Supporting Information

How does the nickel catalyst control the doubly enantioconvergent coupling of racemic alkyl nucleophiles and electrophiles? the rebound mechanism

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Table of Contents

SI1: Results for Using LiCl Additive to Aid the Dissociation of $ZnBr_2$

Comparing eq a and eq b in **Fig. S1**, two LiCl molecules are energetically more advantageous to remove $ZnBr_2$ than one LiCl. Thus, in the precatalyst initiation stage, we used two LiCl molecules to remove $ZnBr_2$ generated from the two transmetalation steps. The exergonicity of -29.8 kcal/mol in eq b was used to construct the energy profile in **Fig. 1** in main text. Because the experimental studies only used 1.2 equiv LiCl additive and precatalyst initiation uses 0.4 equiv LiCl, we could not use two LiCl molecules to remove $ZnBr_2$ involved in the catalytic cycle, otherwise there would not be enough LiCl to complete the reaction. Interestingly, we found that $[ZnBr_2(LiCl)_2]$ (**IM^{Zn1}**) generated from precatalyst initiation stage could serve as a nucleus to effectively stabilize a $ZnBr_2$···LiCl unit in a form of $[ZnBr_2(LiCl)_2]@(ZnBr_2LiCl)_n$ aggregates with stabilization energies, -21.8(n=1, eq c), -21.0(n=2, eq d), -21.2 kcal/mol(n=3, eq e). Thus, we used the value of -21.8 kcal/mol to construct **Fig. 3A** and **3D** in the main text, **Fig. S3** in **SI3** and **Fig. S5** in **SI5**. It should be noted that the value does not affect the mechanism essentially as far as the dissociation of $ZnBr_2$ could take place with feasible energetics.

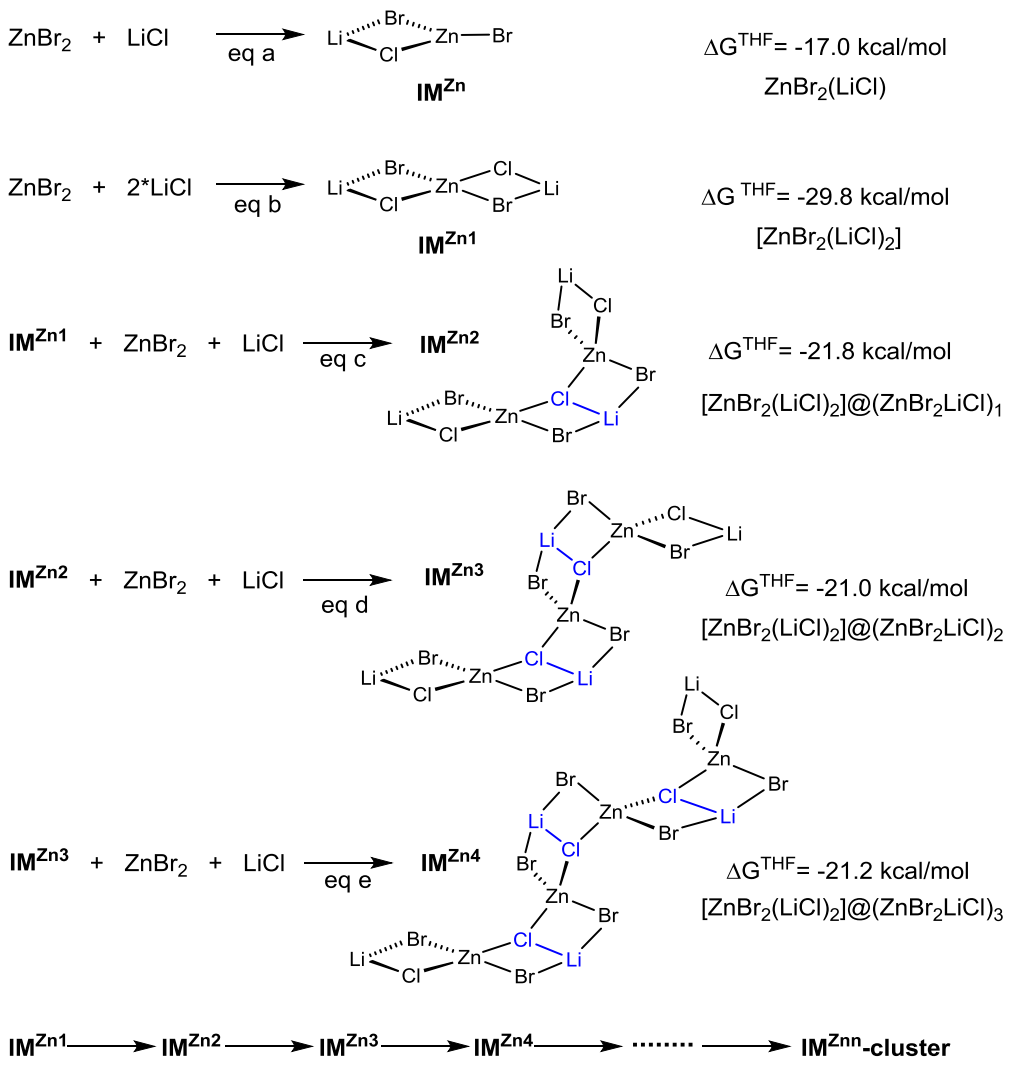


Fig. S1. Energetic results for stabilizing $ZnBr_2$ with LiCl additive.

SI2: Comparison of IM6-*S* and IM6-*S′* in Transmetallation

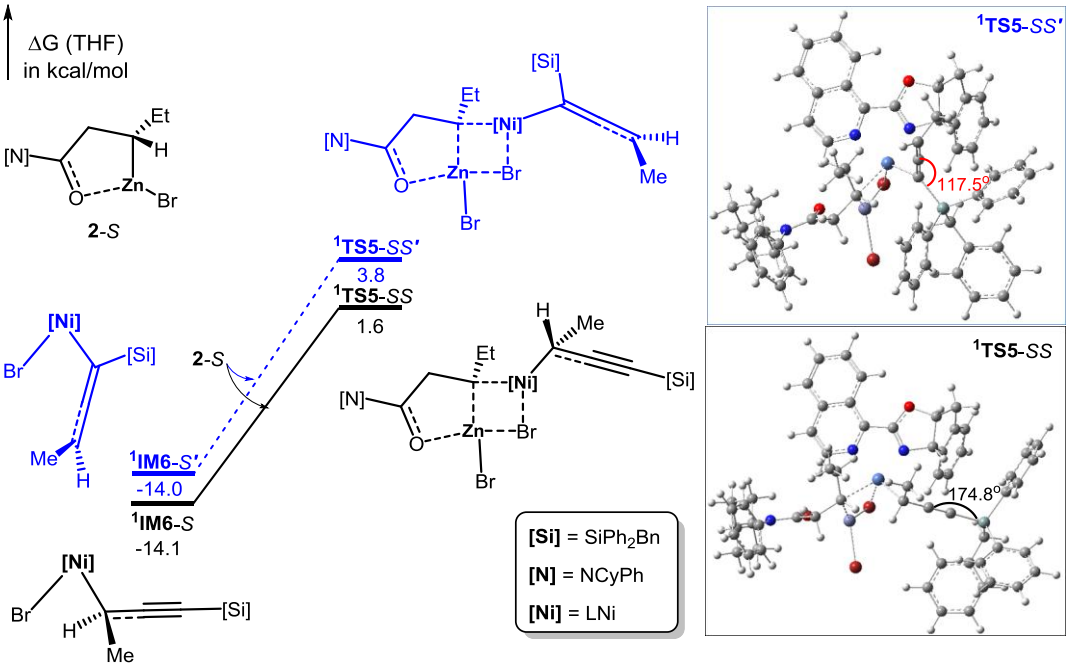


Fig. S2. Energetic results for comparing of **IM6**-*S* and **IM6**-*S′* in transmetallation.

SI3: Mechanism for the Control Reaction

To deepen our understanding to the eq 1 reaction, we further computed the mechanism of the control reaction (eq 2 in the main text), using substrate **1** (R=Me, i.e. eq 3 in the main text) instead of **1**$^{\mathbf{nBu}}$ (R=^{n}Bu, i.e. eq 2). The use of **1** has the advantage allowing us to take most results from the calculations of the main reaction (eq 1). We first considered the reaction with substrates in the (*S*)-chirality. **Fig. S3** shows the intercepting mechanism of TEMPO when ^{1}**IM6**-*S* is formed. After ^{1}**IM6**-*S* undergoes homolytic Ni-C bond cleavage to give radical **1**$^{\bullet}$ and the **LNi^{I}Br** species (i.e. ^{2}**IM9** in main text), TEMPO captures **1**$^{\bullet}$ by crossing ^{1}**TS12**, resulting in **5**. Subsequently, the resultant **LNi^{I}Br** undergoes transmetalation with **2**-*S* via ^{2}**TS13**-*S*, giving ^{2}**IM11**-*S*. After removing $ZnBr_2$ with LiCl (**SI1**), ^{2}**IM12**-*S* is generated, which can react with **1**-*S* via outer-sphere oxidative addition (^{2}**TS14**-*SS*), giving a Ni^{III} species ^{2}**IM14**-*SS*. Starting from ^{2}**IM14**-*SS*, there are three pathways, namely, **PIII-A**, **B**, and **C**, respectively. The reductive elimination pathway **PIII-A** gives the coupling product **4** (i.e **3**-*SS*) and **LNi^{I}Br**. The later can act as a catalyst to start next catalytic cycle. Along **PIII-B**, ^{2}**IM14**-*SS* first homolytically breaks the Ni-C (the carbon of **2**) bond via ^{2}**TS16**-*SS*, giving radical **2**$^{\bullet}$ and **IM6**-*S*. Then TEMPO captures **2**$^{\bullet}$ radical via ^{1}**TS17** to give **6**. **PIII-B** results in **IM6**-*S* which can be transformed convert to **LNi^{I}Br** to start starting next catalytic cycle. **PIII-C** homolytically break a Ni-C (the carbon of **1**) bond, resulting in **5**.

If taking the stereochemistry into account, as shown in **Fig. S5** in **SI5**, **LNi^{I}Br** can catalyze the coupling of racemic **1** and **2**. The coupling proceeds via three stages including

transmetalation, outer-sphere oxidative addition, and elimination. In principle, the oxidative addition could result in ^{2}**IM14**-*SS*, ^{2}**IM14**-*SR*, ^{2}**IM14**-*RS*, and ^{2}**IM14**-*RR*. However, as stated in **SI4**, the energetic results indicate that only ^{2}**IM14**-*SS* and ^{2}**IM14**-*RR* need to be considered. A rebound process can convert ^{2}**IM14**-*RR* to more stable (5.6 kcal/mol) ^{2}**IM14**-*SS*. In the presence of TEMPO, the coupling and radical capture compete, giving **4**-**6**. Because the rebound pathway (**Fig. S5B**) has highest barrier lower (0.2 kcal/mol) than ^{2}**TS15**-*SS*, the energetics in **Fig. S5** can be used to predict the yields of **4**(i.e **3**-*SS*), **5** and **6**. The energy difference (0.2 kcal/mol) between ^{2}**TS15**-*SS* and ^{1}**TS17** predicts the ratio of **4**:**6** to be 52:48. Considering the precatalyst initiation consumes 20% **2**, the ideal yields of **4** and **6** would be 41.6% and 38.4%, respectively. **PIII-C** pathway is not competitive with **PIII-A** and **PIII-B**, thus **5** could not be obtained from **PIII-C**. However, the resulting ^{1}**IM6**-*S* needs to convert to **LNi^{I}Br** for the next cycle and the conversion releases **5**. In addition, when **2** was consumed completely, the remaining 20% of **1** can be covert to ^{1}**IM6**, which can react with TEMPO to give **5**. Thus the ideal yield of **5** should be 58.4%. Taken together, we predict the ideal yields of **4**-**6** are 41.6%, 58.4%, and 38.4%, respectively, Note that eq 2 only converts 75% **1**^{nBu}, 40% **2** and 73% TEMPO to the products **4**^{nBu}, **5**^{nBu}, and **6**^{nBu}, while in our ideal scenario, 80% of **1**, 80% of **2**, and 96.8% of TEMPO appear in **4**-**6**. The difference could be due to some unknown side reactions (e.g. probably self-coupling of **1**˙ and **2**˙ or cross-coupling of **1**˙ and **2**˙). Considering these side reactions we did not take into account and the substitution difference between R=Me and R=nBu, our predicted ideal yields are reasonably in agreement with the experimental values. The success of elucidating the control reaction affirms our rebound mechanism for resetting the chirality of substrates.

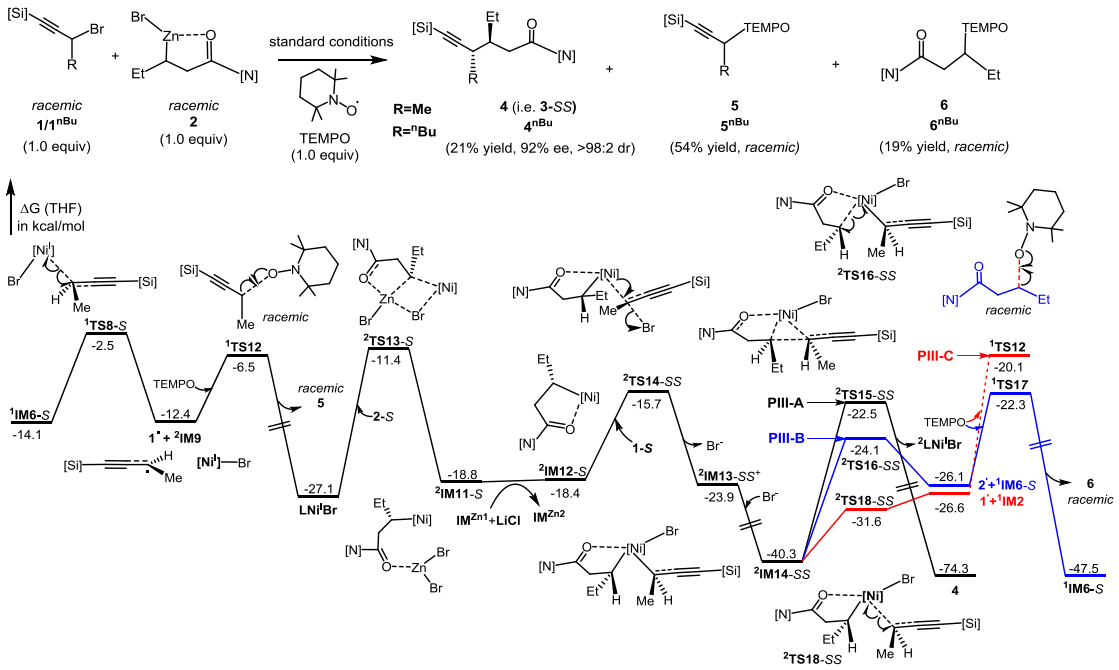


Fig. S3. Free energy profile for rationalizing the control reaction.

SI4: Results for Interconversions of the Four Stereoisomers of ^{1}IM8 via Rebound Mechanism

In our studied reaction, the chiralities of **1** and **2** are erased and reset at **IM6** for **1**(from ^{1}**IM6**-*R* to ^{1}**IM6**-*S*) and ^{1}**IM8** for **2** (from ^{1}**IM8**-*SR* to ^{1}**IM8**-*SS*), separately. We were further interested if the chiralities of **1** and **2** can be erased and reset at ^{1}**IM8**. The energetic results shown in **Fig. S4** indicate that the four stereoisomers of ^{1}**IM8** can be indeed interconverted with highest barrier at ^{1}**TS9**-*SR* which is lower than ^{1}**TS6**-*SR*. The feasible interconversions further ensure the doubly enantioconvergent coupling.

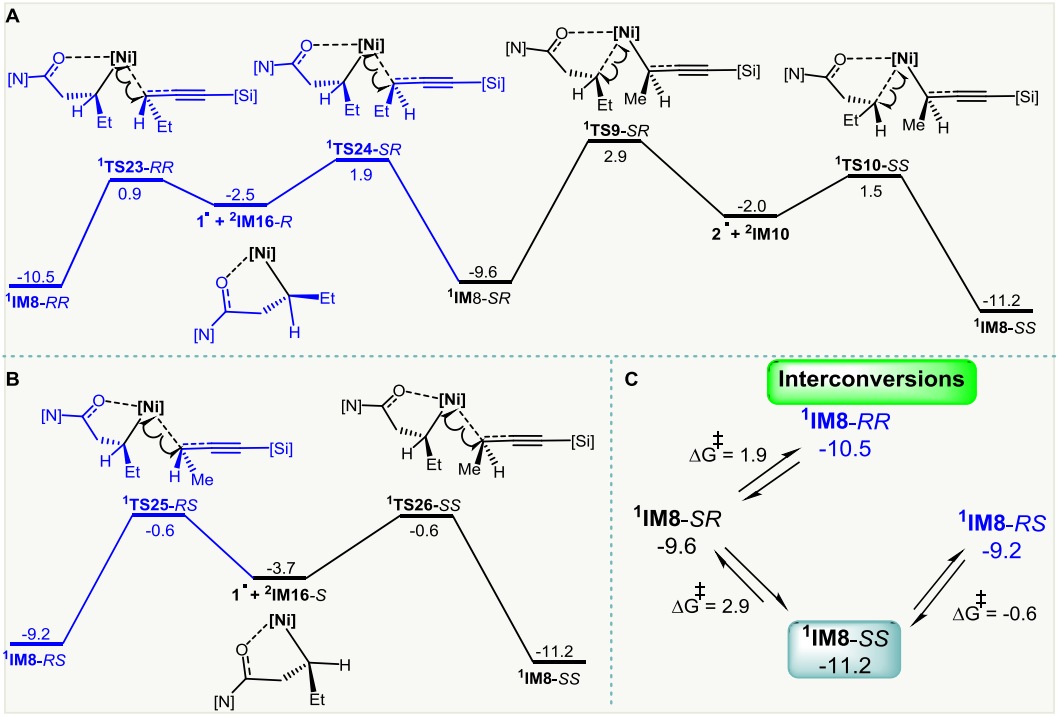
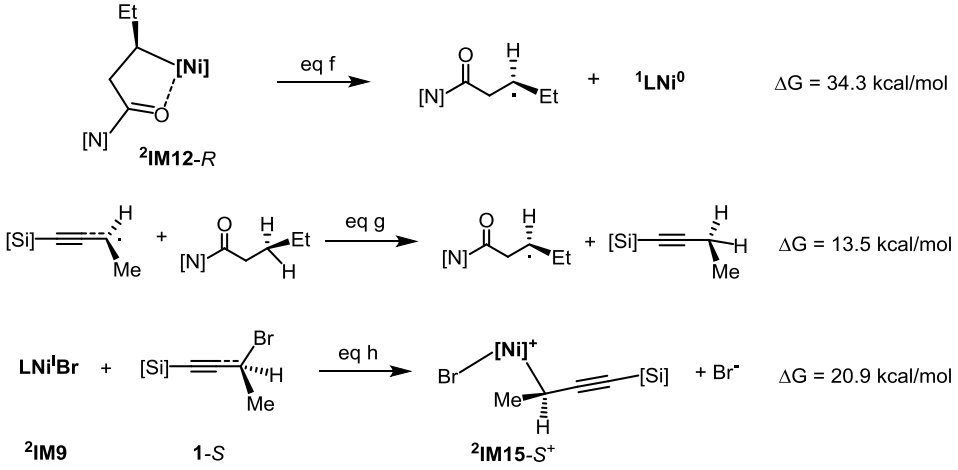


Fig. S4. Free energy profiles for the interconversions of the four stereoisomers of ^{1}**IM8** via rebound processes. Values are relative energies in kcal/mol.

SI5: Results for Catalytic Cycle via Ni^{I}/Ni^{III} Redox Manifold

In the main text, we analyzed that the present catalytic conditions generate Ni^0 as an active catalyst in the main text. However, Ni^I species was also used as or proposed to be an active species to catalyze cross-coupling reactions. Therefore, we were interested in if a Ni^I active species such as **LNi^{I}Br** could also control the doubly enantioconvergent coupling. **Fig. S5** shows the coupling reaction pathways with **LNi^{I}Br** as an active species. The coupling can be fulfilled via transmetalation, outer-sphere oxidative addition, and reductive elimination. Note that the sequence of the Ni^I species is different from the sequence of Ni^0 in the main text, which proceeds via outer-sphere oxidative addition, transmetalation, and reductive elimination.

On the basis of the energy profiles, because ^{2}**TS14**-*SS* is much lower than its three stereoisomers, the reaction consumes **1**-*S* and **2**-*S* first via **PIV**-*SS* pathway. If not considering the resetting of the chiralities of the substrates, the coupling reaction gives racemic **3** (**3**-*SS* and **3**-*RR*). Thus, to achieve doubly enantioconvergence, the (*R*)-chirality of **1** and **2** must be reset to (*S*)-chirality. On the basis of the rebound mechanism in the main text, we first considered a rebound process between ^{2}**IM12**-*R* and ^{2}**IM12**-*S*. However, the homolytic dissociation products (**2**$^{\bullet}$ + ^{1}**LNi^0**) of ^{2}**IM12**-*R* are even 20.5 kcal/mol higher than ^{2}**TS14**-*RR*. Thus, the rebound process cannot take place at ^{2}**IM12** in this Ni^I case. This is reasonable, because **2**$^{\bullet}$ radical lacks p-π conjugation and the dissociation loses a Ni-O coordination, making the homolytic Ni-C bond cleavage unfavorable, as shown by eqs f and g below. This also emphasizes the importance of triple bond in **1** substrate for the chirality resetting.



Next, we considered a rebound pathway to convert ^{2}**IM14**-*RR* to ^{2}**IM14**-*SS* as shown in **Fig. S5B**. Because the rate-determining barrier of the rebound process is lower than ^{2}**TS15**-*SS*, the ratio of **3**-*SS* and **3**-*RR* is actually determined by the barrier difference (1.0 kcal/mol) between ^{2}**TS15**-*SS* and ^{2}**TS15**-*RR*, which corresponds to a ratio of 84:16. The energetic results indicate that the Ni^I species (**LNi^{I}Br**) can also control the stereoselectivity of the reaction, but somewhat inferior to the Ni^0 species in the main text. When Ni^0 is used as the active catalyst, the energy difference to control the stereoselectivity is 1.5 kcal/mol.

On the basis of the results of Ni^0 in the main text and of Ni^I, we proposed that the rebound strategy should be considered to be a ground to develop enantioconvergent coupling reactions. Thus metals with oxidation states to feasibly undergo homolytic metal-bond cleavage could be the good choice for developing such enantioconvergent coupling.

With **LNi^{I}Br** as the active catalyst, we also considered the coupling via S_N2 mechanism. To allow the mechanism, **1** must dissociate Br^-, converting **2** to **2**Br^- for inversion the chirality of **2**. While we were not able to locate the dissociation transition state, the dissociation (20.9 kcal/mol, eq h) allows us to exclude the dissociation process, because it is already 5.2 kcal/mol higher than **^{2}TS13-***S* in **Fig. S5A.** Therefore, the S_N2 coupling pathway can be excluded.

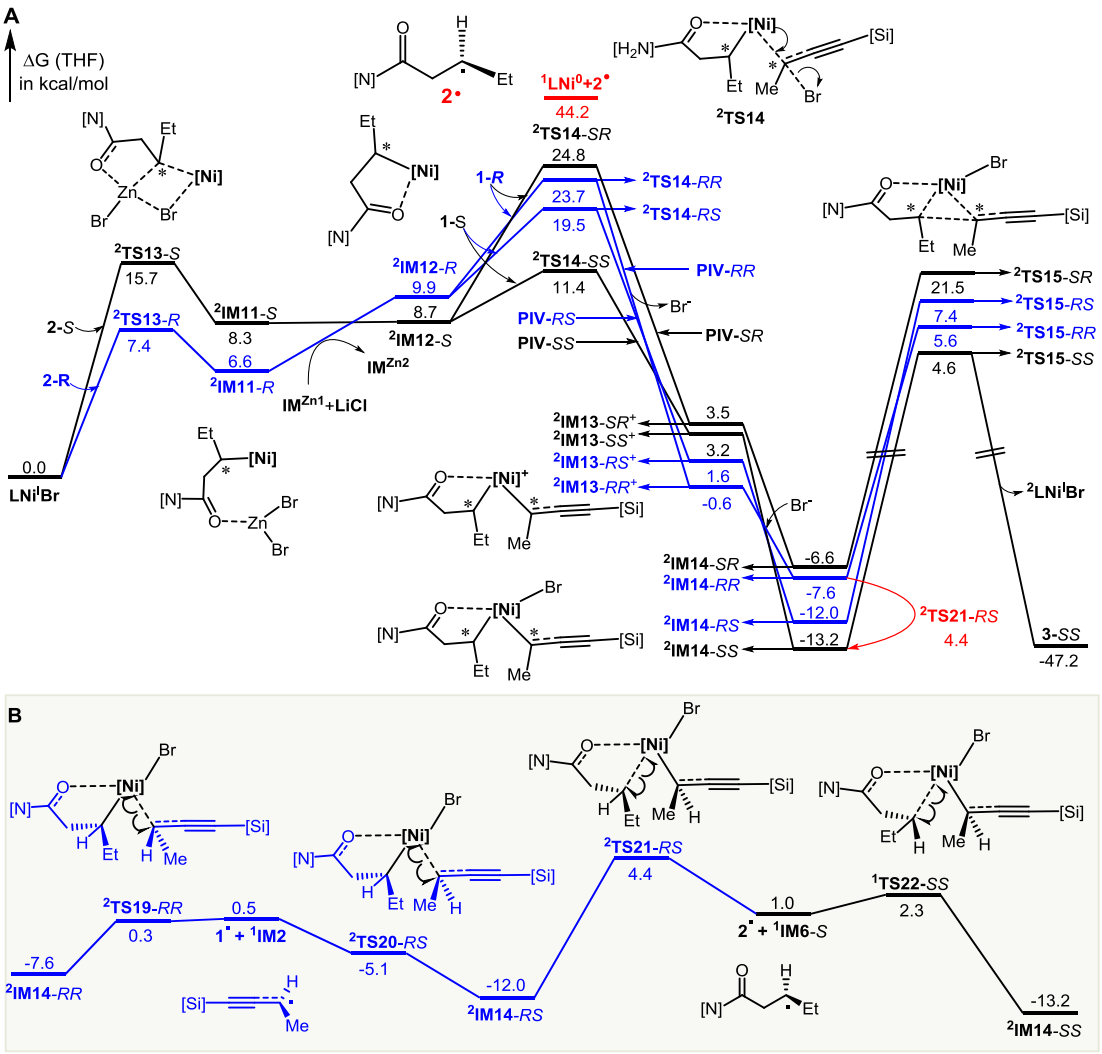


Fig. S5. Free energy profiles for the coupling mechanism involving **Ni^I/Ni^{III}** (**A**), and the rebound processes (**B**) to convert **^{2}IM14-***RR* to **^{2}IM14-***SS*.

SI6: Examining the other conformations of ^{1}TS6-SS

Using ^{1}**TS6**-SS as an example, we examined the reasonability of our considerations by considering other conformations of the transition state hierarchically (see **Fig. S6**).

(1) As shown by the structure of ^{1}**TS6**-*SS*, the LNi moiety is rigid without freedoms with respect to dihedral angle and bond rotation. However, referring to **TS6**-*SS*, the isoquinoline group of the ligand may lie on the right side. We optimized the transition state (i.e. ^{1}**TS6A**-*SS*) which is 3.6 kcal/mol higher than ^{1}**TS6**-*SS*. Thus, we assumed that the orientation of the ligand in **TS6**-*SS* is favored and keep the orientation unchanged for the next steps 2 and 3.

(2) In ^{1}**TS6**-*SS*, the carbonyl group coordinates to the Ni-center. This coordination fixes the five-membered ring, but the Ph and Cy groups in [N] can rotate around C-N bond. As shown by ^{1}**TS6B**-*SS*. The transition state is higher than ^{1}**TS6**-*SS* by 3.1 kcal/mol.

(3) With the orientations of the ligand and [N] group fixed, we next considered the rotation of the [Si] group. As show by ^{1}**TS6C**-*SS* and ^{1}**TS6D**-*SS*, the two conformations are slightly higher than ^{1}**TS6**-*SS*.

(4) In the above transition states, the carbonyl group coordinates to Ni-center. Alternatively, we considered the coordination of propargyl group to the Ni-center. In this scenario, because of the bulky [Si] group, the [Si] group must lie in the side of the isoquinoline part of the ligand, as shown by ^{1}**TS6E**-*SS*. It is higher than ^{1}**TS6**-*SS* by 7.2 kcal/mol.

The above results indicate that we considered the orientations of the ligand, [N] and [Si] groups, and the coordination of nickel center in ^{1}**TS6**-SS properly.

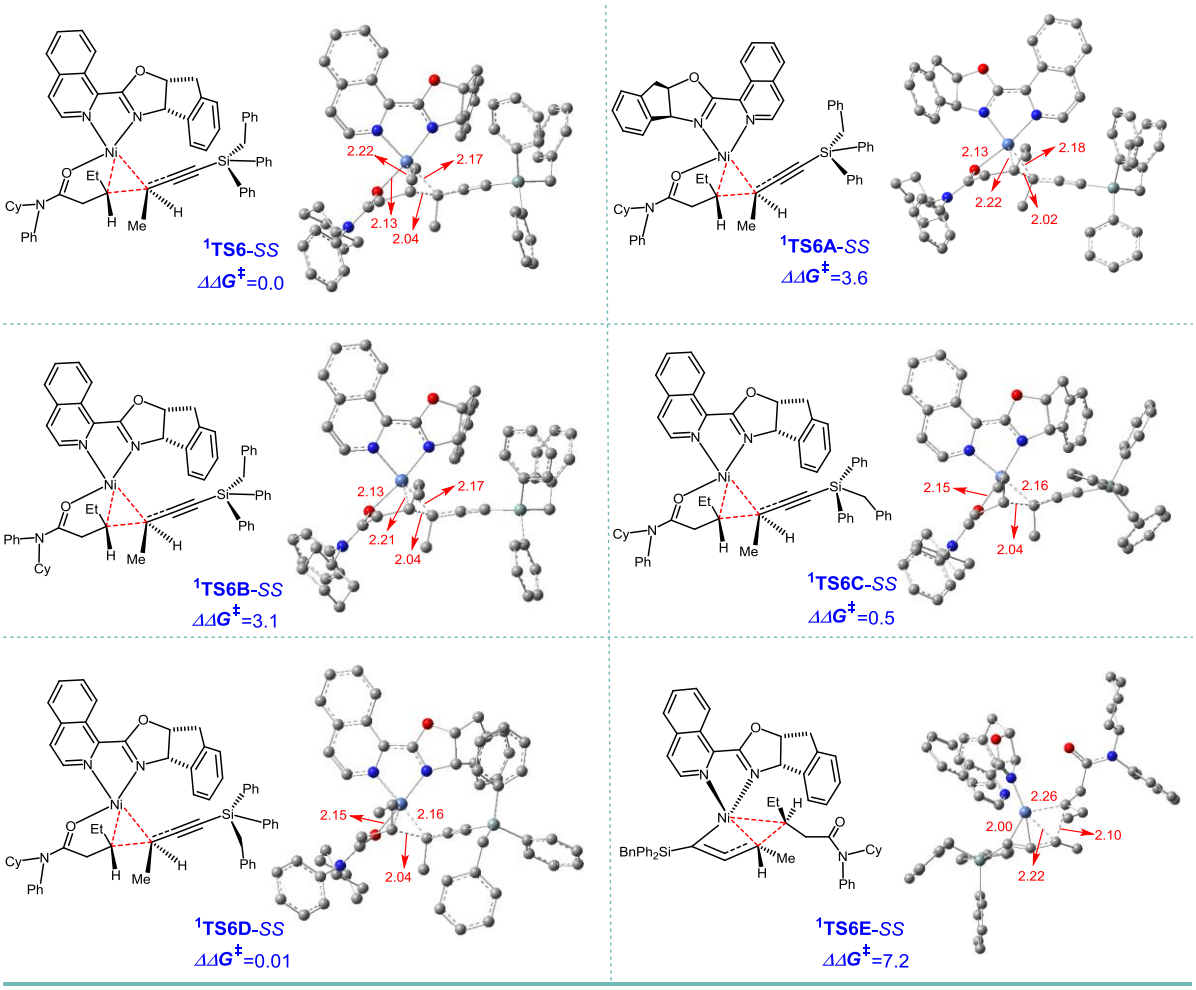


Fig. S6. Energetic comparisons of **^{1}TS6**-*SS* with its other five conformations.

SI7: Results for Spin Contamination Corrections

Attentions were paid to the spin contaminations of open shell wavefunctions. **Table S1** lists the $<S^2>$ values of the species. Compared to the standard $<S^2>$ values, the spin contaminations after annihilation are generally small, but some species, in particular those involved in rebound processes, are somewhat large. To estimate the energetic influences of the spin contaminations, we used the following formula[1] to correct the energies of the open shell singlet, where S_0 and S_1 are the annihilated spin contamination values of the open-shell singlet and triplet states, respectively. E_0 and E_1 are the energies of calculated open-shell singlet and triplet at the same geometry.

$$E \approx \frac{S_1^2 E_0 - S_0^2 E_1}{S_1^2 - S_0^2}$$

Table S2 shows the energy corrections (**ΔE**) due to spin contaminations. It could be found that exception for **^{1}TS9**-*SR* and **^{1}TS10**-*SS*, the corrections are small. **Figure S7** compares the energy profiles of the two rebound processes (**Figure 3B** and **3C** in main text) with or without spin contamination corrections. In terms of the spin contamination corrected energetics, the rebound processes are even more favorable. Thus, the spin contaminations would not affect our proposed mechanism. In the main text, we used the energies without spin contamination corrections.

