	-5.90088000	-1.52358500	1.07316300
H	-5.20674600	-0.16903200	2.86059000
H	-6.74133300	0.62644100	2.56964900
H	-5.69057500	2.50505400	1.48658400
H	-4.65052500	2.11908800	2.83715200

im3a

SCF Energy (a.u.) = -1356.764525

Thermal correction to Gibbs free energy (a.u.) = 0.399753

Charge = 0, Multiplicity = 1

C	3.72452900	-0.06541000	-0.66418300
C	4.23804500	0.96913200	0.13235000
C	5.59803400	1.06380400	0.40167800
C	6.50332100	0.12171200	-0.11865200
C	5.98406900	-0.91064400	-0.91620700
C	4.62094100	-1.00426500	-1.18377700
H	3.55638700	1.71151200	0.54123100
H	5.96146700	1.87949000	1.01941800
H	6.66336100	-1.65275500	-1.32868200
H	4.24431600	-1.82332300	-1.78982000
C	7.95033700	0.17146200	0.13272000
C	8.62018700	1.07674200	0.85697400

H	8.51733900	-0.63288300	-0.33587500
H	9.69727400	1.01141100	0.97450200
H	8.13163700	1.90965000	1.35508200
C	1.54212200	-0.98232300	0.24919700
C	2.23912900	-0.18587100	-0.88685400
H	1.79542500	0.81388400	-0.93670000
H	2.04085200	-0.68190100	-1.84387300
H	1.84881200	-0.50763300	1.19126400
C	0.02152000	-0.91788300	0.19166300
C	-0.71344900	-1.42150500	1.27393300
C	-0.68161600	-0.38067200	-0.89060100
C	-2.10697100	-1.34272500	1.30705800
H	-0.18492900	-1.88345200	2.10471600
C	-2.07771600	-0.29795100	-0.87632300
H	-0.15091900	-0.00575300	-1.75883900
C	-2.77530600	-0.73643200	0.24387200
H	-2.65072600	-1.73698800	2.16070000
H	-2.59946900	0.13444000	-1.72346500
Br	-5.36640300	-1.89034100	-1.01048400
C	3.08767700	-5.02633600	0.24977700
C	3.58820300	-4.08363900	1.14795000
C	3.07103700	-2.78742400	1.16146200
C	2.04882000	-2.41595300	0.28265900
C	1.54963000	-3.37015200	-0.61264700
C	2.06549600	-4.66514400	-0.63145800
H	3.48763800	-6.03635200	0.23749700
H	4.38385100	-4.35388700	1.83673000
H	3.47658100	-2.04901900	1.84798900
H	0.74461100	-3.09682800	-1.28951700
H	1.66541200	-5.39461100	-1.33031200
Ni	-4.56980800	-0.29228800	0.37574600
C	-4.31039300	1.68779100	1.11605200
C	-4.58677100	0.76266200	2.11100400
H	-5.61318600	0.61339300	2.44360900

H	-3.81636600	0.38911400	2.77709700
H	-5.15401200	2.16587100	0.61514900
C	-2.99625100	2.25183600	0.78194900
C	-1.85242400	2.00287600	1.55720100
C	-2.86071400	3.01198400	-0.38942600
C	-0.60253800	2.45626400	1.15394100
H	-1.92735400	1.42398300	2.46962600
C	-1.61668500	3.48108500	-0.80574400
H	-3.73707100	3.21578800	-0.99923200
C	-0.50160100	3.18407700	-0.02932300
H	0.27845900	2.23879300	1.74604900
H	-1.51853400	4.05527500	-1.71968300
Br	1.25754000	3.79303400	-0.61417400

TS2a

SCF Energy (a.u.) = -1356.747612

Thermal correction to Gibbs free energy (a.u.) = 0.398522

Charge = 0, Multiplicity = 1

C	-5.18473800	1.66280000	0.02904900
C	-5.88674000	2.09650100	-1.10471000
C	-7.26337000	2.28283300	-1.07246500
C	-7.99607100	2.04128000	0.10330500
C	-7.28790700	1.60905500	1.23595400
C	-5.90890900	1.42191600	1.20047400
H	-5.34163500	2.29109700	-2.02602100
H	-7.77430000	2.62251400	-1.96817500
H	-7.83156500	1.41327200	2.15689900
H	-5.38941700	1.06736200	2.08617400
C	-9.45187800	2.21984400	0.19583000
C	-10.28471300	2.62423200	-0.77128900
H	-9.87343300	1.98873900	1.17393600
H	-11.35008200	2.71917200	-0.58671100
H	-9.94605000	2.87501700	-1.77275700
C	-3.40095300	-0.03217400	-0.57804000

C	-3.70288400	1.39359000	-0.04402600
H	-3.22166100	2.12551400	-0.70430200
H	-3.25609700	1.50609800	0.95023400
H	-3.91633100	-0.12038300	-1.54343400
C	-1.92394700	-0.29743100	-0.83011000
C	-1.56822300	-1.44768800	-1.55164700
C	-0.90178700	0.53461100	-0.35812000
C	-0.23569500	-1.76809800	-1.79542200
H	-2.35279200	-2.10468000	-1.91844800
C	0.44142800	0.23012800	-0.59228800
H	-1.14248400	1.43373500	0.19876500
C	0.77822400	-0.94875100	-1.27152800
H	0.01340500	-2.65941600	-2.36460500
H	1.21864200	0.89178500	-0.22027500
Br	3.47230600	-3.14968300	0.81360200
C	-5.16375500	-2.92604800	2.11782100
C	-5.81651800	-2.57933300	0.93468300
C	-5.23415300	-1.66398100	0.05709200
C	-3.99530900	-1.08476400	0.34789400
C	-3.34576300	-1.44024800	1.53647400
C	-3.92531900	-2.35314500	2.41664500
H	-5.61403400	-3.63980100	2.80176700
H	-6.78097500	-3.01777900	0.69418200
H	-5.75426500	-1.37957900	-0.85368400
H	-2.37683700	-1.00632100	1.76897600
H	-3.40699500	-2.62165900	3.33288200
Ni	2.31574900	-1.81274000	-0.64824200
C	3.70376700	-1.05717200	-1.80029400
C	2.48137000	-0.88586600	-2.51380200
H	2.21426000	-1.63356600	-3.25517100
H	2.14181500	0.11243400	-2.76301300
H	4.30487900	-1.93483000	-2.02937200
C	4.42563200	0.03814700	-1.12541700
C	3.96356700	1.36470600	-1.11473500

C	5.62457200	-0.25564200	-0.45363400
C	4.66919600	2.36835400	-0.45501300
H	3.04820200	1.63244900	-1.63227500
C	6.34217600	0.73410400	0.20976100
H	5.97808000	-1.28155800	-0.42699700
C	5.85148700	2.03740800	0.20011000
H	4.30639800	3.38974800	-0.45698600
H	7.26125600	0.49309300	0.73097100
Br	6.84724600	3.43766100	1.12533800

im4a

SCF Energy (a.u.) = -1356.784160

Thermal correction to Gibbs free energy (a.u.) = 0.403055

Charge = 0, Multiplicity = 1

C	4.60656900	1.75114000	0.08798900
C	5.55151200	2.17984400	1.03096900
C	6.89226900	2.32111800	0.69422800
C	7.34201000	2.03748300	-0.60759200
C	6.39100400	1.61004600	-1.54793600
C	5.04863100	1.46793500	-1.20780300
H	5.22737700	2.40701100	2.04448500
H	7.59650500	2.65813200	1.44865500
H	6.71366400	1.38233300	-2.56083400
H	4.33774600	1.11678400	-1.95028400
C	8.74642800	2.16817100	-1.02047800
C	9.78106100	2.56569600	-0.26951900
H	8.93725400	1.90454000	-2.06058600
H	10.78229300	2.62336200	-0.68462300
H	9.67654800	2.84748900	0.77461100
C	2.95166500	0.11972400	1.09159300
C	3.16944800	1.53145600	0.48855000
H	2.86887800	2.28334600	1.22883800
H	2.51795700	1.65102900	-0.38447400
H	3.65657500	0.01652300	1.92728600

C	1.55515200	-0.11110300	1.64181300
C	1.32196300	-1.29398200	2.38592300
C	0.48253000	0.73474000	1.39081800
C	0.05278300	-1.64833500	2.79709900
H	2.15918900	-1.95540500	2.58922300
C	-0.82658200	0.38969800	1.79934800
H	0.62587500	1.66261900	0.84957900
C	-1.06339200	-0.82668000	2.49009500
H	-0.10969600	-2.57672700	3.33721700
H	-1.63086700	1.10344900	1.65351700
Br	-1.53773200	-2.29850600	-1.55409800
C	3.94537500	-2.90176600	-1.84841600
C	4.86422000	-2.55916800	-0.85539100
C	4.53563800	-1.59750800	0.10109300
C	3.28909100	-0.96482200	0.07435000
C	2.37514700	-1.31134100	-0.92862200
C	2.69743700	-2.27549200	-1.88234200
H	4.19757000	-3.65570800	-2.58867800
H	5.83823200	-3.03941700	-0.82318100
H	5.25807800	-1.32172900	0.86473300
H	1.39648000	-0.84161700	-0.96497200
H	1.96490700	-2.54106900	-2.63864800
Ni	-1.41623600	-1.20401200	0.45327700
C	-3.08862400	-1.43945200	1.37133300
C	-2.49781100	-1.26339300	2.77414100
H	-2.49224400	-2.21471700	3.31281000
H	-3.03598600	-0.53721900	3.39264800
H	-3.35862600	-2.46819500	1.12856400
C	-4.05211700	-0.45621200	0.82886200
C	-4.31485600	0.78710900	1.43062800
C	-4.73584700	-0.76372400	-0.36490500
C	-5.21643900	1.69195000	0.87058800
H	-3.82666900	1.06263400	2.35965300
C	-5.63855700	0.12448400	-0.93669600

H	-4.52661900	-1.70564000	-0.86198900
C	-5.86581400	1.34782700	-0.30901200
H	-5.41099800	2.64397700	1.35119700
H	-6.15082500	-0.12783100	-1.85796000
Br	-7.12962100	2.60826900	-1.10312400

im5a

SCF Energy (a.u.) = -1497.827002

Thermal correction to Gibbs free energy (a.u.) = 0.468592

Charge = 0, Multiplicity = 1

C	-4.56082500	-1.72820000	0.07567200
C	-5.56765000	-2.10881000	0.97431200
C	-6.89493100	-2.19957900	0.57296700
C	-7.26869600	-1.91123100	-0.75166000
C	-6.25620900	-1.53212300	-1.64745900
C	-4.92739500	-1.44080700	-1.24263600
H	-5.30290700	-2.33847300	2.00434400
H	-7.64830500	-2.50075700	1.29438800
H	-6.51942800	-1.30235400	-2.67699100
H	-4.16708200	-1.12733100	-1.95232800
C	-8.65536300	-1.98929800	-1.23220200
C	-9.74163400	-2.33321500	-0.52920800
H	-8.78352800	-1.73205100	-2.28348800
H	-10.72268600	-2.35508600	-0.99307000
H	-9.70074100	-2.60457100	0.52209000
C	-2.89202000	-0.15259800	1.14143900
C	-3.13708400	-1.56182700	0.54416700
H	-2.90199700	-2.31446900	1.30698200
H	-2.44999800	-1.71939100	-0.29469900
H	-3.63739400	-0.00561000	1.93397200
C	-1.51571000	0.03399200	1.75474000
C	-1.28423700	1.20258600	2.51940100
C	-0.44559600	-0.81580200	1.50903200
C	-0.01259600	1.55649600	2.92399900

H	-2.12161900	1.86059200	2.73460400
C	0.86613300	-0.46793700	1.91068000
H	-0.58899400	-1.74046800	0.96158500
C	1.10550300	0.75092700	2.58854400
H	0.15043600	2.48028400	3.47224100
H	1.67577900	-1.17353100	1.75058400
C	-3.57155200	2.89079100	-1.87088200
C	-4.55520600	2.60807700	-0.92251600
C	-4.32908100	1.63555800	0.05315900
C	-3.12155300	0.93236500	0.09253300
C	-2.14200700	1.21807300	-0.86808500
C	-2.36255700	2.19176600	-1.84097500
H	-3.74384700	3.65219100	-2.62635200
H	-5.50052500	3.14331600	-0.93979600
H	-5.10238700	1.40840600	0.78220200
H	-1.19035100	0.69469900	-0.85693700
H	-1.58325600	2.40430700	-2.56662300
Ni	1.38418800	1.10171900	0.49477200
C	3.05453700	1.43298100	1.37207000
C	2.53745300	1.22743200	2.80409300
H	2.53046900	2.17287200	3.35399800
H	3.12645200	0.51390600	3.39083900
H	3.29627300	2.47283200	1.13952100
C	4.04461000	0.49116100	0.79254400
C	4.41029100	-0.72554900	1.39215900
C	4.63522700	0.80979800	-0.44709900
C	5.32548700	-1.59176700	0.79053100
H	3.99033300	-1.01456900	2.35019800
C	5.54891100	-0.03790500	-1.06083500
H	4.33606500	1.72575800	-0.94669200
C	5.88339000	-1.23459200	-0.42940100
H	5.59833300	-2.52413100	1.27195500
H	5.98802900	0.22347300	-2.01690500
Br	7.16943300	-2.43916800	-1.28292300

O	1.50495400	1.83266500	-1.11238900
C	1.39007200	3.22020100	-1.31328200
C	1.46509800	3.52822400	-2.80720900
H	2.20558400	3.75833900	-0.79625000
H	0.44095000	3.61295600	-0.90833200
H	1.37638200	4.60578800	-2.99333200
H	2.41634500	3.17504000	-3.22006500
H	0.65770000	3.01434200	-3.34137700

im6a

SCF Energy (a.u.) = -2101.559003

Thermal correction to Gibbs free energy (a.u.) = 0.696164

Charge = 0, Multiplicity = 1

C	-5.00768600	-1.53219100	-0.66529000
C	-6.10565900	-2.26329200	-0.19624500
C	-7.39378700	-1.98635700	-0.63084000
C	-7.63563100	-0.95974700	-1.55712900
C	-6.53310000	-0.23302500	-2.02615300
C	-5.24332500	-0.51287500	-1.58864900
H	-5.94477500	-3.06355300	0.51963900
H	-8.21864100	-2.57568600	-0.24865900
H	-6.69318200	0.56667600	-2.74160000
H	-4.41148000	0.07870400	-1.95353200
C	-8.97730000	-0.62037700	-2.04953200
C	-10.13497400	-1.19991000	-1.71812100
H	-9.00152700	0.19985600	-2.76342700
H	-11.06897700	-0.86107600	-2.14901500
H	-10.19726000	-2.02326000	-1.01558600
C	-3.35892900	-1.02823200	1.18710600
C	-3.62356900	-1.79341900	-0.13334600
H	-3.48387000	-2.86361300	0.04746300
H	-2.88469700	-1.49165000	-0.87653300
H	-4.13441800	-1.32900600	1.89901000
C	-2.01493800	-1.34047400	1.81453500

C	-1.83413200	-1.06609200	3.18848000
C	-0.93102300	-1.80290200	1.08674400
C	-0.59745400	-1.17676200	3.78645100
H	-2.68262700	-0.72258000	3.77029000
C	0.34384000	-1.91757700	1.67948200
H	-1.02776200	-2.05644200	0.04088400
C	0.53445600	-1.57257600	3.03539000
H	-0.47401700	-0.93192500	4.83543900
H	1.14881300	-2.34619000	1.09797800
C	-3.81649100	3.21556200	0.48576800
C	-4.78912200	2.51353500	1.19343700
C	-4.62869500	1.15015600	1.43368800
C	-3.49619700	0.47444600	0.97789000
C	-2.52084400	1.18890400	0.27681100
C	-2.68190600	2.54756000	0.02669600
H	-3.94098500	4.27515200	0.29358300
H	-5.67655400	3.02257800	1.55196500
H	-5.39944400	0.60135600	1.96393800
H	-1.62852500	0.69248800	-0.08373500
H	-1.91669700	3.07289900	-0.52833500
Ni	1.06498600	0.13133700	1.83653700
C	2.63995600	-0.46800500	2.75246000
C	1.94287600	-1.52864300	3.61066200
H	1.90176900	-1.21429500	4.65445000
H	2.42730100	-2.50838200	3.58510800
H	2.98565500	0.39943200	3.31321000
C	3.60558100	-0.87556000	1.70479600
C	3.81696000	-2.20646200	1.31502300
C	4.31996900	0.12326300	1.02011200
C	4.68948500	-2.53237200	0.27893800
H	3.29854900	-3.01451900	1.81507400
C	5.18914000	-0.18179900	-0.01553800
H	4.14079600	1.15865200	1.28035600
C	5.35916300	-1.51305300	-0.38075200

H	4.83732200	-3.56441800	-0.01050500
H	5.70574900	0.60369600	-0.54996000
Br	6.53996800	-1.95037200	-1.85816500
O	1.43185600	1.84395100	1.45210100
C	1.34514600	2.82113000	2.45815100
C	-0.03487200	2.90910200	3.10804300
H	1.59159900	3.79526600	2.00504300
H	2.10765600	2.65243700	3.23823400
H	-0.07702000	3.72372900	3.83936500
H	-0.80393400	3.07799500	2.34992900
H	-0.27555900	1.97328200	3.62231600
C	0.12297700	-2.87951600	-2.34997300
C	1.38073800	-2.58795300	-1.82128700
C	1.74601600	-1.26566400	-1.58349600
C	0.85759400	-0.21279500	-1.84564700
C	-0.40523600	-0.52446300	-2.37057500
C	-0.76829000	-1.84347700	-2.63280300
H	-0.15968000	-3.90759600	-2.54784600
H	2.07999900	-3.38859100	-1.60677200
H	2.72825000	-1.03827400	-1.19098200
H	-1.10101700	0.28006600	-2.58086800
H	-1.74143400	-2.06769500	-3.05572800
C	3.03656800	2.84376500	-1.05354500
C	0.68495300	3.57455700	-1.22002200
C	2.11934900	3.92790300	-1.63389000
H	3.03647100	2.89591100	0.03717200
H	-0.02825000	4.23989500	-1.71496600
B	1.28732400	1.26487800	-1.57403200
O	2.61522000	1.52842400	-1.41777400
O	0.32400600	2.23626700	-1.57520700
H	4.05741400	2.96680900	-1.42574200
H	0.57033300	3.67112400	-0.13798000
C	2.49564900	5.28401000	-1.02888700
H	2.41615800	5.26933800	0.06161300

H	3.52313300	5.55349900	-1.29014200
H	1.84028100	6.07437600	-1.40657000
C	2.24096500	3.97510700	-3.16438000
H	1.57707600	4.73843700	-3.58034100
H	3.26521800	4.21829300	-3.46075200
H	1.97969500	3.01831000	-3.61988800

TS3a

SCF Energy (a.u.) = -2101.554274

Thermal correction to Gibbs free energy (a.u.) = 0.704984

Charge = 0, Multiplicity = 1

C	-5.15593800	-1.04872000	-1.24214700
C	-6.32595200	-1.81646200	-1.15814100
C	-7.57098400	-1.26535200	-1.43671400
C	-7.69409900	0.08408600	-1.81248500
C	-6.51898300	0.84816700	-1.89608600
C	-5.27333800	0.29388100	-1.61608700
H	-6.25568000	-2.86345600	-0.87060500
H	-8.45641100	-1.88958000	-1.36435400
H	-6.58769500	1.89489400	-2.18206500
H	-4.38199500	0.91275400	-1.66814600
C	-8.98314400	0.72036500	-2.11776100
C	-10.19555900	0.15254700	-2.10035500
H	-8.91336200	1.77467700	-2.38515000
H	-11.08407500	0.72602800	-2.34496200
H	-10.35227400	-0.89225100	-1.84661100
C	-3.54093500	-1.53375600	0.65032500
C	-3.81795600	-1.63479300	-0.87173700
H	-3.76991800	-2.69009900	-1.16837400
H	-3.02477400	-1.10792900	-1.41002200
H	-4.35685700	-2.05529200	1.16767300
C	-2.22962300	-2.17058300	1.07441200
C	-2.01191400	-2.39194300	2.45534600
C	-1.19071400	-2.43446900	0.19061300

C	-0.76877100	-2.74853200	2.93748700
H	-2.82911300	-2.21381600	3.14907400
C	0.08903900	-2.80696500	0.66494700
H	-1.31600400	-2.30048400	-0.87627500
C	0.32781900	-2.91637800	2.05508600
H	-0.60722300	-2.86505900	4.00567600
H	0.86437000	-3.05462100	-0.05265400
C	-3.61829100	2.63282500	1.84093800
C	-4.71544800	1.80970400	2.10226200
C	-4.68628800	0.46241200	1.73655000
C	-3.56032100	-0.07800700	1.10870600
C	-2.46457100	0.75515300	0.85668100
C	-2.48804000	2.10244100	1.21377900
H	-3.64435400	3.68120900	2.12564200
H	-5.59917900	2.21596500	2.58673600
H	-5.55126200	-0.16937800	1.92136800
H	-1.57954000	0.35897000	0.37436200
H	-1.61814100	2.71456900	0.99532800
Ni	0.83070900	-0.91138700	1.39757700
C	2.39332800	-1.71221300	2.18297200
C	1.75544300	-3.05622400	2.56475000
H	1.75328800	-3.19639000	3.64986300
H	2.26488700	-3.91974000	2.12459300
H	2.62120600	-1.08194900	3.04568100
C	3.45882200	-1.65547000	1.15763400
C	3.69650100	-2.68079400	0.22518200
C	4.23271400	-0.48444900	1.05106400
C	4.65104800	-2.54305800	-0.78202200
H	3.12568000	-3.60264000	0.26639000
C	5.18539700	-0.32595600	0.05204900
H	4.04200000	0.33512000	1.73544500
C	5.37999000	-1.36154800	-0.85779300
H	4.81774700	-3.34176800	-1.49593600
H	5.74790800	0.59633200	-0.03028900

Br	6.69957700	-1.14385300	-2.28469900
O	1.06471000	0.87442100	1.49887900
C	1.20787300	1.54082000	2.73046600
C	0.19371700	1.09438500	3.78114800
H	1.07710800	2.61475800	2.54561400
H	2.23348400	1.40976400	3.12121900
H	0.31096800	1.67085800	4.70801800
H	-0.82377300	1.23594000	3.40310900
H	0.32144300	0.03141000	4.01860200
C	-0.05359000	-1.24691300	-3.02151500
C	1.21076600	-1.35996400	-2.43731700
C	1.67220700	-0.36437800	-1.57390700
C	0.88235800	0.75453200	-1.25756400
C	-0.38050100	0.85352200	-1.86321900
C	-0.84668900	-0.13087200	-2.73750700
H	-0.41127000	-2.01082500	-3.70759400
H	1.84680900	-2.21150000	-2.66693300
H	2.66786700	-0.43846600	-1.15524400
H	-0.99588200	1.72288800	-1.65170100
H	-1.82035300	-0.02245600	-3.20962900
C	3.37128000	3.18704600	0.32024900
C	1.14742300	4.25480700	0.28843100
C	2.61566800	4.44950800	-0.12296900
H	3.35483300	3.10966100	1.41869400
H	0.52340900	5.04021200	-0.15640400
B	1.43678600	1.89959600	-0.31780200
O	2.81840700	2.01872500	-0.25514400
O	0.61167200	3.00548300	-0.12420500
H	4.42119600	3.24274700	0.00684500
H	1.05866900	4.34586300	1.38068100
C	3.18732000	5.67558700	0.59658600
H	3.14528700	5.55813100	1.68632700
H	4.23395800	5.83998000	0.31462100
H	2.62721400	6.58086600	0.33352000

C	2.72637800	4.62345000	-1.64582500
H	2.19473100	5.52612000	-1.96923200
H	3.77563900	4.72122500	-1.94839100
H	2.30145600	3.76878300	-2.17852500

im7a

SCF Energy (a.u.) = -2101.556368

Thermal correction to Gibbs free energy (a.u.) = 0.698647

Charge = 0, Multiplicity = 1

C	-5.09900700	-0.99815500	-1.35995000
C	-6.25098800	-1.79336200	-1.35266800
C	-7.50462600	-1.24573100	-1.58392400
C	-7.65512800	0.12751900	-1.83306600
C	-6.49820000	0.91818100	-1.84373600
C	-5.24340500	0.36659000	-1.61115600
H	-6.16112800	-2.85878100	-1.16372500
H	-8.37390900	-1.89225400	-1.57344300
H	-6.58737600	1.98281600	-2.03211000
H	-4.36765900	1.00554500	-1.60433400
C	-8.95667500	0.76193300	-2.08071000
C	-10.15513000	0.17154700	-2.11243800
H	-8.90968300	1.83454000	-2.25464800
H	-11.05237100	0.74640000	-2.30565400
H	-10.28802000	-0.89221500	-1.95084500
C	-3.50705800	-1.66390900	0.49323400
C	-3.75206500	-1.58620900	-1.03356000
H	-3.66928600	-2.59268700	-1.45577200
H	-2.96879900	-0.97636200	-1.48643600
H	-4.29719700	-2.28907000	0.92345500
C	-2.17216300	-2.28093300	0.86657800
C	-1.94699800	-2.58450200	2.22967800
C	-1.13304800	-2.46457400	-0.03141500
C	-0.69881700	-2.93708700	2.68796000
H	-2.76620400	-2.47364400	2.93133500

C	0.15491700	-2.84081700	0.41711000
H	-1.26416000	-2.26831800	-1.08615900
C	0.39708800	-3.02661900	1.79680600
H	-0.53377800	-3.11644700	3.74434300
H	0.92773100	-3.04289300	-0.31427700
C	-3.84421300	2.30432900	2.18593900
C	-4.90051100	1.40245300	2.30511200
C	-4.78830600	0.11644000	1.77872600
C	-3.61798600	-0.28355100	1.13244000
C	-2.56368600	0.62570200	1.02832900
C	-2.66983900	1.91375900	1.54265200
H	-3.93674900	3.30537300	2.59183100
H	-5.81730500	1.70109100	2.80077500
H	-5.62251500	-0.57283000	1.85227900
H	-1.64778900	0.33761300	0.53228700
H	-1.82990900	2.58937400	1.42599500
Ni	0.88205100	-0.98350200	1.21023000
C	2.43537500	-1.80492700	2.02377200
C	1.82322700	-3.18243500	2.29770300
H	1.82623000	-3.41085900	3.36483300
H	2.34498900	-3.99323200	1.78647600
H	2.59578900	-1.21606900	2.92626600
C	3.53938800	-1.65644000	1.05708200
C	3.82001500	-2.60323900	0.05861700
C	4.30252800	-0.47673500	1.07242700
C	4.80864400	-2.38154900	-0.89329500
H	3.25478400	-3.52470700	0.00159500
C	5.28907400	-0.23678100	0.12762600
H	4.08012800	0.29016500	1.80209700
C	5.52810200	-1.19404400	-0.85076800
H	5.00840600	-3.11723500	-1.66093100
H	5.84178700	0.69239800	0.13707500
Br	6.88297100	-0.85906600	-2.19731100
O	1.04054200	0.84739000	1.52644400

C	1.24271900	1.43087100	2.81210500
C	0.32369600	0.80596900	3.84774400
H	1.03112700	2.49800900	2.72165800
H	2.29630800	1.32372500	3.10055400
H	0.47073700	1.28056600	4.82241800
H	-0.71976500	0.92944000	3.55108000
H	0.52145900	-0.26390600	3.95643800
C	0.16979500	-0.90763000	-3.14169400
C	1.42377100	-1.02184400	-2.54360600
C	1.77647200	-0.17207100	-1.49493500
C	0.88783300	0.79492900	-0.99573800
C	-0.35798200	0.90557400	-1.63255600
C	-0.71578900	0.07289700	-2.69154800
H	-0.10485600	-1.55483200	-3.96777800
H	2.13644700	-1.75510600	-2.90667700
H	2.77230500	-0.22925000	-1.07893400
H	-1.04143700	1.67682500	-1.29741300
H	-1.67830000	0.19434200	-3.17812000
C	3.16050600	3.39523800	0.46792300
C	0.84658000	4.21421400	0.51984700
C	2.22289900	4.46330500	-0.11190400
H	3.26052600	3.56530200	1.55359500
H	0.10027200	4.87947600	0.06877600
B	1.30296100	1.77415000	0.23105600
O	2.70997100	2.08609400	0.20693200
O	0.39068800	2.88686900	0.36120000
H	4.16106300	3.49577000	0.03034100
H	0.90279500	4.47036900	1.59116600
C	2.72049900	5.85666200	0.28154800
H	2.80389500	5.96112900	1.36783700
H	3.70494800	6.05488300	-0.15290900
H	2.03733200	6.63152500	-0.07961100
C	2.14618300	4.33536400	-1.63985000
H	1.47035500	5.08992400	-2.05384500

H	3.13372600	4.48156500	-2.08786900
H	1.78304300	3.35232200	-1.94010300

TS4a

SCF Energy (a.u.) = -2101.551689

Thermal correction to Gibbs free energy (a.u.) = 0.705920

Charge = 0, Multiplicity = 1

C	-5.22595100	0.19571100	-1.47254800
C	-6.29905800	-0.34406800	-2.19585100
C	-7.60118900	0.09559700	-1.99085000
C	-7.88301300	1.10035600	-1.04829600
C	-6.80485500	1.64018800	-0.32899200
C	-5.50185300	1.19711600	-0.53650800
H	-6.10606300	-1.12271700	-2.93081900
H	-8.40769700	-0.34433100	-2.56966300
H	-6.99643400	2.41728800	0.40710200
H	-4.68939200	1.61711700	0.04990100
C	-9.23904100	1.60296100	-0.78807300
C	-10.37754100	1.21921400	-1.37920000
H	-9.29386900	2.37546100	-0.02100900
H	-11.32806200	1.66406900	-1.10198200
H	-10.41048900	0.45753000	-2.15334500
C	-3.58299700	-1.62963200	-0.82368000
C	-3.82925800	-0.34103500	-1.65289800
H	-3.65115900	-0.56333500	-2.71172500
H	-3.09402300	0.41176100	-1.35079700
H	-4.28763200	-2.38591300	-1.19709700
C	-2.17042100	-2.18540300	-0.97870900
C	-1.79158500	-3.29665800	-0.21166200
C	-1.21939100	-1.63102500	-1.83829600
C	-0.49895000	-3.80832200	-0.27297600
H	-2.51675400	-3.74625300	0.46165400
C	0.07494400	-2.14546000	-1.90123800
H	-1.46426900	-0.76825500	-2.44536800

C	0.46347900	-3.22279400	-1.10310900
H	-0.22688500	-4.66211400	0.34449300
H	0.80065800	-1.67698700	-2.56276800
C	-4.60436000	-0.81358400	3.30431400
C	-5.44623800	-1.59876300	2.51784300
C	-5.10523600	-1.87880500	1.19256100
C	-3.92397700	-1.38127500	0.63795600
C	-3.08210800	-0.59171200	1.43306200
C	-3.42119700	-0.31040700	2.75556000
H	-4.86631500	-0.59366600	4.33558700
H	-6.37102100	-1.99156100	2.93149000
H	-5.77288900	-2.47583500	0.57668000
H	-2.16623800	-0.19897800	1.00292900
H	-2.75973200	0.30185400	3.36367900
Ni	2.29181200	-0.97007400	0.04966600
C	2.67524100	-2.94092400	0.07278200
C	1.91454900	-3.65169800	-1.04515000
H	1.97868500	-4.73676200	-0.88439500
H	2.39516100	-3.45361000	-2.00959500
H	2.58314100	-3.41815300	1.04863900
C	3.88739800	-2.20996700	-0.14380500
C	3.93100700	-1.31434100	-1.26333100
C	4.89839800	-2.04987600	0.86419300
C	4.99279100	-0.37735900	-1.40213500
H	3.30541200	-1.49351500	-2.13341100
C	5.90552900	-1.12876500	0.72550600
H	4.86845500	-2.69640100	1.73661100
C	5.94000400	-0.29670000	-0.42025300
H	5.01952000	0.27670700	-2.26488500
H	6.67403400	-1.03281600	1.48451600
Br	7.38594700	1.00856100	-0.56649800
O	0.69524700	-0.79612600	1.05004600
C	0.43513500	-1.44356500	2.30787300
C	1.57636900	-1.28542100	3.29954700

H	0.25686500	-2.49208500	2.05993400
H	-0.49427400	-1.02709700	2.70548900
H	1.34853100	-1.83432100	4.22143500
H	2.50808600	-1.68420200	2.88322200
H	1.72539200	-0.23059200	3.54057400
C	3.75448400	3.15886400	-1.34680000
C	4.00692800	2.74838800	-0.03444200
C	3.26532100	1.70467200	0.51858700
C	2.25947700	1.03718700	-0.20964000
C	2.01748400	1.48871200	-1.52283200
C	2.75081200	2.53237900	-2.09123900
H	4.33121300	3.97013800	-1.78314900
H	4.78326600	3.23815600	0.54692000
H	3.46507300	1.40123400	1.54388700
H	1.23210400	1.00950800	-2.10419800
H	2.54358700	2.85941400	-3.10759900
C	-0.44400300	2.35885000	2.20281500
C	-0.93659100	2.26285400	-0.24862400
C	-0.69109200	3.21793000	0.95370300
H	-1.37281700	1.83509000	2.47323100
H	-0.43437400	2.65728400	-1.14233400
B	0.51096300	0.63274800	0.86296900
O	0.60407100	1.41385900	2.02319200
O	-0.51498800	0.92071600	-0.04312600
H	-0.16344600	2.99794800	3.04705400
H	-2.00906500	2.20636600	-0.46933900
C	-1.94366300	4.07740700	1.18129300
H	-2.81841300	3.45477200	1.40630600
H	-1.79807900	4.77461500	2.01500600
H	-2.17414300	4.67201400	0.28942200
C	0.52020600	4.12721300	0.69387800
H	0.36018700	4.73506900	-0.20431900
H	0.67579400	4.80978200	1.53842100
H	1.43409200	3.54915600	0.55262900

im8a

SCF Energy (a.u.) = -2101.571514

Thermal correction to Gibbs free energy (a.u.) = 0.702894

Charge = 0, Multiplicity = 1

C	-6.01146900	-0.13894100	-1.19665700
C	-7.02242300	-0.95033900	-1.73177100
C	-8.36209200	-0.71470700	-1.44787000
C	-8.74609200	0.34911200	-0.61201100
C	-7.73051200	1.15939700	-0.07990900
C	-6.38922000	0.92010300	-0.36546100
H	-6.75019400	-1.77934900	-2.38149100
H	-9.11837400	-1.36154000	-1.88197600
H	-8.00091400	1.98694800	0.57148600
H	-5.62263800	1.55072600	0.07640700
C	-10.14589100	0.64496800	-0.27649700
C	-11.23788400	-0.00975400	-0.69061800
H	-10.27975300	1.49929000	0.38699600
H	-12.22856600	0.30114100	-0.37432900
H	-11.19239400	-0.86985200	-1.35292200
C	-4.00697600	-1.51433900	-0.46581000
C	-4.55962600	-0.45140400	-1.45392300
H	-4.42698100	-0.82399400	-2.47664700
H	-3.96448100	0.46427200	-1.36182100
H	-4.66462200	-2.38966600	-0.54465800
C	-2.59020700	-1.96805200	-0.78845700
C	-2.10382500	-3.13830700	-0.18721600
C	-1.72253600	-1.24787200	-1.61374000
C	-0.79608800	-3.56446100	-0.39765800
H	-2.76118200	-3.71190800	0.46216100
C	-0.40914000	-1.67394300	-1.82021500
H	-2.05472800	-0.33585300	-2.09781900
C	0.07812100	-2.83028000	-1.21130100
H	-0.44467100	-4.47804400	0.07755900

H	0.25265700	-1.07229900	-2.43618400
C	-4.32406000	0.06519800	3.55681100
C	-5.28593300	-0.82440900	3.07678800
C	-5.17532800	-1.35187100	1.78843300
C	-4.10373900	-0.99932400	0.96347100
C	-3.14535500	-0.10651700	1.45520400
C	-3.24927400	0.42472800	2.73931900
H	-4.40888500	0.47297600	4.56021000
H	-6.12658200	-1.10844300	3.70378900
H	-5.93676500	-2.03014900	1.41292300
H	-2.30169400	0.16065800	0.83014300
H	-2.48429600	1.10797500	3.09722800
Ni	2.57747600	-0.71506900	-0.17018400
C	2.34877000	-2.78356000	-0.14999800
C	1.53093200	-3.23252700	-1.35135800
H	1.59851900	-4.32713800	-1.45392700
H	1.93756800	-2.81278200	-2.27724300
H	2.03755400	-3.25573200	0.78283600
C	3.71179600	-2.38603200	-0.19326300
C	4.14963800	-1.50692200	-1.24922300
C	4.57816200	-2.49561100	0.95667600
C	5.44377900	-0.90040500	-1.19885400
H	3.65419900	-1.52574300	-2.21708300
C	5.79462800	-1.87026500	1.00369600
H	4.25438300	-3.11799700	1.78659800
C	6.22112100	-1.07523100	-0.09377100
H	5.77194900	-0.28232900	-2.02560800
H	6.43832800	-1.98013300	1.86963800
Br	7.96327000	-0.19625000	0.02786300
O	0.86542000	-0.19863500	0.72088400
C	0.54953200	-0.84398700	1.98197000
C	1.64216400	-0.59189700	3.00323700
H	0.44283100	-1.90289000	1.74450600
H	-0.41286000	-0.46411700	2.32599900

H	1.39991200	-1.10693800	3.94018200
H	2.60722900	-0.96301100	2.64192100
H	1.73736800	0.47891900	3.20681200
C	4.41905600	3.65548900	-0.57036800
C	4.43721100	2.97087900	0.64489000
C	3.85945500	1.69876100	0.74332300
C	3.24524400	1.07349100	-0.35590300
C	3.23678500	1.79093100	-1.56680500
C	3.81232100	3.05879700	-1.67956100
H	4.87262300	4.63971100	-0.65434000
H	4.90582900	3.42284400	1.51665800
H	3.90463100	1.18228600	1.70111700
H	2.76981200	1.35021400	-2.44679400
H	3.79392200	3.58120500	-2.63446400
C	-1.12637800	2.87144200	0.93300500
C	-0.28170500	2.58263000	-1.37608000
C	-0.43788300	3.59588400	-0.23032200
H	-2.14431700	2.56566300	0.65633800
H	0.41104000	2.96586200	-2.13180600
B	0.22953200	0.98451800	0.36375300
O	-0.39736300	1.70596000	1.34003500
O	0.23052900	1.31953500	-0.94840900
H	-1.19464700	3.52271600	1.80947400
H	-1.25199900	2.39937100	-1.85703100
C	-1.33126100	4.74935700	-0.70404700
H	-2.32906200	4.39763700	-0.99314500
H	-1.45057400	5.49755500	0.08766500
H	-0.88534900	5.25245100	-1.56948700
C	0.93253800	4.13092400	0.21457700
H	1.42108800	4.66547900	-0.60517500
H	0.81436900	4.82567200	1.05459400
H	1.61243800	3.33475800	0.52539800

im9a

SCF Energy (a.u.) = -1887.137864

Thermal correction to Gibbs free energy (a.u.) = 0.665694

Charge = 0, Multiplicity = 1

C	6.51413000	-1.38408100	0.79577300
C	7.15963300	-2.39718200	0.07122000
C	8.49253000	-2.28078500	-0.30218600
C	9.23893400	-1.13781500	0.03590100
C	8.58953700	-0.12724300	0.76217900
C	7.25316500	-0.24676400	1.13526400
H	6.60408400	-3.29251800	-0.19966100
H	8.96023100	-3.08721200	-0.85869200
H	9.14485000	0.76623300	1.03721200
H	6.77571700	0.55696500	1.68787500
C	10.65072600	-0.96006100	-0.33123200
C	11.42805500	-1.81266900	-1.01045500
H	11.08789600	-0.01815500	-0.00013500
H	12.46447800	-1.57266700	-1.22575000
H	11.07096000	-2.77195800	-1.37474800
C	4.14914700	-1.03437400	-0.04257300
C	5.04817700	-1.50556000	1.13106000
H	4.79420500	-2.54888000	1.35011900
H	4.81875500	-0.93045600	2.03426300
H	4.47763200	-1.59421200	-0.92607300
C	2.67810400	-1.36036600	0.16823100
C	1.95014800	-1.98558000	-0.85168700
C	1.99720600	-1.02546300	1.34416000
C	0.58463300	-2.23049600	-0.71699300
H	2.46101900	-2.27779800	-1.76634100
C	0.62832600	-1.26035600	1.47189000
H	2.53140400	-0.56714500	2.17123000
C	-0.10947000	-1.84534400	0.43736700
H	0.04291900	-2.71278100	-1.52764500
H	0.12187000	-0.97967100	2.39027500
C	4.61587300	3.16974400	-1.02223400

C	4.74679200	2.19164200	-2.00804100
C	4.60986600	0.84215900	-1.67766100
C	4.33569200	0.44337100	-0.36511100
C	4.20924500	1.43589400	0.61609200
C	4.35016000	2.78503300	0.29370900
H	4.72526700	4.22062500	-1.27399900
H	4.96020800	2.47618500	-3.03455800
H	4.71890400	0.08451200	-2.44936600
H	3.99615400	1.15812800	1.64351700
H	4.25188500	3.53697300	1.07198700
Ni	-1.84782300	0.88004200	0.06720300
C	-2.31464300	-0.97748800	-0.40068700
C	-1.60981600	-1.99144300	0.51719200
H	-1.89689100	-3.01323200	0.22038800
H	-1.93412600	-1.86170600	1.55335100
H	-1.85108300	-1.05072700	-1.39353800
C	-3.78328100	-1.17597100	-0.55745100
C	-4.58041100	-1.76790400	0.43641100
C	-4.43564100	-0.71742400	-1.71580900
C	-5.96279400	-1.88120200	0.29771800
H	-4.12386100	-2.11624600	1.35595700
C	-5.81655200	-0.81387800	-1.87564000
H	-3.84876800	-0.26562000	-2.51212000
C	-6.56359000	-1.39522500	-0.85663500
H	-6.55877800	-2.32895900	1.08491400
H	-6.29737700	-0.44959000	-2.77677300
Br	-8.51185900	-1.53300500	-1.05727000
C	-4.76332600	0.87666900	3.76759500
C	-5.19600300	1.25404400	2.49399500
C	-4.31785100	1.20285400	1.40970900
C	-2.98436400	0.78546900	1.56472500
C	-2.56597300	0.42477200	2.85372100
C	-3.44361600	0.46143400	3.94363000
H	-5.44795600	0.90414000	4.61109400

H	-6.22410800	1.57329500	2.33961400
H	-4.69366700	1.45568900	0.42043000
H	-1.54005100	0.10671000	3.02404400
H	-3.09164600	0.16564500	4.92969000
C	-1.65025100	3.24914100	0.29006400
C	-0.64080500	2.63599100	0.96837200
C	0.77623900	2.39164100	0.50904000
C	0.95492800	2.11551400	-1.00135300
C	-0.08315200	1.17367400	-1.56773200
C	-1.28677300	1.51014800	-2.10441700
C	-1.91715100	2.87880900	-2.22115700
C	-1.56361500	3.86880100	-1.08723000
H	-2.59007600	3.38393600	0.82035100
H	-0.84301100	2.36981400	2.00352000
H	1.15862600	1.52711500	1.05927300
H	1.41639300	3.23837900	0.79558200
H	0.96220100	3.05249700	-1.56300600
H	1.94136600	1.66748500	-1.14218700
H	0.21461000	0.13020600	-1.62470000
H	-1.83965300	0.72123300	-2.60843200
H	-3.00477600	2.73644900	-2.23570500
H	-1.65832100	3.32835700	-3.19168900
H	-0.57022900	4.29225300	-1.25053900
H	-2.26618200	4.70792400	-1.13867800

TS5a

SCF Energy (a.u.) = -1887.110945

Thermal correction to Gibbs free energy (a.u.) = 0.662516

Charge = 0, Multiplicity = 1

C	6.43432700	-1.56396000	0.60671100
C	7.11318700	-2.47695800	-0.21313300
C	8.41733800	-2.24050700	-0.63055600
C	9.09789000	-1.07271300	-0.24283700
C	8.41391100	-0.16159500	0.57778800

C	7.10737500	-0.40087500	0.99473100
H	6.60776800	-3.38832900	-0.52541800
H	8.91358400	-2.97161100	-1.26146500
H	8.91776700	0.74973500	0.89066400
H	6.59763700	0.32916500	1.61688100
C	10.47605100	-0.76973100	-0.65337300
C	11.27874400	-1.51594800	-1.42243900
H	10.86190200	0.17649300	-0.27421100
H	12.28531100	-1.18787000	-1.66191200
H	10.97248500	-2.47149600	-1.83915200
C	4.01883300	-1.23456000	-0.07150900
C	4.99552200	-1.80180100	0.99157800
H	4.80364800	-2.87567200	1.10189600
H	4.79006400	-1.33480600	1.96092500
H	4.32349100	-1.65640600	-1.03727500
C	2.56458300	-1.60921200	0.15650200
C	1.69412700	-1.62918300	-0.94143800
C	2.02157100	-1.84323300	1.42248600
C	0.32429800	-1.79380500	-0.77160700
H	2.09861500	-1.48089300	-1.94020000
C	0.64564000	-2.01738600	1.58934600
H	2.66528700	-1.87584500	2.29598100
C	-0.23412900	-1.95037600	0.50541100
H	-0.32236900	-1.78664200	-1.64530400
H	0.24855300	-2.19038200	2.58593700
C	4.44666400	3.07230000	-0.34966500
C	4.91066400	2.25221300	-1.37846400
C	4.76516400	0.86628100	-1.28942200
C	4.15205600	0.28056900	-0.17878600
C	3.68521700	1.11329400	0.84673700
C	3.83379900	2.49651800	0.76652400
H	4.55996700	4.15068300	-0.41541600
H	5.39174600	2.68859100	-2.24942700
H	5.14425000	0.22980600	-2.08459000

H	3.18844100	0.67547000	1.70784100
H	3.45992600	3.12601900	1.56912100
Ni	-1.77784800	1.15679100	-0.11023800
C	-2.47984800	-0.84180000	0.05346200
C	-1.73411600	-2.03341300	0.68928000
H	-2.10716200	-2.94814600	0.20533100
H	-1.96770200	-2.12933200	1.75422500
H	-1.98316300	-0.65328800	-0.91204700
C	-3.92331500	-1.07714700	-0.21295800
C	-4.76781800	-1.61886900	0.77000000
C	-4.49181500	-0.74361500	-1.45251000
C	-6.12670500	-1.82162300	0.53050400
H	-4.36101100	-1.87042500	1.74385800
C	-5.84801000	-0.93293300	-1.71260300
H	-3.85867500	-0.33203600	-2.23410300
C	-6.64837100	-1.47096100	-0.70941000
H	-6.76610700	-2.23765200	1.30090400
H	-6.26840100	-0.67444200	-2.67792900
Br	-8.55833100	-1.74301600	-1.05633400
C	-3.29988000	1.40556100	4.06960900
C	-4.08448000	1.62439700	2.93774100
C	-3.66945800	1.15666800	1.68752900
C	-2.41179700	0.52741500	1.52560000
C	-1.64235200	0.29280100	2.68601300
C	-2.08227800	0.72560200	3.93355300
H	-3.63554400	1.74110700	5.04656100
H	-5.04373600	2.12881100	3.02724900
H	-4.33040800	1.27413100	0.83354500
H	-0.67089700	-0.17777000	2.59853700
H	-1.46105900	0.54795100	4.80885700
C	-0.74317900	2.92032500	0.52466000
C	0.16507200	1.96246200	0.12964800
C	0.84217300	1.87822900	-1.22022900
C	-0.06980900	2.18671500	-2.44236300

C	-1.48672900	1.67379500	-2.30081000
C	-2.53083200	2.35374400	-1.73056900
C	-2.49230500	3.75179400	-1.14505700
C	-1.21522900	4.08248800	-0.32692400
H	-1.01869500	2.95127300	1.57576500
H	0.58126900	1.30841300	0.89348700
H	1.23846100	0.86596100	-1.32151400
H	1.71601300	2.54412600	-1.24953900
H	-0.08941500	3.26311200	-2.63427600
H	0.38690600	1.73170800	-3.32864300
H	-1.71309900	0.73594100	-2.80657500
H	-3.52929300	1.93236100	-1.84822500
H	-3.36332500	3.85375900	-0.48822200
H	-2.61918700	4.50017000	-1.94261800
H	-0.41442500	4.41089400	-0.99520400
H	-1.43862600	4.93697700	0.32155400

im10a

SCF Energy (a.u.) = -1887.161801

Thermal correction to Gibbs free energy (a.u.) = 0.665697

Charge = 0, Multiplicity = 1

C	6.14422600	-1.86549100	0.84294600
C	6.75469700	-2.94604600	0.18996500
C	8.08730300	-2.89386100	-0.20027700
C	8.86673400	-1.75009500	0.04761000
C	8.25104100	-0.67077300	0.70138800
C	6.91576800	-0.72559400	1.09162900
H	6.17209900	-3.84232000	-0.01213700
H	8.52810600	-3.75108600	-0.69996800
H	8.83194500	0.22582600	0.90377800
H	6.46165800	0.13046700	1.58223100
C	10.27923900	-1.63812900	-0.34216500
C	11.02767900	-2.55885300	-0.96245100
H	10.74406900	-0.68645800	-0.08478700

H	12.06794100	-2.36313600	-1.20268900
H	10.64217200	-3.53248900	-1.25218800
C	3.79400100	-1.40648900	0.02470100
C	4.67844500	-1.91278000	1.19505800
H	4.37894400	-2.93902700	1.43825600
H	4.49128500	-1.30151300	2.08457200
H	4.09356000	-1.97573100	-0.86372600
C	2.30634200	-1.63948000	0.23187900
C	1.48248500	-1.80632300	-0.88995000
C	1.69949600	-1.62699900	1.49132700
C	0.10207100	-1.91124300	-0.75985700
H	1.93390200	-1.83115600	-1.87880200
C	0.31270700	-1.73250800	1.62048300
H	2.30398300	-1.52594600	2.38723400
C	-0.51263100	-1.85088300	0.49921900
H	-0.51289900	-2.03018800	-1.64902100
H	-0.13021900	-1.71601400	2.61255900
C	4.62570900	2.76985600	-0.79448200
C	5.02672900	1.78297900	-1.69610700
C	4.75199100	0.44003800	-1.43096900
C	4.07199500	0.06308700	-0.26901700
C	3.67578100	1.06112300	0.62950800
C	3.95127300	2.40284000	0.37249500
H	4.83619100	3.81593200	-0.99844000
H	5.55565400	2.05599700	-2.60497900
H	5.07803200	-0.32698300	-2.12847000
H	3.12380000	0.79063000	1.52409500
H	3.62421200	3.16295300	1.07601900
Ni	-1.56119200	1.99215200	-0.20263300
C	-2.78448100	-0.70178400	0.04231100
C	-2.01574600	-1.92712200	0.61037800
H	-2.36641000	-2.80182400	0.04959000
H	-2.31718100	-2.09787900	1.64915900
H	-2.38867000	-0.52181300	-0.96635400

C	-4.24668500	-1.10138200	-0.12139700
C	-5.12344000	-1.08778100	0.97077900
C	-4.73022200	-1.53493900	-1.35934400
C	-6.44764700	-1.50256200	0.83748800
H	-4.77158300	-0.72892800	1.93354600
C	-6.05425900	-1.95057200	-1.51839800
H	-4.06448400	-1.54804100	-2.21935800
C	-6.89210400	-1.92936300	-0.41038700
H	-7.12059800	-1.48624200	1.68728600
H	-6.42093300	-2.27863200	-2.48442000
Br	-8.75453800	-2.50610600	-0.61245000
C	-3.31957800	2.80201900	2.53591600
C	-3.73941500	2.81134600	1.22373300
C	-3.44608300	1.72777800	0.33510700
C	-2.68004600	0.60635600	0.84525300
C	-2.35313600	0.59890400	2.24027200
C	-2.63639600	1.66990200	3.05660100
H	-3.55338200	3.63921100	3.18797000
H	-4.32939300	3.64520800	0.85041100
H	-4.07053900	1.60235400	-0.54895200
H	-1.85749400	-0.26817700	2.66132900
H	-2.35310900	1.64463600	4.10524400
C	0.26514300	2.52113400	0.68683300
C	0.50075600	1.49518200	-0.19995800
C	0.95419200	1.62229500	-1.63470400
C	0.31176000	2.80795700	-2.39598400
C	-1.14292600	3.04024200	-2.02846400
C	-1.60005200	3.92623700	-1.07939700
C	-0.75640100	4.73281800	-0.11704200
C	0.50342800	3.99402400	0.41449400
H	0.06878500	2.25074700	1.72379000
H	0.52014500	0.49201900	0.20472300
H	0.68339200	0.68836900	-2.14059800
H	2.04857600	1.69314000	-1.69520000

H	0.88642300	3.72199000	-2.22319100
H	0.37910200	2.61109200	-3.47246500
H	-1.88170000	2.62986000	-2.71773000
H	-2.65504200	4.18861600	-1.09986300
H	-1.39749600	4.98391700	0.73641700
H	-0.45167400	5.69039000	-0.56722800
H	1.33600800	4.11002500	-0.28468200
H	0.81655800	4.48329300	1.34435800

P2

SCF Energy (a.u.) = -1404.060869

Thermal correction to Gibbs free energy (a.u.) = 0.492006

Charge = 0, Multiplicity = 1

C	-5.72737100	-0.91283500	-0.80636700
C	-6.49670700	-1.95150700	-0.26188100
C	-7.83946800	-1.76967900	0.04570100
C	-8.47011300	-0.53321200	-0.18100000
C	-7.69617700	0.50297300	-0.72723900
C	-6.35068500	0.31811000	-1.03332200
H	-6.03102000	-2.91737600	-0.07790300
H	-8.40525000	-2.59683200	0.46352600
H	-8.15961800	1.46948500	-0.90985400
H	-5.77067000	1.14300200	-1.43743200
C	-9.88546600	-0.28309500	0.12509500
C	-10.77210000	-1.14533900	0.63805600
H	-10.22384800	0.72803400	-0.10105900
H	-11.79870800	-0.84586600	0.82399000
H	-10.51722700	-2.17106600	0.88990800
C	-3.40303700	-0.84878600	0.21104600
C	-4.25450100	-1.10327400	-1.06434200
H	-4.05839200	-2.12438800	-1.41287700
H	-3.92906900	-0.42028100	-1.85630100
H	-3.82399600	-1.48366900	1.00071500
C	-1.94043500	-1.22518300	0.04985800

C	-1.19547800	-1.55869200	1.18920800
C	-1.27515500	-1.17910900	-1.17886600
C	0.17251000	-1.79918100	1.10824000
H	-1.69602600	-1.60771700	2.15339200
C	0.09793200	-1.41069100	-1.25787300
H	-1.81986400	-0.93839100	-2.08599500
C	0.84591900	-1.70470900	-0.11633100
H	0.73091000	-2.04049100	2.01032000
H	0.60172100	-1.32263400	-2.21653900
C	-3.94793900	3.27784800	1.42470200
C	-4.67819300	2.25981000	2.03805900
C	-4.48097800	0.93131100	1.65881500
C	-3.55234500	0.59817500	0.66734100
C	-2.81827100	1.62625100	0.06174200
C	-3.01754600	2.95531300	0.43400000
H	-4.10028100	4.31326400	1.71621500
H	-5.40569800	2.49772100	2.80917500
H	-5.06733200	0.14334800	2.12370000
H	-2.07519100	1.38485200	-0.69231000
H	-2.44455600	3.74174500	-0.05074200
C	2.98684300	-0.45599500	0.33638900
C	2.35066500	-1.77738100	-0.17656500
H	2.72640000	-2.60996000	0.43107800
H	2.66973400	-1.95466900	-1.20975400
H	2.67645000	-0.35077700	1.38443800
C	4.50936100	-0.45198500	0.31848700
C	5.18034700	0.64762500	0.87497500
C	5.27667000	-1.48318500	-0.22943300
C	6.56998600	0.72166300	0.89305700
H	4.59992100	1.46660200	1.29131400
C	6.67467800	-1.42990800	-0.22544000
H	4.79699800	-2.35064800	-0.66887100
C	7.29950700	-0.32665400	0.33742700
H	7.07421000	1.57732000	1.32750900

H	7.25729700	-2.23700000	-0.65475700
Br	9.25595400	-0.23784200	0.35049300
C	1.21589200	2.82274000	-1.86975700
C	0.76788500	2.51684500	-0.58420300
C	1.36152400	1.47820700	0.13357500
C	2.40923600	0.73385600	-0.41788600
C	2.85745900	1.05278900	-1.70512300
C	2.26424300	2.08735800	-2.42800500
H	0.75566200	3.63038000	-2.43213700
H	-0.04550300	3.07963500	-0.13586100
H	0.98909900	1.22519100	1.12213800
H	3.68005000	0.49021400	-2.13887100
H	2.62327200	2.32260800	-3.42623300

im3b

SCF Energy (a.u.) = -1356.765959

Thermal correction to Gibbs free energy (a.u.) = 0.400558

Charge = 0, Multiplicity = 1

Ni	-4.87709300	-0.96864400	0.00535600
C	-4.00204700	0.63366100	-0.31015000
C	-2.72127500	0.82261200	0.20826000
C	-1.97340500	1.92463200	-0.19741000
C	-2.49497000	2.86148000	-1.10546600
C	-3.81493600	2.68639400	-1.55174700
C	-4.57407100	1.58212300	-1.15625600
H	-2.28428800	0.10613300	0.89527700
H	-0.97365900	2.04915400	0.19934800
H	-4.24989600	3.41535000	-2.23203300
H	-5.58958300	1.46516900	-1.52346900
C	-1.71057700	3.99954100	-1.60526300
C	-0.38813700	4.17474800	-1.48486800
H	-2.28661500	4.75209000	-2.14399900
H	0.09727700	5.05537800	-1.89446500
H	0.25112900	3.45588400	-0.98085900

Br	-5.64500600	-0.48535100	2.08113800
C	0.30854700	-1.36017800	-1.45666400
C	-0.59704500	-0.58881100	-2.19536800
C	-1.95468000	-0.88370900	-2.20964500
C	-2.45900700	-1.95605900	-1.45767700
C	-1.54915000	-2.74592000	-0.73457700
C	-0.18966900	-2.45912700	-0.74277700
H	-0.23569700	0.27352100	-2.74846600
H	-2.62921600	-0.24324400	-2.76688100
H	-1.91963500	-3.58727300	-0.15398700
H	0.48868600	-3.09324000	-0.17902400
C	-3.88932800	-2.25542700	-1.34489100
C	-4.95269500	-1.59129100	-1.93803700
H	-4.10867900	-3.20264400	-0.84623400
H	-5.92848400	-2.07131400	-1.99062600
H	-4.80030700	-0.75143400	-2.60665400
C	2.38340100	-0.89418900	-0.02630700
C	1.78041800	-1.01808500	-1.44512800
H	2.34068200	-1.79109300	-1.98895900
H	1.92929200	-0.07829500	-1.98800700
H	2.17048800	-1.83382200	0.49735500
C	3.89899100	-0.73554700	-0.02684600
C	4.63766300	-0.38974300	-1.16161300
C	4.58720300	-0.91611800	1.18170000
C	6.02589300	-0.22929600	-1.10263600
H	4.14364100	-0.24033400	-2.11542400
C	5.96829400	-0.76437600	1.26408800
H	4.02732500	-1.16958600	2.07821300
C	6.67023800	-0.42020000	0.11139800
H	6.58684300	0.03878400	-1.99064800
H	6.48686600	-0.90954300	2.20486100
Br	8.61234700	-0.20106900	0.20837400
C	0.54132400	2.25557100	2.31851700
C	0.16075000	0.92631500	2.50514100

C	0.74909000	-0.08299300	1.74019300
C	1.72283300	0.21761600	0.78143700
C	2.09087100	1.55617700	0.59524700
C	1.50734100	2.56761400	1.35841400
H	0.08514000	3.04284900	2.91088300
H	-0.59356600	0.67341600	3.24458800
H	0.45085600	-1.11660500	1.89180200
H	2.86116900	1.80316600	-0.13023500
H	1.81071600	3.59976100	1.20834000

TS2b

SCF Energy (a.u.) = -1356.752232

Thermal correction to Gibbs free energy (a.u.) = 0.402628

Charge = 0, Multiplicity = 1

Ni	-3.74972800	-1.09564200	0.41336400
C	-4.53620700	0.40102200	-0.38854800
C	-3.62698600	1.42813200	-0.70830300
C	-3.99977800	2.75597200	-0.54545700
C	-5.29335500	3.10325200	-0.10835800
C	-6.20177200	2.06442500	0.15736000
C	-5.84337500	0.72596100	0.00237100
H	-2.62026800	1.18941600	-1.03454000
H	-3.27393600	3.53317500	-0.76383800
H	-7.20750400	2.31181000	0.48793600
H	-6.56888400	-0.05645600	0.20631700
C	-5.73121400	4.49349600	0.06998800
C	-5.00567600	5.60157100	-0.12719000
H	-6.76269300	4.60493900	0.40244200
H	-5.43381100	6.58477900	0.03917400
H	-3.97021800	5.57765200	-0.45501800
Br	-2.81036200	-2.16412400	2.21845500
C	0.74312400	-1.80244000	-1.87107200
C	-0.16533400	-0.90782600	-2.44705100
C	-1.53416800	-1.07553500	-2.28248300

C	-2.03867600	-2.14630800	-1.52581600
C	-1.12859700	-3.09625300	-1.03045700
C	0.23827800	-2.92724700	-1.20526600
H	0.20816500	-0.03609700	-2.97611700
H	-2.20828500	-0.34334900	-2.71466500
H	-1.50206800	-3.93044400	-0.44434900
H	0.92715100	-3.64534200	-0.76724600
C	-3.45506600	-2.25161400	-1.14378800
C	-4.46294000	-1.32796500	-1.55378300
H	-3.77639400	-3.22435000	-0.77540600
H	-5.49902700	-1.64784200	-1.49172100
H	-4.26363100	-0.65947800	-2.38338800
C	2.53446900	-0.88583900	-0.38152500
C	2.20620300	-1.45687900	-1.79301500
H	2.83412200	-2.33707300	-1.97672300
H	2.45189000	-0.70843200	-2.55437200
H	2.36075200	-1.70535200	0.32823800
C	3.98294300	-0.44676900	-0.21448000
C	4.92631500	-0.49054900	-1.24421900
C	4.39493400	0.02682300	1.04072800
C	6.24674500	-0.07663200	-1.03840800
H	4.65002500	-0.85137100	-2.22873200
C	5.70367800	0.44097700	1.26980500
H	3.67153600	0.08206600	1.84953800
C	6.61453600	0.38292900	0.21771200
H	6.96774800	-0.11500000	-1.84700700
H	6.00719100	0.80370800	2.24519500
Br	8.45884700	0.96741800	0.52039900
C	-0.35379000	2.21698100	0.50572700
C	-0.49910400	0.94357400	1.05965700
C	0.45167000	-0.04342100	0.79796700
C	1.55621800	0.22495800	-0.01859000
C	1.69664500	1.50631300	-0.56483100
C	0.74759600	2.49599400	-0.30737400

H	-1.09207800	2.98681500	0.71243600
H	-1.34941200	0.70639800	1.69183900
H	0.31058400	-1.03692300	1.21320500
H	2.55804900	1.72995000	-1.18906400
H	0.87253500	3.48689000	-0.73602000

im4b

SCF Energy (a.u.) = -1356.784883

Thermal correction to Gibbs free energy (a.u.) = 0.405401

Charge = 0, Multiplicity = 1

Ni	-3.63634200	-0.48896900	0.45437600
C	-4.80045100	-0.26649500	-1.27528100
C	-3.75852400	0.69652400	-1.37696800
C	-3.98792100	2.03114400	-0.99882000
C	-5.22769600	2.44103100	-0.50248100
C	-6.27224100	1.48598400	-0.44062800
C	-6.06478400	0.16836600	-0.80530200
H	-2.80850500	0.44024500	-1.83243500
H	-3.18289300	2.74799800	-1.11236100
H	-7.24661400	1.79502600	-0.07276900
H	-6.87368300	-0.55276900	-0.72960400
C	-5.48721700	3.81515300	-0.05180000
C	-4.56221100	4.73490400	0.24863900
H	-6.53903600	4.07322600	0.06369700
H	-4.84749300	5.72828000	0.57937500
H	-3.49636300	4.53046400	0.19491500
Br	-2.96473900	-0.81376600	2.62184700
C	0.71687700	-2.36658700	-1.05637300
C	-0.09081400	-1.84297800	-2.06933600
C	-1.47622100	-1.83796700	-1.94905500
C	-2.10363900	-2.34307600	-0.79658500
C	-1.28780000	-2.96483500	0.17071400
C	0.09211700	-2.98072900	0.03875500
H	0.37315800	-1.37854600	-2.93489700

H	-2.06649800	-1.40001800	-2.74747600
H	-1.75099600	-3.37092300	1.06448100
H	0.69980000	-3.41974300	0.82653900
C	-3.53575500	-2.15636800	-0.50545900
C	-4.51663500	-1.73152800	-1.59905200
H	-3.93496500	-2.88718800	0.19964300
H	-5.44362400	-2.30818200	-1.53682400
H	-4.11712200	-1.85267500	-2.61170600
C	2.49702700	-0.94183300	-0.02796300
C	2.19626400	-2.08927300	-1.03698900
H	2.76865900	-2.97839900	-0.74518800
H	2.53108800	-1.79257200	-2.03711500
H	2.24051300	-1.33252400	0.96539800
C	3.96099400	-0.52497300	0.01872100
C	4.94575600	-1.07516700	-0.80585100
C	4.34473600	0.46267900	0.93898800
C	6.27892700	-0.65922900	-0.72310600
H	4.69193600	-1.84266200	-1.52852200
C	5.66520800	0.89020900	1.04138300
H	3.59047800	0.91197400	1.57915700
C	6.61735900	0.31847100	0.20094800
H	7.03217800	-1.09416100	-1.37010900
H	5.94646400	1.65355300	1.75783300
Br	8.47927700	0.91267800	0.32680400
C	-0.20873500	2.33894700	-0.84905700
C	-0.45803000	1.47596700	0.21943900
C	0.43042200	0.43593100	0.49746800
C	1.57603300	0.24561900	-0.28316300
C	1.81902300	1.11942300	-1.34998800
C	0.93249000	2.15734800	-1.63471500
H	-0.88677700	3.16180200	-1.06160700
H	-1.33734900	1.60108800	0.84440100
H	0.20903500	-0.24332200	1.31511100
H	2.71299400	0.98914700	-1.95445400

H 1.13699900 2.83010300 -2.46325100

im5b

SCF Energy (a.u.) = -1497.827499

Thermal correction to Gibbs free energy (a.u.) = 0.472407

Charge = 0, Multiplicity = 1

Ni	-3.72093300	-0.47427900	0.57516400
C	-5.00659200	-0.20230600	-1.10640200
C	-4.00087100	0.79914800	-1.15766600
C	-4.27757300	2.10526900	-0.71125900
C	-5.53076300	2.44610400	-0.19948700
C	-6.54173900	1.45430700	-0.19454300
C	-6.28577600	0.16572500	-0.62615800
H	-3.04773700	0.60578300	-1.63802000
H	-3.49943000	2.85659000	-0.79027200
H	-7.52901500	1.71096900	0.17988900
H	-7.07085000	-0.58495500	-0.59621700
C	-5.84016600	3.78718600	0.31696100
C	-4.95070800	4.72134200	0.67421700
H	-6.90148100	4.00494000	0.43070200
H	-5.27301300	5.68785600	1.04803300
H	-3.87807300	4.55497100	0.62344400
C	0.59746600	-2.26232200	-1.23987000
C	-0.24891900	-1.61798100	-2.14547400
C	-1.62865900	-1.62768600	-1.96988200
C	-2.21432600	-2.26857900	-0.86487300
C	-1.36475600	-3.02412800	-0.03343400
C	0.01136200	-3.01734500	-0.21501600
H	0.18173400	-1.04341800	-2.96098900
H	-2.24651000	-1.08360200	-2.67720900
H	-1.79493300	-3.57132400	0.79986700
H	0.64633500	-3.56141600	0.48112300
C	-3.62804300	-2.08462800	-0.47727100
C	-4.66710300	-1.63347000	-1.51008200

H	-3.98606000	-2.87573800	0.18712800
H	-5.56783400	-2.25233400	-1.45556600
H	-4.29727900	-1.68159700	-2.54096200
C	2.38639200	-0.93262900	-0.10596800
C	2.07337100	-1.96566100	-1.22989600
H	2.66780100	-2.87118900	-1.05562500
H	2.37572700	-1.55220900	-2.19867900
H	2.16947900	-1.44063800	0.84307500
C	3.84305800	-0.49190600	-0.05434300
C	4.81511400	-0.93751600	-0.95389400
C	4.23523300	0.40529800	0.95119200
C	6.14326400	-0.50757300	-0.86189100
H	4.55432500	-1.63228400	-1.74438600
C	5.55094600	0.84474700	1.06454300
H	3.49028800	0.77451800	1.65067500
C	6.48987400	0.37788800	0.14802600
H	6.88624000	-0.86080400	-1.56787800
H	5.83846100	1.53768900	1.84705800
Br	8.34556900	0.99056800	0.28871500
C	-0.42560900	2.34133700	-0.47000500
C	-0.62278800	1.35181600	0.49433500
C	0.30347100	0.31686500	0.62823300
C	1.43396100	0.25438900	-0.19325200
C	1.62558200	1.25547800	-1.15355300
C	0.70179000	2.29067200	-1.29448900
H	-1.13579800	3.15830700	-0.57184300
H	-1.49052400	1.36556400	1.14641200
H	0.11709800	-0.46167500	1.36053300
H	2.50640000	1.22442100	-1.78983000
H	0.86562600	3.06175200	-2.04265300
O	-2.87797900	-0.76426800	2.09558600
C	-2.91981800	-1.85488700	2.97034000
C	-1.55018200	-2.07374200	3.61221200
H	-3.21844000	-2.77695100	2.44153700

H	-3.67582300	-1.69232900	3.75862800
H	-1.57296700	-2.90482700	4.32885200
H	-0.80478300	-2.29545400	2.84034400
H	-1.23285900	-1.16779900	4.14040800

im6b

SCF Energy (a.u.) = -2101.541156

Thermal correction to Gibbs free energy (a.u.) = 0.696468

Charge = 0, Multiplicity = 1

C	-7.73596000	-2.93592500	-1.32883200
C	-8.74266500	-2.08013400	-1.11131600
H	-7.94806000	-4.00482600	-1.29810900
C	-6.33011700	-2.58965900	-1.58101100
C	-5.34050800	-3.57937200	-1.45603400
C	-5.91799100	-1.29223800	-1.93181100
C	-3.99210800	-3.27610500	-1.63500700
H	-5.63676700	-4.59571500	-1.20607500
C	-4.57243200	-0.99044100	-2.10058400
H	-6.65808000	-0.50937100	-2.05820600
C	-3.58422600	-1.97336000	-1.94422800
H	-3.24410800	-4.05823900	-1.52358900
H	-4.26656100	0.02811800	-2.31734200
Ni	-2.76209600	-0.39384500	0.43922300
C	-1.55643500	-1.45753800	-0.58948200
C	-2.12055200	-1.60288700	-2.00387100
H	-1.55271700	-2.36142800	-2.56609300
H	-2.01781200	-0.65380500	-2.53534900
H	-1.67086100	-2.40443500	-0.03841700
C	-0.17885300	-0.93641700	-0.43434900
C	0.46442700	-0.15491100	-1.40969700
C	0.51980300	-1.17146200	0.76596100
C	1.73812500	0.36537500	-1.18935200
H	-0.04265700	0.06499900	-2.34245800
C	1.78901400	-0.65016500	0.98368200

H	0.04448400	-1.77092700	1.53952900
C	2.42300900	0.13017400	0.00740600
H	2.20850900	0.96967300	-1.96268100
H	2.30990500	-0.86714100	1.91252700
C	4.87778400	-0.32624700	-0.43214000
C	3.83193200	0.63100800	0.20073500
H	3.94569000	1.62227100	-0.25505900
H	4.04441100	0.73705000	1.27087200
H	4.59377600	-0.44153000	-1.48626700
C	6.30129000	0.21136500	-0.40759600
C	6.69653200	1.30646500	0.36548100
C	7.27468500	-0.43746400	-1.18154700
C	8.02279700	1.75109000	0.37121000
H	5.97321600	1.83464700	0.97693300
C	8.60004600	-0.01199200	-1.19443300
H	6.98852800	-1.30008200	-1.77772900
C	8.95420100	1.08350100	-0.41098700
H	8.31564500	2.60217000	0.97544500
H	9.34086000	-0.52213500	-1.79949500
Br	10.81515000	1.69573100	-0.41490600
C	4.49340400	-4.20299600	1.45958400
C	3.87927700	-3.95515900	0.23156100
C	4.02765600	-2.71318200	-0.38666100
C	4.79014900	-1.70376500	0.20976600
C	5.40564300	-1.96260300	1.44032100
C	5.25785400	-3.20164300	2.06270100
H	4.38070100	-5.16967700	1.94246400
H	3.28126300	-4.72655900	-0.24576400
H	3.52954700	-2.51486900	-1.33174100
H	6.01134000	-1.19074700	1.90744100
H	5.74418800	-3.38738100	3.01652900
O	-2.56263300	1.12892800	-0.50247200
C	-1.63958700	2.05782200	0.01253400
C	-1.35829300	3.13028800	-1.03808900

H	-0.68718700	1.57234100	0.27637000
H	-2.02936100	2.53232600	0.93196200
H	-0.68509500	3.90243700	-0.64492200
H	-0.89531400	2.67741300	-1.92140400
H	-2.29127100	3.61156200	-1.35639700
C	-2.94009100	-1.76660500	3.07370000
C	-3.80542200	-2.01638800	1.99202400
C	-4.59466200	-0.97575700	1.46949200
C	-4.46392100	0.34578000	1.98028700
C	-3.59862800	0.55609300	3.06989900
C	-2.86179300	-0.49179400	3.63461500
H	-2.33294300	-2.57517900	3.47104600
H	-3.88590400	-3.01207000	1.56783400
H	-5.29835000	-1.17461800	0.66881400
H	-3.48010300	1.56688100	3.44817800
H	-2.19810700	-0.30406300	4.47285100
C	-6.09620000	2.33460000	-0.83623400
C	-4.97662400	3.92048900	0.69453500
C	-6.23889300	3.70303800	-0.15421500
H	-5.25821300	2.34594000	-1.54456200
H	-5.09160600	4.80110900	1.33566200
B	-5.04927900	1.55257000	1.16920500
O	-5.86081300	1.28784000	0.10483000
O	-4.68463400	2.81210300	1.54834900
H	-7.01033500	2.07993300	-1.38343200
H	-4.10697000	4.08094300	0.04633300
C	-6.31980600	4.79791900	-1.22439800
H	-5.43980100	4.78503300	-1.87808700
H	-7.20947000	4.66478100	-1.85075200
H	-6.38445400	5.79028000	-0.76311200
C	-7.49409500	3.72826100	0.73224700
H	-7.59970100	4.70229800	1.22350400
H	-8.39415800	3.55246200	0.13185200
H	-7.45450700	2.96037100	1.51010100

H	-8.59642500	-1.00351200	-1.09159200
H	-9.75229900	-2.43583200	-0.93100500

TS3b

SCF Energy (a.u.) = -2101.533966

Thermal correction to Gibbs free energy (a.u.) = 0.698000

Charge = 0, Multiplicity = 1

C	-7.78495700	-2.82481100	-1.37873200
C	-8.78329700	-1.98314100	-1.08254100
H	-7.99476600	-3.89450400	-1.38847700
C	-6.39016500	-2.46661500	-1.67318400
C	-5.41039000	-3.47355400	-1.68957500
C	-5.97817100	-1.14602800	-1.92280200
C	-4.06873100	-3.17022800	-1.91139000
H	-5.70777100	-4.50515200	-1.51580200
C	-4.63960500	-0.84449900	-2.13944600
H	-6.70406100	-0.34025200	-1.92045900
C	-3.66022100	-1.84889000	-2.12840400
H	-3.32761800	-3.96665100	-1.90834600
H	-4.33836100	0.18854200	-2.27507600
Ni	-2.84501300	-0.55267300	0.33590900
C	-1.60237600	-1.35892300	-0.82685000
C	-2.19482500	-1.48952200	-2.22867900
H	-1.64705500	-2.23910300	-2.82068000
H	-2.09549800	-0.53290800	-2.75246000
H	-1.75802500	-2.30603100	-0.25571300
C	-0.21470700	-0.88354400	-0.67055700
C	0.48809200	-0.21720700	-1.68958500
C	0.43126200	-1.02720000	0.57488600
C	1.76298000	0.29787400	-1.46331600
H	0.03200000	-0.08926900	-2.66541000
C	1.70198800	-0.51383400	0.79565900
H	-0.08666000	-1.54642600	1.37867300
C	2.39116500	0.16315300	-0.22088500

H	2.28041700	0.81467100	-2.26891300
H	2.18046700	-0.65489300	1.76074800
C	4.85251600	-0.38739300	-0.47599300
C	3.80052500	0.65600900	-0.01203900
H	3.96032700	1.58635200	-0.57033000
H	3.96081300	0.87942200	1.04887000
H	4.62439300	-0.61257000	-1.52600300
C	6.28652700	0.12044600	-0.42651900
C	6.66638300	1.29065000	0.23620500
C	7.28452800	-0.63609700	-1.05824600
C	8.00211900	1.70447800	0.27126400
H	5.92446700	1.90319400	0.73664500
C	8.61971700	-0.24316000	-1.03930500
H	7.00965500	-1.55716600	-1.56567000
C	8.95860400	0.92963500	-0.36898800
H	8.28297900	2.61457200	0.78895300
H	9.37989500	-0.83704800	-1.53381900
Br	10.83233000	1.49719400	-0.33026000
C	4.25526800	-4.01911600	1.80530900
C	3.74329800	-3.90909000	0.51222000
C	3.96116300	-2.74736700	-0.22950800
C	4.69215100	-1.68283400	0.30691800
C	5.20692300	-1.80424000	1.60332800
C	4.98897400	-2.96204500	2.34898700
H	4.08782800	-4.92256300	2.38486500
H	3.17137400	-4.72543900	0.07988300
H	3.54267300	-2.65521200	-1.22817100
H	5.78901400	-0.98948600	2.02554400
H	5.39652800	-3.04152400	3.35307800
O	-2.88795500	1.22053900	-0.15394200
C	-1.71709800	2.02589400	-0.06138000
C	-1.48694800	2.76085500	-1.37582200
H	-0.84505800	1.40516600	0.16698100
H	-1.84779400	2.73110500	0.76820300

H	-0.60915900	3.41494000	-1.30583400
H	-1.31847000	2.04476500	-2.18644000
H	-2.35640200	3.37408700	-1.63832400
C	-3.82981600	-2.09526900	3.31025800
C	-4.67753900	-2.09953500	2.19987200
C	-4.90911200	-0.90962400	1.49046800
C	-4.26474600	0.29659500	1.85827400
C	-3.42312700	0.26988800	2.99416400
C	-3.21662000	-0.90305800	3.71838800
H	-3.65224200	-3.01430500	3.86213100
H	-5.16887600	-3.01576700	1.88511900
H	-5.59283600	-0.90514000	0.64859000
H	-2.93099900	1.19131200	3.29215400
H	-2.56841400	-0.89869700	4.59047800
C	-5.63845300	2.70953400	-0.77332800
C	-4.35150500	4.02302600	0.88059900
C	-5.68002400	3.97198400	0.10505100
H	-4.84063600	2.80881500	-1.52703000
H	-4.38250200	4.82173400	1.63178200
B	-4.37440200	1.60022200	0.92948100
O	-5.42474500	1.54329900	-0.00170200
O	-4.06021000	2.81180200	1.56320200
H	-6.58941300	2.58678600	-1.30698100
H	-3.53479300	4.25936600	0.18191500
C	-5.79653100	5.21527000	-0.78270400
H	-4.97006400	5.27424500	-1.50159400
H	-6.73556600	5.20417700	-1.34889400
H	-5.78394100	6.13106200	-0.17944900
C	-6.86359700	3.89554800	1.08046700
H	-6.90061000	4.78924300	1.71489300
H	-7.81229700	3.82921200	0.53413500
H	-6.78268600	3.01915300	1.72823900
H	-8.64305400	-0.90716000	-1.02692300
H	-9.78280400	-2.35192100	-0.87451300

im7b

SCF Energy (a.u.) = -2101.545485

Thermal correction to Gibbs free energy (a.u.) = 0.703357

Charge = 0, Multiplicity = 1

C	-8.04005800	-1.34344500	-1.78326500
C	-8.64516300	-0.89338100	-2.88896000
H	-8.65177600	-1.58983200	-0.91750600
C	-6.60112500	-1.57322600	-1.60108100
C	-6.15862900	-2.25332400	-0.46768600
C	-5.63481000	-1.14283500	-2.54169200
C	-4.79966000	-2.56121800	-0.28794500
H	-6.87830900	-2.56873600	0.28073100
C	-4.29686100	-1.43195300	-2.37425700
H	-5.94874200	-0.56548800	-3.40488200
C	-3.84657400	-2.18044600	-1.25933900
H	-4.50637200	-3.19906100	0.54139600
H	-3.56922400	-1.09326800	-3.10574000
Ni	-3.36005300	-0.78757600	0.37629400
C	-1.93434200	-2.07334300	0.24861300
C	-2.39332400	-2.60788900	-1.11171800
H	-2.29457400	-3.70035900	-1.18975600
H	-1.80335100	-2.16878000	-1.92036900
H	-2.13070700	-2.79239000	1.05365800
C	-0.56648900	-1.51857300	0.35043700
C	-0.09771800	-0.54796500	-0.55301200
C	0.29693700	-1.92600800	1.37746300
C	1.18023700	-0.01768900	-0.43162000
H	-0.76516100	-0.17240100	-1.32257600
C	1.58160600	-1.39811400	1.49338100
H	-0.04184600	-2.67426800	2.09007600
C	2.04374300	-0.43374400	0.59287000
H	1.51297600	0.74454200	-1.13307300
H	2.23956700	-1.74873700	2.28370300

C	4.41365500	-0.67077900	-0.27398100
C	3.45193700	0.09895200	0.67042300
H	3.46683000	1.16080800	0.39607200
H	3.82120400	0.02174400	1.69934600
H	3.97634300	-0.61061500	-1.27920400
C	5.80945800	-0.06952400	-0.35518900
C	6.28411700	0.89630900	0.53633800
C	6.67456800	-0.52295300	-1.36185600
C	7.58342200	1.40405500	0.43300000
H	5.64571700	1.27231400	1.32822400
C	7.97066200	-0.03079800	-1.48637000
H	6.32744500	-1.28491200	-2.05492500
C	8.40658300	0.93172100	-0.57914400
H	7.93872100	2.15340500	1.13113100
H	8.62732600	-0.38912100	-2.27093000
Br	10.22769700	1.63460900	-0.73781700
C	4.42442400	-4.83752900	0.90556200
C	3.63508600	-4.41116300	-0.16282900
C	3.65446300	-3.07252200	-0.55607600
C	4.46091200	-2.14330500	0.10862800
C	5.25278100	-2.58098200	1.17711300
C	5.23425500	-3.91718300	1.57502200
H	4.41203500	-5.87931400	1.21335300
H	3.00098000	-5.11877500	-0.68981900
H	3.02268500	-2.73838400	-1.37469000
H	5.89381900	-1.87103500	1.69275000
H	5.85626900	-4.24134900	2.40488900
O	-2.41487300	0.56296000	1.28343000
C	-2.05393500	0.46201100	2.66609400
C	-0.72200000	1.14033600	2.94437600
H	-1.98128500	-0.60498300	2.90416700
H	-2.83952700	0.90681000	3.28632800
H	-0.41019200	0.93193700	3.97555300
H	0.04793200	0.76649900	2.26600700

H	-0.80508500	2.22209400	2.82728000
C	-7.65201900	0.55383600	1.05634700
C	-7.17448800	1.24310000	-0.06416400
C	-5.81416000	1.50306100	-0.19340700
C	-4.88587600	1.12637200	0.80016500
C	-5.39580800	0.41883200	1.90815100
C	-6.75898500	0.12707200	2.03612500
H	-8.71510900	0.35002500	1.15857300
H	-7.86687700	1.55800400	-0.83931000
H	-5.43957200	2.02505900	-1.06833700
H	-4.72712400	0.11754900	2.70964800
H	-7.12002200	-0.41164300	2.90888000
C	-1.90723700	2.64274900	-0.98961300
C	-2.25337000	3.86843200	1.11899800
C	-2.11951700	4.04817600	-0.40363800
H	-0.96629000	2.22446000	-0.59482900
H	-2.54177200	4.81994300	1.58606500
B	-3.35344800	1.70983800	0.71180400
O	-2.99252700	1.79232900	-0.68893800
O	-3.21800800	2.90438500	1.49096300
H	-1.81461400	2.69679300	-2.08324100
H	-1.26202100	3.59964700	1.51857500
C	-0.89917600	4.92282300	-0.70867000
H	0.02555800	4.46340600	-0.33771200
H	-0.78877500	5.07776200	-1.78904900
H	-0.99524800	5.91002900	-0.24018000
C	-3.39194500	4.68429600	-0.98020800
H	-3.51293100	5.70873700	-0.60713200
H	-3.34668900	4.72653100	-2.07573500
H	-4.27833300	4.11328900	-0.69502800
H	-8.10217400	-0.63978300	-3.79495300
H	-9.72259700	-0.76733500	-2.92304900

TS4b

SCF Energy (a.u.) = -2101.524464

Thermal correction to Gibbs free energy (a.u.) = 0.704099

Charge = 0, Multiplicity = 1

C	-7.75206400	-2.38080000	-1.53602600
C	-8.38374600	-2.41900900	-2.71507800
H	-8.34601000	-2.28614300	-0.62882500
C	-6.30358900	-2.47091100	-1.31133000
C	-5.82373600	-2.66476500	-0.01677800
C	-5.35988800	-2.36953700	-2.35921400
C	-4.44963700	-2.79422700	0.23872000
H	-6.52626600	-2.72651400	0.80853100
C	-4.00498700	-2.48654300	-2.11701000
H	-5.70450100	-2.17772600	-3.37030400
C	-3.51410500	-2.72440600	-0.81433300
H	-4.11950200	-3.04650800	1.24263000
H	-3.29699200	-2.40439100	-2.93746100
Ni	-3.10769600	-0.73674700	0.46057400
C	-1.65080500	-2.03912700	0.65918700
C	-2.03385800	-2.92581400	-0.53727700
H	-1.81657200	-3.99040200	-0.35840100
H	-1.46466700	-2.63648900	-1.42599900
H	-1.80747500	-2.57659400	1.60374600
C	-0.28994200	-1.44891600	0.62428400
C	0.14745000	-0.67050400	-0.46398800
C	0.59743100	-1.60009600	1.70227100
C	1.40656500	-0.08195700	-0.47017700
H	-0.52779300	-0.49482700	-1.29735600
C	1.85861800	-1.00743600	1.69743000
H	0.29239400	-2.20096700	2.55634600
C	2.28583500	-0.23802200	0.61088800
H	1.71041800	0.52384700	-1.32153700
H	2.53038100	-1.16271200	2.53755600
C	4.65696900	-0.57669000	-0.21873000
C	3.67676100	0.34189700	0.55940500

H	3.65754900	1.32442200	0.07185900
H	4.05556400	0.48936200	1.57736400
H	4.20944800	-0.73949000	-1.20791700
C	6.03125100	0.03672600	-0.44438400
C	6.48351300	1.17767800	0.22405900
C	6.90050900	-0.58582300	-1.35232200
C	7.76435200	1.69253000	-0.00209500
H	5.84112800	1.68740300	0.93369600
C	8.17847300	-0.09080500	-1.59618500
H	6.57131300	-1.48306700	-1.87001400
C	8.59185600	1.04883700	-0.91087600
H	8.10230500	2.57856700	0.52319400
H	8.83838800	-0.58157000	-2.30245700
Br	10.38776800	1.75921300	-1.23975700
C	4.81616500	-4.40749200	1.79494100
C	3.98906000	-4.22940900	0.68557800
C	3.96080400	-3.00127900	0.02418500
C	4.75644800	-1.93627100	0.45864600
C	5.58561200	-2.12505000	1.57082400
C	5.61509800	-3.35020100	2.23606000
H	4.84074300	-5.36304300	2.31128100
H	3.36169200	-5.04452500	0.33559000
H	3.29861300	-2.85778400	-0.82528900
H	6.21777900	-1.30904200	1.91041000
H	6.26585400	-3.48111200	3.09638200
O	-2.21413100	0.75694800	1.16509000
C	-1.69558200	0.82223300	2.51146500
C	-0.53056900	1.79380000	2.56268400
H	-1.36608300	-0.18586300	2.76112400
H	-2.50262000	1.12236700	3.18446400
H	-0.11558700	1.82235400	3.57732100
H	0.25471600	1.47864000	1.87087400
H	-0.85622600	2.80410800	2.29632800
C	-7.45706200	0.75528500	-0.57224300

C	-6.47068300	0.82809300	-1.55655100
C	-5.12520900	0.72282500	-1.19916900
C	-4.71639100	0.54307800	0.13709600
C	-5.74124600	0.47216400	1.10450300
C	-7.09061300	0.57518700	0.76523100
H	-8.50554900	0.83834400	-0.84532100
H	-6.75327900	0.96272200	-2.59781000
H	-4.36472200	0.79817800	-1.97294600
H	-5.47132000	0.36104400	2.15338900
H	-7.85602000	0.52592600	1.53654800
C	-3.36813800	3.51520300	-1.01377300
C	-3.58726900	3.99527700	1.42875500
C	-4.13970500	4.35776700	0.04320900
H	-2.58368000	4.12602100	-1.47577700
H	-4.15875400	4.50971300	2.20927000
B	-3.14178000	1.78002800	0.68735800
O	-2.70945700	2.36343300	-0.50236100
O	-3.67748200	2.60100500	1.68937100
H	-4.06018900	3.20768400	-1.80999100
H	-2.53890600	4.32408800	1.50780900
C	-3.89877200	5.85003500	-0.22671000
H	-2.83392600	6.10321500	-0.15752900
H	-4.24460600	6.12383100	-1.23076200
H	-4.44484800	6.47312500	0.49163800
C	-5.64824300	4.06648100	0.00134100
H	-6.17882200	4.70529900	0.71840300
H	-6.05520400	4.27027100	-0.99587400
H	-5.86519100	3.02775000	0.25020800
H	-7.85818100	-2.52612100	-3.65987700
H	-9.46531000	-2.34820100	-2.77176000

im8b

SCF Energy (a.u.) = -2101.540692

Thermal correction to Gibbs free energy (a.u.) = 0.703474

Charge = 0, Multiplicity = 1

C	-8.02011200	-1.91411300	-1.35623800
C	-8.70325500	-1.51294800	-2.43466600
H	-8.56311300	-2.06630900	-0.42467200
C	-6.57732300	-2.16764600	-1.27027500
C	-6.03202000	-2.59788300	-0.06249700
C	-5.69704500	-1.96655800	-2.35914500
C	-4.65117400	-2.80669700	0.08223700
H	-6.68516600	-2.75580600	0.79085900
C	-4.33785400	-2.17128500	-2.23007000
H	-6.09282900	-1.62196400	-3.30889300
C	-3.77265800	-2.59781600	-1.00628900
H	-4.27131800	-3.22181400	1.01082500
H	-3.67983800	-2.00137300	-3.07838600
Ni	-3.33116200	-0.81719900	0.39599500
C	-1.85266400	-2.17235600	0.46164700
C	-2.28439600	-2.86404500	-0.84429600
H	-2.07664000	-3.94638900	-0.85595500
H	-1.75393500	-2.43624100	-1.70165100
H	-2.00080800	-2.85377700	1.31035200
C	-0.48271700	-1.61697100	0.49970500
C	-0.03865200	-0.67111400	-0.44769700
C	0.41704200	-1.95813100	1.52465500
C	1.22626800	-0.10110100	-0.36403800
H	-0.71737600	-0.34880400	-1.23297200
C	1.68708100	-1.38931500	1.60514500
H	0.11163000	-2.68967900	2.26979000
C	2.11500200	-0.44728000	0.66449500
H	1.53138000	0.63547800	-1.10564500
H	2.36504500	-1.69571300	2.39801800
C	4.46942900	-0.65053500	-0.25742800
C	3.51316900	0.11627700	0.69588600
H	3.50229200	1.17303600	0.40002800
H	3.91029900	0.06761800	1.71653200

H	4.00011300	-0.62741100	-1.24954600
C	5.84365700	-0.01310100	-0.39804600
C	6.33100500	0.96249900	0.47614800
C	6.67702700	-0.44029100	-1.44223200
C	7.61074800	1.50503700	0.31969600
H	5.71663000	1.31780000	1.29612800
C	7.95337600	0.08636100	-1.62019900
H	6.32059000	-1.20913800	-2.12289300
C	8.40176800	1.05762600	-0.72874700
H	7.97613300	2.26125900	1.00516900
H	8.58520700	-0.25222000	-2.43342000
Br	10.19558200	1.81061000	-0.96291900
C	4.62910100	-4.78652400	1.01739000
C	3.76058200	-4.39657200	-0.00260600
C	3.73222500	-3.06812500	-0.42743900
C	4.56888500	-2.11182500	0.15766500
C	5.43845600	-2.51257100	1.17897800
C	5.46853800	-3.83929700	1.60763600
H	4.65378900	-5.82070700	1.34936700
H	3.10054900	-5.12451500	-0.46616900
H	3.03806500	-2.76220100	-1.20524700
H	6.10166500	-1.78178800	1.63376800
H	6.15125600	-4.13453700	2.39984400
O	-2.31804800	0.57808300	1.39269800
C	-2.08802000	0.33621600	2.80693100
C	-0.74608600	0.87237700	3.27574400
H	-2.12173400	-0.74916800	2.90587800
H	-2.92189600	0.77445900	3.36374800
H	-0.57241900	0.53546900	4.30466300
H	0.05876000	0.48197700	2.64895800
H	-0.72720300	1.96343600	3.26214200
C	-7.30287300	1.80530900	-0.15148200
C	-6.45348700	1.59375200	-1.23989000
C	-5.26018200	0.88760600	-1.07053000

C	-4.88013700	0.34310100	0.17092100
C	-5.74239500	0.59868200	1.25179100
C	-6.93705300	1.31410500	1.10255000
H	-8.23388000	2.35208300	-0.27796500
H	-6.72188500	1.98313700	-2.22053500
H	-4.61395500	0.74643700	-1.93448600
H	-5.49314300	0.21185900	2.24147000
H	-7.58344900	1.48218300	1.96203400
C	-2.50597300	3.25629600	-1.09792400
C	-2.24397000	4.23190400	1.16498000
C	-3.03685200	4.34180000	-0.14286200
H	-1.54082300	3.56424700	-1.51989800
H	-2.62428000	4.93827800	1.90897100
B	-2.34266500	1.86892400	0.87542500
O	-2.31114100	1.98318900	-0.47572500
O	-2.35507100	2.92450800	1.73787900
H	-3.20833700	3.10285100	-1.92350400
H	-1.18116300	4.45335100	0.99461600
C	-2.78764100	5.71738400	-0.77513700
H	-1.71965700	5.89879900	-0.94624600
H	-3.30309200	5.79821800	-1.73903400
H	-3.16952100	6.51583800	-0.12895300
C	-4.53580800	4.15566200	0.14093100
H	-4.88779800	4.93517200	0.82727200
H	-5.11556800	4.22855900	-0.78374500
H	-4.76038600	3.18494800	0.58663400
H	-8.23161200	-1.33149300	-3.39614300
H	-9.77407300	-1.34345700	-2.38511100

im9b

SCF Energy (a.u.) = -1887.122164

Thermal correction to Gibbs free energy (a.u.) = 0.663798

Charge = 0, Multiplicity = 1

Ni	-3.15400100	-0.36833800	-0.25461700
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C	-4.06784300	2.62692600	-1.26871500
C	-4.66210900	2.44862900	-0.00877500
C	-4.55603500	3.41377100	0.98418000
C	-3.85655200	4.61388200	0.75412800
C	-3.30149600	4.80778400	-0.52027200
C	-3.40630700	3.83322800	-1.51189400
H	-5.20498600	1.53119400	0.18897900
H	-5.02878900	3.23978400	1.94630800
H	-2.76981000	5.73283900	-0.73033500
H	-2.94204900	3.99906600	-2.48069300
C	-3.69333000	5.65819500	1.77459500
C	-4.07915900	5.60841200	3.05585900
H	-3.19267900	6.56014400	1.42257900
H	-3.90534600	6.44559000	3.72446500
H	-4.57632100	4.74357700	3.48655000
C	1.08451800	0.76788500	-0.95525200
C	0.10782600	1.51195800	-0.29836400
C	-1.24706000	1.43306100	-0.65032300
C	-1.67863700	0.57508200	-1.69341200
C	-0.67688000	-0.21498200	-2.31840000
C	0.65813900	-0.10484200	-1.97820600
H	0.40200400	2.19075700	0.49901300
H	-1.94824100	2.09483300	-0.16184900
H	-0.97822600	-0.90044000	-3.10611300
H	1.38492400	-0.70170000	-2.51956100
C	-3.09997100	0.35470300	-2.01770200
C	-4.07082400	1.51531400	-2.28869800
H	-3.20881400	-0.38849900	-2.80980700
H	-5.07301600	1.07613300	-2.35705800
H	-3.84465900	1.94233500	-3.27712500
C	3.45901300	-0.26022000	-0.76605000
C	2.54459600	0.97035300	-0.60793700
H	2.95033600	1.77188700	-1.24210300
H	2.60520700	1.33873600	0.42282000

H	3.34126000	-0.63260400	-1.79024100
C	4.94037500	0.07173200	-0.60434000
C	5.40688900	1.25550800	-0.02605300
C	5.88460300	-0.87528500	-1.02602200
C	6.77564800	1.49735500	0.12859400
H	4.71028700	2.01445800	0.31259000
C	7.25186000	-0.65573100	-0.88497000
H	5.54065000	-1.80923500	-1.46291600
C	7.67794600	0.53631400	-0.30470800
H	7.12372700	2.42040700	0.57799500
H	7.96974300	-1.39647100	-1.21816000
Br	9.59677400	0.86240900	-0.09638400
C	2.51191300	-3.54989400	1.89484500
C	2.29415500	-3.67474900	0.52325000
C	2.57941700	-2.60646400	-0.32965600
C	3.08355800	-1.40230600	0.17126100
C	3.28886800	-1.28416700	1.55175100
C	3.00592100	-2.34708800	2.40760400
H	2.29364600	-4.37959300	2.56075000
H	1.90094800	-4.60121800	0.11510700
H	2.41308100	-2.71262100	-1.39838900
H	3.70216100	-0.36310400	1.95420200
H	3.17919800	-2.24072900	3.47486200
C	-6.67753600	-3.20127200	-1.60810500
C	-5.34738700	-3.48755900	-1.92433400
C	-4.32968400	-2.60713900	-1.55032000
C	-4.59750300	-1.42764000	-0.83138300
C	-5.94472300	-1.15033100	-0.54592600
C	-6.97176500	-2.02372500	-0.92075700
H	-7.47256300	-3.88215600	-1.90020500
H	-5.10157800	-4.39631100	-2.47005100
H	-3.30300800	-2.84999300	-1.81453900
H	-6.21550300	-0.24733200	-0.00205700
H	-8.00277100	-1.78014800	-0.67279200

C	-2.35890500	-3.37332200	1.05527100
C	-1.30217800	-2.68246100	0.61297300
C	-0.51419100	-1.59820400	1.29906100
C	-1.22540800	-0.72101600	2.35037600
C	-2.56679700	-0.12873000	1.95673900
C	-3.79120200	-0.73082700	1.96979600
C	-4.17523800	-2.14091300	2.34015600
C	-3.06003500	-3.20603800	2.37728400
H	-2.81234100	-4.09162400	0.37594600
H	-0.93398800	-2.92293700	-0.38401100
H	-0.12570400	-0.94196400	0.51937600
H	0.37369500	-2.03453500	1.77163400
H	-1.33230700	-1.26884600	3.29130500
H	-0.54991300	0.11415300	2.56899200
H	-2.58049000	0.95375700	1.83306700
H	-4.65136200	-0.07446600	1.84577100
H	-4.95860400	-2.46240600	1.64467400
H	-4.65314200	-2.09641300	3.33159900
H	-2.34858800	-2.97896800	3.17462200
H	-3.53003400	-4.15729800	2.65461400

TS5b

SCF Energy (a.u.) = -1887.110832

Thermal correction to Gibbs free energy (a.u.) = 0.665709

Charge = 0, Multiplicity = 1

Ni	-2.91720100	-0.39650700	-0.11213200
C	-4.19458700	2.46462600	-1.28038300
C	-4.86822900	2.28166700	-0.06315500
C	-4.84003500	3.25160700	0.93107700
C	-4.14022900	4.45803100	0.74660100
C	-3.50046200	4.65552700	-0.48699000
C	-3.52841200	3.67786600	-1.47938100
H	-5.41095900	1.36121700	0.11492300
H	-5.37207400	3.07101900	1.86002700

H	-2.96532100	5.58535500	-0.66382400
H	-3.00337000	3.84831400	-2.41580200
C	-4.05842200	5.50569000	1.77365800
C	-4.51326200	5.44369500	3.03136300
H	-3.55955700	6.41916300	1.45019400
H	-4.39675500	6.28326500	3.70934200
H	-5.01020100	4.56521100	3.43359800
C	0.95626700	0.65711100	-0.92619800
C	-0.03863400	1.35241600	-0.25684800
C	-1.40216700	1.24181600	-0.60193500
C	-1.79768400	0.39359300	-1.67578600
C	-0.76591500	-0.34536900	-2.32524600
C	0.55965700	-0.20971700	-1.97260200
H	0.23548500	2.03710500	0.54258900
H	-2.09277400	1.94576200	-0.16208000
H	-1.03837700	-1.00334600	-3.14660500
H	1.31082300	-0.75829200	-2.53398100
C	-3.21108200	0.17902900	-2.09646300
C	-4.14302500	1.38440800	-2.33284700
H	-3.18519900	-0.37318800	-3.03380000
H	-5.14800700	0.99075700	-2.52054800
H	-3.81293200	1.84103500	-3.27513200
C	3.34021700	-0.30403200	-0.59417500
C	2.41466300	0.92957900	-0.62410400
H	2.80636800	1.62094700	-1.38421200
H	2.47944600	1.45790100	0.33393100
H	3.18249400	-0.85983600	-1.52568900
C	4.82172700	0.05956700	-0.55909100
C	5.29558000	1.31889700	-0.18040600
C	5.76026400	-0.92959200	-0.88509000
C	6.66576600	1.59346900	-0.12884500
H	4.60221700	2.11138100	0.07925800
C	7.12912500	-0.67923800	-0.84380400
H	5.41121300	-1.92004600	-1.16569800

C	7.56213200	0.58810500	-0.46293700
H	7.01971100	2.57487600	0.16566500
H	7.84269700	-1.45357300	-1.10133400
Br	9.48363700	0.95935000	-0.39849900
C	2.52272600	-3.04937700	2.65664800
C	2.25744700	-3.42405200	1.34078700
C	2.50602300	-2.53060500	0.29655000
C	3.01735500	-1.25536500	0.55059000
C	3.27370800	-0.88599800	1.87761100
C	3.02855200	-1.77361400	2.92257000
H	2.33353600	-3.74277900	3.47099300
H	1.84969500	-4.40683800	1.12402700
H	2.29834000	-2.82691600	-0.72858200
H	3.69367500	0.09381700	2.08908400
H	3.23867200	-1.47379200	3.94549500
C	-5.81405300	-3.56008000	-1.82629800
C	-4.42850100	-3.66014900	-1.99082200
C	-3.61397100	-2.55125200	-1.78075800
C	-4.14522600	-1.31733200	-1.34678100
C	-5.54413500	-1.22505400	-1.23240600
C	-6.36469700	-2.33166400	-1.45775800
H	-6.45310900	-4.42124200	-1.99832000
H	-3.98298300	-4.60476500	-2.29407300
H	-2.54241800	-2.63879100	-1.93828100
H	-6.00586100	-0.29205500	-0.92622700
H	-7.44060700	-2.23184800	-1.33555600
C	-1.96280800	-3.14990800	0.97203000
C	-0.94824100	-2.27771900	0.91633600
C	-0.54540400	-1.26209700	1.95651700
C	-1.67409500	-0.52246300	2.71029000
C	-2.89255700	-0.09151100	1.90233500
C	-3.98756700	-0.88245600	1.55244500
C	-4.22214700	-2.35510900	1.82405800
C	-2.98341100	-3.24619500	2.07082000

H	-2.11878900	-3.81127700	0.12336100
H	-0.30754600	-2.30257600	0.03855200
H	0.07741800	-0.52030900	1.45409700
H	0.11239500	-1.73855900	2.69551100
H	-2.00645200	-1.12066700	3.56630400
H	-1.22845000	0.38061500	3.14531700
H	-3.08870800	0.98060100	1.92942500
H	-4.92191100	-0.35412300	1.36391600
H	-4.79215400	-2.76616800	0.98293400
H	-4.88150200	-2.43939800	2.70275200
H	-2.53245500	-3.00113800	3.03578300
H	-3.33486500	-4.28235200	2.15278300

im10b

SCF Energy (a.u.) = -1887.161223

Thermal correction to Gibbs free energy (a.u.) = 0.668780

Charge = 0, Multiplicity = 1

Ni	-2.67081900	-1.04309300	0.27724800
C	-4.20119900	1.99046600	-1.58732900
C	-5.46685000	1.74838900	-1.03325500
C	-5.93059800	2.46930500	0.06104800
C	-5.13760900	3.46437000	0.65770000
C	-3.88292200	3.72717100	0.08367600
C	-3.42572800	3.00936300	-1.01829700
H	-6.10340100	0.98597800	-1.47308100
H	-6.91915800	2.25776800	0.45643100
H	-3.25764200	4.50692800	0.51212500
H	-2.45519700	3.24233400	-1.44451700
C	-5.55875200	4.22039200	1.84492800
C	-6.59206300	3.94298700	2.64987200
H	-4.93391200	5.08128800	2.08285900
H	-6.81655500	4.56826000	3.50828100
H	-7.24218700	3.08682300	2.49232300
C	1.26470700	1.35955100	-1.28287400

C	0.21884700	1.23090900	-0.36463700
C	-1.06022300	0.87220000	-0.78065300
C	-1.33269500	0.60686000	-2.12710200
C	-0.29780700	0.78504700	-3.05108500
C	0.97929600	1.16501000	-2.63892200
H	0.41916100	1.37763700	0.69309500
H	-1.86535500	0.79580000	-0.04476100
H	-0.48763800	0.59633900	-4.10536800
H	1.77182800	1.27206600	-3.37647400
C	-2.68228500	0.08171200	-2.57798400
C	-3.72060700	1.22490400	-2.79531700
H	-2.52263500	-0.30816000	-3.59483500
H	-4.58517000	0.80564300	-3.32014100
H	-3.25266900	1.92671100	-3.49626900
C	3.51733800	0.27106600	-0.96230800
C	2.68210600	1.57063800	-0.81402800
H	3.17051700	2.36662900	-1.39029900
H	2.67704100	1.88310500	0.23622100
H	3.50067200	0.01558900	-2.02974500
C	4.97979100	0.42908500	-0.56861000
C	5.48494700	1.55767700	0.08214300
C	5.86616200	-0.61880600	-0.85961600
C	6.83555000	1.64911200	0.43519000
H	4.83301400	2.38965400	0.32424300
C	7.21421700	-0.54964700	-0.52060200
H	5.48808000	-1.51108800	-1.35165600
C	7.67974800	0.59221900	0.12699300
H	7.21387200	2.53070700	0.93998200
H	7.88737000	-1.36683600	-0.75338500
Br	9.57285600	0.70603700	0.61429500
C	1.62859500	-3.02410600	1.13060500
C	1.43662600	-2.85907300	-0.24144300
C	2.05112900	-1.79969500	-0.91100000
C	2.86457100	-0.89170700	-0.22352500

C	3.04125200	-1.05940700	1.15527900
C	2.42862700	-2.11631300	1.82827200
H	1.15170400	-3.84651900	1.65534700
H	0.81050500	-3.55452400	-0.79336300
H	1.89019900	-1.66865000	-1.97722800
H	3.67970000	-0.36893300	1.69972700
H	2.57929900	-2.23464500	2.89761400
C	-3.84867800	-3.87189800	-1.31018800
C	-2.54294400	-3.46869000	-1.16921000
C	-2.15317300	-2.10402800	-1.35678100
C	-3.15102400	-1.13409400	-1.75661100
C	-4.48729400	-1.62325800	-1.95853600
C	-4.83503100	-2.92938800	-1.71475700
H	-4.12457100	-4.91079300	-1.15137500
H	-1.77369100	-4.19731000	-0.92101300
H	-1.09999500	-1.89492200	-1.52733300
H	-5.24640200	-0.94009400	-2.32495100
H	-5.86165600	-3.25359400	-1.86341800
C	-1.97813800	-2.34021100	1.88676800
C	-1.24458800	-1.18092800	1.90665800
C	-1.49269000	0.02595700	2.78493700
C	-2.98486100	0.41770100	2.92416500
C	-3.76638900	0.22676800	1.64011800
C	-4.46460100	-0.91067800	1.28695000
C	-4.53219000	-2.20855900	2.06492900
C	-3.19788500	-2.63575600	2.73691200
H	-1.56607500	-3.17785800	1.33319000
H	-0.29564900	-1.18790900	1.37732200
H	-0.95006700	0.87337200	2.35001000
H	-1.05380700	-0.12914100	3.78299600
H	-3.44844600	-0.15074000	3.73574500
H	-3.04475300	1.47070400	3.22283400
H	-3.97103900	1.12664200	1.07386900
H	-5.19557700	-0.82207400	0.48793000

H	-4.83375100	-2.98951900	1.35850100
H	-5.32060600	-2.16083300	2.83316000
H	-3.09692900	-2.15332900	3.71325200
H	-3.24357500	-3.71289900	2.93403900

im3c

SCF Energy (a.u.) = -1897.572019

Thermal correction to Gibbs free energy (a.u.) = 0.599178

Charge = 0, Multiplicity = 1

C	1.34350200	2.54003500	0.40045500
C	1.91611700	2.08463300	-0.79548900
C	3.23885300	2.35117900	-1.11119000
C	4.05037300	3.09393000	-0.23954800
C	3.46632900	3.58271500	0.93554800
C	2.13921300	3.30477200	1.25277900
H	1.31495500	1.50575700	-1.48922400
H	3.64985600	1.98051400	-2.04228200
H	4.06613900	4.17719100	1.61677800
H	1.71552400	3.68721900	2.17489700
C	5.47146500	3.35226600	-0.50590700
C	6.25394600	2.67337400	-1.34840600
H	5.91223700	4.15602500	0.07936600
H	7.30018000	2.92447100	-1.46556300
H	5.89127500	1.83036200	-1.92512100
C	-1.14780000	2.69727000	-0.22324900
C	-0.07051700	2.16758600	0.76046200
H	-0.14611200	1.07826000	0.78356500
H	-0.29667500	2.52094100	1.76920300
H	-0.73617000	2.59791300	-1.23230800
C	-2.41058900	1.85236000	-0.19362200
C	-3.24609700	1.82388600	-1.31312100
C	-2.75331800	1.05937900	0.90283200
C	-4.34887200	0.97040200	-1.37358700
H	-3.02035000	2.46119300	-2.16270600

C	-3.85035900	0.20104700	0.85804400
H	-2.15222100	1.07885900	1.80315300
C	-4.60847800	0.12293200	-0.30229100
H	-4.96799900	0.95509600	-2.26303900
H	-4.07886600	-0.42097800	1.71420200
Br	-7.45146300	-0.40372300	0.80379600
C	-1.71493200	6.92049400	0.52432400
C	-0.71883200	6.48413100	-0.34672300
C	-0.55922800	5.12377800	-0.60008200
C	-1.38972000	4.17996500	0.01153400
C	-2.38848100	4.62732200	0.88008800
C	-2.54979300	5.98710200	1.13590600
H	-1.84386900	7.97875200	0.71985000
H	-0.06709600	7.20216500	-0.83153000
H	0.22163500	4.78919900	-1.27402400
H	-3.05275100	3.90912400	1.34647500
H	-3.33392800	6.31775000	1.80758600
Ni	-5.79235700	-1.29333800	-0.43850200
C	-4.34705600	-2.77270000	-1.03825600
C	-5.09874200	-2.26343800	-2.08063900
H	-6.00712300	-2.77164100	-2.39381400
H	-4.68531300	-1.55855000	-2.79035200
H	-4.75181900	-3.61740100	-0.48292400
C	-2.95458000	-2.44197500	-0.71838900
C	-2.17440700	-1.61013700	-1.53399700
C	-2.38217700	-2.93708100	0.46041800
C	-0.88639400	-1.26527600	-1.16110000
H	-2.58332100	-1.20987500	-2.45154600
C	-1.08590200	-2.59343900	0.82642300
H	-2.96807100	-3.58414800	1.10457700
C	-0.32024800	-1.74234000	0.02697200
H	-0.30855700	-0.60347000	-1.79764900
H	-0.66094100	-2.99189100	1.74042900
C	2.14923300	-2.24937700	-0.30901900

C	1.09061000	-1.36373700	0.39185600
H	1.27076000	-0.32872000	0.10080300
H	1.22740200	-1.42658300	1.47464000
H	1.90881300	-2.23972500	-1.37803200
C	3.56989700	-1.71645500	-0.17183500
C	3.90873200	-0.61451300	0.61346900
C	4.59158400	-2.36174500	-0.87989700
C	5.22753900	-0.16312400	0.69859100
H	3.15234900	-0.07194300	1.16402000
C	5.90984600	-1.92781300	-0.81146000
H	4.35220400	-3.22733000	-1.48810700
C	6.20982000	-0.82829600	-0.01454300
H	5.47053500	0.70297100	1.29786400
H	6.68891900	-2.43712000	-1.36295400
Br	8.05295200	-0.22290000	0.10398400
C	1.66830100	-6.30562500	1.10803600
C	1.13800100	-5.92566000	-0.12200200
C	1.31612500	-4.62374700	-0.58691600
C	2.02636900	-3.68756400	0.16573600
C	2.55923000	-4.07945700	1.39724100
C	2.38102800	-5.37724000	1.86699300
H	1.53280700	-7.31754100	1.47170900
H	0.58403500	-6.64033100	-0.71988900
H	0.88849900	-4.32714800	-1.53848200
H	3.12634600	-3.36591900	1.98498100
H	2.80307100	-5.66709500	2.82254900

TS2c

SCF Energy (a.u.) = -1897.551115

Thermal correction to Gibbs free energy (a.u.) = 0.599178

Charge = 0, Multiplicity = 1

C	-7.11304900	2.83811400	-0.30943600
C	-7.65666800	3.28156100	-1.52361900
C	-8.88411500	3.93129300	-1.56930200

C	-9.62017300	4.16485800	-0.39401900
C	-9.07051700	3.72028500	0.81900100
C	-7.84122500	3.06838400	0.86166400
H	-7.10538100	3.11318300	-2.44640600
H	-9.27383600	4.26332600	-2.52671000
H	-9.62109100	3.88648100	1.74166700
H	-7.44925000	2.71712600	1.81193700
C	-10.92257100	4.84557100	-0.38156200
C	-11.59169300	5.34063200	-1.43023000
H	-11.37078900	4.94371000	0.60703000
H	-12.55392800	5.82561700	-1.29982700
H	-11.21493400	5.28570900	-2.44785700
C	-6.03699900	0.55607000	-0.55484600
C	-5.81643000	2.06887300	-0.28626900
H	-5.13285700	2.46466600	-1.04736800
H	-5.32918500	2.19273300	0.68741700
H	-6.58020400	0.48348100	-1.50620400
C	-4.74786200	-0.23742900	-0.70984400
C	-4.82816900	-1.54646600	-1.21001700
C	-3.48923500	0.26312000	-0.35621200
C	-3.69328100	-2.33978100	-1.35185000
H	-5.80062500	-1.94892600	-1.48244600
C	-2.33877700	-0.51772400	-0.49160400
H	-3.39117100	1.27233200	0.02918000
C	-2.44399400	-1.83960300	-0.94703500
H	-3.78100300	-3.34702100	-1.74964000
H	-1.37123500	-0.10811300	-0.21568200
Br	-0.62651400	-4.42221200	1.59827600
C	-8.60348000	-1.04220300	2.54511600
C	-9.13364600	-0.70115700	1.30063700
C	-8.29938400	-0.20844300	0.29642000
C	-6.92827200	-0.05088000	0.52025000
C	-6.40399100	-0.39827300	1.77143700
C	-7.23466800	-0.88915000	2.77790700

H	-9.25036200	-1.42788600	3.32794500
H	-10.19716400	-0.81490400	1.11013400
H	-8.71801600	0.07595700	-0.66524700
H	-5.33791200	-0.29275000	1.95427400
H	-6.81194100	-1.15820300	3.74185800
Ni	-1.27972300	-3.04987200	-0.12083200
C	0.24197600	-3.03142300	-1.34939500
C	-0.87203600	-2.57464400	-2.11599400
H	-1.40266700	-3.30085500	-2.72530900
H	-0.84633500	-1.58189400	-2.54982100
H	0.49363300	-4.08890700	-1.40456500
C	1.31985700	-2.15527900	-0.85818100
C	1.33342600	-0.76554500	-1.06747400
C	2.38058400	-2.72657000	-0.13452600
C	2.36825100	0.01767300	-0.56600700
H	0.53706900	-0.28739800	-1.62922100
C	3.41176600	-1.94005900	0.36160600
H	2.37237200	-3.79511600	0.05714500
C	3.42239300	-0.55374300	0.15733500
H	2.36115500	1.09102800	-0.74145100
H	4.22753000	-2.40484900	0.90694500
C	5.65900100	0.46580400	-0.46009800
C	4.57225300	0.29532600	0.63558000
H	4.20890900	1.28779500	0.92759700
H	5.02432900	-0.16239400	1.52236200
H	5.15102100	0.87676000	-1.34242700
C	6.76283300	1.44315200	-0.08107500
C	6.95886800	1.91717400	1.21877100
C	7.64557500	1.87239900	-1.08291500
C	8.00255500	2.79828200	1.52027700
H	6.29832600	1.60844600	2.02160200
C	8.68946200	2.75091200	-0.80740400
H	7.51775500	1.50147100	-2.09656900
C	8.85182700	3.20242600	0.50009600

H	8.14339800	3.15832100	2.53301900
H	9.36278300	3.07584300	-1.59236400
Br	10.31524700	4.43755000	0.90626500
C	7.15534400	-3.45786100	-1.51504400
C	6.22037400	-2.82034400	-2.33063500
C	5.76013900	-1.54466500	-2.00128500
C	6.22671000	-0.88929700	-0.85783400
C	7.17016700	-1.53402700	-0.04860600
C	7.62985000	-2.80978800	-0.37205800
H	7.51475000	-4.45114700	-1.76819500
H	5.84545100	-3.31578900	-3.22188100
H	5.01634400	-1.05822300	-2.62699700
H	7.55169100	-1.02839700	0.83440600
H	8.36215900	-3.29694600	0.26571400

im4c

SCF Energy (a.u.) = -1897.587197

Thermal correction to Gibbs free energy (a.u.) = 0.604134

Charge = 0, Multiplicity = 1

C	-6.96216600	2.53767800	-0.21317100
C	-7.84893800	3.05317600	-1.16910600
C	-9.09944800	3.53745500	-0.80469600
C	-9.51331900	3.52505600	0.53915700
C	-8.62064200	3.00897800	1.49214900
C	-7.36902300	2.52323500	1.12439600
H	-7.55068300	3.07447000	-2.21527400
H	-9.76001300	3.93185200	-1.57075800
H	-8.91787400	2.98593300	2.53766000
H	-6.70625400	2.11126500	1.87999400
C	-10.82291800	4.02298700	0.98286700
C	-11.79034000	4.55435400	0.22508400
H	-10.99855100	3.93684400	2.05502500
H	-12.72392900	4.88936100	0.66586800
H	-11.69484200	4.67750400	-0.85021000

C	-5.77837300	0.45972100	-1.04651100
C	-5.63953100	1.94795200	-0.63357300
H	-5.23091900	2.51378500	-1.48006300
H	-4.92043300	2.02344500	0.18992500
H	-6.54017900	0.41678200	-1.83643800
C	-4.50430700	-0.14883200	-1.60642800
C	-4.58203100	-1.44382200	-2.17590600
C	-3.26048700	0.46252800	-1.52150800
C	-3.44938300	-2.12464300	-2.57431100
H	-5.55376800	-1.92359300	-2.24916000
C	-2.08630200	-0.21717000	-1.92154200
H	-3.16361500	1.46355900	-1.11770200
C	-2.16416500	-1.53868000	-2.43215500
H	-3.52736900	-3.13072700	-2.97662700
H	-1.13957000	0.31295400	-1.91377500
Br	-1.75862900	-2.51067100	1.76657900
C	-7.22981300	-1.86095100	2.31036400
C	-8.11227500	-1.43747500	1.31550100
C	-7.63965200	-0.70453500	0.22600300
C	-6.28306200	-0.38299400	0.11959200
C	-5.40547400	-0.80835200	1.12473700
C	-5.87282900	-1.54533500	2.21172600
H	-7.59573100	-2.43802000	3.15488500
H	-9.16983000	-1.67658800	1.38529500
H	-8.33085400	-0.36336100	-0.54015300
H	-4.34518500	-0.58215800	1.05945500
H	-5.16956800	-1.88039300	2.96826700
Ni	-1.75507400	-1.69786500	-0.37699300
C	-0.23981400	-2.42084700	-1.31542000
C	-0.87965800	-2.31682900	-2.70351500
H	-1.12657700	-3.30870400	-3.09170700
H	-0.24480900	-1.81943500	-3.44456000
H	-0.17909000	-3.43884200	-0.92738700
C	0.94130100	-1.60430100	-0.96453300

C	1.41437000	-0.53895400	-1.75208600
C	1.62862600	-1.88305600	0.23420800
C	2.51910600	0.21122500	-1.35577000
H	0.92863500	-0.29270800	-2.69108300
C	2.73017200	-1.13471500	0.62263600
H	1.26691200	-2.68499600	0.87006400
C	3.19451500	-0.07019700	-0.16350300
H	2.86598400	1.02665500	-1.98684700
H	3.24966200	-1.38306800	1.54345700
C	5.70759300	0.10980500	-0.43829300
C	4.43156900	0.70089300	0.21992500
H	4.33157100	1.74871400	-0.08778300
H	4.55074000	0.68900000	1.30906900
H	5.52191600	0.09582000	-1.52030200
C	6.95962700	0.94435800	-0.20814900
C	7.03683100	1.97312700	0.73443000
C	8.10437900	0.65143800	-0.96382800
C	8.21835100	2.69769500	0.92320400
H	6.17376700	2.22955800	1.33900100
C	9.29034000	1.36047500	-0.79582700
H	8.06730900	-0.15617400	-1.69033100
C	9.32754100	2.37961100	0.15267400
H	8.26457800	3.49323500	1.65812300
H	10.16667900	1.12423900	-1.38857500
Br	10.98763300	3.38713100	0.40358500
C	6.13575400	-3.99407600	0.87381700
C	5.59812700	-3.71057500	-0.38175100
C	5.48677300	-2.38772500	-0.81194700
C	5.91041500	-1.33295600	0.00220200
C	6.45484500	-1.62718400	1.25816000
C	6.56492300	-2.94716600	1.69306300
H	6.22228800	-5.02266500	1.21205500
H	5.26092000	-4.51764800	-1.02615800
H	5.04790300	-2.16801300	-1.78167400

H	6.80106900	-0.81668600	1.89389700
H	6.98938400	-3.15935600	2.67041500

im5c

SCF Energy (a.u.) = -2038.629708

Thermal correction to Gibbs free energy (a.u.) = 0.668952

Charge = 0, Multiplicity = 1

C	7.08849000	2.44450500	0.20892400
C	8.06728600	2.88504200	1.11119300
C	9.31478100	3.30988200	0.67045700
C	9.63338000	3.31060500	-0.69921200
C	8.64917700	2.86961000	-1.59821200
C	7.40056500	2.44347000	-1.15400200
H	7.84377400	2.89477900	2.17596900
H	10.04788800	3.64732800	1.39671800
H	8.87147800	2.85851600	-2.66240700
H	6.66437500	2.08971400	-1.87014800
C	10.93508700	3.74787400	-1.22280100
C	11.98162500	4.20397700	-0.52333200
H	11.03049200	3.68199000	-2.30650000
H	12.89972800	4.49933300	-1.02130700
H	11.96843400	4.30224800	0.55865800
C	5.85008900	0.41325300	1.07563700
C	5.76694300	1.91715900	0.70807500
H	5.44934400	2.47995200	1.59464200
H	4.99830100	2.05478400	-0.06063000
H	6.66962000	0.30460100	1.79821700
C	4.58869900	-0.14098700	1.71390200
C	4.64595300	-1.43913900	2.27561400
C	3.36143300	0.50676000	1.67424600
C	3.50163900	-2.09876000	2.67738900
H	5.60689300	-1.94332700	2.32952700
C	2.17652200	-0.15361300	2.07841900
H	3.28207400	1.51639700	1.28747100

C	2.22812000	-1.48847800	2.54563000
H	3.56130400	-3.11211900	3.06494700
H	1.23888500	0.39367600	2.08717700
C	6.88131700	-1.92025800	-2.42993700
C	7.86425900	-1.57118600	-1.50304800
C	7.52640100	-0.83083800	-0.36890300
C	6.20611100	-0.42756800	-0.14751800
C	5.22656300	-0.77749700	-1.08668200
C	5.55977500	-1.52086400	-2.21795300
H	7.14197400	-2.50230600	-3.30945600
H	8.89576800	-1.87406600	-1.66035400
H	8.29659100	-0.54929100	0.34430800
H	4.19011500	-0.48985900	-0.93669700
H	4.78034500	-1.79139000	-2.92405400
Ni	1.83686000	-1.54201200	0.44325800
C	0.34012600	-2.33930300	1.33701200
C	0.93285700	-2.26499300	2.75271300
H	1.16113700	-3.26487800	3.13334600
H	0.27363000	-1.77990800	3.48104700
H	0.28728000	-3.35600600	0.93943900
C	-0.86307100	-1.54497900	0.98856700
C	-1.37850400	-0.51115400	1.78891800
C	-1.51874700	-1.80677100	-0.23086200
C	-2.49410700	0.22295500	1.38734900
H	-0.91422800	-0.27091900	2.74056400
C	-2.62960000	-1.07583300	-0.62556100
H	-1.12267200	-2.58291300	-0.87864700
C	-3.13897500	-0.04396100	0.17649200
H	-2.87156000	1.01532600	2.03070200
H	-3.12318400	-1.31306200	-1.56388200
C	-5.66187400	0.06958900	0.41107100
C	-4.38924200	0.70334200	-0.21283800
H	-4.32165000	1.74728000	0.11679800
H	-4.49066800	0.71113800	-1.30408800

H	-5.49150700	0.03451200	1.49506400
C	-6.92922700	0.88071200	0.18203100
C	-7.01811800	1.92429300	-0.74323700
C	-8.07610600	0.55053400	0.91894500
C	-8.21268300	2.62682800	-0.93330600
H	-6.15353600	2.20935200	-1.33257900
C	-9.27521500	1.23691400	0.74951300
H	-8.02976800	-0.26861200	1.63189700
C	-9.32337300	2.27142600	-0.18155000
H	-8.26770100	3.43422600	-1.65458900
H	-10.15294100	0.97179200	1.32784200
Br	-11.00247700	3.24779300	-0.43471800
C	-5.98322800	-4.01209500	-0.99899400
C	-5.44693200	-3.74354000	0.26054200
C	-5.36959000	-2.42889100	0.72176100
C	-5.82633600	-1.36685600	-0.06486100
C	-6.36762400	-1.64623800	-1.32551000
C	-6.44408400	-2.95813300	-1.79136200
H	-6.04433700	-5.03457600	-1.36082900
H	-5.08421500	-4.55594000	0.88414800
H	-4.93069400	-2.22003600	1.69369800
H	-6.73831400	-0.83066600	-1.94056900
H	-6.86761200	-3.15843000	-2.77172800
O	1.73709000	-1.98805600	-1.26632000
C	1.98635700	-3.28572000	-1.74153600
C	1.87137100	-3.30561900	-3.26448100
H	1.25747700	-4.00237700	-1.32023700
H	2.98974500	-3.64240300	-1.44778900
H	2.06235500	-4.31001200	-3.66280100
H	0.86946100	-2.98710000	-3.57222800
H	2.59430800	-2.61145100	-3.70840500

im6c

SCF Energy (a.u.) = -2642.348983

Thermal correction to Gibbs free energy (a.u.) = 0.899610

Charge = 0, Multiplicity = 1

C	-8.36626700	-1.08572900	-1.61902900
C	-8.99494500	-2.19097700	-2.21050700
C	-10.32556500	-2.49175500	-1.94588400
C	-11.08480700	-1.69386600	-1.07182400
C	-10.45084900	-0.58901700	-0.48105500
C	-9.11778300	-0.28974300	-0.74804400
H	-8.42780200	-2.82287500	-2.89064200
H	-10.78048700	-3.35363100	-2.42459900
H	-11.01561600	0.04237500	0.20070900
H	-8.64833800	0.56159100	-0.26369100
C	-12.49433700	-1.96268800	-0.75501400
C	-13.26097700	-2.95301500	-1.22863800
H	-12.94029700	-1.25956000	-0.05155700
H	-14.29681700	-3.05350600	-0.92015700
H	-12.89509700	-3.69407700	-1.93396300
C	-5.99939200	-1.56269500	-0.84711300
C	-6.90348200	-0.81396700	-1.86396500
H	-6.62220400	-1.12835800	-2.87587300
H	-6.71111700	0.26208900	-1.79407000
H	-6.29591100	-2.61829100	-0.88130700
C	-4.51890600	-1.49342500	-1.18829800
C	-3.67947800	-2.55403300	-0.81812600
C	-3.93421700	-0.38260900	-1.80516100
C	-2.30528500	-2.49614900	-1.03935200
H	-4.11365400	-3.43205100	-0.34484700
C	-2.55638900	-0.31604500	-2.00889700
H	-4.54951100	0.45682400	-2.11110100
C	-1.71704600	-1.36524700	-1.62237300
H	-1.67684400	-3.33393400	-0.74406900
H	-2.11480500	0.57960500	-2.43458500
C	-6.80220000	-0.12382800	3.16373500
C	-7.22715200	-1.39434200	2.77450100

C	-6.95757400	-1.85934300	1.48568900
C	-6.26132500	-1.06622800	0.56946700
C	-5.84353400	0.21061800	0.96691800
C	-6.10893700	0.67747400	2.25322800
H	-7.00786900	0.23859100	4.16708800
H	-7.77138700	-2.02518600	3.47205700
H	-7.30296500	-2.84432800	1.18238500
H	-5.28389000	0.83956200	0.28310800
H	-5.76468900	1.66649500	2.54434900
Ni	-0.60903500	0.32336000	0.54640400
C	0.41461700	-0.99927600	-0.36929700
C	-0.21504900	-1.23410700	-1.74290500
H	0.21545200	-2.13474600	-2.21004000
H	0.00977300	-0.38803600	-2.39633900
H	0.19900600	-1.84917300	0.29727600
C	1.85206000	-0.65012600	-0.30377600
C	2.55291900	-0.05992000	-1.37002700
C	2.55948800	-0.85343300	0.89726700
C	3.89000800	0.30813300	-1.23567900
H	2.04336900	0.13186100	-2.30763700
C	3.89203100	-0.48333500	1.02915900
H	2.04131300	-1.30670000	1.73973500
C	4.58370100	0.10549300	-0.03791900
H	4.40447900	0.76560000	-2.07862600
H	4.41521600	-0.67322600	1.96264000
C	6.94061600	-0.71151000	-0.48976100
C	6.05166900	0.43270600	0.06805800
H	6.27482300	1.35096400	-0.48900200
H	6.31660600	0.61371300	1.11620500
H	6.60702000	-0.88803300	-1.52065900
C	8.42219500	-0.36890500	-0.55038100
C	8.98310700	0.73656100	0.09488800
C	9.27569700	-1.21708900	-1.27129100
C	10.35550900	0.99855000	0.02687900