References:

(1) K. S. Chan, X. Z. Li, W. I. Dzik, B. de Bruin, Towards comprehensive assessment of mitral regurgitation using cardiovascular magnetic resonance, *J. Am. Chem. Soc.*, 2008, **130**, 2051−2061. (b) Q. Knijnenburg, D. Hetterscheid, T. M. Kooistra, P. H. M. Budzelaar, The Electronic Structure of (Diiminopyridine)cobalt(I) Complexes, *Eur. J. Inorg. Chem.*, 2004, **2004**, 1204−1211. (c) X. Zhang, Z. Ke, N. J. DeYonker, H. Xu, Z. F. Li, X. Xu, X. Zhang, C. Y. Su, D. L. Phillips, C. Zhao, Mechanism and enantioselectivity of dirhodium-catalyzed intramolecular C-H amination of sulfamate, *J. Org. Chem.*, 2013, **78**, 12460-8.

Table S1. **$<S^2>$** values of the structures in the main text.

	Spin contaminant [S*(S+1)]		**Spin state**
	Before annihilation	**After annihilation**	
^{1}NiBr$_2$·glyme	0.9814	0.0269	OS
^{3}NiBr$_2$·glyme	2.0089	2.0000	Triplet
^{1}LNiBr$_2$	0.4867	0.0077	OS
^{3}LNiBr$_2$	2.0116	2.0001	Triplet
^{1}TS1	0.7445	0.0237	OS
^{3}TS1	2.0124	2.0001	Triplet
^{1}IM1	0.9984	0.0908	OS
^{3}IM1	2.0177	2.0001	Triplet
^{1}IM2	1.0040	0.0696	OS

^{3}**IM2**	2.0211	2.0002	Triplet
^{1}**TS2**	0.6060	0.0124	OS
^{3}**TS2**	2.0120	2.0001	Triplet
^{1}**IM3**	1.0834	0.743	OS
^{3}**IM3**	2.0120	2.0001	Triplet
^{1}**TS3**	1.0194	0.2381	OS
^{3}**TS3**	2.0342	2.0001	Triplet
^{1}**IM4**-*S*	0.0000	0.0000	CS
^{3}**IM4**-*S*	2.0283	2.0004	Triplet
^{1}**IM4**-*R*	0.0000	0.0000	CS
^{3}**IM4**-*R*	2.0290	2.0005	Triplet
^{1}**TS4**-*S*	0.2556	0.0112	OS
^{1}**TS4**-*R*	0.3493	0.0202	OS
^{1}**IM5**-S^{+}	0.0000	0.0000	CS
^{1}**IM5**-R^{+}	0.0000	0.0000	CS
^{1}**IM6**-*S*	0.0000	0.0000	CS
^{1}**IM6**-*R*	0.0000	0.0000	CS
^{1}**TS5**-*SS*	0.4777	0.0093	OS
^{1}**TS5**-*RS*	0.4426	0.0079	OS
^{1}**TS5**-*SR*	0.4777	0.0063	OS
^{1}**TS5**-*RR*	0.5413	0.0124	OS
^{1}**IM7**-*SS*	0.0000	0.0000	CS
^{1}**IM7**-*RS*	0.0000	0.0000	CS
^{1}**IM7**-*SR*	0.0000	0.0000	CS
^{1}**IM7**-*RR*	0.0000	0.0000	CS
^{1}**IM8**-*SS*	0.9062	0.4481	OS
^{1}**IM8**-*SR*	0.9597	0.6376	OS
^{1}**IM8**-*RS*	0.8858	0.3583	OS
^{1}**IM8**-*RR*	0.5836	0.1611	OS
^{1}**TS6**-*SS*	1.0252	0.2614	OS
^{1}**TS6**-*SR*	1.0283	0.2979	OS
^{1}**TS6**-*RS*	1.0212	0.2141	OS
^{1}**TS6**-*RR*	1.0120	0.2808	OS
^{1}**TS7**-*R*	0.9837	0.3473	OS
^{1}**TS8**-*S*	1.0248	0.4534	OS
^{1}**TS9**-*SR*	1.2474	1.7115	OS
^{1}**TS10**-*SS*	1.1908	1.5110	OS
^{2}**IM9**	0.7844	0.7507	doublet
^{2}**IM10**	0.7618	0.7501	doublet
^{1}**TS11**-*SR*	0.7991	0.0781	OS
^{1}**TS11**-*SS*	0.8259	0.0857	OS
^{1}**TS11**-*RS*	0.8436	0.0921	OS
^{1}**TS11**-*RR*	0.7874	0.0748	OS

Table S2. Spin contamination corrected energies of the key transition states.

TS_s	E_0 (a.u.)	S_0	E_1(a.u.)	S_1	E	$\Delta E=E-E_0$ (kcal/mol)
^{1}**TS7**-*R*	-2279.258783	0.3473	-2279.255581	2.0017	-2279.258882	-0.06
^{1}**TS8**-*S*	-2279.253359	0.4534	-2279.252816	2.0020	-2279.253388	-0.02
^{1}**TS9**-*SR*	-3057.720640	1.7115	-3057.71978	2.0070	-3057.722933	-1.44
^{1}**TS10**-*SS*	-3057.724327	1.5110	-3057.720897	2.0052	-3057.728834	-2.83
^{1}**TS6**-*SS*	-3057.721300	0.2614	-3057.721781	2.0006	-3057.721292	0.01
^{1}**TS6**-*SR*	-3057.717435	0.2979	-3057.71804	2.0009	-3057.717421	0.01
^{1}**TS6**-*RS*	-3057.705634	0.0921	-3057.706769	2.0006	-3057.705632	0.00
^{1}**TS6**-*RR*	-3057.713307	0.0748	-3057.71320	3.0008	-3057.713307	0.00
^{1}**TS11**-*SR*	-3311.779507	0.0781	-3311.784442	2.0004	-3311.779499	0.01
^{1}**TS11**-*SS*	-3311.778779	0.0857	-3311.783782	2.0004	-3317.868356	0.01
^{1}**TS11**-*RS*	-3311.776347	0.0921	-3311.779974	2.0004	-3311.776339	0.01
^{1}**TS11**-*RR*	-3311.777464	0.0748	-3311.780314	2.0004	-3311.777460	0.00

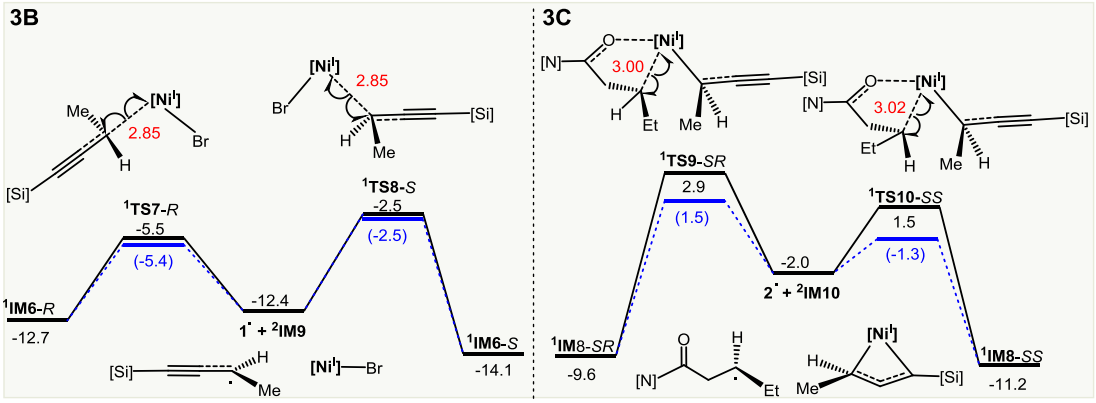


Fig. S7. Comparison of free energy profiles of the two rebound processes (**Fig. 3B** and **3C**) with (blue pathways) or without (black pathways) spin contamination corrections. Relative energies are given in kcal/mol.

Table S3. Comparing the reductive elimination and rebound process barriers (in kcal mol^{-1}) at the various levels.

To examine the effect of dispersions on energy corrections, we recalculated the transition states which are crucial for our proposed mechanism, including those for reductive elimination and rebound process in Figure 3 of the main text at the other two levels (M06(SMD)/ 6-311++G**)// B3LYP-D3BJ(SMD)/6-31G** and B3LYP-D3BJ(SMD)/ 6-311++G**)// B3LYP-D3BJ(gas)/6-31G**). As compared in the table below, in spite of some numerical differences, overall, the energetic results agree with each other well. The four stereoisomers of the reductive elimination states (**TS6**) are in the same order at the three levels. For the two transition states (^{1}**TS9**-*SR* **a**nd ^{1}**TS10**-*SS*) of rebound process, Level B and level C predict that the two

transition states are lower than ^{1}**TS6-***SS* more significantly, indicating that the rebound process takes place even more favorable at the two levels. Thus, the new results do not change our conclusions.

	M06(SMD)/BSII// B3LYP(gas)/BSI	M06(SMD)/ BSII// B3LYP-D3BJ(SMD)/BSI	B3LYP-D3BJ(SMD)/BSII //B3LYP-D3BJ(gas)/BSI
^{1}**TS6**-*SS*	0.0	0.0	0.0
^{1}**TS6**-*SR*	1.8	1.6	1.6
^{1}**TS6**-*RR*	5.0	5.6	4.1
^{1}**TS6**-*RS*	9.9	10.7	10.3
^{1}**TS9**-*SR*	0.3	-0.5	-6.4
^{1}**TS10**-*SS*	-1.1	-1.8	-8.3

SMD calculations used THF as solvent.

BSI denotes a basis with SDD for Ni, Br, Zn and 6-31G** for other atoms.

BSII denotes a basis with SDD for Ni, Br, Zn and 6-311++G** for other atoms.

SI8: Cartesian Coordinates in Å, SCF Energies and Free Energies (in a.u.) at 298.15 K and 1 atm for the Optimized Structures [BSI= 6-31G(d,p), BSII=6-311++G(d,p)]

$^{1}NiBr_2$·glyme

B3LYP/BSI SCF energy: -506.697496a.u.

M06/BSII SCF energy in solution: -506.539596a.u.

M06/BSII free energy in solution: -506.435723a.u.

C	-1.254345	-1.255342	2.354062
H	-1.013237	-0.347370	2.905937
H	-1.140818	-2.127574	3.006802
H	-2.274225	-1.192601	1.962905
O	-0.304059	-1.344476	1.277321
C	-0.450674	-2.517684	0.466632
H	-0.276883	-3.412104	1.078057
H	-1.462754	-2.553994	0.043285
C	0.588895	-2.427706	-0.631347
H	0.493446	-3.280138	-1.314866
H	1.602078	-2.401334	-0.211160
O	0.332666	-1.210570	-1.350239
C	1.231532	-0.978849	-2.452424
H	1.138574	-1.804131	-3.166040
H	0.913956	-0.047526	-2.920116
H	2.260920	-0.884939	-2.094839
Ni	-0.008391	0.312229	0.005914
Br	2.196311	1.039979	0.486494
Br	-2.222809	1.040797	-0.409173

$^{3}NiBr_2$·glyme

B3LYP/BSI SCF energy: -506.722892a.u.

M06/BSII SCF energy in solution: -506.564481a.u.

M06/BSII free energy in solution: -506.461159a.u.

C	1.224221	1.095228	2.425982
H	0.923102	0.176982	2.929244
H	1.126754	1.943589	3.111347
H	2.252027	1.001759	2.063378
O	0.313833	1.275062	1.323939
C	0.542494	2.472621	0.565452
H	0.415893	3.346704	1.215836
H	1.560062	2.461730	0.154916
C	-0.487821	2.492974	-0.544534
H	-0.332825	3.366684	-1.189253
H	-1.505227	2.513571	-0.133811
O	-0.298638	1.293676	-1.310965
C	-1.222082	1.145144	-2.406558
H	-1.108646	1.995641	-3.086793
H	-0.948776	0.223112	-2.918659
H	-2.248994	1.075243	-2.036177
Ni	-0.004078	-0.301521	-0.001734
Br	-2.221150	-1.041871	0.435028
Br	2.207390	-1.056647	-0.446666

glyme

B3LYP/BSI SCF energy: -308.86377a.u.

M06/BSII SCF energy in solution: -308.750078a.u.

M06/BSII free energy in solution: -308.640059a.u.

C	-1.233960	-2.715758	0.000000
H	-2.276964	-3.041925	0.000000
H	-0.733323	-3.125576	0.891798
H	-0.733323	-3.125576	-0.891798
O	-1.233960	-1.305091	0.000000
C	0.068864	-0.757412	0.000000
H	0.637666	-1.077575	0.888375
H	0.637666	-1.077575	-0.888375
C	-0.068864	0.757412	0.000000
H	-0.637666	1.077575	0.888375
H	-0.637666	1.077575	-0.888375
O	1.233960	1.305091	0.000000
C	1.233960	2.715758	0.000000
H	0.733323	3.125576	0.891798
H	2.276964	3.041925	0.000000
H	0.733323	3.125576	-0.891798

(S,R)-L

B3LYP/BSI SCF energy: -917.182967a.u.

M06/BSII SCF energy in solution: -916.75545a.u.

M06/BSII free energy in solution: -916.51459a.u.

C	-0.107471	-0.025708	-0.523624
N	0.772113	0.426990	-1.326219
C	1.883364	-0.539403	-1.312648
H	2.117381	-0.832730	-2.342585
O	0.119014	-1.236729	0.086174
C	-1.377904	0.671659	-0.165601
C	-2.626530	-0.025860	-0.026750
C	-2.799096	-1.424715	-0.222146
C	-3.776233	0.764911	0.300143
C	-2.351700	2.706200	0.299973
C	-4.041735	-2.002707	-0.089936
H	-1.938371	-2.034631	-0.462391
C	-5.043126	0.135668	0.435223
C	-3.602338	2.160530	0.467210
H	-2.188013	3.774870	0.418032
C	-5.173424	-1.219696	0.244041
H	-4.156977	-3.071894	-0.241998
H	-5.905614	0.746935	0.686677
H	-4.453246	2.787077	0.719555
H	-6.145051	-1.694412	0.346129
N	-1.252546	1.979105	-0.012632
C	1.388084	-1.725418	-0.423675
H	1.179533	-2.646931	-0.974194
C	3.103547	-0.013386	-0.582460
C	3.883569	1.093933	-0.912971
C	3.385779	-0.776970	0.554824
C	4.963651	1.427451	-0.093554
H	3.643751	1.693248	-1.786378
C	4.466236	-0.443290	1.372909
C	5.253454	0.662072	1.042048
H	5.580742	2.288025	-0.335652
H	4.693241	-1.031573	2.258485
H	6.095898	0.931591	1.672952
C	2.414681	-1.929139	0.709924
H	1.910999	-1.937735	1.682585
H	2.919804	-2.897458	0.603764

^{1}LNiBr$_2$

B3LYP/BSI SCF energy: -1115.048776a.u.

M06/BSII SCF energy in solution: -1114.5822a.u.

M06/BSII free energy in solution: -1114.345116a.u.

C	0.753032	1.059842	-0.617661
N	-0.427927	0.546909	-0.661918
C	-1.378490	1.612302	-1.037410
H	-2.027396	1.235989	-1.831111
C	-0.441959	2.784197	-1.458575
H	-0.340760	2.926530	-2.536400
O	0.885196	2.338635	-0.986054
C	-0.889801	4.042537	-0.701532
H	-1.388508	4.733522	-1.392671
H	-0.027352	4.575971	-0.287877
C	-1.848022	3.521086	0.348528
C	-2.443704	4.225061	1.394917
C	-2.147610	2.168536	0.148330
C	-3.337516	3.557552	2.235576
H	-2.218228	5.275942	1.556411
C	-3.046176	1.498004	0.979737
C	-3.637421	2.206221	2.028674
H	-3.805693	4.093646	3.056131
H	-3.278354	0.451354	0.808458
H	-4.337197	1.701633	2.687971
C	1.884243	0.227772	-0.170195
C	3.246876	0.634599	-0.083570
C	3.728656	1.932079	-0.421848
C	4.184733	-0.350903	0.378181
C	2.360417	-1.925920	0.587634
C	5.067333	2.224662	-0.303417
H	3.036043	2.684405	-0.771876
C	5.559749	-0.009793	0.487735
C	3.700012	-1.635570	0.708526
H	1.936295	-2.892151	0.835799
C	5.991102	1.251105	0.153995
H	5.423596	3.216414	-0.564311
H	6.258089	-0.763680	0.838664
H	4.384516	-2.400485	1.061127
H	7.042647	1.507836	0.238431
N	1.466199	-1.004249	0.155688
Ni	-0.545701	-1.359000	-0.196846
Br	-0.592226	-3.483142	0.875376
Br	-2.652353	-1.600939	-1.295399

^{3}LNiBr$_2$

B3LYP/BSI SCF energy: -1115.071073a.u.

M06/BSII SCF energy in solution: -1114.595507a.u.

M06/BSII free energy in solution: -1114.362211a.u.

C	0.381827	0.987990	-0.628325
N	-0.639768	0.208264	-0.675331
C	-1.745915	0.931156	-1.323231
H	-2.146461	0.307044	-2.127750
C	-1.070085	2.245417	-1.823552
H	-0.879962	2.278026	-2.897968
O	0.256010	2.203033	-1.182901
C	-1.901847	3.429473	-1.304750
H	-2.424163	3.912758	-2.139641
H	-1.255792	4.189754	-0.852972
C	-2.874224	2.804430	-0.326402
C	-3.783140	3.449321	0.512584
C	-2.806259	1.407209	-0.347929
C	-4.613964	2.678343	1.328637
H	-3.844973	4.534139	0.534957
C	-3.632745	0.632095	0.465768
C	-4.538783	1.280885	1.306869
H	-5.323315	3.168419	1.989238
H	-3.559608	-0.450996	0.467725
H	-5.184842	0.694600	1.952961
C	1.648021	0.525426	-0.015946
C	2.822720	1.308748	0.189796
C	2.953462	2.682560	-0.159994
C	3.940034	0.643808	0.802214
C	2.626868	-1.378934	0.919001
C	4.131727	3.350146	0.083523
H	2.121710	3.197153	-0.619754
C	5.139922	1.367043	1.036165
C	3.808215	-0.718480	1.158910
H	2.477199	-2.419773	1.181845
C	5.233563	2.691991	0.683734
H	4.219400	4.397560	-0.188169
H	5.977287	0.853110	1.498670
H	4.637701	-1.241022	1.624104
H	6.152745	3.240660	0.864938
N	1.572982	-0.760252	0.339568
Ni	-0.234084	-1.677034	-0.062755
Br	-1.137494	-2.219326	2.081910
Br	0.071507	-2.791433	-2.169336

1-*R*

B3LYP/BSI SCF energy:-1191.967096a.u.

M06/BSII SCF energy in solution: -1191.44854a.u.

M06/BSII free energy in solution: -1191.142744a.u.

C	-0.821777	-0.108641	-0.415281
C	-1.940045	-0.593921	-0.429798
Si	0.870652	0.614586	-0.382400
C	1.580588	0.385405	1.349046
C	1.358024	-0.800214	2.074903
C	2.373412	1.383625	1.944450
C	1.911885	-0.983490	3.342268
H	0.738997	-1.585118	1.649433
C	2.930814	1.202755	3.211660
H	2.548946	2.318848	1.419064
C	2.701172	0.017735	3.912331
H	1.724758	-1.905185	3.886439
H	3.537072	1.988744	3.653653
H	3.130032	-0.123144	4.900733
C	0.754209	2.440187	-0.837652
C	1.873084	3.139989	-1.328754
C	-0.448723	3.153068	-0.680818
C	1.796917	4.497912	-1.643736
H	2.820133	2.624532	-1.472927
C	-0.529725	4.510273	-0.996175
H	-1.333481	2.639499	-0.314092
C	0.593519	5.185561	-1.477187
H	2.673635	5.016654	-2.021813
H	-1.469991	5.039425	-0.868261
H	0.531013	6.241824	-1.723936
C	1.923221	-0.287088	-1.699876
H	1.499490	-0.023218	-2.676093
H	2.928109	0.151879	-1.665744
C	2.002728	-1.786393	-1.543759
C	3.002445	-2.382131	-0.759183
C	1.066021	-2.624886	-2.168687
C	3.064909	-3.767769	-0.605024
H	3.740471	-1.753418	-0.267935
C	1.126752	-4.010450	-2.016416
H	0.287820	-2.184077	-2.786495
C	2.126716	-4.589141	-1.232237
H	3.851420	-4.205144	0.003896
H	0.396095	-4.639457	-2.518143
H	2.177694	-5.667951	-1.116549
C	-3.235317	-1.223034	-0.465492
H	-3.683190	-1.152286	-1.457404
C	-3.254392	-2.650581	0.067730
H	-2.579745	-3.260847	-0.543678

H	-2.907244	-2.684056	1.102133
H	-4.261169	-3.069619	0.012833
Br	-4.579389	-0.086421	0.644132

2-*R*

B3LYP/BSI SCF energy: -1032.89201a.u.

M06/BSII SCF energy in solution: -1032.50943a.u.

M06/BSII free energy in solution: -1032.183469a.u.

C	0.448556	-0.325426	-0.027784
O	-0.430293	0.569302	-0.033078
N	1.762734	0.002332	-0.043748
C	0.041419	-1.799044	0.020308
H	0.784063	-2.405461	-0.511182
H	0.117446	-2.104130	1.074871
C	-1.392780	-2.044219	-0.481577
H	-1.361045	-2.094644	-1.580516
C	-1.968584	-3.368122	0.039290
H	-1.293480	-4.199290	-0.225135
H	-2.000787	-3.351684	1.137963
C	-3.365513	-3.685564	-0.501684
H	-3.364778	-3.723803	-1.597239
H	-3.725018	-4.653360	-0.136512
H	-4.091625	-2.922279	-0.198756
Zn	-2.390705	-0.363951	-0.097151
Br	-4.089685	1.187726	0.270332
C	2.792897	-1.001292	0.060981
C	3.497158	-1.398184	-1.081188
C	3.124934	-1.537619	1.309054
C	4.524466	-2.335823	-0.972917
H	3.230621	-0.976512	-2.045531
C	4.150580	-2.478932	1.411021
H	2.579327	-1.215059	2.190548
C	4.851499	-2.878542	0.271862
H	5.066066	-2.644874	-1.861895
H	4.403001	-2.895904	2.381325
H	5.649997	-3.609803	0.353123
C	2.225458	1.427210	-0.087183
C	1.778181	2.162757	-1.362440
C	1.856010	2.208848	1.186205
H	3.317567	1.344563	-0.120240
C	2.371399	3.581672	-1.397983
H	0.686449	2.216371	-1.383237
H	2.095727	1.593891	-2.244918
C	2.443505	3.629812	1.134655
H	0.766735	2.258429	1.271644
H	2.232125	1.673368	2.066425
C	2.007087	4.376130	-0.134882
H	2.017765	4.103728	-2.294258
H	3.466028	3.520152	-1.484590
H	2.139001	4.184634	2.029312
H	3.541423	3.573091	1.161944
H	2.468668	5.369959	-0.166524
H	0.920432	4.534025	-0.107297

LiCl

B3LYP/BSI SCF energy: -467.792911a.u.

M06/BSII SCF energy in solution: -467.824731a.u.

M06/BSII free energy in solution: -467.84402a.u.

Cl	0.000000	0.000000	0.308295
Li	0.000000	0.000000	-1.747003

TEMPO

B3LYP/BSI SCF energy: -483.736133a.u.

M06/BSII SCF energy in solution: -483.505374a.u.

M06/BSII free energy in solution: -483.279449a.u.

C	-1.247052	1.403204	-0.483227
C	-1.331340	-0.068697	-0.029785
C	1.331399	-0.068719	-0.029786
C	1.246925	1.403051	-0.483635
C	0.000070	2.130029	0.023807
H	-1.245733	1.434544	-1.580756
H	-2.161246	1.912670	-0.157277
H	2.161337	1.912632	-0.158494
H	1.244886	1.433826	-1.581183
H	0.000258	2.186245	1.119011
H	0.000063	3.165265	-0.336015
N	0.000026	-0.742525	-0.206554
C	-2.339061	-0.825407	-0.910683
H	-2.411553	-1.868689	-0.601341
H	-3.325020	-0.356837	-0.828440
H	-2.030221	-0.799582	-1.960170
C	-1.761180	-0.185072	1.448277
H	-2.799954	0.141334	1.564031
H	-1.684064	-1.227349	1.767236
H	-1.142085	0.425352	2.111013

C	1.761065	-0.184749	1.448330
H	1.684137	-1.226999	1.767475
H	2.799697	0.141937	1.564314
H	1.141538	0.425460	2.110867
C	2.339310	-0.825497	-0.910360
H	3.325316	-0.357084	-0.827781
H	2.411505	-1.868788	-0.600987
H	2.030882	-0.799604	-1.959969
O	-0.000092	-2.018190	-0.050410

^{1}TS1

B3LYP/BSI SCF energy: -2147.92293a.u.

M06/BSII SCF energy in solution: -2147.0946a.u.

M06/BSII free energy in solution: -2146.506299a.u.

C	3.040592	0.270992	-0.194707
O	2.289846	0.326738	0.806911
N	4.326662	0.691262	-0.132830
C	2.495635	-0.278659	-1.503589
H	2.906420	0.316972	-2.327766
H	2.898923	-1.290678	-1.634490
C	0.946348	-0.309378	-1.585131
H	0.625429	0.737034	-1.602539
C	0.514120	-0.981607	-2.901293
H	0.767536	-2.046803	-2.868733
H	-0.578240	-0.958870	-2.988057
C	1.093847	-0.345047	-4.179500
H	2.175457	-0.487704	-4.267331
H	0.636270	-0.794694	-5.067414
H	0.896052	0.734148	-4.215298
Zn	0.892961	-1.366520	0.439888
Br	2.406503	-3.194428	0.724331
C	5.236693	0.471896	-1.229516
C	5.671925	1.556029	-1.999371
C	5.723021	-0.814276	-1.488205
C	6.587472	1.351269	-3.032072
H	5.287604	2.549431	-1.787609
C	6.633743	-1.012792	-2.527337
H	5.381981	-1.646920	-0.879947
C	7.067412	0.066975	-3.298912
H	6.921653	2.193901	-3.630213
H	7.005915	-2.012709	-2.729099
H	7.777615	-0.090953	-4.105091
C	4.930235	1.201867	1.139400
C	4.240442	2.474381	1.662008
C	5.028932	0.113338	2.222777
H	5.950091	1.479553	0.849911
C	4.968615	3.004539	2.909053
H	3.202494	2.240011	1.913835
H	4.228130	3.235864	0.871603
C	5.741843	0.658097	3.472073
H	4.023488	-0.228961	2.482253
H	5.569255	-0.751917	1.822860
C	5.063690	1.930116	4.002636
H	4.449814	3.893036	3.288061
H	5.981672	3.330726	2.631813
H	5.761969	-0.116238	4.246899
H	6.790585	0.883716	3.228763
H	5.611923	2.319992	4.868432
H	4.053162	1.681667	4.354496
C	-3.509843	1.144365	-0.953552
N	-3.213994	-0.105871	-0.866543
C	-4.442917	-0.879541	-1.130073
H	-4.207685	-1.700450	-1.811046
C	-5.414338	0.189957	-1.708655
H	-5.502298	0.194902	-2.797625
O	-4.748538	1.460869	-1.352403
C	-6.753021	0.056995	-0.972678
H	-7.484092	-0.435509	-1.626749
H	-7.163806	1.041007	-0.722961
C	-6.421834	-0.794713	0.234432
C	-7.232298	-1.085385	1.331500
C	-5.136189	-1.341147	0.142203
C	-6.736389	-1.923685	2.332765
H	-8.232193	-0.666426	1.409826
C	-4.634320	-2.178515	1.139267
C	-5.449225	-2.464790	2.237224
H	-7.355387	-2.155246	3.194925
H	-3.631560	-2.585757	1.064312
H	-5.074670	-3.110589	3.025508
C	-2.505293	2.158728	-0.575984
C	-2.737639	3.559139	-0.434135
C	-3.963107	4.213555	-0.747073
C	-1.643638	4.344841	0.064439
C	-0.310710	2.331173	0.195583
C	-4.084905	5.573312	-0.575367
H	-4.795460	3.636010	-1.123730
C	-1.809290	5.745643	0.231273

C	-0.434315	3.687426	0.386294
H	0.593411	1.788829	0.448149
C	-3.004540	6.346768	-0.082752
H	-5.023019	6.061901	-0.819961
H	-0.975697	6.328160	0.612237
H	0.399365	4.252017	0.791371
H	-3.126696	7.417867	0.046599
N	-1.329234	1.585375	-0.298923
Ni	-1.268639	-0.496728	-0.546750
Br	-0.841304	-0.723499	2.132991
Br	-1.547810	-2.884351	-0.973894

^{3}TS1

B3LYP/BSI SCF energy: -2147.93722a.u.

M06/BSII SCF energy in solution: -2147.10497a.u.

M06/BSII free energy in solution: -2146.520373a.u.

C	-3.107121	0.312755	0.187025
O	-2.510958	0.128182	-0.901629
N	-4.385009	0.758403	0.214411
C	-2.356511	0.054430	1.483315
H	-2.806301	0.649849	2.285656
H	-2.514573	-0.996358	1.766954
C	-0.851604	0.378262	1.330085
H	-0.808605	1.402834	0.942435
C	-0.179686	0.360911	2.724078
H	-0.423627	-0.578968	3.230348
H	0.925571	0.339085	2.647266
C	-0.522836	1.564648	3.620614
H	-1.596884	1.626316	3.823810
H	-0.011448	1.494084	4.587229
H	-0.220496	2.506799	3.148596
Zn	-1.020954	-1.358991	-0.537451
Br	-2.491588	-3.229678	-0.653017
C	-5.140327	0.785692	1.441569
C	-5.513159	2.012398	2.002018
C	-5.545611	-0.411904	2.040401
C	-6.283192	2.038963	3.164815
H	-5.192298	2.935238	1.528013
C	-6.309143	-0.378038	3.208588
H	-5.259519	-1.357618	1.590104
C	-6.680227	0.844551	3.771001
H	-6.568394	2.992448	3.599541
H	-6.617695	-1.309457	3.673644
H	-7.277467	0.867585	4.677622
C	-5.154137	1.031468	-1.042208
C	-4.513536	2.123566	-1.916562
C	-5.447565	-0.249847	-1.842806
H	-6.110660	1.424737	-0.679561
C	-5.410052	2.429179	-3.128393
H	-3.532924	1.782828	-2.259021
H	-4.358063	3.029593	-1.316929
C	-6.328301	0.068193	-3.062731
H	-4.503851	-0.699784	-2.163153
H	-5.946033	-0.979560	-1.194644
C	-5.705249	1.161116	-3.944093
H	-4.929480	3.187094	-3.758148
H	-6.358297	2.866991	-2.783665
H	-6.489800	-0.846404	-3.644036
H	-7.320184	0.401347	-2.723195
H	-6.370261	1.397657	-4.783189
H	-4.769366	0.785208	-4.379520
C	3.648904	1.030450	0.778767
N	3.130815	-0.144055	0.834266
C	4.178786	-1.073440	1.299463
H	3.759678	-1.720201	2.074197
C	5.314357	-0.124904	1.782886
H	5.367542	0.019866	2.864590
O	4.908920	1.177255	1.220619
C	6.629705	-0.603582	1.153988
H	7.241658	-1.103661	1.915655
H	7.217649	0.241846	0.780892
C	6.188896	-1.567896	0.073321
C	6.970147	-2.174647	-0.909944
C	4.821943	-1.854587	0.164894
C	6.364017	-3.065902	-1.798441
H	8.032668	-1.958544	-0.987044
C	4.210645	-2.745580	-0.718038
C	4.996725	-3.349196	-1.702464
H	6.960006	-3.542865	-2.571402
H	3.149117	-2.956060	-0.641458
H	4.538289	-4.042786	-2.400802
C	2.879833	2.169204	0.220473
C	3.412599	3.455936	-0.103012
C	4.752154	3.870772	0.146626
C	2.513619	4.383692	-0.731623
C	0.783308	2.704549	-0.632381
C	5.163858	5.136432	-0.203147

H	5.443386	3.185828	0.616068
C	2.975954	5.680936	-1.079738
C	1.189485	3.965866	-0.998219
H	-0.216467	2.339996	-0.837034
C	4.273806	6.049958	-0.819711
H	6.187195	5.439975	-0.004691
H	2.285151	6.370579	-1.555826
H	0.497745	4.637858	-1.496276
H	4.623144	7.042458	-1.087827
N	1.611878	1.830928	-0.014897
Ni	1.057826	-0.261193	0.517939
Br	0.859497	-0.754343	-2.063846
Br	0.945605	-2.657109	1.333582

^{1}IM1

B3LYP/BSI SCF energy: -2147.95434a.u.

M06/BSII SCF energy in solution: -2147.12266a.u.

M06/BSII free energy in solution: -2146.538119a.u.