H	8.35627100	1.41593100	0.66193800
C	10.64403000	-0.97573800	-1.35580300
H	8.85927300	-2.09008500	-1.76715700
C	11.16462300	0.13666800	-0.69937500
H	10.77734000	1.85992700	0.53213300
H	11.29090600	-1.63908500	-1.91855600
Br	13.08839200	0.49160000	-0.80521200
C	6.11751000	-4.30232000	1.78692600
C	5.49827100	-4.09313500	0.55428000
C	5.78684000	-2.94748500	-0.18793500
C	6.69611700	-1.99718100	0.28768200
C	7.31541800	-2.21719100	1.52386600
C	7.02798500	-3.35967100	2.26989900
H	5.89560500	-5.19416800	2.36632600
H	4.78724300	-4.81920300	0.16986700
H	5.28569100	-2.77542100	-1.13656300
H	8.03336600	-1.49242000	1.89816900
H	7.51901100	-3.51670000	3.22647700
O	-0.24897600	1.69247200	-0.56731800
C	0.79340000	2.55152700	-0.17389200
C	1.16168600	3.46891100	-1.33841200
H	1.69074400	1.98453700	0.11928900
H	0.49449500	3.16262900	0.69797900
H	1.93566800	4.18946700	-1.04560200
H	1.53470100	2.87518900	-2.17993100
H	0.28109900	4.02520100	-1.68296400
C	-0.90584300	-0.69672400	3.38229400
C	-1.78163600	-0.97607800	2.31657000
C	-2.44748000	0.07331800	1.65952100
C	-2.17811500	1.42484800	2.01765100
C	-1.30334000	1.66662500	3.09173300
C	-0.69086700	0.61883700	3.79041700
H	-0.39915600	-1.51423500	3.88756600
H	-1.97439300	-2.00021500	2.01422200

H	-3.17231300	-0.14705800	0.88590800
H	-1.07800500	2.69598300	3.35370600
H	-0.01841200	0.83187800	4.61558800
C	-3.58443600	3.25472900	-1.02272500
C	-2.32071400	4.87575000	0.34738200
C	-3.59859700	4.69273900	-0.48642400
H	-2.74276800	3.10705200	-1.71050800
H	-2.35163900	5.82375800	0.89513700
B	-2.62520800	2.58792200	1.06943500
O	-3.46279600	2.29868900	0.02951800
O	-2.13306300	3.83746400	1.31155300
H	-4.51489800	3.03196900	-1.55618300
H	-1.44047400	4.88736600	-0.30638200
C	-3.57737800	5.67563600	-1.66261900
H	-2.70437400	5.51207300	-2.30523500
H	-4.47739300	5.56482800	-2.27839100
H	-3.54545800	6.71143400	-1.30516000
C	-4.84655600	4.92272200	0.38096200
H	-4.86327800	5.94719100	0.76982600
H	-5.75882600	4.76835600	-0.20673900
H	-4.87801200	4.23804200	1.23356500

TS3c

SCF Energy (a.u.) = -2642.342687

Thermal correction to Gibbs free energy (a.u.) = 0.901795

Charge = 0, Multiplicity = 1

C	-8.38603800	-0.89972800	-1.67879700
C	-9.05355100	-1.99832800	-2.23923700
C	-10.38566200	-2.26140100	-1.94365300
C	-11.10715900	-1.43070400	-1.06824700
C	-10.43436900	-0.33257800	-0.50868100
C	-9.09997900	-0.07093900	-0.80669500
H	-8.51599200	-2.65510900	-2.91987700
H	-10.87135600	-3.11916800	-2.39897200

H	-10.96958400	0.32389600	0.17321500
H	-8.60028300	0.77627900	-0.34621500
C	-12.51624100	-1.65899800	-0.71927200
C	-13.31637700	-2.63770000	-1.16059900
H	-12.93055500	-0.93332300	-0.01938200
H	-14.34799000	-2.70714500	-0.83016200
H	-12.98301400	-3.39935000	-1.86009600
C	-6.01838400	-1.41606900	-0.93838700
C	-6.92201200	-0.66894800	-1.95688900
H	-6.66744700	-1.01408300	-2.96587200
H	-6.70233400	0.40322200	-1.91666300
H	-6.34169700	-2.46423600	-0.94147100
C	-4.54421700	-1.39393000	-1.31103300
C	-3.73357400	-2.49055700	-0.98518800
C	-3.93599400	-0.28754700	-1.91324100
C	-2.36191000	-2.47112200	-1.22951500
H	-4.18668700	-3.36641000	-0.52604900
C	-2.56241400	-0.26083400	-2.14379900
H	-4.52718400	0.58092300	-2.18235100
C	-1.74952200	-1.34452900	-1.79756800
H	-1.75607900	-3.33552600	-0.96564100
H	-2.10478800	0.63263800	-2.55608800
C	-6.69334600	0.11585000	3.06191800
C	-7.12504200	-1.16507000	2.71640900
C	-6.89832100	-1.65696300	1.42943200
C	-6.23862100	-0.88122400	0.47182100
C	-5.81283700	0.40552500	0.82688100
C	-6.03530600	0.89920800	2.11114700
H	-6.86430100	0.49919100	4.06399800
H	-7.64093000	-1.78293700	3.44642600
H	-7.24869700	-2.65015400	1.16009000
H	-5.26215900	1.01710500	0.12040100
H	-5.67868400	1.89266500	2.36837800
Ni	-0.69081900	-0.00180500	0.52117600

C	0.41273800	-1.05866100	-0.58233100
C	-0.24551000	-1.25570300	-1.94702100
H	0.15384200	-2.15154600	-2.44870600
H	-0.01063800	-0.40112800	-2.58870700
H	0.19331300	-1.92768600	0.08006800
C	1.84614200	-0.71265400	-0.51560400
C	2.56812900	-0.19837600	-1.60684800
C	2.52727300	-0.82368500	0.71446700
C	3.89565600	0.20174700	-1.46588300
H	2.08783300	-0.09850400	-2.57414200
C	3.84983500	-0.42476000	0.85077200
H	1.99549800	-1.22565800	1.57445700
C	4.55925400	0.09992400	-0.23913700
H	4.42652400	0.60140300	-2.32752300
H	4.35166900	-0.53883100	1.80759700
C	6.94268900	-0.71153100	-0.53681900
C	6.01750400	0.46306300	-0.11844800
H	6.24325400	1.32911800	-0.75237100
H	6.24382300	0.74686700	0.91570800
H	6.64859900	-0.98991200	-1.55725300
C	8.41997800	-0.34738100	-0.57857300
C	8.93950200	0.82561800	-0.02444600
C	9.31203800	-1.24496100	-1.18360300
C	10.30921900	1.10579700	-0.06993300
H	8.28244700	1.54472500	0.45221600
C	10.67852700	-0.98674600	-1.24352600
H	8.92774400	-2.16958000	-1.60644400
C	11.15771300	0.19355100	-0.68063500
H	10.69884800	2.01968600	0.36384100
H	11.35567200	-1.68890200	-1.71637800
Br	13.07760900	0.57304600	-0.75380100
C	6.09539000	-4.08684200	2.04000300
C	5.53843200	-4.02030200	0.76262000
C	5.83573200	-2.94426900	-0.07458100

C	6.69164700	-1.92310500	0.34971800
C	7.25013700	-2.00080600	1.63127700
C	6.95344800	-3.07278700	2.47205200
H	5.86623600	-4.92367200	2.69374200
H	4.86955300	-4.80356300	0.41686300
H	5.38306000	-2.88316500	-1.06060400
H	7.92781300	-1.22041700	1.96693900
H	7.39625500	-3.11938800	3.46321500
O	-0.58360100	1.67362000	-0.20468200
C	0.63994900	2.38877600	-0.17914300
C	0.90776000	3.01534400	-1.54347000
H	1.47349600	1.72652500	0.08117300
H	0.58105000	3.16213900	0.59986900
H	1.82655300	3.61463600	-1.52549200
H	1.01996900	2.23401400	-2.30215600
H	0.07713100	3.66410400	-1.84520900
C	-1.65169600	-1.13336800	3.65045300
C	-2.43741600	-1.24794900	2.50101800
C	-2.64453600	-0.12761900	1.67947800
C	-2.03661400	1.11668700	1.97998600
C	-1.26018300	1.20367700	3.15543400
C	-1.07711000	0.09953500	3.98623100
H	-1.49577300	-1.99767400	4.29027900
H	-2.91150000	-2.19071500	2.24498100
H	-3.29913400	-0.20636700	0.82083700
H	-0.79629500	2.15518100	3.39843100
H	-0.47583800	0.18879300	4.88681200
C	-3.27801100	3.29061600	-0.91191600
C	-1.88315000	4.69685800	0.56564300
C	-3.21655600	4.65232500	-0.20146900
H	-2.47505000	3.21860000	-1.66023600
H	-1.84761400	5.58063400	1.21365200
B	-2.13257600	2.32190400	0.94771900
O	-3.15711900	2.22192700	0.00928700

O	-1.68068400	3.55812200	1.39338300
H	-4.23777100	3.17343800	-1.43051900
H	-1.05293500	4.77530500	-0.15006600
C	-3.24254000	5.77845100	-1.23991400
H	-2.42063500	5.67922800	-1.95932200
H	-4.18475900	5.77041500	-1.80065500
H	-3.15188900	6.75914700	-0.75779200
C	-4.39716800	4.79037400	0.77166200
H	-4.37097200	5.76282500	1.27727600
H	-5.35175300	4.71192800	0.23761100
H	-4.37111300	4.00910500	1.53599600

im7c

SCF Energy (a.u.) = -2642.373886

Thermal correction to Gibbs free energy (a.u.) = 0.909125

Charge = 0, Multiplicity = 1

C	-7.01409700	2.44921700	-1.06354100
C	-7.88696500	2.90230500	-2.06221500
C	-9.20428600	3.23553700	-1.77070600
C	-9.70055200	3.12942800	-0.45950400
C	-8.81989900	2.67943000	0.53737300
C	-7.50162000	2.34519700	0.24274000
H	-7.52580500	2.99233100	-3.08475600
H	-9.85353500	3.58296600	-2.56861400
H	-9.18044300	2.58565100	1.55876500
H	-6.85018000	1.97341100	1.02810000
C	-11.08343000	3.46483500	-0.09256000
C	-12.05240000	3.91787900	-0.89788100
H	-11.31833100	3.31765700	0.96150600
H	-13.04425800	4.13167300	-0.51226600
H	-11.90111200	4.09304300	-1.95948900
C	-5.54198800	0.54635900	-1.90304800
C	-5.61010400	2.02214800	-1.40869600
H	-5.21579200	2.68550400	-2.18664000

H	-4.96124000	2.12217400	-0.53177800
H	-6.11206100	0.50303600	-2.84239200
C	-4.11651300	0.09113000	-2.21036900
C	-3.80578000	-1.27378000	-2.20224200
C	-3.08341900	0.99721600	-2.50236500
C	-2.50461000	-1.72096800	-2.43576500
H	-4.58161900	-1.99453400	-1.97163600
C	-1.78139700	0.56314000	-2.73105400
H	-3.28336000	2.06180500	-2.52715800
C	-1.45718100	-0.80785100	-2.70264400
H	-2.29554800	-2.78736900	-2.44546600
H	-0.99747700	1.28711300	-2.93811200
C	-7.59274200	-1.89870600	1.01258000
C	-8.22021500	-1.56631800	-0.18841900
C	-7.54299600	-0.80408900	-1.14165300
C	-6.23875500	-0.36247300	-0.90344900
C	-5.61502100	-0.70065400	0.30471200
C	-6.28674100	-1.46741600	1.25543400
H	-8.11401400	-2.49873100	1.75349800
H	-9.23589100	-1.89809300	-0.38617900
H	-8.03949600	-0.53041800	-2.06922800
H	-4.59177400	-0.39180100	0.49357700
H	-5.77871300	-1.73983800	2.17401700
Ni	-1.00090800	-1.03878400	-0.52070800
C	0.43433900	-1.82830500	-1.52391800
C	-0.03263300	-1.31390600	-2.90079200
H	-0.00513900	-2.10174500	-3.66408900
H	0.60154300	-0.49475000	-3.25152400
H	0.34967000	-2.91834400	-1.44733600
C	1.75053500	-1.35189900	-1.02978400
C	2.06976300	0.01870600	-0.99320800
C	2.70711800	-2.25053700	-0.53117300
C	3.27929900	0.46300100	-0.47102600
H	1.34529600	0.74501000	-1.35447100

C	3.91901900	-1.80451000	-0.00967100
H	2.49604100	-3.31657200	-0.55955800
C	4.22457600	-0.44047900	0.03425800
H	3.49429000	1.52934000	-0.44571100
H	4.64711100	-2.52529700	0.35177000
C	6.57401500	0.24383200	-0.62612500
C	5.56130100	0.04635000	0.53357400
H	5.44083900	1.00084200	1.06025400
H	5.97245600	-0.67296200	1.25080800
H	6.09885300	0.92890100	-1.34055000
C	7.88642700	0.88356400	-0.19600300
C	8.27392200	1.02188400	1.13951000
C	8.76498400	1.33800500	-1.19051200
C	9.50074000	1.59913300	1.48364000
H	7.62277800	0.68256400	1.93760400
C	9.98963400	1.91818000	-0.87254600
H	8.48701000	1.22429300	-2.23512800
C	10.33964400	2.03950600	0.46999600
H	9.78885000	1.70043500	2.52377100
H	10.65754500	2.26675600	-1.65198800
Br	12.05922500	2.85199000	0.93631200
C	7.11256200	-3.56299200	-2.61848900
C	6.25196600	-2.60470100	-3.15441400
C	6.10143400	-1.36926400	-2.52345000
C	6.80683200	-1.07311000	-1.35296200
C	7.67189500	-2.03911400	-0.82488700
C	7.82298800	-3.27593100	-1.45055400
H	7.23212600	-4.52553400	-3.10769700
H	5.69414800	-2.81824600	-4.06198700
H	5.41419900	-0.63244600	-2.93070100
H	8.23607600	-1.81544400	0.07653700
H	8.49951400	-4.01436800	-1.02912200
O	-0.48226600	-1.24343500	1.29308300
C	0.35334600	-2.20416300	1.94236300

C	1.42368900	-1.49931600	2.75938800
H	0.80564100	-2.83483400	1.17352800
H	-0.27982000	-2.83688400	2.57425900
H	2.07581500	-2.23439700	3.24679700
H	2.03914200	-0.86607200	2.11348600
H	0.95677500	-0.87898700	3.52990200
C	-4.47336600	-4.39625700	2.55068500
C	-4.22072900	-3.49853400	3.58936600
C	-3.39350200	-2.39290700	3.37374500
C	-2.78937700	-2.15487000	2.12889200
C	-3.05221200	-3.08116400	1.10626900
C	-3.88470200	-4.18278500	1.30259700
H	-5.12261400	-5.25319300	2.71075100
H	-4.67131500	-3.65746500	4.56637200
H	-3.20345300	-1.69184100	4.18090600
H	-2.60203200	-2.93344600	0.12670600
H	-4.07797600	-4.87318000	0.48485200
C	-2.05010900	1.35656700	0.71352200
C	-1.34165700	1.22043900	3.06265000
C	-2.23858100	2.00239400	2.08939600
H	-1.00921000	1.51357500	0.38979800
H	-1.42565500	1.63701800	4.07475200
B	-1.85594500	-0.86346800	1.91038100
O	-2.35021500	-0.04648600	0.71267200
O	-1.71758800	-0.13389200	3.12373100
H	-2.70285500	1.82327400	-0.02970200
H	-0.28966200	1.32410100	2.74605900
C	-1.77797800	3.46210500	2.01045400
H	-0.72409000	3.53552600	1.71458400
H	-2.37430100	4.02491100	1.28175600
H	-1.88946800	3.95627000	2.98246800
C	-3.70816700	1.92635800	2.52892000
H	-3.83652900	2.38181000	3.51798000
H	-4.35278900	2.46701000	1.82461700

H -4.05316500 0.89182800 2.58596700

TS4c

SCF Energy (a.u.) = -2642.323047

Thermal correction to Gibbs free energy (a.u.) = 0.904016

Charge = 0, Multiplicity = 1

C -8.22969100 -2.53423600 -1.11502400
C -8.81622200 -3.19592100 -0.02632800
C -10.19556300 -3.23854400 0.13450200
C -11.04890500 -2.61566600 -0.79352800
C -10.45721100 -1.95530400 -1.88207600
C -9.07471200 -1.91400400 -2.04072300
H -8.17647100 -3.68603000 0.70456500
H -10.61472800 -3.76314600 0.98766800
H -11.09525200 -1.46494200 -2.61330900
H -8.64517200 -1.38149100 -2.88411300
C -12.51358400 -2.62720600 -0.67486200
C -13.24770700 -3.20704900 0.28297400
H -13.03479300 -2.09514200 -1.47059600
H -14.33145400 -3.14863900 0.26792000
H -12.80721400 -3.75698300 1.11004200
C -6.16472700 -1.22566100 -0.42328400
C -6.72937800 -2.43736600 -1.22768700
H -6.25983300 -3.35003400 -0.84308800
H -6.43127400 -2.34205500 -2.27765300
H -6.53879300 -1.33725400 0.60034000
C -4.64766500 -1.30813600 -0.33627600
C -4.03419400 -1.44577900 0.90474200
C -3.82803300 -1.36827200 -1.48215300
C -2.65732200 -1.70552700 1.01641100
H -4.63359400 -1.38030000 1.80798600
C -2.46501800 -1.59227900 -1.38386200
H -4.26686000 -1.26828300 -2.46861000
C -1.85074400 -1.81492600 -0.13478200

H	-2.24359000	-1.93131400	1.99572900
H	-1.85953200	-1.64958300	-2.28461300
C	-7.90285600	2.47200100	-1.87971400
C	-8.20266000	1.99193700	-0.60459900
C	-7.62528100	0.80638400	-0.15119300
C	-6.73772500	0.07992700	-0.95124300
C	-6.46302900	0.56008200	-2.23776800
C	-7.03390700	1.74679300	-2.69729700
H	-8.34652900	3.39699900	-2.23641700
H	-8.88607000	2.53939000	0.03846100
H	-7.86272500	0.43790100	0.84270800
H	-5.79602600	0.01372600	-2.89525700
H	-6.79849600	2.10512600	-3.69564400
Ni	-0.95993000	0.11808900	1.02939200
C	0.26730100	-1.41687700	1.10003600
C	-0.38880100	-2.22366900	-0.02869400
H	-0.31253000	-3.31159800	0.12907500
H	0.10258500	-2.01526900	-0.98413100
H	0.11567900	-1.91440500	2.06754700
C	1.69677700	-1.06909400	0.92610000
C	2.16813800	-0.42953600	-0.23688900
C	2.63023600	-1.30284000	1.94982300
C	3.50090400	-0.05712100	-0.36608700
H	1.46730400	-0.18499000	-1.03038700
C	3.96547600	-0.92534000	1.82167700
H	2.30030700	-1.79885600	2.86023800
C	4.42578000	-0.29691600	0.66041300
H	3.83113400	0.44350600	-1.27440300
H	4.66638500	-1.14309500	2.62341700
C	6.63903900	-1.06371600	-0.30967400
C	5.88351800	0.04165500	0.47617600
H	5.98512100	0.98814800	-0.06933800
H	6.36037800	0.17543000	1.45408900
H	6.09277900	-1.20155900	-1.25191800

C	8.07045600	-0.69591300	-0.67206800
C	8.75348400	0.38440500	-0.10673900
C	8.75074000	-1.49351300	-1.60403200
C	10.07710500	0.67102600	-0.45693000
H	8.26173600	1.02421800	0.61774400
C	10.06694100	-1.22687500	-1.97052300
H	8.24027800	-2.34702200	-2.04264500
C	10.71269900	-0.14057400	-1.38555300
H	10.59500700	1.51239000	-0.01072200
H	10.57904200	-1.85103000	-2.69394800
Br	12.56580900	0.24967400	-1.88803700
C	6.34778200	-4.76067000	1.92718600
C	5.46774200	-4.50287200	0.87569000
C	5.58220600	-3.32225100	0.14121600
C	6.57492900	-2.38468700	0.44409200
C	7.45524000	-2.65305200	1.49911600
C	7.34280700	-3.83088200	2.23706300
H	6.26135100	-5.67965900	2.50016600
H	4.68818700	-5.21803000	0.62804300
H	4.88082900	-3.11293100	-0.66180800
H	8.23837100	-1.93810800	1.73651400
H	8.03552500	-4.02512800	3.05144600
O	0.30739400	1.46814100	1.41774800
C	0.89368000	1.58863600	2.73234900
C	2.21501900	2.32930600	2.63345000
H	1.05200800	0.56979900	3.08785200
H	0.19110300	2.10378900	3.39276600
H	2.68334300	2.38740500	3.62325200
H	2.89218900	1.80196000	1.95646700
H	2.05897000	3.34842700	2.26734300
C	-5.06009500	2.32993600	1.51848900
C	-4.56140700	2.24156400	0.21671200
C	-3.23340100	1.86827900	0.00648300
C	-2.36204400	1.59567700	1.07569400

C	-2.89471300	1.70435900	2.37719600
C	-4.22606200	2.05532400	2.60485200
H	-6.09487200	2.61813800	1.67998400
H	-5.20802300	2.46770200	-0.62429200
H	-2.84732800	1.81939600	-1.00886500
H	-2.24935600	1.52184300	3.23648700
H	-4.60912900	2.13184300	3.62022800
C	-0.02689000	3.94322300	-1.09372000
C	-0.29634200	4.97995600	1.13819200
C	-0.66160700	5.12774600	-0.34608200
H	1.06831200	4.06326800	-1.09831100
H	-0.85478200	5.70609100	1.74032600
B	-0.47748900	2.56479100	0.84955800
O	-0.35157500	2.67776500	-0.53609400
O	-0.57322100	3.68886600	1.66441900
H	-0.36122500	3.93635800	-2.13795200
H	0.77632700	5.19267600	1.27334000
C	-0.06230700	6.43389400	-0.88436400
H	1.02970000	6.45051100	-0.78496000
H	-0.30717300	6.56514700	-1.94500600
H	-0.46436700	7.29840300	-0.34300200
C	-2.18686500	5.14179200	-0.51900800
H	-2.61602400	6.02939800	-0.03852100
H	-2.45630500	5.17047400	-1.58188000
H	-2.65102000	4.26042300	-0.07560500

im8c

SCF Energy (a.u.) = -2642.342395

Thermal correction to Gibbs free energy (a.u.) = 0.904301

Charge = 0, Multiplicity = 1

C	-8.41740800	-2.26061600	-1.08566800
C	-8.99191800	-2.93106100	0.00445600
C	-10.36169200	-2.89759300	0.23293600
C	-11.21831400	-2.18644000	-0.62612100

C	-10.63939100	-1.51833100	-1.71655200
C	-9.26597100	-1.55352200	-1.94303500
H	-8.34977100	-3.48953400	0.68231900
H	-10.77116200	-3.43137300	1.08514300
H	-11.28008400	-0.96105300	-2.39574200
H	-8.84654400	-1.01474500	-2.78711900
C	-12.67353400	-2.11549700	-0.43483800
C	-13.39597300	-2.69062500	0.53468800
H	-13.19806600	-1.51977000	-1.18182000
H	-14.47353000	-2.56675800	0.57611700
H	-12.95155100	-3.30039100	1.31646800
C	-6.23229900	-1.14195000	-0.42848900
C	-6.92061300	-2.25821500	-1.27001100
H	-6.50121200	-3.22163900	-0.95797900
H	-6.66313900	-2.12984600	-2.32708300
H	-6.57227000	-1.28548500	0.60318500
C	-4.72453200	-1.33980000	-0.41557600
C	-4.08838400	-1.70644900	0.76250500
C	-3.94055300	-1.23684700	-1.58399400
C	-2.71061300	-1.99048900	0.79467100
H	-4.66496700	-1.78954300	1.67958400
C	-2.58342500	-1.50322500	-1.56708300
H	-4.40369800	-0.93883000	-2.51789900
C	-1.93236100	-1.91135600	-0.38252100
H	-2.27614600	-2.38696400	1.70745800
H	-2.00252400	-1.42094900	-2.48217300
C	-7.66971100	2.79034800	-1.56556400
C	-7.76432500	2.34647700	-0.24755500
C	-7.27801400	1.08768500	0.10376600
C	-6.69757300	0.24460100	-0.84745600
C	-6.61687400	0.69828100	-2.17103100
C	-7.09120800	1.95984200	-2.52755200
H	-8.04715400	3.77026900	-1.84377500
H	-8.21354600	2.98029600	0.51172400

H	-7.34665100	0.75397900	1.13522200
H	-6.20034900	0.05966100	-2.94356600
H	-7.01775900	2.29002300	-3.56028500
Ni	-1.17374600	-0.15835200	0.93589800
C	0.15419900	-1.66724300	0.89237800
C	-0.46486600	-2.31016700	-0.35903700
H	-0.36176400	-3.40769600	-0.38791600
H	0.01682600	-1.93079500	-1.26657600
H	-0.00291100	-2.31975600	1.76213300
C	1.58137400	-1.29087900	0.80866500
C	2.07004900	-0.44073800	-0.20540400
C	2.50670700	-1.71643800	1.77821200
C	3.40110500	-0.04120200	-0.23685400
H	1.38042700	-0.05437800	-0.95064400
C	3.84231700	-1.31937800	1.74279900
H	2.16797600	-2.37851600	2.57234200
C	4.31506500	-0.47118500	0.73646400
H	3.74111000	0.62536900	-1.02804300
H	4.53389800	-1.68857500	2.49613600
C	6.54796500	-1.01986300	-0.33576900
C	5.77259300	-0.09667100	0.64297200
H	5.87544300	0.93977900	0.29718800
H	6.23617800	-0.15677500	1.63459000
H	6.00958800	-0.97811100	-1.29154300
C	7.97626300	-0.57172100	-0.60720600
C	8.65013700	0.36529200	0.18114700
C	8.66434800	-1.14306100	-1.68765500
C	9.97186000	0.73096700	-0.09426100
H	8.15187700	0.82840200	1.02574700
C	9.97904400	-0.79347300	-1.98353300
H	8.16125000	-1.88478900	-2.30266100
C	10.61513900	0.14498100	-1.17497800
H	10.48259000	1.45918300	0.52549600
H	10.49718300	-1.24204300	-2.82347900

Br	12.46572100	0.64971100	-1.57548100
C	6.28649000	-5.08411400	1.13747100
C	5.39873800	-4.62997100	0.16156600
C	5.50420500	-3.32817500	-0.32869900
C	6.49551500	-2.46296400	0.14614100
C	7.38318800	-2.92797400	1.12374400
C	7.27987000	-4.22801000	1.61769500
H	6.20695800	-6.09775000	1.52032500
H	4.61972500	-5.28634100	-0.21626600
H	4.79668000	-2.96922800	-1.07097300
H	8.16485100	-2.26946200	1.49264700
H	7.97840700	-4.57422200	2.37469600
O	0.11998300	1.15256500	1.69090400
C	0.47701000	1.00654900	3.09096400
C	1.92251400	1.38009400	3.37291900
H	0.30755500	-0.04978500	3.30352300
H	-0.22328500	1.60741800	3.67917800
H	2.16139200	1.09730800	4.40507000
H	2.59429300	0.83437300	2.70696100
H	2.08589300	2.45280600	3.26049700
C	-4.65163500	3.13672100	0.94593400
C	-4.17255900	2.64709300	-0.27096800
C	-3.14781800	1.69904900	-0.28992600
C	-2.57854400	1.18641300	0.89130800
C	-3.07715900	1.70710800	2.09934300
C	-4.09717300	2.66638400	2.13611700
H	-5.45082000	3.87221200	0.96217100
H	-4.60894900	2.99835100	-1.20260800
H	-2.78765000	1.34524200	-1.25321900
H	-2.66814800	1.35440000	3.04767800
H	-4.45729100	3.04316400	3.09185000
C	0.01542600	3.52578100	-1.09017600
C	0.79934300	4.67698900	0.95891200
C	-0.16358600	4.78970900	-0.22923500

H	0.94372100	3.59319400	-1.67206500
H	0.66893800	5.52009000	1.64400600
B	0.24748400	2.35970300	1.01580100
O	0.07425300	2.31655000	-0.32971800
O	0.56200400	3.48553600	1.71630500
H	-0.82105000	3.42205800	-1.78874400
H	1.84281800	4.67412000	0.61433400
C	0.20771000	6.01703400	-1.07138100
H	1.24885000	5.97526200	-1.41360000
H	-0.43638400	6.08772900	-1.95540200
H	0.07618500	6.93837000	-0.49279400
C	-1.60699600	4.91435600	0.28221100
H	-1.71260400	5.81591900	0.89753600
H	-2.30786100	4.98856100	-0.55444400
H	-1.91335800	4.05674100	0.88370300

im9c

SCF Energy (a.u.) = -2427.929536

Thermal correction to Gibbs free energy (a.u.) = 0.862353

Charge = 0, Multiplicity = 1

C	-9.00524700	-1.95980100	-1.00778400
C	-9.38506900	-3.26703900	-0.67014200
C	-10.67376000	-3.55575900	-0.23794100
C	-11.64033500	-2.54073100	-0.12458100
C	-11.25570000	-1.23356100	-0.46332600
C	-9.96383600	-0.94731000	-0.89583900
H	-8.65427000	-4.06900300	-0.74984000
H	-10.93327800	-4.58013600	0.01174500
H	-11.98387400	-0.43012100	-0.38151900
H	-9.68871100	0.07619000	-1.13388300
C	-13.01698700	-2.78632300	0.32674400
C	-13.56174500	-3.95707700	0.68106400
H	-13.64330500	-1.89515400	0.36842300
H	-14.59719900	-4.01697700	1.00125000

H	-13.00780800	-4.89169000	0.66663900
C	-6.68208900	-1.37065800	-0.17081700
C	-7.58411800	-1.65287800	-1.40581400
H	-7.15412100	-2.49443600	-1.96150300
H	-7.56688200	-0.78265200	-2.07056400
H	-6.80548000	-2.22512600	0.50622600
C	-5.20500300	-1.27949500	-0.51851700
C	-4.25457600	-1.69354900	0.42379000
C	-4.73773500	-0.76902100	-1.73305600
C	-2.89153000	-1.59657200	0.16318400
H	-4.59327400	-2.09780300	1.37521100
C	-3.37092800	-0.66410600	-1.98942100
H	-5.43856700	-0.43883600	-2.49348900
C	-2.42378600	-1.06690700	-1.04697800
H	-2.18203500	-1.94069700	0.91189100
H	-3.03640700	-0.23639600	-2.92905200
C	-8.20600600	2.13367800	1.87405200
C	-8.45330900	0.85880100	2.38326500
C	-7.94183200	-0.26581700	1.73344400
C	-7.17602700	-0.13624500	0.57091500
C	-6.93239100	1.14755600	0.06805900
C	-7.44298800	2.27387300	0.71203700
H	-8.60235800	3.01103800	2.37761300
H	-9.04783200	0.73675000	3.28459100
H	-8.15290200	-1.25836700	2.12269000
H	-6.32107600	1.26587900	-0.82022800
H	-7.23934900	3.26273500	0.30907800
Ni	0.39334000	1.58813700	-0.32446000
C	-0.13059300	-0.27255700	-0.26235100
C	-0.94230300	-0.97476400	-1.34324300
H	-0.54927000	-1.99865000	-1.46615900
H	-0.80653000	-0.47755900	-2.30944400
H	-0.53297700	-0.42983800	0.74121700
C	1.32692400	-0.32560900	-0.31585300

C	2.06452800	-0.55613600	-1.51268600
C	2.06149600	0.10108600	0.81931700
C	3.43408800	-0.37412700	-1.54899800
H	1.53643800	-0.87333300	-2.40594600
C	3.45290800	0.26104300	0.76979600
H	1.53856600	0.22061800	1.76391100
C	4.15691300	0.04390300	-0.40917800
H	3.97363300	-0.55688000	-2.47601900
H	3.99075000	0.54281300	1.67045600
C	6.34228900	-1.22084800	-0.19614100
C	5.65964500	0.14971300	-0.45565000
H	5.98070700	0.52307400	-1.43559000
H	6.00280100	0.86852500	0.29693600
H	5.93339400	-1.91898800	-0.93834400
C	7.85277900	-1.19985000	-0.38186700
C	8.53661800	-2.42377700	-0.42236300
C	8.59892000	-0.02326200	-0.48996400
C	9.91933400	-2.48182700	-0.57110900
H	7.97419900	-3.34870300	-0.32463500
C	9.98948200	-0.05641900	-0.63738100
H	8.10751000	0.94317300	-0.46316300
C	10.62826300	-1.28760100	-0.67640100
H	10.43414000	-3.43526400	-0.60297900
H	10.55624400	0.86392400	-0.72033500
Br	12.57361600	-1.34970200	-0.88421400
C	5.11472800	-2.59110500	3.72300500
C	4.50096100	-3.09860400	2.57755600
C	4.91971100	-2.67640400	1.31492800
C	5.95456200	-1.74593400	1.17872300
C	6.56961900	-1.24739400	2.33357600
C	6.15222000	-1.66406000	3.59698300
H	4.79106200	-2.91784600	4.70709400
H	3.69393800	-3.82066600	2.66442200
H	4.42574400	-3.05733900	0.42494600

H	7.38547200	-0.53562600	2.23970100
H	6.64047700	-1.26931000	4.48372200
C	-4.01597300	2.83856700	-1.45849400
C	-3.03369500	2.76225800	-2.44651800
C	-1.73808700	2.34863300	-2.11872800
C	-1.38050100	2.02160400	-0.79991100
C	-2.39649700	2.07282200	0.16917800
C	-3.69294700	2.48208600	-0.14734600
H	-5.02311800	3.16298700	-1.70871600
H	-3.27333200	3.02310000	-3.47554300
H	-0.99452600	2.29481800	-2.91318000
H	-2.17769800	1.78169300	1.19313500
H	-4.45691200	2.50184500	0.62492000
C	2.07935100	3.10263900	-0.34964600
C	1.03269800	3.66840800	-1.02074800
C	0.17410700	4.84942100	-0.64193700
C	0.12139600	5.25868600	0.84677700
C	-0.29807100	4.13425500	1.75354200
C	0.51338500	3.25282800	2.34750800
C	2.02096100	3.19646000	2.28661700
C	2.70303100	3.58610100	0.95091600
H	2.68188600	2.38593100	-0.90739800
H	0.88905100	3.34812700	-2.05177700
H	-0.84186100	4.64093500	-0.99295100
H	0.52503100	5.71327100	-1.22805800
H	1.08288100	5.67315000	1.16023100
H	-0.60289900	6.07758200	0.93176700
H	-1.36976300	4.00529000	1.87935500
H	0.05039500	2.48352400	2.96524500
H	2.32665000	2.17761200	2.54028600
H	2.44999200	3.83141800	3.07686000
H	2.80852100	4.67378000	0.90069100
H	3.72452800	3.19158000	0.98693300

TS5c

SCF Energy (a.u.) = -2427.918802

Thermal correction to Gibbs free energy (a.u.) = 0.864917

Charge = 0, Multiplicity = 1

C	-8.97992200	-2.08092300	-0.88665700
C	-9.39292700	-3.30759300	-0.34653100
C	-10.69048600	-3.49262600	0.11490700
C	-11.63261300	-2.45034000	0.05453300
C	-11.21470200	-1.22435000	-0.48724600
C	-9.91387400	-1.04175400	-0.94829100
H	-8.68172800	-4.12889000	-0.28947500
H	-10.97625100	-4.45700800	0.52386500
H	-11.92353900	-0.40167700	-0.54290600
H	-9.61260100	-0.07678700	-1.34591200
C	-13.01707300	-2.58779400	0.52756600
C	-13.59090500	-3.67274500	1.06273100
H	-13.62224300	-1.68784000	0.41828200
H	-14.62906600	-3.65648100	1.37923400
H	-13.05920800	-4.60948200	1.20538900
C	-6.64667300	-1.43787300	-0.12630200
C	-7.54925800	-1.87407300	-1.31437300
H	-7.14049800	-2.79934600	-1.73744300
H	-7.50607100	-1.11107700	-2.09896200
H	-6.79529600	-2.18011900	0.66782500
C	-5.16552300	-1.42449900	-0.46555900
C	-4.23110300	-1.66263700	0.55157000
C	-4.68014800	-1.13239200	-1.74295900
C	-2.86505900	-1.58464400	0.30504300
H	-4.58580000	-1.90179400	1.55148900
C	-3.30932400	-1.04470300	-1.98662500
H	-5.36971600	-0.95541100	-2.56232100
C	-2.38031200	-1.24850300	-0.96639700
H	-2.16561100	-1.77585100	1.11583700
H	-2.95953000	-0.78343800	-2.98035400

C	-8.07035300	2.37205000	1.37373000
C	-8.37952200	1.19028800	2.04726900
C	-7.90140600	-0.03198900	1.57195800
C	-7.10779800	-0.09364900	0.42249300
C	-6.80187800	1.09805100	-0.24638600
C	-7.27951000	2.32110500	0.22309100
H	-8.44052900	3.32497800	1.74138700
H	-8.99614900	1.21681600	2.94148900
H	-8.16027100	-0.95220800	2.08891500
H	-6.16811800	1.06962100	-1.12688100
H	-7.02933800	3.23637400	-0.30737800
Ni	0.68029500	1.82085200	-0.30331800
C	-0.19238400	-0.08401600	-0.31475600
C	-0.89703500	-1.10733400	-1.21824800
H	-0.40167100	-2.07366800	-1.03676600
H	-0.72884100	-0.86595000	-2.27124800
H	-0.56059000	-0.16130700	0.70910300
C	1.28374900	-0.10725500	-0.35989300
C	2.02566100	-0.39628200	-1.54225600
C	2.01422600	0.33742500	0.77629700
C	3.39898000	-0.25601400	-1.56807800
H	1.50116600	-0.72621200	-2.43308900
C	3.41597300	0.45674800	0.72661500
H	1.50546500	0.44028300	1.73045700
C	4.12214000	0.18292200	-0.43467700
H	3.94210400	-0.48613500	-2.48244100
H	3.95444900	0.74822400	1.62387400
C	6.26591500	-1.14749400	-0.18795600
C	5.62812800	0.24034900	-0.46820000
H	5.97072400	0.59262300	-1.44891700
H	5.98655600	0.95678500	0.27953600
H	5.84119600	-1.84094500	-0.92574600
C	7.77769600	-1.17795400	-0.36082500
C	8.42248100	-2.42340100	-0.38302300

C	8.56227100	-0.02712300	-0.47478100
C	9.80382000	-2.52747600	-0.51948600
H	7.82977400	-3.32871000	-0.28041300
C	9.95224300	-0.10628800	-0.61015500
H	8.10136100	0.95445200	-0.46195100
C	10.55127800	-1.35766400	-0.63109300
H	10.28810300	-3.49715700	-0.53710900
H	10.54894100	0.79450800	-0.69775000
Br	12.49595300	-1.48440600	-0.82201400
C	4.96544400	-2.43821500	3.73534800
C	4.33615400	-2.92734000	2.59021300
C	4.77724000	-2.53108600	1.32685100
C	5.85057700	-1.64528000	1.18898100
C	6.47996600	-1.16461300	2.34357900
C	6.04038600	-1.55526900	3.60785800
H	4.62459800	-2.74503400	4.72012000
H	3.49980100	-3.61525700	2.67807900
H	4.27154000	-2.89641000	0.43696700
H	7.32409700	-0.48680000	2.24901200
H	6.54038200	-1.17438100	4.49415900
C	-3.65883000	2.50991300	-1.81822000
C	-2.62084600	2.23939800	-2.71648300
C	-1.40588900	1.73452900	-2.25734300
C	-1.17346900	1.53695700	-0.88151900
C	-2.24473800	1.76818800	-0.00148500
C	-3.46776500	2.25851200	-0.45872600
H	-4.60932800	2.89466200	-2.17799900
H	-2.76114300	2.41859300	-3.78008000
H	-0.61206700	1.52408200	-2.97105600
H	-2.12001800	1.56129600	1.05657200
H	-4.27779400	2.42457800	0.24529800
C	1.95199600	3.38421300	-0.34947600
C	0.75113900	3.75293100	-0.95876300
C	-0.30501200	4.73080900	-0.49342000

C	-0.34507300	5.08093100	1.01059100
C	-0.48749700	3.88266700	1.90737600
C	0.50908700	3.15862500	2.43048300
C	1.99576700	3.38384600	2.29308900
C	2.52968600	3.93903000	0.95039600
H	2.70672700	2.95527800	-1.01238400
H	0.68649500	3.56517600	-2.03096800
H	-1.28358900	4.33848700	-0.79411900
H	-0.17329900	5.67103200	-1.05192000
H	0.54249900	5.65823800	1.28156600
H	-1.20106700	5.74822500	1.16978800
H	-1.50736700	3.56463700	2.11106500
H	0.23265800	2.31593000	3.06532400
H	2.49236200	2.42811100	2.48550800
H	2.33880800	4.05345700	3.09744400
H	2.43527500	5.03028600	0.94377600
H	3.60805100	3.74121500	0.93933100

im10c

SCF Energy (a.u.) = -2427.968971

Thermal correction to Gibbs free energy (a.u.) = 0.866031

Charge = 0, Multiplicity = 1

C	-9.07434600	-1.59889600	-1.17479600
C	-9.64182800	-2.87825700	-1.08314900
C	-10.96524400	-3.05462000	-0.69825500
C	-11.77898800	-1.95045800	-0.38756000
C	-11.20692900	-0.67184000	-0.48214900
C	-9.88027700	-0.49838800	-0.86702600
H	-9.03197900	-3.74784800	-1.31876900
H	-11.37231600	-4.05958700	-0.64121400
H	-11.81436700	0.19823000	-0.24486000
H	-9.45775000	0.50132800	-0.91310600
C	-13.18342700	-2.07629600	0.02608000
C	-13.89234700	-3.20313800	0.16907800

H	-13.67871800	-1.12796200	0.23444100
H	-14.93077600	-3.17323700	0.48368700
H	-13.47494700	-4.18850400	-0.01896400
C	-6.70368800	-1.56394500	-0.27030900
C	-7.61703500	-1.42923300	-1.52057900
H	-7.31072800	-2.18294600	-2.25590500
H	-7.45922300	-0.44593900	-1.97644400
H	-6.96232400	-2.51827500	0.20554800
C	-5.22153200	-1.60274800	-0.60172200
C	-4.34115100	-2.21251700	0.30282000
C	-4.67850000	-0.99161900	-1.73555000
C	-2.96612100	-2.18592400	0.09531800
H	-4.74460200	-2.69671100	1.18911200
C	-3.29880700	-0.95775800	-1.93841500
H	-5.32754500	-0.51632800	-2.46379400
C	-2.42084200	-1.53937500	-1.02180300
H	-2.30294600	-2.65628700	0.81840400
H	-2.89749600	-0.43997200	-2.80531300
C	-7.70185000	1.60359600	2.51546300
C	-8.22738900	0.32290800	2.68759900
C	-7.88530200	-0.69890700	1.80056400
C	-7.01389900	-0.45966100	0.73324400
C	-6.48723900	0.82801400	0.57073200
C	-6.83047200	1.85226600	1.45230000
H	-7.96631000	2.40112400	3.20418400
H	-8.90724600	0.11749700	3.50991000
H	-8.31257200	-1.69018500	1.92602700
H	-5.78937600	1.02421200	-0.23753800
H	-6.41432300	2.84663400	1.31122900
Ni	0.43598300	2.43184400	-0.15566000
C	-0.39767200	-0.25171000	-0.22544500
C	-0.93076100	-1.37132700	-1.16405300
H	-0.40271600	-2.30293900	-0.92381500
H	-0.69017900	-1.12213400	-2.20244800

H	-0.64243000	-0.55494000	0.79966500
C	1.11757000	-0.10214800	-0.29113600
C	1.84721300	-0.19283200	-1.48891300
C	1.83959900	0.10139400	0.89557400
C	3.23417000	-0.06869700	-1.49601500
H	1.33062100	-0.36672000	-2.42714500
C	3.22930700	0.21873000	0.88702900
H	1.30298800	0.14313300	1.83806800
C	3.94789200	0.14293500	-0.30852600
H	3.77353900	-0.13961300	-2.43800800
H	3.76373200	0.34597300	1.82374700
C	6.08956900	-1.21172800	-0.23060900
C	5.45474500	0.20201900	-0.31676000
H	5.80581000	0.69027200	-1.23367000
H	5.80439600	0.80490700	0.52897300
H	5.67713000	-1.78975600	-1.06802600
C	7.60409900	-1.21608800	-0.38298000
C	8.25271500	-2.44637200	-0.56490200
C	8.38658900	-0.05959600	-0.32819400
C	9.63607300	-2.52934800	-0.69457900
H	7.66137900	-3.35786400	-0.59450900
C	9.77856200	-0.11818200	-0.45316600
H	7.92295000	0.91082000	-0.18878500
C	10.38160000	-1.35442100	-0.63552800
H	10.12345600	-3.48712600	-0.83680700
H	10.37366300	0.78682600	-0.40891600
Br	12.32891200	-1.45205700	-0.81410500
C	4.73882800	-3.06469800	3.44186000
C	4.13837900	-3.39455800	2.22663700
C	4.59548500	-2.81672000	1.04143500
C	5.65604000	-1.90567800	1.05262800
C	6.25739500	-1.58592700	2.27601400
C	5.80157700	-2.15818100	3.46282500
H	4.38504900	-3.51263900	4.36609700

H	3.31165000	-4.09895100	2.19944900
H	4.11168300	-3.05804300	0.09865300
H	7.09219000	-0.89040900	2.29532400
H	6.27908200	-1.90046900	4.40415700
C	-2.83894100	3.16572800	-1.28197200
C	-1.73137800	2.86267700	-2.04510500
C	-0.83848200	1.81367200	-1.67444600
C	-1.10951500	1.07738300	-0.47209200
C	-2.31260400	1.36113200	0.24313200
C	-3.14420500	2.39098700	-0.13306800
H	-3.50111400	3.97392200	-1.58058300
H	-1.53539300	3.41528600	-2.96093500
H	-0.17057900	1.41505600	-2.43290500
H	-2.57055700	0.73694000	1.09444800
H	-4.04091800	2.59920200	0.44260900
C	2.29431000	3.34224900	-0.43421000
C	1.36785300	3.98904600	-1.22997900
C	0.56932800	5.21300300	-0.83853300
C	0.12541800	5.22349400	0.64965400
C	-0.24718600	3.84805000	1.18148100
C	0.61384500	3.01749600	1.87999800
C	2.07533400	3.31305400	2.14087600
C	2.83425700	3.85074100	0.89472500
H	2.87084300	2.54599400	-0.90134400
H	1.30805400	3.70467300	-2.27857900
H	-0.32763600	5.23349400	-1.46750000
H	1.12455200	6.13831300	-1.05879100
H	0.91228100	5.66128300	1.27119600
H	-0.74144000	5.88747800	0.74540400
H	-1.31135700	3.63123400	1.22413200
H	0.17348300	2.21385400	2.46862900
H	2.55267100	2.38510200	2.46994800
H	2.19588600	4.02692600	2.97105500
H	2.82666300	4.94504100	0.89755100

H	3.88788500	3.55827800	0.97591100
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P2a

SCF Energy (a.u.) = -1944.863370

Thermal correction to Gibbs free energy (a.u.) = 0.692866

Charge = 0, Multiplicity = 1

C	-8.95187100	0.96972300	-0.86295500
C	-9.58423800	0.78224000	-2.10078400
C	-10.89047600	0.31523400	-2.18010200
C	-11.62092600	0.01533400	-1.01628100
C	-10.98426000	0.20609200	0.22034200
C	-9.67491800	0.67306700	0.29654800
H	-9.03945200	1.00767200	-3.01511300
H	-11.34951300	0.18479600	-3.15538100
H	-11.52662800	-0.02073800	1.13504300
H	-9.20007400	0.79313100	1.26621300
C	-13.00349200	-0.48207000	-1.03914900
C	-13.76594700	-0.71876100	-2.11404100
H	-13.43074700	-0.67170800	-0.05449400
H	-14.78067400	-1.08928000	-2.00802200
H	-13.41736200	-0.55520300	-3.13004200
C	-6.53298100	0.20376200	-0.93458700
C	-7.51020800	1.40465100	-0.79627300
H	-7.29214800	2.12170900	-1.59683800
H	-7.32321200	1.91226300	0.15605000
H	-6.81806000	-0.32834400	-1.85088900
C	-5.07845200	0.61752600	-1.07651000
C	-4.18282900	-0.25703400	-1.70696000
C	-4.56816500	1.80042000	-0.53379000
C	-2.82119100	0.02350900	-1.75879200
H	-4.56108700	-1.17949400	-2.14136200
C	-3.20156300	2.07621200	-0.57775100
H	-5.23119100	2.50917800	-0.04836000
C	-2.30509500	1.18629800	-1.17227200

H	-2.14447800	-0.67996500	-2.23937800
H	-2.82186000	2.97874600	-0.10670700
C	-7.18633200	-2.49156600	2.39818300
C	-7.78367200	-2.74020500	1.16233300
C	-7.55081300	-1.88123000	0.08737900
C	-6.71815900	-0.76604300	0.22708900
C	-6.11706100	-0.52778100	1.46990500
C	-6.35254300	-1.38089800	2.54755800
H	-7.36648600	-3.15751900	3.23745400
H	-8.43507300	-3.60023200	1.03357600
H	-8.03482300	-2.06641300	-0.86775200
H	-5.44776800	0.31875800	1.59039400
H	-5.88298700	-1.17854400	3.50690300
C	-0.21274200	0.50541400	0.05667000
C	-0.81685100	1.39925800	-1.06138800
H	-0.31495700	1.16534400	-2.00850400
H	-0.61241900	2.45117000	-0.83357600
H	-0.41915200	-0.53323700	-0.23374800
C	1.29605800	0.63712100	0.20869100
C	2.05427600	1.62555400	-0.42489200
C	1.96598500	-0.27195200	1.04107200
C	3.43660500	1.69900900	-0.23426400
H	1.57609000	2.35031400	-1.07510700
C	3.34120500	-0.20089800	1.22727800
H	1.39243000	-1.04099400	1.55239200
C	4.10158800	0.78974300	0.59087400
H	4.00461400	2.47829900	-0.73819800
H	3.83878700	-0.93045900	1.86015200
C	6.31272000	0.05269200	-0.40931300
C	5.60309200	0.83116200	0.73052900
H	5.95265500	1.87054400	0.71455900
H	5.89713100	0.40232500	1.69534600
H	5.94510500	0.47878600	-1.35189500
C	7.82723300	0.20471400	-0.40837300

C	8.54245300	-0.22810100	-1.53463200
C	8.54712400	0.73164600	0.66730100
C	9.93003400	-0.13696700	-1.59722700
H	8.00032400	-0.65483800	-2.37452000
C	9.94187700	0.83079700	0.62893100
H	8.03058600	1.07697100	1.55614100
C	10.61157900	0.39478800	-0.50533100
H	10.46915600	-0.47352600	-2.47541000
H	10.48791700	1.24169500	1.47045900
Br	12.56415600	0.52941800	-0.57467000
C	5.03038800	-4.08055300	-0.25016300
C	4.45224900	-3.20000100	-1.16469000
C	4.88587400	-1.87531200	-1.23008100
C	5.90098100	-1.41262200	-0.38714400
C	6.47884000	-2.30469900	0.52437400
C	6.04630800	-3.62821800	0.59516100
H	4.69488700	-5.11242100	-0.19717400
H	3.66054000	-3.54145700	-1.82578600
H	4.41869700	-1.18548600	-1.92776000
H	7.27848400	-1.96074000	1.17490000
H	6.50592400	-4.30847100	1.30693400
C	-2.40163200	1.28001700	3.71372500
C	-1.36678300	2.13237900	3.32138600
C	-0.63998800	1.86535700	2.16143700
C	-0.93945000	0.74844000	1.37266700
C	-1.97547100	-0.10056100	1.77569400
C	-2.70176500	0.15957900	2.93811700
H	-2.96558100	1.48625900	4.61922100
H	-1.12199800	3.00392300	3.92259700
H	0.17347200	2.52284100	1.86636600
H	-2.23276400	-0.95826000	1.16067000
H	-3.50136900	-0.51461100	3.23112500

im3d

SCF Energy (a.u.) = -2438.376267

Thermal correction to Gibbs free energy (a.u.) = 0.810526

Charge = 0, Multiplicity = 1

C	-3.05045200	-2.80847900	-2.91531300
C	-1.68293700	-2.91991200	-3.19689400
C	-0.88010100	-3.83220200	-2.52022900
C	-1.42609400	-4.64726900	-1.51495300
C	-2.81148800	-4.57942000	-1.27686700
C	-3.60856200	-3.68186800	-1.97140700
H	-1.23759000	-2.25725400	-3.93332000
H	0.17998300	-3.88569300	-2.74432300
H	-3.25113700	-5.21790400	-0.51487900
H	-4.67196500	-3.62829900	-1.75385200
C	-0.62496200	-5.51669000	-0.65306000
C	0.74940200	-5.63541300	-0.55320800
H	-1.22043100	-6.22616000	-0.06852700
H	1.18490100	-6.47913000	-0.02423300
H	1.42168100	-5.07283400	-1.19012600
C	-4.24119000	-0.65124500	-2.43317300
C	-3.88883400	-1.70855600	-3.51347000
H	-3.34561100	-1.22862800	-4.33459800
H	-4.81829500	-2.11783500	-3.92834500
H	-4.80110200	-1.18222700	-1.65200900
C	-2.98384100	-0.10361600	-1.77462100
C	-2.58164600	-0.54857100	-0.51113700
C	-2.20725200	0.86800700	-2.41194700
C	-1.46334600	-0.00856000	0.11983200
H	-3.15857900	-1.31600000	-0.00222400
C	-1.09214000	1.41038700	-1.77690800
H	-2.50777200	1.23949500	-3.38816200
C	-0.71063700	1.00253300	-0.49278700
H	-1.20125100	-0.36410900	1.10940300
H	-0.52697800	2.19729500	-2.27136500
C	-6.77877500	2.62366700	-3.72327900

C	-6.36951000	1.67049500	-4.65239100
C	-5.55284700	0.60536000	-4.25751400
C	-5.13484200	0.47966800	-2.93009600
C	-5.55017600	1.45059600	-2.00384800
C	-6.36472300	2.50937500	-2.39228700
H	-7.41279400	3.45085000	-4.03007500
H	-6.68201600	1.74983800	-5.69020300
H	-5.24723400	-0.12448100	-5.00008700
H	-5.21525100	1.38195200	-0.97227800
H	-6.67013100	3.24502900	-1.65416100
C	0.10642300	2.31023600	1.61186600
C	0.42956600	1.70890600	0.20327700
H	1.29908800	1.05598600	0.30151100
H	0.75961400	2.52980800	-0.44010100
C	-1.36217100	2.71339900	1.69145200
C	-1.82937100	3.73781800	0.85822200
C	-2.28984500	2.02384300	2.47674000
C	-3.18515300	4.04756800	0.77282800
H	-1.12463900	4.28626700	0.23823400
C	-3.65387100	2.31757000	2.41270900
H	-1.95089700	1.23130900	3.13525200
C	-4.07955700	3.31810300	1.54926400
H	-3.53594700	4.83063100	0.11045700
H	-4.36550300	1.76435400	3.01498800
Br	-5.99798100	3.70927600	1.41094700
C	1.52095400	0.05259100	5.03694400
C	1.39728000	-0.58472000	3.80407900
C	0.92539600	0.11579400	2.69056500
C	0.57049600	1.46418600	2.78922500
C	0.68751100	2.08997200	4.04000500
C	1.15803600	1.39791100	5.15316900
H	1.89105600	-0.49188700	5.90114700
H	1.65890300	-1.63160300	3.69404700
H	0.86054000	-0.40895300	1.74566600

H	0.41103100	3.13781000	4.13292400
H	1.24541500	1.90717500	6.10927300
H	0.69672400	3.23348000	1.66844900
C	6.69048400	0.30728900	-1.07405300
C	7.02734100	0.21979900	-2.43255800
C	7.86662300	1.15263400	-3.02945400
C	8.40474400	2.21788400	-2.28577800
C	8.06460200	2.30122000	-0.92609200
C	7.22341300	1.36533800	-0.33060900
H	6.62339700	-0.59600000	-3.02838200
H	8.10902500	1.05154800	-4.08298400
H	8.46610800	3.11679600	-0.32954500
H	6.96343000	1.46431100	0.71937200
C	9.29626600	3.23357800	-2.86292900
C	9.73120900	3.31141800	-4.12683400
H	9.62439200	3.99807300	-2.15875300
H	10.39151500	4.11337000	-4.44153900
H	9.45309400	2.58996300	-4.89017500
C	4.24893200	-0.20703400	-0.64020700
C	5.72031500	-0.67027400	-0.46043100
H	5.83337900	-1.65868600	-0.92165000
H	5.93610900	-0.78329200	0.60752700
H	4.11055600	-0.01409200	-1.71122500
C	3.22554400	-1.25847700	-0.23716900
C	1.96092700	-1.24074500	-0.83846300
C	3.46775700	-2.21469800	0.75629200
C	0.96258200	-2.14652700	-0.46938500
H	1.73457900	-0.49099000	-1.59271000
C	2.48165100	-3.13285600	1.13312400
H	4.43198800	-2.25528900	1.25359500
C	1.23690300	-3.10533100	0.50195200
H	-0.01547900	-2.07725900	-0.92760800
H	2.69489400	-3.85806800	1.91302600
Br	-0.80262000	-3.46453100	2.87136700

C	3.62385600	3.55043600	1.42487000
C	3.73852400	3.52311600	0.03358800
C	3.93372700	2.31000000	-0.62798900
C	4.01154100	1.11016400	0.08646700
C	3.90027200	1.14955000	1.48122300
C	3.70896400	2.35857100	2.14797200
H	3.46902800	4.49308300	1.94254200
H	3.67985500	4.44568000	-0.53756000
H	4.03549200	2.29229400	-1.70984800
H	3.92633500	0.22649800	2.05118800
H	3.59660900	2.36223600	3.22737300
Ni	0.01040900	-4.41263100	0.97921200

TS2d

SCF Energy (a.u.) = -2438.367385

Thermal correction to Gibbs free energy (a.u.) = 0.814150

Charge = 0, Multiplicity = 1

C	-4.00059600	-3.12216800	-2.15951700
C	-2.72392100	-3.16172100	-2.73007000
C	-1.70270800	-3.89941000	-2.14430600
C	-1.92422700	-4.61105300	-0.95304900
C	-3.23561800	-4.66308000	-0.44773900
C	-4.25536600	-3.93722800	-1.04752900
H	-2.51282400	-2.55318300	-3.60470300
H	-0.71655900	-3.88196500	-2.59624200
H	-3.42726600	-5.21323100	0.46847200
H	-5.24796000	-3.94251900	-0.60405000
C	-0.83153100	-5.18300300	-0.15187900
C	0.54618900	-5.14365900	-0.53461400
H	-1.12544200	-5.89880600	0.61356700
H	1.22290400	-5.83836700	-0.04549900
H	0.79953500	-4.95149900	-1.57083600
C	-5.00049100	-0.90829000	-1.55997200
C	-4.99982400	-2.08118500	-2.58721200

H	-4.74339800	-1.69519800	-3.58002900
H	-6.00982300	-2.50402600	-2.64461500
H	-5.35025200	-1.34006500	-0.61225500
C	-3.58559200	-0.40222200	-1.30799800
C	-2.83072500	-0.89810300	-0.23905700
C	-2.99376900	0.54625800	-2.14754000
C	-1.53793200	-0.44102700	0.00368900
H	-3.24903800	-1.65055900	0.42239600
C	-1.70608000	1.01580300	-1.89312300
H	-3.56156700	0.95495000	-2.97883500
C	-0.95956700	0.54858600	-0.80440000
H	-1.01148200	-0.82605400	0.86836100
H	-1.28673900	1.79172200	-2.52928500
C	-7.69273000	2.37652200	-2.46370400
C	-7.66821100	1.26131100	-3.29742000
C	-6.80447900	0.19540900	-3.02517000
C	-5.95429700	0.22707800	-1.91586700
C	-5.98789400	1.35963500	-1.08544000
C	-6.84555700	2.42245700	-1.35238400
H	-8.36074900	3.20630800	-2.67710900
H	-8.31856300	1.21477800	-4.16687100
H	-6.80338700	-0.66041200	-3.69180100
H	-5.31436200	1.41322500	-0.23460600
H	-6.84181000	3.28993900	-0.69950500
C	0.37135100	1.97602600	0.89000200
C	0.35946200	1.20570400	-0.46625600
H	1.18756600	0.49452800	-0.47060400
H	0.58856500	1.93749400	-1.24841600
C	-0.89706500	2.80860600	0.99398200
C	-0.95643100	4.05496900	0.36301400
C	-2.05929000	2.31410000	1.59920600
C	-2.14204800	4.79090500	0.30990200
H	-0.06314100	4.45674000	-0.10982500
C	-3.25534700	3.02945700	1.55969000

H	-2.03543700	1.35378000	2.10088200
C	-3.27738300	4.25695800	0.90681000
H	-2.17697100	5.75405200	-0.18635900
H	-4.14995900	2.63333400	2.02680500
Br	-4.95812500	5.26544000	0.83245000
C	1.36561400	-0.26823400	4.47763400
C	1.46554000	-0.88364300	3.23156700
C	1.12249000	-0.18793300	2.07097600
C	0.65997100	1.13106300	2.12725600
C	0.56459000	1.73777200	3.38890500
C	0.91355900	1.05164900	4.55068500
H	1.62779200	-0.81077200	5.38126200
H	1.80492800	-1.91197400	3.15281100
H	1.23463600	-0.69171400	1.12011800
H	0.21203200	2.76310200	3.45726400
H	0.82793000	1.54675500	5.51422500
H	1.21510000	2.67388800	0.81316900
C	7.17205900	-0.00722500	-0.83822300
C	7.72032600	-0.09137600	-2.12603200
C	8.63941300	0.84623000	-2.58120600
C	9.04751300	1.91260600	-1.76063000
C	8.49529600	1.99230600	-0.47211600
C	7.57486700	1.05175100	-0.01813100
H	7.42077400	-0.90834500	-2.77914000
H	9.04651300	0.74765500	-3.58285400
H	8.79354600	2.80835600	0.18151500
H	7.15201900	1.14803100	0.97761900
C	10.01499700	2.93306200	-2.18782200
C	10.64545200	3.01325600	-3.36619200
H	10.22299600	3.69845800	-1.44033700
H	11.34386300	3.81826100	-3.57183900
H	10.49593300	2.29090800	-4.16392700
C	4.69656800	-0.52163100	-0.77711600
C	6.12247400	-0.99230800	-0.38731700

H	6.30390600	-1.97374700	-0.84172600
H	6.17841500	-1.12181400	0.69901700
H	4.71827300	-0.31090200	-1.85346500
C	3.61672200	-1.56645700	-0.54779600
C	2.44400200	-1.49615100	-1.31736100
C	3.71366000	-2.57188600	0.42030100
C	1.38419500	-2.37260800	-1.11219400
H	2.35802300	-0.72591200	-2.07941200
C	2.66916100	-3.47956400	0.62293800
H	4.61304500	-2.66747200	1.01993200
C	1.47696300	-3.35270400	-0.10680600
H	0.47650800	-2.26730100	-1.69610200
H	2.77784100	-4.26821300	1.36270600
Br	-1.52379200	-3.38538800	2.64847400
C	3.81351800	3.20408100	1.25015300
C	4.01873400	3.18814100	-0.13080500
C	4.28283200	1.98350100	-0.78476300
C	4.34713300	0.78291200	-0.07077400
C	4.13284200	0.80945200	1.31206500
C	3.86911000	2.00878200	1.97079600
H	3.60528300	4.13975500	1.76139500
H	3.97950100	4.11300500	-0.69964700
H	4.46192400	1.97652100	-1.85670600
H	4.14693100	-0.11584000	1.87908000
H	3.67839900	2.00253000	3.03920900
Ni	-0.06958600	-3.71624500	0.90086500

Im4d

SCF Energy (a.u.) = -2438.396920

Thermal correction to Gibbs free energy (a.u.) = 0.815135

Charge = 0, Multiplicity = 1

C	-4.09258300	-3.39133700	-1.21048400
C	-3.14385300	-3.41427500	-2.23628700
C	-1.89649400	-3.99807700	-2.05051100

C	-1.53364300	-4.55403400	-0.81052000
C	-2.52344100	-4.60296100	0.19273600
C	-3.77998700	-4.05095500	-0.01216600
H	-3.37289800	-2.93204800	-3.18273900
H	-1.19302100	-3.99268800	-2.87644900
H	-2.27080200	-5.03504900	1.15667100
H	-4.50935600	-4.07250500	0.79377800
C	-0.16832500	-5.01536900	-0.50488900
C	0.83204200	-5.27513800	-1.63084300
H	-0.12734100	-5.73645000	0.31196400
H	1.40744200	-6.18362200	-1.43334000
H	0.35885600	-5.38931600	-2.61258900
C	-5.26493800	-1.28700000	-0.40157200
C	-5.32624000	-2.53675400	-1.34420600
H	-5.41965900	-2.19536900	-2.38070500
H	-6.23091100	-3.11075600	-1.11062800
H	-5.52873800	-1.65050500	0.60146800
C	-3.84524800	-0.75503700	-0.29700100
C	-3.07788700	-1.05165000	0.83127800
C	-3.23912800	-0.03429500	-1.33212300
C	-1.75179800	-0.64309300	0.93853900
H	-3.51865900	-1.62525600	1.64143400
C	-1.91736000	0.39248200	-1.21904500
H	-3.81346100	0.21783600	-2.21951100
C	-1.15175700	0.10769200	-0.07885200
H	-1.19810000	-0.90246100	1.82992900
H	-1.48035100	0.99128800	-2.01464500
C	-8.18066600	1.79171500	-1.36706100
C	-8.39480500	0.47608500	-1.77543700
C	-7.45572200	-0.51490600	-1.48141300
C	-6.28559800	-0.21289600	-0.77295700
C	-6.08741400	1.11463300	-0.36336100
C	-7.02038800	2.10717600	-0.65750100
H	-8.90722700	2.56455500	-1.60179200

H	-9.29286000	0.21562500	-2.32926900
H	-7.64717100	-1.53071200	-1.81120700
H	-5.18205400	1.37463200	0.17428000
H	-6.83150900	3.12926200	-0.34267200
C	0.25406100	1.97574600	1.01367400
C	0.22069200	0.71974500	0.08299700
H	0.95759200	-0.00781900	0.43405000
H	0.56857000	1.05751700	-0.89981200
C	-0.91491100	2.88256300	0.66364500
C	-0.79392600	3.81003900	-0.37463700
C	-2.16266500	2.73728300	1.28392500
C	-1.88485700	4.56857400	-0.80644800
H	0.16748000	3.93926800	-0.86663200
C	-3.26506200	3.48431800	0.87350800
H	-2.27733100	2.02161900	2.09011100
C	-3.10806200	4.38619000	-0.17396000
H	-1.77969200	5.28311500	-1.61491500
H	-4.22628800	3.36213200	1.35973800
Br	-4.65547600	5.43184200	-0.77009800
C	0.72383900	1.34589700	5.28835600
C	0.79060300	0.25601600	4.42299700
C	0.62406100	0.43526700	3.04791100
C	0.36680900	1.69855600	2.50982900
C	0.30240000	2.78801300	3.39316700
C	0.48309200	2.61911800	4.76415500
H	0.85643500	1.20905000	6.35798100
H	0.98050400	-0.74388300	4.80339000
H	0.72598600	-0.43300900	2.41143300
H	0.10777700	3.78084600	2.99664800
H	0.43110500	3.48102600	5.42407800
H	1.17546200	2.50652300	0.74155100
C	6.61930600	0.48134500	-1.49705100
C	6.73028200	1.18904100	-2.70264200
C	7.38857200	2.41121400	-2.76248500

C	7.96578800	2.97629500	-1.61113200
C	7.85403400	2.26210400	-0.40758100
C	7.19236400	1.03853400	-0.35005700
H	6.29257400	0.77178400	-3.60714300
H	7.45829900	2.93068100	-3.71325400
H	8.28996000	2.67839800	0.49719400
H	7.10311500	0.51723300	0.59883500
C	8.67159100	4.26537400	-1.61436500
C	8.87698500	5.07702400	-2.65908700
H	9.05994000	4.56959900	-0.64258400
H	9.41511200	6.01228400	-2.54176400
H	8.52418000	4.84782600	-3.66084500
C	4.31266100	-0.54033600	-1.24675600
C	5.83343000	-0.80340700	-1.43261900
H	5.97888100	-1.38196100	-2.35331400
H	6.19655200	-1.41514400	-0.59962900
H	4.01441300	0.15342100	-2.04270000
C	3.45879300	-1.78745600	-1.39839800
C	2.11782000	-1.64853000	-1.74362100
C	3.95870200	-3.08744800	-1.17003600
C	1.26034700	-2.76156900	-1.83583000
H	1.71708800	-0.66025800	-1.94305500
C	3.13501100	-4.19753600	-1.25777600
H	5.00219700	-3.22702900	-0.91076300
C	1.76538200	-4.06758600	-1.58917900
H	0.25022900	-2.61290000	-2.19905600
H	3.53644700	-5.18899600	-1.06775400
Br	0.43559400	-3.42120900	2.44367000
C	3.72097100	1.47770300	2.54050700
C	3.81170600	2.20977300	1.35720600
C	3.97303900	1.55185000	0.13607200
C	4.04989200	0.15637500	0.08191500
C	3.96056700	-0.57118900	1.27610300
C	3.79912300	0.08451500	2.49532600

H	3.55752300	1.98247500	3.48726600
H	3.75176300	3.29439700	1.38124000
H	4.06066400	2.12621200	-0.78223200
H	4.00022100	-1.65674200	1.25455100
H	3.70420200	-0.49390300	3.40865500
Ni	0.79033900	-3.48803300	0.17664400

im5d

SCF Energy (a.u.) = -2579.441448

Thermal correction to Gibbs free energy (a.u.) = 0.883168

Charge = 0, Multiplicity = 1

C	-4.13295100	-3.39995900	-1.20395500
C	-3.11074100	-3.38182000	-2.15659800
C	-1.86285500	-3.93098500	-1.88777500
C	-1.56869500	-4.49274900	-0.63299600
C	-2.63351700	-4.60340400	0.28232700
C	-3.88916200	-4.07773600	-0.00137200
H	-3.28176700	-2.88758700	-3.10919500
H	-1.10223000	-3.88813300	-2.66003500
H	-2.45311200	-5.07759800	1.24310500
H	-4.67618300	-4.14255000	0.74679200
C	-0.20378500	-4.89992500	-0.23557400
C	0.81471600	-5.28424100	-1.31662000
H	-0.20830700	-5.57829000	0.62196700
H	1.33758000	-6.20643000	-1.04604600
H	0.35556100	-5.44232000	-2.29986200
C	-5.32836000	-1.26596400	-0.51881400
C	-5.36475500	-2.55584000	-1.40996400
H	-5.42595400	-2.25590300	-2.46179800
H	-6.27729600	-3.11858800	-1.17950400
H	-5.61153300	-1.59139300	0.49229000
C	-3.90911400	-0.73413700	-0.40786600
C	-3.13799000	-1.07243800	0.70633600
C	-3.29799800	-0.00074100	-1.43053900

C	-1.79989400	-0.70912900	0.80414500
H	-3.58666400	-1.65288100	1.50673300
C	-1.96496100	0.39316300	-1.32050100
H	-3.87420000	0.28245400	-2.30715300
C	-1.19369200	0.05294800	-0.20068600
H	-1.23144000	-1.02691800	1.66547300
H	-1.52228200	1.00248900	-2.10493900
C	-8.21823600	1.77915300	-1.64948200
C	-8.39836000	0.46088000	-2.06499100
C	-7.46734900	-0.52118500	-1.71839800
C	-6.33990200	-0.20705400	-0.94937900
C	-6.17561000	1.12379800	-0.53384700
C	-7.10002600	2.10714000	-0.87991800
H	-8.93828300	2.54474300	-1.92478900
H	-9.26314300	0.19102500	-2.66541200
H	-7.63131300	-1.53949500	-2.05492300
H	-5.30135600	1.39332500	0.04953900
H	-6.93659200	3.13123500	-0.55735500
C	0.27258000	1.83616100	0.94864300
C	0.19691800	0.61936000	-0.03087200
H	0.91215600	-0.14198300	0.29169500
H	0.54868000	0.98135600	-1.00377200
C	-0.89156900	2.77147000	0.66306000
C	-0.78609000	3.73320500	-0.34523600
C	-2.12638300	2.61400300	1.30576800
C	-1.88139700	4.51130900	-0.72875500
H	0.16501800	3.87201000	-0.85431600
C	-3.23337600	3.37787000	0.94194100
H	-2.22879800	1.87161900	2.08892200
C	-3.09279400	4.31240200	-0.07878600
H	-1.78914800	5.25128100	-1.51563100
H	-4.18603200	3.24204100	1.44133600
Br	-4.64911200	5.37937700	-0.61231000
C	0.83269200	1.04498800	5.18622400

C	0.83922200	-0.01670000	4.28415900
C	0.64145900	0.20778100	2.91889900
C	0.41484300	1.49735400	2.43002000
C	0.40733800	2.55852400	3.34978100
C	0.61758400	2.34116600	4.70960100
H	0.99042300	0.86923600	6.24681700
H	1.00707500	-1.03337800	4.62901300
H	0.68213300	-0.65218600	2.26394400
H	0.23457900	3.56922200	2.98967700
H	0.60892600	3.18257400	5.39742700
H	1.19582600	2.36499100	0.67878300
C	6.86487400	0.21866100	-1.33704100
C	7.10508800	0.82270700	-2.57947000
C	7.81393700	2.01394500	-2.67649100
C	8.31319000	2.65135700	-1.52668800
C	8.07089700	2.04144700	-0.28545600
C	7.35958500	0.84855000	-0.19088900
H	6.72937800	0.34800900	-3.48349200
H	7.98413800	2.45221100	-3.65509600
H	8.44423600	2.51562200	0.61887400
H	7.16968000	0.40922000	0.78428700
C	9.06767900	3.91185600	-1.56836200
C	9.39634400	4.62744000	-2.65113100
H	9.38148300	4.28225300	-0.59258300
H	9.95922700	5.55098800	-2.55996100
H	9.12375300	4.32809600	-3.65940000
C	4.51195900	-0.70420000	-1.17300100
C	6.02823300	-1.03205000	-1.24190400
H	6.20960500	-1.67459700	-2.11230200
H	6.31418200	-1.60039800	-0.34994800
H	4.28896500	-0.06521400	-2.03670000
C	3.61344900	-1.92623900	-1.27491600
C	2.28347000	-1.74555800	-1.63712500
C	4.05398000	-3.23498200	-0.98225300

C	1.37210400	-2.81984500	-1.66680700
H	1.93154200	-0.75164300	-1.89391300
C	3.17796000	-4.30765800	-1.01695500
H	5.09045100	-3.41009000	-0.71562000
C	1.81315100	-4.13078800	-1.34434500
H	0.37321000	-2.64259800	-2.04745600
H	3.53418600	-5.30700500	-0.78150100
C	3.76936600	1.61785800	2.40791200
C	3.87251300	2.24904400	1.16874300
C	4.08441200	1.49456200	0.01239000
C	4.19646000	0.10276000	0.07947700
C	4.08936200	-0.52319900	1.32851200
C	3.88077900	0.22797800	2.48338200
H	3.57426100	2.19583800	3.30528700
H	3.78859500	3.33017800	1.09856300
H	4.18611500	1.99135000	-0.94881800
H	4.15721400	-1.60585700	1.39641900
H	3.77675500	-0.27087000	3.44120300
Ni	0.81528100	-3.37509800	0.36589500
O	0.34001700	-2.98224300	2.01843300
C	-0.18458900	-3.74884500	3.06377100
C	-1.49469600	-3.15899100	3.58758100
H	0.54904600	-3.80100400	3.88772400
H	-0.36091400	-4.79065600	2.74500600
H	-1.88651400	-3.74890900	4.42639800
H	-1.33938200	-2.13030100	3.93090300
H	-2.24438400	-3.14299900	2.79020400

im6d

SCF Energy (a.u.) = -3183.171370

Thermal correction to Gibbs free energy (a.u.) = 1.115907

Charge = 0, Multiplicity = 1

C	-2.45829300	-4.00858200	-0.97259500
C	-1.49507100	-4.12520300	-1.97930500

C	-0.15419300	-4.36676000	-1.68013800
C	0.28412000	-4.48911700	-0.35101800
C	-0.68966900	-4.36111200	0.65912900
C	-2.02450200	-4.13565700	0.35642500
H	-1.80015200	-4.03076300	-3.01877600
H	0.55188800	-4.45533000	-2.49983500
H	-0.37089300	-4.41867100	1.69508000
H	-2.74212400	-4.04897200	1.16791900
C	1.69631700	-4.70713800	0.04290800
C	2.72493700	-5.17164700	-0.99667400
H	1.77534600	-5.23313800	0.99677000
H	3.33138900	-5.99403800	-0.60559400
H	2.27305800	-5.51417400	-1.93450400
C	-4.58280100	-2.61025600	-0.59055500
C	-3.91685200	-3.80190600	-1.31444100
H	-4.01719600	-3.66770900	-2.39779800
H	-4.47295800	-4.71458700	-1.06075600
H	-4.49880700	-2.80198700	0.48759100
C	-3.85752500	-1.30250600	-0.85951700
C	-3.14598200	-0.65862100	0.15330400
C	-3.93410100	-0.68258100	-2.11151100
C	-2.54574900	0.57810400	-0.06624900
H	-3.04294300	-1.13184200	1.12388200
C	-3.34354700	0.56025700	-2.32432800
H	-4.50189900	-1.15383900	-2.90965900
C	-2.64940800	1.22040400	-1.30328100
H	-2.00154300	1.04810500	0.74218500
H	-3.44252100	1.04029000	-3.29500800
C	-8.82193200	-2.06703600	-1.39690100
C	-8.16111600	-3.17469900	-1.92192800
C	-6.79796600	-3.36778900	-1.67459900
C	-6.07418700	-2.45837400	-0.89735200
C	-6.75384200	-1.34407900	-0.37770500
C	-8.10975700	-1.14784300	-0.62068000

H	-9.87936000	-1.91406100	-1.59389300
H	-8.70103800	-3.89395800	-2.53215300
H	-6.30791900	-4.23615600	-2.10129000
H	-6.20029800	-0.61015800	0.20126100
H	-8.60675300	-0.26975000	-0.21899400
C	-2.58928100	3.70996800	-0.57318300
C	-2.08339300	2.60059900	-1.54928800
H	-0.98884700	2.57841000	-1.55325800
H	-2.37839300	2.91052400	-2.55761400
C	-4.10367000	3.59803100	-0.45773200
C	-4.91291700	4.18001300	-1.43844700
C	-4.71994600	2.82291900	0.53312400
C	-6.29580100	3.98673000	-1.45610000
H	-4.45653700	4.78830400	-2.21592100
C	-6.09843100	2.61465300	0.53771800
H	-4.11745000	2.36794800	1.30978300
C	-6.86519900	3.19680700	-0.46530500
H	-6.90999200	4.44032000	-2.22556100
H	-6.56133100	2.00649500	1.30667300
Br	-8.80303900	2.89870800	-0.47662200
C	-0.49285700	4.13932600	3.21672700
C	0.05537600	3.35011600	2.20754300
C	-0.62307400	3.18628100	0.99773700
C	-1.86115500	3.79797400	0.76898600
C	-2.39723600	4.59392600	1.79380000
C	-1.72483000	4.76227500	3.00315400
H	0.02944500	4.26697600	4.16111100
H	0.99847100	2.83338100	2.35200200
H	-0.17101900	2.55878800	0.24120900
H	-3.35491500	5.08315900	1.64206000
H	-2.16547500	5.38168700	3.77983100
H	-2.38108300	4.66111600	-1.08456300
C	7.96648500	1.09583300	-1.15463100
C	8.30837900	1.60674300	-2.41510200

C	8.85559500	2.87638300	-2.55382900
C	9.08485900	3.68950500	-1.42940100
C	8.74359500	3.17193200	-0.16979900
C	8.19374700	1.90014900	-0.03405900
H	8.14039100	0.99642700	-3.29999100
H	9.11014000	3.23941100	-3.54487600
H	8.90863600	3.78168600	0.71510200
H	7.91936000	1.53282600	0.95082500
C	9.65872800	5.03964600	-1.51579500
C	10.04686000	5.68939500	-2.62020400
H	9.76836500	5.54537700	-0.55658400
H	10.45869800	6.69196200	-2.56220400
H	9.97287000	5.25674800	-3.61411300
C	5.76661800	-0.16263300	-1.25845100
C	7.29985900	-0.25027100	-1.02870100
H	7.72428500	-0.94897000	-1.76036900
H	7.48875900	-0.66442300	-0.03193500
H	5.62027200	0.31935900	-2.23355700
C	5.07587700	-1.51684900	-1.31112700
C	3.77447200	-1.57603300	-1.79954900
C	5.66507500	-2.70694700	-0.83452500
C	3.02296000	-2.76506200	-1.74705200
H	3.30469500	-0.68297700	-2.19379200
C	4.94492500	-3.89076800	-0.78186500
H	6.68917600	-2.70023500	-0.47773900
C	3.59653000	-3.94181000	-1.20383700
H	2.03766500	-2.78239300	-2.19820900
H	5.40704900	-4.79200500	-0.38791200
C	4.04261300	2.42728800	1.75800700
C	4.38835100	2.93782200	0.50545600
C	4.92347100	2.09524200	-0.47014400
C	5.11986600	0.73491800	-0.20950900
C	4.76541000	0.23194800	1.04802300
C	4.23017700	1.06972300	2.02484000

H	3.61672700	3.07984100	2.51483700
H	4.24030300	3.99139800	0.28570200
H	5.20684900	2.49873600	-1.43835400
H	4.88575100	-0.82553500	1.26138700
H	3.93821100	0.65539900	2.98391800
Ni	2.47874200	-2.99055100	0.37098500
O	2.07296100	-2.68747200	2.09003600
C	2.74155600	-3.38997600	3.10079800
C	4.22032500	-3.01702300	3.22380800
H	2.65593200	-4.48287400	2.95435800
H	2.24007700	-3.17398100	4.06168400
H	4.70384100	-3.55683800	4.04882800
H	4.75158700	-3.25543100	2.29396100
H	4.32345800	-1.94083000	3.40547500
C	0.92281800	0.42426900	-2.81951200
C	1.62183800	1.17353600	-1.86672400
C	1.52531700	0.84309300	-0.51435700
C	0.71093700	-0.21833800	-0.08508800
C	0.02705000	-0.96655000	-1.05754300
C	0.13519600	-0.65661700	-2.41254500
H	0.99114900	0.68323400	-3.87334900
H	2.24831800	2.00648500	-2.17488200
H	2.07736400	1.41844300	0.21963700
H	-0.61783100	-1.77544600	-0.74140600
H	-0.42053200	-1.23802000	-3.14264300
C	1.00377500	-0.03459800	3.74019600
C	-0.69219500	-1.73007400	3.13974000
C	-0.39637400	-0.56311300	4.09316400
H	1.76451000	-0.77363100	4.01826800
H	-1.72802800	-2.06901700	3.26334600
B	0.47089900	-0.49555500	1.43482000
O	1.15647400	0.25228100	2.35499800
O	-0.52922300	-1.36160400	1.77729000
H	1.20599100	0.89415900	4.28721600

H	-0.01885400	-2.56919900	3.34125900
C	-0.39069200	-1.07575900	5.53767100
H	0.34754500	-1.87480600	5.67568900
H	-0.15105300	-0.26740100	6.23876800
H	-1.37465600	-1.47267300	5.81412900
C	-1.45025000	0.54272800	3.92572100
H	-2.45164400	0.15493100	4.14831600
H	-1.25094400	1.38026700	4.60317000
H	-1.45850400	0.94515900	2.91056800

TS3d

SCF Energy (a.u.) = -3183.170200

Thermal correction to Gibbs free energy (a.u.) = 1.117795

Charge = 0, Multiplicity = 1

C	2.57226700	3.97449900	-0.75657200
C	1.61424300	4.10309900	-1.76768300
C	0.26570600	4.29698600	-1.47160500
C	-0.18779900	4.35442800	-0.14265600
C	0.77981800	4.21199500	0.87074900
C	2.12355400	4.03596300	0.57153400
H	1.93054400	4.05474300	-2.80685100
H	-0.43895600	4.38787900	-2.29250900
H	0.45752500	4.22916000	1.90753500
H	2.83781700	3.94176000	1.38555700
C	-1.61008600	4.51157200	0.23671400
C	-2.60028100	5.15228200	-0.74834000
H	-1.71463800	4.90009000	1.25242300
H	-3.11607000	6.00492900	-0.29527000
H	-2.11973900	5.50741800	-1.66572700
C	4.70268500	2.56839500	-0.45702100
C	4.04020000	3.81726600	-1.08535900
H	4.16473100	3.78039200	-2.17381200
H	4.58057900	4.70743900	-0.73546500
H	4.54747100	2.63848400	0.62790500

C	4.02166000	1.28726200	-0.91195000
C	3.07414900	0.66398100	-0.09820700
C	4.32869200	0.69875900	-2.14380600
C	2.46088500	-0.52091500	-0.49273900
H	2.78277900	1.11487100	0.84330500
C	3.72371700	-0.49594300	-2.52849800
H	5.07642200	1.15654600	-2.78573800
C	2.78761000	-1.13320100	-1.70547700
H	1.72613100	-0.97224000	0.15896000
H	4.00328900	-0.95738800	-3.47267700
C	8.99221800	2.20801200	-1.04163900
C	8.31698700	3.29468600	-1.59134100
C	6.93617500	3.43280500	-1.41318600
C	6.21069600	2.48873900	-0.68106600
C	6.90494400	1.39596200	-0.13634800
C	8.27766700	1.25361600	-0.31078100
H	10.06364400	2.09826800	-1.18429300
H	8.85952300	4.04027700	-2.16660700
H	6.43363600	4.28529900	-1.85730600
H	6.34891500	0.63673200	0.40715000
H	8.78656500	0.39118100	0.10914300
C	2.62749400	-3.64789500	-1.13056300
C	2.22533700	-2.48087800	-2.09242100
H	1.13584400	-2.43918600	-2.19329300
H	2.61187000	-2.74182500	-3.08352300
C	4.11608600	-3.53235000	-0.83182600
C	5.04549400	-4.06920900	-1.72721200
C	4.59580500	-2.78846500	0.25450600
C	6.41788400	-3.86237600	-1.56874200
H	4.69526200	-4.65136000	-2.57646400
C	5.95989700	-2.56743300	0.43427500
H	3.89629600	-2.36543800	0.96533300
C	6.85098300	-3.10511400	-0.48796400
H	7.12749400	-4.28069400	-2.27338400

H	6.31757100	-1.98356200	1.27482300
Br	8.77187100	-2.78871100	-0.25104900
C	0.14556900	-4.34109100	2.37741800
C	-0.31003100	-3.49828000	1.36610100
C	0.48762000	-3.24686900	0.24662600
C	1.75749900	-3.82113000	0.11644900
C	2.20093700	-4.66891000	1.14492300
C	1.40801700	-4.92756800	2.26115600
H	-0.47303200	-4.53810200	3.24899000
H	-1.27539800	-3.01170700	1.44846200
H	0.09860600	-2.58198600	-0.51377300
H	3.18114200	-5.12986800	1.06804600
H	1.77842100	-5.58821100	3.04063500
H	2.49082000	-4.56844100	-1.71640400
C	-8.22275900	-0.76410600	-0.97586800
C	-8.59855100	-1.26611500	-2.23037200
C	-9.20171500	-2.51137800	-2.35686400
C	-9.45563200	-3.30799900	-1.22578400
C	-9.08075100	-2.79914300	0.02770900
C	-8.47463400	-1.55181200	0.15109900
H	-8.41249900	-0.66840200	-3.12023000
H	-9.48125000	-2.86809600	-3.34344300
H	-9.26409800	-3.39636200	0.91753400
H	-8.17603900	-1.19130100	1.13145800
C	-10.08829000	-4.63237800	-1.29943200
C	-10.51231400	-5.27129600	-2.39692300
H	-10.21262500	-5.12705200	-0.33626800
H	-10.96687500	-6.25463100	-2.32961000
H	-10.42664900	-4.84844400	-3.39409800
C	-5.97322000	0.40018400	-1.12676200
C	-7.49662700	0.55188600	-0.86268900
H	-7.90550300	1.27207300	-1.58245200
H	-7.64686600	0.96840900	0.13931000
H	-5.86698600	-0.10013200	-2.09738400

C	-5.23179500	1.72399700	-1.20744900
C	-3.99042100	1.75707400	-1.83543600
C	-5.69879800	2.90196800	-0.58545800
C	-3.15534600	2.88949300	-1.75217800
H	-3.62135100	0.87688400	-2.34801800
C	-4.89636300	4.02779200	-0.49727700
H	-6.68379800	2.92130400	-0.13212400
C	-3.58707400	4.03073000	-1.03099000
H	-2.21676000	2.89667800	-2.29608000
H	-5.25498400	4.91383700	0.01973000
C	-4.23158700	-2.20048300	1.87653100
C	-4.68784300	-2.72615400	0.66603800
C	-5.23022200	-1.88195700	-0.30446500
C	-5.33105100	-0.50468800	-0.07764400
C	-4.86962600	0.01093900	1.13968400
C	-4.31875100	-0.82667400	2.10778200
H	-3.79137500	-2.85299700	2.62509000
H	-4.61557200	-3.79266200	0.47197300
H	-5.59160300	-2.29643900	-1.24148200
H	-4.90434500	1.07960800	1.32398800
H	-3.92216100	-0.39861900	3.02166700
Ni	-2.43959500	2.77586100	0.30421900
O	-2.00651100	2.09183500	1.91304900
C	-2.19742300	2.76430800	3.12625000
C	-3.62786400	3.26763700	3.31941600
H	-1.49527300	3.61290900	3.22169100
H	-1.95234600	2.07000600	3.94458300
H	-3.74603400	3.76983300	4.28841700
H	-3.89731800	3.97432700	2.52571500
H	-4.33210500	2.42907200	3.27425200
C	-1.19383200	-0.24201900	-2.72417700
C	-1.92616600	-0.97630700	-1.78453400
C	-1.77406800	-0.71528900	-0.42226800
C	-0.87950400	0.26577200	0.03714000

C	-0.17211100	1.00707900	-0.92425700
C	-0.32618100	0.76289200	-2.28962400
H	-1.29880900	-0.45343600	-3.78576200
H	-2.61412200	-1.75277300	-2.10927000
H	-2.34078900	-1.29130900	0.29762100
H	0.53982600	1.75027300	-0.59463200
H	0.25911400	1.33344500	-3.00553500
C	-0.60886600	-0.61153200	3.77257400
C	1.01727000	1.17467300	3.24070300
C	0.86079900	-0.18472800	3.93837600
H	-1.24709700	0.00172900	4.42494000
H	2.06929700	1.48603900	3.25030700
B	-0.54525400	0.42392800	1.56998200
O	-1.08177900	-0.50694800	2.43841900
O	0.60366000	1.12668600	1.88701300
H	-0.72981800	-1.65818200	4.07759300
H	0.43777100	1.94191900	3.77300300
C	1.17853600	-0.03364900	5.43018800
H	0.54290600	0.72511400	5.90280800
H	1.02462000	-0.98123300	5.96003400
H	2.22412700	0.26153000	5.57774200
C	1.80072900	-1.21993000	3.30071700
H	2.84037600	-0.87255400	3.34363700
H	1.73806100	-2.17882800	3.82514500
H	1.54689400	-1.40728200	2.25657400

im7d

SCF Energy (a.u.) = -3183.171602

Thermal correction to Gibbs free energy (a.u.) = 1.119602

Charge = 0, Multiplicity = 1

C	2.68459900	3.96683900	-0.76811200
C	1.73381900	4.03786900	-1.79309900
C	0.38162100	4.22209700	-1.51505500
C	-0.08200500	4.32489000	-0.19072900

C	0.87905600	4.24603900	0.83555800
C	2.22751400	4.08375500	0.55259800
H	2.05946300	3.94400900	-2.82590600
H	-0.32133400	4.25759600	-2.34178200
H	0.55179200	4.30376300	1.86872100
H	2.93809200	4.03488300	1.37359800
C	-1.51062900	4.44671400	0.16434300
C	-2.49656800	5.09550200	-0.81530800
H	-1.65090000	4.79377400	1.19051400
H	-2.96481700	5.98662000	-0.38444500
H	-2.01967800	5.39343100	-1.75374700
C	4.76974200	2.51471500	-0.43672200
C	4.15504900	3.78805200	-1.06847000
H	4.30518500	3.76047900	-2.15374400
H	4.70491800	4.66104900	-0.69184600
H	4.56335400	2.56670300	0.64060500
C	4.08782500	1.25451400	-0.94877800
C	3.03795900	0.68091000	-0.22850100
C	4.48827200	0.64175300	-2.14188800
C	2.41874100	-0.48227500	-0.67530400
H	2.66775900	1.14901000	0.67673100
C	3.87139000	-0.52861800	-2.57975900
H	5.31360400	1.06144700	-2.71033400
C	2.83339600	-1.11818200	-1.84810600
H	1.60884600	-0.89566800	-0.09244600
H	4.22189600	-1.00981300	-3.48984500
C	9.07464200	2.10000900	-0.82450300
C	8.43630400	3.18097800	-1.42697900
C	7.05074900	3.33744900	-1.31158000
C	6.28420700	2.41793400	-0.59036600
C	6.94144600	1.33051100	0.00790600
C	8.31858000	1.16987900	-0.10407600
H	10.14991200	1.97595100	-0.91798800
H	9.01167600	3.90759300	-1.99457800

H	6.57692000	4.18464600	-1.79593000
H	6.35336700	0.59042800	0.54414600
H	8.79914300	0.31212200	0.35661800
C	2.58437700	-3.63158100	-1.30584100
C	2.25428400	-2.44661200	-2.27440500
H	1.17101500	-2.37604300	-2.41834100
H	2.67671700	-2.70967800	-3.25028900
C	4.05560900	-3.54162100	-0.92417800
C	5.02728100	-4.08806300	-1.76688700
C	4.48075200	-2.80810700	0.19164700
C	6.39103400	-3.90079200	-1.52794100
H	4.71889900	-4.66217200	-2.63762300
C	5.83477200	-2.60629600	0.45083800
H	3.74627500	-2.37817200	0.86184000
C	6.77032300	-3.15327800	-0.42063800
H	7.13488600	-4.32657700	-2.19163300
H	6.15073500	-2.03029600	1.31325100
Br	8.67914100	-2.86534600	-0.07089400
C	-0.05197200	-4.29981000	2.09257600
C	-0.43883200	-3.41781600	1.08667300
C	0.40224000	-3.17932200	-0.00384900
C	1.65158000	-3.80193900	-0.10456100
C	2.02450100	-4.69099900	0.91724200
C	1.18591900	-4.94044300	2.00128200
H	-0.70383200	-4.48234800	2.94268400
H	-1.38263400	-2.88941900	1.15446100
H	0.06485200	-2.48315800	-0.76122500
H	2.98804900	-5.18904900	0.86180600
H	1.50308100	-5.63251200	2.77703200
H	2.46529200	-4.54371200	-1.90833500
C	-8.31326900	-0.63704800	-0.86709800
C	-8.71674500	-1.13726000	-2.11360400
C	-9.35747000	-2.36520000	-2.22388100
C	-9.62205900	-3.14555500	-1.08402500

C	-9.21829400	-2.63887400	0.16140900
C	-8.57488200	-1.40886800	0.26875300
H	-8.52322000	-0.55183600	-3.01001500
H	-9.65799900	-2.72092000	-3.20460500
H	-9.40911000	-3.22391200	1.05769900
H	-8.25566100	-1.04991800	1.24315700
C	-10.29429200	-4.45119100	-1.14056100
C	-10.75098200	-5.08409400	-2.22835000
H	-10.42075300	-4.93582100	-0.17261300
H	-11.23325900	-6.05319500	-2.14880300
H	-10.66577900	-4.67020300	-3.22931500
C	-6.02906100	0.45117100	-1.02559300
C	-7.54797200	0.65820000	-0.77186900
H	-7.92978500	1.37913000	-1.50550500
H	-7.69085300	1.09537500	0.22231300
H	-5.93558600	-0.07681100	-1.98227600
C	-5.24526400	1.74689500	-1.13828500
C	-4.05298000	1.75686700	-1.85496700
C	-5.62907900	2.92474900	-0.46038400
C	-3.17995100	2.86509000	-1.81268200
H	-3.74953400	0.87827500	-2.41175900
C	-4.78901400	4.02370200	-0.40655000
H	-6.58082800	2.96348200	0.05836600
C	-3.52646100	4.00280800	-1.04094400
H	-2.29226000	2.86730500	-2.43750900
H	-5.08336100	4.90999800	0.14923200
C	-4.34109000	-2.12669600	2.02783900
C	-4.78350600	-2.66143500	0.81655300
C	-5.31551700	-1.82487200	-0.16621100
C	-5.41724200	-0.44608900	0.04773500
C	-4.97721200	0.07793600	1.26953800
C	-4.43810700	-0.75213900	2.25093100
H	-3.90257600	-2.77140200	2.78365900
H	-4.70561400	-3.72881900	0.63017700

H	-5.66329700	-2.24580900	-1.10551500
H	-5.01864800	1.14835300	1.44374500
H	-4.05050400	-0.32162500	3.16770900
Ni	-2.24561100	2.65538200	0.15672000
O	-1.79581500	1.96994700	1.84059300
C	-1.92603600	2.64760100	3.08018100
C	-3.33627100	3.19075100	3.25831300
H	-1.18604600	3.45852700	3.14408100
H	-1.70069600	1.93388800	3.87779500
H	-3.42645700	3.73058400	4.20852100
H	-3.59739700	3.87537000	2.44387500
H	-4.06108400	2.37022600	3.25338400
C	-1.29809100	-0.37545600	-2.62728000
C	-2.07418800	-0.98088200	-1.63161800
C	-1.92531500	-0.59774200	-0.29780200
C	-0.98941300	0.37859300	0.09137800
C	-0.23530000	0.98422300	-0.93215700
C	-0.38367200	0.61870500	-2.27358300
H	-1.40227900	-0.68126700	-3.66574500
H	-2.79174800	-1.75519500	-1.89091300
H	-2.52438000	-1.07689400	0.46450700
H	0.51927000	1.70988700	-0.66387400
H	0.24359400	1.08452700	-3.02918400
C	-0.49711800	-0.54742300	3.75998000
C	1.15461900	1.18712600	3.14170800
C	1.00799700	-0.21561000	3.75239600
H	-0.97875300	0.03458900	4.56701100
H	2.21992700	1.44444500	3.05258600
B	-0.74288600	0.75402600	1.65313700
O	-1.14714600	-0.30996600	2.53188300
O	0.58621600	1.27253700	1.85727400
H	-0.63612700	-1.60885300	4.00955200
H	0.70388300	1.92853500	3.82526900
C	1.53658400	-0.20907800	5.19054900

H	1.02992600	0.54657200	5.80400100
H	1.38636300	-1.18553000	5.66711000
H	2.61189700	0.00632900	5.21035600
C	1.77972800	-1.24114000	2.91214500
H	2.82896400	-0.93948600	2.79975400
H	1.75501900	-2.23082600	3.38018600
H	1.34386500	-1.34033300	1.91913100

TS4d

SCF Energy (a.u.) = -3183.144771

Thermal correction to Gibbs free energy (a.u.) = 1.120241

Charge = 0, Multiplicity = 1

C	1.87943300	4.28203500	-1.16789300
C	0.63061200	4.04577700	-1.72743300
C	-0.55247900	4.32338800	-1.02414900
C	-0.51523600	4.87131900	0.28928500
C	0.78174900	5.07555500	0.85938500
C	1.92917500	4.80194900	0.14823300
H	0.56131300	3.62857600	-2.72777800
H	-1.50683300	4.15648400	-1.50987200
H	0.84531700	5.47971500	1.86651000
H	2.89653100	5.00307200	0.60256800
C	-1.70977400	4.95237600	1.11670200
C	-3.08816300	5.20044900	0.48540900
H	-1.54928200	5.47583000	2.06001800
H	-3.66779900	5.83808600	1.16387000
H	-2.98571400	5.76583800	-0.45061100
C	4.16574900	3.08104600	-1.30227400
C	3.16226400	4.08105400	-1.94107600
H	2.92723700	3.77660400	-2.96600800
H	3.66532600	5.05378100	-2.01361800
H	4.05124000	3.14959300	-0.21468000
C	3.92001600	1.62508500	-1.68280900
C	3.77315900	0.64064300	-0.70528800

C	3.94018100	1.21334000	-3.02332300
C	3.65469000	-0.71033300	-1.04370800
H	3.74329800	0.92558200	0.34327000
C	3.83340400	-0.13142100	-3.35874700
H	4.07258400	1.94818300	-3.81259100
C	3.69868000	-1.12563700	-2.37524700
H	3.52391800	-1.43220700	-0.25220900
H	3.86686700	-0.42258700	-4.40669800
C	8.33483500	3.92583900	-2.16575800
C	7.35409700	4.26155000	-3.09878300
C	6.00791000	4.01112000	-2.82572600
C	5.61979200	3.42197700	-1.61687800
C	6.61439900	3.08615900	-0.69006100
C	7.95921800	3.33558400	-0.95714900
H	9.38202800	4.12271400	-2.37697400
H	7.63440200	4.72149500	-4.04257700
H	5.25838200	4.28123100	-3.56373300
H	6.32753000	2.61673700	0.24792100
H	8.71365500	3.07009500	-0.22168500
C	3.54857800	-3.72193400	-1.80763900
C	3.63042500	-2.57079200	-2.84049600
H	2.78361300	-2.68428000	-3.53000500
H	4.52131300	-2.75430400	-3.45389600
C	4.74255200	-3.71017900	-0.84731000
C	6.03066200	-3.86716400	-1.37576900
C	4.61956200	-3.53661700	0.53537300
C	7.16509800	-3.82924800	-0.56655000
H	6.15877200	-4.02123100	-2.44411900
C	5.73994000	-3.49475800	1.36702500
H	3.63777700	-3.42693400	0.98011200
C	6.99992400	-3.63704200	0.80078800
H	8.15411000	-3.94920600	-0.99377600
H	5.62520000	-3.35168300	2.43553200
Br	8.58124900	-3.57356600	1.95474700

C	-0.32702900	-4.34569100	0.05177400
C	-0.13472700	-3.25169800	-0.78922900
C	1.11501200	-3.02502600	-1.37232100
C	2.18790500	-3.89072300	-1.13911400
C	1.97285000	-4.99973600	-0.30392800
C	0.73483900	-5.22195200	0.29483900
H	-1.29268500	-4.51450300	0.51978200
H	-0.94368900	-2.55531600	-0.98194100
H	1.24318000	-2.14385000	-1.98724900
H	2.79067100	-5.69077200	-0.11662200
H	0.59678700	-6.08303400	0.94318800
H	3.68017200	-4.62869200	-2.41734900
C	-8.30069600	-1.01545000	-0.03834000
C	-9.36384500	-0.73761800	-0.90978200
C	-10.17749100	-1.75070300	-1.40216200
C	-9.95729600	-3.09163800	-1.04085500
C	-8.89140500	-3.36510900	-0.16880700
C	-8.07800500	-2.34818900	0.32349900
H	-9.55385600	0.29254800	-1.20346000
H	-10.99367200	-1.49796200	-2.07218000
H	-8.69892900	-4.39437600	0.12438700
H	-7.25079500	-2.59125900	0.98394100
C	-10.78431400	-4.20370000	-1.52944600
C	-11.84049800	-4.13412200	-2.34947200
H	-10.47973600	-5.18533800	-1.16650800
H	-12.37763300	-5.02980500	-2.64521600
H	-12.21006100	-3.19595400	-2.75419600
C	-6.21539800	0.32255300	-0.56726000
C	-7.38556400	0.08869000	0.42822100
H	-7.94342500	1.02657700	0.53243200
H	-6.98025100	-0.15745900	1.41541500
H	-6.67219600	0.46310000	-1.55436000
C	-5.41792600	1.58278700	-0.26679000
C	-4.89517700	2.33486400	-1.32511000

C	-5.16690200	2.03012800	1.03626800
C	-4.15371700	3.49255200	-1.09368000
H	-5.07315700	2.00827200	-2.34684300
C	-4.41864300	3.18250500	1.26632000
H	-5.55909900	1.48282600	1.88764100
C	-3.89562100	3.93790300	0.20772200
H	-3.77876000	4.06383600	-1.93989700
H	-4.24044800	3.50284300	2.28641300
C	-3.80389900	-3.27110900	-0.83892100
C	-4.58563000	-2.86075700	-1.91868100
C	-5.34754200	-1.69505300	-1.82555200
C	-5.33880700	-0.91965200	-0.66113600
C	-4.55014600	-1.34093300	0.41727800
C	-3.78917000	-2.50573500	0.32908000
H	-3.20510000	-4.17408100	-0.91096400
H	-4.60699300	-3.44840900	-2.83222600
H	-5.96926600	-1.38762600	-2.66233400
H	-4.50454000	-0.74711500	1.32532500
H	-3.17405700	-2.80591900	1.17180500
Ni	-1.27824200	2.99278200	1.09405600
O	-1.67979700	2.15948800	2.89158000
C	-1.36935400	2.88951100	4.09826500
C	-2.55327600	3.75170300	4.48924500
H	-0.46896600	3.49053800	3.93631600
H	-1.14889600	2.15974300	4.88475600
H	-2.33226700	4.28739800	5.41960100
H	-2.77128900	4.48854900	3.71190600
H	-3.44388400	3.13478700	4.64634100
C	-0.67539300	-0.06526300	-2.18235200
C	-1.88934100	-0.02031900	-1.49196900
C	-1.95213600	0.62383100	-0.25477600
C	-0.82430400	1.23530300	0.32674600
C	0.39218200	1.12238800	-0.36575200
C	0.46974300	0.49769300	-1.61292200

H	-0.61829500	-0.54695900	-3.15619300
H	-2.78245300	-0.47277500	-1.91308600
H	-2.90346200	0.67346100	0.25956900
H	1.28616600	1.58536600	0.04324900
H	1.41225400	0.46946300	-2.14698300
C	-0.83621100	-1.39534800	2.35576400
C	0.83853000	-0.14934200	3.75311600
C	0.62040200	-1.42299800	2.92559100
H	-1.41688200	-2.22959400	2.76237500
H	1.89896800	-0.03799200	4.00139400
B	-0.88450200	0.98066400	2.62711200
O	-1.57215800	-0.21354200	2.67968300
O	0.44359400	1.02257300	3.04132700
H	-0.81742500	-1.49676500	1.26642000
H	0.27531000	-0.21245800	4.69634800
C	0.81058900	-2.65288000	3.82521400
H	0.08827400	-2.66198700	4.65052300
H	0.67694900	-3.57257800	3.24379200
H	1.81935100	-2.67626900	4.25609500
C	1.64463400	-1.46373000	1.78468200
H	2.66605100	-1.44898700	2.18765700
H	1.52344200	-2.37143100	1.19024900
H	1.52423300	-0.61012000	1.11528400

im8d

SCF Energy (a.u.) = -3183.162135

Thermal correction to Gibbs free energy (a.u.) = 1.118357

Charge = 0, Multiplicity = 1

C	2.33302900	4.26324100	-0.87048200
C	1.05205600	4.20125800	-1.36173500
C	-0.08756700	4.45413500	-0.54077600
C	0.08892300	4.87822000	0.82961200
C	1.44937600	4.94099700	1.31299200
C	2.50776600	4.65714300	0.49527800

H	0.88390100	3.91615300	-2.39584600
H	-1.04625800	4.59696000	-1.03125100
H	1.61789600	5.27201000	2.33475700
H	3.51795000	4.75525000	0.88704700
C	-1.03034600	4.95003000	1.68922200
C	-2.42835300	5.31334600	1.20764800
H	-0.82071300	5.14168500	2.73876400
H	-2.92532100	5.89614200	1.99460900
H	-2.36560700	5.97801000	0.33594500
C	4.51856100	2.91864700	-1.18130200
C	3.55045400	4.00784000	-1.73068300
H	3.23292400	3.75244400	-2.74710400
H	4.11806400	4.94453500	-1.80630200
H	4.42327900	2.91763800	-0.08999500
C	4.21232800	1.49655500	-1.64398600
C	3.96824600	0.47840900	-0.72143800
C	4.28065800	1.13906400	-2.99805200
C	3.82277400	-0.85398900	-1.11979100
H	3.89407900	0.72170000	0.33573100
C	4.14137200	-0.18611600	-3.39516200
H	4.47824000	1.90013100	-3.74780000
C	3.92594600	-1.21766900	-2.46449000
H	3.63994800	-1.60256200	-0.36290200
H	4.21600900	-0.43354000	-4.45213500
C	8.71165900	3.64620100	-2.03874300
C	7.73755500	4.06486400	-2.94502000
C	6.38490400	3.85222600	-2.67243800
C	5.98266500	3.21736200	-1.49133300
C	6.97077100	2.79809800	-0.59195400
C	8.32233100	3.01051700	-0.85791200
H	9.76402600	3.81482200	-2.24892700
H	8.02838600	4.56119000	-3.86696500
H	5.64020000	4.18849600	-3.38784500
H	6.67259900	2.29339800	0.32405600

H	9.07143400	2.68153400	-0.14277100
C	3.48564200	-3.84635600	-2.11499700
C	3.89306300	-2.64124600	-3.00437900
H	3.24153000	-2.66423100	-3.88669200
H	4.89823600	-2.85418300	-3.39194200
C	4.25514500	-3.91388200	-0.79193600
C	5.64957300	-3.76947300	-0.79115400
C	3.61538800	-4.11402400	0.43532600
C	6.38504800	-3.79560700	0.39214500
H	6.17905400	-3.61637700	-1.72675200
C	4.33121500	-4.14208600	1.63423800
H	2.54008800	-4.23345700	0.46603400
C	5.70888100	-3.97569700	1.59473700
H	7.46182200	-3.67168500	0.37599600
H	3.81741500	-4.28796900	2.57795600
Br	6.72451000	-3.99556600	3.26921500
C	-0.78183100	-4.49904900	-1.66960500
C	-0.30534700	-3.21149400	-1.91242000
C	1.06734900	-2.98363500	-2.05104900
C	1.98278900	-4.03561700	-1.95713400
C	1.48813300	-5.32753500	-1.71867400
C	0.12230100	-5.56084000	-1.57023900
H	-1.84816300	-4.67817200	-1.56066900
H	-0.98844600	-2.37279000	-1.99811200
H	1.41014300	-1.97241100	-2.22983400
H	2.18711100	-6.15787900	-1.64591500
H	-0.23627400	-6.57014300	-1.38737700
H	3.82356300	-4.72063900	-2.69091100
C	-7.97303100	-0.57739500	0.55610600
C	-9.21760300	-0.06341800	0.16394100
C	-10.22181900	-0.89307300	-0.31985900
C	-10.01883700	-2.27979700	-0.43291500
C	-8.77131100	-2.78993500	-0.03938900
C	-7.76718700	-1.95665600	0.44567400

H	-9.39809300	1.00657700	0.24207500
H	-11.17412000	-0.46013400	-0.61079100
H	-8.58842000	-3.85889300	-0.11902900
H	-6.80617600	-2.37753400	0.72613800
C	-11.04250800	-3.20530600	-0.93772700
C	-12.28128400	-2.90477600	-1.34750900
H	-10.72937000	-4.24882000	-0.97176800
H	-12.95439100	-3.67808500	-1.70409200
H	-12.67190000	-1.89090500	-1.34473700
C	-6.02289400	0.86507500	-0.18398400
C	-6.87322800	0.34886200	1.01100600
H	-7.29771800	1.21545800	1.53102300
H	-6.22190200	-0.16757500	1.72412500
H	-6.73170800	1.28338300	-0.90871100
C	-5.07977600	1.99213200	0.20641500
C	-4.86868800	3.04814100	-0.68917300
C	-4.38992900	2.02237400	1.42390800
C	-4.00582000	4.09714100	-0.38091700
H	-5.38308200	3.04119300	-1.64717100
C	-3.52935800	3.07521800	1.73577100
H	-4.51483600	1.22057100	2.14428700
C	-3.32473800	4.13545400	0.84137700
H	-3.86302200	4.90320500	-1.09695000
H	-3.01218300	3.07307100	2.68883600
C	-4.18722900	-2.55189100	-2.12124400
C	-5.15602500	-1.79957200	-2.78441100
C	-5.72120900	-0.68592400	-2.16053500
C	-5.32294700	-0.29745900	-0.87737200
C	-4.33258200	-1.04691800	-0.22928800
C	-3.77935400	-2.17070400	-0.84165800
H	-3.74512500	-3.42089900	-2.60057900
H	-5.48116400	-2.08255700	-3.78165300
H	-6.49711300	-0.11948500	-2.66880800
H	-3.97764800	-0.74051900	0.74985800

H	-3.01706600	-2.74514100	-0.32588800
Ni	-0.71977200	2.94403200	0.83503000
O	-0.67073100	1.86777700	2.80361300
C	0.04936800	2.55517100	3.85282000
C	-0.91634400	3.03445500	4.92144500
H	0.56508200	3.38769600	3.37457700
H	0.79581400	1.87731800	4.27068700
H	-0.37311900	3.57352200	5.70619300
H	-1.66543900	3.70852000	4.49463600
H	-1.43332100	2.18639600	5.38333000
C	-0.60745400	0.04136400	-2.88579400
C	-1.80718500	0.36488300	-2.24680600
C	-1.79013300	1.12592500	-1.07349500
C	-0.58988300	1.58655100	-0.50269100
C	0.59922900	1.20318400	-1.13761300
C	0.60078900	0.45150500	-2.31588000
H	-0.61281400	-0.52743000	-3.81292400
H	-2.75712000	0.03837200	-2.66211400
H	-2.73622200	1.37595400	-0.61035500
H	1.55181100	1.54365700	-0.74715800
H	1.54420600	0.22010500	-2.80047000
C	-1.22345100	-1.47958700	1.49543700
C	0.18530800	-1.60950200	3.52410200
C	0.10453400	-2.02317100	2.04995700
H	-2.06049000	-2.09730900	1.84598900
H	1.12632200	-1.94447400	3.97207300
B	-0.66929100	0.48285100	2.78472200
O	-1.48647900	-0.12980200	1.89348900
O	0.14265000	-0.18618200	3.65889000
H	-1.21803100	-1.48572500	0.40289000
H	-0.64310400	-2.05060000	4.09599900
C	0.10926000	-3.55331200	1.94896600
H	-0.71326600	-3.99688400	2.52355000
H	0.00898800	-3.87606100	0.90842200

H	1.04861400	-3.96172700	2.34017500
C	1.29191300	-1.43411400	1.27115600
H	2.24107300	-1.74972600	1.71934700
H	1.26870100	-1.77792500	0.23583300
H	1.27263900	-0.34187100	1.24056500

im9d

SCF Energy (a.u.) = -2968.740283

Thermal correction to Gibbs free energy (a.u.) = 1.076770

Charge = 0, Multiplicity = 1

C	1.23510500	1.32080800	-2.44953500
C	0.78882800	0.64802000	-1.30291900
C	-0.21473800	-0.30025300	-1.39057200
C	-0.79522400	-0.64948700	-2.62010400
C	-0.38446000	0.05791000	-3.75493900
C	0.61397400	1.03158700	-3.66771600
H	1.23485700	0.87494400	-0.34156500
H	-0.55407000	-0.81364000	-0.49901600
H	-0.82306800	-0.18244100	-4.72075900
H	0.93151500	1.55710700	-4.56614600
C	-1.71437900	-1.81118400	-2.71228200
C	-1.15688000	-3.16706800	-2.26057100
H	-2.23589400	-1.86759800	-3.66862900
H	-1.74152100	-3.55193700	-1.35053900
H	-1.38225300	-3.93047900	-3.01320200
C	1.75178500	3.77113800	-1.99011300
C	2.31388000	2.36535400	-2.34089100
H	3.02959800	2.06164800	-1.57158000
H	2.86332200	2.44325100	-3.28673900
H	1.01601200	4.01665100	-2.76690200
C	1.00581700	3.73869500	-0.66322000
C	-0.37163500	3.49425900	-0.62550100
C	1.68028800	3.87613300	0.55336800
C	-1.05476600	3.40198300	0.58535800

H	-0.91770800	3.35324900	-1.55406700
C	0.99745400	3.77498400	1.76389500
H	2.74713900	4.07462500	0.55220400
C	-0.38386700	3.54753500	1.80742200
H	-2.11922200	3.20468900	0.56899300
H	1.54520600	3.89115700	2.69635500
C	4.69507100	6.95890000	-1.97604500
C	5.11399000	5.63510600	-1.85615000
C	4.18100700	4.59439600	-1.87315200
C	2.81376000	4.86105200	-2.00769300
C	2.40608200	6.19740300	-2.12627200
C	3.33239400	7.23714500	-2.11282500
H	5.42081900	7.76728100	-1.96518000
H	6.17122700	5.40563900	-1.75115200
H	4.52836900	3.57159700	-1.77868300
H	1.34544200	6.41774300	-2.22179900
H	2.99273500	8.26486500	-2.20950500
C	-1.79108800	2.19864300	3.57548700
C	-1.08482600	3.51809900	3.14975200
H	-0.33332900	3.72068100	3.92026300
H	-1.80600500	4.34167800	3.22161100
C	-3.15805600	1.92962000	2.94674800
C	-3.91123500	2.91166900	2.29398300
C	-3.74645400	0.66779200	3.11887900
C	-5.18277500	2.64172400	1.78234800
H	-3.51190200	3.90992600	2.15773600
C	-5.02444300	0.38451400	2.64157800
H	-3.19532900	-0.11181700	3.63532800
C	-5.72053000	1.37514600	1.95825300
H	-5.73416800	3.40701600	1.24899400
H	-5.46267700	-0.59426800	2.79419400
Br	-7.48138700	0.96987400	1.21865100
C	0.99725700	-1.10930400	3.30691700
C	0.24805400	-0.73916400	2.18716500

C	-0.65540100	0.32054600	2.26213800
C	-0.83424700	1.02093500	3.46343800
C	-0.07505700	0.64222100	4.57598800
C	0.83831700	-0.41117100	4.50323600
H	1.70050000	-1.93547100	3.24396600
H	0.37932000	-1.27402300	1.25301300
H	-1.22799000	0.60185200	1.38566900
H	-0.20469900	1.17791200	5.51384700
H	1.41429100	-0.68969100	5.38129500
H	-1.99116700	2.33024900	4.64901700
C	6.31782900	-3.01159400	1.01311500
C	7.32335300	-3.71889900	0.33859900
C	8.66808000	-3.44078200	0.55183800
C	9.06229000	-2.43647000	1.45359300
C	8.05177100	-1.73085000	2.12626100
C	6.70547500	-2.01144900	1.91088900
H	7.04282100	-4.50056000	-0.36417100
H	9.41986200	-4.01071400	0.01437100
H	8.33037700	-0.94731100	2.82679800
H	5.94460800	-1.43667700	2.43111500
C	10.46762900	-2.09848300	1.71874800
C	11.55620400	-2.66499800	1.18324300
H	10.60935800	-1.29083600	2.43684400
H	12.55171600	-2.32907200	1.45582000
H	11.50291400	-3.47580500	0.46194900
C	4.35316400	-2.42787900	-0.48153800
C	4.86333300	-3.27578400	0.71659000
H	4.70803500	-4.33568800	0.48260500
H	4.26050100	-3.04721900	1.60228500
H	5.03293100	-2.62558000	-1.31935500
C	2.95072600	-2.80101000	-0.93352900
C	2.60207900	-2.62645700	-2.28062800
C	1.95915000	-3.24695500	-0.05515500
C	1.30012900	-2.82437600	-2.72061200

H	3.35955600	-2.28971200	-2.98389300
C	0.64537600	-3.43123500	-0.49460200
H	2.19376200	-3.42911400	0.98912900
C	0.28867900	-3.18662700	-1.82086200
H	1.04732900	-2.62553900	-3.75740600
H	-0.12012700	-3.72390800	0.22009100
C	4.74888600	1.75744000	0.58191800
C	5.62865700	1.17913100	-0.33409700
C	5.48166400	-0.16117400	-0.69958900
C	4.45769500	-0.94167900	-0.15594200
C	3.57561600	-0.34726800	0.75413600
C	3.71590000	0.98832100	1.12498000
H	4.86250800	2.80035500	0.86286100
H	6.43613800	1.76802400	-0.76096500
H	6.18315500	-0.61184200	-1.39660800
H	2.76301700	-0.92843400	1.17221400
H	3.00720800	1.42791500	1.82020300
Ni	-2.82229500	-2.16665900	-1.21730900
C	-5.18265800	1.81661700	-2.21362100
C	-4.08755900	1.84774600	-1.34862800
C	-3.37558700	0.68008500	-1.06577300
C	-3.73256000	-0.55370500	-1.63396300
C	-4.82413200	-0.55989400	-2.51822500
C	-5.54722400	0.60424400	-2.79965200
H	-5.73863300	2.72422500	-2.43309900
H	-3.78467500	2.78690600	-0.89253900
H	-2.51659800	0.74573000	-0.40399600
H	-5.12215400	-1.48852600	-2.99886300
H	-6.39190700	0.56228700	-3.48418300
C	-5.31757700	-4.02575600	-1.61700700
C	-4.20000400	-4.75238100	-1.74348000
C	-3.39589800	-5.41404200	-0.64839600
C	-3.30119800	-4.67378900	0.71007200
C	-3.09764300	-3.16168500	0.69418600

C	-4.07592800	-2.20444900	0.58061000
C	-5.55234200	-2.38017700	0.32722300
C	-6.02651000	-3.69547900	-0.33070300
H	-5.75448000	-3.61004100	-2.52268900
H	-3.81631500	-4.90792300	-2.75134000
H	-2.37936600	-5.57095900	-1.02826700
H	-3.78711900	-6.42446200	-0.45683000
H	-4.18822000	-4.89849800	1.30907600
H	-2.46051500	-5.11472000	1.25854600
H	-2.15181200	-2.81811100	1.11644200
H	-3.81703600	-1.20229600	0.90683500
H	-5.88072700	-1.53249100	-0.28204200
H	-6.07650000	-2.27237100	1.28886000
H	-5.93670600	-4.52504800	0.37528300
H	-7.09863800	-3.58715600	-0.53296700

TS5d

SCF Energy (a.u.) = -2968.722566

Thermal correction to Gibbs free energy (a.u.) = 1.077622

Charge = 0, Multiplicity = 1

C	-1.11825200	1.10241400	2.34623600
C	-0.62108200	0.52986800	1.16689200
C	0.37698700	-0.43300400	1.21300600
C	0.89786100	-0.87845000	2.43434000
C	0.44631600	-0.26714900	3.60637000
C	-0.54799600	0.71184300	3.56116400
H	-1.03879300	0.83448100	0.21377500
H	0.74550000	-0.89071600	0.30169000
H	0.84384300	-0.58992200	4.56610900
H	-0.90598700	1.15765600	4.48669300
C	1.79928600	-2.07269900	2.49818100
C	1.03182100	-3.43742600	2.12953200
H	2.14520400	-2.21044400	3.51992000
H	1.52801000	-4.05469500	1.31914900

H	1.12331100	-4.07658800	3.01235800
C	-1.67275100	3.57619300	2.09902000
C	-2.21502100	2.13417400	2.29388000
H	-2.89889300	1.89061300	1.47487000
H	-2.79755900	2.10783200	3.22238600
H	-0.94169300	3.75247200	2.89850800
C	-0.93382800	3.69097000	0.77409900
C	0.46269300	3.65274900	0.71386800
C	-1.64264300	3.76694600	-0.42778500
C	1.13339000	3.68489100	-0.50904900
H	1.03442700	3.58563700	1.63584200
C	-0.97589600	3.76959000	-1.64941000
H	-2.72510900	3.81639500	-0.40346800
C	0.42195000	3.72871600	-1.71647700
H	2.21761800	3.66171600	-0.51927500
H	-1.54961200	3.81180300	-2.57242600
C	-4.66857400	6.70049900	2.38947100
C	-5.06230800	5.39237300	2.11323300
C	-4.11215100	4.37087400	2.03131500
C	-2.75265800	4.64237100	2.22136700
C	-2.36947800	5.96237900	2.49708100
C	-3.31359500	6.98261500	2.58272600
H	-5.40790200	7.49377700	2.45552300
H	-6.11338300	5.16013000	1.96215300
H	-4.43996900	3.36061200	1.81352200
H	-1.31464600	6.18710000	2.63691700
H	-2.99369900	7.99801600	2.80064800
C	1.96738500	2.50817300	-3.44243000
C	1.10062800	3.74975900	-3.06739200
H	0.32896800	3.83634400	-3.83995000
H	1.71823700	4.65046100	-3.16154400
C	3.28463400	2.41226900	-2.66877400
C	4.05960000	3.56112100	-2.44489100
C	3.80760000	1.18581300	-2.24572300

C	5.29401500	3.50002200	-1.80015500
H	3.70508600	4.53233900	-2.77395400
C	5.04069900	1.09844100	-1.59504600
H	3.25117800	0.27442000	-2.42580800
C	5.76602900	2.26146200	-1.37954300
H	5.87423300	4.40053200	-1.63346800
H	5.41710500	0.14142600	-1.25977600
Br	7.49633700	2.15832200	-0.46973000
C	-0.51149200	-1.05228200	-3.52988500
C	-0.12228300	-0.50950800	-2.30333300
C	0.68351400	0.62939600	-2.25715100
C	1.12422200	1.24220900	-3.44108400
C	0.72848100	0.68329800	-4.66211900
C	-0.08382200	-0.45097800	-4.71291700
H	-1.13990300	-1.93841600	-3.55924600
H	-0.45078300	-0.97798800	-1.38212500
H	0.97355100	1.03990300	-1.29697200
H	1.06264100	1.14457100	-5.58867700
H	-0.37505400	-0.86416800	-5.67454400
H	2.25657800	2.68161400	-4.48898300
C	-6.48189700	-2.72663700	-0.94580600
C	-7.50776900	-3.29002000	-0.17328800
C	-8.83516000	-2.92329200	-0.35909800
C	-9.19090200	-1.97149500	-1.33123100
C	-8.16037300	-1.41090000	-2.10268000
C	-6.83147700	-1.77986500	-1.91408600
H	-7.25711100	-4.02857200	0.58519700
H	-9.60384200	-3.38255100	0.25497300
H	-8.40890700	-0.67078900	-2.85949500
H	-6.05250100	-1.31496800	-2.51174800
C	-10.57635100	-1.54426100	-1.57098300
C	-11.67955800	-1.96870100	-0.94210000
H	-10.68797600	-0.79547500	-2.35514000
H	-12.65742600	-1.57801800	-1.20538900

H	-11.65610800	-2.71290500	-0.15081900
C	-4.42533800	-2.19240400	0.44380100
C	-5.04018800	-3.07712800	-0.67922500
H	-4.95070200	-4.12723700	-0.37722300
H	-4.45524700	-2.95230100	-1.59668000
H	-5.08274300	-2.29348200	1.31577100
C	-3.03910300	-2.64565300	0.86593800
C	-2.66669400	-2.54839800	2.21346100
C	-2.08747500	-3.12347400	-0.04130600
C	-1.38128900	-2.87043400	2.63242800
H	-3.39329200	-2.19252500	2.93966000
C	-0.79017200	-3.42422500	0.37481600
H	-2.34551900	-3.25226600	-1.08824200
C	-0.40735100	-3.27308100	1.70994200
H	-1.11412600	-2.75433100	3.67839700
H	-0.05338500	-3.74636300	-0.35414300
C	-4.66669300	1.92061700	-0.89992400
C	-5.55947500	1.43785600	0.05734800
C	-5.45021400	0.12417400	0.51807500
C	-4.45565000	-0.72708800	0.02692900
C	-3.55687800	-0.22637700	-0.92319200
C	-3.65728100	1.08454500	-1.38490100
H	-4.75580100	2.94084800	-1.26169500
H	-6.34930800	2.07927400	0.43891200
H	-6.16360900	-0.25479900	1.24480600
H	-2.76882200	-0.86354100	-1.30769100
H	-2.93844200	1.45098500	-2.11126800
Ni	2.59687400	-2.76395500	0.79961600
C	5.90876000	-0.06883700	2.47158700
C	4.85575400	0.53134500	1.77625600
C	3.67375400	-0.16746900	1.53842100
C	3.52571700	-1.49861400	1.96633100
C	4.56785100	-2.06798300	2.72322500
C	5.75388500	-1.37155700	2.95247000

H	6.82944100	0.47945200	2.64691300
H	4.96030800	1.54590400	1.40444800
H	2.87205100	0.31624200	0.99109800
H	4.45291400	-3.07400300	3.11730700
H	6.55540400	-1.84482200	3.51461700
C	5.11205200	-4.62479600	0.62450600
C	4.00833200	-5.37711800	0.72719400
C	3.01777200	-5.75632700	-0.34867400
C	2.80255400	-4.75953200	-1.50900100
C	2.59480500	-3.29540100	-1.12633300
C	3.58540900	-2.33330100	-0.85753400
C	5.09064900	-2.51087600	-0.82225300
C	5.63690500	-3.94142100	-0.60923900
H	5.68520600	-4.45132500	1.53277600
H	3.78691000	-5.79680800	1.70931100
H	2.04807500	-5.91869400	0.14137700
H	3.29160700	-6.73557100	-0.77219200
H	3.62172900	-4.84605700	-2.23006500
H	1.90873600	-5.09455200	-2.05011600
H	1.65735200	-2.87777500	-1.49913100
H	3.29589900	-1.29911100	-1.03873200
H	5.49365700	-1.85953900	-0.03746200
H	5.50869800	-2.13960300	-1.77189200
H	5.44062200	-4.54751000	-1.49633600
H	6.72834000	-3.86543300	-0.53159500

im10d

SCF Energy (a.u.) = -2968.767920

Thermal correction to Gibbs free energy (a.u.) = 1.081280

Charge = 0, Multiplicity = 1

C	1.44868100	1.39424300	-2.42078700
C	0.73294400	0.80219100	-1.36989500
C	-0.33640400	-0.04465100	-1.62683200
C	-0.71621700	-0.34749500	-2.94112800

C	-0.03698700	0.27989400	-3.98567300
C	1.03113600	1.14206100	-3.72932200
H	1.03034900	1.00496200	-0.34771500
H	-0.87474700	-0.51238900	-0.80959500
H	-0.31979300	0.06260200	-5.01350000
H	1.56135900	1.60549100	-4.55856000
C	-1.73141800	-1.43388800	-3.22216800
C	-1.14792700	-2.87864300	-2.88780700
H	-1.91017100	-1.42315900	-4.30608200
H	-1.80992000	-3.36480500	-2.15620800
H	-1.19427300	-3.48706300	-3.79847500
C	2.15793200	3.78128200	-1.90427800
C	2.60785000	2.31365600	-2.13791300
H	3.14917600	1.95599900	-1.25747700
H	3.30914800	2.29816200	-2.98045200
H	1.56259000	4.07280500	-2.77946100
C	1.24780600	3.87381800	-0.68847800
C	-0.14315200	3.89780300	-0.82751800
C	1.77969700	3.86836600	0.60461900
C	-0.98045000	3.92084700	0.28811500
H	-0.57821100	3.88592700	-1.82340200
C	0.94440100	3.87750600	1.71770000
H	2.85629200	3.86055500	0.73668600
C	-0.44982700	3.91120500	1.58457000
H	-2.05485500	3.93628900	0.13993800
H	1.38027200	3.86602700	2.71387700
C	5.39192000	6.65204800	-1.55183300
C	5.65929100	5.29258100	-1.40253600
C	4.63234100	4.35241400	-1.52626400
C	3.32143900	4.75782300	-1.79794400
C	3.06507200	6.12868400	-1.94413300
C	4.08590700	7.06816100	-1.82526000
H	6.19087400	7.38221500	-1.45781700
H	6.67092200	4.95615600	-1.19046500