C	-2.723179	0.022356	0.483343
O	-2.077682	-0.669868	-0.337445
N	-3.884866	0.602264	0.083124
C	-2.207312	0.249054	1.885815
H	-2.987070	0.706071	2.500266
H	-1.998761	-0.739280	2.307173
C	-0.925662	1.113159	1.928407
H	-1.142783	2.062403	1.416545
C	-0.534679	1.448743	3.383081
H	-0.460279	0.521040	3.963715
H	0.472283	1.892527	3.395035
C	-1.481017	2.429812	4.101457
H	-2.496462	2.030916	4.191519
H	-1.123373	2.645215	5.114518
H	-1.546005	3.381448	3.560966
Zn	-0.631964	-2.144452	-0.391785
Br	-1.769438	-4.226136	-0.414351
C	-4.706947	1.381626	0.975363
C	-4.584129	2.774333	1.002454
C	-5.672988	0.749645	1.766251
C	-5.417726	3.531238	1.827387
H	-3.835473	3.254924	0.380332
C	-6.502416	1.510755	2.590742
H	-5.760221	-0.331975	1.736925
C	-6.376843	2.901320	2.622635
H	-5.316017	4.612249	1.848878
H	-7.246319	1.015848	3.207808
H	-7.023746	3.491384	3.264832
C	-4.440568	0.396214	-1.296164
C	-3.529730	0.960525	-2.401634
C	-4.843817	-1.065141	-1.565131
H	-5.358571	0.994592	-1.295018
C	-4.205205	0.818608	-3.776474
H	-2.577529	0.423886	-2.401077
H	-3.316671	2.017480	-2.191708
C	-5.505234	-1.192298	-2.948059
H	-3.961551	-1.708426	-1.515020
H	-5.534727	-1.401831	-0.782924
C	-4.601637	-0.638232	-4.059580
H	-3.529012	1.189407	-4.555430
H	-5.103236	1.452954	-3.813123
H	-5.745740	-2.243799	-3.139478
H	-6.460422	-0.646344	-2.951878
H	-5.107271	-0.709637	-5.029836
H	-3.694787	-1.253348	-4.129413
C	3.293253	1.437236	0.589242
N	2.808060	0.339178	1.051060
C	3.925042	-0.404474	1.670716
H	3.603926	-0.781731	2.645330
C	5.067120	0.653247	1.741515
H	5.189574	1.135051	2.714838
O	4.587629	1.706514	0.827076
C	6.347120	0.004549	1.202504
H	7.020645	-0.230842	2.036649
H	6.888168	0.692011	0.543608
C	5.856762	-1.248603	0.510243
C	6.586070	-2.129275	-0.287972
C	4.505104	-1.493267	0.780577
C	5.944637	-3.253292	-0.813278
H	7.635863	-1.945033	-0.501295
C	3.860416	-2.613775	0.257191
C	4.592785	-3.492904	-0.543210
H	6.499377	-3.945080	-1.440679
H	2.809401	-2.788272	0.454419
H	4.102047	-4.364110	-0.965751
C	2.415398	2.348606	-0.168733
C	2.849166	3.390714	-1.038962
C	4.209223	3.771034	-1.222986
C	1.833936	4.078057	-1.785367

C	0.180313	2.663215	-0.738819
C	4.531411	4.786309	-2.093740
H	4.985348	3.257636	-0.672889
C	2.205079	5.120855	-2.674453
C	0.490631	3.671564	-1.618162
H	-0.835996	2.322228	-0.599739
C	3.526564	5.467933	-2.824311
H	5.571343	5.068255	-2.226260
H	1.427741	5.631521	-3.235085
H	-0.297296	4.149657	-2.191103
H	3.806769	6.263945	-3.507473
N	1.124663	2.023428	-0.004529
Ni	0.764341	0.442152	1.173876
Br	0.863883	-1.235994	-2.042493
Br	0.500526	-1.826830	2.004013

^{3}IM1

B3LYP/BSI SCF energy: -2147.967559a.u.

M06/BSII SCF energy in solution: -2147.12681a.u.

M06/BSII free energy in solution: -2146.541868a.u.

C	-2.650799	0.494003	0.892774
O	-2.791431	-0.630164	0.351037
N	-3.601857	1.436258	0.667546
C	-1.484963	0.804148	1.806244
H	-1.822199	1.542086	2.541576
H	-1.272710	-0.121092	2.349138
C	-0.191090	1.306741	1.105668
H	-0.472100	2.068448	0.361464
C	0.740040	1.966987	2.139152
H	0.978966	1.238113	2.927662
H	1.695688	2.208612	1.655844
C	0.229479	3.264109	2.795673
H	-0.679948	3.108603	3.384394
H	0.984289	3.682180	3.472476
H	0.001952	4.022774	2.038542
Zn	-1.695869	-2.253696	-0.186806
Br	-3.123608	-4.065445	-0.659329
C	-3.552746	2.747630	1.263427
C	-3.000013	3.815725	0.550379
C	-4.131643	2.970867	2.517950
C	-3.018382	5.100994	1.095315
H	-2.563024	3.632564	-0.425882
C	-4.141646	4.256037	3.061168
H	-4.565328	2.136011	3.059865
C	-3.586274	5.322907	2.350953
H	-2.587998	5.927707	0.537808
H	-4.586960	4.423329	4.037370
H	-3.598131	6.322853	2.774198
C	-4.802784	1.165691	-0.193023
C	-4.445300	0.915980	-1.668879
C	-5.710698	0.061898	0.379378
H	-5.365791	2.104829	-0.148624
C	-5.723871	0.757029	-2.510112
H	-3.834035	0.014146	-1.750216
H	-3.843664	1.752572	-2.045518
C	-6.979700	-0.084334	-0.477467
H	-5.167481	-0.886123	0.396615
H	-5.976847	0.308934	1.414634
C	-6.634654	-0.346272	-1.951092
H	-5.450688	0.538091	-3.548605
H	-6.274977	1.709116	-2.525839
H	-7.596478	-0.897500	-0.078585
H	-7.583349	0.832413	-0.402891
H	-7.551667	-0.417237	-2.547962
H	-6.125052	-1.315133	-2.036283
C	3.592530	0.757208	0.291791
N	2.844390	-0.208853	0.701502
C	3.648869	-1.018049	1.638217
H	3.041376	-1.269809	2.511131
C	4.869531	-0.104937	1.947542
H	4.800404	0.462022	2.879259
O	4.804944	0.884176	0.858289
C	6.139058	-0.954423	1.824536
H	6.509032	-1.210479	2.825724
H	6.938298	-0.399059	1.322615
C	5.678719	-2.183340	1.071219
C	6.460876	-3.199482	0.523066
C	4.282260	-2.239037	0.983138
C	5.829167	-4.268601	-0.116256
H	7.545169	-3.161078	0.588313
C	3.646671	-3.306510	0.347322
C	4.433639	-4.321280	-0.202789
H	6.426683	-5.065023	-0.550589
H	2.564557	-3.346642	0.283823
H	3.954272	-5.157463	-0.702790
C	3.125714	1.688713	-0.758448
C	3.868371	2.782901	-1.305266

C	5.179166	3.163868	-0.900759
C	3.225523	3.539310	-2.343923
C	1.294501	2.104000	-2.138612
C	5.809421	4.231591	-1.499226
H	5.677697	2.608032	-0.119850
C	3.908771	4.632596	-2.939332
C	1.920637	3.166727	-2.745208
H	0.299545	1.776259	-2.418634
C	5.174879	4.972217	-2.525754
H	6.809357	4.509429	-1.180240
H	3.411200	5.192750	-3.725675
H	1.418218	3.717083	-3.534545
H	5.692930	5.809047	-2.984315
N	1.891663	1.378622	-1.165082
Ni	0.867090	-0.096784	0.036565
Br	-0.402698	-1.073417	-2.032491
Br	0.174858	-2.350752	1.462963

$ZnBr_2$

B3LYP/BSI SCF energy: -254.020927a.u.

M06/BSII SCF energy in solution: -254.003471a.u.

M06/BSII free energy in solution: -254.030224.u.

Zn	0.000000	0.000000	0.000000
Br	0.000000	0.000000	2.258590
Br	0.000000	0.000000	-2.258590

IM^{Zn}

B3LYP/BSI SCF energy: -721.87023a.u.

M06/BSII SCF energy in solution: -721.869021a.u.

M06/BSII free energy in solution: -721.901265a.u.

Zn	-0.160845	0.265438	-0.000292
Br	-2.357036	-0.407175	0.000095
Br	1.905016	-1.083292	0.000081
Li	2.658833	1.215253	-0.000150
Cl	0.745266	2.385732	0.000180

IM^{Zn1}

B3LYP/BSI SCF energy: -1189.720784a.u.

M06/BSII SCF energy in solution: -1189.73194a.u.

M06/BSII free energy in solution: -1189.76573a.u.

Zn	0.000000	0.000000	0.365215
Br	-1.394377	-1.579939	-0.983988
Br	1.394377	1.579939	-0.983988
Li	0.000000	2.940682	0.420578
Cl	-1.229205	1.531649	1.629390
Li	0.000000	-2.940682	0.420578
Cl	1.229205	-1.531649	1.629390

IM^{Zn2}

B3LYP/BSI SCF energy:-1911.622033a.u.

M06/BSII SCF energy in solution: -1911.62636a.u.

M06/BSII free energy in solution:-1911.674712a.u.

Zn	-2.259370	-0.080359	-0.406669
Br	-2.453870	2.281909	0.130574
Br	-2.676030	-1.798941	1.333735
Li	-3.976525	-2.458769	-0.582531
Cl	-3.562148	-0.920710	-2.143201
Zn	2.088324	-0.066431	0.161423
Br	2.240012	2.329136	0.535013
Br	3.867263	-1.231780	-1.125048
Li	3.489371	-2.550556	0.856178
Cl	1.894319	-1.480240	1.990166
Cl	0.051470	-0.099497	-1.196845
Li	-0.045740	2.209323	-0.371734

IM^{Zn3}

B3LYP/BSI SCF energy: -2633.523375a.u.

M06/BSII SCF energy in solution: -2633.52055a.u.

M06/BSII free energy in solution:-2633.582295a.u.

Zn	-0.000682	0.002761	0.597410
Br	-0.127928	-2.153022	1.691668
Br	0.127583	2.162934	1.682859
Li	2.216225	2.269103	0.372874
Cl	1.862129	0.232243	-0.936848
Zn	-4.228865	0.078319	-0.299260
Br	-4.672917	-2.186366	0.450414
Br	-5.391927	1.049695	-2.257310
Li	-5.379428	2.765139	-0.554045
Cl	-4.394050	1.822264	1.215595
Cl	-1.862139	-0.233132	-0.936842
Li	-2.213322	-2.267731	0.377627
Zn	4.228211	-0.081295	-0.299245
Br	4.675619	2.183954	0.447215

Br	5.391425	-1.055953	-2.255629
Li	5.379523	-2.768313	-0.549332
Cl	4.392068	-1.823233	1.218028

IM^{Zn4}

B3LYP/BSI SCF energy: -3355.424229a.u.

M06/BSII SCF energy in solution: -3355.41535a.u.

M06/BSII free energy in solution: -3355.490265a.u.

Zn	-1.661709	-0.131955	-0.408946
Br	-1.130384	2.138954	0.222228
Br	-1.708437	-1.042436	-2.651755
Li	-0.000158	-2.530241	-1.678088
Cl	-0.211543	-1.797994	0.637795
Zn	-5.866640	0.480370	0.186304
Br	-5.676398	2.620953	1.309488
Br	-7.601184	-1.176779	0.781901
Li	-7.520361	-1.118308	-1.634876
Cl	-5.997764	0.441669	-2.128563
Cl	-3.678500	-0.451207	0.873591
Li	-3.313044	1.930752	1.365163
Zn	2.233477	-1.885737	0.468633
Br	2.400977	-3.065566	-1.637418
Br	3.191312	-2.575307	2.579566
Li	4.145073	-0.294123	2.428811
Cl	2.912614	0.414627	0.429830
Zn	5.205323	1.137924	-0.204385
Br	4.979898	3.292431	-1.390675
Br	6.212943	0.970621	1.993525
Cl	5.944043	-0.234903	-1.916138
Li	5.625358	1.663323	-3.057363

^{1}IM2

B3LYP/BSI SCF energy: -1893.894894a.u.

M06/BSII SCF energy in solution: -1893.05572a.u.

M06/BSII free energy in solution: -1892.463289a.u.

C	-2.487944	0.223523	0.280644
O	-1.610348	0.473534	-0.578582
N	-3.807695	0.303189	-0.025869
C	-2.061423	-0.169412	1.684701
H	-2.723555	0.312022	2.418810
H	-2.224294	-1.249295	1.781206
C	-0.580180	0.140735	1.908055
H	-0.427132	1.223109	2.018627
C	0.047204	-0.611581	3.073166
H	-0.046964	-1.690931	2.899368
H	1.122925	-0.393516	3.102347
C	-0.549976	-0.263769	4.452383
H	-1.611339	-0.528064	4.511607
H	-0.032183	-0.804083	5.253410
H	-0.462380	0.809056	4.662033
C	-4.811839	-0.142706	0.906703
C	-5.633880	0.792509	1.544828
C	-5.000378	-1.510830	1.131530
C	-6.637740	0.359158	2.411425
H	-5.476659	1.851564	1.363152
C	-6.002203	-1.937558	2.004775
H	-4.358627	-2.226989	0.626945
C	-6.822153	-1.005653	2.644044
H	-7.271774	1.087886	2.907951
H	-6.142555	-2.999859	2.180943
H	-7.602216	-1.340984	3.321130
C	-4.287001	0.644010	-1.400638
C	-3.852462	2.046459	-1.859135
C	-3.927940	-0.437774	-2.435417
H	-5.378369	0.660139	-1.300782
C	-4.461259	2.376926	-3.232265
H	-2.761869	2.078190	-1.925636
H	-4.159659	2.789075	-1.112236
C	-4.521580	-0.089458	-3.811311
H	-2.839707	-0.525402	-2.501299
H	-4.305959	-1.407704	-2.092982
C	-4.097331	1.311088	-4.277087
H	-4.120023	3.366591	-3.558470
H	-5.555715	2.439540	-3.144451
H	-4.215790	-0.845205	-4.543612
H	-5.619411	-0.133566	-3.759050
H	-4.565098	1.549266	-5.239835
H	-3.011194	1.323665	-4.442914
C	2.975896	0.405351	0.532704
N	2.243583	-0.655001	0.410799
C	3.084699	-1.811002	0.767270
H	2.513978	-2.484124	1.412352
C	4.325600	-1.161899	1.447889
H	4.302539	-1.160960	2.541213
O	4.222729	0.240606	1.028356
C	5.583370	-1.808577	0.855293

H	6.003573	-2.526965	1.571203
H	6.358685	-1.059021	0.664314
C	5.080456	-2.500745	-0.393100
C	5.829384	-3.094685	-1.408854
C	3.681267	-2.525207	-0.438367
C	5.160857	-3.711307	-2.468976
H	6.916001	-3.077320	-1.379578
C	3.007885	-3.142267	-1.493358
C	3.762173	-3.735066	-2.509079
H	5.732075	-4.175814	-3.268102
H	1.922171	-3.155995	-1.513289
H	3.254923	-4.219207	-3.338692
C	2.442704	1.720118	0.171425
C	3.146249	2.967897	0.227315
C	4.495528	3.120221	0.649923
C	2.425316	4.136808	-0.189489
C	0.493570	2.744040	-0.603377
C	5.091129	4.364121	0.653831
H	5.053529	2.250480	0.966912
C	3.069796	5.399154	-0.172378
C	1.076413	3.986606	-0.606416
H	-0.536766	2.582911	-0.898066
C	4.378737	5.512779	0.241216
H	6.123246	4.461547	0.977239
H	2.510775	6.274149	-0.492251
H	0.510124	4.855012	-0.928795
H	4.866355	6.483067	0.250591
N	1.162160	1.624848	-0.232699
Ni	0.254354	-0.260162	0.102462
Br	-0.499617	-2.665261	-0.264665

^{3}IM2

B3LYP/BSI SCF energy: -1893.911955a.u.

M06/BSII SCF energy in solution: -1893.07152a.u.

M06/BSII free energy in solution: -1892.479664a.u.

C	-2.510550	0.145668	0.294776
O	-1.655952	0.435191	-0.575975
N	-3.837723	0.248913	0.020634
C	-2.055624	-0.326269	1.666225
H	-2.737638	0.069156	2.432454
H	-2.183627	-1.417066	1.676877
C	-0.576413	0.003419	1.901211
H	-0.470065	1.079697	2.109350
C	0.043209	-0.800681	3.042228
H	-0.020533	-1.871878	2.805798
H	1.115221	-0.564713	3.104428
C	-0.577028	-0.556177	4.432521
H	-1.632968	-0.846910	4.460670
H	-0.058870	-1.131627	5.209255
H	-0.519113	0.504044	4.707983
C	-4.828883	-0.220896	0.954998
C	-5.631509	0.699776	1.637638
C	-5.030232	-1.593621	1.135793
C	-6.627323	0.247691	2.503789
H	-5.464698	1.762716	1.490582
C	-6.023703	-2.039886	2.008812
H	-4.404933	-2.299131	0.597079
C	-6.823841	-1.122240	2.692137
H	-7.245508	0.965700	3.034779
H	-6.173314	-3.106135	2.150276
H	-7.597551	-1.472506	3.368960
C	-4.344083	0.642502	-1.329929
C	-3.908050	2.055812	-1.753214
C	-4.019054	-0.408794	-2.406843
H	-5.432860	0.665394	-1.205662
C	-4.542263	2.434747	-3.102102
H	-2.819047	2.081056	-1.841932
H	-4.193262	2.776252	-0.976451
C	-4.635894	-0.010849	-3.758592
H	-2.933490	-0.507318	-2.497113
H	-4.402639	-1.384698	-2.088209
C	-4.207682	1.400194	-4.187438
H	-4.200108	3.431998	-3.403544
H	-5.634245	2.502193	-2.990311
H	-4.351835	-0.745084	-4.520927
H	-5.732903	-0.046381	-3.686080
H	-4.691289	1.673123	-5.133017
H	-3.124744	1.408668	-4.373453
C	2.959246	0.451254	0.546360
N	2.282427	-0.632436	0.372452
C	3.148014	-1.758555	0.765818
H	2.570599	-2.450745	1.384078
C	4.331840	-1.067669	1.506067
H	4.263613	-1.083218	2.597014
O	4.184423	0.336995	1.103166
C	5.639833	-1.651980	0.957983
H	6.069469	-2.349684	1.688442

H	6.383825	-0.864931	0.794981
C	5.217100	-2.366071	-0.307644
C	6.031188	-2.933566	-1.287871
C	3.823292	-2.448378	-0.411187
C	5.432760	-3.581851	-2.370750
H	7.114058	-2.872884	-1.213297
C	3.219548	-3.097270	-1.488914
C	4.039060	-3.663127	-2.468723
H	6.055129	-4.026684	-3.142374
H	2.136826	-3.153706	-1.554689
H	3.586957	-4.171368	-3.315577
C	2.385892	1.758732	0.188865
C	3.055887	3.022384	0.258413
C	4.403778	3.205736	0.676531
C	2.301630	4.176402	-0.142176
C	0.411979	2.735961	-0.576946
C	4.963831	4.464514	0.694240
H	4.986871	2.347795	0.979579
C	2.911410	5.457026	-0.109690
C	0.959409	3.995182	-0.560376
H	-0.612668	2.547151	-0.874136
C	4.217102	5.599651	0.300527
H	5.994360	4.586858	1.013921
H	2.327475	6.320373	-0.415982
H	0.368112	4.852014	-0.868378
H	4.678548	6.582430	0.322008
N	1.114030	1.634601	-0.216925
Ni	0.241960	-0.300372	0.055077
Br	-0.395720	-2.668777	-0.578155

^{1}TS2

B3LYP/BSI SCF energy: -2926.77357a.u.

M06/BSII SCF energy in solution: -2925.58089a.u.

M06/BSII free energy in solution: -2924.638133a.u.

C	3.124272	-0.849685	-0.305016
O	2.483546	-1.747932	0.270749
N	4.364033	-0.492452	0.136433
C	2.568092	-0.137381	-1.544573
H	2.612362	0.942456	-1.351618
H	3.303683	-0.302806	-2.342440
C	1.181619	-0.624879	-2.022557
H	0.473881	0.212234	-1.810227
C	1.136800	-0.791612	-3.556977
H	1.875339	-1.551545	-3.840184
H	0.168455	-1.210699	-3.853134
C	1.379469	0.488688	-4.373984
H	2.356837	0.936595	-4.156713
H	1.346121	0.286927	-5.450993
H	0.612964	1.245206	-4.159544
Zn	0.916286	-2.466115	-1.110731
Br	2.074090	-4.299474	-2.243412
C	5.124383	0.550042	-0.502521
C	4.998033	1.874959	-0.069581
C	6.030382	0.235007	-1.522012
C	5.768812	2.878353	-0.659313
H	4.295273	2.110912	0.723737
C	6.800677	1.241288	-2.106596
H	6.120791	-0.794919	-1.853134
C	6.671148	2.563805	-1.677468
H	5.666517	3.904942	-0.319207
H	7.500057	0.990718	-2.898691
H	7.271746	3.345220	-2.133767
C	5.057779	-1.245758	1.227718
C	4.351192	-1.111375	2.587970
C	5.318520	-2.717663	0.856870
H	6.030681	-0.747531	1.313766
C	5.152318	-1.827679	3.688134
H	3.351788	-1.547579	2.510444
H	4.229740	-0.048911	2.833285
C	6.108849	-3.424616	1.970707
H	4.365229	-3.226598	0.690741
H	5.873089	-2.763487	-0.087816
C	5.406954	-3.299769	3.331017
H	4.617299	-1.751757	4.642608
H	6.116537	-1.318037	3.831931
H	6.245831	-4.479166	1.706915
H	7.115916	-2.987545	2.043852
H	6.006073	-3.780969	4.113397
H	4.448230	-3.834417	3.293163
C	0.459975	2.684857	-0.034890
N	-0.453338	2.477479	-0.909593
C	-0.292549	3.523620	-1.939532
H	-0.303343	3.058659	-2.929705
O	1.353410	3.680787	-0.259449
C	0.604265	1.848421	1.182522
C	1.226769	2.286167	2.394256
C	1.784440	3.581879	2.599781

C	1.256115	1.350300	3.482268	C	-5.040647	1.231830	1.998939
C	0.101907	-0.241997	2.081975	H	-6.028520	-0.651158	2.215228
C	2.350908	3.913557	3.809225	C	-4.464465	-0.345884	4.452147
H	1.761212	4.304274	1.796445	H	-3.045990	-0.592985	2.826768
C	1.854129	1.727034	4.715432	H	-4.121323	-1.972383	3.044332
C	0.679746	0.075235	3.287383	C	-5.429444	1.746870	3.395244
H	-0.330114	-1.217905	1.884611	H	-4.054104	1.614080	1.723341
C	2.392344	2.981086	4.875188	H	-5.752663	1.592367	1.246404
H	2.770270	4.905140	3.950255	C	-4.496854	1.189773	4.481613
H	1.872471	1.005204	5.526674	H	-3.763984	-0.729683	5.202809
H	0.697024	-0.659493	4.086010	H	-5.456153	-0.732780	4.727680
H	2.847009	3.263968	5.819833	H	-5.412208	2.842921	3.400541
N	0.061585	0.637541	1.046655	H	-6.464150	1.451233	3.621707
Ni	-1.057472	0.113966	-0.653576	H	-4.812326	1.544363	5.470079
C	1.061023	4.213170	-1.591382	H	-3.481110	1.576407	4.317748
H	1.899385	3.923049	-2.228662	Br	-0.913229	-3.292068	0.368711
C	-3.606537	-0.630726	-0.052748	C	-1.312232	4.642431	-1.810929
O	-2.709315	0.108763	0.445753	C	-2.701332	4.554260	-1.898309
N	-4.744793	-0.879083	0.630065	C	-0.686142	5.869058	-1.561885
C	-3.364149	-1.225408	-1.419711	C	-3.461770	5.713327	-1.730347
H	-3.047956	-2.262368	-1.257418	H	-3.180787	3.599629	-2.088199
H	-4.302321	-1.270450	-1.987856	C	-1.447290	7.026448	-1.395318
C	-2.232763	-0.449229	-2.120075	C	-2.838797	6.941109	-1.479556
H	-1.674992	-1.140170	-2.761659	H	-4.544750	5.661311	-1.794116
C	-2.742869	0.726333	-2.962416	H	-0.967564	7.982563	-1.202682
H	-3.376645	1.375640	-2.339892	H	-3.442002	7.835127	-1.350125
H	-1.893489	1.346268	-3.276827	C	0.821393	5.730689	-1.544911
C	-3.524570	0.321208	-4.226045	H	1.293762	6.177218	-0.663538
H	-4.414943	-0.270375	-3.986388	H	1.275738	6.207671	-2.422512
H	-3.857814	1.201371	-4.788608				
H	-2.898631	-0.284087	-4.890898	**^{3}TS2**			
C	-5.677576	-1.874280	0.158010	B3LYP/BSI SCF energy:-2926.785877a.u.			
C	-5.335845	-3.229917	0.204878	M06/BSII SCF energy in solution: -2925.58975a.u.			
C	-6.940691	-1.480357	-0.295892	M06/BSII free energy in solution:-2924.647735a.u.			
C	-6.258234	-4.188210	-0.218644				
H	-4.352167	-3.524924	0.558499	C	3.379617	-0.639792	-0.289588
C	-7.860117	-2.444780	-0.709053	O	2.803558	-1.547089	0.338341
H	-7.191588	-0.424284	-0.329824	N	4.617813	-0.216240	0.094699
C	-7.519534	-3.798959	-0.673085	C	2.733696	0.024158	-1.514258
H	-5.987661	-5.239265	-0.189270	H	2.677715	1.099908	-1.297344
H	-8.838989	-2.137346	-1.065045	H	3.461654	-0.049802	-2.332307
H	-8.234944	-4.547812	-0.999653	C	1.380231	-0.582622	-1.952241
C	-5.014201	-0.306509	1.985072	H	0.609516	0.189303	-1.763973
C	-4.075553	-0.877660	3.062769	C	1.319753	-0.846149	-3.472024

H	2.112745	-1.555803	-3.739283	C	1.443609	1.791026	3.292473
H	0.380643	-1.364710	-3.702743	C	0.332132	-0.047572	2.186937
C	1.426873	0.399988	-4.366753	C	2.314452	4.458407	3.235728
H	2.369041	0.939203	-4.208161	H	1.508008	4.568063	1.263446
H	1.376872	0.137514	-5.430060	C	2.114039	2.354607	4.412283
H	0.606760	1.101966	-4.164359	C	0.976387	0.458034	3.291900
Zn	1.215580	-2.371453	-0.953409	H	-0.017639	-1.072875	2.130848
Br	2.329968	-4.297053	-1.956697	C	2.541929	3.659738	4.384244
C	5.308960	0.839140	-0.598622	H	2.650433	5.490921	3.228457
C	5.136023	2.169891	-0.201635	H	2.276414	1.733182	5.288001
C	6.199281	0.532965	-1.634517	H	1.131835	-0.173530	4.160798
C	5.843694	3.187644	-0.843417	H	3.052634	4.085752	5.242575
H	4.448369	2.398143	0.607295	N	0.118730	0.699133	1.075323
C	6.906557	1.553501	-2.271464	Ni	-1.051633	-0.013594	-0.602501
H	6.326289	-0.501943	-1.936834	C	0.281909	4.075414	-1.965116
C	6.729738	2.881748	-1.878247	H	1.085562	3.863304	-2.673678
H	5.705187	4.218878	-0.531411	C	-3.590150	-0.843547	0.057437
H	7.593821	1.309574	-3.076145	O	-2.755742	-0.018389	0.519949
H	7.281028	3.674453	-2.375430	N	-4.744308	-1.086740	0.724386
C	5.371205	-0.888644	1.198706	C	-3.286659	-1.567160	-1.243470
C	4.691523	-0.724612	2.569972	H	-2.939400	-2.566061	-0.958767
C	5.689412	-2.362667	0.886635	H	-4.218133	-1.716123	-1.804996
H	6.322470	-0.344794	1.237796	C	-2.178033	-0.847331	-2.037478
C	5.549787	-1.355059	3.679654	H	-1.571008	-1.597845	-2.559490
H	3.711470	-1.207927	2.536859	C	-2.749182	0.110424	-3.093190
H	4.527224	0.341591	2.771304	H	-3.454534	0.809892	-2.620601
C	6.537477	-2.982882	2.009680	H	-1.940269	0.727689	-3.505555
H	4.756159	-2.919944	0.769056	C	-3.455921	-0.575504	-4.277365
H	6.222424	-2.426252	-0.069353	H	-4.305148	-1.185375	-3.950360
C	5.861800	-2.829067	3.380306	H	-3.837273	0.157687	-4.998455
H	5.034830	-1.260353	4.643489	H	-2.763054	-1.238382	-4.807386
H	6.493295	-0.797746	3.776101	C	-5.621929	-2.156801	0.317858
H	6.716798	-4.040953	1.788859	C	-5.243325	-3.488666	0.516842
H	7.524747	-2.498095	2.038740	C	-6.875701	-1.857101	-0.225685
H	6.499225	-3.248603	4.167885	C	-6.115441	-4.517064	0.156190
H	4.927239	-3.406081	3.388881	H	-4.269072	-3.711842	0.941190
C	0.153858	2.634041	-0.227617	C	-7.746009	-2.889636	-0.575891
N	-0.784169	2.172002	-0.976606	H	-7.157235	-0.819382	-0.378162
C	-0.954460	3.136736	-2.083399	C	-7.366537	-4.220559	-0.387759
H	-1.002284	2.594138	-3.030520	H	-5.814450	-5.549732	0.304098
O	0.803474	3.743696	-0.634863	H	-8.716930	-2.653845	-1.001602
C	0.538224	1.964369	1.036045	H	-8.043112	-5.023232	-0.665564
C	1.223001	2.593299	2.122068	C	-5.089593	-0.399940	2.005878
C	1.672556	3.946005	2.131608	C	-4.153881	-0.797870	3.161749

C	-5.206455	1.127388	1.859133
H	-6.088891	-0.780912	2.244897
C	-4.611434	-0.146584	4.477611
H	-3.134586	-0.482794	2.919635
H	-4.141127	-1.889369	3.260152
C	-5.661847	1.762332	3.184026
H	-4.236850	1.537212	1.563818
H	-5.918559	1.363543	1.058735
C	-4.729951	1.378988	4.343613
H	-3.912617	-0.408238	5.280584
H	-5.587815	-0.559143	4.770382
H	-5.707128	2.852097	3.073131
H	-6.683965	1.431250	3.418570
H	-5.092297	1.816291	5.281646
H	-3.733300	1.805217	4.161588
Br	-0.613974	-3.052279	0.609338
C	-2.135497	4.075395	-1.885868
C	-3.486158	3.751849	-1.757662
C	-1.713118	5.408889	-1.829741
C	-4.412565	4.780576	-1.575403
H	-3.810348	2.717684	-1.792045
C	-2.639766	6.435976	-1.649337
C	-3.992628	6.114192	-1.522245
H	-5.467448	4.542964	-1.474056
H	-2.316051	7.472646	-1.606687
H	-4.723710	6.904889	-1.380413
C	-0.215684	5.527103	-2.012381
H	0.272324	6.134440	-1.242748
H	0.038431	5.978339	-2.979722

^{1}IM3

B3LYP/BSI SCF energy: -2672.724421a.u.

M06/BSII SCF energy in solution:-2671.52917a.u.

M06/BSII free energy in solution: -2670.576005a.u.