H	4.86155400	3.30031500	-1.40347600
H	2.04760500	6.45632900	-2.14443100
H	3.86433800	8.12521600	-1.94550300
C	-2.12005300	2.65686400	3.15967100
C	-1.30901900	3.94588600	2.82903300
H	-0.64917100	4.11618500	3.68619600
H	-1.98983300	4.80436400	2.80673100
C	-3.42682900	2.46631000	2.38972600
C	-4.09212300	3.51745300	1.74761600
C	-4.07109300	1.22054600	2.43407800
C	-5.35224200	3.34419000	1.16892100
H	-3.64345900	4.50245000	1.69452800
C	-5.33064600	1.02428700	1.86985500
H	-3.58119600	0.38307800	2.91954200
C	-5.95724000	2.09748400	1.24738300
H	-5.84924700	4.17242200	0.67668000
H	-5.80811000	0.05299000	1.91583000
Br	-7.73422300	1.84777700	0.46460000
C	0.60807400	-0.70897000	3.13859600
C	-0.00665300	-0.30570500	1.95111600
C	-0.90270600	0.76314300	1.94624400
C	-1.20297000	1.44387100	3.13409100
C	-0.58055000	1.03045500	4.31722100
C	0.32099100	-0.03517300	4.32510300
H	1.30592200	-1.54170500	3.13628000
H	0.21938100	-0.82481100	1.02603000
H	-1.37003800	1.06955100	1.01645000
H	-0.80583900	1.55138800	5.24526000
H	0.78974800	-0.34082600	5.25628300
H	-2.42987500	2.78737900	4.20697500
C	6.04803700	-3.12289300	0.93012600
C	7.08769100	-3.73831900	0.21802600
C	8.41846700	-3.52786400	0.55815100
C	8.76411300	-2.68713700	1.63111200

C	7.71978800	-2.07412400	2.34174300
C	6.38762100	-2.28648800	1.99843900
H	6.84494300	-4.39282700	-0.61639100
H	9.19735600	-4.02334300	-0.01345700
H	7.96068800	-1.41723900	3.17408900
H	5.60074600	-1.78270000	2.55272300
C	10.15273600	-2.42616700	2.03485800
C	11.26787300	-2.92059200	1.48278900
H	10.25603800	-1.74878300	2.88253700
H	12.24702300	-2.65427400	1.86819400
H	11.25311700	-3.60211000	0.63672700
C	4.20768700	-2.28155000	-0.60661500
C	4.61449500	-3.29918800	0.49937800
H	4.45309000	-4.31122700	0.11010700
H	3.95208300	-3.17440300	1.36265600
H	4.93615000	-2.39538800	-1.41851400
C	2.83287900	-2.56315000	-1.18809200
C	2.61688500	-2.37503900	-2.55987200
C	1.74653400	-2.97576700	-0.40899200
C	1.35838500	-2.54975100	-3.12443200
H	3.44877600	-2.06918300	-3.18966200
C	0.47782900	-3.12293400	-0.97173900
H	1.87483100	-3.17142700	0.65170300
C	0.25437000	-2.88490300	-2.33012800
H	1.22095500	-2.37227800	-4.18698500
H	-0.36196600	-3.38756100	-0.33985900
C	4.72313100	1.67717100	1.08358200
C	5.66695300	1.16186400	0.19380200
C	5.47585100	-0.09557500	-0.38266500
C	4.34499900	-0.85927200	-0.07633800
C	3.40036000	-0.32519100	0.80731900
C	3.58202800	0.92956300	1.38604400
H	4.87347200	2.65583700	1.53020000
H	6.55883300	1.73445800	-0.04635000

H	6.22698000	-0.50176900	-1.05466500
H	2.50903600	-0.89231900	1.04243600
H	2.82531100	1.32052500	2.05928900
Ni	-3.44148100	-2.74154800	-0.75596800
C	-5.72544800	-0.68709600	-1.65028800
C	-4.76792900	0.33999600	-1.66335000
C	-3.47928700	0.08771600	-2.11438500
C	-3.09287600	-1.19363900	-2.56852400
C	-4.08948900	-2.22058600	-2.63533100
C	-5.39904700	-1.94402100	-2.15045000
H	-6.72635000	-0.49033500	-1.27953300
H	-5.02959100	1.32889400	-1.30261000
H	-2.74701500	0.88702800	-2.11679000
H	-3.92757600	-3.10615300	-3.24838300
H	-6.15920700	-2.71717900	-2.21704000
C	-4.80797900	-4.77597800	-0.08406600
C	-3.56816300	-5.21390100	-0.40898400
C	-2.37808700	-5.34539000	0.51595300
C	-2.20937200	-4.21342600	1.56716000
C	-2.53974200	-2.81344100	1.06361900
C	-3.80420500	-2.20535100	1.10392300
C	-5.09960100	-2.83355100	1.57975100
C	-5.26312800	-4.35264900	1.29249400
H	-5.56237600	-4.76524000	-0.86848400
H	-3.41068500	-5.56214200	-1.42958800
H	-1.47975800	-5.37422300	-0.11154700
H	-2.40756300	-6.31541400	1.03618300
H	-2.80292800	-4.44314500	2.45804800
H	-1.16504600	-4.23008700	1.90346600
H	-1.69364300	-2.13181900	1.02081700
H	-3.82625800	-1.11693700	1.06701100
H	-5.92273200	-2.29614000	1.09221000
H	-5.23039500	-2.67813800	2.66378700
H	-4.72698500	-4.92962000	2.04984700

H -6.32288900 -4.60783300 1.41184100

P3

SCF Energy (a.u.) = -2485.673045

Thermal correction to Gibbs free energy (a.u.) = 0.906279

Charge = 0, Multiplicity = 1

C	0.27628500	0.78830800	-2.36037000
C	-0.16231100	0.17062500	-1.18091600
C	-0.90777200	-1.00112200	-1.22222100
C	-1.20344100	-1.62434700	-2.44101400
C	-0.79979700	-0.98984500	-3.61719200
C	-0.07848000	0.20454600	-3.57890600
H	0.10828300	0.60686000	-0.22672200
H	-1.21744900	-1.46856900	-0.29374900
H	-1.02189000	-1.45369900	-4.57572800
H	0.24432400	0.66864200	-4.50818900
C	-1.84969800	-2.99589000	-2.49676700
C	-1.25282300	-3.98335900	-1.43563500
H	-1.61155100	-3.41007500	-3.48519100
H	-1.80751300	-3.87053700	-0.49765900
H	-1.45323000	-5.00595700	-1.77935500
C	0.28451400	3.33122000	-2.06745000
C	1.11223000	2.04116500	-2.30586800
H	1.85433100	1.93896400	-1.50851800
H	1.66470900	2.15566900	-3.24567300
H	-0.47158600	3.37883700	-2.86203600
C	-0.45806800	3.26560200	-0.74087600
C	-1.83368400	3.02150600	-0.69025100
C	0.23479300	3.39225200	0.46810100
C	-2.50115800	2.90122400	0.52962200
H	-2.38897500	2.91272300	-1.61828900
C	-0.42544600	3.25000400	1.68501300
H	1.29993300	3.60058900	0.45189800
C	-1.80334600	3.00172200	1.73977200

H	-3.57082800	2.71530600	0.53842600
H	0.13475200	3.33391900	2.61309200
C	2.57250900	7.01611200	-2.25298300
C	3.24049200	5.79682200	-2.16137100
C	2.52134900	4.59876400	-2.11402400
C	1.12291900	4.60186700	-2.15403200
C	0.46305300	5.83609400	-2.24462600
C	1.17549000	7.03106800	-2.29611400
H	3.13167800	7.94671400	-2.29161200
H	4.32659100	5.77142300	-2.12887100
H	3.06213100	3.66178900	-2.04465300
H	-0.62407500	5.85225700	-2.26378900
H	0.64235400	7.97515600	-2.36889700
C	-2.95446000	1.39296400	3.44624500
C	-2.48853300	2.84034400	3.07560400
H	-1.80082900	3.16166100	3.86536400
H	-3.35522400	3.50823800	3.13226300
C	-4.17719200	0.92769300	2.65011700
C	-5.31561000	1.74898000	2.61139700
C	-4.25762200	-0.32058300	2.02340900
C	-6.48448500	1.35612400	1.96343600
H	-5.30379800	2.71527000	3.10692900
C	-5.41978100	-0.73970000	1.36870700
H	-3.41055800	-0.99483500	2.04875400
C	-6.51729700	0.10885900	1.34800200
H	-7.35290200	2.00490600	1.94821500
H	-5.45493700	-1.70743600	0.88353800
Br	-8.16671500	-0.46359100	0.45724600
C	0.43079000	-1.31181600	3.51417800
C	-0.07101200	-0.85439900	2.29403600
C	-1.16056400	0.01440400	2.26423500
C	-1.78229900	0.43013600	3.45104200
C	-1.26887600	-0.03732600	4.66604600
C	-0.16921600	-0.89730100	4.70310000

H	1.28051700	-1.98918700	3.53618700
H	0.38232500	-1.17750400	1.36428600
H	-1.53763700	0.36628300	1.31201400
H	-1.73754300	0.27551600	5.59632500
H	0.21043000	-1.24691300	5.65913800
H	-3.29737200	1.47273500	4.48727900
C	6.35072600	-2.33237900	1.06808200
C	7.40834800	-2.93593200	0.37252200
C	8.69505600	-2.41344900	0.42059500
C	8.97622400	-1.25774600	1.17059200
C	7.91411900	-0.65694500	1.86519300
C	6.62600300	-1.18248000	1.81544000
H	7.21528800	-3.83129400	-0.21451600
H	9.49025800	-2.90930800	-0.12774500
H	8.10502400	0.23894500	2.45110200
H	5.82029600	-0.68671800	2.34918500
C	10.31596700	-0.66029500	1.25786800
C	11.44068300	-1.09476000	0.67565100
H	10.36988800	0.23791900	1.87298400
H	12.37949900	-0.56723600	0.81180800
H	11.47385200	-1.98159200	0.04880800
C	4.20229300	-2.26333100	-0.27606500
C	4.94731300	-2.87015900	0.94519600
H	4.96461400	-3.96034800	0.83124800
H	4.38546900	-2.64980500	1.85928300
H	4.84056700	-2.43587000	-1.15096400
C	2.85911200	-2.91781000	-0.55262000
C	2.42788700	-3.06796200	-1.87698400
C	1.97830200	-3.29941400	0.46450200
C	1.14029400	-3.50215900	-2.17305400
H	3.10063600	-2.79765400	-2.68730000
C	0.67685400	-3.70598600	0.16687700
H	2.28553200	-3.24356700	1.50459700
C	0.21953500	-3.77228700	-1.15204900

H	0.82779700	-3.55828000	-3.21127200
H	-0.01068100	-3.92190400	0.98129400
C	3.88463700	2.03172100	0.27258000
C	4.74810800	1.50632900	-0.68960600
C	4.83067500	0.12493600	-0.88121000
C	4.05751500	-0.75241900	-0.11581700
C	3.19013000	-0.21199800	0.84195500
C	3.09923800	1.16428000	1.03712900
H	3.81995000	3.10609000	0.41968900
H	5.36535100	2.17051200	-1.28869600
H	5.51861900	-0.27763100	-1.61991400
H	2.57637100	-0.87082700	1.44394500
H	2.40713900	1.55387000	1.77779500
C	-6.18107200	-3.00493100	-2.17716500
C	-5.46612100	-1.84189200	-1.89443200
C	-4.07295200	-1.82720400	-1.99099100
C	-3.37127200	-2.97110100	-2.38622000
C	-4.10192200	-4.13165900	-2.68129700
C	-5.49141600	-4.15350000	-2.57338100
H	-7.26410100	-3.01305600	-2.09457400
H	-5.99311200	-0.94157100	-1.59651100
H	-3.53035400	-0.91518300	-1.76744800
H	-3.57529800	-5.02714500	-3.00365800
H	-6.03632300	-5.06451800	-2.80594900

im1f

SCF Energy (a.u.) = -1887.167088

Thermal correction to Gibbs free energy (a.u.) = 0.662331

Charge = 0, Multiplicity = 1

C	-7.37713400	1.00259500	-0.90887000
C	-8.20937800	0.57072500	-1.95196000
C	-9.58227700	0.44878200	-1.77605600
C	-10.18114100	0.75622100	-0.54124500
C	-9.34408300	1.18864100	0.49960300

C	-7.96866600	1.30885300	0.32062100
H	-7.76915900	0.32745800	-2.91664800
H	-10.19639900	0.11414300	-2.60656800
H	-9.78218300	1.43002300	1.46505800
H	-7.34234700	1.62796500	1.14889500
C	-11.62610100	0.64610900	-0.29752500
C	-12.57134600	0.26428300	-1.16554700
H	-11.93431400	0.91168800	0.71367300
H	-13.61496400	0.21961800	-0.87049500
H	-12.34933100	-0.01487900	-2.19185100
C	-5.21071600	-0.31906000	-0.83716000
C	-5.88225400	1.05925000	-1.09372500
H	-5.63725000	1.37828700	-2.11389100
H	-5.45537400	1.80000600	-0.40916000
H	-5.73276700	-1.04521200	-1.47276700
C	-3.73916400	-0.35527400	-1.21178400
C	-3.15405000	-1.58294900	-1.55065700
C	-2.91457500	0.77260900	-1.16116800
C	-1.78806600	-1.68517700	-1.79488000
H	-3.77958100	-2.47104600	-1.60244500
C	-1.54379800	0.66709000	-1.39560800
H	-3.33213100	1.74381600	-0.91595100
C	-0.95572200	-0.56274100	-1.69723300
H	-1.35598000	-2.65270600	-2.04145600
H	-0.91529900	1.54902500	-1.30518900
C	-5.92156300	-1.44658400	3.28868200
C	-6.72450400	-1.95832000	2.26926100
C	-6.47596700	-1.60942700	0.94099500
C	-5.42328000	-0.75026000	0.60946100
C	-4.61786200	-0.24648700	1.63902400
C	-4.86745200	-0.58801700	2.96782300
H	-6.11316100	-1.71495800	4.32383400
H	-7.54814100	-2.62627700	2.50582000
H	-7.11695900	-1.99335200	0.15196500

H	-3.78061700	0.40171900	1.39852500
H	-4.23656100	-0.18333600	3.75522000
C	1.13749100	-1.29645700	-0.47801200
C	0.54239000	-0.70093500	-1.78409000
H	0.82359000	-1.34762800	-2.62415400
H	0.99447300	0.28159500	-1.96207200
H	0.72674400	-2.31138000	-0.38025900
C	2.65440400	-1.40264700	-0.49020900
C	3.28193800	-1.96212400	0.66954200
C	3.44333500	-1.00093400	-1.54457900
C	4.64403400	-2.03167000	0.78714700
H	2.65358200	-2.32445200	1.47852100
C	4.87925300	-1.03639300	-1.48817400
H	2.99130200	-0.65725500	-2.46947300
C	5.45573400	-1.45793800	-0.23934500
H	5.11312900	-2.46710800	1.66319700
H	5.44480200	-1.06828900	-2.41579900
Br	7.38428900	-2.05038400	-0.29043800
C	-0.32915500	1.03949200	2.86785000
C	-0.97533400	-0.14104200	2.49810000
C	-0.48689500	-0.90444800	1.43714500
C	0.65244900	-0.50469000	0.73126500
C	1.30012400	0.67425300	1.11814600
C	0.81329000	1.44442500	2.17368900
H	-0.70787600	1.63583900	3.69332700
H	-1.86196100	-0.47270000	3.03032500
H	-1.01040800	-1.80829800	1.13949100
H	2.20074900	0.97480300	0.59352500
H	1.32807900	2.35880800	2.45817800
Ni	5.57065400	0.48014000	-0.38191500
C	6.33601500	2.21900500	-1.34428000
C	4.96262100	2.27155600	-1.36525700
C	4.08866700	2.97087900	-0.34843300
C	4.55940800	2.81690700	1.12756700

C	5.18860500	1.47117400	1.44535000
C	6.53244100	1.17763600	1.37472400
C	7.63304800	2.08113100	0.86290800
C	7.22860000	2.94972900	-0.35763400
H	6.83517600	1.77732000	-2.20681300
H	4.45044600	1.90487600	-2.25208100
H	3.07891200	2.55893800	-0.44597100
H	3.99975900	4.04239900	-0.58359100
H	5.25862400	3.61881400	1.37963700
H	3.68994400	2.95896400	1.77909800
H	4.54365600	0.74992500	1.94480300
H	6.87167900	0.25913700	1.84864400
H	8.47118500	1.43650700	0.57386800
H	8.01202500	2.73525000	1.66311800
H	6.73494500	3.86602500	-0.02275700
H	8.14136200	3.26884000	-0.87321400

TS1f

SCF Energy (a.u.) = -1887.163810

Thermal correction to Gibbs free energy (a.u.) = 0.662948

Charge = 0, Multiplicity = 1

C	-7.58387200	-0.09206900	-1.25598500
C	-8.47252500	-1.15995800	-1.44858700
C	-9.82606200	-1.03277000	-1.16147100
C	-10.34780900	0.17605400	-0.66703400
C	-9.45458300	1.24238500	-0.47699000
C	-8.09870300	1.11157200	-0.76457900
H	-8.09240900	-2.10506600	-1.83053200
H	-10.48552100	-1.87958700	-1.32544300
H	-9.83253200	2.18695400	-0.09328400
H	-7.42671400	1.94710200	-0.58998700
C	-11.76880600	0.36802200	-0.34551500
C	-12.75890200	-0.52504600	-0.46745100
H	-12.01530300	1.35970300	0.03376000

H	-13.77815600	-0.26903800	-0.19585300
H	-12.59890200	-1.53372100	-0.83824900
C	-5.38203600	-0.88154800	-0.27066200
C	-6.10722100	-0.26922400	-1.50147000
H	-5.94146500	-0.92703900	-2.36311100
H	-5.65549000	0.69979500	-1.73933500
H	-5.92451600	-1.79943600	-0.01154800
C	-3.93702000	-1.26197200	-0.54320100
C	-3.33431400	-2.24811000	0.24990800
C	-3.14761100	-0.61470700	-1.49812100
C	-1.98191900	-2.54724200	0.12014600
H	-3.93341500	-2.76842200	0.99354800
C	-1.78961000	-0.90877900	-1.62117900
H	-3.58066600	0.14501100	-2.14066900
C	-1.18111300	-1.86259500	-0.80323500
H	-1.53413700	-3.30464400	0.76005900
H	-1.18538500	-0.35890300	-2.33770000
C	-5.78195800	1.85867600	3.06556500
C	-6.63991500	0.76550900	2.94406600
C	-6.49136900	-0.12551400	1.88026000
C	-5.48526400	0.05737200	0.92602700
C	-4.62372800	1.15404400	1.05967900
C	-4.77364100	2.04966900	2.11792500
H	-5.89575100	2.55506600	3.89163000
H	-7.42883500	0.60646500	3.67400600
H	-7.17514500	-0.96376500	1.77722000
H	-3.82134400	1.29824100	0.34232700
H	-4.10102800	2.89941200	2.20359900
C	0.96224100	-1.30679200	0.39382900
C	0.31564300	-2.04369300	-0.81075800
H	0.58888800	-3.10490800	-0.75993600
H	0.72597700	-1.64385600	-1.74434600
H	0.53663700	-1.75781800	1.29952900
C	2.47216300	-1.43935700	0.47259100

C	3.09793300	-1.14032400	1.71309800
C	3.27042300	-1.79062500	-0.60469900
C	4.46848200	-1.09934300	1.85306800
H	2.46998600	-0.89897300	2.56786100
C	4.68316100	-1.76802000	-0.51255400
H	2.82225300	-2.12443600	-1.53523600
C	5.25097100	-1.28393000	0.69186400
H	4.93554200	-0.83404000	2.79520700
H	5.28944300	-2.23405400	-1.27987400
Br	7.37080600	-1.79600700	0.90243100
C	-0.30685700	2.83886600	0.28994600
C	-0.92756600	1.93443000	1.15221400
C	-0.50105800	0.60648000	1.19937900
C	0.55268000	0.16302000	0.39411400
C	1.17530000	1.07984600	-0.46205300
C	0.74623700	2.40566100	-0.51941400
H	-0.63828700	3.87266600	0.24899800
H	-1.74740600	2.25510300	1.78831100
H	-1.00920600	-0.09938800	1.85021400
H	2.00445700	0.75004900	-1.08176800
H	1.23350100	3.10173600	-1.19731600
Ni	5.99463800	0.03952700	-0.37432000
C	7.22724700	1.04802100	-1.78530700
C	5.97217700	0.85829400	-2.32097700
C	4.82153100	1.84366400	-2.28984700
C	4.69537300	2.64648600	-0.96712900
C	5.01436600	1.82450300	0.26875100
C	6.25305300	1.73518700	0.87242700
C	7.54006100	2.37223600	0.39122500
C	7.73303600	2.33069700	-1.14783200
H	7.98008200	0.29177200	-2.00478900
H	5.82523400	-0.00835000	-2.96363100
H	3.89969500	1.26969700	-2.44055000
H	4.88748100	2.54370600	-3.13710800

H	5.33430200	3.53297500	-1.00350500
H	3.66754100	3.01535400	-0.88432400
H	4.15508500	1.44268100	0.81463500
H	6.29330900	1.31073300	1.87387100
H	8.36706300	1.82910900	0.86198300
H	7.61986100	3.41449900	0.73747600
H	7.24401000	3.19027700	-1.61406600
H	8.80149000	2.43639200	-1.36637200

im2f

SCF Energy (a.u.) = -1887.200889

Thermal correction to Gibbs free energy (a.u.) = 0.662682

Charge = 0, Multiplicity = 1

C	8.16510200	-0.51689200	1.10028800
C	8.92633100	-1.69115400	1.00548100
C	10.26791800	-1.65414300	0.64575500
C	10.90570400	-0.43255200	0.36484200
C	10.14005500	0.74016400	0.46225700
C	8.79566200	0.69971400	0.82177700
H	8.45494500	-2.64827300	1.21830500
H	10.82723100	-2.58279000	0.58499500
H	10.60904100	1.69737800	0.24748100
H	8.22187800	1.62087100	0.87071800
C	12.32016500	-0.33270700	-0.02075100
C	13.19933500	-1.33318900	-0.15825300
H	12.66491300	0.68371700	-0.21084100
H	14.22609400	-1.13777600	-0.45116500
H	12.93781500	-2.37373200	0.01319300
C	5.83252300	-0.84496700	0.15217100
C	6.69334500	-0.58047200	1.41928500
H	6.49584500	-1.37961400	2.14381200
H	6.37619900	0.36180500	1.87870200
H	6.24568700	-1.74213400	-0.32571100
C	4.37039500	-1.11877400	0.45892200

C	3.61254600	-1.86271300	-0.45580900
C	3.71725700	-0.59232600	1.57716100
C	2.24415400	-2.04064200	-0.27853100
H	4.10343400	-2.28676300	-1.32871600
C	2.34360900	-0.76307200	1.74888100
H	4.27147700	-0.02121000	2.31499800
C	1.58227700	-1.47126900	0.81714400
H	1.67535000	-2.60812000	-1.01199000
H	1.84922700	-0.30416300	2.60081400
C	6.37485200	2.46528200	-2.59545300
C	7.10905100	1.28972700	-2.75345100
C	6.91307300	0.21975100	-1.87921300
C	5.98195100	0.30401400	-0.83876000
C	5.24393800	1.48576400	-0.69193600
C	5.44179100	2.55886700	-1.56022900
H	6.52558100	3.30051700	-3.27371200
H	7.83809200	1.20441300	-3.55457500
H	7.50164400	-0.68656900	-1.99318100
H	4.49784200	1.56003100	0.09348500
H	4.86460600	3.47070900	-1.42908200
C	-0.55685500	-0.48273400	-0.07664900
C	0.07808200	-1.50058000	0.91116500
H	-0.31388700	-2.49940600	0.68345000
H	-0.22803100	-1.25381300	1.93357300
H	-0.23383600	-0.78594100	-1.08091100
C	-2.07828100	-0.48334000	-0.07313000
C	-2.74917600	0.14456900	-1.13294200
C	-2.84898400	-1.05482500	0.94192500
C	-4.14031700	0.20336900	-1.17821900
H	-2.16717800	0.59476700	-1.93439900
C	-4.24848700	-0.99244400	0.90764000
H	-2.37161300	-1.56428500	1.77312400
C	-4.90315100	-0.35888500	-0.14831000
H	-4.62814800	0.66976400	-2.03045500

H	-4.81625000	-1.46420300	1.70653500
Br	-6.87029100	-2.09095100	-1.54919300
C	1.17491500	3.41106300	0.71220800
C	1.65118000	2.62879200	-0.34059600
C	1.07268600	1.38738700	-0.60650000
C	0.01041600	0.90963900	0.16840300
C	-0.46553500	1.70503900	1.21739100
C	0.11316400	2.94430100	1.49078300
H	1.62372300	4.37791100	0.92300800
H	2.47440600	2.97805300	-0.95721500
H	1.46672000	0.77080000	-1.40935900
H	-1.29937800	1.34973000	1.81722300
H	-0.26748300	3.54869200	2.31005200
Ni	-6.78137700	-0.23534600	-0.12739300
C	-9.14412300	0.29144000	-0.42420700
C	-9.00445200	-0.57996200	0.60602800
C	-8.84722700	-0.26062700	2.07463900
C	-8.00689500	1.00229400	2.37451900
C	-6.78172800	1.14379700	1.48755100
C	-6.71671200	1.80687500	0.27547200
C	-7.84335300	2.46447400	-0.48738000
C	-9.22762000	1.79572200	-0.32578600
H	-9.25027500	-0.13608000	-1.41868400
H	-9.05135200	-1.63770700	0.36095300
H	-8.36334400	-1.12360900	2.54584400
H	-9.83363800	-0.16930000	2.55213400
H	-8.62544500	1.90003700	2.29809600
H	-7.67329800	0.95252800	3.41632100
H	-5.82963200	0.90766400	1.95506800
H	-5.72390400	2.06287800	-0.08563200
H	-7.56780400	2.45798200	-1.54889400
H	-7.90652800	3.52476300	-0.19884700
H	-9.69009600	2.09402400	0.61744600
H	-9.88339400	2.16675700	-1.12072500

im3f

SCF Energy (a.u.) = -1897.567666

Thermal correction to Gibbs free energy (a.u.) = 0.601278

Charge = 0, Multiplicity = 1

C	7.67223400	-0.48048100	-1.18857400
C	8.35941000	0.54322000	-1.85717700
C	9.66095100	0.88437000	-1.51039600
C	10.33130900	0.21017600	-0.47405200
C	9.63981700	-0.81459300	0.19131100
C	8.33528200	-1.15328900	-0.15761200
H	7.86174400	1.07894600	-2.66275500
H	10.16340000	1.68031100	-2.05163100
H	10.13506500	-1.34964500	0.99798900
H	7.81703000	-1.93757800	0.38684100
C	11.70607100	0.52805300	-0.06370200
C	12.51520700	1.46088800	-0.58125700
H	12.08333300	-0.08047400	0.75813600
H	13.51829800	1.60729500	-0.19322500
H	12.21771000	2.10810300	-1.40171000
C	5.24841700	0.14769500	-0.77528100
C	6.23577800	-0.78796800	-1.52647200
H	6.06690100	-0.67576300	-2.60425600
H	6.01203200	-1.82850200	-1.26784300
H	5.56723400	1.17604600	-0.98738100
C	3.80701200	0.00744000	-1.23326600
C	2.92066800	1.07099900	-1.01146200
C	3.29526300	-1.16965100	-1.78614600
C	1.56455100	0.94636100	-1.29295300
H	3.30095500	1.99735500	-0.58708600
C	1.93299300	-1.29768100	-2.06020100
H	3.95146300	-2.01106300	-1.98327900
C	1.04550700	-0.25267300	-1.80017700
H	0.89366300	1.77748500	-1.08677800

H	1.54928800	-2.23987000	-2.44218000
C	5.68908700	-0.50578300	3.48821100
C	6.34344400	0.55796600	2.86677200
C	6.18057400	0.77601400	1.49796400
C	5.36233300	-0.05959800	0.73094000
C	4.70451100	-1.12223200	1.36435000
C	4.86950000	-1.34581800	2.73073500
H	5.81400500	-0.67843200	4.55351200
H	6.98452100	1.21770400	3.44496900
H	6.70786800	1.59347300	1.01364800
H	4.04663000	-1.76682700	0.78889200
H	4.35550500	-2.17704400	3.20680700
C	-1.06790700	-0.68164300	-0.50963500
C	-0.44357200	-0.45310000	-1.91350000
H	-0.92370200	0.42212600	-2.37039400
H	-0.65554000	-1.31457500	-2.55626500
H	-0.79233800	0.19496500	0.08936500
C	-2.58647800	-0.73709800	-0.51623100
C	-3.25896900	-0.50689800	0.69280100
C	-3.34900400	-0.98422600	-1.65991800
C	-4.64835900	-0.45498900	0.75109800
H	-2.67931900	-0.34980700	1.59906300
C	-4.75079100	-0.93360700	-1.62041300
H	-2.86359700	-1.19369800	-2.60809100
C	-5.38316800	-0.61499600	-0.42502600
H	-5.14481200	-0.25426800	1.69455400
H	-5.32146300	-1.11335600	-2.52705300
Br	-7.94952400	-2.02834300	0.56943800
C	0.82583800	-4.11947000	1.32130000
C	1.26303600	-2.82895100	1.62327100
C	0.63436100	-1.72487700	1.04765500
C	-0.44030700	-1.89212500	0.16659100
C	-0.87595100	-3.18935400	-0.12575700
C	-0.24668100	-4.29611100	0.44453200

H	1.31255900	-4.98130400	1.76936700
H	2.09183900	-2.67576700	2.30865200
H	0.99533100	-0.72386200	1.26644400
H	-1.72101900	-3.33118200	-0.79414200
H	-0.59900000	-5.29677600	0.20948100
Ni	-7.17040300	-0.12929500	-0.37506600
C	-2.90499800	2.97350100	0.54053600
C	-3.14032800	2.60066600	-0.78010000
C	-4.44344200	2.32975900	-1.17748800
C	-5.50851200	2.40902500	-0.26615300
C	-5.23984500	2.83506600	1.04352600
C	-3.93994900	3.11710700	1.45845300
H	-2.32058300	2.50604300	-1.48218800
H	-4.62261800	2.02127400	-2.20018600
H	-6.05433700	2.91010600	1.75932800
H	-3.73762200	3.42022700	2.47913100
C	-6.86977700	1.98440600	-0.61688800
C	-7.25582400	1.33470400	-1.77870300
H	-7.65216100	2.34521800	0.05258300
H	-8.30898100	1.29581400	-2.05476400
H	-6.55167700	1.11453600	-2.57419500
Br	-1.06367800	3.26468000	1.11768900

TS2f

SCF Energy (a.u.) = -1897.551216

Thermal correction to Gibbs free energy (a.u.) = 0.601040

Charge = 0, Multiplicity = 1

C	9.07384400	-0.60052100	0.28195500
C	9.97667100	-1.00717000	-0.71136500
C	11.25398400	-0.46596300	-0.79035900
C	11.68158000	0.51009900	0.12747800
C	10.77482800	0.91270100	1.12080700
C	9.49526300	0.36940100	1.19676200
H	9.66898300	-1.76145100	-1.43248800

H	11.92777300	-0.80679900	-1.57055400
H	11.08035400	1.66751400	1.84133100
H	8.80760600	0.71323300	1.96429500
C	13.01901100	1.11797500	0.09183400
C	14.00832500	0.85842700	-0.77221000
H	13.19717600	1.86158900	0.86855300
H	14.96084100	1.37405800	-0.70144200
H	13.91339700	0.13153300	-1.57416200
C	6.72537800	-0.35653800	-0.64719600
C	7.66715500	-1.14166000	0.30800500
H	7.66000700	-2.19718200	0.01056500
H	7.27169000	-1.08763600	1.32793100
H	7.20658400	-0.35846900	-1.63323500
C	5.35355400	-0.98924700	-0.80439500
C	4.61833900	-0.73464600	-1.97017800
C	4.75050800	-1.75511700	0.19772500
C	3.31369700	-1.19657300	-2.11197300
H	5.07260800	-0.14741200	-2.76475800
C	3.43911200	-2.20938200	0.05926800
H	5.29219200	-1.98574400	1.10923200
C	2.69468100	-1.92223400	-1.08626600
H	2.75896000	-0.97178300	-3.02063900
H	2.97516400	-2.76215600	0.87152200
C	6.52342100	3.76017500	0.69796100
C	7.37717900	3.39993400	-0.34471800
C	7.42048000	2.07740100	-0.78823900
C	6.61238500	1.09736400	-0.20281300
C	5.75309200	1.46934000	0.83919800
C	5.71212800	2.78870300	1.28893400
H	6.48868600	4.78837200	1.04702500
H	8.01436500	4.14596000	-0.81153100
H	8.10284800	1.79642600	-1.58589500
H	5.10092300	0.72726600	1.28986400
H	5.04498600	3.05934700	2.10342900

C	0.36027700	-1.00275800	-0.86406600
C	1.22662100	-2.25850800	-1.15702800
H	0.96268900	-2.64836500	-2.14811900
H	0.99150500	-3.03824800	-0.42399300
H	0.59384200	-0.27433200	-1.65217000
C	-1.13984900	-1.25466800	-0.91702300
C	-2.00435900	-0.15461300	-0.77636200
C	-1.70216700	-2.52231300	-1.09355100
C	-3.38521900	-0.30937100	-0.80754600
H	-1.57857400	0.83426000	-0.62737100
C	-3.08996100	-2.69897800	-1.12418900
H	-1.06577200	-3.39180200	-1.21569200
C	-3.93378300	-1.59854400	-0.93380200
H	-4.03296300	0.55585700	-0.69827500
H	-3.50334400	-3.69276700	-1.27302100
Br	-6.63818000	-2.42167100	1.97400600
C	1.67268300	0.69842200	2.89541900
C	2.10495300	1.24592200	1.68693500
C	1.65720100	0.71189300	0.47839100
C	0.77308900	-0.37146400	0.45903300
C	0.33959200	-0.91075500	1.67601600
C	0.78709300	-0.38183700	2.88636600
H	2.01876700	1.11209700	3.83845400
H	2.79297400	2.08605400	1.67757900
H	2.01944700	1.12325800	-0.45947300
H	-0.35640200	-1.74567300	1.67472400
H	0.44034800	-0.81032500	3.82257500
Ni	-5.49039700	-1.92066200	0.05163200
C	-8.45384600	2.43461200	-0.49800200
C	-7.31420700	2.31578200	-1.28769200
C	-6.79953700	1.04558800	-1.53688000
C	-7.40970400	-0.10283900	-1.00574800
C	-8.55965900	0.05869800	-0.21412900
C	-9.08743600	1.31934300	0.04440100

H	-6.83831000	3.19512800	-1.70614200
H	-5.91720800	0.96013800	-2.16263600
H	-9.02401800	-0.81676200	0.22877600
H	-9.97013800	1.43115800	0.66310300
C	-6.89176600	-1.46500200	-1.23433700
C	-5.73646900	-1.75903400	-2.01645200
H	-7.61078600	-2.26574700	-1.07324100
H	-5.63585800	-2.76207800	-2.42114400
H	-5.30909500	-0.99094900	-2.65017800
Br	-9.18296600	4.21020500	-0.14595700

im4f

SCF Energy (a.u.) = -1897.586131

Thermal correction to Gibbs free energy (a.u.) = 0.605207

Charge = 0, Multiplicity = 1

C	8.37369300	-0.18917700	0.81235600
C	9.42792600	-0.90861700	0.23085900
C	10.69732100	-0.35668100	0.10974500
C	10.96411200	0.94559500	0.56889600
C	9.90594100	1.66118500	1.15132700
C	8.63481300	1.10592700	1.27029500
H	9.24605800	-1.91832300	-0.13117000
H	11.49059700	-0.94363400	-0.34310600
H	10.08569500	2.67094800	1.51230500
H	7.82975800	1.68914200	1.70832100
C	12.28547700	1.58047600	0.46683400
C	13.40417300	1.05377500	-0.04678900
H	12.32981100	2.59536400	0.86185600
H	14.32902000	1.62149900	-0.06967000
H	13.44611800	0.04937100	-0.45903000
C	6.20292300	-0.53879200	-0.45396800
C	6.98531700	-0.77363900	0.86818600
H	7.03478600	-1.85327900	1.05422800
H	6.43061800	-0.32455000	1.69896000

H	6.83703000	-0.91780000	-1.26527300
C	4.87996100	-1.28211100	-0.51884800
C	4.33078600	-1.57989900	-1.77359800
C	4.13814500	-1.61467500	0.61840500
C	3.06838000	-2.15332900	-1.88725100
H	4.89566500	-1.33556300	-2.67010300
C	2.86830500	-2.18024800	0.50392700
H	4.53477900	-1.41230100	1.60784900
C	2.30679400	-2.44006500	-0.74734000
H	2.65771600	-2.35963000	-2.87357700
H	2.29003100	-2.38484600	1.40073200
C	5.74251100	3.73202300	-1.04063300
C	6.76027700	3.03627400	-1.69329100
C	6.88890600	1.65768700	-1.51824400
C	6.00453200	0.95348900	-0.69472500
C	4.98106400	1.65905100	-0.04860700
C	4.85383200	3.03751400	-0.21654800
H	5.64073300	4.80549100	-1.17311200
H	7.45871400	3.56536700	-2.33573900
H	7.69629900	1.12274700	-2.01099800
H	4.27023100	1.12570800	0.57549100
H	4.05865100	3.57136500	0.29757900
C	-0.03996300	-1.67101700	-1.22676900
C	0.86945400	-2.87836100	-0.87053500
H	0.76249800	-3.64843100	-1.64515700
H	0.53402700	-3.31440700	0.07711900
H	0.29564300	-1.30277400	-2.20542900
C	-1.51698800	-2.01730500	-1.35108700
C	-2.40925700	-1.00292600	-1.70093600
C	-2.03688500	-3.29782300	-1.07228200
C	-3.79893700	-1.21808700	-1.70016200
H	-2.02691000	-0.01320000	-1.93177300
C	-3.40482100	-3.53090300	-1.06298800
H	-1.36637300	-4.11110100	-0.82094500

C	-4.32183900	-2.49327900	-1.34881900
H	-4.46117800	-0.42663900	-2.03552000
H	-3.78700500	-4.51442200	-0.80462600
Br	-4.13712400	-0.93733300	2.67068600
C	0.59146300	1.51315200	1.64174400
C	1.23529700	1.54407100	0.40370900
C	1.01622900	0.52582100	-0.52502300
C	0.15492800	-0.53513900	-0.22859100
C	-0.48331900	-0.56064900	1.01762100
C	-0.27138900	0.45777700	1.94623200
H	0.75445900	2.30948900	2.36246400
H	1.90689400	2.35977200	0.15247300
H	1.53594100	0.54461600	-1.47884000
H	-1.16592900	-1.36817400	1.26759600
H	-0.79437200	0.42730200	2.89724700
Ni	-4.29073800	-1.36009500	0.42340600
C	-8.11868500	2.00646300	-0.37289500
C	-7.70052300	1.35123600	-1.52502500
C	-7.05824700	0.11933700	-1.40268300
C	-6.82715200	-0.46742800	-0.14588900
C	-7.27109500	0.23192700	0.99495000
C	-7.91385200	1.45955300	0.89242200
H	-7.87515100	1.78618800	-2.50252200
H	-6.75127600	-0.38783300	-2.31141300
H	-7.07699400	-0.18851400	1.97657800
H	-8.24323900	1.98454100	1.78163900
C	-6.12845900	-1.75877300	0.03857900
C	-5.82600900	-2.66378900	-1.16068400
H	-6.46569100	-2.29542200	0.92611100
H	-6.05213900	-3.70704800	-0.92460100
H	-6.38621200	-2.40066900	-2.06413200
Br	-9.01800500	3.73346400	-0.53264200

SCF Energy (a.u.) = -2038.628845

Thermal correction to Gibbs free energy (a.u.) = 0.669341

Charge = 0, Multiplicity = 1

C	8.28357000	-0.19014000	0.80008300
C	9.33955100	-0.89685900	0.20628700
C	10.60516700	-0.33612700	0.08601600
C	10.86624800	0.96257700	0.55836500
C	9.80636800	1.66542500	1.15307600
C	8.53903800	1.10137300	1.27119800
H	9.16206600	-1.90353500	-0.16619700
H	11.39995500	-0.91335000	-0.37658600
H	9.98169500	2.67223800	1.52433600
H	7.73242200	1.67499100	1.71892000
C	12.18339300	1.60639200	0.45771200
C	13.30273900	1.09234500	-0.06719400
H	12.22360400	2.61687600	0.86429500
H	14.22412000	1.66576600	-0.08773100
H	13.34860200	0.09313400	-0.49145900
C	6.10880800	-0.53690100	-0.46019600
C	6.89889200	-0.78336400	0.85521900
H	6.95550800	-1.86490700	1.02770400
H	6.34556500	-0.34777700	1.69407800
H	6.74123500	-0.90201800	-1.27913100
C	4.78976200	-1.28685800	-0.52806900
C	4.23635100	-1.57222100	-1.78392300
C	4.05455100	-1.63649100	0.60828400
C	2.97608400	-2.14999700	-1.89891600
H	4.79604700	-1.31441700	-2.67990800
C	2.78657100	-2.20605700	0.49229900
H	4.45467800	-1.44400500	1.59833600
C	2.22030300	-2.45344100	-0.75931300
H	2.56183200	-2.34620700	-2.88574400
H	2.21291900	-2.42397400	1.38905000
C	5.61718100	3.73744600	-0.99391800

C	6.63588600	3.05622800	-1.66026100
C	6.77490100	1.67660700	-1.50192200
C	5.90009400	0.95698000	-0.68161500
C	4.87592600	1.64820300	-0.02119900
C	4.73817300	3.02753800	-0.17257100
H	5.50705000	4.81155300	-1.11384200
H	7.32683100	3.59742200	-2.30072400
H	7.58282700	1.15284600	-2.00567600
H	4.17276900	1.10265300	0.60111200
H	3.94214700	3.55013500	0.35174700
C	-0.13835800	-1.69656200	-1.21901400
C	0.78538500	-2.89872600	-0.88175000
H	0.68027800	-3.65951300	-1.66571500
H	0.45758900	-3.34983800	0.06150600
H	0.19814200	-1.30409200	-2.18778800
C	-1.60986000	-2.06287200	-1.35190000
C	-2.51336200	-1.06034500	-1.70260400
C	-2.11851000	-3.34361500	-1.05737400
C	-3.90298300	-1.27894600	-1.66423800
H	-2.14112600	-0.07156800	-1.95452200
C	-3.48568000	-3.57929000	-1.01548500
H	-1.44039100	-4.15373200	-0.81520600
C	-4.41213800	-2.54534800	-1.27549500
H	-4.57610800	-0.49410300	-1.99459800
H	-3.85851900	-4.56303800	-0.74340700
C	0.40968000	1.45684100	1.70614000
C	1.11629900	1.48106800	0.50259300
C	0.92670000	0.47158600	-0.44186300
C	0.03316200	-0.57645800	-0.19675400
C	-0.66647600	-0.59549900	1.01654700
C	-0.48547800	0.41547700	1.95981100
H	0.54760300	2.24859400	2.43713700
H	1.81165200	2.28751400	0.28859600
H	1.49205500	0.48878400	-1.36927300

H	-1.38044200	-1.38744800	1.22502300
H	-1.06205500	0.39312500	2.87958800
Ni	-4.33216500	-1.31874700	0.47733800
C	-8.24623100	1.96032100	-0.34661000
C	-7.85280700	1.26495000	-1.48189300
C	-7.18683600	0.04733600	-1.32940800
C	-6.90692000	-0.48568300	-0.05986500
C	-7.32880900	0.25476300	1.06274900
C	-7.99264700	1.46832000	0.93236100
H	-8.06257600	1.65655800	-2.47090100
H	-6.89475000	-0.48860300	-2.22670400
H	-7.10382200	-0.12457700	2.05470600
H	-8.30418800	2.02389000	1.80958400
C	-6.17064500	-1.75534700	0.15887200
C	-5.90561100	-2.70674300	-1.01813300
H	-6.50634900	-2.26742800	1.06347300
H	-6.11831900	-3.74157000	-0.73479800
H	-6.50283200	-2.48388100	-1.90965500
Br	-9.18312500	3.66778100	-0.54619500
O	-4.21588800	-0.75649100	2.14588400
C	-4.59620300	-1.48628400	3.27979000
C	-3.96848800	-0.85839700	4.52293800
H	-4.28933500	-2.54585400	3.21398900
H	-5.69620100	-1.48363700	3.39583200
H	-4.26841400	-1.39553700	5.43126400
H	-2.87534300	-0.88457700	4.44754800
H	-4.27773600	0.18838200	4.61288500

im6f

SCF Energy (a.u.) = -2642.358953

Thermal correction to Gibbs free energy (a.u.) = 0.905384

Charge = 0, Multiplicity = 1

C	-9.21019500	-0.09194400	-0.64126800
C	-10.27701600	-0.85958400	-0.15161800

C	-11.50284900	-0.28013800	0.15208800
C	-11.71136300	1.09960800	-0.02320300
C	-10.64092900	1.86352100	-0.51476000
C	-9.41347900	1.28029500	-0.81718800
H	-10.13989100	-1.92926900	-0.00809700
H	-12.30768500	-0.90550900	0.52627400
H	-10.77580000	2.93301700	-0.65705100
H	-8.59647200	1.89852100	-1.17831400
C	-12.98476800	1.76665400	0.28174000
C	-14.10636800	1.20482800	0.74979600
H	-12.98674200	2.84079900	0.09675000
H	-14.99252300	1.80209200	0.94001200
H	-14.18867100	0.14192200	0.95950400
C	-7.00415500	-0.79400500	0.39742100
C	-7.86458600	-0.72239300	-0.89473800
H	-7.98896000	-1.73981200	-1.28467900
H	-7.32573900	-0.14571300	-1.65414500
H	-7.61863700	-1.29410000	1.15650100
C	-5.72707200	-1.59991200	0.23490800
C	-5.13843600	-2.17345700	1.37047800
C	-5.05933700	-1.72808500	-0.98642500
C	-3.90689300	-2.81579900	1.29416100
H	-5.64607200	-2.09105700	2.32863400
C	-3.81941200	-2.36284300	-1.06022400
H	-5.48932800	-1.30947400	-1.89049900
C	-3.21524900	-2.89787300	0.07871600
H	-3.46270900	-3.23704400	2.19365300
H	-3.29539800	-2.40633300	-2.01120200
C	-6.24730300	3.24434800	1.78224800
C	-7.27031000	2.48451800	2.34959300
C	-7.49485700	1.17749700	1.91470600
C	-6.70233900	0.60886600	0.91249200
C	-5.67356400	1.37731700	0.35216500
C	-5.45034400	2.68544000	0.78036500

H	-6.07035800	4.26231000	2.11784600
H	-7.89801400	2.90854900	3.12848400
H	-8.30613300	0.59612100	2.34445400
H	-5.03357900	0.94444800	-0.41092500
H	-4.65159700	3.27059300	0.33167700
C	-0.80725900	-2.35736200	0.58476900
C	-1.80061200	-3.41569200	0.03058500
H	-1.69964100	-4.33695900	0.61846600
H	-1.53385200	-3.65468100	-1.00477000
H	-1.10907600	-2.15616900	1.62052100
C	0.63986700	-2.82264300	0.61576800
C	1.56344300	-2.06327500	1.32872400
C	1.10574800	-3.95177200	-0.08841600
C	2.93924100	-2.35831400	1.29547800
H	1.23234000	-1.20028800	1.89444500
C	2.45703900	-4.25958200	-0.13466700
H	0.40662900	-4.58220800	-0.62658100
C	3.40967400	-3.45491100	0.52887200
H	3.61068400	-1.78558300	1.92567800
H	2.80040400	-5.11787000	-0.70596800
C	-1.28196000	1.32919800	-1.64337000
C	-1.96540700	1.13928700	-0.44095300
C	-1.79341100	-0.04065200	0.28353200
C	-0.93743600	-1.04510600	-0.18106800
C	-0.25415600	-0.84407600	-1.38582800
C	-0.42357900	0.33355500	-2.11212700
H	-1.40267200	2.25281900	-2.20197600
H	-2.62864600	1.90907500	-0.05742600
H	-2.34524300	-0.19100200	1.20691600
H	0.43191300	-1.60220700	-1.75186100
H	0.13213500	0.48031400	-3.03235200
Ni	3.62685500	-1.65703000	-0.65994600
C	7.48788200	0.70592500	1.72053200
C	6.96226200	-0.34297000	2.46481000

C	6.28391100	-1.36553500	1.80048500
C	6.12521300	-1.35652200	0.40404300
C	6.68427600	-0.27807300	-0.30837400
C	7.36051100	0.75125000	0.33414400
H	7.07304600	-0.36594600	3.54307600
H	5.87476100	-2.17575100	2.39473200
H	6.53542900	-0.23333700	-1.38163000
H	7.75861300	1.58592100	-0.23057900
C	5.36822800	-2.38677300	-0.34802500
C	4.90632200	-3.66799000	0.35541100
H	5.08051400	-4.54161700	-0.27930200
H	5.40958900	-3.85573900	1.31103500
Br	8.40838200	2.16462700	2.64339300
O	3.87234700	-0.72853000	-2.16820100
C	3.98202800	-1.41242600	-3.38742700
C	2.70193300	-2.14734300	-3.78994100
H	4.82212400	-2.13151800	-3.37001100
H	4.23117200	-0.67543300	-4.17158800
H	2.80796700	-2.63337900	-4.76879600
H	2.45313600	-2.91512900	-3.04639200
H	1.86353800	-1.44272800	-3.84038200
H	5.78736000	-2.55765100	-1.34159700
C	1.98760700	0.99099300	3.27277700
C	3.34293400	0.93379000	2.93316300
C	3.74333500	1.19805700	1.62303900
C	2.80163600	1.50278600	0.62523700
C	1.44281300	1.53773700	0.98051700
C	1.03739200	1.29685500	2.29332500
H	1.67385500	0.79987500	4.29617500
H	4.08757400	0.69713400	3.68895300
H	4.79521100	1.17213500	1.36407000
H	0.70235900	1.75626800	0.21920400
H	-0.01855900	1.33540000	2.54789200
C	2.68997100	2.15236300	-3.15205100

C	5.04680500	2.17946400	-2.40840400
C	4.02240000	2.90429300	-3.29494600
H	2.76905600	1.15799500	-3.60552100
H	5.98492400	2.74596500	-2.37002400
B	3.25965600	1.82516100	-0.83381100
O	2.29881000	1.98699300	-1.79479200
O	4.59222600	2.02441000	-1.06848000
H	1.88694100	2.70226300	-3.65779200
H	5.24933700	1.18090500	-2.80903300
C	4.48367700	2.84522200	-4.75535500
H	4.60530900	1.80943100	-5.09425200
H	3.75732400	3.33449100	-5.41525800
H	5.44458700	3.35779000	-4.88246700
C	3.86242100	4.36473900	-2.84448900
H	4.81375400	4.90249700	-2.93208000
H	3.12206100	4.88249300	-3.46578800
H	3.53415300	4.43030800	-1.80338000

TS3f

SCF Energy (a.u.) = -2642.353372

Thermal correction to Gibbs free energy (a.u.) = 0.906902

Charge = 0, Multiplicity = 1

C	9.31537700	0.09250700	0.56311700
C	10.38018600	-0.78389900	0.30772900
C	11.59534900	-0.31949300	-0.18051600
C	11.79472100	1.04936300	-0.43427100
C	10.72639400	1.92278100	-0.17571800
C	9.50961300	1.45436500	0.31243000
H	10.25000600	-1.84738900	0.49662800
H	12.39892600	-1.02623400	-0.36395400
H	10.85429300	2.98568200	-0.36580600
H	8.69350600	2.15019300	0.48547800
C	13.05657000	1.59702500	-0.95128000
C	14.17489900	0.92362500	-1.24889200

H	13.05205300	2.67676100	-1.10012900
H	15.05216000	1.43824400	-1.62804200
H	14.26319800	-0.15259600	-1.12858000
C	7.09978500	-0.90071900	-0.17303200
C	7.97979800	-0.43602000	1.02053000
H	8.11961100	-1.28596600	1.69931500
H	7.44791100	0.34250600	1.57784000
H	7.70631300	-1.60670300	-0.75408900
C	5.83177500	-1.62214400	0.24936300
C	5.22631400	-2.51078500	-0.64989600
C	5.18731800	-1.37806400	1.46551800
C	4.00015400	-3.10077200	-0.36096600
H	5.71590200	-2.71956500	-1.59818100
C	3.95305200	-1.96221200	1.75038600
H	5.63076200	-0.70690900	2.19376500
C	3.33138600	-2.81456600	0.83621100
H	3.54211800	-3.77245500	-1.08407300
H	3.44682300	-1.71803700	2.68037400
C	6.29079500	2.52172800	-2.70891200
C	7.31199800	1.62886800	-3.03411700
C	7.55293800	0.51696700	-2.22578900
C	6.77874300	0.27746100	-1.08593800
C	5.75114700	1.17596600	-0.77025800
C	5.51190400	2.29111000	-1.57253200
H	6.10125300	3.38884700	-3.33530300
H	7.92560200	1.79803400	-3.91465700
H	8.36304500	-0.16465000	-2.47068700
H	5.12436800	0.99329500	0.09755800
H	4.71485300	2.98235400	-1.31065100
C	0.92210700	-2.43071500	0.23116100
C	1.91785400	-3.28786900	1.06143700
H	1.80046700	-4.34097100	0.77613100
H	1.67250200	-3.20602100	2.12568300
H	1.21266900	-2.54625200	-0.82008300

C	-0.52687200	-2.87395100	0.34580900
C	-1.41261200	-2.53255500	-0.67094500
C	-1.03024400	-3.57769600	1.46022000
C	-2.79135200	-2.80858400	-0.57299200
H	-1.04917700	-2.01203800	-1.54846800
C	-2.38023200	-3.86788100	1.57341300
H	-0.35800000	-3.89096300	2.25170400
C	-3.29626700	-3.47158000	0.57337900
H	-3.43238800	-2.60252100	-1.42456200
H	-2.75247200	-4.39875100	2.44548900
C	1.46617400	1.74854600	1.24221100
C	2.06155500	1.21544800	0.09753700
C	1.86829400	-0.12641200	-0.23115800
C	1.07543300	-0.95252000	0.57260700
C	0.48298500	-0.40921400	1.71732700
C	0.67607200	0.93090100	2.05181500
H	1.60546200	2.79565900	1.49477800
H	2.67425900	1.84003800	-0.54578400
H	2.35417100	-0.54114200	-1.10978400
H	-0.15196400	-1.02934400	2.34203900
H	0.19007500	1.34160000	2.93083300
Ni	-3.62915800	-1.32280800	0.81144100
C	-7.67842000	-0.12217900	-1.89909400
C	-7.05605000	-1.29884700	-2.29839200
C	-6.30666600	-2.01384500	-1.36409100
C	-6.16927000	-1.56976200	-0.03798100
C	-6.82598100	-0.37618100	0.32402800
C	-7.57620200	0.35019300	-0.59231600
H	-7.14722900	-1.65351400	-3.31887000
H	-5.81496300	-2.92421500	-1.69125300
H	-6.68426700	0.01386100	1.32549900
H	-8.05067400	1.27991400	-0.30130600
C	-5.30792800	-2.23693300	0.96318700
C	-4.79567100	-3.66160600	0.73941600

H	-5.00028900	-4.29608200	1.60718500
H	-5.23652000	-4.15249700	-0.13462100
Br	-8.70981400	0.90305500	-3.20750600
O	-4.05834800	0.11516800	1.83479800
C	-4.03783700	-0.00792000	3.23680300
C	-2.65262800	-0.32291500	3.79780700
H	-4.75181800	-0.78609300	3.55980800
H	-4.40112200	0.93689000	3.66708600
H	-2.66270600	-0.35092600	4.89528300
H	-2.30917300	-1.29830800	3.43088800
H	-1.94135000	0.43759900	3.46402600
H	-5.64293800	-2.05369200	1.98503700
C	-2.08638100	0.02312500	-2.99560600
C	-3.45104700	0.04506800	-2.69605900
C	-3.88971600	0.58676600	-1.48630800
C	-2.98039100	1.09342700	-0.53722600
C	-1.61121700	1.04663100	-0.85344400
C	-1.16776100	0.52873400	-2.07145400
H	-1.74198100	-0.37520400	-3.94725200
H	-4.17677800	-0.33542300	-3.41027100
H	-4.95151300	0.65115500	-1.28259600
H	-0.89317300	1.44332100	-0.14535900
H	-0.10461500	0.52102900	-2.29539900
C	-2.87547600	3.27839800	2.62168600
C	-5.17958100	3.24937500	1.72553400
C	-4.05625000	4.17717000	2.21795400
H	-3.12373300	2.73868200	3.54768800
H	-6.02442000	3.84294600	1.35490400
B	-3.49438300	1.82589500	0.77008200
O	-2.51733500	2.34701200	1.61514300
O	-4.74855600	2.41436100	0.66809000
H	-1.98977100	3.89243900	2.82998000
H	-5.54754400	2.63278200	2.56044200
C	-4.53622400	4.96779400	3.43927700

H	-4.86158000	4.30068700	4.24701300
H	-3.73619900	5.60700200	3.83193100
H	-5.38029100	5.61672100	3.17721100
C	-3.63333500	5.13384000	1.09255100
H	-4.47849500	5.75630200	0.77560800
H	-2.83124100	5.79946900	1.43337200
H	-3.27268300	4.58428000	0.21932600

im7f

SCF Energy (a.u.) = -2642.355767

Thermal correction to Gibbs free energy (a.u.) = 0.908019

Charge = 0, Multiplicity = 1

C	-9.25154500	-0.09104600	-0.45472200
C	-10.29234600	-0.96934400	-0.11934900
C	-11.50133500	-0.49851600	0.37798700
C	-11.71841700	0.87896400	0.56066500
C	-10.67418300	1.75414500	0.22206100
C	-9.46350800	1.27934000	-0.27502100
H	-10.14807600	-2.03947400	-0.25219900
H	-12.28622700	-1.20711100	0.62439300
H	-10.81604800	2.82379000	0.35613200
H	-8.66563500	1.97781200	-0.51093700
C	-12.97470900	1.43373500	1.08359600
C	-14.07135900	0.75954300	1.45173500
H	-12.98581000	2.52008000	1.17151900
H	-14.94666600	1.27995600	1.82747800
H	-14.14319200	-0.32309400	1.39460800
C	-6.99813700	-1.00450400	0.26993700
C	-7.92009400	-0.62214600	-0.92107000
H	-8.06387000	-1.51102200	-1.54714200
H	-7.41831000	0.13255000	-1.53611700
H	-7.57514500	-1.68603300	0.90757500
C	-5.72988700	-1.72780400	-0.14863400
C	-5.07525900	-2.54215200	0.78594100

C	-5.13152800	-1.55180100	-1.39950500
C	-3.84597300	-3.12419200	0.49470700
H	-5.52840900	-2.69699500	1.76225300
C	-3.89399300	-2.12767100	-1.68739100
H	-5.61347500	-0.93912300	-2.15428700
C	-3.22338100	-2.90408400	-0.74082200
H	-3.34886200	-3.73635300	1.24438400
H	-3.42387800	-1.93468000	-2.64787600
C	-6.17169900	2.56676500	2.58534200
C	-7.17296800	1.68227500	2.98661700
C	-7.41947800	0.52333700	2.24917500
C	-6.67077900	0.22824400	1.10531500
C	-5.66325600	1.11923100	0.71274800
C	-5.41847300	2.28084500	1.44425600
H	-5.97762300	3.47014300	3.15667300
H	-7.76654200	1.89428900	3.87160900
H	-8.21420500	-0.15263100	2.55302400
H	-5.05624600	0.89485000	-0.15937700
H	-4.63685400	2.96501300	1.12385900
C	-0.80643900	-2.41591100	-0.25286300
C	-1.80648500	-3.35926600	-0.98038400
H	-1.65055000	-4.38336000	-0.61848300
H	-1.59992000	-3.35551200	-2.05577000
H	-1.06461900	-2.45102700	0.81206600
C	0.64518100	-2.84152400	-0.37593200
C	1.53151900	-2.53398700	0.65010700
C	1.15259900	-3.48895400	-1.52222500
C	2.91468100	-2.78509400	0.53065500
H	1.16712800	-2.05818900	1.55239200
C	2.50555700	-3.75062700	-1.65931800
H	0.47852300	-3.77870600	-2.32131500
C	3.41975900	-3.39008300	-0.64728300
H	3.55542900	-2.62678900	1.39293300
H	2.87940600	-4.23622600	-2.55665900

C	-1.43527000	1.67235400	-1.55148600
C	-2.01250000	1.20814900	-0.36779600
C	-1.79710800	-0.10560700	0.04734900
C	-0.99664300	-0.97187500	-0.70650100
C	-0.42422700	-0.49748300	-1.89112800
C	-0.64162700	0.81398500	-2.31254500
H	-1.59009300	2.69901900	-1.87047900
H	-2.62597200	1.86675400	0.23996100
H	-2.26794400	-0.46721100	0.95706500
H	0.22303500	-1.14294200	-2.47718600
H	-0.16653400	1.17201600	-3.21952400
Ni	3.75591200	-1.14492300	-0.69684700
C	7.80865000	-0.08295300	1.88302300
C	7.15891200	-1.25226700	2.26194900
C	6.40520900	-1.94071200	1.31303500
C	6.28805200	-1.47846800	-0.01035100
C	6.97641200	-0.29628300	-0.35279100
C	7.73139400	0.40443900	0.57989500
H	7.23245700	-1.62032200	3.27904700
H	5.89082600	-2.84376400	1.62469200
H	6.87110300	0.10355300	-1.35522100
H	8.23441800	1.32319600	0.30202600
C	5.40331000	-2.10820800	-1.01228300
C	4.91753600	-3.54666100	-0.83507400
H	5.12663600	-4.14799700	-1.72514100
H	5.37777300	-4.05683000	0.01743500
Br	8.84961800	0.90185700	3.21134100
O	4.18591700	0.35222800	-1.74133000
C	4.34761000	0.30669700	-3.15423400
C	3.18554800	-0.38331800	-3.85831900
H	5.29180900	-0.21038500	-3.37386300
H	4.45667800	1.33715100	-3.50807100
H	3.34056000	-0.39534500	-4.94446500
H	3.09033400	-1.41933200	-3.51094300

H	2.25708800	0.14391600	-3.62839900
H	5.69653700	-1.87811600	-2.03671600
C	2.15113400	0.13863100	2.93777600
C	3.51050900	0.18974600	2.61928300
C	3.91360400	0.62843100	1.35416700
C	2.97549500	1.00265800	0.36457700
C	1.61269600	0.92847200	0.71231500
C	1.20332300	0.51648700	1.98190200
H	1.83350400	-0.18053000	3.92772400
H	4.25877700	-0.08554300	3.35834800
H	4.97276400	0.73026800	1.14292100
H	0.87657100	1.22453800	-0.02510900
H	0.14341500	0.48884900	2.22167700
C	2.26353000	3.10028200	-2.67227000
C	4.42098700	3.78297800	-1.71575400
C	2.99746000	4.27996900	-2.01831000
H	2.70624100	2.91754100	-3.66967500
H	4.99168700	4.56963900	-1.20241500
B	3.44579500	1.60954600	-1.07340100
O	2.30165700	1.93159600	-1.89250800
O	4.43119500	2.64011600	-0.89671200
H	1.20683500	3.35939700	-2.83658300
H	4.93690800	3.58805800	-2.67516300
C	3.05446700	5.45816800	-2.99528800
H	3.56586000	5.18406700	-3.92647800
H	2.04565800	5.80244200	-3.25465300
H	3.59130200	6.30674200	-2.55432200
C	2.28754800	4.69356100	-0.72079300
H	2.82141200	5.51864100	-0.23390300
H	1.26450100	5.02948300	-0.93171000
H	2.23380600	3.86112400	-0.01547600

TS4f

SCF Energy (a.u.) = -2642.331521

Thermal correction to Gibbs free energy (a.u.) = 0.908937

Charge = 0, Multiplicity = 1

C	9.22799000	-0.30506400	0.32664700
C	10.25261000	-0.96848800	-0.36407800
C	11.43844400	-0.32195200	-0.69043000
C	11.64767100	1.02290000	-0.33615500
C	10.61960200	1.68226800	0.35619800
C	9.43206900	1.03216500	0.68073800
H	10.11421800	-2.00944600	-0.64845800
H	12.21141100	-0.86745600	-1.22316500
H	10.75564700	2.72320700	0.63940000
H	8.64543700	1.57222200	1.20008700
C	12.87984900	1.75738800	-0.65515900
C	13.95945800	1.29554800	-1.29846100
H	12.88702600	2.79386800	-0.31800300
H	14.81744200	1.93526700	-1.47956400
H	14.03391900	0.27572700	-1.66579100
C	6.94342200	-0.90753000	-0.59915800
C	7.91861100	-0.99725200	0.60733100
H	8.08976600	-2.05603600	0.83620600
H	7.44568800	-0.54592500	1.48615500
H	7.48917100	-1.28562900	-1.47274700
C	5.69200900	-1.75284200	-0.43604600
C	4.99321900	-2.15588400	-1.58254000
C	5.15092200	-2.07867700	0.81081600
C	3.77587300	-2.82168000	-1.48488600
H	5.40182400	-1.91868600	-2.56200400
C	3.92531500	-2.73808600	0.90790300
H	5.66896600	-1.79684600	1.72166800
C	3.20910700	-3.10049800	-0.23425300
H	3.24332400	-3.10561800	-2.39014700
H	3.50031800	-2.93633300	1.88821400
C	6.03714700	3.26887500	-1.33145500
C	7.00914800	2.61495700	-2.08865300

C	7.28039000	1.26466100	-1.86315300
C	6.58552500	0.54682200	-0.88443200
C	5.60596600	1.20966100	-0.13335000
C	5.33743000	2.56046500	-0.35177500
H	5.82461100	4.32032300	-1.50322700
H	7.56113300	3.15513200	-2.85283700
H	8.05337200	0.76451600	-2.44037300
H	5.03925300	0.66250300	0.61417500
H	4.57975500	3.06238000	0.24466900
C	0.78036100	-2.48693500	-0.41318100
C	1.79989600	-3.62570100	-0.12724900
H	1.62079200	-4.44211900	-0.83766000
H	1.63519100	-4.02520300	0.87892100
H	0.98615300	-2.13576700	-1.43120800
C	-0.67303000	-2.92840500	-0.37587000
C	-1.60645100	-2.26947100	-1.17893400
C	-1.14335300	-3.93013600	0.48620000
C	-2.97397500	-2.56151100	-1.09797800
H	-1.27492000	-1.49008600	-1.85714500
C	-2.50170400	-4.22380300	0.57991700
H	-0.44521600	-4.48357400	1.10650300
C	-3.44595900	-3.53840100	-0.19441800
H	-3.65753700	-2.07201700	-1.78726900
H	-2.84075100	-4.98767500	1.27503700
C	1.49984500	0.89073800	2.21278300
C	1.99123800	0.89252400	0.90634000
C	1.75707300	-0.19847600	0.06894700
C	1.02276600	-1.30201800	0.51628500
C	0.54959000	-1.30154200	1.83317300
C	0.78335700	-0.21469100	2.67583000
H	1.67191700	1.74252900	2.86450500
H	2.55299000	1.74270300	0.53096600
H	2.15601600	-0.19683600	-0.94123000
H	-0.03434200	-2.14220400	2.19401800

H	0.38996300	-0.22396700	3.68811000
Ni	-4.10995900	-1.01036100	0.49361100
C	-7.63758200	0.40600200	-1.79834700
C	-6.99631100	-0.64676500	-2.43982000
C	-6.34957000	-1.61272300	-1.67070700
C	-6.33132000	-1.55083100	-0.25788700
C	-7.02667300	-0.47087700	0.34624400
C	-7.66979900	0.50160600	-0.40743700
H	-6.98894600	-0.71197800	-3.52204200
H	-5.84736400	-2.42543600	-2.18467500
H	-7.01481600	-0.38105800	1.42737300
H	-8.17037800	1.33071900	0.07891800
C	-5.49159400	-2.42194900	0.58102400
C	-4.93393300	-3.73167500	0.01691300
H	-5.09540600	-4.55159700	0.72460000
H	-5.42817100	-4.03016000	-0.91660800
Br	-8.51006500	1.79002700	-2.87134700
O	-4.43308600	-0.20729900	2.21779800
C	-4.14013000	-0.90464800	3.44281100
C	-2.84231200	-1.69288700	3.38861300
H	-4.99423500	-1.56619700	3.61746300
H	-4.10950300	-0.15743100	4.24175900
H	-2.69049400	-2.22702200	4.33507800
H	-2.87169100	-2.42716500	2.57695100
H	-2.00279700	-1.01761400	3.21829600
H	-5.85487800	-2.50839500	1.60603000
C	-1.89252700	1.85561100	-2.34249700
C	-3.28677300	1.76950400	-2.27716800
C	-3.89459600	1.19431700	-1.15895200
C	-3.13543900	0.65675100	-0.09470500
C	-1.73689800	0.76919800	-0.18689800
C	-1.11778700	1.36594200	-1.28819900
H	-1.41460600	2.31766200	-3.20289200
H	-3.89738900	2.16602100	-3.08505800

H	-4.98039400	1.17739100	-1.10639600
H	-1.12225300	0.38479200	0.61904100
H	-0.03491200	1.44413000	-1.32154700
C	-1.96701800	2.55197900	2.60002700
C	-4.33676600	3.32457100	2.38621100
C	-2.87266600	3.74024500	2.17203500
H	-1.59281300	2.71461900	3.61804600
H	-5.00568400	4.10832700	2.01434600
B	-3.78198600	1.06469300	1.90611400
O	-2.61310700	1.28263500	2.62501600
O	-4.66865800	2.12545200	1.69894000
H	-1.09785300	2.48383500	1.93386700
H	-4.53132200	3.20226100	3.46393500
C	-2.55667500	4.95431400	3.05832400
H	-2.74736300	4.73981900	4.11693000
H	-1.50379800	5.24472100	2.95813000
H	-3.16590100	5.81936200	2.77094300
C	-2.64914900	4.11478000	0.69820700
H	-3.25624800	4.98914700	0.43310400
H	-1.59773500	4.36726100	0.51807800
H	-2.92122700	3.30007000	0.02823400

im8f

SCF Energy (a.u.) = -2642.364127

Thermal correction to Gibbs free energy (a.u.) = 0.907914

Charge = 0, Multiplicity = 1

C	9.48178400	0.60457800	0.93232000
C	10.56771500	-0.23060200	1.23316800
C	11.86289500	0.10778500	0.86084300
C	12.12493800	1.30352400	0.16836100
C	11.03496700	2.13680100	-0.12933800
C	9.73817200	1.79434800	0.24392300
H	10.38995900	-1.16084600	1.76858000
H	12.67988900	-0.56150000	1.11280500

H	11.21058800	3.06578700	-0.66639500
H	8.91085600	2.44852800	-0.01631700
C	13.47266500	1.71253600	-0.25086100
C	14.62203000	1.05540800	-0.05111100
H	13.51016500	2.66285000	-0.78335600
H	15.56441100	1.45732200	-0.40968800
H	14.67254100	0.10385700	0.47092300
C	7.45752400	-0.73935600	0.19400800
C	8.07511300	0.18792800	1.27798200
H	8.06216600	-0.34450600	2.23667300
H	7.44570200	1.07728300	1.39008500
H	8.16591900	-1.56438200	0.04661800
C	6.12501900	-1.34443300	0.60109000
C	5.70357200	-2.53171100	-0.01308400
C	5.25579700	-0.73060100	1.50740800
C	4.44316100	-3.06315100	0.23955800
H	6.36798500	-3.02851800	-0.71621000
C	3.98885300	-1.25968600	1.75392600
H	5.55046600	0.18265300	2.01395200
C	3.55420400	-2.41941500	1.10998100
H	4.13322400	-3.97597700	-0.26486500
H	3.31379700	-0.73960500	2.42775900
C	7.23041200	1.47197800	-3.52823500
C	8.30182000	0.61299500	-3.28219100
C	8.35622500	-0.11391900	-2.09228400
C	7.34394400	0.00153400	-1.13357700
C	6.26730400	0.85946200	-1.39277400
C	6.21367600	1.59217700	-2.57819800
H	7.18567300	2.04076600	-4.45281500
H	9.09893500	0.51031100	-4.01336500
H	9.20295200	-0.76579500	-1.89494300
H	5.45755300	0.94117000	-0.67413900
H	5.37386900	2.25763900	-2.76065000
C	1.30981800	-2.47602100	-0.03075700

C	2.12415800	-2.88285300	1.22976100
H	2.08140300	-3.97231100	1.34557100
H	1.65818300	-2.44240700	2.11886300
H	1.74131400	-3.04278900	-0.86760100
C	-0.16960500	-2.84360800	0.03977000
C	-1.04231300	-2.34003800	-0.93525200
C	-0.70578300	-3.70060300	1.00722100
C	-2.39031200	-2.68664700	-0.94953300
H	-0.66180200	-1.66093500	-1.69188600
C	-2.06148900	-4.04200600	0.99732500
H	-0.07056100	-4.11590600	1.78240400
C	-2.93019000	-3.54847900	0.01992200
H	-3.01864200	-2.29100500	-1.74022100
H	-2.44593900	-4.71758800	1.75847100
C	2.05975100	1.71202500	-0.85141500
C	2.60104400	0.72517500	-1.67552100
C	2.33637900	-0.62157000	-1.42055600
C	1.52950700	-1.00360100	-0.34561800
C	0.99042200	-0.00506300	0.47469900
C	1.25113700	1.34131700	0.22653200
H	2.26236600	2.76133400	-1.04701000
H	3.23545000	0.99667200	-2.51380100
H	2.77881200	-1.38607300	-2.05307900
H	0.36584900	-0.28418100	1.31590300
H	0.81601400	2.10111000	0.86965700
Ni	-4.55048000	-0.94792200	0.13781000
C	-7.69506800	-0.23921400	-1.83907600
C	-6.60547300	-0.84728300	-2.40971200
C	-5.84207700	-1.75719700	-1.64216500
C	-6.22525700	-2.10096600	-0.29857600
C	-7.36567400	-1.40505100	0.24031300
C	-8.08677000	-0.50805800	-0.50824000
H	-6.31113800	-0.62554700	-3.42868400
H	-5.07539300	-2.33145000	-2.14968400

H	-7.65731900	-1.61219500	1.26569400
H	-8.94600000	-0.00150500	-0.08332200
C	-5.33742600	-2.84023000	0.53627500
C	-4.40401700	-3.92353800	0.00084900
H	-4.54081000	-4.83637000	0.59364200
H	-4.68714100	-4.18629600	-1.02657600
Br	-8.73081100	1.06271800	-2.86792200
O	-4.24315400	-0.49097300	2.20440900
C	-3.27939900	-1.21897600	2.99723700
C	-1.86374800	-0.85449300	2.60140000
H	-3.48131300	-2.27399800	2.80446600
H	-3.47160100	-1.00011600	4.05117900
H	-1.14738800	-1.44909500	3.17904700
H	-1.70772000	-1.06986400	1.54352300
H	-1.67693800	0.20712700	2.78480400
H	-5.65905300	-2.97053300	1.56829500
C	-2.90853700	3.10291200	-1.77821400
C	-4.28432700	2.86594800	-1.70319200
C	-4.76245300	1.68521300	-1.12945700
C	-3.89858800	0.69881900	-0.61725200
C	-2.51911500	0.97027700	-0.69877000
C	-2.02558900	2.14996500	-1.27023100
H	-2.53171100	4.01860800	-2.22764400
H	-4.98540600	3.60088200	-2.09492000
H	-5.83756500	1.52719000	-1.08741400
H	-1.79801800	0.25042400	-0.31928100
H	-0.95134800	2.31214500	-1.32094400
C	-4.33165000	2.73662500	3.93028300
C	-5.94441700	2.74043200	2.05165100
C	-4.79565300	3.53096700	2.70198800
H	-5.13965100	2.66423800	4.67135000
H	-6.14267000	3.11535200	1.04296000
B	-4.60581300	0.79787600	2.57136000
O	-3.91197400	1.41420800	3.57325900

O	-5.66344500	1.34386000	1.92428000
H	-3.47511100	3.22366200	4.40668900
H	-6.86084600	2.84160300	2.64705000
C	-5.32418000	4.89849200	3.15298800
H	-6.12838300	4.79958700	3.89214800
H	-4.52203000	5.49638800	3.60042000
H	-5.71755900	5.46009600	2.29816900
C	-3.62873800	3.71307400	1.71724000
H	-3.94018600	4.31591200	0.86005100
H	-2.79200700	4.22244800	2.21037500
H	-3.26227000	2.76531400	1.31589800

im9f

SCF Energy (a.u.) = -2427.933853

Thermal correction to Gibbs free energy (a.u.) = 0.868540

Charge = 0, Multiplicity = 1

C	8.54058900	-0.83847800	1.24474900
C	9.64694200	-1.53769800	0.74038200
C	10.93256300	-1.01924800	0.83541700
C	11.16406100	0.22767800	1.44332700
C	10.05376900	0.92315000	1.94787200
C	8.76667800	0.40156400	1.85006400
H	9.49286000	-2.50443500	0.26574800
H	11.76590500	-1.58929000	0.43600800
H	10.20563000	1.89080400	2.42000300
H	7.92318900	0.97007800	2.23142200
C	12.50034100	0.82542100	1.57132900
C	13.66586600	0.30997300	1.16062400
H	12.51339400	1.79969900	2.05991100
H	14.59720400	0.84729400	1.30934200
H	13.74085300	-0.65500500	0.66694800
C	6.54745400	-1.00862500	-0.31893600
C	7.14505900	-1.37951000	1.06706100
H	7.14683300	-2.47210400	1.16168900

H	6.49494800	-0.98478400	1.85520700
H	7.27401300	-1.33857400	-1.07228100
C	5.22782700	-1.69933300	-0.61666400
C	4.82639500	-1.84508300	-1.95171600
C	4.34712800	-2.12182300	0.38299100
C	3.57219900	-2.35324700	-2.27348100
H	5.50034400	-1.52844300	-2.74436700
C	3.08647200	-2.62418900	0.05939100
H	4.62628500	-2.03816900	1.42828900
C	2.66969200	-2.72733100	-1.26918300
H	3.27619600	-2.43547600	-3.31716000
H	2.40035100	-2.90056500	0.85533500
C	6.26068500	3.30989500	-0.58047200
C	7.35254400	2.64068600	-1.13373900
C	7.42713100	1.24882700	-1.06625000
C	6.41509900	0.50469500	-0.45065100
C	5.31812400	1.18437900	0.09495200
C	5.24410300	2.57561500	0.03455700
H	6.19962700	4.39347000	-0.63046300
H	8.14972600	3.20036100	-1.61527400
H	8.28921400	0.73268900	-1.48011000
H	4.50916400	0.62251600	0.55220000
H	4.38880200	3.08786300	0.46757500
C	0.45109100	-1.77413000	-1.94206000
C	1.23955900	-3.06853100	-1.60518200
H	1.17742100	-3.74844200	-2.46347300
H	0.77389900	-3.57582700	-0.75419800
H	0.93031500	-1.33517500	-2.82542200
C	-1.01922600	-1.97566400	-2.25614600
C	-1.65561300	-1.05778900	-3.10188600
C	-1.81326900	-2.91647700	-1.59405700
C	-3.04222000	-0.99678200	-3.17082400
H	-1.05639400	-0.33617200	-3.65218600
C	-3.20533700	-2.84605300	-1.65433100

H	-1.35953600	-3.67578500	-0.96490000
C	-3.84049000	-1.83700100	-2.38092700
H	-3.51422100	-0.23029700	-3.78017700
H	-3.79638900	-3.54215700	-1.07122100
C	0.87570000	1.10932300	1.27998400
C	1.54969500	1.29539000	0.07237200
C	1.40540800	0.36773900	-0.96154200
C	0.58178600	-0.75165500	-0.81322200
C	-0.09574700	-0.92706500	0.40126600
C	0.05323100	-0.00968000	1.44082500
H	0.98512300	1.82995800	2.08537700
H	2.19026600	2.16041900	-0.07086400
H	1.95166500	0.50865000	-1.88982300
H	-0.75938200	-1.77661400	0.52766200
H	-0.48033600	-0.16433500	2.37537400
Ni	-5.90577800	-0.27922200	0.61677100
C	-2.93644700	3.00342800	-0.97984200
C	-2.51879700	1.74441600	-0.55785100
C	-3.38912300	0.66881700	-0.70726200
C	-4.67706900	0.81699400	-1.27120200
C	-5.03103200	2.10566400	-1.71549300
C	-4.17922200	3.20249400	-1.57023800
H	-1.53623500	1.59479900	-0.12666700
H	-3.05995900	-0.30951300	-0.38840000
H	-5.99331400	2.25492300	-2.19892100
H	-4.47775500	4.18542000	-1.91755200
C	-5.65538900	-0.31933000	-1.32763300
C	-5.31113700	-1.54380200	-2.22550200
H	-5.83657500	-2.42565700	-1.84746900
H	-5.73021300	-1.33238500	-3.22059400
Br	-1.72872500	4.53156300	-0.75124200
H	-6.61844100	0.06036800	-1.69121800
C	-3.89872300	-4.41525000	1.65520800
C	-3.16018700	-3.24388900	1.83256400

C	-3.69966300	-2.00853200	1.46384400
C	-4.97977300	-1.90099100	0.89566900
C	-5.70598800	-3.09364700	0.72851100
C	-5.18143500	-4.33348900	1.10822500
H	-3.48230600	-5.37761700	1.93999600
H	-2.15897200	-3.28977900	2.25639600
H	-3.08944900	-1.11975300	1.60863600
H	-6.69887500	-3.06230300	0.28298000
H	-5.77123100	-5.23656600	0.96692100
C	-6.11975300	-0.08119500	2.96319800
C	-5.26306100	0.84319700	2.44292200
C	-5.54003400	2.28376400	2.07625800
C	-6.96144300	2.56710500	1.53534900
C	-7.41578000	1.54541600	0.51592900
C	-8.03067000	0.34561400	0.73638000
C	-8.47697700	-0.25008200	2.05388900
C	-7.58794100	0.10291300	3.26750900
H	-5.69438900	-1.04025200	3.24326900
H	-4.21190400	0.56618100	2.40084800
H	-4.81192100	2.57470300	1.31195600
H	-5.34323200	2.92787500	2.94674500
H	-7.67822300	2.64110100	2.35666600
H	-6.94590100	3.55108400	1.05485700
H	-7.31162100	1.84974000	-0.51864600
H	-8.40802200	-0.17916600	-0.14011700
H	-8.49614400	-1.33999200	1.93864000
H	-9.51491900	0.05500900	2.25729800
H	-7.79206900	1.12023400	3.60762300
H	-7.86202400	-0.55844500	4.09649700

TS5f

SCF Energy (a.u.) = -2427.907304

Thermal correction to Gibbs free energy (a.u.) = 0.866620

Charge = 0, Multiplicity = 1

C	-8.51124900	-0.76765400	-1.36730100
C	-9.63477200	-1.48692300	-0.93427000
C	-10.90875800	-0.93467000	-0.98613000
C	-11.11063900	0.36779400	-1.47685100
C	-9.98314000	1.08330000	-1.91021200
C	-8.70778000	0.52769300	-1.85585100
H	-9.50376600	-2.49665000	-0.55100400
H	-11.75621700	-1.52150500	-0.64505800
H	-10.11206400	2.09340200	-2.29147900
H	-7.85047600	1.11107000	-2.17966100
C	-12.43349700	1.00294100	-1.55465500
C	-13.61160500	0.47687600	-1.19678500
H	-12.42366200	2.01770700	-1.95240600
H	-14.53083200	1.04494900	-1.29931800
H	-13.70919200	-0.52720900	-0.79329800
C	-6.52988700	-1.12564800	0.17993200
C	-7.12825200	-1.35261100	-1.23630000
H	-7.15229800	-2.43125400	-1.43305200
H	-6.46623600	-0.89960100	-1.98206800
H	-7.26495800	-1.51219200	0.89719500
C	-5.22377700	-1.86518600	0.41366300
C	-4.82774000	-2.14141900	1.72968100
C	-4.34934200	-2.21045300	-0.62048800
C	-3.58358300	-2.69979400	2.00352100
H	-5.49740700	-1.88744300	2.54802500
C	-3.09850600	-2.76320200	-0.34447200
H	-4.62517500	-2.02669400	-1.65370800
C	-2.68605500	-2.99504300	0.96895700
H	-3.29162800	-2.88356600	3.03535000
H	-2.41675900	-2.97840200	-1.16275200
C	-6.16909500	3.14313800	0.84819300
C	-7.27203200	2.44318900	1.33778200
C	-7.37020000	1.06538700	1.13937200
C	-6.37095300	0.36572500	0.45468300

C	-5.26264000	1.07521500	-0.02616800
C	-5.16519200	2.45317300	0.16484900
H	-6.08993400	4.21603400	0.99964600
H	-8.05968800	2.96831100	1.87106100
H	-8.24111400	0.52717300	1.50361000
H	-4.46362300	0.54578000	-0.53652000
H	-4.30189800	2.98959900	-0.22030700
C	-0.46415700	-2.14224200	1.74531500
C	-1.26100200	-3.38674600	1.27186300
H	-1.20905800	-4.15449200	2.05343900
H	-0.79855200	-3.80638300	0.37254000
H	-0.93811400	-1.80003800	2.67300000
C	1.00755500	-2.37644800	2.03173800
C	1.65209100	-1.51827800	2.93195300
C	1.79379700	-3.28292000	1.31318500
C	3.03845900	-1.46354900	2.99551600
H	1.05880200	-0.83050400	3.52944300
C	3.18809100	-3.22609400	1.37768900
H	1.32782200	-4.01060300	0.65556300
C	3.83049200	-2.25518100	2.15104600
H	3.51516200	-0.73535700	3.64615800
H	3.78116300	-3.89957300	0.76931000
C	-0.86792100	1.08927900	-1.13000900
C	-1.51631700	1.15697000	0.10376400
C	-1.37981200	0.11691700	1.02576000
C	-0.59004000	-0.99943900	0.73755500
C	0.06063000	-1.05600700	-0.50244800
C	-0.07956900	-0.02536700	-1.43133400
H	-0.97032600	1.89770300	-1.84810800
H	-2.13103900	2.01604300	0.35432400
H	-1.90605600	0.16753200	1.97458500
H	0.69068100	-1.90881300	-0.73812100
H	0.43270600	-0.08806700	-2.38794000
Ni	5.38547400	0.27050500	-0.74145200

C	2.84686100	2.59333700	1.45184500
C	2.44806200	1.45013400	0.77958800
C	3.34423400	0.37809200	0.68337500
C	4.64678700	0.45418900	1.24537500
C	4.99384500	1.64259200	1.93177800
C	4.10770200	2.70542900	2.04594300
H	1.45665400	1.36708500	0.35236300
H	2.99208500	-0.54794700	0.24803600
H	5.98064200	1.72037600	2.38151600
H	4.38837300	3.60641600	2.57975000
C	5.60427300	-0.67861300	1.11465700
C	5.29479200	-1.94052900	1.99248200
H	5.85038400	-2.79837900	1.60568800
H	5.71260900	-1.70381000	2.98110600
Br	1.59658500	4.09527100	1.59563100
H	6.61733100	-0.35883500	1.37100200
C	6.54360700	-4.07850400	-1.84603800
C	5.20190400	-3.69258500	-1.75459300
C	4.85039400	-2.48281400	-1.15790100
C	5.83131300	-1.60043400	-0.65466200
C	7.17408100	-2.02333700	-0.72872900
C	7.52709100	-3.23404700	-1.32794900
H	6.81471900	-5.02332200	-2.30803800
H	4.42284500	-4.33703500	-2.15647800
H	3.80264200	-2.20314700	-1.11202900
H	7.95576500	-1.38898900	-0.31780000
H	8.57512500	-3.51899400	-1.38512500
C	5.34966300	0.32661100	-2.86415400
C	4.33315700	1.09795300	-2.32845100
C	4.30349900	2.60112200	-2.14723400
C	5.67211300	3.27139800	-1.86982400
C	6.49342800	2.53663700	-0.83811900
C	7.39139800	1.54827600	-1.07457200
C	7.80340400	0.99438200	-2.42110400

C	6.65652300	0.83663400	-3.44912300
H	5.09794500	-0.69735400	-3.12224500
H	3.35552800	0.62520200	-2.23398200
H	3.63307100	2.82081300	-1.30801700
H	3.84673000	3.07427600	-3.03155300
H	6.23616800	3.37673500	-2.79955300
H	5.48149000	4.28998000	-1.51269600
H	6.36708500	2.86920500	0.18669000
H	7.97031800	1.18543600	-0.22484600
H	8.25123500	0.01054500	-2.25393400
H	8.59411800	1.62303700	-2.85924700
H	6.48667400	1.78249100	-3.97158500
H	6.99005900	0.12874900	-4.21590600

im10f

SCF Energy (a.u.) = -2427.969605

Thermal correction to Gibbs free energy (a.u.) = 0.871181

Charge = 0, Multiplicity = 1

C	8.30534800	-0.40810100	1.43304600
C	9.46251300	-1.12880700	1.10322800
C	10.70727800	-0.51309200	1.05742800
C	10.84476800	0.85730300	1.34221900
C	9.68387100	1.57410300	1.67313200
C	8.43786600	0.95459700	1.71695200
H	9.38132300	-2.19029100	0.87899400
H	11.58217500	-1.10253700	0.80049300
H	9.76283600	2.63568300	1.89472300
H	7.55313500	1.53765300	1.95663300
C	12.13421500	1.56129300	1.30881400
C	13.33679800	1.04488100	1.02618400
H	12.07401200	2.62372500	1.54476000
H	14.22647400	1.66669700	1.03109100
H	13.48419400	-0.00363300	0.78242700
C	6.34454700	-1.09859100	-0.02432700

C	6.95321400	-1.07361400	1.40519500
H	7.03162100	-2.10621000	1.76640700
H	6.26906900	-0.54385700	2.07682000
H	7.09824700	-1.55461900	-0.67883300
C	5.07595900	-1.92719600	-0.13216000
C	4.67884200	-2.39360900	-1.39313900
C	4.23151700	-2.17268800	0.95383900
C	3.45947600	-3.03866600	-1.56916000
H	5.32554000	-2.21839400	-2.24967800
C	3.00492400	-2.81338500	0.77507900
H	4.50969700	-1.84028000	1.94854100
C	2.58840500	-3.23397200	-0.48915100
H	3.16404100	-3.36918700	-2.56269700
H	2.34348300	-2.94866000	1.62642900
C	5.76190100	2.98905600	-1.34759800
C	6.90561300	2.28301300	-1.72124100
C	7.07623500	0.96032600	-1.31056200
C	6.10995300	0.32230600	-0.52564200
C	4.96076600	1.03634000	-0.16136400
C	4.79059100	2.36009400	-0.56547900
H	5.62584700	4.01902400	-1.66534300
H	7.66837100	2.76099100	-2.32975700
H	7.97784400	0.42019200	-1.58658900
H	4.18691400	0.54987800	0.42501000
H	3.89556500	2.90149900	-0.27036800
C	0.32733000	-2.57710400	-1.32880000
C	1.17823900	-3.71997000	-0.71611900
H	1.15084800	-4.58113500	-1.39486100
H	0.74330300	-4.04207500	0.23581800
H	0.78509700	-2.32746000	-2.29328200
C	-1.13310700	-2.90557700	-1.57936500
C	-1.81477000	-2.16895000	-2.55614300
C	-1.87698000	-3.77685900	-0.77700500
C	-3.20089500	-2.19008300	-2.62952200

H	-1.25447700	-1.50916600	-3.21359400
C	-3.27234100	-3.79593500	-0.85238200
H	-1.37920100	-4.41609500	-0.05399500
C	-3.95831500	-2.93704100	-1.71666300
H	-3.70552200	-1.54604100	-3.34286900
H	-3.83413100	-4.44673000	-0.18708200
C	0.56664000	0.99534100	1.12995800
C	1.17643200	0.96080400	-0.12464800
C	1.09812400	-0.19080600	-0.91111400
C	0.40186900	-1.31781300	-0.46608200
C	-0.21152200	-1.27157500	0.79276700
C	-0.12434600	-0.13024800	1.58877900
H	0.62357000	1.88980200	1.74346300
H	1.71221500	1.82773600	-0.49877300
H	1.59152300	-0.21519600	-1.87834800
H	-0.77209300	-2.13182000	1.14730700
H	-0.60098000	-0.11571000	2.56527900
Ni	-4.94990000	0.89037700	0.69310500
C	-2.98085300	1.57783000	-2.06823200
C	-2.64578400	0.81744300	-0.98088600
C	-3.59495000	-0.10462700	-0.44194000
C	-4.89539000	-0.20014600	-1.05595800
C	-5.13809800	0.55431700	-2.24611600
C	-4.21731500	1.44667200	-2.74531700
H	-1.65926200	0.87906400	-0.53892300
H	-3.19261800	-0.90866100	0.16184100
H	-6.08697300	0.42101800	-2.76253100
H	-4.42428200	2.03455600	-3.63213300
C	-5.80867900	-1.38913000	-0.75912400
C	-5.43834800	-2.67867700	-1.59216600
H	-5.95485200	-3.53570700	-1.14520800
H	-5.86095600	-2.53228300	-2.59302200
Br	-1.67364100	2.87108500	-2.76692400
H	-6.80655300	-1.10429800	-1.11304700

C	-6.37201700	-1.95949500	3.51962000
C	-5.20009100	-2.41840400	2.91365200
C	-4.99639000	-2.24343900	1.54558400
C	-5.96085300	-1.60840200	0.74350900
C	-7.13335100	-1.15550900	1.37072100
C	-7.33964700	-1.32632200	2.74102200
H	-6.52964300	-2.09868900	4.58531600
H	-4.43834000	-2.91556900	3.50821400
H	-4.08133800	-2.60754500	1.09869500
H	-7.89533100	-0.66699700	0.77015800
H	-8.26019100	-0.97052600	3.19501600
C	-4.70122400	1.26735800	2.74661000
C	-3.57170300	1.69617000	2.08049600
C	-3.33697500	3.09044400	1.54256700
C	-4.60891200	3.76972400	0.96109100
C	-5.54151000	2.80897400	0.23798200
C	-6.63268800	2.17612600	0.81128800
C	-7.02828600	2.26291900	2.26962500
C	-5.82595200	2.16019500	3.24661100
H	-4.68387400	0.25719400	3.15322000
H	-2.71238700	1.03179500	2.04470200
H	-2.58896300	3.01126000	0.74610300
H	-2.89984000	3.74424000	2.31327500
H	-5.15395100	4.28619000	1.75674400
H	-4.28859700	4.54560600	0.25693000
H	-5.47506000	2.82046200	-0.84744200
H	-7.38052800	1.75620500	0.13961000
H	-7.71854100	1.43929700	2.47753800
H	-7.58612400	3.18937800	2.47875400
H	-5.43276500	3.15790400	3.46244800
H	-6.18658400	1.76502300	4.20345100

im10f

SCF Energy (a.u.) = -1944.859109

Thermal correction to Gibbs free energy (a.u.) = 0.695950

Charge = 0, Multiplicity = 1

C	7.48567000	-1.04328500	0.95001400
C	8.49388700	-1.79326100	0.32686200
C	9.81523600	-1.36359700	0.32412000
C	10.18293700	-0.15863200	0.94931200
C	9.17050900	0.58781200	1.57284200
C	7.84716100	0.15529900	1.57274300
H	8.23380700	-2.72909600	-0.16322800
H	10.57015900	-1.97094600	-0.16589200
H	9.42832900	1.52455300	2.06102800
H	7.08062400	0.76235200	2.04608800
C	11.56301000	0.34538500	0.97744600
C	12.65044600	-0.22880500	0.44777500
H	11.68497100	1.29705000	1.49465300
H	13.62577300	0.24032900	0.53051600
H	12.61612700	-1.17675600	-0.08207000
C	5.36039000	-1.02747100	-0.43791600
C	6.04634400	-1.48527200	0.87938100
H	5.98138500	-2.57828300	0.94150700
H	5.49428600	-1.07656400	1.73250900
H	5.99618800	-1.37760400	-1.26089400
C	3.97635900	-1.61942500	-0.64065800
C	3.45802300	-1.70010100	-1.94055000
C	3.15384600	-2.01146500	0.41925300
C	2.15065500	-2.11732500	-2.16806600
H	4.08463700	-1.40597600	-2.77929500
C	1.84016100	-2.42155800	0.19088600
H	3.52273300	-1.97587100	1.43912000
C	1.31128000	-2.46142100	-1.10045300
H	1.76593400	-2.15234100	-3.18515500
H	1.20394500	-2.67471500	1.03463300
C	5.34598600	3.30692300	-0.54907600
C	6.33644000	2.58747000	-1.21792800

C	6.32220100	1.19217600	-1.19702700
C	5.32072400	0.49487600	-0.51336100
C	4.32591800	1.22540200	0.14976300
C	4.34103900	2.61972700	0.13562100
H	5.35452800	4.39321300	-0.56253200
H	7.12389300	3.11034200	-1.75371300
H	7.10712900	0.63555800	-1.70190200
H	3.52591300	0.70153600	0.66443000
H	3.56533800	3.17195900	0.65999800
C	-0.90639300	-1.37656000	-1.56194600
C	-0.15811600	-2.71493500	-1.32452400
H	-0.32188200	-3.36930400	-2.18981100
H	-0.58109400	-3.21859600	-0.44854000
H	-0.46818900	-0.92675600	-2.46199400
C	-2.40260400	-1.51505900	-1.78861000
C	-3.10464100	-0.38777300	-2.23797500
C	-3.13657900	-2.66041400	-1.47114700
C	-4.49116500	-0.37433500	-2.27418100
H	-2.55194900	0.50888200	-2.50664100
C	-4.53492400	-2.64611800	-1.51147800
H	-2.62943000	-3.56906400	-1.16334800
C	-5.23592900	-1.48684500	-1.85224900
H	-5.00785700	0.53035700	-2.57979000
H	-5.08539900	-3.54120500	-1.23350000
C	-0.13235800	1.33651300	1.73443300
C	0.55662800	1.47905200	0.52942200
C	0.29960900	0.60978800	-0.53195000
C	-0.65227000	-0.40706800	-0.41075800
C	-1.34014100	-0.54178500	0.80175000
C	-1.08011000	0.31817300	1.86866500
H	0.06473500	2.01245900	2.56159000
H	1.29533600	2.26597600	0.40900100
H	0.85690500	0.71198800	-1.45876500
H	-2.09326700	-1.31852000	0.90346300

H	-1.62031000	0.19670800	2.80410100
C	-4.86141400	2.92984800	0.06905600
C	-4.41892800	1.76289700	0.67990600
C	-5.20831600	0.61796700	0.58229500
C	-6.41719500	0.62069700	-0.12373000
C	-6.83656400	1.82181200	-0.70709100
C	-6.06819700	2.98432600	-0.61926900
H	-3.46745100	1.73046100	1.19771800
H	-4.85386500	-0.29313500	1.04817200
H	-7.77460800	1.85106800	-1.25672400
H	-6.40309000	3.90688600	-1.07969800
C	-7.21991900	-0.64883000	-0.37811400
C	-6.73182700	-1.37277300	-1.69285100
H	-7.20437300	-2.36026600	-1.72720700
H	-7.13365700	-0.79299900	-2.53210400
Br	-3.74865900	4.53928500	0.17619500
H	-8.24230000	-0.32691500	-0.60762800
C	-7.67303500	-3.15986200	3.13634700
C	-6.46888700	-3.17512000	2.43240400
C	-6.30232500	-2.38011900	1.29758400
C	-7.33803900	-1.55260100	0.83943900
C	-8.54153200	-1.54965600	1.55779400
C	-8.71213900	-2.34108900	2.69320900
H	-7.80071000	-3.77943300	4.01943800
H	-5.65116800	-3.80858600	2.76574500
H	-5.36044800	-2.41284900	0.76515600
H	-9.35706200	-0.91399700	1.22097000
H	-9.65695200	-2.31837400	3.22928300

im3e

SCF Energy (a.u.) = -2438.367508

Thermal correction to Gibbs free energy (a.u.) = 0.812479

Charge = 0, Multiplicity = 1

C	8.10890400	-1.99413300	0.65823100
C	9.04182500	-2.83834500	0.03887400
C	10.32888200	-2.40197400	-0.25093200
C	10.73568300	-1.09440900	0.06848000
C	9.79806800	-0.25291600	0.68827600
C	8.50924200	-0.69261400	0.97762600
H	8.75031400	-3.85468800	-0.21737400
H	11.02610500	-3.08419500	-0.72774900
H	10.08732700	0.76357400	0.94391400
H	7.79985500	-0.01463800	1.44338100
C	12.08224400	-0.57820100	-0.21411600
C	13.10128100	-1.23185700	-0.78597900
H	12.24033700	0.45748400	0.08652200
H	14.05762900	-0.74410600	-0.94629200
H	13.02766900	-2.26538000	-1.11300800
C	5.78926000	-2.20060700	-0.33118400
C	6.69511000	-2.46008900	0.90021900
H	6.68222200	-3.53375000	1.12288800
H	6.27928500	-1.94295900	1.77182200
H	6.29076400	-2.65500200	-1.19483000
C	4.40037200	-2.80998000	-0.22487100
C	3.66574100	-3.00502500	-1.40396300
C	3.76948900	-3.07591500	0.99282100
C	2.32776600	-3.37669600	-1.36085500
H	4.14441500	-2.81933900	-2.36255300
C	2.42078100	-3.43815100	1.03508800
H	4.31119900	-2.95904500	1.92593800
C	1.66976200	-3.55448000	-0.13519700
H	1.76946200	-3.48463700	-2.28842600
H	1.93307800	-3.57211400	1.99683600
C	5.46320600	2.05658000	-1.10662600
C	6.24148000	1.24946900	-1.93605200
C	6.34410400	-0.12112600	-1.68671700
C	5.66852300	-0.70588100	-0.61245500

C	4.89370100	0.11389600	0.21910600
C	4.79367400	1.48356400	-0.02179100
H	5.37148100	3.12135400	-1.29874800
H	6.77181900	1.68452500	-2.77867100
H	6.96297300	-0.74356800	-2.32774000
H	4.35402400	-0.32998500	1.05057100
H	4.19434300	2.11161700	0.63201700
C	-0.48717300	-2.29058400	-0.41841100
C	0.16738600	-3.66932900	-0.09866000
H	-0.18901600	-4.39734300	-0.83796400
H	-0.16146100	-4.01181000	0.88820100
H	-0.03618300	-1.95211000	-1.35996700
C	-1.98699400	-2.36416000	-0.64354200
C	-2.60093700	-1.36802500	-1.40978300
C	-2.80934800	-3.32177600	-0.04076500
C	-3.98950300	-1.29020800	-1.52340100
H	-1.98583100	-0.61425500	-1.89757400
C	-4.20424600	-3.25507100	-0.14221800
H	-2.37403200	-4.11703400	0.55638200
C	-4.79939900	-2.21622400	-0.86786600
H	-4.41728500	-0.47305100	-2.08671000
H	-4.80804100	-3.99018300	0.37666100
Br	-7.16304200	-2.38138800	1.42534800
C	0.56117400	0.63113800	2.62613100
C	1.45828500	0.32053100	1.60321600
C	1.11054300	-0.59600800	0.61170600
C	-0.13440600	-1.24610200	0.64365000
C	-1.02073600	-0.93218100	1.68091600
C	-0.68365500	0.00611800	2.65774600
H	0.82505500	1.36710200	3.38018600
H	2.42440500	0.81225700	1.56222800
H	1.81405900	-0.81042500	-0.18665800
H	-1.99759200	-1.40057200	1.71472600
H	-1.40796900	0.25943800	3.42507800

Ni	-6.65748300	-2.09494000	-0.79695500
C	-5.01754100	2.70824700	-1.33050400
C	-5.00315100	2.12897600	-2.60743400
C	-5.85454700	1.07513100	-2.92388700
C	-6.74440100	0.57554900	-1.95893000
C	-6.86832800	1.25790000	-0.73627100
C	-6.01179100	2.30655400	-0.42660000
H	-4.27385700	2.46861300	-3.33853700
H	-5.79931500	0.60264600	-3.90035500
H	-7.56695900	0.89213500	0.01098100
H	-6.05935500	2.76503200	0.55537500
C	-7.42571400	-0.71309200	-2.12008000
C	-6.96922300	-1.81352800	-2.83260100
H	-8.42858500	-0.77156300	-1.68355500
H	-7.64798500	-2.62431800	-3.08720800
H	-6.03198300	-1.78299300	-3.37759300
C	-2.76533800	2.67640300	-0.24423400
C	-3.87174500	3.57844800	-0.88956500
H	-3.44060400	4.10254600	-1.74953300
H	-4.19942300	4.33235900	-0.16590800
H	-2.68553000	1.78901500	-0.88240300
C	-1.39342200	3.32562800	-0.23731200
C	-1.19904900	4.70712800	-0.13024600
C	-0.26784700	2.49897500	-0.32981400
C	0.08602900	5.25696800	-0.11610400
H	-2.05177300	5.37578000	-0.05961000
C	1.02232100	3.02464400	-0.33118200
H	-0.39590000	1.42227500	-0.38293800
C	1.17607300	4.40165300	-0.22056600
H	0.22827000	6.32819900	-0.02928900
H	1.88211300	2.37090900	-0.41332700
Br	2.98834800	5.15436400	-0.20216000
C	-4.12354400	1.30524700	3.63812500
C	-4.28363200	0.50020900	2.50907400

C	-3.81294800	0.93910500	1.27129500
C	-3.19267100	2.18629000	1.13490500
C	-3.03061700	2.98267200	2.27444500
C	-3.49028800	2.54544200	3.51724000
H	-4.48678000	0.96933600	4.60539800
H	-4.77672200	-0.46532800	2.57985500
H	-3.93284600	0.30267500	0.40371400
H	-2.52920800	3.94300000	2.19335000
H	-3.35240800	3.17403300	4.39292400

TS2e

SCF Energy (a.u.) = -2438.354735

Thermal correction to Gibbs free energy (a.u.) = 0.805805

Charge = 0, Multiplicity = 1

C	9.45924800	-0.13822700	0.87357200
C	10.58322800	-0.73952600	0.28851900
C	11.77656900	-0.04404500	0.13731100
C	11.89355300	1.28955600	0.56838300
C	10.76623700	1.88651600	1.15472900
C	9.57151700	1.18745600	1.30384300
H	10.51725800	-1.77064000	-0.05218800
H	12.62759800	-0.54221900	-0.31703500
H	10.83009800	2.91741600	1.49445100
H	8.70911500	1.68019400	1.74389800
C	13.12886100	2.07397700	0.43344800
C	14.29359000	1.67421400	-0.09218300
H	13.05917900	3.09361100	0.81224600
H	15.14442300	2.34649900	-0.13997400
H	14.44722100	0.67503500	-0.49037700
C	7.32954400	-0.76944800	-0.35353200
C	8.15067200	-0.88126200	0.96153800
H	8.32951700	-1.94327400	1.16834500
H	7.55706600	-0.48291900	1.79129900
H	7.99414100	-1.08825600	-1.16624900

C	6.10467800	-1.66693200	-0.38314000
C	5.59320500	-2.07695400	-1.62194100
C	5.41006600	-2.04262900	0.77050800
C	4.40859900	-2.80179500	-1.70568300
H	6.12351700	-1.80228100	-2.53073200
C	4.21723800	-2.76047900	0.68542900
H	5.78211900	-1.75735600	1.74911600
C	3.68801500	-3.13360100	-0.55132500
H	4.02419600	-3.09385500	-2.68081300
H	3.67028000	-3.00005200	1.59321300
C	6.36450900	3.40498700	-1.01896200
C	7.44964700	2.81904600	-1.67093900
C	7.74058100	1.46898200	-1.47015900
C	6.95361100	0.68358800	-0.62146400
C	5.86143000	1.27842900	0.02342900
C	5.57212400	2.62888700	-0.16992200
H	6.13663500	4.45626100	-1.17109500
H	8.07454000	3.41226100	-2.33281000
H	8.59986900	1.02183100	-1.96259100
H	5.22433900	0.67924700	0.66698900
H	4.72575600	3.07685200	0.34454100
C	1.26624300	-2.67378400	-1.06201300
C	2.31295600	-3.74415000	-0.64964300
H	2.29960900	-4.55675300	-1.38671600
H	2.02680900	-4.17322400	0.31721400
H	1.55296800	-2.32602800	-2.06377400
C	-0.16161100	-3.19457800	-1.14341800
C	-1.17557700	-2.28119500	-1.48343200
C	-0.52592500	-4.51170500	-0.85075600
C	-2.51374700	-2.64760200	-1.46926700
H	-0.90411500	-1.25453800	-1.71478100
C	-1.87109000	-4.90511600	-0.83985500
H	0.23186000	-5.24932600	-0.61012600
C	-2.86804900	-3.95014500	-1.07630800

H	-3.28363700	-1.91868200	-1.69651600
H	-2.13222800	-5.93117900	-0.59564700
Br	-5.14004800	-4.11045500	2.28280500
C	1.53833600	0.73287700	1.60415600
C	2.16486800	0.76393300	0.35778800
C	2.06270200	-0.32886000	-0.50411600
C	1.33698900	-1.46535200	-0.13482700
C	0.71454300	-1.48905400	1.11983600
C	0.81188700	-0.39844300	1.98326000
H	1.61048300	1.58457100	2.27462800
H	2.73443100	1.63553900	0.04929200
H	2.56976600	-0.30683700	-1.46449300
H	0.13942500	-2.36245700	1.41627200
H	0.31354100	-0.42903400	2.94801600
Ni	-4.27914600	-4.08144200	0.14782800
C	-6.54068100	0.21606200	-1.34136300
C	-5.93966600	-0.43770500	-2.42297100
C	-5.74004500	-1.81545600	-2.40264500
C	-6.14229500	-2.58329600	-1.29614800
C	-6.84146000	-1.93785500	-0.26154100
C	-7.02942100	-0.56304400	-0.28527800
H	-5.58987700	0.14165100	-3.27436700
H	-5.25668700	-2.29130800	-3.25068600
H	-7.15165700	-2.51283000	0.60483700
H	-7.50425400	-0.07577400	0.56058700
C	-5.76078100	-4.00105500	-1.12454000
C	-4.68984900	-4.60362500	-1.85866900
H	-6.48971900	-4.65169500	-0.64442900
H	-4.62605500	-5.68842800	-1.87994800
H	-4.33403700	-4.13173300	-2.76693000
C	-5.09759400	2.21745500	-0.83861200
C	-6.51912200	1.71897300	-1.23482000
H	-6.80874100	2.18531500	-2.18435000
H	-7.24011900	2.04334900	-0.47665900

H	-4.44661000	2.00435400	-1.69783900
C	-5.02233000	3.71802200	-0.58018000
C	-6.09940000	4.58669700	-0.77700800
C	-3.80691800	4.26220600	-0.13726100
C	-5.97817400	5.96038600	-0.54311900
H	-7.05646200	4.20806000	-1.11802200
C	-3.66174400	5.62636900	0.09824500
H	-2.96319400	3.60099900	0.03853800
C	-4.75832300	6.45903600	-0.10952000
H	-6.82344100	6.62138400	-0.69724200
H	-2.71648700	6.03153000	0.44102800
Br	-4.57333700	8.38004200	0.22364000
C	-3.71939300	-0.25587500	2.43548700
C	-3.14022700	-0.37949900	1.17290300
C	-3.56059600	0.44930100	0.13134200
C	-4.55765500	1.40820600	0.33193400
C	-5.10910600	1.54660200	1.61127700
C	-4.69808100	0.71715600	2.65384600
H	-3.41643700	-0.91758300	3.24067900
H	-2.36857700	-1.12080700	0.99360800
H	-3.12098700	0.34039000	-0.85682700
H	-5.87009900	2.30310100	1.78657800
H	-5.14613000	0.82467600	3.63770700

im4e

SCF Energy (a.u.) = -2438.393983

Thermal correction to Gibbs free energy (a.u.) = 0.811022

Charge = 0, Multiplicity = 1

C	9.05480700	0.66004200	0.64137800
C	10.21764500	0.43600000	-0.11012700
C	11.25941700	1.35540800	-0.11826100
C	11.17852400	2.54337300	0.63015200
C	10.01320400	2.76236300	1.38188100
C	8.97055400	1.83981200	1.38718500

H	10.30367200	-0.47625200	-0.69667400
H	12.14641600	1.14765500	-0.70897000
H	9.92508500	3.67422700	1.96752200
H	8.07228200	2.04366400	1.96311000
C	12.24751900	3.55131200	0.65887300
C	13.42025000	3.51268400	0.01396300
H	12.03325500	4.41814200	1.28392900
H	14.13735100	4.32175100	0.11065200
H	13.71199000	2.68555800	-0.62734400
C	6.97649600	-0.03729200	-0.63651500
C	7.90330200	-0.31087300	0.58057100
H	8.27694200	-1.33930400	0.50702600
H	7.31588300	-0.24238800	1.50243500
H	7.62093000	-0.02138100	-1.52444300
C	5.92224700	-1.10922800	-0.85197100
C	5.37449200	-1.27358000	-2.13168400
C	5.40783400	-1.88941500	0.18762300
C	4.32184200	-2.15531900	-2.35452900
H	5.76667900	-0.68166900	-2.95530600
C	4.34587100	-2.76622600	-0.03409700
H	5.81509000	-1.80170500	1.18949700
C	3.77394000	-2.89772200	-1.30067900
H	3.90235200	-2.25104800	-3.35396000
H	3.93027500	-3.32572200	0.79945800
C	5.25913000	3.91937500	-0.19694600
C	6.37481200	3.72120400	-1.01051200
C	6.90877100	2.44120100	-1.16588800
C	6.33740600	1.34176500	-0.51699200
C	5.21259800	1.54870400	0.29222900
C	4.68079000	2.82753900	0.45463800
H	4.84224900	4.91478700	-0.07200000
H	6.83456600	4.56254200	-1.52165200
H	7.79112900	2.29432700	-1.78290500
H	4.74041300	0.70378100	0.78454000

H	3.81246800	2.97240800	1.09231500
C	1.28283100	-2.74287300	-1.55095400
C	2.50770900	-3.69349300	-1.49479000
H	2.54785700	-4.28065400	-2.42115600
H	2.38389300	-4.39649500	-0.66376800
H	1.43097800	-2.08816600	-2.41952600
C	-0.05628000	-3.44214200	-1.72496700
C	-1.18858000	-2.64905700	-1.90917500
C	-0.22736600	-4.83685000	-1.61937200
C	-2.47972900	-3.20150800	-1.89591700
H	-1.07472000	-1.57387500	-2.01415900
C	-1.49487700	-5.40388500	-1.60281200
H	0.63646800	-5.48121600	-1.50323500
C	-2.65500200	-4.60093700	-1.70736600
H	-3.33357000	-2.56298700	-2.08856000
H	-1.60780100	-6.47650400	-1.47304600
Br	-2.48817800	-3.84853600	2.50205800
C	1.22449800	-0.22451200	1.97482400
C	1.69563700	0.27776500	0.76101200
C	1.70197800	-0.53101900	-0.37633300
C	1.23522200	-1.84773600	-0.31676100
C	0.76031400	-2.34252800	0.90438400
C	0.75494200	-1.53831300	2.04359200
H	1.21293900	0.40643000	2.85901800
H	2.05857000	1.29887200	0.69190000
H	2.09295900	-0.14272200	-1.31259700
H	0.37231000	-3.35485300	0.97209800
H	0.36378500	-1.93973000	2.97343800
Ni	-2.77739700	-3.76754700	0.22153700
C	-6.54173900	-0.69064700	-0.21807500
C	-6.33034200	-1.36831800	-1.42354600
C	-5.74450600	-2.63067800	-1.44108400
C	-5.34793000	-3.26249900	-0.24705000
C	-5.66904000	-2.62048500	0.96692600

C	-6.24954400	-1.36089700	0.97681600
H	-6.58822500	-0.88461100	-2.36325400
H	-5.57497800	-3.11395800	-2.39812900
H	-5.37611000	-3.08842800	1.90128600
H	-6.41331400	-0.85702100	1.92450300
C	-4.51178900	-4.48035300	-0.20347000
C	-4.05962700	-5.16572100	-1.49582000
H	-4.74474900	-5.15536400	0.62038500
H	-4.00040400	-6.24806600	-1.35614200
H	-4.71529500	-4.97742200	-2.35342300
C	-5.61863300	1.62051800	-0.52886700
C	-6.88772000	0.77482100	-0.21160000
H	-7.66285600	1.00153400	-0.95381700
H	-7.27684100	1.06135900	0.77158100
H	-5.33594700	1.37332500	-1.56139500
C	-5.84984900	3.12565200	-0.47439500
C	-7.09049500	3.70414500	-0.19334600
C	-4.76505300	3.97915900	-0.72777100
C	-7.25596700	5.09296100	-0.16588600
H	-7.95428600	3.08100300	0.00957500
C	-4.90637500	5.36364000	-0.70978900
H	-3.78839100	3.54802900	-0.92928400
C	-6.15932400	5.90154900	-0.42654000
H	-8.22403100	5.52737700	0.05612900
H	-4.05869900	6.00984800	-0.90737900
Br	-6.37506800	7.84796600	-0.39154000
C	-2.45759700	0.20258800	2.06569400
C	-2.44150400	-0.11804500	0.70831700
C	-3.44030900	0.37237300	-0.13425400
C	-4.46211600	1.18927100	0.36287700
C	-4.45199100	1.52765800	1.72072400
C	-3.46067300	1.03337000	2.56802900
H	-1.69230100	-0.19796400	2.72041000
H	-1.65191000	-0.75227200	0.31866600

H	-3.44476400	0.09979100	-1.18712900
H	-5.22960000	2.17735000	2.11469700
H	-3.47301600	1.29467400	3.62265500

im5e

SCF Energy (a.u.) = -2579.435872

Thermal correction to Gibbs free energy (a.u.) = 0.875102

Charge = 0, Multiplicity = 1

C	9.04275800	0.76665900	0.63819500
C	10.20856000	0.58117600	-0.11918800
C	11.23155500	1.52143700	-0.11039700
C	11.12805900	2.69235800	0.66170600
C	9.95972400	2.87291800	1.41895600
C	8.93593900	1.92955100	1.40730100
H	10.31187700	-0.31723200	-0.72402200
H	12.12139700	1.34361800	-0.70657800
H	9.85417600	3.77107300	2.02262900
H	8.03465500	2.10379900	1.98821100
C	12.17670100	3.72074700	0.70942600
C	13.35046300	3.71696200	0.06524800
H	11.94478600	4.57180500	1.34967300
H	14.05115700	4.53837200	0.17699600
H	13.65918900	2.90727700	-0.59020500
C	6.97469400	0.05316700	-0.64814100
C	7.91123200	-0.22624900	0.56019500
H	8.30570300	-1.24500700	0.46416100
H	7.32559500	-0.18910700	1.48499900
H	7.61544900	0.10064600	-1.53758700
C	5.94205600	-1.03584100	-0.88204600
C	5.39469400	-1.18750000	-2.16354400
C	5.44598700	-1.84561300	0.14372200
C	4.35999500	-2.08662000	-2.40091200
H	5.77263200	-0.57232500	-2.97671600
C	4.40167200	-2.73962600	-0.09255000

H	5.85354300	-1.76808500	1.14633800
C	3.82959900	-2.85971200	-1.36017200
H	3.94024800	-2.17232300	-3.40109800
H	3.99929600	-3.32307900	0.73112800
C	5.17698800	3.96324900	-0.12134500
C	6.29342700	3.80520400	-0.94259100
C	6.85345000	2.54013200	-1.12611000
C	6.30771700	1.41592200	-0.49800700
C	5.18214700	1.58272100	0.31939100
C	4.62421900	2.84645700	0.50983300
H	4.73960800	4.94684100	0.02513200
H	6.73335700	4.66626300	-1.43808800
H	7.73614800	2.42446700	-1.74925000
H	4.72987500	0.71807300	0.79593500
H	3.75531400	2.96010800	1.15302900
C	1.33018600	-2.76526400	-1.60333400
C	2.58233300	-3.68123500	-1.56714800
H	2.63567500	-4.24918300	-2.50475300
H	2.47820000	-4.40355400	-0.75003400
H	1.45816000	-2.08887700	-2.45841800
C	0.01288400	-3.50439600	-1.78340500
C	-1.14760100	-2.74573100	-1.92418400
C	-0.11357400	-4.90535800	-1.69811200
C	-2.42182000	-3.33602700	-1.85875300
H	-1.07062400	-1.66619100	-2.01971700
C	-1.36333300	-5.50786200	-1.63626700
H	0.77219200	-5.52651700	-1.62764100
C	-2.54816400	-4.73721900	-1.66479300
H	-3.30281300	-2.72206100	-2.00752800
H	-1.43999900	-6.58560000	-1.52021400
C	1.16601900	-0.30897700	1.96722000
C	1.69273500	0.20673700	0.78211500
C	1.73642700	-0.58301000	-0.36761500
C	1.25502900	-1.89610300	-0.35021900

C	0.72862700	-2.40485600	0.84407800
C	0.68096500	-1.61834000	1.99446600
H	1.12124500	0.30933700	2.85931100
H	2.06601600	1.22575500	0.74367200
H	2.16477500	-0.18118500	-1.28143900
H	0.32469200	-3.41255600	0.87971500
H	0.23873200	-2.02800700	2.89720800
Ni	-2.59728100	-3.84978600	0.27548800
C	-6.58948400	-0.94826600	-0.09979900
C	-6.37432700	-1.64265700	-1.29234400
C	-5.71468300	-2.87136400	-1.29829500
C	-5.23950800	-3.44563400	-0.10664900
C	-5.55816700	-2.78984900	1.09906400
C	-6.21460400	-1.56923500	1.09987100
H	-6.68558800	-1.19878700	-2.23595000
H	-5.54429500	-3.36520700	-2.25002600
H	-5.19694700	-3.20877500	2.03295400
H	-6.37431700	-1.04954400	2.04014600
C	-4.32712800	-4.61571800	-0.05827700
C	-3.92071200	-5.33028500	-1.35575700
H	-4.53239100	-5.28697700	0.77853400
H	-3.82049200	-6.40594100	-1.18630800
H	-4.62766000	-5.19398300	-2.18295500
C	-5.79717100	1.40205900	-0.48102400
C	-7.01177300	0.49759000	-0.11401000
H	-7.81619000	0.67003700	-0.83973400
H	-7.39025300	0.78537500	0.87330800
H	-5.52901800	1.14773000	-1.51564100
C	-6.10341000	2.89410200	-0.45097600
C	-7.36264000	3.41504500	-0.14115100
C	-5.07312500	3.79629000	-0.75800900
C	-7.59889500	4.79392700	-0.13705300
H	-8.18562500	2.75269400	0.10285100
C	-5.28494200	5.17189800	-0.76394500

H	-4.08259700	3.41086900	-0.98316300
C	-6.55430800	5.65113900	-0.45038200
H	-8.58057700	5.18336100	0.10757900
H	-4.47867500	5.85598200	-1.00305500
Br	-6.86912800	7.58519200	-0.44811000
C	-2.51379400	0.18156700	2.06010000
C	-2.53209500	-0.19188300	0.71641000
C	-3.56861500	0.24050200	-0.11130900
C	-4.59724700	1.04803400	0.38723400
C	-4.55393000	1.43923500	1.73007000
C	-3.52229000	1.00551400	2.56259000
H	-1.71723600	-0.17377900	2.70391200
H	-1.74228100	-0.82636100	0.32759000
H	-3.60204700	-0.07798300	-1.15038000
H	-5.33782900	2.08096200	2.12458800
H	-3.50862200	1.30876100	3.60616800
O	-2.43207100	-3.60697700	2.02101200
C	-2.61500200	-4.57732500	3.01233700
C	-2.15119200	-4.02349600	4.35878600
H	-2.06053600	-5.50791900	2.79093600
H	-3.68153200	-4.85921500	3.09338800
H	-2.30442000	-4.75378300	5.16311800
H	-1.08494800	-3.77198900	4.31696900
H	-2.70609900	-3.11022800	4.59940700

im6e

SCF Energy (a.u.) = -3183.160338

Thermal correction to Gibbs free energy (a.u.) = 1.110250

Charge = 0, Multiplicity = 1

C	11.14387200	1.00028000	0.88212000
C	12.32112600	0.85721900	0.13319300
C	13.39951700	1.71465100	0.31354000
C	13.34269800	2.75616900	1.25695600
C	12.16283900	2.89445200	2.00515200

C	11.08352100	2.03449700	1.82126800
H	12.38891300	0.05855800	-0.60243500
H	14.29624900	1.57259300	-0.28194100
H	12.09272600	3.69339300	2.73937100
H	10.17540000	2.17638800	2.40037000
C	14.45070500	3.69286500	1.49000900
C	15.64308700	3.71121900	0.88120300
H	14.25036400	4.44799700	2.25007200
H	16.38898800	4.45718400	1.13686800
H	15.92310800	2.99419200	0.11441300
C	9.08363600	0.62890500	-0.55448300
C	9.95634600	0.10915300	0.62217000
H	10.28974300	-0.90765500	0.38220200
H	9.34024700	0.04569700	1.52548100
H	9.75870300	0.76637800	-1.40856400
C	7.99611500	-0.34283300	-0.97878100
C	7.48927400	-0.26670800	-2.28324600
C	7.41432600	-1.26283200	-0.10178900
C	6.41222200	-1.05144300	-2.68253100
H	7.93361600	0.43682600	-2.98349500
C	6.32910700	-2.04333900	-0.50039200
H	7.78778200	-1.36241000	0.91220200
C	5.79708400	-1.93546000	-1.78666600
H	6.02516500	-0.95893800	-3.69513400
H	5.86368600	-2.71723600	0.21343000
C	7.52378800	4.52922700	0.51993600
C	8.66581000	4.42023900	-0.27382200
C	9.14841800	3.16185400	-0.63565000
C	8.49934700	1.99586100	-0.21593100
C	7.34801100	2.11481400	0.57330800
C	6.86739200	3.37091200	0.94225600
H	7.14663900	5.50726400	0.80559300
H	9.18576600	5.31356100	-0.60874700
H	10.05069900	3.08079600	-1.23577100

H	6.81452000	1.22240300	0.88620400
H	5.97698000	3.44483100	1.56133100
C	3.32664100	-1.62173700	-2.10647700
C	4.50770700	-2.62805000	-2.15045200
H	4.56397200	-3.06470200	-3.15509400
H	4.31441800	-3.44735700	-1.44904500
H	3.53584600	-0.86876700	-2.87844400
C	1.96771400	-2.22894800	-2.43052000
C	0.85260600	-1.37868200	-2.45610200
C	1.75989300	-3.58069700	-2.70937300
C	-0.41763400	-1.85899600	-2.74707300
H	0.98249700	-0.32574200	-2.22929900
C	0.48025300	-4.06440600	-3.00614800
H	2.59127400	-4.27768200	-2.69642000
C	-0.62953400	-3.21935400	-3.03273200
H	-1.24417900	-1.15582900	-2.76109400
H	0.34729300	-5.12286600	-3.21593300
C	3.40009900	0.43358000	1.70789600
C	3.77835200	1.10214500	0.54258800
C	3.73476600	0.44210200	-0.68751100
C	3.30984400	-0.88661300	-0.77346900
C	2.93103100	-1.54808400	0.40071300
C	2.97807700	-0.89684900	1.63212600
H	3.43157200	0.94325400	2.66675400
H	4.11557400	2.13351900	0.58525500
H	4.05613700	0.95871400	-1.58764600
H	2.59099000	-2.57669500	0.34790300
H	2.67879500	-1.42653800	2.53248200
Ni	-2.47956000	-2.49425800	-0.78729900
C	-6.01695700	-0.53173700	-1.97120900
C	-4.90819500	-0.38525000	-2.80212200
C	-3.95976900	-1.40389200	-2.93895200
C	-4.09858800	-2.62732200	-2.24414100
C	-5.23988900	-2.76513600	-1.40228800

C	-6.16718800	-1.74958400	-1.27195700
H	-4.78021800	0.53736600	-3.36376400
H	-3.13138200	-1.26369200	-3.62403400
H	-5.35917500	-3.68781600	-0.84198400
H	-7.02076200	-1.88362300	-0.61526600
C	-3.02906500	-3.62836500	-2.20483000
C	-2.01687800	-3.75147900	-3.35099000
H	-3.33498600	-4.58360300	-1.78054900
H	-1.92648900	-4.80752000	-3.62668500
H	-2.40087000	-3.24052800	-4.24468100
C	-6.82433200	1.42733900	-0.54049900
C	-7.02017900	0.58605700	-1.82831000
H	-6.94063300	1.25516100	-2.69268000
H	-8.03514400	0.17190000	-1.83755400
H	-5.76364300	1.70574100	-0.50122100
C	-7.62995800	2.72068000	-0.53876900
C	-8.76231500	2.91781300	-1.33447000
C	-7.24306200	3.75032300	0.33004200
C	-9.49399900	4.10748100	-1.27283200
H	-9.09175000	2.14481800	-2.02063700
C	-7.95441600	4.94496300	0.40692900
H	-6.37286100	3.60944000	0.96600800
C	-9.07652100	5.10420600	-0.40163100
H	-10.36983400	4.24845100	-1.89592200
H	-7.64195200	5.73395900	1.08144400
Br	-10.08877200	6.77799600	-0.30837200
C	-7.67404300	-0.90671300	3.00966400
C	-6.39087900	-0.41150800	2.78725500
C	-6.12196700	0.34768900	1.64661700
C	-7.12583200	0.62116300	0.71604800
C	-8.41820100	0.13348700	0.95645900
C	-8.69041100	-0.62949100	2.08959000
H	-7.88626700	-1.49945100	3.89524100
H	-5.59022200	-0.62179800	3.48659900

H	-5.11607100	0.71777200	1.47672600
H	-9.21760900	0.36091000	0.25593800
H	-9.69668100	-1.00229700	2.26017400
O	-2.15096600	-3.80695800	0.44298500
C	-1.04246300	-4.65593900	0.32416000
C	0.29072000	-3.94900500	0.55779600
H	-1.02295900	-5.14283200	-0.66613800
H	-1.15804800	-5.46712100	1.06533000
H	1.13251700	-4.64515300	0.44331600
H	0.41260900	-3.14000700	-0.16665500
H	0.31897900	-3.51568500	1.56222200
C	-0.97824200	1.18406700	-0.66615500
C	-0.11070400	0.53922300	0.22756900
C	-0.58999000	-0.47628800	1.04555900
C	-1.94515100	-0.87142600	1.01160100
C	-2.80347600	-0.21046600	0.10215500
C	-2.31660600	0.80790500	-0.73359800
H	-0.60354400	1.97806400	-1.30726500
H	0.93529700	0.82443800	0.27635300
H	0.08321100	-0.97818100	1.73090800
H	-3.86069700	-0.45963100	0.08953500
H	-2.99259700	1.29956600	-1.42665300
C	-2.09436300	-3.61928500	3.68814100
C	-4.33208300	-3.35841100	2.65779700
C	-3.60162100	-3.58301900	3.99194600
H	-1.85308900	-4.51847100	3.10807000
H	-5.40382800	-3.20461900	2.82398400
B	-2.48971200	-1.98886200	1.98003700
O	-1.65439900	-2.48119300	2.95165900
O	-3.84554500	-2.21023800	1.97115000
H	-1.51828000	-3.64580500	4.62010600
H	-4.19248900	-4.22490800	2.00092200
C	-4.03166600	-4.93004000	4.58325000
H	-3.82184200	-5.75454100	3.89178200