C	2.829644	-0.394813	-0.863378
O	1.921905	-1.064858	-0.346326
N	4.135611	-0.526099	-0.460445
C	2.524486	0.494629	-2.061409
H	3.378619	1.132427	-2.303471
H	2.435130	-0.216160	-2.897752
C	1.233750	1.312827	-1.952788
H	1.403852	2.156443	-1.274711
C	0.782103	1.861215	-3.305886
H	0.659420	1.041939	-4.026628
H	-0.204748	2.320439	-3.185110
C	1.733958	2.911474	-3.909972
H	2.721585	2.492829	-4.132358
H	1.330995	3.312400	-4.847160
H	1.878172	3.752645	-3.222247
C	5.117889	0.485678	-0.745377
C	5.004780	1.750663	-0.155231
C	6.212870	0.195312	-1.567913
C	5.973004	2.724204	-0.406937
H	4.161077	1.960843	0.496268
C	7.184153	1.168074	-1.804136
H	6.291170	-0.786355	-2.025843
C	7.064434	2.435069	-1.227953
H	5.875784	3.705701	0.047470
H	8.029648	0.938895	-2.446289
H	7.818987	3.192551	-1.418166
C	4.570222	-1.629113	0.445523
C	4.045951	-1.496658	1.886325
C	4.272069	-3.022470	-0.135623
H	5.660322	-1.522086	0.485346
C	4.642586	-2.596538	2.780396
H	2.955880	-1.581532	1.872750
H	4.294449	-0.503719	2.278240
C	4.860915	-4.121085	0.765257
H	3.188765	-3.150569	-0.220651
H	4.688431	-3.094078	-1.147778
C	4.361012	-3.996199	2.212216
H	4.238575	-2.507913	3.795501
H	5.729422	-2.452107	2.865072
H	4.610684	-5.107649	0.357401
H	5.958335	-4.052197	0.756370
H	4.826521	-4.763747	2.841894
H	3.278037	-4.183093	2.238184
C	-1.296058	2.900634	-0.151767
N	-1.672453	1.907026	-0.939041
C	-2.814674	2.397214	-1.712947
H	-2.734098	2.092074	-2.761635
O	-1.955576	4.087298	-0.343477
C	-0.278201	2.761961	0.831247
C	0.143963	3.758061	1.798451
C	-0.335164	5.088326	1.847246
C	1.113779	3.357095	2.778363
C	1.171866	1.154990	1.754506

C	0.117843	5.981941	2.811279	C	-2.293013	-2.623044	4.155996
H	-1.066311	5.413603	1.120746	H	-1.117354	-1.703566	2.581056
C	1.552539	4.286460	3.743642	H	-0.781798	-3.423842	2.808679
C	1.604934	2.011714	2.742799	C	-4.460195	-1.978328	3.012711
H	1.547249	0.140231	1.688888	H	-3.395035	-1.025984	1.382583
C	1.064310	5.585599	3.765667	H	-4.469002	-2.326075	0.863380
H	-0.270817	6.996808	2.820824	C	-3.472558	-1.639761	4.139822
H	2.285973	3.963051	4.478756	H	-1.574927	-2.346204	4.936486
H	2.313393	1.672055	3.491905	H	-2.661581	-3.626943	4.413610
H	1.412617	6.288163	4.517921	H	-5.272537	-1.243362	2.982151
N	0.283805	1.496499	0.804543	H	-4.926509	-2.952828	3.220546
Ni	-0.151776	0.365494	-0.871848	H	-3.985879	-1.647848	5.108681
C	-2.764666	3.939837	-1.533424	H	-3.091962	-0.620149	3.992373
H	-2.259886	4.469809	-2.348961	C	-4.183590	2.034001	-1.141132
C	-1.300195	-2.113948	-0.280218	C	-4.700252	0.770441	-0.856682
O	-1.295119	-0.975250	0.239096	C	-4.947247	3.181234	-0.892160
N	-1.911167	-3.157845	0.340153	C	-5.990152	0.663449	-0.330364
C	-0.589833	-2.301226	-1.604383	H	-4.100301	-0.117891	-1.023442
H	0.413625	-2.667998	-1.363147	C	-6.233270	3.076057	-0.361971
H	-1.072496	-3.083180	-2.203222	C	-6.753481	1.809855	-0.084375
C	-0.474445	-0.952599	-2.347478	H	-6.401975	-0.316710	-0.105361
H	0.391591	-1.008350	-3.012982	H	-6.823430	3.966922	-0.161307
C	-1.714458	-0.623300	-3.182160	H	-7.753637	1.715306	0.329608
H	-2.610329	-0.642859	-2.548871	C	-4.194594	4.435950	-1.279637
H	-1.631797	0.402591	-3.553958	H	-4.211531	5.212093	-0.507463
C	-1.936018	-1.548322	-4.394096	H	-4.606676	4.882081	-2.194619
H	-2.081622	-2.593393	-4.099119				
H	-2.822082	-1.244904	-4.963525	**^{3}IM3**			
H	-1.076555	-1.516137	-5.074049	B3LYP/BSI SCF energy: -2672.725797a.u.			
C	-1.822590	-4.495252	-0.184288	M06/BSII SCF energy in solution: -2671.53016a.u.			
C	-0.642753	-5.233026	-0.039457	M06/BSII free energy in solution:-2670.579068a.u.			
C	-2.939347	-5.080113	-0.792151				
C	-0.577939	-6.544320	-0.513179	C	2.818019	-0.273315	-0.815693
H	0.215152	-4.774670	0.442713	O	1.888019	-0.913328	-0.298390
C	-2.871896	-6.393471	-1.257892	N	4.118598	-0.459044	-0.419432
H	-3.850051	-4.499077	-0.901041	C	2.540494	0.636389	-2.004731
C	-1.691247	-7.127077	-1.121268	H	3.390966	1.294080	-2.202509
H	0.341535	-7.111414	-0.401485	H	2.496404	-0.057601	-2.859185
H	-3.740425	-6.841231	-1.731786	C	1.228076	1.421455	-1.923678
H	-1.639881	-8.148398	-1.486604	H	1.358814	2.274326	-1.247885
C	-2.579133	-3.006735	1.671329	C	0.783703	1.943845	-3.288795
C	-1.580070	-2.671567	2.794205	H	0.681530	1.111494	-3.997554
C	-3.760207	-2.022002	1.644009	H	-0.211019	2.390034	-3.186346
H	-2.985179	-4.004080	1.876106	C	1.727877	2.997860	-3.899170

H	2.724004	2.589621	-4.102776	C	1.535340	2.170688	2.727968
H	1.330877	3.377695	-4.847737	H	1.528858	0.276731	1.718031
H	1.852118	3.852324	-3.223911	C	0.886569	5.743827	3.684565
C	5.144269	0.505229	-0.716763	H	-0.490198	7.095088	2.712030
C	5.101627	1.772254	-0.121453	H	2.158192	4.173648	4.426915
C	6.212583	0.164438	-1.554513	H	2.257098	1.868168	3.480528
C	6.113120	2.697712	-0.382920	H	1.215173	6.472471	4.420603
H	4.275645	2.022574	0.538520	N	0.203466	1.565643	0.820949
C	7.227871	1.088870	-1.800425	Ni	-0.144942	0.406242	-0.862730
H	6.236101	-0.818255	-2.016212	C	-2.940999	3.876718	-1.529327
C	7.178558	2.357894	-1.218759	H	-2.469395	4.458446	-2.329357
H	6.070249	3.681509	0.074888	C	-1.237129	-2.111640	-0.286075
H	8.052514	0.820481	-2.454348	O	-1.277143	-0.972225	0.228325
H	7.967063	3.077936	-1.416391	N	-1.801003	-3.177315	0.344117
C	4.512772	-1.579582	0.484000	C	-0.523519	-2.284841	-1.612525
C	4.003884	-1.424411	1.928024	H	0.479779	-2.653687	-1.371616
C	4.154587	-2.960149	-0.093678	H	-1.003500	-3.070657	-2.209864
H	5.606561	-1.517378	0.516954	C	-0.412801	-0.934714	-2.351639
C	4.560667	-2.547393	2.819331	H	0.478372	-0.970333	-2.985489
H	2.911104	-1.463142	1.922848	C	-1.628679	-0.641366	-3.235048
H	4.297088	-0.442712	2.317563	H	-2.550424	-0.715230	-2.643715
C	4.706510	-4.080328	0.803938	H	-1.579350	0.394920	-3.584201
H	3.066412	-3.045112	-0.169541	C	-1.755493	-1.551248	-4.471948
H	4.559293	-3.049117	-1.109149	H	-1.848678	-2.608884	-4.200798
C	4.220998	-3.935156	2.253866	H	-2.637213	-1.289159	-5.068464
H	4.166126	-2.442243	3.836560	H	-0.875565	-1.455744	-5.119007
H	5.652831	-2.446337	2.897892	C	-1.681049	-4.510311	-0.185519
H	4.415696	-5.056683	0.398432	C	-0.490250	-5.227559	-0.027524
H	5.805675	-4.053968	0.787758	C	-2.778305	-5.112721	-0.811475
H	4.660095	-4.719812	2.881391	C	-0.395266	-6.535513	-0.505252
H	3.131684	-4.079780	2.287039	H	0.352815	-4.755407	0.467423
C	-1.406163	2.912078	-0.167970	C	-2.680652	-6.422410	-1.282326
N	-1.697906	1.921720	-0.989124	H	-3.697614	-4.547447	-0.930493
C	-2.884442	2.339228	-1.740580	C	-1.489151	-7.135353	-1.131784
H	-2.791279	2.059327	-2.795092	H	0.532614	-7.086607	-0.383228
O	-2.150197	4.051600	-0.329450	H	-3.534157	-6.883509	-1.770531
C	-0.385903	2.817186	0.821475	H	-1.414115	-8.153899	-1.500806
C	0.012551	3.847315	1.761049	C	-2.455611	-3.050329	1.684038
C	-0.502311	5.165653	1.780352	C	-1.457130	-2.664466	2.791087
C	0.999107	3.498685	2.743600	C	-3.680379	-2.120304	1.669549
C	1.122240	1.280107	1.763576	H	-2.813362	-4.063866	1.899514
C	-0.072803	6.091706	2.723325	C	-2.152002	-2.638880	4.162931
H	-1.244405	5.453845	1.049409	H	-1.040586	-1.678451	2.565690
C	1.412819	4.459901	3.688460	H	-0.626035	-3.380587	2.798368

C	-4.361672	-2.099110	3.048121
H	-3.364938	-1.110516	1.396530
H	-4.386141	-2.461186	0.901543
C	-3.373969	-1.708887	4.158174
H	-1.435773	-2.325557	4.931327
H	-2.471816	-3.656439	4.431918
H	-5.207097	-1.402071	3.025453
H	-4.780122	-3.092306	3.268993
H	-3.872212	-1.732724	5.134639
H	-3.040920	-0.674568	3.998379
C	-4.219931	1.871098	-1.165732
C	-4.644031	0.570696	-0.895520
C	-5.063399	2.957737	-0.901372
C	-5.923426	0.365639	-0.372362
H	-3.980875	-0.269496	-1.070041
C	-6.338762	2.754561	-0.374067
C	-6.767384	1.450944	-0.113680
H	-6.263970	-0.644085	-0.159599
H	-6.990741	3.598634	-0.162901
H	-7.758552	1.279634	0.297244
C	-4.402149	4.267777	-1.271460
H	-4.474005	5.030585	-0.489242
H	-4.843696	4.695758	-2.181378

^{1}TS3

B3LYP/BSI SCF energy:-2672.688465a.u.

M06/BSII SCF energy in solution: -2671.51272a.u.

M06/BSII free energy in solution:-2670.557389a.u.

C	1.927591	1.602285	-1.730438
O	2.942098	0.991588	-1.370901
N	1.659081	2.867272	-1.273343
C	0.979563	0.986363	-2.766365
H	0.634463	1.783542	-3.434306
H	1.604875	0.326927	-3.378807
C	-0.281549	0.247935	-2.279551
H	-0.755620	0.882722	-1.516865
C	-1.281660	0.072132	-3.433089
H	-0.738885	-0.204525	-4.348419
H	-1.952054	-0.761513	-3.210785
C	-2.136073	1.318411	-3.706369
H	-1.527651	2.198958	-3.935913
H	-2.804320	1.148083	-4.558050
H	-2.752050	1.564661	-2.836072
C	0.469415	3.602867	-1.622258
C	-0.650786	3.553127	-0.785228
C	0.459993	4.431395	-2.751375
C	-1.778630	4.321896	-1.082427
H	-0.633270	2.920250	0.095624
C	-0.671628	5.193219	-3.047855
H	1.338633	4.473628	-3.388628
C	-1.791292	5.140109	-2.213646
H	-2.641966	4.273631	-0.425482
H	-0.675045	5.832427	-3.926192
H	-2.668866	5.737224	-2.443881
C	2.611111	3.576313	-0.365424
C	2.755324	2.905888	1.012024
C	3.979605	3.826184	-1.026625
H	2.143956	4.554553	-0.204456
C	3.674984	3.734608	1.924596
H	3.167343	1.902133	0.874626
H	1.765753	2.795484	1.468252
C	4.890221	4.649238	-0.100419
H	4.445237	2.862424	-1.250705
H	3.834161	4.349680	-1.979634
C	5.044399	3.984928	1.275837
H	3.795264	3.224590	2.887800
H	3.198742	4.701306	2.144151
H	5.870603	4.785915	-0.572261
H	4.466478	5.655572	0.031022
H	5.668038	4.606646	1.929546
H	5.569763	3.026754	1.157832
C	-3.317150	0.088732	0.181775
N	-2.774966	-0.857396	-0.574876
C	-3.885313	-1.533872	-1.248434
H	-3.636040	-1.750067	-2.294856
O	-4.663211	0.278879	0.003577
C	-2.575812	0.842056	1.131343
C	-3.076789	1.901915	1.988987
C	-4.389856	2.427333	1.941766
C	-2.162989	2.460780	2.946200
C	-0.439455	0.972238	2.102169
C	-4.788379	3.449666	2.796651
H	-5.095905	2.021149	1.230958
C	-2.599476	3.493811	3.802218
C	-0.826062	1.949781	2.995481
H	0.574037	0.583066	2.102233
C	-3.894901	3.986513	3.733599

H	-5.804817	3.829422	2.735542
H	-1.894557	3.901986	4.522707
H	-0.122362	2.339486	3.724261
H	-4.212987	4.782455	4.401439
N	-1.252371	0.435650	1.176633
Ni	-0.675530	-0.765513	-0.430643
C	-5.071598	-0.539990	-1.116087
H	-5.205968	0.116357	-1.983381
C	1.947309	-1.885391	-0.114171
O	1.038155	-1.379367	0.575892
N	3.049838	-2.433318	0.463669
C	1.818008	-1.880684	-1.620030
H	2.441656	-1.052944	-1.968038
H	2.256247	-2.791793	-2.042926
C	0.379652	-1.707980	-2.126425
H	0.474811	-1.568574	-3.205164
C	-0.498223	-2.968868	-1.958174
H	-0.532461	-3.287423	-0.909212
H	-1.527193	-2.731188	-2.239694
C	-0.032462	-4.153281	-2.829422
H	0.959405	-4.517421	-2.542991
H	-0.728540	-4.993788	-2.735179
H	0.008150	-3.870798	-3.887866
C	4.194546	-2.810012	-0.325258
C	4.953013	-1.832298	-0.979932
C	4.576408	-4.155186	-0.390337
C	6.084125	-2.209692	-1.706204
H	4.642934	-0.792813	-0.930035
C	5.713827	-4.522097	-1.109575
H	3.977710	-4.904726	0.118804
C	6.468998	-3.550166	-1.770082
H	6.668482	-1.450185	-2.217353
H	6.005596	-5.567100	-1.158653
H	7.352788	-3.837410	-2.332107
C	3.225234	-2.479265	1.948119
C	3.453401	-1.082788	2.553180
C	2.104549	-3.245957	2.671930
H	4.150260	-3.050630	2.084858
C	3.730306	-1.179954	4.062788
H	2.564148	-0.471304	2.376415
H	4.291211	-0.596180	2.039991
C	2.404186	-3.335633	4.178223
H	1.151822	-2.734484	2.514165
H	2.012056	-4.250263	2.240041
C	2.616204	-1.944091	4.793646
H	3.843614	-0.173200	4.481560
H	4.688942	-1.693465	4.226510
H	1.583005	-3.856219	4.684031
H	3.305972	-3.944220	4.340352
H	2.854213	-2.033213	5.860206
H	1.680053	-1.373447	4.725723
C	-4.411181	-2.783821	-0.544753
C	-3.713847	-3.933286	-0.173647
C	-5.778927	-2.666843	-0.266483
C	-4.397444	-4.967077	0.471107
H	-2.650486	-4.019879	-0.370457
C	-6.461649	-3.697169	0.379840
C	-5.764190	-4.850695	0.745840
H	-3.862606	-5.865486	0.766839
H	-7.521669	-3.603638	0.602742
H	-6.284369	-5.658864	1.252531
C	-6.328403	-1.345828	-0.760328
H	-6.936017	-0.819817	-0.016749
H	-6.954804	-1.481150	-1.652215

^{3}TS3

B3LYP/BSI SCF energy: -2672.688769a.u.

M06/BSII SCF energy in solution: -2671.51297a.u.

M06/BSII free energy in solution:-2670.558723a.u.

C	1.907785	1.622087	-1.713192
O	2.923487	1.009239	-1.360461
N	1.639151	2.883116	-1.245929
C	0.957763	1.012761	-2.751151
H	0.609682	1.814279	-3.412384
H	1.581714	0.358496	-3.370295
C	-0.301379	0.271037	-2.266143
H	-0.774535	0.897791	-1.496846
C	-1.303649	0.095674	-3.416884
H	-0.763364	-0.177198	-4.334780
H	-1.972054	-0.738858	-3.192571
C	-2.161335	1.341366	-3.683263
H	-1.555494	2.224251	-3.910785
H	-2.831218	1.172806	-4.533994
H	-2.775710	1.582014	-2.810329
C	0.449189	3.621001	-1.589226
C	-0.668895	3.568938	-0.749587
C	0.437284	4.452892	-2.715832

C	-1.797637	4.338274	-1.041879	H	-4.182353	4.832400	4.319734
H	-0.648918	2.934772	0.130284	N	-1.264103	0.395793	1.174934
C	-0.695125	5.215446	-3.007425	Ni	-0.680488	-0.778119	-0.436132
H	1.314465	4.497053	-3.354971	C	-5.095670	-0.580928	-1.097559
C	-1.812889	5.159589	-2.170850	H	-5.251953	0.072846	-1.963232
H	-2.659361	4.287647	-0.382976	C	1.952755	-1.882812	-0.129909
H	-0.700633	5.857285	-3.883837	O	1.041112	-1.390011	0.566758
H	-2.691120	5.757129	-2.397477	N	3.060699	-2.427393	0.439936
C	2.591602	3.585267	-0.333094	C	1.818471	-1.866289	-1.635446
C	2.739616	2.902255	1.037795	H	2.434193	-1.030620	-1.978618
C	3.958358	3.843499	-0.994601	H	2.261947	-2.770483	-2.067730
H	2.123011	4.561090	-0.162045	C	0.376833	-1.699407	-2.131942
C	3.659521	3.724294	1.956145	H	0.459745	-1.544361	-3.209042
H	3.153328	1.900643	0.890339	C	-0.494211	-2.964668	-1.967100
H	1.751084	2.785621	1.494740	H	-0.527001	-3.287790	-0.919261
C	4.869534	4.659449	-0.062669	H	-1.524283	-2.731247	-2.248678
H	4.425075	2.882546	-1.228313	C	-0.021907	-4.144553	-2.841044
H	3.810259	4.375439	-1.942505	H	0.970774	-4.505484	-2.553585
C	5.027319	3.982866	1.307227	H	-0.715024	-4.987912	-2.750648
H	3.782451	3.205815	2.914488	H	0.019651	-3.858384	-3.898417
H	3.182070	4.688155	2.185292	C	4.205874	-2.788330	-0.355825
H	5.848819	4.801907	-0.535095	C	4.955263	-1.798717	-1.002927
H	4.444545	5.663894	0.078694	C	4.597068	-4.130013	-0.435302
H	5.651116	4.599680	1.965418	C	6.087049	-2.160719	-1.735973
H	5.554119	3.026721	1.179525	H	4.637643	-0.762117	-0.942008
C	-3.328534	0.070378	0.171225	C	5.735054	-4.481554	-1.161322
N	-2.786239	-0.860736	-0.604316	H	4.005254	-4.888870	0.068070
C	-3.900010	-1.560959	-1.247357	C	6.481358	-3.497680	-1.814187
H	-3.669437	-1.782035	-2.297289	H	6.664455	-1.392000	-2.241211
O	-4.679809	0.243081	0.015678	H	6.034183	-5.523883	-1.221590
C	-2.582865	0.822860	1.115505	H	7.365591	-3.772963	-2.381473
C	-3.071731	1.904271	1.952660	C	3.241097	-2.485373	1.923437
C	-4.373241	2.454988	1.882260	C	3.462252	-1.092982	2.540366
C	-2.158250	2.459273	2.912050	C	2.127828	-3.265849	2.643998
C	-0.448209	0.938719	2.095080	H	4.170257	-3.051915	2.051940
C	-4.762942	3.493861	2.721687	C	3.745636	-1.202548	4.047922
H	-5.078523	2.053418	1.167842	H	2.568416	-0.485682	2.372428
C	-2.585307	3.508703	3.751948	H	4.294962	-0.596137	2.028718
C	-0.828455	1.929251	2.976128	C	2.433881	-3.367977	4.148173
H	0.560994	0.538776	2.104625	H	1.171426	-2.758665	2.494894
C	-3.871184	4.023988	3.663749	H	2.039782	-4.266529	2.202862
H	-5.771508	3.891344	2.644412	C	2.639585	-1.980999	4.775954
H	-1.880893	3.912635	4.475366	H	3.853998	-0.199101	4.475809
H	-0.125503	2.314155	3.708204	H	4.708249	-1.711297	4.202877

H	1.617929	-3.898436	4.652166
H	3.340046	-3.972392	4.301089
H	2.882748	-2.078789	5.840590
H	1.699503	-1.415784	4.717633
C	-4.397429	-2.812259	-0.524773
C	-3.679911	-3.950349	-0.157136
C	-5.761914	-2.710820	-0.224613
C	-4.339387	-4.987725	0.506796
H	-2.619229	-4.025808	-0.371730
C	-6.420623	-3.744594	0.440705
C	-5.702622	-4.886449	0.803697
H	-3.788291	-5.877125	0.799932
H	-7.477939	-3.662704	0.680410
H	-6.203989	-5.697170	1.325062
C	-6.336430	-1.401075	-0.719875
H	-6.941516	-0.878287	0.027972
H	-6.972237	-1.551338	-1.602704

7

B3LYP/BSI SCF energy:-1584.576262a.u.

M06/BSII SCF energy in solution: -1583.80118a.u.

M06/BSII free energy in solution:-1583.113378a.u.

C	-3.036617	-0.954746	-0.123250
O	-3.455790	-2.085550	-0.359582
N	-3.898177	0.115152	0.034083
C	-1.533772	-0.670336	0.002767
H	-1.217913	-0.255489	-0.962066
H	-1.359169	0.125889	0.733852
C	-0.702120	-1.929477	0.335391
C	-3.437264	1.469984	0.143143
C	-2.913358	2.137284	-0.971065
C	-3.560741	2.155062	1.359153
C	-2.502982	3.467062	-0.865521
H	-2.835211	1.609078	-1.916477
C	-3.160666	3.487790	1.458493
H	-3.967113	1.633688	2.220641
C	-2.627573	4.145905	0.347846
H	-2.094408	3.974189	-1.734783
H	-3.259945	4.010041	2.405762
H	-2.313547	5.182493	0.427445
C	-5.374764	-0.077175	-0.059401
C	-5.827369	-0.496374	-1.471074
C	-5.927288	-1.027078	1.018759
H	-5.790300	0.918267	0.137370
C	-7.359500	-0.600942	-1.548133
H	-5.370556	-1.460852	-1.709922
H	-5.459053	0.233455	-2.202678
C	-7.459514	-1.121488	0.928507
H	-5.482152	-2.015692	0.880865
H	-5.624647	-0.668376	2.010378
C	-7.916025	-1.548262	-0.474794
H	-7.657332	-0.938186	-2.548031
H	-7.802871	0.396529	-1.412466
H	-7.830639	-1.825885	1.682287
H	-7.904614	-0.144987	1.170240
H	-9.011141	-1.578468	-0.525573
H	-7.562320	-2.569009	-0.674573
C	-0.593879	-2.170129	1.856952
H	-0.031701	-1.349038	2.325091
H	0.011379	-3.072074	2.013714
C	-1.928817	-2.335891	2.593965
H	-2.532577	-3.131774	2.148235
H	-1.758172	-2.583586	3.647311
H	-2.528150	-1.419049	2.570036
H	-1.250220	-2.779367	-0.087466
C	3.036614	-0.954739	0.123424
O	3.455813	-2.085520	0.359815
N	3.898163	0.115148	-0.034050
C	1.533754	-0.670348	-0.002491
H	1.217943	-0.255518	0.962364
H	1.359099	0.125884	-0.733555
C	0.702092	-1.929488	-0.335094
C	3.437260	1.469984	-0.143113
C	2.913533	2.137358	0.971135
C	3.560598	2.155002	-1.359170
C	2.503176	3.467141	0.865582
H	2.835509	1.609204	1.916587
C	3.160546	3.487736	-1.458521
H	3.966839	1.633575	-2.220688
C	2.627618	4.145920	-0.347835
H	2.094739	3.974323	1.734877
H	3.259712	4.009938	-2.405828
H	2.313612	5.182513	-0.427442
C	5.374757	-0.077193	0.059257
C	5.827540	-0.496328	1.470894
C	5.927129	-1.027155	-1.018928
H	5.790279	0.918235	-0.137618

C	7.359680	-0.600909	1.547757
H	5.370747	-1.460789	1.709850
H	5.459328	0.233540	2.202512
C	7.459365	-1.121579	-0.928871
H	5.481997	-2.015757	-0.880927
H	5.624363	-0.668500	-2.010527
C	7.916055	-1.548288	0.474392
H	7.657642	-0.938108	2.547633
H	7.803042	0.396551	1.411982
H	7.830385	-1.826019	-1.682663
H	7.904445	-0.145095	-1.170712
H	9.011177	-1.578500	0.525028
H	7.562368	-2.569022	0.674268
C	0.593818	-2.170139	-1.856651
H	0.031655	-1.349028	-2.324777
H	-0.011476	-3.072062	-2.013398
C	1.928730	-2.335949	-2.593700
H	2.532478	-3.131848	-2.147984
H	1.758042	-2.583646	-3.647039
H	2.528096	-1.419127	-2.569801
H	1.250186	-2.779382	0.087760

^{1}IM4-*R*

B3LYP/BSI SCF energy: -2280.179427a.u.

M06/BSII SCF energy in solution:-2279.25604a.u.

M06/BSII free energy in solution:-2278.682229a.u.

C	-3.436957	0.184105	-0.709453
N	-2.545100	-0.734318	-0.923673
C	-3.266358	-1.993157	-1.168613
H	-2.842232	-2.493259	-2.044904
C	-4.743715	-1.541081	-1.366262
H	-5.066336	-1.484542	-2.409402
O	-4.734326	-0.169437	-0.855880
C	-5.631415	-2.444099	-0.496891
H	-6.168273	-3.162142	-1.129863
H	-6.388779	-1.854879	0.030410
C	-4.654819	-3.140907	0.427249
C	-4.935429	-3.949796	1.528687
C	-3.328973	-2.902908	0.047156
C	-3.875845	-4.511204	2.244944
H	-5.962326	-4.138666	1.830576
C	-2.268083	-3.456292	0.764066
C	-2.551094	-4.264188	1.867482
H	-4.081884	-5.140789	3.105772
H	-1.240825	-3.243630	0.485214
H	-1.736552	-4.699406	2.438629
C	-2.999009	1.517994	-0.324313
C	-3.830486	2.667623	-0.140457
C	-5.244463	2.673685	-0.293227
C	-3.175887	3.891303	0.220101
C	-1.057218	2.722307	0.156831
C	-5.962770	3.833416	-0.093548
H	-5.754346	1.759774	-0.565353
C	-3.946783	5.064515	0.419166
C	-1.764653	3.880134	0.361066
H	0.018067	2.687514	0.266053
C	-5.314921	5.037978	0.265577
H	-7.042103	3.821355	-0.213154
H	-3.436124	5.983345	0.693446
H	-1.237311	4.787384	0.637736
H	-5.899662	5.940069	0.418952
N	-1.653589	1.545143	-0.175202
Ni	-0.707632	-0.143552	-0.642630
C	1.180304	-0.223600	-0.545966
C	0.682946	-1.275178	-1.127162
Si	2.732047	0.661379	-0.050925
C	2.313539	2.018358	1.208841
C	1.623701	1.695640	2.395575
C	2.657468	3.367181	1.003138
C	1.288551	2.676801	3.329608
H	1.338446	0.665868	2.590175
C	2.323687	4.354327	1.935495
H	3.188010	3.654520	0.099431
C	1.636814	4.010588	3.100788
H	0.756155	2.400609	4.235853
H	2.601876	5.388949	1.751277
H	1.376373	4.775369	3.827879
C	3.494062	1.459314	-1.594345
C	4.795399	1.997472	-1.566954
C	2.783803	1.541559	-2.806027
C	5.361860	2.593030	-2.695431
H	5.382979	1.954210	-0.652481
C	3.344513	2.136130	-3.938463
H	1.780698	1.127657	-2.863471
C	4.635605	2.663697	-3.885710
H	6.369481	2.997383	-2.646850
H	2.774491	2.184645	-4.862711

H	5.074891	3.124069	-4.766594
C	4.036838	-0.525191	0.700967
H	4.155368	-1.340153	-0.021481
H	4.985857	0.024839	0.719101
C	3.736168	-1.071344	2.075119
C	4.237426	-0.444805	3.227006
C	2.937840	-2.215460	2.241615
C	3.951870	-0.938795	4.500581
H	4.860272	0.440168	3.122136
C	2.649998	-2.709933	3.514650
H	2.554148	-2.725082	1.362683
C	3.153597	-2.073842	4.651475
H	4.356459	-0.436306	5.375300
H	2.036199	-3.601205	3.617273
H	2.932683	-2.462182	5.641821
C	0.787388	-2.505480	-1.888656
H	0.170791	-3.303251	-1.475327
C	0.565957	-2.338142	-3.388047
H	0.651481	-3.295893	-3.905617
H	-0.437486	-1.928924	-3.553065
H	1.293091	-1.639335	-3.807465
Br	2.694975	-3.459964	-1.686633

^{3}IM4-*R*

B3LYP/BSI SCF energy:-2280.173874a.u.

M06/BSII SCF energy in solution: -2279.24171a.u.

M06/BSII free energy in solution:-2278.672092a.u.

C	-3.192391	-0.121599	-1.002177
N	-2.081739	-0.789491	-1.265178
C	-2.451473	-2.151756	-1.666854
H	-1.991031	-2.393110	-2.632338
C	-4.012104	-2.109589	-1.734226
H	-4.412271	-2.146549	-2.750880
O	-4.349695	-0.803483	-1.197178
C	-4.557321	-3.236692	-0.834574
H	-5.053355	-4.006554	-1.438653
H	-5.308705	-2.840299	-0.143404
C	-3.333662	-3.790154	-0.135513
C	-3.278561	-4.773565	0.853404
C	-2.155809	-3.214350	-0.623437
C	-2.033637	-5.176754	1.342215
H	-4.190243	-5.223432	1.238346
C	-0.910559	-3.625456	-0.147665
C	-0.855017	-4.609979	0.842072
H	-1.979400	-5.942083	2.111483
H	0.007127	-3.190450	-0.534284
H	0.110283	-4.933229	1.219344
C	-3.144351	1.231482	-0.549353
C	-4.257731	2.071474	-0.180990
C	-5.614505	1.667514	-0.219240
C	-3.957662	3.404791	0.253740
C	-1.598602	2.938868	-0.061241
C	-6.626509	2.541142	0.147560
H	-5.860928	0.664938	-0.541067
C	-5.011332	4.269132	0.621309
C	-2.588458	3.815977	0.303447
H	-0.551390	3.224619	-0.021789
C	-6.329475	3.848213	0.569773
H	-7.659757	2.207970	0.107310
H	-4.767433	5.276787	0.947925
H	-2.335946	4.819001	0.631341
H	-7.130315	4.524338	0.854940
N	-1.842615	1.678255	-0.489029
Ni	-0.466945	0.293077	-0.958830
C	1.450813	0.463882	-0.540468
C	1.291612	0.448401	-1.798882
Si	2.350450	0.592151	1.081909
C	1.158881	0.170032	2.481640
C	0.428715	-1.035046	2.458148
C	0.959645	1.034671	3.573168
C	-0.462001	-1.362362	3.480945
H	0.547121	-1.728858	1.631684
C	0.071442	0.709346	4.600888
H	1.495555	1.978324	3.619677
C	-0.641319	-0.489408	4.556373
H	-1.016347	-2.295336	3.431204
H	-0.067923	1.395599	5.431854
H	-1.336590	-0.740474	5.352843
C	2.997877	2.359248	1.257501
C	3.841975	2.697578	2.333649
C	2.685230	3.371395	0.332760
C	4.343139	3.991371	2.484938
H	4.115213	1.944787	3.070108
C	3.184743	4.667303	0.478340
H	2.052162	3.141712	-0.519843
C	4.013453	4.980584	1.556490
H	4.992058	4.225935	3.324284

H	2.929695	5.430342	-0.252049
H	4.403809	5.987977	1.670852
C	3.864287	-0.579122	1.047174
H	4.498506	-0.221926	0.227204
H	4.419096	-0.393919	1.975726
C	3.585913	-2.053680	0.892517
C	3.444813	-2.886779	2.013177
C	3.466160	-2.631681	-0.382666
C	3.196483	-4.252794	1.867714
H	3.538987	-2.461067	3.008877
C	3.214223	-3.996515	-0.530092
H	3.589762	-2.006711	-1.263202
C	3.078982	-4.814899	0.594666
H	3.104000	-4.878990	2.751086
H	3.139008	-4.424035	-1.526400
H	2.898151	-5.879857	0.479139
C	1.606102	0.475354	-3.213482
H	1.322275	-0.455828	-3.702927
C	1.108904	1.697866	-3.973712
H	1.417418	1.647630	-5.019570
H	0.014834	1.726598	-3.926112
H	1.499659	2.617572	-3.532584
Br	3.717647	0.382805	-3.480486

^{1}IM4-*S*

B3LYP/BSI SCF energy:-2280.180242a.u.

M06/BSII SCF energy in solution: -2279.25938a.u.

M06/BSII free energy in solution:-2278.682982a.u.

C	-3.116978	0.225974	0.640631
N	-1.878796	0.572815	0.469363
C	-1.753077	1.968371	0.932922
H	-0.860505	2.068625	1.553325
C	-3.084409	2.223308	1.697415
H	-3.006395	2.145267	2.785000
O	-3.930859	1.109884	1.258001
C	-3.658337	3.562471	1.213232
H	-3.496004	4.334421	1.976394
H	-4.739776	3.491761	1.055886
C	-2.876172	3.860035	-0.048572
C	-3.098605	4.868904	-0.986192
C	-1.796829	2.981725	-0.199349
C	-2.230714	4.986138	-2.074744
H	-3.935594	5.553662	-0.875579
C	-0.928598	3.096232	-1.284154
C	-1.153058	4.105771	-2.222709
H	-2.395049	5.766731	-2.812302
H	-0.096026	2.412502	-1.403916
H	-0.482296	4.204140	-3.071196
C	-3.566789	-1.073780	0.159122
C	-4.894289	-1.602616	0.240438
C	-5.992633	-0.931764	0.844939
C	-5.116585	-2.898137	-0.332288
C	-2.779920	-2.970777	-0.948777
C	-7.239142	-1.520865	0.875553
H	-5.842469	0.045915	1.281334
C	-6.410744	-3.472856	-0.284172
C	-4.016013	-3.562555	-0.934894
H	-1.924403	-3.457947	-1.399414
C	-7.454842	-2.797721	0.309037
H	-8.067333	-0.995327	1.341613
H	-6.562796	-4.454839	-0.723430
H	-4.153769	-4.540944	-1.384573
H	-8.444432	-3.243430	0.342895
N	-2.538068	-1.743915	-0.409548
Ni	-0.771816	-0.855638	-0.298165
C	1.103799	-0.649204	-0.385649
C	0.731760	-1.812235	-0.830404
Si	2.471964	0.548916	-0.052255
C	1.934739	1.682460	1.374449
C	1.530360	1.115714	2.601084
C	1.911933	3.085028	1.271195
C	1.129023	1.913404	3.674435
H	1.524652	0.036111	2.721138
C	1.509092	3.889397	2.341549
H	2.201654	3.561577	0.339200
C	1.117858	3.305361	3.547102
H	0.828321	1.448783	4.609922
H	1.499018	4.970570	2.230842
H	0.808069	3.928559	4.382021
C	2.793566	1.570429	-1.618390
C	3.790986	2.565452	-1.644917
C	2.080407	1.335902	-2.808305
C	4.053283	3.304395	-2.799751
H	4.377652	2.772158	-0.752161
C	2.339695	2.070526	-3.968400
H	1.318581	0.561567	-2.827519
C	3.324746	3.059362	-3.965610

H	4.827739	4.066802	-2.791173
H	1.777233	1.864262	-4.875232
H	3.529416	3.630433	-4.867181
C	4.145726	-0.283241	0.385738
H	4.367778	-0.953999	-0.451673
H	4.893450	0.519688	0.352579
C	4.243000	-1.022856	1.696135
C	4.605219	-0.358761	2.879348
C	3.979241	-2.400558	1.769816
C	4.691371	-1.041846	4.093165
H	4.825520	0.705186	2.845957
C	4.063052	-3.085511	2.983084
H	3.727659	-2.938091	0.859988
C	4.416251	-2.409272	4.152589
H	4.978589	-0.504138	4.993026
H	3.862423	-4.153499	3.011762
H	4.486604	-2.943155	5.096150
C	1.030351	-3.135913	-1.347370
Br	2.992255	-3.264560	-2.186800
C	0.923720	-4.261570	-0.324638
H	-0.102606	-4.298118	0.058646
H	1.169282	-5.225209	-0.775661
H	1.589855	-4.079420	0.521129
H	0.466643	-3.355285	-2.254472

^{3}IM4-*S*

B3LYP/BSI SCF energy: -2280.172168a.u.