H	-3.50351400	-5.13256000	5.52264100
H	-5.10671900	-4.93525400	4.79923600
C	-3.91447100	-2.44578000	4.97621800
H	-4.99157800	-2.38856400	5.17396300
H	-3.40487200	-2.60978300	5.93305500
H	-3.58669300	-1.47873800	4.58412600

TS3e

SCF Energy (a.u.) = -3183.160845

Thermal correction to Gibbs free energy (a.u.) = 1.112268

Charge = 0, Multiplicity = 1

C	11.14982900	0.99882700	0.89314400
C	12.33003100	0.84475000	0.15107400
C	13.40963700	1.70162800	0.32670000
C	13.35111300	2.75368400	1.25824400
C	12.16835300	2.90288800	1.99973100
C	11.08781400	2.04346500	1.82057200
H	12.39918000	0.03782300	-0.57534900
H	14.30869500	1.55083600	-0.26309800
H	12.09690200	3.71005400	2.72476800
H	10.17750100	2.19385400	2.39405600
C	14.46022500	3.69045900	1.48566000
C	15.65459900	3.70046300	0.88057400
H	14.25887900	4.45353300	2.23748100
H	16.40115900	4.44745000	1.13128500
H	15.93563500	2.97539300	0.12175800
C	9.09536300	0.61668600	-0.54872800
C	9.96127300	0.10778400	0.63762200
H	10.29322900	-0.91243600	0.41046100
H	9.34083600	0.05585500	1.53869900
H	9.77472000	0.74303100	-1.40113100
C	8.00717000	-0.35672800	-0.96741800
C	7.50500800	-0.29172100	-2.27429900
C	7.42013400	-1.26696400	-0.08378400

C	6.42722800	-1.07734000	-2.66975700
H	7.95350300	0.40406600	-2.97962000
C	6.33416800	-2.04838500	-0.47864900
H	7.78988900	-1.35787200	0.93237200
C	5.80666000	-1.95112400	-1.76760900
H	6.04375900	-0.99334900	-3.68446700
H	5.86455500	-2.71423800	0.23995400
C	7.54033400	4.53244700	0.47530500
C	8.68584400	4.41192100	-0.31172900
C	9.16699400	3.14844100	-0.65739100
C	8.51297300	1.98875100	-0.22800400
C	7.35816200	2.11921000	0.55431800
C	6.87899000	3.38047900	0.90714100
H	7.16430000	5.51449600	0.74839400
H	9.20964700	5.30021700	-0.65394500
H	10.07193400	3.05855600	-1.25222700
H	6.82086600	1.23164200	0.87441600
H	5.98582300	3.46340500	1.52107600
C	3.33877100	-1.63174400	-2.09793000
C	4.51614300	-2.64278700	-2.12921500
H	4.57430800	-3.08833400	-3.12982800
H	4.31761800	-3.45530500	-1.42136400
H	3.55355200	-0.88636500	-2.87572500
C	1.97846800	-2.23617000	-2.42162800
C	0.86563700	-1.38300200	-2.44970000
C	1.76733800	-3.58779600	-2.69869500
C	-0.40519800	-1.86026500	-2.74265300
H	0.99748600	-0.33026600	-2.22303800
C	0.48682600	-4.06844000	-2.99701500
H	2.59679300	-4.28703000	-2.68322600
C	-0.62043500	-3.22027100	-3.02731400
H	-1.22936000	-1.15424900	-2.75789800
H	0.35144600	-5.12682200	-3.20580900
C	3.40303500	0.45815200	1.69772300

C	3.78457300	1.11595600	0.52741300
C	3.74451300	0.44462600	-0.69669400
C	3.31975400	-0.88477100	-0.77158900
C	2.93779400	-1.53547400	0.40758800
C	2.98136400	-0.87296900	1.63307500
H	3.43162700	0.97665500	2.65191200
H	4.12151800	2.14774100	0.56152900
H	4.06820900	0.95299100	-1.60068800
H	2.59800300	-2.56460100	0.36333700
H	2.67947000	-1.39424200	2.53745000
Ni	-2.50178000	-2.45164800	-0.81288900
C	-6.01505100	-0.53619100	-1.97700100
C	-4.89606300	-0.38118200	-2.79055800
C	-3.94610600	-1.40011900	-2.92708800
C	-4.09843300	-2.63351900	-2.25131300
C	-5.25037100	-2.77849000	-1.42354400
C	-6.17591600	-1.76252300	-1.29294900
H	-4.75941800	0.54743800	-3.34000600
H	-3.11314500	-1.25569400	-3.60554100
H	-5.37822700	-3.70742600	-0.87567800
H	-7.03760300	-1.90138600	-0.64790800
C	-3.02475900	-3.62715600	-2.20849200
C	-2.00854900	-3.74799200	-3.35086800
H	-3.31884500	-4.58025600	-1.77146500
H	-1.92034300	-4.80305800	-3.63136200
H	-2.38865200	-3.23169100	-4.24300600
C	-6.83357200	1.41493100	-0.54198500
C	-7.02008600	0.58009600	-1.83516000
H	-6.93534700	1.25363800	-2.69559300
H	-8.03445700	0.16486200	-1.85344500
H	-5.77403000	1.69671500	-0.49600900
C	-7.64354100	2.70560100	-0.53741000
C	-8.77107400	2.90432400	-1.33950500
C	-7.26578600	3.73081900	0.34063600

C	-9.50690200	4.09131100	-1.27521700
H	-9.09348900	2.13478900	-2.03285200
C	-7.98138900	4.92271900	0.42032000
H	-6.39955200	3.58849900	0.98166900
C	-9.09846700	5.08369400	-0.39484500
H	-10.37894200	4.23355300	-1.90331900
H	-7.67600600	5.70830200	1.10201800
Br	-10.11655900	6.75372800	-0.29777700
C	-7.69215500	-0.93798800	2.99344500
C	-6.41034200	-0.43508400	2.78075800
C	-6.13872900	0.32976400	1.64457900
C	-7.13832200	0.60115400	0.70883600
C	-8.42946000	0.10550600	0.93937500
C	-8.70437100	-0.66303100	2.06811200
H	-7.90658800	-1.53516300	3.87549300
H	-5.61246900	-0.64335200	3.48385100
H	-5.13398400	0.70649000	1.48291200
H	-9.22587200	0.33131200	0.23489900
H	-9.70962200	-1.04189700	2.23122500
O	-2.15761300	-3.73280500	0.45415400
C	-1.06264600	-4.60201500	0.34535700
C	0.28394100	-3.91668100	0.56357500
H	-1.05702000	-5.10112200	-0.63851300
H	-1.18990600	-5.40095400	1.09738700
H	1.11152400	-4.62879200	0.44476700
H	0.41366600	-3.11420300	-0.16641600
H	0.32947800	-3.47972400	1.56550000
C	-0.99201300	1.20201700	-0.66424500
C	-0.11612600	0.55037000	0.21718100
C	-0.58654900	-0.47305700	1.02973400
C	-1.94106600	-0.87207700	1.00333800
C	-2.80859000	-0.20180700	0.10964200
C	-2.33019700	0.82571300	-0.72148100
H	-0.62397700	2.00237000	-1.30127300

H	0.92968500	0.83759300	0.26078000
H	0.09310700	-0.97821200	1.70609100
H	-3.86650100	-0.44885300	0.10742900
H	-3.01380800	1.32461200	-1.40187300
C	-2.07886400	-3.60780000	3.69777900
C	-4.32021500	-3.35027300	2.67355300
C	-3.58506700	-3.56368500	4.00735000
H	-1.84295200	-4.51783600	3.13166800
H	-5.39178700	-3.19767900	2.84253100
B	-2.47502200	-2.00716900	1.96144600
O	-1.63827100	-2.48184800	2.94492300
O	-3.83732700	-2.20683700	1.97885900
H	-1.49954700	-3.62410200	4.62813300
H	-4.18312400	-4.22314300	2.02392300
C	-4.01685700	-4.90243400	4.61562800
H	-3.81374100	-5.73542000	3.93226700
H	-3.48459000	-5.09684100	5.55445700
H	-5.09081500	-4.90139000	4.83717300
C	-3.89015300	-2.41420500	4.97960900
H	-4.96594400	-2.35328400	5.18368000
H	-3.37476700	-2.56704100	5.93523900
H	-3.56368800	-1.45296500	4.57266600

im7e

SCF Energy (a.u.) = -3183.164238

Thermal correction to Gibbs free energy (a.u.) = 1.113090

Charge = 0, Multiplicity = 1

C	11.19267200	1.01099800	0.84205500
C	12.36289600	0.88432400	0.07931500
C	13.43901900	1.74432600	0.26104000
C	13.38684200	2.77200500	1.21977200
C	12.21412100	2.89367100	1.98194800
C	11.13705300	2.03121300	1.79666500
H	12.42698400	0.09661000	-0.66836100

H	14.33035000	1.61509100	-0.34536900
H	12.14772100	3.68162000	2.72827600
H	10.23422500	2.16042300	2.38689700
C	14.49253800	3.71095800	1.45476000
C	15.67771500	3.74523600	0.83272800
H	14.29692400	4.45320200	2.22861400
H	16.42256800	4.49118700	1.09146200
H	15.95266300	3.04177800	0.05166800
C	9.12079400	0.65205900	-0.57988900
C	10.00637200	0.11857300	0.58075600
H	10.34157700	-0.89330300	0.32301900
H	9.39914700	0.03966600	1.48885600
H	9.78710700	0.80361000	-1.43845800
C	8.03156400	-0.31626700	-1.00768500
C	7.50850400	-0.21867200	-2.30432300
C	7.46355600	-1.25361900	-0.14013300
C	6.42892800	-0.99950500	-2.70413400
H	7.94192900	0.49873700	-2.99725400
C	6.37563700	-2.03032000	-0.53900100
H	7.84973800	-1.36984400	0.86725900
C	5.82751200	-1.90095600	-1.81640000
H	6.02906600	-0.89012300	-3.71008800
H	5.92101100	-2.71785500	0.16871600
C	7.55959500	4.53172500	0.56442100
C	8.69244200	4.43768800	-0.24426000
C	9.17535700	3.18608600	-0.62849800
C	8.53560600	2.01224100	-0.21654400
C	7.39336200	2.11620900	0.58786200
C	6.91255100	3.36543800	0.97917900
H	7.18231400	5.50440800	0.86759600
H	9.20508800	5.33737400	-0.57335000
H	10.07082500	3.11640700	-1.24015200
H	6.86703700	1.21768400	0.89541800
H	6.02948100	3.42779500	1.60988800

C	3.35387100	-1.58463100	-2.09758800
C	4.53472400	-2.58905300	-2.17712700
H	4.58017800	-3.00458500	-3.19127300
H	4.35125700	-3.42319000	-1.49051100
H	3.55291800	-0.81720900	-2.85791600
C	1.99103800	-2.18420500	-2.42063000
C	0.87100200	-1.34071600	-2.38685000
C	1.78576400	-3.52210100	-2.76385000
C	-0.39819800	-1.81213300	-2.69762500
H	0.99319300	-0.30193200	-2.09865900
C	0.50547400	-3.99891700	-3.06920100
H	2.62104400	-4.21365100	-2.79576100
C	-0.60768500	-3.15801300	-3.04933700
H	-1.22366000	-1.10636100	-2.67498700
H	0.37669500	-5.04671600	-3.32977700
C	3.47298400	0.40230400	1.75041700
C	3.82740900	1.09433800	0.59143600
C	3.76868000	0.45614400	-0.64930500
C	3.35297500	-0.87416600	-0.75153000
C	2.99965400	-1.55962200	0.41650800
C	3.06056000	-0.92995700	1.65837700
H	3.51469300	0.89530200	2.71746200
H	4.15706800	2.12749500	0.64706800
H	4.07076800	0.99121800	-1.54532100
H	2.66992300	-2.59113200	0.35132200
H	2.77828900	-1.47655800	2.55394900
Ni	-2.55450400	-2.29745200	-0.92961400
C	-6.00266300	-0.48100800	-2.00797200
C	-4.85404000	-0.29822200	-2.76856600
C	-3.90949000	-1.32451500	-2.92360200
C	-4.10803300	-2.59246000	-2.31756300
C	-5.28243700	-2.75551600	-1.52102300
C	-6.19692500	-1.73412500	-1.37791500
H	-4.68829900	0.65184100	-3.27037200

H	-3.07035400	-1.16964800	-3.59203300
H	-5.43701000	-3.70330500	-1.01434300
H	-7.07814900	-1.88569300	-0.76322600
C	-3.02698000	-3.57137600	-2.27186200
C	-1.99437000	-3.67725800	-3.39987500
H	-3.29754900	-4.52264000	-1.81410200
H	-1.90625900	-4.72763000	-3.69805200
H	-2.36151100	-3.14380100	-4.28696900
C	-6.86902900	1.44971200	-0.56525700
C	-7.01879200	0.62641200	-1.86997600
H	-6.92691300	1.30884400	-2.72271400
H	-8.02677300	0.19772900	-1.90997300
H	-5.82542400	1.78704400	-0.52112200
C	-7.74722100	2.69494100	-0.53570000
C	-8.84286600	2.88423800	-1.38242500
C	-7.46351300	3.68760700	0.41308900
C	-9.63846100	4.03090800	-1.29418500
H	-9.09489500	2.13983600	-2.13002400
C	-8.23928400	4.83880500	0.51746500
H	-6.62485000	3.54978300	1.09059700
C	-9.32216100	4.99204300	-0.34450300
H	-10.48542400	4.16574400	-1.95725900
H	-8.00664600	5.59910400	1.25428500
Br	-10.42430300	6.60522800	-0.21280600
C	-7.53644200	-1.07291200	2.88914800
C	-6.28430000	-0.50219500	2.67023800
C	-6.08321000	0.33175800	1.56885700
C	-7.11687200	0.59356500	0.66867700
C	-8.37884700	0.03172100	0.90745000
C	-8.58701800	-0.79815500	2.00715500
H	-7.69759000	-1.72508800	3.74302800
H	-5.45317200	-0.71641400	3.33109700
H	-5.10403300	0.76883700	1.40392300
H	-9.20245400	0.25129800	0.23252400

H	-9.56971800	-1.22884400	2.17941500
O	-2.14018600	-3.47207200	0.51971500
C	-1.10352500	-4.44697200	0.45642700
C	0.30479400	-3.87395700	0.50637500
H	-1.24845900	-5.00006900	-0.47909700
H	-1.25443500	-5.15240200	1.28273300
H	1.03826400	-4.66941900	0.32392100
H	0.43162700	-3.11009800	-0.26265700
H	0.49636000	-3.42783600	1.48399400
C	-1.02773400	1.30457000	-0.39843600
C	-0.10545400	0.57980800	0.37568400
C	-0.51135500	-0.55572300	1.06481500
C	-1.84893700	-1.00800600	1.03173400
C	-2.76640900	-0.24669900	0.26790500
C	-2.35429900	0.89509200	-0.44925500
H	-0.70537500	2.18867500	-0.94273100
H	0.93086500	0.90112300	0.42953000
H	0.21057700	-1.10619700	1.65677400
H	-3.81955400	-0.51442000	0.29512700
H	-3.08295500	1.45607600	-1.02900100
C	-1.98975500	-3.78871800	3.69951500
C	-4.23484800	-3.44726600	2.71489700
C	-3.47981700	-3.60670200	4.04850800
H	-1.85661100	-4.78728800	3.24811900
H	-5.30217500	-3.26772400	2.89938200
B	-2.31579600	-2.39888900	1.73120300
O	-1.49161300	-2.78598000	2.83692100
O	-3.73441000	-2.36158900	1.97011100
H	-1.38531000	-3.76886700	4.61643200
H	-4.15016600	-4.38291800	2.13520900
C	-3.98745100	-4.84750900	4.78889100
H	-3.88346500	-5.75093700	4.17514600
H	-3.43007700	-5.00761600	5.72017100
H	-5.04720200	-4.73982200	5.05108200

C	-3.66712000	-2.35336000	4.91442800
H	-4.72903100	-2.18909800	5.13786600
H	-3.13654100	-2.45661900	5.86896100
H	-3.28024400	-1.46868300	4.40268200

TS4e

SCF Energy (a.u.) = -3183.136846

Thermal correction to Gibbs free energy (a.u.) = 1.112203

Charge = 0, Multiplicity = 1

C	10.96984800	1.37516000	-0.53353500
C	11.76990800	1.90066800	-1.55864500
C	12.75157700	2.84770700	-1.29382000
C	12.97322300	3.30968100	0.01589000
C	12.17051200	2.77997100	1.03868800
C	11.18701800	1.83189800	0.77014100
H	11.61748800	1.55830300	-2.58000000
H	13.35444100	3.23051400	-2.11166500
H	12.32040100	3.12247300	2.05971400
H	10.56782400	1.45275400	1.57823000
C	13.99561200	4.30932000	0.35494100
C	14.85041800	4.91454800	-0.47914000
H	14.03970600	4.56830600	1.41276800
H	15.56677300	5.64294800	-0.11248000
H	14.87337300	4.71260400	-1.54647400
C	8.55281800	1.13310100	-1.26701100
C	9.86005700	0.40458600	-0.84782100
H	10.15975000	-0.26476800	-1.66313000
H	9.65867200	-0.21981600	0.02919800
H	8.82140200	1.81464900	-2.08379100
C	7.47354500	0.19805100	-1.78418300
C	6.49952300	0.70309500	-2.65679900
C	7.35410600	-1.13013200	-1.36502400
C	5.42299700	-0.07924800	-3.06187100
H	6.57943600	1.73152600	-3.00107100

C	6.26821900	-1.91028000	-1.76285300
H	8.09621800	-1.56229100	-0.70160200
C	5.27686500	-1.39360200	-2.59904100
H	4.67038300	0.34201100	-3.72504200
H	6.17066600	-2.92469600	-1.38532100
C	7.19382000	3.55728500	2.06123800
C	7.91196100	4.13556000	1.01456000
C	8.32758300	3.35412500	-0.06457900
C	8.03067100	1.98857600	-0.11816100
C	7.30372500	1.41739200	0.93454800
C	6.89264400	2.19393400	2.01734500
H	6.87014800	4.16236800	2.90344100
H	8.15397300	5.19449200	1.03780200
H	8.90536100	3.80398000	-0.86746200
H	7.04448500	0.36343500	0.89909000
H	6.33560000	1.73392800	2.82969200
C	2.84614800	-1.67034700	-1.97200000
C	4.01518500	-2.17021700	-2.87360400
H	3.70682400	-2.06953900	-3.92136600
H	4.19299100	-3.23433700	-2.68698000
H	2.70713300	-0.60857800	-2.20606800
C	1.53121300	-2.36906500	-2.26674400
C	0.34072800	-1.64262100	-2.27460800
C	1.45342700	-3.75589500	-2.48142000
C	-0.90062900	-2.27789700	-2.44072300
H	0.36390900	-0.56936100	-2.11423900
C	0.22965100	-4.39951400	-2.62749800
H	2.36239200	-4.34880800	-2.51555600
C	-0.97333600	-3.68052100	-2.59450000
H	-1.79935100	-1.67027800	-2.52173000
H	0.19820000	-5.47819800	-2.75737400
C	3.96709600	-1.81475300	2.22282300
C	4.17606800	-0.65982100	1.46671000
C	3.81276500	-0.62947900	0.12103100

C	3.22661800	-1.74280900	-0.49471300
C	3.03850100	-2.90008300	0.26841200
C	3.40403000	-2.93773900	1.61526500
H	4.24056600	-1.83974100	3.27387900
H	4.61511200	0.22392400	1.92021700
H	3.98953200	0.27004800	-0.46094200
H	2.57227500	-3.77155000	-0.17779800
H	3.23349700	-3.84259700	2.19186000
Ni	-1.85243700	-2.76430700	-0.27609400
C	-6.39727600	-1.35257200	-1.12615800
C	-5.59856600	-1.42795600	-2.27293500
C	-4.49938100	-2.28046300	-2.33629300
C	-4.15649500	-3.11847800	-1.25309800
C	-4.94870300	-3.00474700	-0.08529600
C	-6.03519100	-2.14181500	-0.02549200
H	-5.85283300	-0.82274400	-3.14107900
H	-3.92050500	-2.31426500	-3.25405400
H	-4.68676900	-3.60221100	0.78203100
H	-6.61797600	-2.07824200	0.88944400
C	-2.98995400	-4.03003800	-1.25527700
C	-2.31544200	-4.38118100	-2.58550500
H	-3.15061100	-4.90232600	-0.61896100
H	-2.15586100	-5.46198000	-2.66128500
H	-2.91881200	-4.09736700	-3.45735500
C	-7.25833400	1.02925500	-0.79931400
C	-7.60734600	-0.45154600	-1.08850400
H	-8.13073900	-0.50154600	-2.05169800
H	-8.30518800	-0.81115900	-0.32370200
H	-6.50159500	1.32401000	-1.53798000
C	-8.43650200	1.98060200	-0.96107200
C	-9.76478200	1.55368900	-1.04229100
C	-8.18111900	3.35904800	-1.00280200
C	-10.81569800	2.46860600	-1.16514900
H	-10.00306100	0.49608700	-1.01298700

C	-9.20970600	4.28862100	-1.12782800
H	-7.15537400	3.70994600	-0.92402300
C	-10.51987900	3.82349300	-1.20717700
H	-11.84159300	2.12378900	-1.22726800
H	-8.99673700	5.35102900	-1.16104300
Br	-11.98109400	5.11701600	-1.38254700
C	-5.42916100	1.38231900	3.10717600
C	-4.64504100	1.45273100	1.95656800
C	-5.24513900	1.35453300	0.70098800
C	-6.62443200	1.17744000	0.57538300
C	-7.40303300	1.10189400	1.73729400
C	-6.81053600	1.20280500	2.99478500
H	-4.96873400	1.47136400	4.08728700
H	-3.57078700	1.57333500	2.02811000
H	-4.63518700	1.40417000	-0.19635600
H	-8.47987700	0.98031600	1.65363200
H	-7.42764700	1.14889400	3.88760000
O	-2.10964800	-3.55468900	1.46593100
C	-1.43375000	-4.79664100	1.75087900
C	-0.01640900	-4.85966600	1.20297000
H	-2.05927100	-5.57568500	1.30564600
H	-1.43587800	-4.92271400	2.83732100
H	0.41962800	-5.84246200	1.42310300
H	-0.01400100	-4.71737800	0.11687500
H	0.60331100	-4.08604600	1.65900900
C	-0.25544200	1.57483800	0.06263100
C	0.63236600	0.61524500	0.55279500
C	0.18923300	-0.68860200	0.79639200
C	-1.14803000	-1.06763100	0.58986200
C	-2.03170700	-0.06394400	0.13209900
C	-1.59456400	1.23140900	-0.15278600
H	0.08740600	2.58748400	-0.13495800
H	1.66958000	0.87566600	0.73828500
H	0.90045300	-1.42285300	1.16068300

H	-3.08485000	-0.30395100	0.00868700
H	-2.29468600	1.97950900	-0.51909300
C	-0.34751900	-1.51457900	4.01996300
C	-2.83652600	-1.25638700	4.04175800
C	-1.51319000	-0.56541600	4.41089500
H	-0.01812000	-2.08289200	4.89819900
H	-3.67856700	-0.58160100	4.22282600
B	-1.78522000	-2.34771100	2.21785300
O	-0.66827600	-2.48442400	3.02856800
O	-2.89211700	-1.63216800	2.67301100
H	0.50877000	-0.92774700	3.66273000
H	-2.97560600	-2.14498300	4.67836600
C	-1.47753100	-0.32405000	5.92723200
H	-1.60146200	-1.25949300	6.48601800
H	-0.52303100	0.12437100	6.22822900
H	-2.27556700	0.36295200	6.23315800
C	-1.39689000	0.78113800	3.68050500
H	-2.20196500	1.45632200	3.99532600
H	-0.44262800	1.26680600	3.91541500
H	-1.45446500	0.65819600	2.59950200

im8e

SCF Energy (a.u.) = -3183.156751

Thermal correction to Gibbs free energy (a.u.) = 1.108274

Charge = 0, Multiplicity = 1

C	11.01088100	1.38252200	-0.30365800
C	11.84726700	1.91405400	-1.29621800
C	12.82868500	2.84821900	-0.98831200
C	13.01374700	3.29052900	0.33383600
C	12.17510100	2.75460800	1.32401800
C	11.19181400	1.81964800	1.01218400
H	11.72327600	1.58703700	-2.32640400
H	13.45996000	3.23640800	-1.78184600
H	12.29612900	3.08220700	2.35374300

H	10.54389500	1.43598300	1.79521900
C	14.03380200	4.27614300	0.71785700
C	14.91887600	4.88534500	-0.08106100
H	14.04765400	4.52011000	1.78009600
H	15.62975600	5.60224000	0.31757300
H	14.97269600	4.69815600	-1.14997500
C	8.61746500	1.17148600	-1.12356600
C	9.90264700	0.42698500	-0.66532200
H	10.22426700	-0.23841300	-1.47554900
H	9.66404700	-0.20261300	0.19854400
H	8.92107500	1.85733700	-1.92449300
C	7.54987900	0.24970000	-1.68725800
C	6.59831000	0.77566200	-2.57187100
C	7.41930700	-1.08776000	-1.30233300
C	5.53275100	0.00365700	-3.02301000
H	6.68602800	1.81234700	-2.88845300
C	6.34559900	-1.85852800	-1.74833100
H	8.14307600	-1.53570000	-0.62921300
C	5.37615100	-1.32194300	-2.59771900
H	4.79672400	0.44159800	-3.69392100
H	6.23914000	-2.88146900	-1.39766000
C	7.17502400	3.57848200	2.18157900
C	7.95527200	4.15327500	1.17818200
C	8.39669300	3.37805800	0.10504100
C	8.06466300	2.02227400	0.01436600
C	7.27419900	1.45511600	1.02238400
C	6.83704100	2.22572700	2.09929500
H	6.83067900	4.17873400	3.01910500
H	8.22521000	5.20442000	1.23064000
H	9.02191100	3.82439700	-0.66353200
H	6.98368800	0.41099300	0.95552600
H	6.22956600	1.76869100	2.87629200
C	2.93815500	-1.59723000	-2.03298100
C	4.11983000	-2.09018700	-2.92022700

H	3.83526700	-1.96963700	-3.97257200
H	4.28851000	-3.15872600	-2.74977000
H	2.79126800	-0.53914400	-2.27729100
C	1.62834300	-2.30314400	-2.33729300
C	0.45239100	-1.56490000	-2.41085500
C	1.54050900	-3.69621000	-2.53082300
C	-0.79122500	-2.17986200	-2.65068400
H	0.48228100	-0.49132900	-2.25627500
C	0.31978900	-4.32127300	-2.74933900
H	2.44144100	-4.30224200	-2.51251900
C	-0.87333500	-3.58093700	-2.82379700
H	-1.65903500	-1.55128300	-2.83185600
H	0.28018700	-5.39940700	-2.88285700
C	4.16021000	-1.70547700	2.12761700
C	4.12062300	-0.49879900	1.42788500
C	3.70343700	-0.47519400	0.09730400
C	3.32197500	-1.64957000	-0.55908000
C	3.37605400	-2.85559300	0.14839400
C	3.78713600	-2.88551700	1.48110700
H	4.47885000	-1.72748200	3.16599200
H	4.41037100	0.42869400	1.91286800
H	3.68306100	0.46678500	-0.44213100
H	3.08372000	-3.78037600	-0.33795200
H	3.81313300	-3.83164200	2.01491100
Ni	-1.84847100	-2.66042600	-0.64568400
C	-6.21933800	-1.23958100	-1.18516100
C	-5.38943500	-1.17963500	-2.31237400
C	-4.34046900	-2.07622400	-2.49066300
C	-4.07307000	-3.10034200	-1.54779500
C	-4.90978500	-3.13235000	-0.40440300
C	-5.94645100	-2.22660100	-0.22927000
H	-5.58094700	-0.42976700	-3.07768800
H	-3.74045700	-2.00287900	-3.39231100
H	-4.72295200	-3.88627400	0.35239000

H	-6.56516500	-2.28858300	0.66269500
C	-2.93506000	-4.01825700	-1.64090300
C	-2.22514800	-4.24831000	-2.97216000
H	-3.06012000	-4.92397400	-1.04630300
H	-2.08917300	-5.31725400	-3.17053400
H	-2.77482800	-3.83922500	-3.83019600
C	-6.98928600	1.15856300	-0.71906400
C	-7.39168300	-0.29961000	-1.04219500
H	-7.96359600	-0.29165800	-1.97920300
H	-8.06593400	-0.67426300	-0.26362800
H	-6.19328800	1.43162200	-1.42267400
C	-8.12243400	2.15866000	-0.91730800
C	-9.47153800	1.79205000	-0.92488000
C	-7.80485300	3.51644600	-1.05990300
C	-10.48242400	2.74659800	-1.07236100
H	-9.75614800	0.75064600	-0.81877500
C	-8.79374400	4.48521300	-1.21099200
H	-6.76181500	3.82201200	-1.04201500
C	-10.12575100	4.08044900	-1.21395100
H	-11.52483700	2.44896800	-1.07784100
H	-8.53301800	5.53141100	-1.32345300
Br	-11.53121900	5.42885500	-1.42538400
C	-5.38167100	1.72461000	3.26437900
C	-4.55513100	1.85721700	2.14873900
C	-5.07265600	1.64680300	0.86929200
C	-6.41485500	1.30778800	0.68370500
C	-7.23133100	1.15648000	1.81263100
C	-6.72052300	1.36032900	3.09305300
H	-4.98693000	1.90288800	4.26091100
H	-3.50683700	2.11235600	2.26354200
H	-4.42709100	1.75164800	0.00329600
H	-8.28176600	0.90823600	1.68527600
H	-7.37038800	1.25106400	3.95707300
O	-1.93247300	-3.76063400	1.09045400

C	-1.02148100	-4.87988000	1.16246100
C	0.42645400	-4.44113600	1.07112100
H	-1.29085500	-5.52288800	0.32093200
H	-1.21568300	-5.41414000	2.09640400
H	1.07887200	-5.32278900	1.06864600
H	0.60114300	-3.88291100	0.14798400
H	0.69709000	-3.80811500	1.91927800
C	-0.29081900	1.52745900	1.07032300
C	0.50141300	0.39704600	1.27450100
C	0.07411700	-0.85364800	0.81396100
C	-1.15376600	-1.03104900	0.15044000
C	-1.93638200	0.12891100	-0.02924500
C	-1.51357500	1.38815300	0.40864300
H	0.04112100	2.50388100	1.41507400
H	1.45794500	0.48359700	1.78259600
H	0.73821200	-1.69994600	0.96264500
H	-2.90189700	0.04708700	-0.52701200
H	-2.13313000	2.26559700	0.22994000
C	-2.16376300	-2.75826500	4.61865300
C	-3.96531900	-1.67652500	3.30341400
C	-2.89134000	-1.42768600	4.37287900
H	-2.83984100	-3.47933300	5.09821300
H	-4.40333700	-0.73689900	2.96429900
B	-2.34170400	-3.11171900	2.25187800
O	-1.66338600	-3.34829000	3.41128100
O	-3.44384800	-2.33414000	2.14741800
H	-1.30307300	-2.61030400	5.27865800
H	-4.77087900	-2.30121200	3.71427100
C	-3.57509000	-0.98616600	5.67327600
H	-4.26975100	-1.74859100	6.04638000
H	-2.83390600	-0.78867900	6.45630700
H	-4.14319500	-0.06382300	5.51125700
C	-1.90230400	-0.35174400	3.89911600
H	-2.41821200	0.60298300	3.76208000

H	-1.10801600	-0.20685700	4.64102800
H	-1.43252300	-0.60597800	2.94754700

im9e

SCF Energy (a.u.) = -2968.736859

Thermal correction to Gibbs free energy (a.u.) = 1.070439

Charge = 0, Multiplicity = 1

C	10.97523300	1.59376700	-0.06231000
C	11.87304000	2.06099800	-1.03335500
C	12.87673200	2.96634000	-0.71154200
C	13.02331100	3.44316100	0.60344500
C	12.12323700	2.97146900	1.57212000
C	11.11777500	2.06527500	1.24631800
H	11.77993100	1.70609600	-2.05754600
H	13.55586100	3.30445200	-1.48828700
H	12.21385900	3.32660900	2.59581600
H	10.42300200	1.73147000	2.01186600
C	14.06462400	4.40065900	1.00135800
C	15.00592500	4.94962200	0.22334300
H	14.04361400	4.67750000	2.05537900
H	15.72748300	5.65088900	0.63047900
H	15.09714200	4.72645700	-0.83608200
C	8.61427400	1.44786900	-0.98464300
C	9.84627600	0.67029100	-0.44260400
H	10.17623900	-0.03539800	-1.21445700
H	9.54380000	0.08135900	0.42988900
H	8.98110200	2.09240100	-1.79335900
C	7.53613100	0.54917100	-1.56487500
C	6.64965900	1.07820200	-2.51300300
C	7.33004300	-0.76503600	-1.13565400
C	5.57107700	0.33493900	-2.98155100
H	6.79809300	2.09598600	-2.86627400
C	6.24336300	-1.50657100	-1.59953900
H	8.00327400	-1.21588500	-0.41381900

C	5.33579600	-0.96351500	-2.51096500
H	4.88619700	0.77591400	-3.70278900
H	6.07658200	-2.50920000	-1.21530600
C	7.12607700	4.02568800	2.16854100
C	7.97780600	4.53168700	1.18640700
C	8.43400800	3.70210200	0.16118200
C	8.04598700	2.35963200	0.09732400
C	7.18371400	1.86203900	1.08310200
C	6.73167600	2.68694500	2.11265800
H	6.77095500	4.66818000	2.96946100
H	8.29259200	5.57109500	1.21884200
H	9.11472800	4.09446600	-0.58943200
H	6.85067800	0.82958300	1.03605700
H	6.06952400	2.28267500	2.87413600
C	2.87529400	-1.08928000	-2.04436000
C	4.05775800	-1.68843900	-2.85125200
H	3.82557700	-1.61600700	-3.92083800
H	4.16629900	-2.75150000	-2.61221900
H	2.79157000	-0.03794000	-2.34699300
C	1.53029400	-1.75002200	-2.29028000
C	0.37279300	-1.04875300	-1.93192600
C	1.37896100	-3.06733400	-2.73189200
C	-0.87594300	-1.66148900	-1.93383900
H	0.46167300	-0.01505200	-1.60375700
C	0.12102100	-3.67335700	-2.75197800
H	2.24503700	-3.64529900	-3.03927800
C	-1.02774200	-3.00093100	-2.31980900
H	-1.73630600	-1.09402400	-1.60642900
H	0.03668300	-4.71078500	-3.06457000
C	3.82730800	-1.11490300	2.18881300
C	3.88898600	0.07405300	1.46067500
C	3.57379300	0.07954000	0.10067100
C	3.18723000	-1.09551500	-0.55055600
C	3.12665100	-2.28344700	0.18943400

C	3.44712800	-2.29620100	1.54624800
H	4.07357300	-1.12327300	3.24693800
H	4.18769400	0.99986800	1.94368600
H	3.64965200	1.00310900	-0.46624600
H	2.81356200	-3.20179500	-0.29985600
H	3.39164000	-3.22690200	2.10427900
Ni	-2.11196600	-3.18069800	0.58237500
C	-6.50467600	-0.64235300	-1.36525100
C	-5.34985200	-0.49133200	-2.13772600
C	-4.29806100	-1.40486900	-2.05828600
C	-4.34936900	-2.51252600	-1.19207100
C	-5.54327600	-2.67964500	-0.46050200
C	-6.58738900	-1.76574100	-0.53312500
H	-5.26946600	0.35325100	-2.81981000
H	-3.43680100	-1.26157500	-2.70135700
H	-5.63709800	-3.54858900	0.18829400
H	-7.47953900	-1.91788700	0.06918900
C	-3.24893700	-3.50934900	-1.02583900
C	-2.35577000	-3.73120800	-2.26870800
H	-3.72369600	-4.46410900	-0.78933600
H	-2.13067700	-4.80023700	-2.32100800
H	-2.93036900	-3.49632700	-3.17925700
C	-7.21855100	1.65199700	-0.56306000
C	-7.59792300	0.39587400	-1.38713500
H	-7.80914700	0.70693400	-2.41802900
H	-8.52109700	-0.03628900	-0.98418600
H	-6.29319100	2.04541100	-1.00395400
C	-8.25342800	2.76892600	-0.62235800
C	-9.52087600	2.61425100	-1.19006600
C	-7.92611100	4.01378500	-0.06437700
C	-10.44234800	3.66668700	-1.20771300
H	-9.81209400	1.66811900	-1.63250000
C	-8.82488200	5.07645700	-0.07278300
H	-6.95086300	4.14774200	0.39632100

C	-10.07823200	4.88294100	-0.64840500
H	-11.42233900	3.53266000	-1.65137800
H	-8.55708700	6.03319300	0.36093700
Br	-11.35738600	6.36609000	-0.66625100
C	-6.30863200	0.53678800	3.52353400
C	-5.28270100	0.88684500	2.64648200
C	-5.57913100	1.24841800	1.33095900
C	-6.90049000	1.28024900	0.87821600
C	-7.92512100	0.93252500	1.76793000
C	-7.63322700	0.55704100	3.07774500
H	-6.08166200	0.25651200	4.54848800
H	-4.24929100	0.87581700	2.97943400
H	-4.77446500	1.49696500	0.64439100
H	-8.95831700	0.96961300	1.43259600
H	-8.43970500	0.29024800	3.75521800
C	-0.79734300	-7.71445800	0.57586600
C	0.09135900	-6.74689100	0.10475200
C	-0.29549300	-5.40496300	0.03694500
C	-1.58021000	-4.99065400	0.42553700
C	-2.46438300	-5.98454800	0.88139900
C	-2.07969700	-7.32610400	0.96743400
H	-0.49708100	-8.75746800	0.63166800
H	1.09123100	-7.03532800	-0.21355600
H	0.41410500	-4.67894300	-0.34810500
H	-3.47639400	-5.71190100	1.17657200
H	-2.78618000	-8.06850400	1.33257700
C	-2.52557400	-0.89113500	1.10146000
C	-3.36369300	-1.72138400	1.78373600
C	-3.25445800	-2.21651600	3.20593600
C	-1.81822000	-2.41967200	3.73214700
C	-0.95155000	-3.14808500	2.73372700
C	-0.16690300	-2.55878800	1.79571600
C	0.01523700	-1.08172700	1.55381200
C	-1.27452600	-0.22530100	1.63827000

H	-2.87911000	-0.55823300	0.12937100
H	-4.31808300	-1.93092000	1.31544100
H	-3.78880200	-3.17271100	3.26261700
H	-3.80279400	-1.52762500	3.86652900
H	-1.36868100	-1.45891900	3.99569400
H	-1.86737500	-3.00274500	4.65857500
H	-0.91304500	-4.23036000	2.82047900
H	0.48708200	-3.20287900	1.21663300
H	0.45060600	-0.97103900	0.56089500
H	0.76579400	-0.68323700	2.25082600
H	-1.44937000	0.08909800	2.67210700
H	-1.10192400	0.69647800	1.07120100

TS5e

SCF Energy (a.u.) = -2968.704027

Thermal correction to Gibbs free energy (a.u.) = 1.070301

Charge = 0, Multiplicity = 1

C	10.98195000	1.44709800	-0.07358100
C	11.87056000	1.92704600	-1.04684600
C	12.87055400	2.83641800	-0.72480300
C	13.02243200	3.30466900	0.59264200
C	12.13163000	2.82013600	1.56356100
C	11.12987700	1.90993800	1.23756400
H	11.77310800	1.57906500	-2.07301200
H	13.54256700	3.18449300	-1.50333900
H	12.22644800	3.16847700	2.58920500
H	10.44205300	1.56632900	2.00503100
C	14.05993100	4.26615800	0.99090300
C	14.99195400	4.82779800	0.21076900
H	14.04431500	4.53460300	2.04718500
H	15.71145300	5.53086000	0.61845400
H	15.07724200	4.61372700	-0.85102700
C	8.61519900	1.29476000	-0.97843100
C	9.85597400	0.51972200	-0.45341800

H	10.18432800	-0.17690300	-1.23416500
H	9.56404600	-0.07889900	0.41607500
H	8.97137600	1.94774000	-1.78513800
C	7.53609900	0.39547900	-1.55616700
C	6.63556400	0.92977000	-2.48800300
C	7.34276200	-0.92462100	-1.13930700
C	5.55627900	0.18516700	-2.95264900
H	6.77359500	1.95246700	-2.83109100
C	6.25524600	-1.66761800	-1.59897200
H	8.02661300	-1.37918000	-0.42992000
C	5.33446000	-1.11992000	-2.49409200
H	4.86046600	0.63000400	-3.66096200
H	6.09812800	-2.67503700	-1.22331600
C	7.13903600	3.83871300	2.20740600
C	7.97414300	4.35916400	1.21861600
C	8.42668400	3.54039100	0.18308200
C	8.05135100	2.19459600	0.11568300
C	7.20603100	1.68224200	1.10855400
C	6.75762900	2.49631600	2.14821200
H	6.78654900	4.47279600	3.01612100
H	8.27874600	5.40151300	1.25373900
H	9.09467900	3.94402500	-0.57299300
H	6.88324700	0.64660400	1.05916400
H	6.10832900	2.08119500	2.91488800
C	2.87923200	-1.27530500	-2.00100500
C	4.05836100	-1.84947300	-2.83105500
H	3.81561600	-1.76039000	-3.89720600
H	4.17717700	-2.91571400	-2.61046900
H	2.78858500	-0.21756200	-2.27904000
C	1.53532700	-1.93356700	-2.26557700
C	0.37945000	-1.28634000	-1.81448600
C	1.38549800	-3.19036600	-2.85879900
C	-0.87334800	-1.88644300	-1.89987300
H	0.46652800	-0.30133000	-1.36332900

C	0.12523700	-3.78204400	-2.96689700
H	2.25120400	-3.72640500	-3.23410600
C	-1.02590100	-3.15561500	-2.47576500
H	-1.73123500	-1.35542200	-1.51028900
H	0.03835200	-4.76534700	-3.42376700
C	3.88128800	-1.39857400	2.21521700
C	3.96082600	-0.19805200	1.50836500
C	3.62702100	-0.16003300	0.15377100
C	3.20491100	-1.31473100	-0.51207200
C	3.12742300	-2.51450000	0.20580900
C	3.46451600	-2.55868700	1.55787200
H	4.13821600	-1.43125400	3.27026600
H	4.28388800	0.71228100	2.00481900
H	3.71487700	0.77202100	-0.39725700
H	2.78367600	-3.41522600	-0.29569100
H	3.38988600	-3.49616600	2.10173200
Ni	-2.35652400	-2.82378700	0.41531900
C	-6.34551600	-0.65323400	-1.33950500
C	-5.17994900	-0.51263700	-2.10027800
C	-4.19965400	-1.50188600	-2.12361900
C	-4.33075900	-2.68368500	-1.36710500
C	-5.53772500	-2.84196400	-0.65281800
C	-6.50503700	-1.84448200	-0.62051300
H	-5.04176100	0.37975600	-2.70802700
H	-3.33423800	-1.35662100	-2.75926100
H	-5.71316700	-3.76578400	-0.10977800
H	-7.41118300	-1.99784000	-0.03945200
C	-3.33540200	-3.81246700	-1.39616500
C	-2.36309800	-3.86077000	-2.58673200
H	-3.93328600	-4.72091300	-1.45036000
H	-2.15551300	-4.91556100	-2.79260200
H	-2.89922200	-3.48460500	-3.47077200
C	-6.95281900	1.68506200	-0.53322500
C	-7.39695800	0.42859100	-1.31768700

H	-7.64323000	0.73240700	-2.34364500
H	-8.31658800	0.02941400	-0.87489000
H	-6.01618000	2.02856400	-0.99119600
C	-7.94052600	2.84369900	-0.61464100
C	-9.23739000	2.71464900	-1.11903200
C	-7.53826700	4.10015500	-0.13820000
C	-10.11494000	3.80341200	-1.15403500
H	-9.58641600	1.76031000	-1.49758100
C	-8.39234300	5.19887600	-0.16550900
H	-6.53915000	4.21536900	0.27391300
C	-9.67671500	5.03014700	-0.67669000
H	-11.11834900	3.68918300	-1.54817100
H	-8.06664000	6.16427100	0.20476100
Br	-10.89361200	6.56467200	-0.72118100
C	-6.06667800	0.74203700	3.60095000
C	-5.04139100	1.10395700	2.72890100
C	-5.32955000	1.40128300	1.39540000
C	-6.64103500	1.35276600	0.91880000
C	-7.66609700	0.99179500	1.80338500
C	-7.38241400	0.68262300	3.13169200
H	-5.84611100	0.50970900	4.63906100
H	-4.01350500	1.14442800	3.07624700
H	-4.52277600	1.66059000	0.71554800
H	-8.69395200	0.96976000	1.45041300
H	-8.18848000	0.40515100	3.80543600
C	-1.96396500	-7.06041700	1.55717600
C	-1.07267700	-6.60647300	0.57979600
C	-1.33106900	-5.44044600	-0.13920900
C	-2.48657100	-4.67040000	0.12430200
C	-3.41566800	-5.18419000	1.06620000
C	-3.14094300	-6.34142600	1.79027700
H	-1.75442400	-7.96920100	2.11372100
H	-0.15707700	-7.16016500	0.38365600
H	-0.60288000	-5.08998700	-0.86114100

H	-4.34394800	-4.65153600	1.24826100
H	-3.85419000	-6.69130800	2.53308200
C	-2.38971600	-0.71987100	1.04247200
C	-3.34254700	-1.52000400	1.65256600
C	-3.30527000	-2.07512000	3.06332200
C	-1.91054000	-2.45956300	3.62007300
C	-1.06441000	-3.21170100	2.62401100
C	-0.19436900	-2.63938800	1.76586700
C	0.11507500	-1.16758900	1.65357900
C	-1.11109200	-0.20969500	1.68339200
H	-2.71124300	-0.20102400	0.14135100
H	-4.33676000	-1.51642900	1.21202600
H	-3.94691600	-2.96369800	3.08460300
H	-3.77454100	-1.35068700	3.74718400
H	-1.38355500	-1.56312200	3.95754300
H	-2.06172700	-3.07987900	4.51145600
H	-1.17338200	-4.29275100	2.60563700
H	0.37629400	-3.29367900	1.11068000
H	0.65795000	-1.02022600	0.72026200
H	0.81583100	-0.86869400	2.44568600
H	-1.32207400	0.07820600	2.71967300
H	-0.81556300	0.71773400	1.17797300

im10e

SCF Energy (a.u.) = -2968.748082

Thermal correction to Gibbs free energy (a.u.) = 1.072292

Charge = 0, Multiplicity = 1

C	10.88539200	1.47953000	-0.31332300
C	11.69022000	2.13844000	-1.25420600
C	12.69418800	3.01347900	-0.85790800
C	12.93442300	3.26572200	0.50466500
C	12.12725200	2.60265400	1.44266400
C	11.12134400	1.72731300	1.04248600
H	11.52355400	1.95908000	-2.31423600

H	13.30018100	3.50374600	-1.61375100
H	12.29122300	2.78232900	2.50243500
H	10.49886800	1.24254100	1.78926100
C	13.98025400	4.18106300	0.98198000
C	14.83921900	4.89282400	0.24149900
H	14.03952800	4.27157000	2.06657000
H	15.57374800	5.54172700	0.70795400
H	14.84768700	4.85940200	-0.84447100
C	8.45989700	1.40301400	-1.05693900
C	9.75222400	0.59190600	-0.76071200
H	10.03335200	0.04536600	-1.66895500
H	9.53985600	-0.15178800	0.01481300
H	8.74047400	2.19255000	-1.76538400
C	7.35805800	0.57818900	-1.69929900
C	6.38180700	1.23021700	-2.46512800
C	7.22080600	-0.79781200	-1.49496600
C	5.28667000	0.53870100	-2.97287800
H	6.47464300	2.29922900	-2.64195500
C	6.11756800	-1.48860000	-1.99651000
H	7.96291800	-1.34120700	-0.91916500
C	5.12443500	-0.83037400	-2.72414200
H	4.53303700	1.07187500	-3.54863800
H	6.00726000	-2.54842400	-1.78351200
C	7.17786000	3.33190300	2.60845900
C	7.91783900	4.03917100	1.66080400
C	8.30767700	3.41917600	0.47283000
C	7.96313900	2.08916900	0.21068500
C	7.21344000	1.38869100	1.16468100
C	6.82810900	2.00341800	2.35557300
H	6.87420400	3.81087200	3.53510200
H	8.19695500	5.07276400	1.84599400
H	8.90246400	3.96681900	-0.25322500
H	6.91472600	0.36344300	0.96762600
H	6.25271100	1.44377400	3.08866900

C	2.70705100	-1.15945300	-2.11265800
C	3.84588000	-1.53637600	-3.09829800
H	3.53237500	-1.27422700	-4.11648600
H	4.00333600	-2.62026600	-3.07296500
H	2.56371300	-0.07464300	-2.20223700
C	1.37287200	-1.82573600	-2.41003300
C	0.25145700	-1.42038400	-1.67588500
C	1.20712500	-2.87446700	-3.31875800
C	-0.97429500	-2.06126600	-1.81160700
H	0.34690100	-0.61151500	-0.95742500
C	-0.02916200	-3.51104500	-3.46110000
H	2.04492600	-3.22056600	-3.91506300
C	-1.14033900	-3.13109800	-2.70165000
H	-1.80069800	-1.73437800	-1.18518300
H	-0.12035400	-4.33913700	-4.16092200
C	4.01807200	-1.94913700	1.94349500
C	4.06438700	-0.65295600	1.42940000
C	3.62726400	-0.39987500	0.12849000
C	3.13455800	-1.43272100	-0.67504200
C	3.08853300	-2.73007500	-0.14938900
C	3.52927200	-2.98831100	1.14815800
H	4.35240700	-2.14874200	2.95757800
H	4.43853900	0.16648100	2.03594200
H	3.68811500	0.60724500	-0.27388200
H	2.68876400	-3.53746800	-0.75680700
H	3.48276300	-3.99979000	1.54235600
Ni	-2.13462400	-2.72250000	0.71900300
C	-6.37830500	-0.86349100	-1.28065700
C	-5.17346500	-0.63953300	-1.95606700
C	-4.20764700	-1.63703000	-2.06479800
C	-4.40172300	-2.90759600	-1.50415300
C	-5.63304200	-3.14224600	-0.87580700
C	-6.58966200	-2.13639700	-0.74374100
H	-4.98661000	0.32468900	-2.42286500

H	-3.30150300	-1.41663500	-2.61523200
H	-5.85825700	-4.13452700	-0.49546900
H	-7.52718600	-2.35294100	-0.23758500
C	-3.38532900	-4.04275800	-1.62380300
C	-2.43683300	-3.90831600	-2.84565900
H	-3.98982000	-4.93343700	-1.85393400
H	-2.17043700	-4.91985800	-3.17174000
H	-3.02912000	-3.48637600	-3.66822500
C	-6.95821400	1.52073200	-0.54780100
C	-7.44247800	0.20661700	-1.19823600
H	-7.80643300	0.43741300	-2.20883000
H	-8.29878200	-0.18449900	-0.63746500
H	-6.07062500	1.84837900	-1.10288100
C	-7.97340100	2.65504100	-0.63710000
C	-9.31265700	2.46422000	-0.98771200
C	-7.55043700	3.95507600	-0.32396300
C	-10.21174700	3.53487500	-1.03111100
H	-9.67955200	1.47450500	-1.23646700
C	-8.42566800	5.03664600	-0.36310700
H	-6.51668000	4.11972800	-0.03137500
C	-9.75226700	4.80614400	-0.71862400
H	-11.24800800	3.37267600	-1.30508000
H	-8.08354100	6.03625900	-0.12050200
Br	-10.99898500	6.31568200	-0.77793500
C	-5.73487600	0.97462600	3.57084700
C	-4.78395000	1.24430700	2.58797100
C	-5.17942100	1.40629600	1.25865100
C	-6.52514100	1.31169300	0.89655400
C	-7.47345900	1.03735000	1.89082200
C	-7.08266400	0.86460600	3.21660800
H	-5.43055100	0.85067500	4.60629000
H	-3.73195500	1.31305900	2.84566900
H	-4.43116000	1.59877900	0.49444900
H	-8.52610700	0.98123100	1.62552800

H	-7.83024500	0.65599300	3.97704800
C	-1.70834800	-6.00017600	1.88649400
C	-0.93731800	-5.85121900	0.72265600
C	-1.39827800	-5.08706200	-0.34102600
C	-2.65768700	-4.40707100	-0.30338800
C	-3.37377900	-4.49840200	0.93571600
C	-2.90910800	-5.31618000	1.98787000
H	-1.35790100	-6.62584100	2.70222400
H	0.02376200	-6.35132000	0.63793400
H	-0.79252700	-5.03371900	-1.23647600
H	-4.37082500	-4.08552000	1.01438800
H	-3.51381900	-5.40311800	2.88660900
C	-2.05968800	-0.78599600	1.26425700
C	-3.09559400	-1.48691400	1.91395400
C	-3.17927700	-1.90116200	3.36865500
C	-1.84887100	-2.07698200	4.13917000
C	-0.87013600	-2.99585300	3.45944300
C	0.05622600	-2.64832700	2.55473000
C	0.38954900	-1.27230300	2.03119100
C	-0.76976400	-0.25862300	1.88939000
H	-2.37775400	-0.22962400	0.37967400
H	-4.08114500	-1.40303700	1.45217400
H	-3.74359700	-2.84173800	3.42102600
H	-3.79024600	-1.16091900	3.90830600
H	-1.39610100	-1.09844600	4.31584800
H	-2.09169300	-2.48007100	5.13069600
H	-0.97056500	-4.05304600	3.69213300
H	0.67687400	-3.44498100	2.14793300
H	0.84925600	-1.41115600	1.04917600
H	1.18010300	-0.82205700	2.64987700
H	-0.98380900	0.20388400	2.86009400
H	-0.39787000	0.56113700	1.26069100

SCF Energy (a.u.) = -1897.569749

Thermal correction to Gibbs free energy (a.u.) = 0.608256

Charge = 0, Multiplicity = 1

Ni	-4.75171300	0.81533900	-0.65307700
C	-4.07612600	0.04661900	0.88536800
C	-2.75236700	0.26570800	1.25324300
C	-2.22976900	-0.39230300	2.36637200
C	-3.02063300	-1.26409800	3.13076300
C	-4.36618900	-1.43001000	2.76338400
C	-4.89559000	-0.79733400	1.63678500
H	-2.12470500	0.92957900	0.67338900
H	-1.19329600	-0.22524900	2.64521800
H	-4.99953000	-2.09427500	3.34704400
H	-5.92544500	-0.98162900	1.34634900
C	-2.48052100	-2.01666000	4.27254100
C	-1.19741000	-2.35323800	4.45084100
H	-3.21686000	-2.34825900	5.00466600
H	-0.87879000	-2.91590600	5.32293500
H	-0.42956700	-2.10372500	3.72400100
Br	-4.62836100	-0.97457800	-2.05996500
C	-0.34471700	4.02656700	-0.07532000
C	-1.21194900	4.00509100	1.02675400
C	-2.54333200	3.62523100	0.88902800
C	-3.05278400	3.26321500	-0.36970600
C	-2.18923300	3.30719100	-1.47836600
C	-0.85893100	3.67562200	-1.33022700
H	-0.83445300	4.28176600	2.00807700
H	-3.19413600	3.61778800	1.75742100
H	-2.56747000	3.02617200	-2.45789000
H	-0.19832300	3.66533700	-2.19156500
C	-4.44441900	2.85576100	-0.58183100
C	-5.39156700	2.48180800	0.36090300
H	-4.79939300	3.01557800	-1.60573600
H	-6.45051800	2.50148000	0.11181500

H	-5.15207100	2.43388300	1.41750600
C	1.90493700	3.08566300	0.62604600
H	1.53330500	2.90530400	1.64496400
C	1.54653100	1.85896400	-0.19407100
C	0.52433500	1.01128200	0.23812600
C	2.15477600	1.58710000	-1.42301600
C	0.11442200	-0.07579300	-0.52589300
H	0.03659200	1.21781100	1.18672800
C	1.76623300	0.47911900	-2.17514400
H	2.96070700	2.22443400	-1.77584400
C	0.74798400	-0.37602500	-1.73824900
H	-0.67238600	-0.71867200	-0.15526200
H	2.28374000	0.25683400	-3.10493000
C	6.20878400	3.57302900	0.94345000
C	5.41219600	4.67919700	0.65664000
C	4.02511900	4.54112400	0.54506100
C	3.41262900	3.29664400	0.72102700
C	4.22843400	2.19066200	1.01094200
C	5.60952700	2.32264500	1.12038600
H	7.28689100	3.67959900	1.02319200
H	5.86610000	5.65591700	0.51250100
H	3.42908900	5.41811600	0.31576600
H	3.77181700	1.21192900	1.12443300
H	6.21724100	1.44696900	1.32984600
C	0.82137000	-2.94325900	-1.68397800
C	0.44568200	-1.65241700	-2.48819700
H	-0.60393200	-1.69878700	-2.79389500
H	1.03559300	-1.66466400	-3.41070000
C	2.24814900	-2.76636700	-1.17909900
C	3.32108100	-3.08271800	-2.01790800
C	2.53040900	-2.14591400	0.04599500
C	4.63865900	-2.77045400	-1.67266700
H	3.12824200	-3.56691300	-2.97243500
C	3.83522200	-1.82539800	0.41408200

H	1.71931700	-1.89245500	0.71701300
C	4.87133400	-2.13381400	-0.46028600
H	5.45896300	-3.01435600	-2.33805700
H	4.03651100	-1.33802800	1.36140200
Br	6.70548500	-1.64759400	0.03413300
C	-2.03090300	-4.15324800	1.37917900
C	-2.44788500	-3.35736800	0.31389900
C	-1.53890400	-2.96769300	-0.67038100
C	-0.19017300	-3.34603600	-0.60747600
C	0.20585700	-4.17156800	0.45577900
C	-0.70036100	-4.56815600	1.43953000
H	-2.72966400	-4.43611100	2.15997400
H	-3.47419900	-3.01204100	0.24753600
H	-1.90866000	-2.33985800	-1.47238700
H	1.23884500	-4.49835900	0.52223400
H	-0.36091400	-5.19499500	2.25975400
H	0.83745100	-3.75745600	-2.42268500
C	1.12470900	4.32418000	0.09364900
H	1.55238800	4.62439400	-0.86919300
H	1.26244600	5.16006400	0.78934000

TS2g

SCF Energy (a.u.) = -1897.557489

Thermal correction to Gibbs free energy (a.u.) = 0.608388

Charge = 0, Multiplicity = 1

Ni	-3.92317900	0.74318100	-0.69234000
C	-4.25031800	0.23540000	1.08166600
C	-3.07196000	0.13171000	1.84562900
C	-2.93775800	-0.89194600	2.77474000
C	-3.98915000	-1.79724800	3.01414700
C	-5.18630300	-1.63201400	2.29693400
C	-5.32687600	-0.62678000	1.34157100
H	-2.26540400	0.84221900	1.69425800
H	-2.01571100	-0.97926300	3.34083400

H	-6.01428900	-2.31158300	2.48317400
H	-6.25967800	-0.52360600	0.79440600
C	-3.87823400	-2.89028600	3.98900500
C	-2.73882500	-3.42194800	4.44940500
H	-4.82587300	-3.30783900	4.32808200
H	-2.74980100	-4.23392700	5.16962900
H	-1.76332500	-3.08671100	4.10899400
Br	-3.38493700	0.39746800	-2.90387200
C	-0.06797600	4.14018700	0.27880000
C	-0.97461500	4.01265500	1.33771100
C	-2.27633400	3.57494200	1.11621000
C	-2.71990800	3.26779100	-0.18215700
C	-1.83532700	3.48517400	-1.25309500
C	-0.53383000	3.90931800	-1.02217500
H	-0.64391000	4.21599200	2.35362600
H	-2.94738000	3.47250300	1.96345000
H	-2.15757500	3.24130900	-2.26058100
H	0.15506700	3.99729500	-1.85673100
C	-4.04672300	2.68193400	-0.45077300
C	-4.87083500	2.12685900	0.57887100
H	-4.52010600	2.96792100	-1.38831000
H	-5.93131400	2.00441200	0.37457300
H	-4.65862000	2.36874800	1.61378800
C	2.02578800	2.97565700	1.03582800
H	1.59224900	2.78118600	2.02736900
C	1.57005500	1.84686700	0.12591800
C	0.45949400	1.06733100	0.46376400
C	2.17883500	1.62682700	-1.11242900
C	-0.03976900	0.10265700	-0.40626700
H	-0.03057300	1.23460500	1.41905300
C	1.70039000	0.63948700	-1.97018100
H	3.04934200	2.21282500	-1.39368600
C	0.59125300	-0.14424700	-1.63327100
H	-0.89857000	-0.48920700	-0.11157200

H	2.21422200	0.45235400	-2.90948800
C	6.33985600	2.98773300	1.54499200
C	5.66528500	4.19204400	1.35626700
C	4.27801000	4.20496700	1.18329700
C	3.54192800	3.01581500	1.19879600
C	4.23548900	1.81004900	1.39200100
C	5.61698900	1.79177100	1.56177700
H	7.41875000	2.97738300	1.67154500
H	6.21595200	5.12866600	1.33636100
H	3.77820800	5.15596900	1.03249700
H	3.68343000	0.87521800	1.38067300
H	6.12884000	0.84251700	1.69190300
C	0.48036600	-2.69883700	-1.87239000
C	0.19450400	-1.30075000	-2.51765900
H	-0.85348300	-1.22542400	-2.81774100
H	0.78241700	-1.24948400	-3.44010000
C	1.90585100	-2.68460500	-1.33726200
C	2.96843700	-2.99314600	-2.19173300
C	2.20898400	-2.22249200	-0.04880800
C	4.29857300	-2.82657100	-1.79706600
H	2.75884900	-3.35391200	-3.19599200
C	3.52648200	-2.04987500	0.36956600
H	1.40563400	-1.97402500	0.63362000
C	4.55398400	-2.34639600	-0.51905200
H	5.11155300	-3.06165400	-2.47449800
H	3.74480800	-1.68338400	1.36627500
Br	6.40971900	-2.07037400	0.05095400
C	-2.52405900	-4.16761100	0.91814100
C	-2.86456500	-3.21610400	-0.04232600
C	-1.90205100	-2.72845200	-0.92662700
C	-0.57241400	-3.17112200	-0.86774000
C	-0.24951700	-4.14203300	0.09182100
C	-1.21012400	-4.63183000	0.97746300
H	-3.26743700	-4.53637900	1.61659100

H	-3.88165400	-2.84099900	-0.10413100
H	-2.20841200	-1.99121700	-1.65868200
H	0.76712300	-4.51761000	0.14979400
H	-0.92859400	-5.37961200	1.71428800
H	0.45492500	-3.41762300	-2.70402600
C	1.40321600	4.32317100	0.54959200
H	1.91739800	4.64601200	-0.36212200
H	1.56683400	5.09262100	1.31313800

im4g

SCF Energy (a.u.) = -1897.589746

Thermal correction to Gibbs free energy (a.u.) = 0.612370

Charge = 0, Multiplicity = 1

Ni	-3.81765000	0.57672500	-0.52538700
C	-5.07177500	1.20656000	1.03304900
C	-3.86559500	0.76045000	1.64391300
C	-3.80786300	-0.50327400	2.26403200
C	-4.92641700	-1.33800700	2.31044200
C	-6.12144800	-0.88632900	1.69504100
C	-6.19388200	0.34250600	1.06964300
H	-3.02020600	1.43238300	1.74810800
H	-2.87690000	-0.81230300	2.72709100
H	-6.99772500	-1.52840600	1.71916700
H	-7.11979300	0.66384200	0.60135900
C	-4.93948500	-2.63902600	2.99282400
C	-3.94235300	-3.18712300	3.69822700
H	-5.87878500	-3.18445500	2.91317700
H	-4.06596500	-4.15298400	4.17745100
H	-2.97485900	-2.71054100	3.82205900
Br	-3.30482000	-0.24325000	-2.60318500
C	-0.08258600	4.06764200	-0.14515100
C	-1.02767300	4.14331800	0.88339700
C	-2.32442400	3.67157800	0.70191300
C	-2.72674600	3.10817300	-0.52398600

C	-1.79196000	3.10820600	-1.57882400
C	-0.50185600	3.58139600	-1.39149400
H	-0.73378300	4.54190400	1.85193400
H	-3.02263100	3.73747600	1.53039200
H	-2.07650900	2.67080000	-2.53087700
H	0.21642500	3.50910600	-2.20247900
C	-4.04501000	2.47981100	-0.73597200
C	-5.12687400	2.56551400	0.33817400
H	-4.41087500	2.57648500	-1.75827200
H	-6.11164700	2.69381900	-0.11858400
H	-4.98181800	3.39058200	1.04521900
C	1.99985000	3.05611400	0.83080200
H	1.52188300	2.98452800	1.81826600
C	1.61152300	1.80800000	0.05566200
C	0.50223000	1.04626600	0.43534200
C	2.28007800	1.46222700	-1.12220800
C	0.06292900	-0.02454500	-0.33937300
H	-0.04399800	1.31631800	1.33547800
C	1.85323700	0.38019200	-1.88603200
H	3.15059200	2.03386300	-1.43169200
C	0.74418400	-0.38631500	-1.50883400
H	-0.80130000	-0.59582000	-0.02022300
H	2.40718600	0.10422900	-2.77943000
C	6.28587300	3.23498800	1.51512300
C	5.60420700	4.38253600	1.11606000
C	4.22574900	4.34118300	0.88601700
C	3.50570300	3.15399300	1.05333400
C	4.20625200	2.00600800	1.45743700
C	5.57890700	2.04146800	1.68526100
H	7.35822100	3.26533900	1.68625500
H	6.14268800	5.31587600	0.97522600
H	3.72035900	5.24742500	0.56969700
H	3.66656100	1.07008400	1.56651100
H	6.09844500	1.13423100	1.97973200