M06/BSII SCF energy in solution: -2279.24169a.u.

M06/BSII free energy in solution: -2278.673129a.u.

C	-3.257753	0.178562	1.073928
N	-2.055569	0.637171	1.395100
C	-2.246860	1.886387	2.140745
H	-1.599927	1.899812	3.025358
C	-3.763343	1.874088	2.495617
H	-3.984866	1.540307	3.513926
O	-4.304191	0.873924	1.588553
C	-4.336716	3.260706	2.167124
H	-4.494251	3.832258	3.091042
H	-5.310918	3.172117	1.675337
C	-3.273200	3.900031	1.300063
C	-3.349893	5.088169	0.572915
C	-2.091722	3.149446	1.305762
C	-2.230485	5.518142	-0.143611
H	-4.266936	5.671802	0.560129
C	-0.970639	3.579480	0.596620
C	-1.047555	4.770542	-0.129837
H	-2.278849	6.440776	-0.715328
H	-0.050740	3.002535	0.603108
H	-0.180015	5.113357	-0.685202
C	-3.408933	-0.980214	0.256633
C	-4.639885	-1.620875	-0.139976
C	-5.931423	-1.180518	0.237766
C	-4.534167	-2.782454	-0.974504
C	-2.119686	-2.560446	-0.919642
C	-7.064795	-1.855381	-0.188871
H	-6.030898	-0.305759	0.865987
C	-5.708136	-3.446147	-1.392476
C	-3.232390	-3.233980	-1.358152
H	-1.119915	-2.881873	-1.198341
C	-6.958305	-2.992985	-1.007449
H	-8.044812	-1.497696	0.114184
H	-5.611421	-4.324708	-2.025114
H	-3.127319	-4.105642	-1.995699
H	-7.853068	-3.513607	-1.336341
N	-2.179875	-1.461872	-0.132667
Ni	-0.613969	-0.469305	0.656284
C	1.304946	-0.734033	0.116593
C	0.945102	-1.607722	0.956685
Si	2.279551	0.164732	-1.184828
C	2.535172	1.942569	-0.606666
C	2.801028	2.235402	0.744826
C	2.547790	3.009590	-1.523585
C	3.064630	3.540050	1.164532
H	2.808653	1.433488	1.478355
C	2.815086	4.316935	-1.108869
H	2.339669	2.821121	-2.573588
C	3.072053	4.584402	0.237110
H	3.267521	3.741241	2.212777
H	2.823064	5.124434	-1.836226
H	3.278546	5.600493	0.561789
C	1.281857	0.124568	-2.785739
C	1.669690	-0.670836	-3.878973
C	0.096537	0.876551	-2.909913
C	0.907414	-0.716625	-5.048579
H	2.575636	-1.268759	-3.824456
C	-0.668122	0.833878	-4.076255
H	-0.234300	1.507833	-2.088874

C	-0.263436	0.035564	-5.148564
H	1.228066	-1.339553	-5.879095
H	-1.578755	1.422143	-4.147165
H	-0.858275	0.000622	-6.057087
C	3.965964	-0.699161	-1.458489
H	3.772893	-1.770618	-1.586082
H	4.348824	-0.328450	-2.417969
C	4.994216	-0.473079	-0.374415
C	5.852251	0.636993	-0.419433
C	5.114121	-1.360078	0.706500
C	6.800848	0.853578	0.580198
H	5.776168	1.336849	-1.247900
C	6.061973	-1.143364	1.708441
H	4.467712	-2.231395	0.758217
C	6.909935	-0.036030	1.650765
H	7.457015	1.717686	0.519945
H	6.141855	-1.849223	2.531006
H	7.651024	0.129207	2.427706
C	0.920703	-2.749568	1.849551
Br	2.326425	-4.217174	1.204236
C	1.226206	-2.434316	3.308009
H	0.459986	-1.750710	3.691048
H	1.213442	-3.347262	3.906152
H	2.202459	-1.954712	3.406937
H	0.006457	-3.328138	1.731060

^{1}TS4-*R*

B3LYP/BSI SCF energy:-2280.16943a.u.

M06/BSII SCF energy in solution:-2279.252139a.u.

M06/BSII free energy in solution:-2278.681147a.u.

C	-3.350516	0.081129	-0.797120
N	-2.436434	-0.804383	-1.022122
C	-3.109181	-2.110923	-1.164816
H	-2.723293	-2.622141	-2.051531
C	-4.617787	-1.732270	-1.266836
H	-5.027345	-1.753233	-2.279378
O	-4.630848	-0.323116	-0.847636
C	-5.390864	-2.603057	-0.266163
H	-5.957549	-3.374141	-0.803052
H	-6.118490	-2.003374	0.290562
C	-4.311979	-3.213143	0.602828
C	-4.469743	-3.971967	1.762440
C	-3.033235	-2.964953	0.090290
C	-3.334773	-4.475572	2.401878
H	-5.459706	-4.169920	2.164776
C	-1.897402	-3.470049	0.724628
C	-2.057701	-4.227141	1.886901
H	-3.444557	-5.066868	3.306243
H	-0.902551	-3.280512	0.335503
H	-1.182238	-4.624486	2.390753
C	-2.955708	1.460415	-0.479438
C	-3.834631	2.566049	-0.276094
C	-5.254542	2.497578	-0.357658
C	-3.224348	3.829946	0.027174
C	-1.057447	2.767611	-0.120995
C	-6.016943	3.623638	-0.143935
H	-5.731008	1.554926	-0.587531
C	-4.044042	4.968896	0.243612
C	-1.813224	3.894181	0.099004
H	0.021748	2.784064	-0.055174
C	-5.412656	4.868128	0.160038
H	-7.098699	3.557437	-0.209146
H	-3.568443	5.917625	0.474329
H	-1.321143	4.831908	0.335545
H	-6.035563	5.741847	0.325612
N	-1.615869	1.563435	-0.403730
Ni	-0.613387	-0.111491	-0.871835
C	1.373999	0.062926	-0.654841
C	1.121005	-0.985289	-1.332556
Si	2.763728	1.019023	0.126694
C	2.040037	2.071596	1.526596
C	1.207734	1.482818	2.500883
C	2.293615	3.451694	1.634632
C	0.652609	2.240700	3.533010
H	0.990169	0.419631	2.454661
C	1.740243	4.214573	2.667077
H	2.926486	3.941808	0.899862
C	0.916944	3.610081	3.618010
H	0.017263	1.761609	4.273092
H	1.954749	5.278422	2.728465
H	0.486359	4.200214	4.422622
C	3.539456	2.139732	-1.184704
C	4.715021	2.863311	-0.902061
C	2.988231	2.272213	-2.471814
C	5.307214	3.690484	-1.857627
H	5.183180	2.781743	0.076675
C	3.576825	3.097432	-3.432344

H	2.094968	1.710578	-2.731351
C	4.736798	3.810357	-3.126448
H	6.215407	4.235265	-1.614459
H	3.133636	3.177650	-4.421347
H	5.198232	4.450030	-3.873690
C	4.099195	-0.186180	0.765738
H	4.424680	-0.767511	-0.104968
H	4.954887	0.430120	1.071262
C	3.688829	-1.108939	1.889534
C	3.788830	-0.702329	3.229799
C	3.196546	-2.395525	1.615728
C	3.404316	-1.551427	4.268655
H	4.177157	0.286756	3.461047
C	2.812512	-3.243617	2.656426
H	3.132125	-2.749428	0.588705
C	2.910937	-2.826583	3.985744
H	3.497166	-1.217516	5.298934
H	2.451553	-4.240845	2.419241
H	2.619144	-3.492099	4.793787
C	0.567585	-1.994837	-2.066690
H	0.225820	-2.884535	-1.552442
C	0.379391	-1.924973	-3.561961
H	0.791108	-2.828717	-4.016240
H	-0.687859	-1.866001	-3.814225
H	0.883407	-1.054138	-3.986128
Br	2.644224	-4.062842	-1.976298

^{1}TS4-*S*

B3LYP/BSI SCF energy:-2280.168876a.u.

M06/BSII SCF energy in solution:-2279.257219a.u.

M06/BSII free energy in solution:-2278.683853a.u.

C	-3.040078	0.123648	0.616390
N	-1.831879	0.511898	0.375667
C	-1.733759	1.922388	0.807148
H	-0.814336	2.067260	1.376957
C	-3.032065	2.139541	1.635519
H	-2.900681	2.077264	2.718219
O	-3.854938	0.978862	1.254220
C	-3.684509	3.443299	1.159189
H	-3.507065	4.235359	1.897633
H	-4.769879	3.330671	1.067766
C	-2.986623	3.741395	-0.150895
C	-3.302760	4.717499	-1.095804
C	-1.880476	2.905206	-0.343073
C	-2.501137	4.843898	-2.233091
H	-4.160117	5.370150	-0.953441
C	-1.077588	3.029140	-1.476109
C	-1.396276	4.006247	-2.421792
H	-2.738383	5.599120	-2.976890
H	-0.221096	2.381991	-1.627669
H	-0.776593	4.113589	-3.306910
C	-3.474562	-1.211203	0.176175
C	-4.800072	-1.734724	0.249660
C	-5.907464	-1.054084	0.830994
C	-5.013662	-3.040110	-0.309148
C	-2.670866	-3.119793	-0.893881
C	-7.150204	-1.645621	0.854484
H	-5.765192	-0.070813	1.256332
C	-6.309800	-3.617029	-0.268234
C	-3.911570	-3.708510	-0.891787
H	-1.810038	-3.611123	-1.327247
C	-7.357332	-2.933625	0.302909
H	-7.985610	-1.116732	1.302885
H	-6.455733	-4.604815	-0.695260
H	-4.042537	-4.690301	-1.335371
H	-8.347249	-3.378427	0.332887
N	-2.444523	-1.890596	-0.358866
Ni	-0.682142	-0.959297	-0.253881
C	1.263412	-0.387041	-0.259789
C	1.177018	-1.631573	-0.498169
Si	2.517978	0.957320	-0.002752
C	1.897109	2.051735	1.416538
C	1.595532	1.469700	2.665990
C	1.690091	3.436572	1.278175
C	1.110572	2.237765	3.726478
H	1.744870	0.404547	2.816151
C	1.205260	4.209778	2.337080
H	1.897692	3.920897	0.328734
C	0.913666	3.611940	3.564037
H	0.892298	1.764541	4.680200
H	1.055315	5.277545	2.201269
H	0.540554	4.211952	4.389841
C	2.704920	1.944678	-1.603258
C	3.538632	3.079248	-1.659183
C	2.088767	1.529347	-2.798392
C	3.729826	3.782349	-2.849588
H	4.053023	3.422084	-0.763912

C	2.278529	2.228349	-3.993036
H	1.464620	0.639836	-2.799246
C	3.095550	3.359653	-4.019670
H	4.377461	4.654714	-2.865362
H	1.797984	1.880930	-4.903506
H	3.247377	3.902220	-4.948674
C	4.223574	0.180800	0.376571
H	4.511780	-0.342710	-0.542776
H	4.923192	1.019332	0.491958
C	4.318018	-0.755206	1.557473
C	4.581351	-0.268901	2.848245
C	4.150207	-2.139701	1.386007
C	4.663279	-1.135297	3.939768
H	4.732027	0.797830	2.996932
C	4.233456	-3.004755	2.478914
H	3.974311	-2.549174	0.392768
C	4.485432	-2.508394	3.759966
H	4.875608	-0.736766	4.928595
H	4.114697	-4.072933	2.319252
H	4.556986	-3.185346	4.606924
C	0.714574	-2.900112	-0.684944
Br	3.127767	-4.038074	-2.117460
C	0.625917	-3.918090	0.426143
H	-0.385829	-4.335406	0.499692
H	1.313475	-4.737160	0.199368
H	0.898047	-3.481419	1.389029
H	0.536459	-3.230726	-1.704283

^{1}TS4'

B3LYP/BSI SCF energy: -2280.137811a.u.

M06/BSII SCF energy in solution: -2279.22138a.u.

M06/BSII free energy in solution:-2278.65125a.u.

C	2.494336	0.475976	1.340375
N	1.774289	-0.593685	1.281884
C	2.707935	-1.746961	1.183820
H	2.403496	-2.509052	1.906926
C	4.100495	-1.124124	1.473293
H	4.474632	-1.295357	2.485588
O	3.837645	0.308381	1.364997
C	5.064398	-1.593444	0.372323
H	5.744581	-2.356094	0.772750
H	5.689409	-0.766295	0.019523
C	4.153739	-2.171139	-0.690758
C	4.485717	-2.590181	-1.979692
C	2.838127	-2.289328	-0.228102
C	3.486258	-3.124180	-2.796921
H	5.505174	-2.501144	-2.346387
C	1.839309	-2.830504	-1.037871
C	2.171885	-3.244825	-2.329828
H	3.731704	-3.448849	-3.804266
H	0.817785	-2.906889	-0.676438
H	1.399165	-3.652223	-2.974743
C	1.977352	1.868003	1.403313
C	2.595460	2.950823	0.691887
C	3.723466	2.823597	-0.165095
C	1.995635	4.243295	0.846502
C	0.350487	3.235855	2.290814
C	4.236950	3.924438	-0.812865
H	4.181873	1.853271	-0.300483
C	2.554329	5.359033	0.167365
C	0.851292	4.357232	1.672361
H	-0.529987	3.290159	2.925016
C	3.653568	5.203557	-0.643465
H	5.099165	3.811706	-1.463444
H	2.092185	6.333730	0.296884
H	0.374385	5.323701	1.807373
H	4.075457	6.059931	-1.161389
N	0.905053	2.007448	2.165213
Ni	-0.108910	-0.919814	1.377478
C	-1.719494	-0.538589	0.489580
C	-1.930655	-1.368434	1.452983
Si	-2.439760	0.464361	-0.885471
C	-1.057532	1.238836	-1.914956
C	0.070384	0.477446	-2.278528
C	-1.126793	2.565301	-2.377512
C	1.083346	1.017161	-3.072817
H	0.165056	-0.546882	-1.932406
C	-0.116205	3.109791	-3.173522
H	-1.975748	3.187466	-2.106635
C	0.991469	2.336052	-3.523093
H	1.941315	0.405086	-3.338365
H	-0.192369	4.138463	-3.516312
H	1.779423	2.758932	-4.140793
C	-3.558043	1.813228	-0.161311
C	-3.492924	2.153101	1.202711
C	-4.483014	2.511604	-0.961500
C	-4.310608	3.147901	1.742855

H	-2.796588	1.624703	1.848061
C	-5.301888	3.508772	-0.427624
H	-4.572879	2.278330	-2.020280
C	-5.216719	3.829458	0.928412
H	-4.243641	3.388635	2.800875
H	-6.007804	4.031009	-1.068027
H	-5.855064	4.602473	1.347714
C	-3.541350	-0.650668	-1.997424
H	-4.345791	-1.027929	-1.354292
H	-4.016623	-0.001330	-2.742984
C	-2.835028	-1.793967	-2.681438
C	-2.286696	-1.644086	-3.965212
C	-2.695028	-3.039773	-2.048063
C	-1.628038	-2.700346	-4.595743
H	-2.380691	-0.689051	-4.475492
C	-2.036249	-4.098261	-2.674735
H	-3.114924	-3.179870	-1.055607
C	-1.499871	-3.934361	-3.954499
H	-1.220152	-2.559609	-5.593167
H	-1.951016	-5.054993	-2.166309
H	-1.000158	-4.762125	-4.450172
C	-2.424608	-2.269910	2.419577
H	-2.682967	-3.259281	2.045343
C	-3.341226	-1.745149	3.501433
H	-4.288493	-1.452794	3.028056
H	-3.543024	-2.506440	4.257087
H	-2.913695	-0.863670	3.982625
Br	-0.601070	-3.050593	3.594844

^{1}IM5-R^{+}

B3LYP/BSI SCF energy:-2266.610163a.u.

M06/BSII SCF energy in solution: -2265.73947a.u.

M06/BSII free energy in solution:-2265.162227a.u.

C	-3.085489	0.627449	-0.647894
N	-2.503245	-0.455225	-1.055227
C	-3.565705	-1.431587	-1.385481
H	-3.338514	-1.914737	-2.339215
C	-4.848723	-0.550915	-1.429258
H	-5.163338	-0.239562	-2.427458
O	-4.411896	0.681802	-0.739894
C	-5.936029	-1.262395	-0.618208
H	-6.661284	-1.723979	-1.299523
H	-6.491470	-0.552584	0.002906
C	-5.175562	-2.305182	0.172364
C	-5.651396	-3.121569	1.198162
C	-3.850644	-2.420838	-0.266031
C	-4.786936	-4.050527	1.780964
H	-6.678738	-3.038249	1.541155
C	-2.986157	-3.350100	0.313613
C	-3.462890	-4.164383	1.342689
H	-5.145579	-4.690534	2.581194
H	-1.956101	-3.440620	-0.016221
H	-2.801974	-4.891071	1.804715
C	-2.266362	1.705455	-0.073461
C	-2.740358	2.956370	0.409645
C	-4.098902	3.382992	0.359714
C	-1.760193	3.841283	0.981122
C	-0.061930	2.183348	0.512496
C	-4.451618	4.617213	0.853457
H	-4.851110	2.735855	-0.068445
C	-2.164983	5.106498	1.483604
C	-0.417868	3.410646	1.024554
H	0.958254	1.834448	0.552217
C	-3.483816	5.485819	1.420322
H	-5.488757	4.934049	0.808929
H	-1.415371	5.763143	1.914220
H	0.345919	4.044132	1.463313
H	-3.792158	6.453415	1.803336
N	-0.969979	1.339270	-0.035595
Ni	-0.597033	-0.376143	-0.960748
C	1.483975	-0.550560	-0.932827
C	0.928425	-1.458418	-1.609910
Si	3.114973	0.086001	-0.263032
C	2.870886	0.462678	1.568983
C	2.163600	-0.431013	2.399326
C	3.407497	1.623446	2.158701
C	1.999270	-0.173639	3.760967
H	1.743155	-1.342145	1.981996
C	3.246674	1.881697	3.522116
H	3.954572	2.337299	1.548607
C	2.541040	0.984111	4.324890
H	1.453732	-0.877781	4.382777
H	3.673986	2.781124	3.956395
H	2.416163	1.183109	5.385344
C	3.596207	1.628747	-1.228410
C	4.888852	2.173084	-1.086344
C	2.712993	2.266254	-2.119304

C	5.276841	3.311762	-1.793632
H	5.610470	1.704768	-0.420561
C	3.097720	3.404420	-2.830466
H	1.714976	1.862797	-2.271714
C	4.379951	3.930755	-2.666591
H	6.278924	3.711255	-1.668204
H	2.400042	3.876278	-3.516731
H	4.681908	4.814442	-3.220971
C	4.423226	-1.273861	-0.562144
H	4.593361	-1.308734	-1.644548
H	5.353753	-0.900381	-0.115190
C	4.099800	-2.649855	-0.031346
C	4.335795	-2.984956	1.311394
C	3.552492	-3.630782	-0.873129
C	4.026684	-4.255832	1.797670
H	4.774871	-2.247434	1.977809
C	3.242375	-4.902753	-0.388471
H	3.392435	-3.402547	-1.924270
C	3.475260	-5.219638	0.950961
H	4.227383	-4.496082	2.837886
H	2.834475	-5.651112	-1.062393
H	3.244650	-6.211693	1.327517
C	-0.208179	-2.029750	-2.150481
H	-0.569777	-2.940116	-1.670777
C	-0.533884	-1.903876	-3.627157
H	-0.066407	-2.720028	-4.191031
H	-1.612462	-1.973145	-3.797221
H	-0.176599	-0.957905	-4.040542

^{1}IM5-S^+

B3LYP/BSI SCF energy: -2266.608998a.u.

M06/BSII SCF energy in solution:-2265.740887a.u.

M06/BSII free energy in solution:-2265.160006a.u.

C	-2.600130	0.302529	0.648924
N	-1.350973	0.391017	0.322798
C	-0.772646	1.502629	1.117276
H	0.189062	1.195667	1.527109
C	-1.856080	1.765296	2.199845
H	-1.665561	1.295728	3.166817
O	-3.039176	1.072568	1.640180
C	-2.103194	3.275338	2.265619
H	-1.609440	3.687869	3.154106
H	-3.170554	3.498234	2.363274
C	-1.477626	3.798856	0.990857
C	-1.557596	5.084578	0.456892
C	-0.712097	2.815046	0.352925
C	-0.864335	5.372513	-0.721240
H	-2.148566	5.853164	0.947161
C	-0.015063	3.100789	-0.820581
C	-0.097018	4.388668	-1.354500
H	-0.919456	6.369771	-1.147167
H	0.586338	2.344887	-1.313008
H	0.444692	4.626434	-2.264759
C	-3.480090	-0.600717	-0.111877
C	-4.887649	-0.738414	0.047332
C	-5.656238	-0.080719	1.050251
C	-5.563022	-1.607155	-0.879343
C	-3.432171	-2.066408	-1.923318
C	-7.015290	-0.283169	1.119348
H	-5.168548	0.574065	1.757990
C	-6.966978	-1.787636	-0.778073
C	-4.793564	-2.250306	-1.873156
H	-2.827885	-2.553116	-2.674990
C	-7.677972	-1.138161	0.202670
H	-7.591836	0.219787	1.889119
H	-7.464085	-2.444688	-1.484970
H	-5.274275	-2.895805	-2.601020
H	-8.751576	-1.277293	0.280308
N	-2.774741	-1.262541	-1.047552
Ni	-0.832991	-0.979985	-0.941822
C	1.270803	-0.888638	-0.980202
C	0.798450	-1.817885	-1.690514
Si	2.877283	-0.146857	-0.348769
C	2.609160	0.467762	1.413244
C	2.141359	-0.419358	2.406328
C	2.848794	1.803711	1.787449
C	1.922012	0.012230	3.715773
H	1.951611	-1.459974	2.159987
C	2.631217	2.237820	3.097788
H	3.199797	2.519195	1.049988
C	2.166985	1.343597	4.063980
H	1.569724	-0.691306	4.464963
H	2.826819	3.272999	3.362500
H	2.004453	1.679078	5.084378
C	3.409218	1.220141	-1.528861
C	4.571031	1.970487	-1.256503
C	2.736462	1.473417	-2.738620

C	5.028194	2.945137	-2.144397
H	5.133643	1.796098	-0.342041
C	3.191238	2.447093	-3.630630
H	1.850709	0.897451	-2.994567
C	4.336191	3.187640	-3.332639
H	5.925277	3.511135	-1.911196
H	2.656692	2.621461	-4.560190
H	4.692740	3.943757	-4.025845
C	4.200395	-1.526387	-0.440762
H	4.324286	-1.746741	-1.507961
H	5.135602	-1.049735	-0.119164
C	3.965961	-2.798674	0.336957
C	4.377991	-2.917576	1.673819
C	3.338743	-3.902696	-0.262212
C	4.158571	-4.094489	2.391148
H	4.884287	-2.083676	2.152822
C	3.117932	-5.080882	0.453214
H	3.046897	-3.846331	-1.308116
C	3.523232	-5.180237	1.785514
H	4.495110	-4.166298	3.421471
H	2.645773	-5.928357	-0.036161
H	3.361530	-6.099453	2.340389
C	-0.262670	-2.571559	-2.150968
C	-0.517248	-3.971373	-1.619059
H	-1.582169	-4.219800	-1.649292
H	0.004465	-4.711157	-2.237903
H	-0.162274	-4.078792	-0.591909
H	-0.569672	-2.395586	-3.184700

Br^-

B3LYP/BSI SCF energy: -13.471995a.u.

M06/BSII SCF energy in solution:-13.51096a.u.

M06/BSII free energy in solution:-13.527136a.u.

Br	0.000000	0.000000	0.000000

^{1}IM6-*R*

B3LYP/BSI SCF energy: -2280.204947a.u.

M06/BSII SCF energy in solution:-2279.275656a.u.

M06/BSII free energy in solution:-2278.703079a.u.

C	-3.351572	0.601099	-0.130707
N	-3.085950	-0.575467	-0.575476
C	-4.102164	-1.500932	-0.043652
H	-4.475445	-2.121768	-0.861281
C	-5.159657	-0.546394	0.587964
H	-6.064005	-0.405611	-0.008169
O	-4.470839	0.755491	0.596485
C	-5.430144	-1.024055	2.022708
H	-6.418168	-1.498425	2.077179
H	-5.445140	-0.178709	2.718757
C	-4.323054	-2.020377	2.295954
C	-4.008650	-2.650176	3.500233
C	-3.597127	-2.314418	1.135909
C	-2.960737	-3.573667	3.527098
H	-4.567956	-2.428244	4.405406
C	-2.553976	-3.241299	1.154472
C	-2.240531	-3.868487	2.363232
H	-2.705683	-4.070454	4.458945
H	-2.004727	-3.465487	0.245277
H	-1.432793	-4.593646	2.397510
C	-2.416052	1.696778	-0.419720
C	-2.569053	3.052197	-0.001666
C	-3.688132	3.552650	0.725389
C	-1.512374	3.960915	-0.341604
C	-0.376526	2.136900	-1.444388
C	-3.739830	4.877701	1.092197
H	-4.496875	2.885507	0.987032
C	-1.596818	5.320427	0.060679
C	-0.412762	3.458777	-1.069763
H	0.471201	1.732052	-1.973844
C	-2.688902	5.769866	0.762998
H	-4.598998	5.246178	1.644418
H	-0.782542	5.990548	-0.198056
H	0.420098	4.106596	-1.323038
H	-2.752119	6.810025	1.068219
N	-1.357866	1.253345	-1.126612
Ni	-1.480411	-0.681726	-1.732092
C	2.153918	-0.109590	-1.072315
C	1.272564	-0.442126	-1.859741
Si	3.339799	0.526352	0.148725
C	2.852423	-0.056240	1.876318
C	1.689517	-0.819435	2.082880
C	3.638742	0.257195	3.002044
C	1.321605	-1.248216	3.360216
H	1.070404	-1.086161	1.230721
C	3.275344	-0.167092	4.281319
H	4.548143	0.843644	2.885370

C	2.113603	-0.921221	4.462027
H	0.418767	-1.839184	3.490613
H	3.898063	0.087615	5.134872
H	1.830278	-1.254246	5.456946
C	3.287842	2.424818	0.051140
C	2.935897	3.234282	1.145313
C	3.588704	3.070166	-1.164747
C	2.888806	4.626942	1.034635
H	2.692468	2.772027	2.097919
C	3.542742	4.460287	-1.283788
H	3.856686	2.479149	-2.038117
C	3.192517	5.243935	-0.180017
H	2.617661	5.228929	1.898132
H	3.785699	4.932294	-2.232300
H	3.164324	6.327048	-0.266361
C	5.120554	-0.024031	-0.274436
H	5.376696	0.433748	-1.237837
H	5.790058	0.428182	0.467948
C	5.322801	-1.519357	-0.329636
C	5.748767	-2.233535	0.800586
C	5.068712	-2.237523	-1.508518
C	5.922401	-3.617284	0.753471
H	5.945407	-1.698385	1.726146
C	5.241409	-3.620866	-1.558172
H	4.730677	-1.705059	-2.393512
C	5.670393	-4.317928	-0.427057
H	6.257073	-4.147459	1.641154
H	5.040157	-4.154361	-2.483168
H	5.806976	-5.394896	-0.465752
C	0.204629	-0.821412	-2.743919
H	0.277068	-1.896141	-2.928031
C	0.157469	-0.090608	-4.096472
H	1.098919	-0.210927	-4.649465
H	-0.647548	-0.511066	-4.705070
H	-0.026257	0.984512	-3.997158
Br	-2.228875	-2.749985	-2.670943

[1]IM6-*S*

B3LYP/BSI SCF energy: -2280.203038a.u.

M06/BSII SCF energy in solution:-2279.27854a.u.

M06/BSII free energy in solution:-2278.705308a.u.

C	3.059720	0.920267	-0.350303
N	1.897242	0.351057	-0.345051
C	0.908476	1.411943	-0.048419
H	0.019183	1.281250	-0.665007
O	3.094954	2.258372	-0.274998
C	4.275094	0.096780	-0.354020
C	5.613804	0.567070	-0.503862
C	5.975942	1.926105	-0.725126
C	6.652354	-0.421101	-0.433411
C	4.953774	-2.116573	-0.121442
C	7.299959	2.276982	-0.858452
H	5.203388	2.680157	-0.784711
C	8.008025	-0.019829	-0.571825
C	6.280603	-1.770421	-0.231947
H	4.619762	-3.137881	0.022495
C	8.324811	1.301468	-0.779327
H	7.564433	3.316436	-1.027074
H	8.784900	-0.776572	-0.513544
H	7.044607	-2.538852	-0.166190
H	9.362400	1.603285	-0.885854
N	3.961919	-1.194133	-0.176553
Ni	1.909426	-1.580865	-0.388162
C	1.694792	2.720273	-0.315484
H	1.542332	3.160358	-1.303862
C	-1.936852	-0.390106	-0.579342
C	-0.949479	-1.053377	-0.881755
Si	-3.421749	0.597570	-0.210307
C	-4.773839	0.200742	-1.466877
C	-5.878572	1.059247	-1.626141
C	-4.740443	-0.975212	-2.236679
C	-6.910071	0.754750	-2.515538
H	-5.931949	1.985358	-1.057672
C	-5.769273	-1.283898	-3.128880
H	-3.897012	-1.652987	-2.137328
C	-6.856474	-0.419853	-3.269236
H	-7.751988	1.433562	-2.623474
H	-5.721492	-2.198377	-3.713971
H	-7.657405	-0.658603	-3.963864
C	-3.003251	2.446846	-0.343629
C	-2.730195	3.238432	0.786694
C	-2.933634	3.070268	-1.605245
C	-2.404463	4.592491	0.666180
H	-2.770118	2.800336	1.780201
C	-2.602878	4.420190	-1.733959
H	-3.153993	2.494723	-2.500919
C	-2.338522	5.186446	-0.595874

H	-2.209724	5.182725	1.557877
H	-2.560803	4.876513	-2.719498
H	-2.093089	6.240892	-0.691929
C	-4.028787	0.238156	1.565484
H	-3.217781	0.503186	2.254107
H	-4.857639	0.926901	1.771630
C	-4.461794	-1.190496	1.797034
C	-5.790734	-1.586479	1.580586
C	-3.541805	-2.164400	2.215153
C	-6.187724	-2.908979	1.780963
H	-6.519311	-0.850015	1.251133
C	-3.935629	-3.487853	2.414857
H	-2.506499	-1.881440	2.385349
C	-5.261975	-3.866356	2.199392
H	-7.223386	-3.190566	1.610196
H	-3.203804	-4.222527	2.739272
H	-5.570599	-4.895979	2.356380
C	0.173316	-1.851102	-1.288718
C	0.518694	-1.678162	-2.782427
H	1.331755	-2.353027	-3.066405
H	-0.347738	-1.913034	-3.415738
H	0.825337	-0.652306	-3.014359
H	-0.059739	-2.897634	-1.081472
C	0.587330	1.496440	1.435922
C	0.073887	0.499869	2.266499
C	0.899179	2.764679	1.940351
C	-0.129860	0.793956	3.617929
H	-0.158977	-0.481614	1.867852
C	0.691169	3.056505	3.288060
C	0.174460	2.062965	4.123901
H	-0.522544	0.028666	4.280878
H	0.931587	4.038759	3.686524
H	0.013328	2.275533	5.176926
C	1.417054	3.676222	0.848954
H	0.651036	4.400776	0.545498
H	2.313621	4.240755	1.124909
Br	2.111360	-3.914438	0.043012

^{1}IM6-*S*'

B3LYP/BSI SCF energy: -2280.205391a.u.

M06/BSII SCF energy in solution: -2279.281172a.u.

M06/BSII free energy in solution: -2278.705301a.u.

C	2.628211	0.128116	0.392692
N	1.600769	-0.582254	0.058438
C	1.835808	-1.951961	0.560254
H	0.917184	-2.345250	0.996318
O	3.533270	-0.439503	1.200987
C	2.780068	1.477164	-0.168473
C	3.793069	2.424038	0.163640
C	4.811824	2.212510	1.135599
C	3.758732	3.674500	-0.540571
C	1.798100	2.899615	-1.728479
C	5.746024	3.192134	1.382894
H	4.846697	1.276404	1.675803
C	4.742061	4.660387	-0.259313
C	2.736203	3.878741	-1.495413
H	0.995817	3.007572	-2.449853
C	5.715182	4.423623	0.681974
H	6.518806	3.020466	2.126000
H	4.707377	5.601493	-0.800296
H	2.689615	4.811639	-2.048550
H	6.464347	5.180464	0.894072
N	1.821596	1.712207	-1.076362
Ni	0.334039	0.259341	-1.110759
C	2.984994	-1.756842	1.586171
H	2.658099	-1.664146	2.622880
C	-1.127433	-0.890977	-0.633263
C	-1.418142	-1.948955	-1.332192
Si	-2.103743	-0.544986	0.947951
C	-2.342471	1.285335	1.361480
C	-2.687873	1.667717	2.673670
C	-2.287236	2.296019	0.384094
C	-2.951242	2.998723	3.000288
H	-2.750393	0.917386	3.458389
C	-2.547516	3.630517	0.707804
H	-2.047814	2.043292	-0.643702
C	-2.877265	3.986260	2.015863
H	-3.214959	3.264163	4.020902
H	-2.499941	4.389333	-0.068878
H	-3.082361	5.023796	2.266653
C	-1.181461	-1.351832	2.415440
C	-1.328359	-2.728750	2.677613
C	-0.313277	-0.628627	3.255619
C	-0.643779	-3.354696	3.721927
H	-1.989251	-3.328194	2.055953
C	0.370262	-1.245315	4.308162

H	-0.183659	0.438742	3.098200
C	0.208847	-2.612723	4.542970
H	-0.782252	-4.417869	3.900270
H	1.019528	-0.655533	4.950988
H	0.733482	-3.093897	5.364128
C	-3.817940	-1.409757	0.844987
H	-3.669261	-2.336420	0.276595
H	-4.100774	-1.700687	1.863483
C	-4.920216	-0.584530	0.224389
C	-5.904321	0.015650	1.023916
C	-4.985437	-0.382953	-1.163595
C	-6.921134	0.787296	0.459652
H	-5.873645	-0.126692	2.101641
C	-6.000563	0.387883	-1.730469
H	-4.229583	-0.829975	-1.801965
C	-6.974729	0.976991	-0.921808
H	-7.672718	1.239174	1.101806
H	-6.028336	0.527870	-2.807742
H	-7.765911	1.576396	-1.363431
C	-1.727371	-3.014482	-2.053825
C	-2.649170	-3.009383	-3.250994
H	-2.144783	-3.425810	-4.132207
H	-3.542130	-3.623708	-3.074933
H	-2.968358	-1.994336	-3.497548
H	-1.280819	-3.973681	-1.785403
C	2.454200	-2.869020	-0.486378
C	1.948584	-3.219398	-1.738764
C	3.690638	-3.359660	-0.047717
C	2.699822	-4.076992	-2.546788
H	0.993596	-2.833468	-2.080326
C	4.435480	-4.218238	-0.855411
C	3.932256	-4.573848	-2.109020
H	2.322648	-4.356351	-3.526150
H	5.395578	-4.601586	-0.519725
H	4.504641	-5.238068	-2.750314
C	4.025319	-2.853355	1.338831
H	3.912599	-3.641631	2.094319
H	5.043663	-2.462464	1.434342
Br	-0.827218	1.158304	-2.982541

2Br$^-$

B3LYP/BSI SCF energy: -1046.39825a.u.

M06/BSII SCF energy in solution: -1046.04565a.u.

M06/BSII free energy in solution:-1045.724682a.u.

C	0.808431	-0.194405	-0.388216
O	0.034401	0.765821	-0.284085
N	2.171689	0.009738	-0.315732
C	0.288541	-1.609843	-0.622163
H	1.016062	-2.165150	-1.235817
H	0.280709	-2.110834	0.357332
C	-1.136428	-1.619014	-1.191292
H	-1.093042	-1.271117	-2.235104
C	-1.715811	-3.036507	-1.172663
H	-1.042718	-3.748326	-1.689998
H	-1.779010	-3.390335	-0.133460
C	-3.103300	-3.135876	-1.816071
H	-3.078209	-2.799482	-2.859918
H	-3.482105	-4.165719	-1.805911
H	-3.824351	-2.502618	-1.288066
Zn	-2.123874	-0.190525	-0.136454
Br	-3.710288	1.518149	-0.905803
C	3.096594	-1.077926	-0.198849
C	4.044626	-1.301461	-1.206368
C	3.105201	-1.888283	0.943945
C	4.984919	-2.323132	-1.074141
H	4.028490	-0.675285	-2.093516
C	4.038252	-2.918732	1.065682
H	2.377225	-1.705194	1.728032
C	4.982377	-3.137453	0.060657
H	5.712856	-2.489723	-1.863636
H	4.030611	-3.545359	1.953144
H	5.710704	-3.937523	0.160050
C	2.731741	1.380189	-0.143675
C	2.373673	2.324498	-1.305656
C	2.378723	1.999285	1.222685
H	3.818945	1.233235	-0.167043
C	3.053551	3.691053	-1.123313
H	1.288682	2.449097	-1.341479
H	2.681369	1.867599	-2.254713
C	3.051521	3.371483	1.390176
H	1.292316	2.097960	1.294494
H	2.696740	1.318919	2.021919
C	2.698830	4.319060	0.233517
H	2.761648	4.360497	-1.941618
H	4.146238	3.573985	-1.191157
H	2.755182	3.812772	2.349274
H	4.144402	3.244226	1.429500

H	3.216597	5.279157	0.355727
H	1.622227	4.533894	0.259675
Br	-2.150598	-0.626756	2.355037

^{1}TS5-*SS*

B3LYP/BSI SCF energy: -3313.066886a.u.

M06/BSII SCF energy in solution:-3311.78532a.u.

M06/BSII free energy in solution:-3310.860798a.u.

C	-4.355823	-1.155166	0.334126
O	-3.759482	-0.803705	-0.713312
N	-5.696578	-1.348693	0.332020
C	-3.548515	-1.411280	1.596513
H	-4.190535	-1.310538	2.475352
H	-3.267201	-2.471105	1.540977
C	-2.254773	-0.556015	1.739266
Zn	-1.664908	-1.097309	-0.348899
Br	-1.343538	-3.503870	-0.339909
C	-6.381736	-1.890022	1.480169
C	-7.186124	-1.056907	2.265105
C	-6.288892	-3.254639	1.773606
C	-7.889504	-1.588329	3.346570
H	-7.249547	0.000692	2.027358
C	-6.990711	-3.779207	2.860104
H	-5.665385	-3.893394	1.155694
C	-7.791757	-2.949018	3.646370
H	-8.509996	-0.938524	3.956551
H	-6.911625	-4.837732	3.088607
H	-8.337805	-3.360278	4.490029
C	-6.515301	-1.209061	-0.914977
C	-6.487023	0.211840	-1.505079
C	-6.167411	-2.274634	-1.970083
H	-7.539633	-1.399146	-0.575299
C	-7.436668	0.307802	-2.711690
H	-5.467392	0.448638	-1.820772
H	-6.774339	0.935574	-0.731429
C	-7.108633	-2.161209	-3.181333
H	-5.129272	-2.141219	-2.287512
H	-6.245034	-3.271702	-1.521281
C	-7.097827	-0.745632	-3.777375
H	-7.386272	1.315729	-3.140150
H	-8.473919	0.164269	-2.375551
H	-6.818558	-2.897201	-3.939375
H	-8.133583	-2.416585	-2.874867
H	-7.805645	-0.679986	-4.611991
H	-6.102188	-0.534440	-4.190544
C	0.430293	3.505367	0.706429
N	0.980836	2.336744	0.700667
C	2.442161	2.565285	0.713480
H	2.943467	1.807597	1.316957
O	1.228701	4.561010	0.924883
C	-0.998963	3.650456	0.372307
C	-1.701880	4.884524	0.218992
C	-1.166044	6.169448	0.518311
C	-3.048765	4.798018	-0.270862
C	-2.818113	2.392283	-0.345923
C	-1.930577	7.299164	0.336078
H	-0.155136	6.251585	0.891597
C	-3.804415	5.987052	-0.452568
C	-3.575853	3.519585	-0.563760
H	-3.192149	1.399074	-0.561319
C	-3.256743	7.211834	-0.154939
H	-1.511452	8.272768	0.571019
H	-4.819955	5.907483	-0.829319
H	-4.581143	3.425087	-0.962140
H	-3.838456	8.118035	-0.294374
N	-1.551871	2.457804	0.129989
Ni	-0.302026	0.813938	0.702637
C	2.566832	4.014922	1.239720
H	2.695140	4.115528	2.320775
C	-2.565515	0.727732	2.545563
H	-3.346420	1.310959	2.040464
H	-1.688757	1.387352	2.579464
C	-2.993573	0.485739	4.006618
H	-2.233794	-0.088191	4.548677
H	-3.127507	1.439404	4.530172
H	-3.937957	-0.061319	4.087826
H	-1.565069	-1.167370	2.324401
C	3.359067	-0.831995	0.645485
C	2.212134	-0.664714	1.046614
Si	5.095332	-1.164559	0.186805
C	5.701874	-2.684804	1.128762
C	7.078573	-2.936955	1.281646
C	4.799955	-3.628925	1.650888
C	7.537138	-4.085327	1.929122
H	7.806011	-2.223328	0.900709
C	5.253725	-4.779391	2.298835
H	3.731573	-3.460202	1.548726

C	6.623252	-5.009809	2.439293
H	8.604900	-4.257518	2.037309
H	4.537393	-5.495585	2.692262
H	6.977466	-5.904701	2.944181
C	6.153011	0.332124	0.686938
C	6.458559	1.363971	-0.219330
C	6.623588	0.467681	2.007670
C	7.198667	2.482359	0.173456
H	6.112194	1.305608	-1.247367
C	7.361526	1.583157	2.407576
H	6.418772	-0.315926	2.732660
C	7.651426	2.595164	1.489382
H	7.423355	3.261298	-0.550429
H	7.715466	1.659691	3.432473
H	8.232818	3.461015	1.795738
C	5.238075	-1.438662	-1.696811
H	4.839510	-0.545821	-2.193046
H	6.306122	-1.485693	-1.943146
C	4.530509	-2.680114	-2.193132
C	5.247699	-3.854848	-2.464034
C	3.137628	-2.697531	-2.371142
C	4.597100	-5.008480	-2.904507
H	6.326757	-3.863837	-2.328631
C	2.483782	-3.850771	-2.806865
H	2.552746	-1.807493	-2.157866
C	3.212152	-5.011383	-3.077461
H	5.175107	-5.905669	-3.110858
H	1.404111	-3.838167	-2.923588
H	2.703648	-5.909356	-3.417168
C	0.901816	-0.499125	1.616138
C	0.995497	-0.097203	3.104915
H	0.006577	-0.037178	3.567850
H	1.583373	-0.828059	3.675651
H	1.482364	0.876639	3.229127
H	0.377405	-1.456061	1.518970
C	3.014360	2.674567	-0.695811
C	2.913525	1.761244	-1.744403
C	3.673058	3.898455	-0.867251
C	3.500325	2.086342	-2.971368
H	2.372059	0.831221	-1.618784
C	4.263293	4.217219	-2.089292
C	4.174843	3.300935	-3.140917
H	3.419869	1.391520	-3.801980
H	4.774338	5.166471	-2.228021
H	4.621747	3.539557	-4.101889
C	3.634783	4.720093	0.402425
H	4.594300	4.677064	0.934473
H	3.394049	5.776724	0.247144
Br	-0.530535	0.083038	-2.175042

^{1}TS5-*SS*'

B3LYP/BSI SCF energy: -3313.064792a.u.

M06/BSII SCF energy in solution: -3311.783843a.u.

M06/BSII free energy in solution: -3310.857277a.u.

C	-3.652151	-0.555798	0.132304
O	-3.231723	0.214884	-0.767199
N	-4.977030	-0.789544	0.277287
C	-2.649760	-1.260595	1.030790
H	-3.116278	-1.499767	1.990201
H	-2.447439	-2.223505	0.545929
C	-1.308240	-0.501138	1.252110
Zn	-1.155458	-0.300320	-1.011857
Br	-1.435055	-2.479778	-2.082309
C	-5.466696	-1.778644	1.206511
C	-6.113130	-1.369379	2.377745
C	-5.345215	-3.140279	0.909986
C	-6.630557	-2.323118	3.254875
H	-6.199678	-0.309286	2.596585
C	-5.859987	-4.089138	1.794753
H	-4.843266	-3.446978	-0.002577
C	-6.503498	-3.683608	2.965462
H	-7.128420	-2.002865	4.165330
H	-5.758409	-5.145547	1.565319
H	-6.904122	-4.424721	3.650606
C	-5.993314	-0.204975	-0.655605
C	-6.032644	1.332965	-0.625740
C	-5.854341	-0.749306	-2.089058
H	-6.948727	-0.561603	-0.254595
C	-7.167398	1.855915	-1.523280
H	-5.074828	1.722624	-0.980950
H	-6.169862	1.676847	0.407328
C	-6.979895	-0.205280	-2.984776
H	-4.879137	-0.460694	-2.491305
H	-5.883676	-1.844572	-2.067358
C	-7.033952	1.329309	-2.960456
H	-7.167939	2.952363	-1.514699

H	-8.137020	1.541695	-1.110408	H	1.179657	-4.558769	-0.603700
H	-6.837192	-0.566370	-4.009322	C	0.392084	-4.561809	3.187978
H	-7.946170	-0.605831	-2.644761	H	1.469465	-2.710550	3.277296
H	-7.867973	1.689844	-3.574031	C	-0.063305	-5.603668	2.376291
H	-6.115109	1.730963	-3.409081	H	-0.124846	-6.394817	0.371354
C	1.534991	3.568251	0.781046	H	0.173320	-4.564230	4.252885
N	1.919408	2.365505	0.523173	H	-0.638018	-6.420000	2.806169
C	3.394144	2.381633	0.493342	C	4.239072	-2.174905	1.242923
H	3.772241	1.492018	0.999470	C	5.229143	-1.268605	0.811621
O	2.486105	4.465853	1.087494	C	4.621284	-3.141735	2.188252
C	0.106599	3.926218	0.700731	C	6.534318	-1.320360	1.302712
C	-0.425201	5.249764	0.794330	H	4.986589	-0.514292	0.065236
C	0.338690	6.419065	1.073933	C	5.925780	-3.198705	2.687401
C	-1.838299	5.389401	0.584562	H	3.891795	-3.865590	2.539573
C	-1.972731	3.000619	0.243239	C	6.886019	-2.288036	2.247316
C	-0.274079	7.649357	1.142221	H	7.277623	-0.612230	0.944891
H	1.403881	6.334874	1.233687	H	6.191622	-3.959682	3.416610
C	-2.435164	6.676363	0.660220	H	7.901703	-2.333811	2.631128
C	-2.589723	4.228637	0.296391	C	2.553652	-2.004357	-1.346374
H	-2.521137	2.098808	0.003679	H	1.559880	-1.737609	-1.719959
C	-1.669006	7.783541	0.933909	H	3.198314	-1.143742	-1.570309
H	0.320753	8.531767	1.357603	C	3.069880	-3.218371	-2.093263
H	-3.504988	6.765573	0.495504	C	4.405876	-3.639365	-1.986864
H	-3.656322	4.304578	0.109475	C	2.217133	-3.938789	-2.946378
H	-2.128817	8.765603	0.990323	C	4.868925	-4.747607	-2.697487
N	-0.643885	2.848398	0.456600	H	5.090540	-3.093140	-1.345282
Ni	0.496263	0.964790	0.514813	C	2.680158	-5.049112	-3.655196
C	3.750476	3.714174	1.199497	H	1.183782	-3.619790	-3.053907
H	3.960638	3.629902	2.268629	C	4.007938	-5.461245	-3.533200
C	-1.468929	0.472877	2.447612	H	5.907675	-5.052073	-2.597688
H	-2.288891	1.176618	2.252653	H	1.999353	-5.587443	-4.309516
H	-0.573490	1.093454	2.576221	H	4.369450	-6.323712	-4.086507
C	-1.711415	-0.217775	3.803867	C	2.236949	0.227275	3.709096
H	-0.917105	-0.940477	4.017434	C	3.428916	1.005490	4.212845
H	-1.721483	0.521717	4.612886	H	3.128914	1.955440	4.677752
H	-2.664927	-0.753546	3.846077	H	3.972398	0.438784	4.979426
H	-0.588669	-1.269679	1.530819	H	4.135796	1.223269	3.407548
C	1.747318	-0.416504	1.207340	H	1.530804	-0.116162	4.466819
C	2.003135	-0.096015	2.441345	C	3.972480	2.566302	-0.903403
Si	2.465233	-2.050299	0.558177	C	3.757137	1.789719	-2.041558
C	1.436239	-3.481953	1.254732	C	4.800659	3.694740	-0.951035
C	0.968258	-4.543010	0.459116	C	4.406904	2.142555	-3.227167
C	1.128010	-3.515154	2.630725	H	3.066822	0.954387	-2.024778
C	0.225978	-5.590212	1.011863	C	5.448957	4.044344	-2.134750

C	5.250732	3.257357	-3.271931
H	4.242878	1.550667	-4.122327
H	6.091771	4.919790	-2.177399
H	5.746170	3.520935	-4.201941
C	4.859606	4.393029	0.390579
H	5.824300	4.236303	0.890753
H	4.703922	5.475375	0.332581
Br	-0.042956	1.282066	-2.504062

^{1}TS5-*RS*

B3LYP/BSI SCF energy: -3313.063365a.u.

M06/BSII SCF energy in solution:-3311.78278a.u.

M06/BSII free energy in solution:-3310.857125a.u.

C	4.381754	-0.664327	-0.253926
O	3.726259	-0.455382	0.794572
N	5.627274	-1.190931	-0.203353
C	3.764344	-0.311847	-1.597169
H	4.554134	0.085215	-2.245033
H	3.426241	-1.244725	-2.066369
C	2.588020	0.695379	-1.484310
Zn	1.690165	-0.518400	0.171881
Br	1.478596	-2.877560	-0.395149
C	6.335190	-1.552308	-1.405564
C	7.428137	-0.785088	-1.823234
C	5.965340	-2.696119	-2.121418
C	8.145265	-1.158239	-2.960258
H	7.705265	0.099849	-1.258076
C	6.683654	-3.060362	-3.261679
H	5.119278	-3.287332	-1.783836
C	7.773081	-2.294840	-3.681809
H	8.991572	-0.559373	-3.283697
H	6.392035	-3.946321	-3.817729
H	8.330969	-2.583031	-4.567810
C	6.256501	-1.608449	1.091455
C	6.461782	-0.436088	2.066822
C	5.511420	-2.783684	1.748784
H	7.249110	-1.965486	0.794371
C	7.192640	-0.915543	3.333073
H	5.487728	-0.019759	2.337111
H	7.034949	0.357943	1.571382
C	6.241387	-3.242729	3.022268
H	4.491761	-2.473522	1.992904
H	5.433270	-3.611477	1.035009
C	6.450241	-2.080433	4.004483
H	7.303454	-0.077702	4.031349
H	8.210839	-1.238191	3.070105
H	5.671948	-4.048928	3.498087
H	7.219555	-3.668200	2.753437
H	7.004076	-2.423160	4.886534
H	5.473050	-1.728419	4.361939
C	-1.040147	3.824833	-0.621107
N	-1.346473	2.571345	-0.669021
C	-2.823947	2.502581	-0.672912
H	-3.169948	1.684035	-1.304854
O	-2.033621	4.708301	-0.798571
C	0.325685	4.233522	-0.238555
C	0.762281	5.573506	-0.010663
C	0.008610	6.738656	-0.330021
C	2.062236	5.733265	0.578260
C	2.298569	3.328266	0.590418
C	0.523998	7.988513	-0.073391
H	-0.969509	6.634355	-0.778215
C	2.556528	7.039728	0.836336
C	2.801224	4.571531	0.897885
H	2.832880	2.419861	0.838363
C	1.803162	8.143702	0.516445
H	-0.057674	8.869844	-0.325668
H	3.538408	7.146797	1.287925
H	3.764818	4.658928	1.389781
H	2.185667	9.140611	0.713536
N	1.090115	3.162303	0.002276
Ni	0.212355	1.351189	-0.772442
C	-3.237771	3.918392	-1.141593
H	-3.387356	4.035146	-2.218217
C	-2.875004	-1.115786	-0.678165
C	-1.863289	-0.624548	-1.167790
Si	-4.441612	-1.921231	-0.190439
C	-4.603448	-3.553558	-1.124606
C	-5.846909	-4.206252	-1.226182
C	-3.482780	-4.182022	-1.696504
C	-5.968352	-5.436876	-1.873346
H	-6.737601	-3.745039	-0.804550
C	-3.599709	-5.413743	-2.343843
H	-2.509419	-3.703449	-1.633847
C	-4.842189	-6.043248	-2.434040
H	-6.939281	-5.920840	-1.941443
H	-2.718882	-5.881011	-2.775880

H	-4.933614	-7.001589	-2.938578
C	-5.872398	-0.770239	-0.681151
C	-6.367853	0.206816	0.202609
C	-6.446190	-0.833988	-1.965381
C	-7.387774	1.082562	-0.177645
H	-5.952683	0.296531	1.202542
C	-7.465633	0.038300	-2.352073
H	-6.097573	-1.583255	-2.671276
C	-7.939628	1.000293	-1.457589
H	-7.752549	1.824144	0.528428
H	-7.893123	-0.036386	-3.348705
H	-8.737429	1.676467	-1.754073
C	-4.513169	-2.209395	1.695523
H	-4.310932	-1.248915	2.184536
H	-5.548923	-2.473495	1.943087
C	-3.567543	-3.272567	2.207701
C	-4.039327	-4.550845	2.540927
C	-2.194209	-3.014947	2.344425
C	-3.169724	-5.540814	3.001052
H	-5.099605	-4.771092	2.439693
C	-1.322402	-4.004349	2.800908
H	-1.794938	-2.038836	2.084361
C	-1.806716	-5.271493	3.133174
H	-3.559645	-6.523218	3.255118
H	-0.263231	-3.780122	2.884018
H	-1.127528	-6.041639	3.488366
C	-0.745166	-0.039483	-1.860166
C	-3.399604	2.439020	0.737173
C	-3.113369	1.521955	1.747201
C	-4.294068	3.494637	0.952741
C	-3.753649	1.669005	2.981662
H	-2.393104	0.728066	1.587454
C	-4.937719	3.633524	2.181558
C	-4.663009	2.711368	3.195299
H	-3.532180	0.971148	3.783621
H	-5.632676	4.451141	2.354818
H	-5.149880	2.812448	4.161129
C	-4.421723	4.361871	-0.280605
H	-5.354810	4.156578	-0.821740
H	-4.393203	5.437413	-0.078278
Br	0.497227	0.360883	2.123120
C	2.141025	1.092394	-2.903503
H	1.712995	0.220766	-3.412880
H	1.329555	1.829413	-2.840191
C	3.231556	1.710052	-3.802350
H	4.000586	0.987612	-4.091197
H	2.788573	2.093768	-4.728270
H	3.731143	2.548613	-3.301651
H	2.993968	1.587009	-1.000419
H	0.010655	-0.816650	-2.017421
C	-1.209426	0.520380	-3.225954
H	-1.685975	-0.270569	-3.819350
H	-1.946472	1.321718	-3.114055
H	-0.377092	0.914558	-3.812002

^{1}TS5-*SR*

B3LYP/BSI SCF energy: -3313.063316a.u.

M06/BSII SCF energy in solution:-3311.778865a.u.

M06/BSII free energy in solution:-3310.855389a.u.

C	4.382128	-0.694670	-0.260892
O	3.722727	-0.484886	0.784890
N	5.639512	-1.193206	-0.204678
C	3.760499	-0.366578	-1.608375
H	4.547531	0.025753	-2.262413
H	3.425247	-1.306491	-2.065041
C	2.580512	0.637695	-1.503770
Zn	1.682433	-0.575162	0.152001
Br	1.491569	-2.934899	-0.413303
C	6.333230	-1.599892	-1.400673
C	7.435537	-0.864385	-1.849740
C	5.938367	-2.758391	-2.078655
C	8.136887	-1.284520	-2.980231
H	7.732056	0.032594	-1.314186
C	6.640223	-3.168897	-3.213294
H	5.085620	-3.324814	-1.716220
C	7.739177	-2.435477	-3.664569
H	8.990634	-0.710442	-3.328119
H	6.328924	-4.066110	-3.739812
H	8.284947	-2.759671	-4.545650
C	6.290888	-1.548242	1.096777
C	6.461337	-0.339356	2.033242
C	5.596220	-2.728709	1.799110
H	7.293992	-1.878148	0.803321
C	7.227514	-0.750466	3.302072
H	5.475486	0.046600	2.305674
H	6.995509	0.460997	1.505461
C	6.360048	-3.120901	3.075015

H	4.569299	-2.446347	2.047179	H	-7.120084	-5.765602	-1.937234
H	5.539437	-3.580523	1.111915	H	-2.881147	-5.924304	-2.655830
C	6.540102	-1.922552	4.018969	H	-5.138563	-6.948069	-2.864277
H	7.314763	0.111706	3.973581	C	-5.891531	-0.675324	-0.657209
H	8.253897	-1.041318	3.034075	C	-6.409774	0.275789	0.241153
H	5.827877	-3.932295	3.584017	C	-6.417392	-0.687858	-1.963550
H	7.349143	-3.518679	2.803877	C	-7.405371	1.176410	-0.145944
H	7.119610	-2.218119	4.901610	H	-6.031591	0.325708	1.258376
H	5.555799	-1.596896	4.381950	C	-7.412023	0.209277	-2.357261
C	-0.985785	3.811455	-0.637509	H	-6.050551	-1.416651	-2.681719
N	-1.319629	2.564909	-0.684385	C	-7.909009	1.145477	-1.447690
C	-2.798042	2.529135	-0.694873	H	-7.788471	1.897670	0.571299
H	-3.159958	1.716674	-1.325939	H	-7.802707	0.174177	-3.371040
O	-1.958031	4.716469	-0.823788	H	-8.687917	1.840916	-1.749811
C	0.386043	4.189701	-0.245141	C	-4.555682	-2.136430	1.724836
C	0.852728	5.519349	-0.017314	H	-4.323155	-1.179743	2.207650
C	0.129605	6.701014	-0.346241	H	-5.595610	-2.372481	1.982928
C	2.151549	5.649601	0.581266	C	-3.633504	-3.223149	2.230575
C	2.330748	3.239518	0.601434	C	-4.133917	-4.491896	2.558331
C	0.672859	7.939059	-0.089936	C	-2.253866	-2.998519	2.362982
H	-0.847267	6.618566	-0.801750	C	-3.286168	-5.504366	3.010164
C	2.674967	6.944785	0.838743	H	-5.199218	-4.686931	2.458362
C	2.860218	4.471403	0.909809	C	-1.403937	-4.010745	2.810748
H	2.840716	2.318240	0.853851	H	-1.832615	-2.030813	2.106215
C	1.950900	8.065438	0.509127	C	-1.916676	-5.267857	3.138397
H	0.114540	8.833216	-0.349672	H	-3.698084	-6.478745	3.260333
H	3.655684	7.029999	1.297445	H	-0.339417	-3.811997	2.891024
H	3.821940	4.537096	1.408667	H	-1.254463	-6.055639	3.486869
H	2.355924	9.053514	0.705676	C	-0.762084	-0.067494	-1.859049
N	1.123126	3.101513	0.004346	C	-1.224513	0.493071	-3.225147
Ni	0.216493	1.312478	-0.775100	H	-0.389322	0.870723	-3.817582
C	-3.177903	3.952338	-1.170033	H	-1.717351	-0.292739	-3.811968
H	-3.319571	4.068772	-2.247741	H	-1.947716	1.306803	-3.112559
C	-2.906107	-1.100640	-0.664296	H	-0.018574	-0.856228	-2.017805
C	-1.887029	-0.631184	-1.159946	C	-3.380697	2.484049	0.713395
Si	-4.490728	-1.860667	-0.163164	C	-3.118313	1.565548	1.728774
C	-4.703774	-3.493772	-1.085316	C	-4.251442	3.560906	0.921390
C	-5.972032	-4.091472	-1.213217	C	-3.757838	1.733983	2.960859
C	-3.597202	-4.178788	-1.618643	H	-2.416866	0.753922	1.574438
C	-6.130654	-5.324429	-1.847967	C	-4.894850	3.720809	2.147722
H	-6.852216	-3.585153	-0.822582	C	-4.643613	2.797922	3.166739
C	-3.751383	-5.412805	-2.253490	H	-3.554474	1.035621	3.767189
H	-2.605759	-3.741996	-1.536225	H	-5.571416	4.554886	2.315149
C	-5.017981	-5.987877	-2.369466	H	-5.130050	2.915307	4.130963

C	-4.354983	4.425702	-0.315969
H	-5.290621	4.239761	-0.859620
H	-4.302454	5.501055	-0.117484
Br	0.479851	0.296067	2.101950
C	2.130266	1.022613	-2.924909
H	1.700262	0.147943	-3.427311
H	1.320029	1.760969	-2.864633
C	3.219088	1.633344	-3.830633
H	3.985529	0.908104	-4.119433
H	2.773465	2.013979	-4.756555
H	3.722300	2.472992	-3.335455
H	2.984680	1.534950	-1.028859

^{1}TS5-*RR*

B3LYP/BSI SCF energy: -3313.057274a.u.

M06/BSII SCF energy in solution:-3311.775723a.u.

M06/BSII free energy in solution:-3310.851897a.u.

C	4.474117	-0.700839	-0.399605
O	3.906577	-0.349862	0.664415
N	5.770554	-1.084090	-0.407011
C	3.688452	-0.665686	-1.703864
H	4.363863	-0.325895	-2.497652
H	3.408129	-1.692831	-1.968856
C	2.444833	0.258183	-1.604786
Zn	1.840042	-0.899114	0.294056
Br	2.212153	-3.300671	0.355753
C	6.365956	-1.663802	-1.585335
C	7.342366	-0.954252	-2.292758
C	6.006010	-2.955550	-1.984295
C	7.953452	-1.535926	-3.403904
H	7.612214	0.047509	-1.971760
C	6.616773	-3.528059	-3.101397
H	5.251330	-3.496957	-1.421195
C	7.590281	-2.821990	-3.810687
H	8.709517	-0.982874	-3.953417
H	6.333667	-4.529406	-3.411712
H	8.065835	-3.272088	-4.677037
C	6.589066	-1.138627	0.846909
C	6.738110	0.234281	1.525370
C	6.096632	-2.217927	1.827228
H	7.583020	-1.436601	0.494316
C	7.673642	0.131134	2.741792
H	5.753754	0.584750	1.847118
H	7.127962	0.961096	0.801332
C	7.027962	-2.300250	3.048456
H	5.077489	-1.981264	2.144719
H	6.053758	-3.184889	1.314005
C	7.187272	-0.935442	3.734769
H	7.746480	1.108520	3.233345
H	8.689126	-0.123138	2.404557
H	6.636669	-3.040168	3.755521
H	8.017461	-2.663269	2.733634
H	7.884026	-1.012930	4.577809
H	6.219525	-0.625737	4.152343
C	-0.712197	3.533970	-0.726205
N	-1.167349	2.325352	-0.706221
C	-2.640689	2.446975	-0.782251
H	-3.066120	1.635375	-1.372386
O	-1.579081	4.518353	-1.013603
C	0.675287	3.818215	-0.312656
C	1.243771	5.118511	-0.137907
C	0.622763	6.339986	-0.525829
C	2.542415	5.172496	0.472043
C	2.536875	2.758292	0.587631
C	1.259955	7.541063	-0.312209
H	-0.351824	6.317980	-0.991958
C	3.164878	6.431626	0.684112
C	3.157985	3.957342	0.848690
H	2.992260	1.812063	0.854305
C	2.536661	7.591782	0.299824
H	0.776855	8.464527	-0.616566
H	4.144609	6.457051	1.152148
H	4.124961	3.968162	1.341715
H	3.016862	8.552055	0.462117
N	1.317904	2.689985	-0.001505
Ni	0.266988	0.875179	-0.649921
C	-2.855951	3.863071	-1.362579
H	-2.948118	3.919451	-2.450662
C	-3.314533	-0.940246	-0.625344
C	-2.190105	-0.684680	-1.044512
Si	-5.025433	-1.396100	-0.182854
C	-5.492101	-2.989152	-1.084622
C	-6.841911	-3.349154	-1.259644
C	-4.510184	-3.879989	-1.552987
C	-7.197532	-4.550074	-1.875958
H	-7.629662	-2.679353	-0.921599
C	-4.860527	-5.082723	-2.169364

H	-3.460278	-3.627404	-1.434495
C	-6.205174	-5.420229	-2.332008
H	-8.246526	-4.805294	-2.002143
H	-4.083400	-5.755634	-2.521744
H	-6.479154	-6.355700	-2.812630
C	-6.192093	-0.008613	-0.748478
C	-6.612181	1.015753	0.119655
C	-6.632247	0.052299	-2.085232
C	-7.433502	2.055338	-0.324878
H	-6.293400	1.014833	1.158316
C	-7.451138	1.088746	-2.536496
H	-6.338516	-0.728409	-2.782246
C	-7.854687	2.094763	-1.655366
H	-7.745690	2.830361	0.370164
H	-7.779161	1.108177	-3.572622
H	-8.498813	2.898860	-2.001860
C	-5.183681	-1.630605	1.705273
H	-4.879094	-0.692475	2.183967
H	-6.247919	-1.769577	1.932497
C	-4.375839	-2.787672	2.249705
C	-4.982926	-4.023173	2.519668
C	-2.995258	-2.664249	2.476634
C	-4.238763	-5.098902	3.006762
H	-6.049975	-4.141674	2.346555
C	-2.248281	-3.739031	2.960802
H	-2.492619	-1.724705	2.265888
C	-2.867812	-4.961592	3.229601
H	-4.732988	-6.045168	3.211310
H	-1.181054	-3.616086	3.121669
H	-2.286720	-5.798147	3.607422
C	-0.876824	-0.507078	-1.607247
C	-3.261583	2.562976	0.606125
C	-3.106914	1.709412	1.697908
C	-4.022005	3.734400	0.709860
C	-3.750104	2.035242	2.896187
H	-2.481497	0.827102	1.626306
C	-4.666668	4.054153	1.903814
C	-4.529129	3.193758	2.996577
H	-3.631840	1.386858	3.759273
H	-5.256476	4.963088	1.990083
H	-5.018271	3.434388	3.936258
C	-4.008765	4.507504	-0.590751
H	-4.941996	4.363401	-1.151177
H	-3.862555	5.585734	-0.470218
Br	0.465051	0.023441	2.114996
C	1.879707	0.523591	-3.019385
H	1.517499	-0.405658	-3.471750
H	1.001561	1.178093	-2.951028
C	2.859957	1.202701	-3.997481
H	3.694102	0.554492	-4.282414
H	2.341153	1.480494	-4.921752
H	3.281365	2.118725	-3.565584
H	2.822651	1.212020	-1.233774
C	-0.307568	-1.905494	-1.926399
H	-0.281447	-2.535443	-1.035754
H	-0.941420	-2.411568	-2.667225
H	0.705429	-1.865137	-2.327082
H	-0.975204	0.071171	-2.539736

^{1}TS5-*SS*'

B3LYP/BSI SCF energy: -3313.064792a.u.