C	0.82585600	-2.95397600	-1.56089400
C	0.40345900	-1.63305700	-2.28767400
H	-0.65827000	-1.66238300	-2.54403900
H	0.94878800	-1.60682000	-3.23696100
C	2.24667300	-2.78061400	-1.04259400
C	3.33218300	-3.04224400	-1.88300900
C	2.50429000	-2.22346500	0.21746200
C	4.64208700	-2.74051500	-1.50083200
H	3.15609900	-3.47475300	-2.86513400
C	3.80080500	-1.91469600	0.62216300
H	1.67874300	-2.00762900	0.88525400
C	4.85209900	-2.17158900	-0.25124800
H	5.47426800	-2.94224200	-2.16560800
H	3.98502000	-1.47532300	1.59592400
Br	6.67698300	-1.71290400	0.29932600
C	-1.94509300	-4.58122000	1.37271000
C	-2.38216000	-3.61394500	0.46884700
C	-1.49908200	-3.06856900	-0.46581000
C	-0.15584600	-3.46590300	-0.50668800
C	0.26706700	-4.44439000	0.40649600
C	-0.61327100	-4.99698300	1.33514900
H	-2.63700300	-5.00938300	2.09114200
H	-3.41546800	-3.28042400	0.48296300
H	-1.88260500	-2.33266000	-1.16204500
H	1.30076500	-4.77615000	0.38894000
H	-0.25721000	-5.75584300	2.02691000
H	0.85880000	-3.72407100	-2.34485300
C	1.37718400	4.30966800	0.13794500
H	1.91741800	4.50585000	-0.79472000
H	1.50745400	5.18307000	0.78753000

im5g

SCF Energy (a.u.) = -2038.634365

Thermal correction to Gibbs free energy (a.u.) = 0.678814

Charge = 0, Multiplicity = 1

Ni	3.66278400	0.57815800	0.53896000
C	4.90122900	1.33541400	-1.02360200
C	3.66900800	0.94849800	-1.61658800
C	3.58724800	-0.23214000	-2.38135400
C	4.70287500	-1.04439500	-2.58411500
C	5.93015900	-0.64430500	-1.99829300
C	6.02666700	0.50246500	-1.23498600
H	2.81762500	1.62058400	-1.60668200
H	2.64139900	-0.48256500	-2.85030200
H	6.81103400	-1.26164700	-2.15443600
H	6.97865800	0.78567200	-0.79432600
C	4.67259500	-2.26130200	-3.40685400
C	3.58142100	-2.89477100	-3.85339200
H	5.65148700	-2.66915600	-3.65629200
H	3.66532300	-3.78586700	-4.46737700
H	2.57431900	-2.57108900	-3.61009300
C	-0.04985200	4.10393700	0.31057300
C	0.91738900	4.25092100	-0.68679800
C	2.21666300	3.78121900	-0.50272200
C	2.59486700	3.13651500	0.68848600
C	1.64157500	3.08122000	1.72348500
C	0.35288200	3.55980200	1.53914000
H	0.64066000	4.69700600	-1.63989800
H	2.92997900	3.89756700	-1.31279100
H	1.90784200	2.58893200	2.65423500
H	-0.37975000	3.43770700	2.33115500
C	3.89901000	2.45760300	0.87244200
C	4.98960700	2.61048200	-0.18879600
H	4.26259900	2.51706500	1.90033300
H	5.97612700	2.65634100	0.28099200
H	4.88375800	3.51021800	-0.80867400
C	-2.07273700	3.05585200	-0.75534900
H	-1.58898600	3.05200300	-1.74265300

C	-1.62003100	1.80075100	-0.02988200
C	-0.48217600	1.10343800	-0.44646800
C	-2.24171700	1.40473800	1.15792300
C	0.04410600	0.06307700	0.31487600
H	0.02369900	1.41106300	-1.35803900
C	-1.72577100	0.35411000	1.90988400
H	-3.13584200	1.92337200	1.49272600
C	-0.57325100	-0.33076000	1.50863100
H	0.93462200	-0.45415900	-0.02510000
H	-2.23462200	0.04535000	2.81941200
C	-6.36150900	3.07661800	-1.45451900
C	-5.71575600	4.25525600	-1.08625700
C	-4.33830400	4.26126400	-0.84945800
C	-3.58145300	3.09153700	-0.97871900
C	-4.24609500	1.91206300	-1.35182500
C	-5.61860400	1.90067800	-1.58635300
H	-7.43343900	3.07041600	-1.63125200
H	-6.28222800	5.17605300	-0.97522900
H	-3.86091700	5.19089600	-0.55834700
H	-3.68027800	0.98883200	-1.43286400
H	-6.10792800	0.96949400	-1.85723200
C	-0.41175900	-2.89729600	1.62151600
C	-0.09927000	-1.52204900	2.30235100
H	0.96676400	-1.43461000	2.51843800
H	-0.61790100	-1.52128900	3.26716100
C	-1.82825100	-2.84231400	1.06712300
C	-2.91495300	-3.11685000	1.90190800
C	-2.08966300	-2.36523200	-0.22428300
C	-4.23055200	-2.89749500	1.48509400
H	-2.73586800	-3.48929600	2.90786200
C	-3.39175700	-2.13680300	-0.66337000
H	-1.26304000	-2.14597100	-0.88953700
C	-4.44462900	-2.39819800	0.20670700
H	-5.06412600	-3.10542200	2.14621700

H	-3.57905200	-1.75292500	-1.65984600
Br	-6.27864800	-2.04396700	-0.39000200
C	2.54032300	-4.46200600	-1.16258100
C	2.87222100	-3.39487400	-0.32879400
C	1.93060600	-2.86408800	0.55661100
C	0.62887200	-3.38096900	0.61221100
C	0.30810500	-4.45377900	-0.23422000
C	1.24941100	-4.99065600	-1.11072200
H	3.27803900	-4.87412500	-1.84348200
H	3.87074400	-2.96764600	-0.36059500
H	2.23807300	-2.04625600	1.19877700
H	-0.69331500	-4.87311300	-0.20368900
H	0.97388400	-5.82510700	-1.75031200
H	-0.41075800	-3.63769300	2.43434700
C	-1.51055600	4.30786400	-0.00237500
H	-2.08319800	4.45187900	0.92065800
H	-1.65545200	5.19861400	-0.62459500
O	3.10361700	-0.11450800	2.07534400
C	3.81479000	-0.02287300	3.28313800
C	3.09053200	-0.80707300	4.37555700
H	3.90247400	1.03059300	3.60429600
H	4.84477300	-0.40825700	3.18109700
H	3.63374400	-0.74725400	5.32674800
H	2.08102800	-0.40820500	4.52320400
H	3.00275100	-1.86210100	4.09251300

im6g

SCF Energy (a.u.) = -2642.347652

Thermal correction to Gibbs free energy (a.u.) = 0.910305

Charge = 0, Multiplicity = 1

Ni	4.01880600	0.00029100	-0.79842700
C	3.53113400	-2.20415200	-2.91692000
C	2.28237700	-2.64019800	-3.37801200
C	1.64821700	-3.74575000	-2.81634200

C	2.25667800	-4.47155600	-1.77955400
C	3.50390300	-4.02361000	-1.31135200
C	4.13243900	-2.91534700	-1.86903900
H	1.79463000	-2.09704300	-4.18433700
H	0.66705800	-4.03961400	-3.17707100
H	3.98953200	-4.56089200	-0.49993900
H	5.08187400	-2.57670300	-1.46860400
C	1.64831100	-5.66697000	-1.17844100
C	0.69892900	-6.44051500	-1.72198000
H	2.04912300	-5.94671600	-0.20388700
H	0.30921300	-7.30705800	-1.19730900
H	0.29486300	-6.25087000	-2.71298000
C	1.24204000	2.92436200	-1.52803000
C	1.01816300	1.55920400	-1.63351200
C	2.02777600	0.67632100	-2.06376800
C	3.31343200	1.16312600	-2.41010900
C	3.54058200	2.56431600	-2.26774000
C	2.53392300	3.40759700	-1.85587400
H	0.05240700	1.14488100	-1.38509100
H	1.78046100	-0.36830000	-2.21117100
H	4.52356600	2.95839200	-2.51091100
H	2.72935500	4.47497700	-1.78060700
C	4.41157700	0.23602100	-2.65852900
C	4.22997700	-1.00877500	-3.53878900
H	5.22914000	-1.33185700	-3.85315700
H	3.69725700	-0.72781200	-4.45867800
C	-1.27390600	3.61833900	-1.40731700
H	-1.29137200	3.20257300	-2.42194300
C	-1.88845700	2.57666200	-0.47943000
C	-2.33086200	1.34583300	-0.96639700
C	-2.02460500	2.82066700	0.89284100
C	-2.81033400	0.35245600	-0.11142600
H	-2.26862500	1.13996500	-2.03243700
C	-2.51612700	1.83721000	1.74556600

H	-1.74116400	3.78741800	1.29954100
C	-2.88602800	0.56892200	1.26863000
H	-3.10694100	-0.59803900	-0.53202700
H	-2.59267000	2.04571700	2.81036900
C	-3.88011600	7.08844600	-1.41853200
C	-2.74688800	7.08051100	-0.60634200
C	-1.88828700	5.97890000	-0.60585700
C	-2.14891700	4.86742700	-1.41562400
C	-3.29229700	4.88705500	-2.22497600
C	-4.15018600	5.98474300	-2.23087800
H	-4.54618600	7.94646500	-1.42119300
H	-2.52538300	7.93400900	0.02860500
H	-1.00821900	5.99488600	0.02966000
H	-3.51061000	4.02641400	-2.85284200
H	-5.02834600	5.98025100	-2.87071200
C	-4.08554400	-1.73596900	1.88664600
C	-3.25800500	-0.49082000	2.29132500
H	-2.31853500	-0.85972300	2.72415200
H	-3.78664600	-0.00185700	3.11903000
C	-5.54202800	-1.45032000	1.55164200
C	-6.46587900	-2.50126600	1.65403200
C	-6.01350200	-0.19656600	1.15038300
C	-7.81558200	-2.32115700	1.36147000
H	-6.11931100	-3.48452800	1.96212200
C	-7.36451100	0.00891800	0.85467600
H	-5.33160700	0.64004000	1.05964000
C	-8.24488100	-1.05866600	0.96221200
H	-8.51651300	-3.14365600	1.44671600
H	-7.71536300	0.98719600	0.54638800
Br	-10.13917400	-0.78381100	0.54725100
C	-1.99321400	-4.19842300	-1.02653100
C	-1.43180300	-3.93605000	0.22397800
C	-2.12117800	-3.15434300	1.15019100
C	-3.38077900	-2.61705300	0.84790600

C	-3.94173000	-2.90520500	-0.40200000
C	-3.25184800	-3.68397900	-1.33361000
H	-1.45168600	-4.80908200	-1.74112100
H	-0.45882700	-4.34835500	0.47317100
H	-1.66929200	-2.95649200	2.11888200
H	-4.91882100	-2.50783200	-0.65517400
H	-3.70434400	-3.88730200	-2.30044100
H	-4.11177600	-2.33804000	2.80649800
C	0.20400600	3.92695000	-1.06300300
H	0.29956900	4.05679300	0.02417400
H	0.45771400	4.89857700	-1.50199600
O	5.60728800	-0.53009000	-0.07765900
C	6.83659100	-0.00852600	-0.50072100
C	7.53453100	-0.89160000	-1.53555500
H	7.49777900	0.07020800	0.37904200
H	6.73551500	1.01723100	-0.89665400
H	8.52340200	-0.49094600	-1.79479400
H	7.66483200	-1.90455400	-1.13769900
H	6.94301700	-0.96430000	-2.45333500
H	5.35913600	0.74156500	-2.85015900
C	0.55276900	-0.73596600	0.81277500
C	1.56289400	-1.66955600	0.60468500
C	2.88597300	-1.35569600	0.95276800
C	3.22016700	-0.08514100	1.47676300
C	2.17821200	0.85616500	1.63409600
C	0.86123600	0.52989100	1.32982900
H	-0.47262600	-0.97926600	0.55621900
H	1.33371200	-2.64019300	0.17739500
H	3.66189100	-2.10844600	0.86951600
H	2.42136600	1.84277400	2.01867500
H	0.06949900	1.25583000	1.47405600
C	6.34264700	1.86912700	2.59011600
C	6.58437100	-0.49642700	3.27584600
C	6.72381400	0.95435500	3.76517300

H	7.11108700	1.81572900	1.80840600
H	6.74590000	-1.19396400	4.10584700
B	4.67227300	0.21803700	2.01110300
O	5.08473900	1.53174000	2.01471700
O	5.29203000	-0.76136800	2.74635800
H	6.27801700	2.91104000	2.92524400
H	7.33695700	-0.71050100	2.50521400
C	8.17872600	1.22234100	4.16544200
H	8.86458900	1.03993100	3.32946200
H	8.31040800	2.26148900	4.48981500
H	8.48006400	0.57455400	4.99706600
C	5.78762300	1.20315800	4.95834800
H	6.04126700	0.53984300	5.79353300
H	5.87556400	2.23833700	5.30873700
H	4.74261700	1.02312300	4.69152100

TS3g

SCF Energy (a.u.) = -2642.347400

Thermal correction to Gibbs free energy (a.u.) = 0.911355

Charge = 0, Multiplicity = 1

Ni	4.00456300	0.04275300	-0.82141300
C	3.53955000	-2.14146300	-2.96199000
C	2.29151800	-2.57313300	-3.42926500
C	1.65411500	-3.68063300	-2.87522300
C	2.25849500	-4.41289900	-1.84048700
C	3.50529200	-3.97022700	-1.36695300
C	4.13718100	-2.86021700	-1.91738700
H	1.80675200	-2.02460900	-4.23375500
H	0.67364200	-3.97141400	-3.24030000
H	3.98848100	-4.51331500	-0.55799100
H	5.08721500	-2.52762000	-1.51352800
C	1.64791500	-5.61229300	-1.24955000
C	0.70599800	-6.38583700	-1.80578100
H	2.04076800	-5.89551700	-0.27278400

H	0.31346500	-7.25577100	-1.28888400
H	0.31093200	-6.19235700	-2.79967600
C	1.22007600	2.95505600	-1.52065800
C	1.00249100	1.59000200	-1.63978400
C	2.01559500	0.71767300	-2.08458900
C	3.29896300	1.21535600	-2.42716900
C	3.51834800	2.61644300	-2.27062700
C	2.50801400	3.44933900	-1.84806600
H	0.03955100	1.16777700	-1.39167500
H	1.77362800	-0.32655700	-2.24329300
H	4.49875500	3.01853000	-2.51096400
H	2.69725800	4.51699300	-1.76215500
C	4.40632700	0.29933200	-2.67965100
C	4.24001200	-0.94020700	-3.57043300
H	5.24381900	-1.25673200	-3.87656400
H	3.71563100	-0.65525700	-4.49384800
C	-1.29796600	3.63147400	-1.37487800
H	-1.32213600	3.22557100	-2.39336100
C	-1.89780600	2.57722800	-0.45192100
C	-2.36745800	1.36181900	-0.95151800
C	-1.99981600	2.79761600	0.92727700
C	-2.84773600	0.36165400	-0.10453600
H	-2.32950100	1.17420200	-2.02208600
C	-2.48770700	1.80641700	1.77246100
H	-1.69319300	3.75236100	1.34542500
C	-2.89162500	0.55451100	1.28029600
H	-3.16988600	-0.57573300	-0.53560200
H	-2.53760700	1.99611900	2.84237200
C	-3.92964000	7.08211000	-1.32690700
C	-2.79186500	7.07185100	-0.52105400
C	-1.92538500	5.97666700	-0.53966100
C	-2.18240300	4.87408400	-1.36262500
C	-3.33020700	4.89592700	-2.16552000
C	-4.19615300	5.98726200	-2.15224400

H	-4.60195600	7.93515600	-1.31458900
H	-2.57307600	7.91855000	0.12385100
H	-1.04203700	5.99078400	0.09134800
H	-3.54571600	4.04210400	-2.80357200
H	-5.07777700	5.98470100	-2.78730300
C	-4.08609600	-1.75879300	1.87264300
C	-3.26873400	-0.51286100	2.29338800
H	-2.33191100	-0.87907500	2.73394200
H	-3.80792100	-0.03155000	3.11889500
C	-5.54539000	-1.47938200	1.54463100
C	-6.46357100	-2.53542500	1.64455300
C	-6.02457900	-0.22579300	1.15190700
C	-7.81516800	-2.36057400	1.35726200
H	-6.11111600	-3.51852400	1.94644000
C	-7.37749500	-0.02550300	0.86173900
H	-5.34704600	0.61465200	1.06360400
C	-8.25211800	-1.09818400	0.96622400
H	-8.51166600	-3.18704400	1.44041400
H	-7.73435800	0.95267300	0.56010700
Br	-10.14907600	-0.83064400	0.55888700
C	-1.98486000	-4.16874100	-1.07831200
C	-1.41310800	-3.90221800	0.16664000
C	-2.10338500	-3.13531100	1.10436900
C	-3.37595900	-2.61901700	0.81992200
C	-3.94657500	-2.91077200	-0.42470900
C	-3.25497600	-3.67346000	-1.36829800
H	-1.44211000	-4.76800200	-1.80154800
H	-0.43175800	-4.30179700	0.40315600
H	-1.64293400	-2.93475000	2.06838500
H	-4.93329200	-2.52934100	-0.66455400
H	-3.71565400	-3.87982400	-2.33062200
H	-4.10644300	-2.37437500	2.78365600
C	0.17988900	3.94836000	-1.04177600
H	0.28540200	4.07326400	0.04497600

H	0.42335500	4.92399800	-1.47769500
O	5.58610200	-0.48036900	-0.06350900
C	6.82378900	0.04049300	-0.47193400
C	7.51381600	-0.82962200	-1.52149900
H	7.48026200	0.09341300	0.41128400
H	6.72967300	1.07426200	-0.84611200
H	8.50614600	-0.43209000	-1.77161300
H	7.63562300	-1.85052100	-1.14189900
H	6.92370400	-0.88020800	-2.44137800
H	5.34953000	0.81583500	-2.86437000
C	0.56896100	-0.64335400	0.86021600
C	1.53666000	-1.61317700	0.61634600
C	2.87955800	-1.35157600	0.92717000
C	3.27938900	-0.10041900	1.45170900
C	2.27872400	0.87764700	1.64739300
C	0.94158500	0.60518300	1.37684800
H	-0.47171200	-0.84426600	0.62926300
H	1.25850600	-2.57075700	0.18822100
H	3.62405500	-2.13077900	0.80949800
H	2.57195800	1.84978600	2.03367500
H	0.18220700	1.35951400	1.54864800
C	6.41523700	1.77388400	2.64990900
C	6.62539000	-0.61576900	3.25518200
C	6.74430900	0.81503600	3.80570600
H	7.22202900	1.75100700	1.90531600
H	6.76003900	-1.34479100	4.06302600
B	4.76743000	0.14525700	1.93239100
O	5.18506400	1.46171900	2.00857500
O	5.35340400	-0.85923400	2.67352100
H	6.33652300	2.80252000	3.02214900
H	7.40992500	-0.79805100	2.50717400
C	8.17952300	1.06532700	4.28084200
H	8.90277200	0.91114700	3.47097700
H	8.29732600	2.09210000	4.64743600

H	8.44257300	0.38782700	5.10177900
C	5.75507500	1.01947400	4.96389400
H	5.96955600	0.32314500	5.78313800
H	5.82827100	2.03991300	5.35838200
H	4.72360800	0.85278700	4.64192000

im7g

SCF Energy (a.u.) = -2642.367163

Thermal correction to Gibbs free energy (a.u.) = 0.910696

Charge = 0, Multiplicity = 1

Ni	3.89638600	0.85575100	-0.81602000
C	2.96034600	-2.28376600	-1.42529200
C	1.73529500	-2.87927200	-1.74904200
C	0.97166000	-3.52864200	-0.78200200
C	1.41547700	-3.59823100	0.54881100
C	2.63235600	-2.97440600	0.87406600
C	3.40504300	-2.34422100	-0.09695500
H	1.36726000	-2.82042200	-2.77082800
H	0.01500200	-3.96448200	-1.05505700
H	2.99020500	-3.00481700	1.90052900
H	4.33610900	-1.86384600	0.19453600
C	0.66595200	-4.31464100	1.59151900
C	-0.14140800	-5.36579800	1.39586900
H	0.83005400	-3.96443600	2.61069800
H	-0.65483700	-5.84739000	2.22256600
H	-0.28777200	-5.79920100	0.41025700
C	0.42263600	2.57173500	-1.29436300
C	0.79467800	1.48588900	-0.52533200
C	1.77585700	0.56956400	-0.96184400
C	2.40998100	0.74852100	-2.23291800
C	2.05760200	1.91436100	-2.98178600
C	1.07838100	2.77177100	-2.53631200
H	0.29498500	1.29369400	0.41514100
H	1.86651300	-0.36504400	-0.42335900

H	2.55629200	2.09224100	-3.93067400
H	0.79406700	3.62535700	-3.14797000
C	3.60248600	-0.01942000	-2.51651500
C	3.75786800	-1.53825700	-2.46915900
H	4.82591600	-1.74180000	-2.32590800
H	3.49841600	-1.93313500	-3.46350400
C	-2.08943200	2.77915600	-1.32150100
H	-2.02027600	2.59590000	-2.40203900
C	-2.24584900	1.42943700	-0.63980000
C	-1.92068200	0.24222100	-1.30473400
C	-2.63801000	1.35666400	0.70069200
C	-2.01662900	-0.99090700	-0.66169900
H	-1.57750800	0.28557200	-2.33508400
C	-2.74810900	0.12515200	1.33871400
H	-2.89463000	2.26730900	1.23469100
C	-2.47031400	-1.06904400	0.66171600
H	-1.77249900	-1.89833200	-1.20270000
H	-3.10800600	0.08162800	2.36327600
C	-5.69758600	5.07750900	-0.60605500
C	-4.49032400	5.51657300	-0.06822100
C	-3.31013700	4.80297200	-0.30370600
C	-3.32133900	3.64070000	-1.07859500
C	-4.54405000	3.21098200	-1.61855800
C	-5.72025200	3.91842900	-1.38876800
H	-6.61401900	5.63007700	-0.42076800
H	-4.46019900	6.41611300	0.54038200
H	-2.38163900	5.16206500	0.12810400
H	-4.56564100	2.30195900	-2.21517900
H	-6.65511400	3.56978800	-1.81937400
C	-4.14674000	-3.01055600	0.70022800
C	-2.82700300	-2.38892300	1.29044900
H	-2.01661500	-3.11426900	1.17398500
H	-2.98174500	-2.25184600	2.36642000
C	-5.31854000	-2.05852800	0.86872200

C	-6.30737800	-2.34642400	1.81601000
C	-5.42131800	-0.84764900	0.16257300
C	-7.36273400	-1.46720100	2.06971400
H	-6.25360400	-3.27592300	2.37749700
C	-6.46146900	0.04920300	0.40206700
H	-4.67699100	-0.58277500	-0.57737700
C	-7.41765300	-0.27586700	1.35710900
H	-8.11843000	-1.70761500	2.80873500
H	-6.50539800	0.99043400	-0.13443000
Br	-8.87676100	0.98468100	1.70890300
C	-3.36456400	-4.61796300	-3.26746300
C	-2.64137900	-5.04843600	-2.15172500
C	-2.92518200	-4.52567700	-0.89278700
C	-3.92401400	-3.55538300	-0.71085900
C	-4.66083700	-3.15863500	-1.83042400
C	-4.38051100	-3.68052300	-3.09679900
H	-3.14521500	-5.01930100	-4.25268600
H	-1.86009800	-5.79623500	-2.26141900
H	-2.35823200	-4.87293200	-0.03473900
H	-5.46469500	-2.44073400	-1.72265800
H	-4.96474700	-3.34883000	-3.95082300
H	-4.35556100	-3.88216100	1.33477000
C	-0.74526400	3.43760500	-0.89591300
H	-0.74693000	3.58592500	0.18962000
H	-0.66640500	4.42605100	-1.36326900
O	5.76995100	0.62685700	-0.70468800
C	6.63170400	1.38855600	-1.55397100
C	7.47737300	0.45313800	-2.40628400
H	7.25544000	2.02909300	-0.92365400
H	6.02468100	2.03892700	-2.19691300
H	8.15798800	1.02293900	-3.05057400
H	8.07515700	-0.20835800	-1.77034500
H	6.83973100	-0.17211800	-3.04094000
H	4.20966000	0.40407300	-3.32117500

C	2.08161000	2.87579700	2.03450700
C	2.31501800	1.57990500	2.51548300
C	3.45112700	0.88374400	2.11834100
C	4.40634200	1.46064200	1.24762300
C	4.13160200	2.76104500	0.76103500
C	2.98207000	3.46289100	1.15090300
H	1.19229400	3.41806700	2.34565400
H	1.60317000	1.12062900	3.19693500
H	3.64379400	-0.11786700	2.48999900
H	4.86560200	3.25499100	0.12769300
H	2.80086100	4.46434300	0.77046500
C	8.19108500	0.85017100	1.42136500
C	7.01198100	-1.31844500	1.39229500
C	8.08953500	-0.50988900	2.13574700
H	8.64010800	0.69098800	0.42489200
H	6.85802300	-2.28877400	1.88307000
B	5.81623300	0.71883900	0.89903800
O	6.94331300	1.50598200	1.30390600
O	5.77510200	-0.64047000	1.37440000
H	8.86503800	1.51728100	1.97487500
H	7.35499400	-1.52051200	0.36224800
C	9.43547600	-1.23572800	2.04850300
H	9.73418500	-1.40365200	1.00612300
H	10.22802400	-0.65451700	2.53560200
H	9.38683000	-2.21223800	2.54559200
C	7.67873500	-0.30982100	3.60114300
H	7.56916500	-1.27612900	4.10902700
H	8.43662600	0.27151400	4.14035800
H	6.72692200	0.22222100	3.66759700

TS4g

SCF Energy (a.u.) = -2642.336796

Thermal correction to Gibbs free energy (a.u.) = 0.910672

Charge = 0, Multiplicity = 1

Ni	4.25441400	0.92762400	-0.45561400
C	4.38040700	-0.66627900	-3.11158400
C	3.30801400	-1.01614300	-3.94256100
C	2.61268200	-2.20876200	-3.75950200
C	2.97341500	-3.10258900	-2.73688700
C	4.04182100	-2.74234200	-1.89904200
C	4.74167700	-1.55545800	-2.09090100
H	3.00339200	-0.33401800	-4.73290500
H	1.77250000	-2.44164100	-4.40710800
H	4.33457200	-3.39853200	-1.08435300
H	5.56211600	-1.31355700	-1.42604200
C	2.29809500	-4.39013100	-2.52449400
C	1.50762400	-5.03720300	-3.39157500
H	2.50658400	-4.86145500	-1.56366200
H	1.06115600	-5.99379500	-3.13864800
H	1.29244100	-4.64890100	-4.38356300
C	1.29442800	3.34902700	-0.56596800
C	1.35869900	2.03089900	-0.96258600
C	2.51388600	1.49324200	-1.58785900
C	3.65702900	2.31595000	-1.83652600
C	3.58196300	3.67321700	-1.37752000
C	2.44087500	4.16380400	-0.79480600
H	0.53311400	1.36015600	-0.77219900
H	2.43391400	0.51007500	-2.03671200
H	4.44192200	4.31954100	-1.53304300
H	2.40638600	5.20769600	-0.49042000
C	4.91281300	1.69603700	-2.17299500
C	5.11270400	0.65067500	-3.27560600
H	6.18869100	0.43957500	-3.31949300
H	4.84974900	1.08697200	-4.25080300
C	-1.29432700	3.62789400	-0.51461400
H	-1.13238800	3.48237000	-1.58896400
C	-1.87485000	2.32861500	0.03677800
C	-1.86607100	1.15442100	-0.72031900

C	-2.41358600	2.26476900	1.32661300
C	-2.28524200	-0.06229600	-0.18461400
H	-1.48861100	1.17869600	-1.73936600
C	-2.88200300	1.06056100	1.84591600
H	-2.48113800	3.16702000	1.92715100
C	-2.79783800	-0.13499900	1.11833400
H	-2.20402200	-0.95189200	-0.79318000
H	-3.29920000	1.04141700	2.85011800
C	-4.27770400	6.75258500	-0.11022700
C	-3.28273500	6.62002900	0.85761700
C	-2.30472500	5.63108700	0.73103600
C	-2.30576500	4.75673500	-0.36244300
C	-3.31297900	4.89916400	-1.32568200
C	-4.28879800	5.88655200	-1.20595100
H	-5.03650800	7.52384900	-0.01391000
H	-3.26323600	7.28816100	1.71434300
H	-1.53575200	5.54580500	1.49304900
H	-3.32988300	4.22185100	-2.17632900
H	-5.05695100	5.98188600	-1.96854000
C	-3.98771700	-2.51144700	1.04368200
C	-3.16367000	-1.43483700	1.80931000
H	-2.23295300	-1.91349400	2.14203800
H	-3.71682600	-1.19573400	2.72477600
C	-5.41786800	-2.07314000	0.78317200
C	-6.47336200	-2.87745900	1.22768500
C	-5.73340900	-0.88228000	0.11180000
C	-7.80683700	-2.51908300	1.02260400
H	-6.25348700	-3.80672500	1.74722000
C	-7.05874800	-0.50277700	-0.10273900
H	-4.94146900	-0.23852300	-0.25079600
C	-8.07739400	-1.32955600	0.35795200
H	-8.61188400	-3.15340100	1.37557000
H	-7.28827400	0.42189200	-0.61993100
Br	-9.94138100	-0.80406400	0.06111600

C	-1.73103700	-3.89063700	-2.40287400
C	-1.19826600	-3.97542700	-1.11442600
C	-1.95515700	-3.56787800	-0.01917800
C	-3.24755400	-3.04436900	-0.18412700
C	-3.78315400	-2.99928000	-1.47450700
C	-3.03017500	-3.41729000	-2.57557600
H	-1.13159100	-4.19503900	-3.25521400
H	-0.18915700	-4.34986800	-0.97380100
H	-1.52560100	-3.63542000	0.97720000
H	-4.78540800	-2.61532700	-1.62742600
H	-3.46288600	-3.36065100	-3.57080000
H	-4.05187200	-3.35143000	1.74896200
C	0.08944600	3.96722200	0.11400700
H	0.08235900	3.67743300	1.17292100
H	0.21690000	5.05464500	0.09134100
O	5.82407000	0.24185400	0.38894500
C	6.97512900	1.06597700	0.65369200
C	8.01248800	0.83091100	-0.42891200
H	7.35401400	0.80174100	1.64358800
H	6.65826000	2.11403600	0.68314900
H	8.89281400	1.45967400	-0.25173000
H	8.32780900	-0.21746900	-0.43640300
H	7.60563600	1.07525000	-1.41435900
H	5.75764800	2.38566500	-2.11377700
C	0.53245300	0.19422700	2.17448100
C	0.93790400	-0.80722300	1.28919400
C	2.22939700	-0.78110100	0.75927600
C	3.14686600	0.24124200	1.07963400
C	2.70803900	1.22958400	1.98338500
C	1.42305400	1.21199900	2.52703900
H	-0.47291000	0.18904500	2.57963100
H	0.24181900	-1.59087100	0.99880600
H	2.53117900	-1.55626500	0.05870500
H	3.39138600	2.02561900	2.27168600

H	1.11000000	1.98744600	3.22277100
C	5.67954300	-1.08452500	3.67914100
C	4.50567000	-2.71019000	2.17921400
C	4.62173700	-2.19850200	3.64497500
H	6.67207900	-1.51170700	3.46757100
H	3.45058600	-2.89780700	1.93858700
B	5.13162600	-0.47068500	1.45128800
O	5.40308900	-0.03959500	2.75170700
O	5.05069600	-1.83752600	1.19656500
H	5.71493000	-0.63165700	4.67579100
H	5.04717900	-3.65685500	2.06832500
C	5.07966800	-3.35149600	4.55076600
H	6.05680800	-3.74164900	4.24128600
H	5.15790600	-3.02498000	5.59465100
H	4.36114400	-4.17920200	4.51726400
C	3.27593800	-1.65576800	4.15113700
H	2.50474300	-2.43356000	4.10535400
H	3.36408600	-1.33071800	5.19528500
H	2.93498500	-0.80677700	3.55926500

im8g

SCF Energy (a.u.) = -2642.362932

Thermal correction to Gibbs free energy (a.u.) = 0.911022

Charge = 0, Multiplicity = 1

Ni	3.57748000	-0.04392900	-1.22001100
C	4.49164500	-2.87827900	-1.79749200
C	3.63673300	-3.96090900	-2.03990200
C	3.01850200	-4.64090600	-0.99477800
C	3.23723700	-4.26280500	0.34123900
C	4.12982700	-3.20578800	0.58085900
C	4.74411100	-2.52482400	-0.46620300
H	3.43512000	-4.25838200	-3.06642800
H	2.35729700	-5.47231200	-1.21987000
H	4.32536300	-2.89047000	1.60128400

H	5.42200500	-1.70834900	-0.24401400
C	2.57570900	-4.91147800	1.48151700
C	1.59129700	-5.81817000	1.44123000
H	2.93816400	-4.58763700	2.45740400
H	1.17316000	-6.23066600	2.35412600
H	1.16307600	-6.17723000	0.50945300
C	0.68754500	1.05003000	-3.09849700
C	0.90027900	-0.24162900	-2.67374400
C	2.19898400	-0.81778900	-2.64996300
C	3.32572400	-0.12097000	-3.21082200
C	3.06290000	1.21061500	-3.69863500
C	1.80593100	1.75557200	-3.63823700
H	0.08741600	-0.83430900	-2.27929500
H	2.27499800	-1.87278500	-2.41807100
H	3.88487600	1.77137000	-4.13763300
H	1.64967000	2.76675000	-4.00899700
C	4.64588000	-0.58342000	-2.93305800
C	5.07371300	-2.05163400	-2.92732600
H	6.16844500	-2.07064900	-2.84711900
H	4.83210400	-2.53521300	-3.88533300
C	-1.95538700	1.08553800	-3.05221600
H	-1.97562300	0.63260000	-4.05153700
C	-2.25293200	-0.01573400	-2.04116100
C	-3.20591400	-0.98997900	-2.36333500
C	-1.66616100	-0.06470100	-0.77295000
C	-3.58367600	-1.96779200	-1.44406300
H	-3.67415800	-0.96995800	-3.34490400
C	-2.02914600	-1.05449000	0.13471100
H	-0.90413400	0.64891900	-0.48326300
C	-3.00840400	-2.00638100	-0.16805600
H	-4.34680500	-2.68874600	-1.71985800
H	-1.55915400	-1.05865700	1.11119100
C	-5.10566200	4.06477700	-2.86767100
C	-4.30690100	3.80899100	-1.74913100

C	-3.30410300	2.84330400	-1.81054800
C	-3.07255200	2.12392500	-2.99168400
C	-3.87365400	2.39041100	-4.10506100
C	-4.88669800	3.35122100	-4.04545900
H	-5.89088600	4.81401900	-2.81927700
H	-4.46391100	4.35960600	-0.82508800
H	-2.70464600	2.63719000	-0.92883200
H	-3.70366600	1.84009500	-5.02763300
H	-5.50217600	3.54081500	-4.92083700
C	-4.74376000	-2.40188900	1.69859300
C	-3.48626200	-2.93531900	0.92406900
H	-3.68232900	-3.94391900	0.54813400
H	-2.68481500	-3.03640500	1.66330600
C	-4.54000400	-0.91615500	1.95657400
C	-3.76932900	-0.49326400	3.04293900
C	-4.95414000	0.04003600	1.02131000
C	-3.37192900	0.83956800	3.17694500
H	-3.43979500	-1.21942300	3.78251500
C	-4.57598000	1.37519900	1.13472100
H	-5.54455600	-0.26720500	0.16575300
C	-3.76987600	1.74776500	2.20379400
H	-2.75734000	1.15413800	4.01276900
H	-4.87491300	2.09305200	0.38159600
Br	-3.14450100	3.60393400	2.31445900
C	-8.67765700	-3.29847800	0.06738600
C	-7.55490200	-3.93172200	-0.46012000
C	-6.28152100	-3.64584800	0.03995700
C	-6.10022200	-2.71756100	1.07049400
C	-7.24399600	-2.09548400	1.59775500
C	-8.51548000	-2.37875800	1.10601200
H	-9.66733000	-3.51831000	-0.32273000
H	-7.66256400	-4.65294000	-1.26569100
H	-5.43127500	-4.16461200	-0.38634700
H	-7.12924600	-1.37193400	2.39956000

H	-9.38064800	-1.87905500	1.53317700
H	-4.73058400	-2.91075900	2.67305300
C	-0.60250600	1.81654400	-2.90018800
H	-0.56451100	2.28026700	-1.90450500
H	-0.62098800	2.65665900	-3.60463200
O	5.10082300	0.89615600	-0.21887000
C	5.69396500	1.99788400	-0.95338300
C	7.15821500	1.71000200	-1.22713700
H	5.56391100	2.91244400	-0.37139700
H	5.11890100	2.08254500	-1.87562000
H	7.59407000	2.51250600	-1.83309100
H	7.71982400	1.64500100	-0.28951100
H	7.26561600	0.76512800	-1.76887300
H	5.43569500	0.09336200	-3.25993000
C	0.23970500	1.25122500	1.93317600
C	0.75480100	-0.04740700	1.96399100
C	1.73334800	-0.44427200	1.04646600
C	2.23867200	0.43463000	0.06996400
C	1.70454600	1.73873000	0.06547300
C	0.72275300	2.14823200	0.97772700
H	-0.53371300	1.55862600	2.63057400
H	0.38555000	-0.75830800	2.70200300
H	2.10755400	-1.46448800	1.09008400
H	2.04553800	2.45196900	-0.68399000
H	0.32801200	3.16162000	0.94098400
C	5.80003100	1.93649200	3.22266900
C	4.68014700	-0.27156500	3.22605100
C	4.65654900	1.13198500	3.85496200
H	6.77211000	1.49132800	3.47627200
H	3.74616500	-0.80081800	3.44104300
B	5.18927100	0.88915200	1.16742800
O	5.68030900	1.99553300	1.79665200
O	4.82232500	-0.25044200	1.80363700
H	5.79329200	2.96893200	3.58503300

H	5.51352400	-0.85810100	3.63419200
C	4.89946600	1.00611400	5.36427300
H	5.87260800	0.54996000	5.58290000
H	4.86893900	1.99032700	5.84512700
H	4.12350200	0.38747100	5.82927200
C	3.31168900	1.82665300	3.58953300
H	2.49418700	1.27292900	4.05967900
H	3.31995700	2.84216600	4.00279300
H	3.07629500	1.89614000	2.52536100

im9g

SCF Energy (a.u.) = -2427.934730

Thermal correction to Gibbs free energy (a.u.) = 0.871929

Charge = 0, Multiplicity = 1

Ni	-3.24754300	-1.79839500	-0.13497300
C	-6.21285400	1.24503000	0.44774900
C	-7.28856500	1.03904200	-0.42954900
C	-8.08520300	2.09202100	-0.86195800
C	-7.83533200	3.40732600	-0.43217900
C	-6.75879100	3.61092200	0.44622400
C	-5.96328200	2.55333700	0.87893800
H	-7.50387500	0.02872600	-0.77284200
H	-8.91226800	1.89160800	-1.53677100
H	-6.54571300	4.61889600	0.79491500
H	-5.13211900	2.74478600	1.55047600
C	-8.64247400	4.56002700	-0.85385300
C	-9.70086300	4.55924100	-1.67444100
H	-8.31923400	5.51329800	-0.43526300
H	-10.22129000	5.48080400	-1.91573800
H	-10.08800300	3.65360500	-2.13337200
C	-1.04707800	3.00250900	-0.04194600
C	-1.60548800	2.51051800	1.14644100
C	-2.60445800	1.54308400	1.13113900
C	-3.11760900	1.04035100	-0.08015700

C	-2.61071300	1.60440800	-1.26231000
C	-1.58381200	2.54530400	-1.24684500
H	-1.22391300	2.86163400	2.10337400
H	-2.97330900	1.15038500	2.07180700
H	-3.03393500	1.30288500	-2.21748700
H	-1.18428600	2.92045300	-2.18608700
C	-4.13723600	-0.05073600	-0.13677200
C	-5.31574000	0.09553600	0.84493900
H	-4.95041300	0.22927600	1.86555000
H	-5.89951500	-0.83337400	0.84586500
C	1.40542200	3.09120600	0.50903200
H	1.14868100	2.78440500	1.53087500
C	1.62301200	1.80605500	-0.27964000
C	1.05615400	0.60763100	0.16924900
C	2.38661100	1.77975500	-1.45069400
C	1.30524900	-0.59459100	-0.48570400
H	0.42257600	0.61933600	1.04925400
C	2.65660000	0.57234800	-2.09321600
H	2.82975900	2.69854400	-1.82367800
C	2.16468500	-0.63917700	-1.59293400
H	0.88831100	-1.51305400	-0.08784900
H	3.32110900	0.56073700	-2.95335800
C	5.18483300	5.20421600	0.76417100
C	4.97922600	4.00288300	1.45041200
C	3.74969200	3.35584600	1.36591600
C	2.69876900	3.88723000	0.60120300
C	2.91403400	5.09198100	-0.07270100
C	4.14843500	5.74575100	0.00739700
H	6.14337700	5.71131200	0.82485700
H	5.77664900	3.57612700	2.05316900
H	3.59426200	2.41683000	1.89269100
H	2.12025300	5.53213300	-0.66733500
H	4.29511400	6.68082000	-0.52625900
C	3.71753200	-2.62664800	-1.08370900

C	2.71112300	-1.95009500	-2.09222100
H	1.90692400	-2.66958800	-2.28431800
H	3.24149100	-1.79586200	-3.03835300
C	4.91954900	-1.74135400	-0.80016400
C	6.18433100	-2.15437200	-1.23659500
C	4.82490200	-0.49231100	-0.16218700
C	7.32127200	-1.36369500	-1.05822400
H	6.28920500	-3.11587900	-1.73312700
C	5.94474900	0.31873400	0.02030300
H	3.87113000	-0.12358500	0.18968000
C	7.17862900	-0.13120100	-0.43288000
H	8.29109700	-1.70223400	-1.40443300
H	5.84110800	1.29058000	0.48931600
Br	8.75498800	1.00705600	-0.18728900
C	1.33922200	-4.11161300	2.23757200
C	1.29185700	-4.71800500	0.97974500
C	2.10264700	-4.24760300	-0.05191300
C	2.97188000	-3.16194900	0.13726500
C	3.04774000	-2.60107700	1.41605400
C	2.23414500	-3.06511500	2.45244500
H	0.69155600	-4.45375700	3.03874100
H	0.62053200	-5.55329000	0.80113200
H	2.05625600	-4.72646700	-1.02769700
H	3.73622900	-1.78876500	1.61056300
H	2.29839100	-2.59859000	3.43140900
H	4.09774200	-3.50563900	-1.61972000
C	0.18047200	3.88101800	-0.02186900
H	0.38481900	4.24086200	-1.03645600
H	0.03413800	4.76397400	0.61398000
H	-4.56814600	-0.05882200	-1.14748500
C	-1.99072400	-1.71124500	4.39938000
C	-3.31272600	-2.02035500	4.07395600
C	-3.73687500	-1.99651300	2.74020700
C	-2.85673800	-1.66035200	1.70088100

C	-1.53032600	-1.35698300	2.05087300
C	-1.09680500	-1.38141300	3.37825900
H	-1.66198500	-1.72846000	5.43515500
H	-4.01913500	-2.28028500	4.85940500
H	-4.77456200	-2.23701200	2.51766600
H	-0.82240700	-1.08920000	1.27397500
H	-0.06086900	-1.14381900	3.60963600
C	-3.99818800	-2.46097300	-2.30568300
C	-2.82188100	-1.78364200	-2.40784200
C	-1.41953900	-2.33519900	-2.50299800
C	-1.18239900	-3.67575700	-1.77148300
C	-1.77653000	-3.70526400	-0.38251800
C	-3.02342400	-4.11643200	-0.02548300
C	-4.14221300	-4.60114700	-0.91690100
C	-4.18709100	-3.96271000	-2.32411100
H	-4.91227900	-1.87042000	-2.31723500
H	-2.87940000	-0.70735800	-2.53164200
H	-0.74461700	-1.57964700	-2.08488800
H	-1.13423300	-2.43988600	-3.56091700
H	-1.55683100	-4.51033400	-2.36894900
H	-0.10197800	-3.82403400	-1.67976800
H	-1.09893600	-3.44510000	0.42601400
H	-3.22576700	-4.18816000	1.04052000
H	-5.08713700	-4.38554300	-0.40304800
H	-4.09744600	-5.69635900	-1.01527300
H	-3.44434900	-4.42800700	-2.97557100
H	-5.16303000	-4.18609600	-2.76920100

TS5g

SCF Energy (a.u.) = -2427.899016

Thermal correction to Gibbs free energy (a.u.) = 0.872955

Charge = 0, Multiplicity = 1

Ni	-3.40271000	-1.91366200	-0.80285700
C	-5.65926200	1.87394000	0.34690200

C	-5.70539600	3.13004800	-0.27709100
C	-5.66694900	4.30791400	0.45721600
C	-5.58298300	4.27840300	1.86017900
C	-5.55933300	3.01997600	2.48277300
C	-5.60135900	1.83974400	1.74443600
H	-5.74925000	3.17896400	-1.36216400
H	-5.69770800	5.25982800	-0.06408600
H	-5.50330600	2.96811200	3.56771500
H	-5.56182100	0.88618400	2.25708700
C	-5.52335300	5.48917100	2.69029900
C	-5.50856500	6.76163800	2.27359500
H	-5.48389100	5.29926300	3.76297000
H	-5.46112200	7.58139000	2.98357000
H	-5.54169300	7.03616400	1.22285900
C	-0.92573000	2.70573200	-1.84418300
C	-1.63702900	2.85576200	-0.64840400
C	-2.70982200	2.02839000	-0.32962000
C	-3.14690300	1.03036400	-1.22226100
C	-2.47115000	0.93567600	-2.45105800
C	-1.37618200	1.74114900	-2.75079200
H	-1.32141200	3.60657200	0.07306200
H	-3.19295700	2.14260000	0.63036400
H	-2.79632800	0.19411500	-3.17522300
H	-0.84763000	1.60166600	-3.69064900
C	-4.23144100	0.05869700	-0.88716000
C	-5.62708400	0.62503400	-0.50244700
H	-6.21114000	-0.17019600	-0.03073400
H	-6.13970400	0.85939800	-1.44553400
C	1.44830500	2.96998400	-1.05949800
H	1.03160100	3.14842600	-0.06028300
C	1.67675700	1.46746100	-1.16881700
C	0.92610500	0.58037000	-0.38690200
C	2.62992500	0.93348600	-2.04062200
C	1.15742800	-0.79163200	-0.42792700

H	0.16120800	0.97379000	0.27452700
C	2.87978400	-0.43742600	-2.06433800
H	3.22389100	1.59913500	-2.65980800
C	2.18069300	-1.31858100	-1.23154400
H	0.58236300	-1.43885600	0.22376500
H	3.67737900	-0.82392900	-2.69371300
C	5.28748900	4.98297300	-1.16928700
C	4.90788500	4.20818100	-0.06854400
C	3.66207600	3.58802500	-0.05187800
C	2.76755500	3.72404500	-1.12535200
C	3.15581400	4.50575400	-2.21630500
C	4.40716500	5.13096000	-2.23858300
H	6.25964400	5.46699900	-1.18791000
H	5.58296000	4.09223300	0.77524600
H	3.37110800	2.97850100	0.80089600
H	2.48540700	4.63347000	-3.06000700
H	4.69006600	5.73354900	-3.09740200
C	3.32558400	-3.03541500	0.31274600
C	2.65377300	-2.74171700	-1.07836500
H	1.83096100	-3.45059400	-1.20711100
H	3.39243500	-2.96451600	-1.85615200
C	4.54242800	-2.15272700	0.53377600
C	5.81477900	-2.73576500	0.55342900
C	4.46127300	-0.75454300	0.65378900
C	6.97544800	-1.96907100	0.67780000
H	5.90807900	-3.81521500	0.46313500
C	5.60634600	0.03251700	0.77066100
H	3.49978800	-0.25846100	0.64510400
C	6.84917600	-0.58932000	0.77890300
H	7.95175400	-2.43995500	0.68920600
H	5.52219200	1.11157900	0.83258400
Br	8.46308200	0.51233400	0.93162900
C	0.19000700	-3.05101400	3.32639100
C	0.20097000	-3.98185500	2.28507600

C	1.23955100	-3.97828700	1.35722400
C	2.28262100	-3.04045700	1.43029800
C	2.28089600	-2.14297800	2.50183400
C	1.24290300	-2.14526200	3.43789400
H	-0.63098500	-3.03405500	4.03583700
H	-0.60136300	-4.70917000	2.19721100
H	1.23438700	-4.70902400	0.55204000
H	3.08820600	-1.42868200	2.60859000
H	1.25940400	-1.42786600	4.25397900
H	3.69687900	-4.06567700	0.23286100
C	0.36825000	3.45048300	-2.06628200
H	0.71830900	3.28339300	-3.09108300
H	0.23135500	4.53210900	-1.93877700
H	-4.44621800	-0.53756600	-1.80000500
C	-3.20551500	-1.07229700	3.55495900
C	-4.45455300	-1.46068300	3.04828900
C	-4.71546800	-1.40432500	1.68279400
C	-3.72355600	-0.97514800	0.76572500
C	-2.48142100	-0.55746600	1.30013600
C	-2.22282400	-0.62793900	2.67155900
H	-3.01189600	-1.10979600	4.62330200
H	-5.22807800	-1.81456600	3.72647200
H	-5.68679800	-1.72861100	1.31754300
H	-1.71452100	-0.17996300	0.63322800
H	-1.24762200	-0.32644300	3.04414200
C	-2.80058500	-2.72503200	-3.12228500
C	-1.67067400	-2.58148300	-2.38407900
C	-0.97194100	-3.63995900	-1.56154800
C	-1.87534700	-4.69219500	-0.87284800
C	-3.10197800	-4.10792900	-0.20329500
C	-4.32655800	-3.90273700	-0.79749600
C	-4.70949900	-4.20668100	-2.23154900
C	-3.60076300	-3.99561400	-3.29884200
H	-3.13667500	-1.86624900	-3.70026800

H	-1.15842000	-1.62050700	-2.42400400
H	-0.40681000	-3.12238300	-0.78300700
H	-0.22552200	-4.15927800	-2.18327100
H	-2.16600200	-5.46981100	-1.58409100
H	-1.26794200	-5.19642100	-0.11278100
H	-3.04119100	-3.96400000	0.87312200
H	-5.16718300	-3.68268600	-0.14116800
H	-5.56466100	-3.56866400	-2.48635300
H	-5.07387100	-5.24289100	-2.31305000
H	-2.92977600	-4.85737500	-3.31350400
H	-4.08444100	-3.97519500	-4.28217900

im10g

SCF Energy (a.u.) = -2427.966602

Thermal correction to Gibbs free energy (a.u.) = 0.872608

Charge = 0, Multiplicity = 1

Ni	-2.91731200	-1.03802600	-1.73299600
C	-5.71599800	1.13146600	1.77082800
C	-5.54820900	2.30414200	2.52429300
C	-5.22998600	2.26154100	3.87646800
C	-5.07030600	1.03231600	4.53929900
C	-5.26502600	-0.13905100	3.78967300
C	-5.58663600	-0.09527800	2.43595500
H	-5.65707100	3.26758800	2.03194300
H	-5.10838900	3.19217300	4.42255700
H	-5.16130900	-1.10415200	4.28008800
H	-5.73762500	-1.02240100	1.89440600
C	-4.72156200	0.92251200	5.96227100
C	-4.45980800	1.92078000	6.81550600
H	-4.67398500	-0.09987100	6.33732600
H	-4.21142000	1.71860100	7.85265900
H	-4.48102100	2.96639400	6.52081600
C	-1.39376000	3.22554000	-1.19934000
C	-1.93161200	2.98711400	0.07174200

C	-3.07438900	2.21113200	0.24538300
C	-3.75416000	1.66847000	-0.85504100
C	-3.24310800	1.94749900	-2.12925600
C	-2.07578900	2.69409000	-2.29750500
H	-1.44677300	3.40306300	0.95085500
H	-3.43318100	2.02524400	1.24879200
H	-3.76474100	1.56808800	-3.00118300
H	-1.69276700	2.86908700	-3.30022300
C	-4.95351900	0.74348700	-0.72477800
C	-6.04333200	1.20604600	0.29715100
H	-6.92622200	0.58438500	0.10403400
H	-6.32255700	2.23487300	0.04078500
C	1.03132600	3.63961000	-0.46324600
H	0.66872300	3.71410500	0.56901900
C	1.43059200	2.18782000	-0.68656300
C	0.97938300	1.17952000	0.17255000
C	2.24510700	1.81943300	-1.76159600
C	1.31866100	-0.15509700	-0.03779300
H	0.33967100	1.43832800	1.01106600
C	2.59773700	0.48618300	-1.96291400
H	2.62967000	2.58533700	-2.42945300
C	2.14306400	-0.52688200	-1.11003600
H	0.93712000	-0.90590100	0.64199000
H	3.24541400	0.22556500	-2.79634900
C	4.55642600	6.16371900	-0.66369200
C	4.37548100	5.25414700	0.38242400
C	3.23164000	4.46289900	0.42734900
C	2.24201200	4.56004100	-0.56254700
C	2.43418200	5.47317700	-1.60352700
C	3.58292500	6.26920600	-1.65425600
H	5.44827700	6.78256400	-0.70306200
H	5.12703200	5.16306200	1.16188600
H	3.09921600	3.74706100	1.23530000
H	1.68881800	5.57580100	-2.38498900

H	3.71163600	6.97260500	-2.47242000
C	3.17130400	-2.80198200	-0.26039700
C	2.51108300	-1.96416500	-1.39939200
H	1.60609200	-2.49532900	-1.71738400
H	3.19699000	-1.98283800	-2.25380500
C	4.52767600	-2.26208500	0.15684700
C	5.64856500	-3.09656800	0.07344600
C	4.71790200	-0.94948500	0.61633700
C	6.92399800	-2.65363600	0.42745400
H	5.52725400	-4.11836900	-0.27730000
C	5.98367200	-0.48463000	0.97485200
H	3.87550600	-0.27412900	0.69578300
C	7.06999300	-1.34608300	0.87350300
H	7.78032300	-3.31420300	0.35401400
H	6.11544500	0.53317200	1.32395200
Br	8.85089600	-0.69947600	1.37242300
C	0.25969300	-3.54769900	2.87878200
C	0.08496300	-4.06229800	1.59115200
C	1.04724700	-3.82943700	0.61140300
C	2.19807800	-3.07481800	0.88628200
C	2.37641300	-2.59181900	2.18614500
C	1.41282400	-2.82066100	3.17209500
H	-0.48985500	-3.72240600	3.64523700
H	-0.79985400	-4.64433400	1.34892300
H	0.89690400	-4.23158800	-0.38683100
H	3.26634500	-2.02349900	2.43160100
H	1.56806800	-2.42704900	4.17279200
H	3.36306900	-3.77858400	-0.72433900
C	-0.13845700	4.04889700	-1.38876700
H	0.18135600	3.96557400	-2.43363400
H	-0.35973600	5.11061100	-1.21133700
H	-5.46783100	0.76987200	-1.69506200
C	-4.18564800	-3.31373600	0.59742500
C	-5.36899000	-2.98686300	-0.12540000

C	-5.53490100	-1.72334800	-0.63760000
C	-4.52463200	-0.71235300	-0.50357800
C	-3.34407600	-1.03950200	0.25599400
C	-3.21835800	-2.35704200	0.79867900
H	-4.06949600	-4.30863300	1.01923300
H	-6.14642200	-3.73504100	-0.25525500
H	-6.45505900	-1.46690300	-1.16010800
H	-2.72495600	-0.25612200	0.68116000
H	-2.33947500	-2.58629300	1.39537900
C	-0.94439400	-0.83460000	-2.45750800
C	-1.04224300	-1.98711400	-1.70788000
C	-1.37147700	-3.36878300	-2.22667400
C	-2.39681600	-3.38279300	-3.39254500
C	-3.50071000	-2.35145500	-3.22876200
C	-3.49225500	-1.08318100	-3.78031400
C	-2.35510100	-0.47894100	-4.57739800
C	-0.95234700	-0.75923000	-3.97338400
H	-0.60061000	0.05900200	-1.94273300
H	-0.71921800	-1.94873900	-0.67281600
H	-1.79081900	-3.93486300	-1.38621900
H	-0.46265800	-3.90721500	-2.54157100
H	-1.88303700	-3.23215400	-4.34619500
H	-2.84730300	-4.38072600	-3.44356300
H	-4.44243100	-2.72937800	-2.83905300
H	-4.44226200	-0.55174100	-3.82947600
H	-2.50937700	0.60502400	-4.61680200
H	-2.37625700	-0.82379300	-5.62304500
H	-0.54340600	-1.68426600	-4.39084900
H	-0.26849800	0.03866100	-4.28503200

ima1

SCF Energy (a.u.) = -1076.873593

Thermal correction to Gibbs free energy (a.u.) = 0.151000

Charge = 0, Multiplicity = 1

C	-0.69219100	1.97865200	0.32621900
C	-1.95750900	1.41699700	0.36373000
C	-2.17766800	0.15662100	-0.20526100
C	-1.13937200	-0.52425500	-0.83027600
C	0.13895800	0.03468400	-0.85587300
C	0.43665200	1.31387600	-0.26507800
H	-0.53935100	2.96277800	0.76511000
H	-2.77788600	1.95712900	0.82633300
H	-1.31646600	-1.48942300	-1.29593000
H	0.93258800	-0.51509500	-1.35778100
C	1.74965500	1.82935000	-0.16394000
C	2.88931900	1.22249900	-0.86445100
Br	-3.96888300	-0.65813400	-0.10741300
H	2.64675900	0.85085600	-1.87526700
H	1.88361700	2.82002400	0.26221500
K	1.66396700	-0.37084800	1.69005500
H	3.73543700	1.91638900	-0.94623900
O	3.41740400	0.00667400	-0.15035800
C	4.44267900	-0.65310600	-0.86611500
H	5.31511200	0.01156300	-0.98083000
H	4.09429000	-0.90522900	-1.88161200
C	4.83756700	-1.91803700	-0.11850900
H	5.63484900	-2.45274500	-0.64667800
H	5.19915200	-1.67620100	0.88793000
H	3.97966400	-2.59632300	-0.02862500

imb1

SCF Energy (a.u.) = -1399.327317

Thermal correction to Gibbs free energy (a.u.) = 0.257324

Charge = 0, Multiplicity = 1

C	1.29100500	0.99459600	-1.97664200
C	0.41471400	1.96088300	-1.49303700
C	0.47899900	2.32942800	-0.14964700
C	1.45544200	1.78520700	0.68830700

C	2.32109600	0.81247200	0.20666200
C	2.25438300	0.32376900	-1.14364500
H	1.26116900	0.74610500	-3.03878300
H	-0.30312400	2.42971500	-2.15944900
H	1.54853500	2.13280400	1.71357100
H	3.10831000	0.44424300	0.85501800
C	2.98502300	-0.80196300	-1.60588500
C	4.04120000	-1.42292600	-0.76384200
Br	-0.81367900	3.63088700	0.57207300
H	3.65401700	-1.69191600	0.23854000
H	4.40521600	-2.35703600	-1.22452100
O	5.17105700	-0.54632800	-0.55825100
C	6.15863800	-1.11723400	0.26776800
H	6.54976500	-2.04967200	-0.18061400
H	5.72855200	-1.39651000	1.24897000
C	7.28132000	-0.10871300	0.45406500
H	8.07050400	-0.51732900	1.09579300
H	7.71954600	0.15515500	-0.51389700
H	6.89584700	0.80761900	0.91302000
C	1.22066300	-2.87178100	2.14144600
C	0.52080700	-1.72766400	2.12779200
H	3.13723700	-0.86371000	-2.68561500
H	2.23347300	-2.90000400	2.52898000
C	-0.83460500	-1.54286600	1.57979900
C	-1.29079000	-0.23707700	1.31980300
C	-1.67073800	-2.62124000	1.22037900
C	-2.50212400	-0.00345500	0.66616400
H	-0.66592400	0.60997900	1.57582300
C	-2.88805800	-2.40478500	0.57510000
H	-1.37434900	-3.63992600	1.45358600
C	-3.28088000	-1.09441900	0.29007900
H	-2.81190300	1.01285300	0.45057100
H	-3.52530500	-3.24034200	0.30657500
H	0.81945600	-3.81444300	1.77569800

H	1.00131600	-0.81736400	2.47819100
K	0.29162900	-1.76184200	-1.36274800
Br	-4.96055900	-0.79425800	-0.65496500

TSb1

SCF Energy (a.u.) = -1399.321850

Thermal correction to Gibbs free energy (a.u.) = 0.260748

Charge = 0, Multiplicity = 1

C	-1.68757400	0.67296100	1.87443400
C	-1.22015100	1.94609900	1.57989000
C	-1.36615900	2.45477600	0.27915900
C	-2.00701100	1.69779700	-0.70672300
C	-2.45766300	0.41287800	-0.41217100
C	-2.34326500	-0.16104400	0.90348300
H	-1.58280900	0.29933100	2.89047000
H	-0.74959700	2.54694600	2.35232000
H	-2.16447100	2.11231400	-1.69853300
H	-3.01369600	-0.12533000	-1.17023800
C	-2.80740300	-1.45124500	1.22111900
C	-3.62596900	-2.22526200	0.24667200
Br	-0.67262500	4.24287400	-0.15311100
H	-3.06189100	-2.39656600	-0.69181300
H	-3.86934700	-3.22060200	0.65355700
O	-4.84697600	-1.55019700	-0.08718100
C	-5.61537300	-2.25666200	-1.03770900
H	-5.88867700	-3.25361600	-0.64758500
H	-5.02631600	-2.42717300	-1.95794700
C	-6.86306700	-1.44623600	-1.34873000
H	-7.48797500	-1.96308700	-2.08577500
H	-7.45191000	-1.29014600	-0.43918500
H	-6.58928200	-0.46448300	-1.74900800
C	-0.96970500	-3.08934400	1.23045300
C	-0.11406700	-3.11573900	0.16047600
H	-2.95096900	-1.67191600	2.27554700

H	-1.80798100	-3.77271900	1.26490700
C	1.18673300	-2.49543400	0.09572400
C	1.89948700	-2.44296300	-1.13439900
C	1.83236200	-1.89956400	1.21688200
C	3.13426600	-1.80830000	-1.25656000
H	1.46054500	-2.91157600	-2.01200700
C	3.06453800	-1.26006000	1.10731100
H	1.35737300	-1.94353700	2.19166100
C	3.70411600	-1.19773400	-0.13531400
H	3.64547000	-1.78555300	-2.21350100
H	3.52769100	-0.81789600	1.98359200
H	-0.67170900	-2.67524800	2.18754400
H	-0.43426200	-3.62879900	-0.74484600
K	0.69288500	0.44538100	-0.37841500
Br	5.41280400	-0.26231800	-0.29848400

imb2

SCF Energy (a.u.) = -1399.353237

Thermal correction to Gibbs free energy (a.u.) = 0.265265

Charge = 0, Multiplicity = 1

C	-1.55906000	0.49134200	1.79508000
C	-1.09817400	1.79047400	1.56061700
C	-1.30281800	2.35044900	0.30095900
C	-1.97535900	1.65504300	-0.70273100
C	-2.42499400	0.35455900	-0.44076900
C	-2.21489600	-0.25725100	0.80476100
H	-1.39387300	0.04916700	2.77355800
H	-0.58892600	2.34703100	2.33984200
H	-2.16006900	2.11787100	-1.66676100
H	-2.97039500	-0.17056600	-1.21442500
C	-2.62996100	-1.68492100	1.11351900
C	-3.54118600	-2.30406100	0.06178900
Br	-0.60975000	4.14550400	-0.08017000
H	-3.01696900	-2.37718900	-0.90537400

H	-3.79510200	-3.33120400	0.36997700
O	-4.71634800	-1.52578600	-0.07102200
C	-5.61903100	-2.04545300	-1.03050300
H	-5.92002500	-3.06908800	-0.75077300
H	-5.12617300	-2.11311400	-2.01629300
C	-6.82821900	-1.12848800	-1.09720600
H	-7.55191100	-1.49948000	-1.83088400
H	-7.31864200	-1.07269600	-0.12026300
H	-6.52567700	-0.11658300	-1.38598900
C	-1.37898100	-2.59850900	1.33175500
C	-0.43970100	-2.68819100	0.16635100
H	-3.19896600	-1.66324000	2.05438500
H	-1.77124300	-3.59052700	1.61464100
C	0.88847500	-2.29827200	0.17155100
C	1.74106000	-2.49466500	-0.99640000
C	1.56417300	-1.61811000	1.27057000
C	3.00239000	-1.94092200	-1.11275400
H	1.35090600	-3.09214100	-1.81791800
C	2.83357400	-1.07299600	1.14601600
H	1.05952900	-1.51797000	2.22605200
C	3.52787800	-1.15051800	-0.07125400
H	3.58601500	-2.11014800	-2.01350800
H	3.28473100	-0.56701000	1.99543000
H	-0.85692300	-2.23398900	2.22255200
H	-0.78932600	-3.23951500	-0.70563800
K	1.08163100	0.42589800	-0.81677900
Br	5.34151600	-0.39671700	-0.22582200