M06/BSII SCF energy in solution: -3311.78384a.u.

M06/BSII free energy in solution: -3310.857277a.u.

C	-3.652151	-0.555798	0.132304
O	-3.231723	0.214884	-0.767199
N	-4.977030	-0.789544	0.277287
C	-2.649760	-1.260595	1.030790
H	-3.116278	-1.499767	1.990201
H	-2.447439	-2.223505	0.545929
C	-1.308240	-0.501138	1.252110
Zn	-1.155458	-0.300320	-1.011857
Br	-1.435055	-2.479778	-2.082309
C	-5.466696	-1.778644	1.206511
C	-6.113130	-1.369379	2.377745
C	-5.345215	-3.140279	0.909986
C	-6.630557	-2.323118	3.254875
H	-6.199678	-0.309286	2.596585
C	-5.859987	-4.089138	1.794753
H	-4.843266	-3.446978	-0.002577
C	-6.503498	-3.683608	2.965462
H	-7.128420	-2.002865	4.165330
H	-5.758409	-5.145547	1.565319
H	-6.904122	-4.424721	3.650606
C	-5.993314	-0.204975	-0.655605
C	-6.032644	1.332965	-0.625740
C	-5.854341	-0.749306	-2.089058
H	-6.948727	-0.561603	-0.254595

C	-7.167398	1.855915	-1.523280	H	-0.588669	-1.269679	1.530819
H	-5.074828	1.722624	-0.980950	C	1.747318	-0.416504	1.207340
H	-6.169862	1.676847	0.407328	C	2.003135	-0.096015	2.441345
C	-6.979895	-0.205280	-2.984776	Si	2.465233	-2.050299	0.558177
H	-4.879137	-0.460694	-2.491305	C	1.436239	-3.481953	1.254732
H	-5.883676	-1.844572	-2.067358	C	0.968258	-4.543010	0.459116
C	-7.033952	1.329309	-2.960456	C	1.128010	-3.515154	2.630725
H	-7.167939	2.952363	-1.514699	C	0.225978	-5.590212	1.011863
H	-8.137020	1.541695	-1.110408	H	1.179657	-4.558769	-0.603700
H	-6.837192	-0.566370	-4.009322	C	0.392084	-4.561809	3.187978
H	-7.946170	-0.605831	-2.644761	H	1.469465	-2.710550	3.277296
H	-7.867973	1.689844	-3.574031	C	-0.063305	-5.603668	2.376291
H	-6.115109	1.730963	-3.409081	H	-0.124846	-6.394817	0.371354
C	1.534991	3.568251	0.781046	H	0.173320	-4.564230	4.252885
N	1.919408	2.365505	0.523173	H	-0.638018	-6.420000	2.806169
C	3.394144	2.381633	0.493342	C	4.239072	-2.174905	1.242923
H	3.772241	1.492018	0.999470	C	5.229143	-1.268605	0.811621
O	2.486105	4.465853	1.087494	C	4.621284	-3.141735	2.188252
C	0.106599	3.926218	0.700731	C	6.534318	-1.320360	1.302712
C	-0.425201	5.249764	0.794330	H	4.986589	-0.514292	0.065236
C	0.338690	6.419065	1.073933	C	5.925780	-3.198705	2.687401
C	-1.838299	5.389401	0.584562	H	3.891795	-3.865590	2.539573
C	-1.972731	3.000619	0.243239	C	6.886019	-2.288036	2.247316
C	-0.274079	7.649357	1.142221	H	7.277623	-0.612230	0.944891
H	1.403881	6.334874	1.233687	H	6.191622	-3.959682	3.416610
C	-2.435164	6.676363	0.660220	H	7.901703	-2.333811	2.631128
C	-2.589723	4.228637	0.296391	C	2.553652	-2.004357	-1.346374
H	-2.521137	2.098808	0.003679	H	1.559880	-1.737609	-1.719959
C	-1.669006	7.783541	0.933909	H	3.198314	-1.143742	-1.570309
H	0.320753	8.531767	1.357603	C	3.069880	-3.218371	-2.093263
H	-3.504988	6.765573	0.495504	C	4.405876	-3.639365	-1.986864
H	-3.656322	4.304578	0.109475	C	2.217133	-3.938789	-2.946378
H	-2.128817	8.765603	0.990323	C	4.868925	-4.747607	-2.697487
N	-0.643885	2.848398	0.456600	H	5.090540	-3.093140	-1.345282
Ni	0.496263	0.964790	0.514813	C	2.680158	-5.049112	-3.655196
C	3.750476	3.714174	1.199497	H	1.183782	-3.619790	-3.053907
H	3.960638	3.629902	2.268629	C	4.007938	-5.461245	-3.533200
C	-1.468929	0.472877	2.447612	H	5.907675	-5.052073	-2.597688
H	-2.288891	1.176618	2.252653	H	1.999353	-5.587443	-4.309516
H	-0.573490	1.093454	2.576221	H	4.369450	-6.323712	-4.086507
C	-1.711415	-0.217775	3.803867	C	2.236949	0.227275	3.709096
H	-0.917105	-0.940477	4.017434	C	3.428916	1.005490	4.212845
H	-1.721483	0.521717	4.612886	H	3.128914	1.955440	4.677752
H	-2.664927	-0.753546	3.846077	H	3.972398	0.438784	4.979426

H	4.135796	1.223269	3.407548
H	1.530804	-0.116162	4.466819
C	3.972480	2.566302	-0.903403
C	3.757137	1.789719	-2.041558
C	4.800659	3.694740	-0.951035
C	4.406904	2.142555	-3.227167
H	3.066822	0.954387	-2.024778
C	5.448957	4.044344	-2.134750
C	5.250732	3.257357	-3.271931
H	4.242878	1.550667	-4.122327
H	6.091771	4.919790	-2.177399
H	5.746170	3.520935	-4.201941
C	4.859606	4.393029	0.390579
H	5.824300	4.236303	0.890753
H	4.703922	5.475375	0.332581
Br	-0.042956	1.282066	-2.504062

[1]IM7-*SR*

B3LYP/BSI SCF energy: -3313.101523a.u.

M06/BSII SCF energy in solution:-3311.811784a.u.

M06/BSII free energy in solution:-3310.886152a.u.

C	-2.028999	-2.473358	0.389104
O	-3.008054	-2.233205	-0.378223
N	-1.817076	-3.748648	0.775917
C	-1.095257	-1.359129	0.830682
H	-0.364354	-1.756314	1.531816
H	-0.536532	-1.096900	-0.078282
C	-1.750976	-0.081612	1.405088
Zn	-3.526566	-0.567462	-1.327255
Br	-1.976519	0.051628	-2.979302
C	-0.689415	-4.128804	1.598195
C	-0.894254	-4.435433	2.947489
C	0.581341	-4.252228	1.029661
C	0.179879	-4.859892	3.730297
H	-1.886176	-4.334147	3.376537
C	1.653060	-4.668376	1.821611
H	0.731219	-4.014134	-0.018332
C	1.453919	-4.974683	3.169139
H	0.020800	-5.094433	4.778693
H	2.642215	-4.744256	1.381796
H	2.289526	-5.301295	3.781213
C	-2.693191	-4.881941	0.324334
C	-4.148672	-4.758591	0.808334
C	-2.605721	-5.135085	-1.191218
H	-2.257392	-5.753637	0.823680
C	-4.947716	-6.012701	0.414174
H	-4.609522	-3.871351	0.366772
H	-4.164773	-4.625362	1.896625
C	-3.419183	-6.383851	-1.572604
H	-2.990714	-4.264039	-1.728667
H	-1.555257	-5.259150	-1.479182
C	-4.876007	-6.277014	-1.097076
H	-5.989552	-5.896488	0.733535
H	-4.551835	-6.885662	0.953470
H	-3.379654	-6.528723	-2.658230
H	-2.956137	-7.273966	-1.122569
H	-5.424313	-7.192635	-1.347905
H	-5.372955	-5.456021	-1.631832
C	-0.163205	4.202237	0.847852
N	0.492554	3.091597	0.837806
C	1.847735	3.408700	0.348013
H	2.594844	2.825808	0.890148
O	0.529659	5.333640	0.616674
C	-1.620040	4.180314	1.035077
C	-2.462333	5.325844	1.165684
C	-1.998654	6.672250	1.200119
C	-3.873076	5.084558	1.270496
C	-3.416969	2.715375	1.160544
C	-2.893366	7.711156	1.320281
H	-0.939085	6.873143	1.127515
C	-4.766722	6.182039	1.386750
C	-4.322390	3.745233	1.255609
H	-3.754494	1.688314	1.146505
C	-4.286595	7.469651	1.410671
H	-2.526400	8.732825	1.344581
H	-5.831779	5.981838	1.457570
H	-5.382786	3.521058	1.309834
H	-4.972451	8.306685	1.500080
N	-2.080371	2.915662	1.043734
Ni	-0.573694	1.476292	1.296556
C	1.949017	4.942736	0.543785
H	2.410340	5.264937	1.481252
C	2.925015	-0.088351	0.696745
C	1.972740	0.202167	1.417278
Si	4.457435	-0.529042	-0.175016
C	5.322301	-1.942818	0.740979
C	6.524654	-2.486647	0.248351

C	4.798950	-2.486615	1.926560
C	7.173912	-3.532405	0.906220
H	6.969964	-2.086272	-0.660382
C	5.446010	-3.531640	2.591891
H	3.874418	-2.083885	2.331022
C	6.633465	-4.058726	2.081942
H	8.100568	-3.934171	0.504980
H	5.024492	-3.930406	3.511236
H	7.137699	-4.871318	2.598035
C	5.618298	0.973327	-0.211458
C	5.478213	1.990609	-1.174975
C	6.634058	1.125436	0.750703
C	6.313378	3.109939	-1.176449
H	4.706600	1.919988	-1.936588
C	7.470933	2.243345	0.755565
H	6.777987	0.356163	1.504705
C	7.312760	3.239230	-0.209700
H	6.185809	3.876168	-1.936834
H	8.248140	2.334292	1.509870
H	7.966452	4.107513	-0.211425
C	4.135610	-1.046910	-1.988268
H	3.765203	-0.161584	-2.516547
H	5.118649	-1.272728	-2.421584
C	3.193384	-2.205447	-2.212013
C	3.642703	-3.533652	-2.123544
C	1.844741	-1.988769	-2.535912
C	2.780510	-4.603412	-2.368005
H	4.681832	-3.728560	-1.872283
C	0.978444	-3.055360	-2.785313
H	1.466451	-0.973593	-2.614959
C	1.444805	-4.370244	-2.706673
H	3.157338	-5.621114	-2.307458
H	-0.053991	-2.848190	-3.053308
H	0.780112	-5.202957	-2.920183
C	0.873966	0.555799	2.276358
C	1.301536	1.460369	3.454741
H	0.441173	1.682290	4.095192
H	2.064685	0.972575	4.077047
H	1.718753	2.413382	3.116850
H	0.461244	-0.361815	2.702617
C	1.963862	3.253673	-1.161885
C	1.678515	2.131373	-1.938329
C	2.378915	4.452471	-1.754342
C	1.833412	2.219082	-3.325178
H	1.332311	1.214942	-1.473129
C	2.541939	4.535399	-3.136785
C	2.269016	3.409708	-3.918665
H	1.601571	1.359888	-3.947291
H	2.862261	5.463378	-3.603331
H	2.380817	3.463247	-4.997715
C	2.598424	5.528847	-0.713116
H	3.667213	5.694697	-0.524545
H	2.160962	6.497354	-0.975705
Br	-5.710565	0.128893	-0.807621
C	-2.378003	-0.263752	2.798543
H	-1.601657	-0.617670	3.491596
H	-2.673607	0.723416	3.178211
C	-3.601183	-1.193484	2.909605
H	-3.349779	-2.235610	2.689377
H	-4.014190	-1.170337	3.925041
H	-4.396210	-0.895424	2.217467
H	-2.545306	0.232903	0.698492

^{1}IM7-*RS*

B3LYP/BSI SCF energy: -3313.101523a.u.

M06/BSII SCF energy in solution:-3311.811782a.u.

M06/BSII free energy in solution:-3310.886171a.u.

C	2.029426	-2.472969	-0.388964
O	3.008556	-2.232833	0.378275
N	1.817537	-3.748212	-0.775919
C	1.095506	-1.358744	-0.830142
H	0.364189	-1.755898	-1.530852
H	0.537292	-1.096453	0.079123
C	1.751003	-0.081263	-1.404845
Zn	3.526684	-0.567206	1.327652
Br	1.976437	0.050724	2.979979
C	0.690240	-4.128171	-1.598811
C	0.895480	-4.433279	-2.948387
C	-0.580529	-4.252885	-1.030593
C	-0.178295	-4.857512	-3.731804
H	1.887417	-4.330972	-3.377150
C	-1.651891	-4.668816	-1.823142
H	-0.730674	-4.015905	0.017615
C	-1.452358	-4.973600	-3.170957
H	-0.018931	-5.090882	-4.780417
H	-2.641086	-4.745681	-1.383585
H	-2.287682	-5.300033	-3.783514

C	2.693557	-4.881587	-0.324401	C	-5.322029	-1.943177	-0.741175
C	4.148921	-4.758657	-0.808913	C	-6.524621	-2.486803	-0.248896
C	2.606594	-5.134404	1.191228	C	-4.798311	-2.487218	-1.926476
H	2.257394	-5.753292	-0.823416	C	-7.173736	-3.532616	-0.906818
C	4.947866	-6.012831	-0.414766	H	-6.970243	-2.086204	0.659586
H	4.610064	-3.871404	-0.367678	C	-5.445227	-3.532298	-2.591863
H	4.164704	-4.625670	-1.897236	H	-3.873608	-2.084621	-2.330682
C	3.419901	-6.383285	1.572572	C	-6.632907	-4.059196	-2.082250
H	2.992001	-4.263345	1.728359	H	-8.100580	-3.934220	-0.505851
H	1.556214	-5.258152	1.479640	H	-5.023418	-3.931249	-3.510995
C	4.876593	-6.276853	1.096553	H	-7.137031	-4.871830	-2.598384
H	5.989621	-5.896877	-0.734489	C	-5.618284	0.972750	0.211802
H	4.551648	-6.885817	-0.953776	C	-5.478583	1.989666	1.175760
H	3.380696	-6.527940	2.658238	C	-6.633843	1.125092	-0.750538
H	2.956511	-7.273380	1.122855	C	-6.313922	3.108867	1.177488
H	5.424776	-7.192550	1.347374	H	-4.707137	1.918860	1.937524
H	5.373887	-5.455870	1.631002	C	-7.470888	2.242873	-0.755152
C	0.162426	4.202233	-0.847656	H	-6.777486	0.356091	-1.504874
N	-0.493038	3.091414	-0.837579	C	-7.313096	3.238392	0.210554
C	-1.848240	3.408124	-0.347576	H	-6.186651	3.874809	1.938210
H	-2.595267	2.825114	-0.889691	H	-8.247932	2.334002	-1.509602
O	-0.530677	5.333436	-0.616270	H	-7.966931	4.106568	0.212483
C	1.619241	4.180666	-1.035137	C	-4.135279	-1.047673	1.988163
C	2.461214	5.326380	-1.166076	H	-3.764824	-0.162483	2.516633
C	1.997176	6.672662	-1.200565	H	-5.118313	-1.273572	2.421451
C	3.871992	5.085428	-1.271213	C	-3.193070	-2.206284	2.211566
C	3.416514	2.716142	-1.160799	C	-3.642425	-3.534451	2.122761
C	2.891592	7.711780	-1.321082	C	-1.844402	-1.989722	2.535465
H	0.937569	6.873280	-1.127725	C	-2.780248	-4.604304	2.366880
C	4.765325	6.183127	-1.387841	H	-4.681570	-3.729269	1.871500
C	4.321654	3.746219	-1.256248	C	-0.978131	-3.056408	2.784534
H	3.754258	1.689147	-1.146618	H	-1.466077	-0.974575	2.614772
C	4.284861	7.470612	-1.411799	C	-1.444528	-4.371262	2.705552
H	2.524367	8.733355	-1.345415	H	-3.157108	-5.621978	2.306064
H	5.830415	5.983192	-1.458918	H	0.054315	-2.849347	3.052570
H	5.382098	3.522327	-1.310707	H	-0.779849	-5.204051	2.918822
H	4.970478	8.307812	-1.501486	C	-0.873875	0.555684	-2.276383
N	2.079906	2.916137	-1.043726	C	-1.964097	3.252879	1.162314
Ni	0.573498	1.476447	-1.296424	C	-1.678384	2.130532	1.938560
C	-1.949928	4.942168	-0.543152	C	-2.379292	4.451515	1.754995
H	-2.411502	5.264352	-1.480500	C	-1.833041	2.218026	3.325447
C	-2.924924	-0.088567	-0.696817	H	-1.332083	1.214232	1.473173
C	-1.972613	0.201847	-1.417347	C	-2.542080	4.534227	3.137479
Si	-4.457243	-0.529462	0.175019	C	-2.268782	3.408490	3.919163

H	-1.600882	1.358805	3.947403
H	-2.862515	5.462077	3.604205
H	-2.380381	3.461871	4.998242
C	-2.599234	5.527973	0.713944
H	-3.668099	5.693585	0.525596
H	-2.161949	6.496552	0.976564
Br	5.710303	0.130566	0.808491
C	2.377990	-0.263549	-2.798314
H	1.601833	-0.618319	-3.491137
H	2.672867	0.723660	-3.178449
C	3.601840	-1.192437	-2.909093
H	3.351279	-2.234656	-2.688360
H	4.014751	-1.169432	-3.924573
H	4.396706	-0.893497	-2.217145
H	2.545353	0.233517	-0.698390
H	-0.460975	-0.361835	-2.702663
C	-1.301517	1.460272	-3.454723
H	-2.064515	0.972385	-4.077140
H	-1.718943	2.413173	-3.116774
H	-0.441136	1.682415	-4.095074

[1]IM7-*SS*

B3LYP/BSI SCF energy: -3313.084387a.u.

M06/BSII SCF energy in solution:-3311.801119a.u.

M06/BSII free energy in solution:-3310.875895a.u.

C	3.416293	-1.669896	-0.466155
O	3.337742	-0.711757	0.353736
N	4.449945	-2.534223	-0.366735
C	2.375500	-1.841349	-1.550626
H	2.721030	-2.594671	-2.263465
H	1.496493	-2.270518	-1.050688
C	1.970374	-0.539321	-2.285053
Zn	1.563651	-0.042458	1.132619
Br	0.388786	-2.025367	1.750122
C	4.531024	-3.724099	-1.180622
C	5.470064	-3.795773	-2.214777
C	3.719723	-4.825116	-0.888192
C	5.587532	-4.967349	-2.963636
H	6.094647	-2.934295	-2.430382
C	3.839448	-5.991976	-1.644725
H	2.997852	-4.757498	-0.080096
C	4.772388	-6.065688	-2.680836
H	6.313136	-5.019428	-3.769831
H	3.203575	-6.843076	-1.420716
H	4.864027	-6.975437	-3.266467
C	5.487711	-2.423886	0.713049
C	6.288399	-1.111091	0.661521
C	4.915619	-2.697207	2.115385
H	6.185077	-3.235589	0.478867
C	7.413068	-1.136649	1.711192
H	5.620117	-0.269793	0.861392
H	6.705338	-0.973714	-0.344211
C	6.043718	-2.701375	3.161230
H	4.178740	-1.929244	2.365358
H	4.392627	-3.660344	2.116145
C	6.860172	-1.400871	3.120045
H	7.959115	-0.186487	1.685830
H	8.139882	-1.920476	1.452558
H	5.615053	-2.852454	4.158063
H	6.712435	-3.554713	2.975936
H	7.680883	-1.445822	3.845531
H	6.218798	-0.561244	3.420225
C	0.085128	3.416868	-0.927746
N	-0.471733	2.262075	-0.780056
C	-1.891265	2.521753	-0.435078
H	-2.538651	1.841954	-0.988570
O	-0.699144	4.503744	-0.886209
C	1.548789	3.522648	-1.045956
C	2.292702	4.740937	-1.088375
C	1.720913	6.040019	-1.215195
C	3.721012	4.628120	-1.003468
C	3.467531	2.230916	-0.877240
C	2.528466	7.153339	-1.253908
H	0.648124	6.145894	-1.283857
C	4.521977	5.800429	-1.038911
C	4.279363	3.338867	-0.865602
H	3.861234	1.235846	-0.742337
C	3.937665	7.037790	-1.162306
H	2.078945	8.136504	-1.354468
H	5.600721	5.697524	-0.966443
H	5.351043	3.220732	-0.741332
H	4.553089	7.932002	-1.189795
N	2.120229	2.311268	-1.004911
Ni	0.753768	0.757651	-1.351233
C	-2.086278	4.019381	-0.789732
H	-2.544891	4.208095	-1.763672
C	3.153079	0.055955	-3.087370

H	4.051237	0.157983	-2.466250
H	2.902599	1.071272	-3.419445
C	3.530970	-0.766946	-4.333530
H	2.679105	-0.856627	-5.017329
H	4.351071	-0.292735	-4.885361
H	3.853947	-1.781272	-4.075447
H	1.279000	-0.893913	-3.054202
C	-3.056828	-0.693598	-0.667337
C	-1.948810	-0.561179	-1.176346
Si	-4.803889	-0.820217	-0.150563
C	-5.694718	-2.017743	-1.310249
C	-7.100347	-2.030186	-1.389859
C	-4.986976	-2.952756	-2.085504
C	-7.772222	-2.940029	-2.207698
H	-7.682013	-1.312576	-0.815181
C	-5.653852	-3.865090	-2.905560
H	-3.901173	-2.962344	-2.046800
C	-7.048213	-3.860933	-2.967932
H	-8.858076	-2.928842	-2.254228
H	-5.084908	-4.578959	-3.495410
H	-7.568671	-4.569795	-3.606504
C	-5.616227	0.889970	-0.317204
C	-5.759803	1.755838	0.782278
C	-6.080580	1.344732	-1.567071
C	-6.344864	3.017539	0.643553
H	-5.408337	1.451572	1.764286
C	-6.661014	2.605728	-1.714246
H	-5.999426	0.697715	-2.436881
C	-6.796889	3.445938	-0.606257
H	-6.449700	3.661649	1.512609
H	-7.015601	2.928821	-2.689642
H	-7.259350	4.423574	-0.715058
C	-4.970848	-1.387648	1.664953
H	-4.320954	-0.745203	2.271138
H	-6.001916	-1.173130	1.972810
C	-4.649232	-2.844081	1.908233
C	-5.666327	-3.810332	1.935638
C	-3.325191	-3.268716	2.097849
C	-5.372918	-5.157326	2.151807
H	-6.698572	-3.502537	1.787086
C	-3.030287	-4.615500	2.314330
H	-2.516423	-2.544346	2.074432
C	-4.052169	-5.566558	2.343553
H	-6.178787	-5.886417	2.172633
H	-1.996622	-4.915968	2.463390
H	-3.822626	-6.614540	2.515957
C	-0.731280	-0.434619	-1.945478
C	-1.097242	0.100550	-3.355670
H	-0.224106	0.141806	-4.014410
H	-1.851761	-0.535096	-3.837239
H	-1.517591	1.110505	-3.298179
H	-0.310610	-1.440590	-2.029781
C	-2.153121	2.478001	1.062911
C	-1.964726	1.412557	1.942992
C	-2.642349	3.707758	1.518494
C	-2.271328	1.596262	3.294016
H	-1.586028	0.459625	1.591098
C	-2.950459	3.888265	2.866510
C	-2.760720	2.824448	3.752421
H	-2.112291	0.780879	3.992974
H	-3.328393	4.842031	3.225907
H	-2.988098	2.954364	4.806706
C	-2.810197	4.691265	0.381571
H	-3.869658	4.820208	0.126373
H	-2.398546	5.685279	0.585426
Br	2.010594	1.832245	2.515821

[1]IM7-*RR*

B3LYP/BSI SCF energy: -3313.078645a.u.

M06/BSII SCF energy in solution:-3311.796858a.u.

M06/BSII free energy in solution:-3310.870099a.u.

C	-3.828765	-0.994130	0.540807
O	-3.437246	-0.391099	-0.495774
N	-4.967562	-1.719995	0.509113
C	-3.040027	-0.878316	1.830590
H	-3.710334	-1.074015	2.673784
H	-2.315430	-1.697806	1.834249
C	-2.364190	0.501555	1.972640
Zn	-1.383596	-0.430096	-0.912953
Br	-0.995334	-2.796061	-0.912841
C	-5.347238	-2.562546	1.616736
C	-6.449862	-2.221616	2.407358
C	-4.644680	-3.747347	1.859906
C	-6.842394	-3.063694	3.448024
H	-6.986740	-1.298993	2.208132
C	-5.040036	-4.581866	2.906834
H	-3.795868	-4.002792	1.232384

C	-6.137527	-4.243101	3.700363	H	2.751908	3.962250	2.474453
H	-7.696006	-2.795993	4.063677	C	2.731243	-0.902995	0.650986
H	-4.490869	-5.499104	3.096863	C	1.677702	-0.565562	1.180770
H	-6.443962	-4.895858	4.512261	Si	4.443528	-1.403308	0.241760
C	-5.801875	-1.852674	-0.731298	C	4.819353	-3.030731	1.122791
C	-6.348676	-0.505960	-1.235047	C	6.146303	-3.417311	1.389320
C	-5.092454	-2.643307	-1.844338	C	3.791308	-3.919017	1.485909
H	-6.660114	-2.447019	-0.398324	C	6.436742	-4.641996	1.992957
C	-7.290399	-0.729091	-2.430804	H	6.966721	-2.750258	1.133997
H	-5.514166	0.131470	-1.538658	C	4.076923	-5.145263	2.089127
H	-6.877034	0.004690	-0.419900	H	2.757175	-3.646192	1.295359
C	-6.035000	-2.843741	-3.043258	C	5.400295	-5.509256	2.344005
H	-4.195312	-2.104630	-2.159527	H	7.469261	-4.917848	2.191131
H	-4.761412	-3.611092	-1.451881	H	3.265787	-5.816249	2.359040
C	-6.592263	-1.507379	-3.556311	H	5.623450	-6.463280	2.814407
H	-7.650647	0.238513	-2.799316	C	5.611241	-0.057500	0.904913
H	-8.178906	-1.286706	-2.100305	C	6.134731	0.950916	0.075509
H	-5.499363	-3.367221	-3.842859	C	5.952464	-0.016958	2.271104
H	-6.871474	-3.494816	-2.749460	C	6.963159	1.954893	0.584657
H	-7.289032	-1.679608	-4.385118	H	5.891671	0.964888	-0.983207
H	-5.768429	-0.901271	-3.957092	C	6.777672	0.983646	2.786939
C	0.455211	3.631237	0.825591	H	5.576455	-0.786769	2.940350
N	0.880300	2.413794	0.767633	C	7.286618	1.973678	1.942682
C	2.357715	2.507030	0.809379	H	7.357669	2.717729	-0.081474
H	2.779937	1.685990	1.388807	H	7.029327	0.987275	3.844378
O	1.350931	4.599276	1.088114	H	7.936586	2.749299	2.339525
C	-0.952726	3.939555	0.513948	C	4.731625	-1.572127	-1.637837
C	-1.488232	5.243482	0.278837	H	4.349773	-0.661974	-2.114995
C	-0.787341	6.463744	0.499800	H	5.818180	-1.571273	-1.790772
C	-2.834146	5.306394	-0.216065	C	4.123167	-2.800497	-2.275349
C	-2.923134	2.894308	-0.133209	C	4.918993	-3.911007	-2.594112
C	-1.396429	7.670561	0.242063	C	2.748985	-2.868748	-2.552505
H	0.225730	6.435812	0.874183	C	4.363742	-5.050400	-3.177970
C	-3.426694	6.570289	-0.478098	H	5.985673	-3.879645	-2.384510
C	-3.522599	4.092687	-0.438350	C	2.190717	-4.007083	-3.135406
H	-3.424036	1.948828	-0.298540	H	2.103646	-2.031541	-2.302943
C	-2.722592	7.728655	-0.252751	C	2.996317	-5.102716	-3.452832
H	-0.851496	8.592984	0.418218	H	5.002124	-5.896592	-3.418814
H	-4.443677	6.600851	-0.858054	H	1.123142	-4.031173	-3.332731
H	-4.525287	4.104616	-0.853735	H	2.562055	-5.988321	-3.908565
H	-3.179556	8.693024	-0.453406	C	0.478203	-0.279100	1.942399
N	-1.662657	2.817483	0.361304	C	2.951426	2.610643	-0.591010
Ni	-0.699321	1.076850	1.093894	C	2.753888	1.762498	-1.679238
C	2.623107	3.915542	1.389504	C	3.738024	3.763170	-0.710829

C	3.381591	2.070375	-2.890187
H	2.106918	0.897740	-1.595424
C	4.368241	4.065344	-1.916854
C	4.188523	3.207814	-3.005956
H	3.225927	1.427246	-3.751042
H	4.978481	4.959476	-2.015696
H	4.665084	3.435686	-3.955231
C	3.768106	4.537984	0.588307
H	4.710955	4.378386	1.128005
H	3.638632	5.618549	0.468599
Br	-0.951074	1.025972	-2.748803
C	-2.179102	0.926358	3.449321
H	-1.625100	0.168726	4.013011
H	-1.560356	1.834266	3.487140
C	-3.495625	1.235981	4.186675
H	-4.157160	0.364366	4.237644
H	-3.300577	1.556504	5.216182
H	-4.046625	2.040737	3.685899
H	-3.072960	1.221056	1.553003
C	0.033069	-1.602841	2.597945
H	-0.274482	-2.331390	1.843802
H	0.874636	-2.043114	3.147498
H	-0.779289	-1.463483	3.311724
H	0.758127	0.426381	2.746761

^{1}IM8-*SS*

B3LYP/BSI SCF energy: -3059.035406a.u.

M06/BSII SCF energy in solution:-3057.744689a.u.

M06/BSII free energy in solution:-3056.813209a.u.

C	-3.550916	0.904653	0.317207
O	-3.004053	-0.121360	0.768311
N	-4.838939	1.208813	0.637951
C	-2.793179	1.815231	-0.644675
H	-3.217620	1.636610	-1.642680
H	-3.034086	2.860563	-0.420306
C	-1.277036	1.557622	-0.654162
C	-5.499085	2.367593	0.091150
C	-6.141782	2.290966	-1.148977
C	-5.544823	3.556434	0.828064
C	-6.818266	3.402770	-1.653470
H	-6.106911	1.362504	-1.710707
C	-6.223402	4.664951	0.320438
H	-5.042985	3.604834	1.789655
C	-6.859872	4.590219	-0.920489
H	-7.312765	3.339578	-2.618219
H	-6.252333	5.586881	0.893534
H	-7.386110	5.454417	-1.314612
C	-5.670674	0.326660	1.513818
C	-5.947315	-1.047810	0.877599
C	-5.112456	0.192317	2.941600
H	-6.627829	0.855885	1.585308
C	-6.890573	-1.876760	1.765681
H	-4.999015	-1.576649	0.742844
H	-6.389021	-0.907669	-0.116549
C	-6.065477	-0.638793	3.817079
H	-4.132706	-0.290933	2.897657
H	-4.967550	1.189758	3.373881
C	-6.345581	-2.014998	3.194803
H	-7.043613	-2.864826	1.316842
H	-7.878381	-1.394532	1.800861
H	-5.638186	-0.751619	4.820158
H	-7.014910	-0.098076	3.943018
H	-7.052499	-2.576047	3.817314
H	-5.414506	-2.597821	3.171724
C	0.494350	-2.395979	-1.000309
N	0.444374	-1.700708	0.128620
C	1.572854	-2.149352	0.956498
H	2.069382	-1.295240	1.424970
O	1.586334	-3.191601	-1.152855
C	-0.543517	-2.281781	-1.962014
C	-0.668649	-3.025497	-3.196004
C	0.308519	-3.923369	-3.688942
C	-1.865473	-2.838846	-3.960029
C	-2.623181	-1.252248	-2.290771
C	0.113841	-4.599801	-4.884244
H	1.216541	-4.081451	-3.123207
C	-2.034973	-3.542670	-5.171401
C	-2.856896	-1.940850	-3.454692
H	-3.366309	-0.565538	-1.904141
C	-1.060298	-4.412171	-5.632220
H	0.879678	-5.282391	-5.241869
H	-2.949284	-3.389389	-5.739250
H	-3.787535	-1.800296	-3.995132
H	-1.203428	-4.947566	-6.566555
N	-1.495902	-1.369325	-1.555014
Ni	-0.937817	-0.269448	0.104003
C	2.491469	-2.898134	-0.046322

H	3.307380	-2.290267	-0.445776
C	-0.163133	0.612335	1.750669
H	0.005053	-0.310631	2.318084
C	-0.632381	1.701092	-2.034142
H	-1.133691	1.050581	-2.760304
H	0.408054	1.358647	-1.979673
C	-0.631984	3.148640	-2.563194
H	-0.085529	3.814308	-1.885758
H	-0.152365	3.205521	-3.546930
H	-1.649708	3.542540	-2.669777
H	-0.791479	2.269414	0.013908
C	-1.053208	1.546545	2.577732
H	-1.971536	1.034282	2.873454
H	-0.535575	1.870207	3.490549
H	-1.325273	2.452817	2.027902
C	1.098887	1.184237	1.375488
C	2.171002	1.665602	1.024234
Si	3.757638	2.335419	0.441669
C	3.624318	4.209991	0.215367
C	3.545157	4.798668	-1.059642
C	3.569437	5.064831	1.332638
C	3.416509	6.181030	-1.213609
H	3.586909	4.170466	-1.945079
C	3.441895	6.446348	1.185537
H	3.619777	4.649726	2.336742
C	3.365453	7.008083	-0.090915
H	3.356910	6.610990	-2.209973
H	3.402399	7.084118	2.064672
H	3.266952	8.083890	-0.208616
C	4.225916	1.504954	-1.190397
C	5.410901	1.849629	-1.868812
C	3.422505	0.496802	-1.752658
C	5.777658	1.215042	-3.057166
H	6.057849	2.630010	-1.472606
C	3.785346	-0.144409	-2.939969
H	2.501015	0.211320	-1.253224
C	4.964804	0.214207	-3.594499
H	6.695847	1.501240	-3.563396
H	3.146334	-0.922048	-3.349881
H	5.249291	-0.281467	-4.518716
C	5.121403	1.991780	1.743170
H	4.867628	2.564200	2.643346
H	6.054959	2.418227	1.355884
C	5.309788	0.534912	2.085971
C	4.560022	-0.069749	3.108327
C	6.224992	-0.262173	1.380365
C	4.725376	-1.419723	3.421207
H	3.843085	0.528183	3.664579
C	6.394611	-1.612037	1.691751
H	6.811529	0.182670	0.580879
C	5.647379	-2.197686	2.716065
H	4.137660	-1.863285	4.220212
H	7.118109	-2.204196	1.137611
H	5.788551	-3.244507	2.970487
C	1.210335	-3.233162	1.966529
C	0.251669	-3.194810	2.978971
C	1.982509	-4.384412	1.765301
C	0.076645	-4.316072	3.794065
H	-0.364830	-2.312771	3.126061
C	1.806950	-5.504491	2.577781
C	0.850457	-5.464284	3.595255
H	-0.669249	-4.297928	4.583792
H	2.400878	-6.401289	2.419583
H	0.702745	-6.332000	4.232200
C	2.957774	-4.196449	0.623169
H	2.967488	-5.028836	-0.088074
H	3.982172	-4.068005	0.994482

^{1}IM8-*RR*

B3LYP/BSI SCF energy: -3059.038239a.u.

M06/BSII SCF energy in solution:-3057.745782a.u.

M06/BSII free energy in solution:-3056.812027a.u.

C	3.740126	1.076212	-0.140345
O	3.001040	0.070575	-0.147357
N	5.090939	0.970504	-0.297579
C	3.112240	2.438334	0.102949
H	3.857275	3.153731	0.467411
H	2.759550	2.830708	-0.861444
C	1.944969	2.255220	1.078848
C	5.918271	2.134249	-0.477336
C	6.820527	2.509768	0.525293
C	5.862937	2.862778	-1.670453
C	7.655106	3.610924	0.335544
H	6.854702	1.941803	1.450093
C	6.693580	3.969836	-1.851885
H	5.170027	2.557918	-2.448674
C	7.591873	4.344702	-0.851598

H	8.349727	3.899945	1.118693	C	0.273652	1.641973	-1.112282
H	6.642123	4.533731	-2.778554	C	-1.160997	1.570651	-1.056688
H	8.240004	5.203890	-0.995622	C	-2.386976	1.511729	-1.030864
C	5.779285	-0.351529	-0.411161	Si	-4.202669	1.479200	-1.078854
C	5.533312	-1.272871	0.796364	C	-4.861545	3.231819	-0.793722
C	5.473147	-1.059248	-1.741733	C	-6.053433	3.478957	-0.089442
H	6.844390	-0.093374	-0.413513	C	-4.176422	4.339363	-1.328312
C	6.358473	-2.564114	0.657916	C	-6.548061	4.775784	0.065887
H	4.469164	-1.514610	0.856313	H	-6.598772	2.650949	0.355855
H	5.800804	-0.744937	1.719973	C	-4.666066	5.637119	-1.176536
C	6.291132	-2.355754	-1.867145	H	-3.239093	4.184450	-1.857546
H	4.404653	-1.288202	-1.776904	C	-5.856175	5.857972	-0.479786
H	5.696194	-0.383705	-2.576429	H	-7.469788	4.940916	0.617648
C	6.061335	-3.284901	-0.665453	H	-4.117354	6.476199	-1.596394
H	6.150001	-3.224410	1.507343	H	-6.238188	6.868030	-0.357923
H	7.430571	-2.322939	0.706129	C	-4.893331	0.291906	0.219074
H	6.033805	-2.866771	-2.802660	C	-6.229058	-0.153051	0.172522
H	7.360360	-2.107751	-1.935665	C	-4.088942	-0.170463	1.276277
H	6.685820	-4.181613	-0.756230	C	-6.740782	-1.019248	1.140565
H	5.017214	-3.624953	-0.666373	H	-6.885955	0.176679	-0.630008
C	-0.544566	-1.641794	1.242464	C	-4.592405	-1.042851	2.244553
N	-0.070956	-1.068604	0.162759	H	-3.054742	0.156643	1.340379
C	-0.553613	-1.852788	-0.986078	C	-5.920357	-1.467688	2.177879
H	-0.947820	-1.182902	-1.753963	H	-7.775608	-1.346694	1.083049
O	-1.361321	-2.706028	1.048674	H	-3.945859	-1.393217	3.044009
C	-0.262764	-1.113495	2.544128	H	-6.314419	-2.146161	2.929783
C	-0.700878	-1.669523	3.800338	C	-4.779572	0.927655	-2.823785
C	-1.409627	-2.891644	3.938282	H	-4.499404	1.737174	-3.508138
C	-0.386220	-0.938503	4.991100	H	-5.876298	0.902734	-2.813102
C	0.729863	0.713901	3.613366	C	-4.225613	-0.387010	-3.312800
C	-1.794438	-3.351468	5.187899	C	-3.016545	-0.437550	-4.026921
H	-1.648540	-3.470037	3.057209	C	-4.892340	-1.597588	-3.064577
C	-0.792617	-1.432390	6.248557	C	-2.497348	-1.649948	-4.482883
C	0.340621	0.282708	4.851704	H	-2.482600	0.486959	-4.229353
H	1.284048	1.638825	3.514017	C	-4.376764	-2.812302	-3.521048
C	-1.490483	-2.623397	6.351781	H	-5.827804	-1.586479	-2.511943
H	-2.335298	-4.290579	5.265192	C	-3.176299	-2.845469	-4.234369
H	-0.544982	-0.858527	7.137925	H	-1.565025	-1.660223	-5.041090
H	0.587474	0.869044	5.731309	H	-4.921143	-3.732913	-3.327065
H	-1.798904	-2.995277	7.324521	H	-2.779076	-3.787997	-4.600369
N	0.461094	0.054134	2.454769	C	0.445185	-2.855420	-1.549352
Ni	0.920980	0.650326	0.530482	C	1.715038	-2.617220	-2.074141
C	-1.661168	-2.755142	-0.378002	C	-0.072867	-4.156417	-1.507000
H	-2.674592	-2.367807	-0.505812	C	2.457437	-3.693572	-2.568115

H	2.125744	-1.613688	-2.080899
C	0.672504	-5.231142	-1.992239
C	1.940623	-4.993008	-2.527078
H	3.444493	-3.519947	-2.987470
H	0.273574	-6.241870	-1.956394
H	2.529652	-5.821500	-2.910746
C	-1.469757	-4.174149	-0.926375
H	-1.610859	-4.925139	-0.141948
H	-2.218246	-4.368136	-1.704240
C	0.860553	1.110172	-2.429945
H	0.590817	0.069112	-2.615176
H	0.498090	1.696418	-3.286056
H	1.952437	1.170414	-2.424217
H	0.570458	2.685230	-0.991611
C	1.185197	3.540251	1.408143
H	0.782547	3.993139	0.493108
H	0.311544	3.287559	2.021676
C	2.014309	4.603665	2.153196
H	2.856376	4.962992	1.551623
H	1.398311	5.473533	2.406283
H	2.424997	4.204834	3.088739
H	2.378465	1.852315	2.004404

^{1}IM8-*SR*

B3LYP/BSI SCF energy: -3059.035055a.u.

M06/BSII SCF energy in solution:-3057.742055a.u.

M06/BSII free energy in solution:-3056.81085a.u.

C	3.483737	1.257123	-0.267005
O	2.891741	0.175491	-0.470880
N	4.828281	1.357955	-0.447253
C	2.687898	2.471946	0.187691
H	3.298387	3.084794	0.862147
H	2.519008	3.097970	-0.696608
C	1.354976	2.056429	0.823516
C	5.506719	2.623428	-0.337545
C	6.292836	2.898721	0.787465
C	5.423729	3.558460	-1.374677
C	6.984760	4.106878	0.875293
H	6.350491	2.167988	1.588508
C	6.112445	4.768745	-1.279148
H	4.821441	3.332316	-2.249286
C	6.893987	5.044592	-0.155948
H	7.590025	4.317279	1.752020
H	6.041334	5.492712	-2.085426
H	7.430694	5.985774	-0.084134
C	5.665798	0.181396	-0.836788
C	5.630640	-0.950251	0.205827
C	5.345870	-0.335066	-2.251425
H	6.686231	0.580760	-0.855310
C	6.588416	-2.083823	-0.197770
H	4.610803	-1.335581	0.286650
H	5.906963	-0.551008	1.189354
C	6.303573	-1.473942	-2.640480
H	4.312815	-0.694097	-2.272171
H	5.423791	0.491319	-2.968480
C	6.277761	-2.610183	-1.607033
H	6.524880	-2.895083	0.536181
H	7.625151	-1.717555	-0.169101
H	6.038821	-1.853274	-3.634304
H	7.327416	-1.080467	-2.721094
H	6.993796	-3.392133	-1.886104
H	5.283631	-3.077492	-1.607457
C	-0.309257	-2.185922	0.929358
N	-0.226708	-1.413651	-0.143338
C	-1.023547	-2.058399	-1.195766
H	-1.623942	-1.318400	-1.732542
O	-1.173158	-3.231390	0.835318
C	0.460375	-1.901770	2.087780
C	0.522407	-2.689936	3.299072
C	-0.275975	-3.832032	3.551785
C	1.459339	-2.283258	4.303415
C	2.094907	-0.425642	2.881973
C	-0.155966	-4.534910	4.742025
H	-0.986631	-4.157620	2.804706
C	1.559716	-3.020404	5.502363
C	2.268413	-1.133385	4.044893
H	2.695393	0.458639	2.692484
C	0.763748	-4.132313	5.724171
H	-0.781920	-5.406548	4.911767
H	2.276167	-2.697118	6.253434
H	3.005624	-0.812829	4.774016
H	0.850613	-4.690071	6.652320
N	1.201521	-0.748472	1.921208
Ni	0.840311	0.258073	0.111240
C	-1.900813	-3.075721	-0.419084
H	-2.900916	-2.708335	-0.174519
C	0.062937	1.034784	-1.595704

H	0.103905	0.090765	-2.148292
C	0.766089	2.094639	-2.449431
H	1.805879	1.809810	-2.637497
H	0.271014	2.185527	-3.425897
H	0.750699	3.086275	-1.993194
C	-1.305735	1.332468	-1.279237
C	-2.474991	1.550356	-0.979508
Si	-4.194162	1.779188	-0.432312
C	-4.508874	3.603609	-0.037369
C	-4.892045	4.042823	1.242031
C	-4.360024	4.576824	-1.044349
C	-5.122726	5.395495	1.504975
H	-5.010553	3.321132	2.045420
C	-4.588101	5.928767	-0.787857
H	-4.051413	4.278366	-2.044089
C	-4.972530	6.341142	0.490327
H	-5.417481	5.709644	2.502798
H	-4.465336	6.660211	-1.582304
H	-5.151488	7.393619	0.693291
C	-4.516212	0.693806	1.080350
C	-5.797464	0.613979	1.660131
C	-3.492320	-0.085368	1.648997
C	-6.044978	-0.206036	2.762717
H	-6.617767	1.201700	1.252272
C	-3.734968	-0.911980	2.749232
H	-2.494577	-0.046665	1.221458
C	-5.012487	-0.972390	3.308390
H	-7.041622	-0.248222	3.194296
H	-2.927106	-1.508050	3.164843
H	-5.203679	-1.613284	4.164865
C	-5.394869	1.281643	-1.840793
H	-5.278705	2.022727	-2.640540
H	-6.413779	1.403179	-1.452609
C	-5.198877	-0.111966	-2.382654
C	-4.339492	-0.350188	-3.467800
C	-5.854581	-1.212892	-1.808479
C	-4.150677	-1.638836	-3.969188
H	-3.819946	0.487043	-3.926391
C	-5.668445	-2.503218	-2.307384
H	-6.521287	-1.054199	-0.965140
C	-4.817076	-2.723097	-3.392827
H	-3.488230	-1.795090	-4.816327
H	-6.198230	-3.336217	-1.852731
H	-4.683859	-3.724232	-3.793466
C	-0.218464	-2.945783	-2.139831
C	0.875632	-2.605754	-2.935616
C	-0.709685	-4.257604	-2.133093
C	1.468336	-3.588283	-3.733106
H	1.275589	-1.596139	-2.926481
C	-0.116860	-5.238736	-2.927688
C	0.974068	-4.896853	-3.730677
H	2.321715	-3.335204	-4.356168
H	-0.493477	-6.258583	-2.920560
H	1.445147	-5.653286	-4.352291
C	-1.899201	-4.391405	-1.206786
H	-1.840438	-5.255644	-0.537094
H	-2.834888	-4.477497	-1.773104
H	1.549635	1.742287	1.852686
C	0.311487	3.167858	0.893820
H	-0.629068	2.745888	1.265803
H	0.082598	3.561456	-0.102176
C	0.718803	4.340266	1.807208
H	-0.082962	5.084099	1.868670
H	0.930488	3.993421	2.825637
H	1.615391	4.851954	1.438508

^{1}IM8-*RS*

B3LYP/BSI SCF energy: -3059.033742a.u.

M06/BSII SCF energy in solution:-3057.741646a.u.

M06/BSII free energy in solution:-3056.81016a.u.

C	-3.633203	0.726491	0.213283
O	-3.097666	-0.120802	0.956270
N	-4.812641	1.314334	0.557183
C	-2.986135	1.075947	-1.122665
H	-3.467840	0.425868	-1.867600
H	-3.247266	2.099360	-1.411982
C	-1.468873	0.838839	-1.137136
C	-5.496550	2.218825	-0.332417
C	-6.268917	1.719591	-1.386455
C	-5.433086	3.598680	-0.107151
C	-6.963147	2.598549	-2.219243
H	-6.319359	0.647352	-1.549090
C	-6.132687	4.473041	-0.939355
H	-4.829518	3.977050	0.712228
C	-6.896975	3.975096	-1.996996
H	-7.557228	2.206192	-3.039220
H	-6.075965	5.543197	-0.763997

H	-7.438274	4.657510	-2.645338	C	1.932508	1.865226	0.587729
C	-5.518865	0.984855	1.833885	Si	3.465547	2.690992	0.060063
C	-6.019740	-0.470528	1.872595	C	3.097724	4.527098	-0.231234
C	-4.699484	1.342712	3.086504	C	3.571364	5.223954	-1.356744
H	-6.400213	1.636167	1.822562	C	2.347883	5.249650	0.716836
C	-6.824751	-0.734423	3.155951	C	3.316027	6.587026	-1.525897
H	-5.159034	-1.144313	1.826420	H	4.140241	4.696164	-2.117370
H	-6.639140	-0.666194	0.988680	C	2.090698	6.611006	0.553868
C	-5.516232	1.070325	4.360907	H	1.946751	4.737094	1.588360
H	-3.783230	0.746712	3.098063	C	2.576920	7.284026	-0.569576
H	-4.402823	2.397643	3.040399	H	3.690886	7.102458	-2.406271
C	-6.014354	-0.381937	4.412190	H	1.508768	7.146318	1.299655
H	-7.138829	-1.784100	3.184000	H	2.376560	8.344139	-0.699977
H	-7.746026	-0.134087	3.140484	C	4.139739	1.896825	-1.516580
H	-4.906193	1.297206	5.242802	C	5.426836	2.201691	-1.999622
H	-6.379915	1.750202	4.397612	C	3.364707	0.987797	-2.258502
H	-6.620006	-0.543397	5.311662	C	5.918084	1.627347	-3.173831
H	-5.151561	-1.058037	4.487624	H	6.060724	2.900144	-1.456976
C	0.458727	-2.691627	-0.751915	C	3.850733	0.407876	-3.432880
N	0.500063	-1.845279	0.271162	H	2.368024	0.732785	-1.908870
C	1.855977	-1.947723	0.827805	C	5.129467	0.727042	-3.892994
H	2.219890	-0.967055	1.143303	H	6.914755	1.880322	-3.525629
O	1.647013	-3.257431	-1.095267	H	3.230310	-0.290443	-3.988408
C	-0.766383	-2.947996	-1.424423	H	5.509683	0.277296	-4.806144
C	-1.010976	-3.934498	-2.450995	C	4.774907	2.584782	1.454173
C	-0.003915	-4.730340	-3.047264	H	4.380307	3.168630	2.294437
C	-2.366046	-4.116697	-2.878555	H	5.665926	3.119610	1.102627
C	-3.041971	-2.374461	-1.331657	C	5.138126	1.191323	1.903785
C	-0.321199	-5.660410	-4.026007	C	4.400964	0.543049	2.908677
H	1.023591	-4.606812	-2.732429	C	6.210834	0.497462	1.322771
C	-2.656663	-5.073092	-3.874470	C	4.726147	-0.749641	3.321135
C	-3.384538	-3.319384	-2.265824	H	3.565035	1.061893	3.370330
H	-3.798025	-1.758927	-0.857422	C	6.540864	-0.794903	1.734709
C	-1.650833	-5.836420	-4.444288	H	6.794751	0.976704	0.541483
H	0.469180	-6.258930	-4.470245	C	5.800159	-1.425559	2.736402
H	-3.689695	-5.201123	-4.188143	H	4.139758	-1.231363	4.098309
H	-4.424088	-3.461743	-2.543534	H	7.383304	-1.305927	1.275779
H	-1.889052	-6.568891	-5.210358	H	6.055134	-2.430003	3.061418
N	-1.772347	-2.147674	-0.925024	C	2.003679	-3.005006	1.924278
Ni	-1.065144	-0.606114	0.203001	C	1.271278	-3.162416	3.100845
C	2.680132	-2.560615	-0.330046	C	3.027723	-3.908081	1.606637
H	3.144896	-1.826243	-0.994450	C	1.591383	-4.210210	3.969382
C	-0.376644	0.834118	1.422274	H	0.448665	-2.495403	3.334213
C	0.869295	1.389339	0.973365	C	3.345698	-4.954747	2.470854

C	2.626042	-5.098324	3.660009
H	1.024589	-4.340397	4.887137
H	4.135604	-5.658261	2.219458
H	2.862077	-5.911973	4.340259
C	3.661082	-3.565433	0.276227
H	3.810314	-4.430650	-0.377843
H	4.636053	-3.080947	0.415414
C	-0.324919	0.257943	2.844993
H	0.516869	-0.423818	2.973928
H	-0.210857	1.060067	3.588052
H	-1.248823	-0.281051	3.079954
H	-1.155751	1.600616	1.371765
H	-0.957387	1.740951	-0.793609
C	-0.926084	0.472883	-2.518078
H	0.115988	0.143609	-2.420641
H	-1.477940	-0.381737	-2.926442
C	-0.971619	1.636626	-3.527190
H	-1.998177	1.974885	-3.709433
H	-0.397386	2.495963	-3.163418
H	-0.548483	1.335801	-4.492235

^{1}TS6-*SS*

B3LYP/BSI SCF energy: -3058.996971a.u.

M06/BSII SCF energy in solution:-3057.7213a.u.

M06/BSII free energy in solution:-3056.791282a.u.

B3LYP-D3(BJ)/BSII free energy in solution: -3059.108679 a.u.

C	3.513343	-1.107445	0.301607
O	3.099581	-0.149299	0.985500
N	4.714836	-1.690130	0.556810
C	2.671810	-1.584653	-0.868415
H	2.957258	-0.931491	-1.704942
H	2.947023	-2.602746	-1.156746
C	1.137077	-1.474792	-0.668257
C	5.253988	-2.725480	-0.288963
C	5.845107	-2.398529	-1.514066
C	5.234616	-4.055875	0.144586
C	6.400808	-3.402772	-2.308331
H	5.863153	-1.362783	-1.839008
C	5.797050	-5.054871	-0.650379
H	4.772924	-4.299109	1.096679
C	6.379067	-4.730653	-1.878033
H	6.853387	-3.145018	-3.261118
H	5.775739	-6.086622	-0.312425
H	6.813529	-5.510087	-2.496636
C	5.609505	-1.201502	1.654699
C	6.140789	0.219120	1.390920
C	4.978855	-1.326855	3.052516
H	6.463996	-1.886552	1.619055
C	7.135415	0.639055	2.486284
H	5.298598	0.916982	1.364338
H	6.625158	0.250031	0.407390
C	5.986702	-0.904704	4.135298
H	4.092174	-0.689420	3.105295
H	4.652223	-2.361117	3.216993
C	6.518054	0.515024	3.887034
H	7.468812	1.666837	2.303823
H	8.032564	0.005629	2.428984
H	5.512724	-0.969223	5.121436
H	6.829969	-1.610549	4.149114
H	7.256860	0.781783	4.651725
H	5.691581	1.232372	3.983204
C	-0.113930	2.741879	-0.849717
N	-0.355927	1.785865	0.034288
C	-1.652318	2.081711	0.647116
H	-2.244619	1.169208	0.766801
O	-1.155735	3.597240	-1.077700
C	1.151410	2.888456	-1.483489
C	1.508545	3.869449	-2.490188
C	0.605970	4.794457	-3.065167
C	2.872255	3.894133	-2.936634
C	3.346033	2.048716	-1.435008
C	1.025103	5.703636	-4.029452
H	-0.427023	4.792277	-2.746324
C	3.267621	4.830313	-3.914122
C	3.793219	2.957861	-2.366057
H	4.034858	1.337692	-0.986157
C	2.359560	5.727668	-4.458008
H	0.306928	6.401565	-4.451535
H	4.305955	4.835666	-4.237433
H	4.835569	2.968474	-2.668889
H	2.681131	6.442717	-5.210321
N	2.074332	1.971852	-0.998578
Ni	1.237361	0.546200	0.232834
C	-2.297461	3.104757	-0.327603
H	-2.999329	2.661601	-1.040990
C	0.278160	-1.160771	1.159112

H	0.350525	-0.207709	1.726954
C	0.389999	-1.026803	-1.932560
H	0.811186	-0.093172	-2.318645
H	-0.650078	-0.820868	-1.668133
C	0.409021	-2.101595	-3.035634
H	-0.048735	-3.034216	-2.686620
H	-0.153088	-1.760432	-3.911227
H	1.427527	-2.331274	-3.369291
H	0.786607	-2.487278	-0.457488
C	0.916439	-2.258759	2.017765
H	1.938197	-1.993057	2.292598
H	0.343717	-2.391374	2.942432
H	0.924833	-3.224324	1.500392
C	-1.097375	-1.427634	0.842752
C	-2.250226	-1.721069	0.552737
Si	-3.935764	-2.269564	0.097275
C	-3.891304	-4.126112	-0.271332
C	-3.903694	-4.615606	-1.590069
C	-3.818834	-5.067630	0.773002
C	-3.846096	-5.985459	-1.855967
H	-3.963928	-3.918623	-2.421355
C	-3.761743	-6.437478	0.513691
H	-3.802639	-4.732112	1.807481
C	-3.775668	-6.899697	-0.804076
H	-3.858067	-6.337772	-2.883971
H	-3.708273	-7.143584	1.338089
H	-3.733128	-7.966046	-1.008672
C	-4.523250	-1.321432	-1.424565
C	-5.766994	-1.623447	-2.012963
C	-3.763508	-0.287570	-1.999503
C	-6.231648	-0.923226	-3.127336
H	-6.382138	-2.423165	-1.605127
C	-4.222367	0.415341	-3.116321
H	-2.800370	-0.028313	-1.569501
C	-5.458562	0.099381	-3.681630
H	-7.193980	-1.176454	-3.564086
H	-3.612473	1.205974	-3.545228
H	-5.817227	0.644311	-4.550519
C	-5.138234	-1.985636	1.556590
H	-4.764990	-2.565538	2.409327
H	-6.094291	-2.440566	1.269020
C	-5.341214	-0.543027	1.953382
C	-4.480497	0.082293	2.869556
C	-6.387180	0.215673	1.405833
C	-4.660664	1.418216	3.231086
H	-3.662280	-0.486655	3.303443
C	-6.571726	1.551158	1.766095
H	-7.064030	-0.246928	0.692247
C	-5.709537	2.158717	2.680980
H	-3.979176	1.881591	3.938117
H	-7.393578	2.115428	1.333341
H	-5.853707	3.196500	2.967492
C	-1.568340	2.858596	1.956416
C	-0.916915	2.500595	3.136184
C	-2.262978	4.071088	1.870050
C	-0.967956	3.364811	4.233189
H	-0.367433	1.565398	3.201675
C	-2.311664	4.936869	2.962823
C	-1.661974	4.577070	4.146597
H	-0.461793	3.097435	5.156756
H	-2.844504	5.882364	2.896873
H	-1.691285	5.244761	5.003281
C	-2.915981	4.230888	0.513870
H	-2.743670	5.209661	0.054491
H	-4.001826	4.086480	0.584753

B3LYP-D3BJ/BSI SCF energy in solution: -3059.401905a.u.

M06/BSII SCF energy in solution: -3057.726458a.u.

M06/BSII free energy in solution: -3056.788569a.u.

C	3.542868	-0.715939	0.336920
O	3.042106	0.317680	0.834047
N	4.821090	-1.068215	0.589593
C	2.709143	-1.564415	-0.599157
H	2.865665	-1.132432	-1.596161
H	3.095384	-2.584632	-0.637627
C	1.194511	-1.576451	-0.300647
C	5.444114	-2.166239	-0.097533
C	5.835336	-2.021022	-1.430754
C	5.688949	-3.358875	0.587953
C	6.462538	-3.082361	-2.084832
H	5.642340	-1.085079	-1.945255
C	6.321970	-4.413660	-0.069526
H	5.374952	-3.453422	1.622559
C	6.707125	-4.277769	-1.405762
H	6.761900	-2.972830	-3.122667

H	6.509120	-5.342698	0.460239	H	0.517044	-0.001352	1.955353
H	7.196589	-5.101729	-1.915860	C	0.315421	-1.448383	-1.545973
C	5.704954	-0.248735	1.466614	H	0.644392	-0.609875	-2.166151
C	6.018010	1.120474	0.846898	H	-0.709767	-1.241196	-1.237502
C	5.176264	-0.130730	2.902082	C	0.311447	-2.740884	-2.375984
H	6.639091	-0.816856	1.507449	H	-0.075236	-3.581127	-1.788214
C	7.006041	1.893771	1.730778	H	-0.326567	-2.625547	-3.259213
H	5.088486	1.688057	0.743401	H	1.316358	-3.006315	-2.724374
H	6.431910	0.975740	-0.157715	H	0.972388	-2.558222	0.115386
C	6.175736	0.646146	3.770740	C	1.312908	-1.924442	2.446895
H	4.214604	0.388123	2.892667	H	2.343056	-1.568724	2.508246
H	5.007998	-1.134010	3.310350	H	0.897300	-1.911561	3.460673
C	6.487227	2.022622	3.168585	H	1.318692	-2.963672	2.103654
H	7.189970	2.883972	1.299076	C	-0.876645	-1.432591	1.347772
H	7.971748	1.369000	1.741211	C	-2.008864	-1.799228	1.066058
H	5.775050	0.753554	4.785044	Si	-3.605136	-2.372793	0.401147
H	7.108177	0.070723	3.859417	C	-3.458616	-4.198732	-0.020102
H	7.220229	2.550316	3.789750	C	-3.056589	-4.602867	-1.306176
H	5.572794	2.631534	3.168952	C	-3.689593	-5.194879	0.944491
C	-0.738893	2.295594	-1.007185	C	-2.884336	-5.952831	-1.615934
N	-0.724376	1.525011	0.062847	H	-2.879716	-3.855674	-2.074764
C	-1.926558	1.819637	0.851975	C	-3.522125	-6.546723	0.638578
H	-2.449966	0.896776	1.112132	H	-4.001590	-4.917184	1.948132
O	-1.878446	3.018626	-1.195437	C	-3.116825	-6.927372	-0.642626
C	0.380387	2.399474	-1.881474	H	-2.572401	-6.244126	-2.615037
C	0.425587	3.100941	-3.144706	H	-3.706986	-7.301680	1.397665
C	-0.680555	3.748421	-3.742961	H	-2.985613	-7.978800	-0.882313
C	1.679965	3.121374	-3.844939	C	-4.003751	-1.404134	-1.158509
C	2.647304	1.795544	-2.055695	C	-5.134767	-1.749778	-1.921375
C	-0.560339	4.392242	-4.970736	C	-3.230269	-0.313157	-1.583982
H	-1.633105	3.747608	-3.231218	C	-5.478753	-1.028360	-3.065499
C	1.770770	3.785944	-5.084747	H	-5.752808	-2.594515	-1.625137
C	2.803802	2.458529	-3.253660	C	-3.566750	0.411513	-2.729788
H	3.486286	1.285225	-1.591155	H	-2.352647	-0.025653	-1.018371
C	0.666636	4.415586	-5.647005	C	-4.694106	0.055182	-3.471315
H	-1.429010	4.880364	-5.403972	H	-6.355535	-1.310713	-3.641661
H	2.728694	3.794563	-5.598745	H	-2.951308	1.253001	-3.033551
H	3.767234	2.475643	-3.752721	H	-4.960552	0.616529	-4.362439
H	0.755485	4.922138	-6.603884	C	-4.971356	-2.087449	1.684635
N	1.489192	1.733924	-1.376901	H	-4.786471	-2.733932	2.549138
Ni	1.053143	0.545426	0.230775	H	-5.920980	-2.403870	1.238204
C	-2.763718	2.759400	-0.067815	C	-5.020069	-0.641899	2.100883
H	-3.665259	2.295123	-0.466337	C	-4.284545	-0.191064	3.208488
C	0.483818	-1.027712	1.529550	C	-5.747254	0.300767	1.358020

C	-4.296869	1.153361	3.579522
H	-3.700646	-0.905583	3.782464
C	-5.759703	1.647365	1.727317
H	-6.308510	-0.025596	0.487052
C	-5.038480	2.079002	2.842441
H	-3.718865	1.481829	4.437743
H	-6.337227	2.358540	1.143185
H	-5.044579	3.125022	3.131036
C	-1.644094	2.659999	2.079271
C	-0.907092	2.306964	3.208697
C	-2.245256	3.919435	1.983635
C	-0.765441	3.234066	4.244770
H	-0.459670	1.321129	3.289462
C	-2.106504	4.845214	3.018141
C	-1.361491	4.497225	4.148606
H	-0.194885	2.972049	5.131222
H	-2.574548	5.823773	2.950013
H	-1.247026	5.210703	4.959672
C	-3.044115	4.058737	0.708860
H	-2.755489	4.931963	0.115091
H	-4.113761	4.152214	0.9243

^{1}TS6-*SR*

B3LYP/BSI SCF energy: -3058.995741a.u.

M06/BSII SCF energy in solution:-3057.717435a.u.

M06/BSII free energy in solution:-3056.788323a.u.

B3LYP-D3(BJ)/BSII free energy in solution: -3059.106174 a.u.

C	3.581964	1.158206	-0.247092
O	3.113211	0.070417	-0.637215
N	4.859266	1.518454	-0.540829
C	2.718077	2.112901	0.560281
H	3.234318	2.333730	1.503699
H	2.671852	3.074481	0.038240
C	1.321890	1.570688	0.861029
C	5.415419	2.761833	-0.069981
C	6.046473	2.818394	1.177608
C	5.368402	3.901051	-0.880736
C	6.619379	4.013707	1.614529
H	6.083802	1.926966	1.796502
C	5.943941	5.093723	-0.440011
H	4.880934	3.845980	-1.849381
C	6.568525	5.152135	0.807477
H	7.105707	4.053735	2.584565
H	5.903104	5.976188	-1.071486
H	7.014741	6.081171	1.149172
C	5.762126	0.645515	-1.355991
C	6.086562	-0.690569	-0.663802
C	5.249206	0.437403	-2.792289
H	6.693082	1.220348	-1.419213
C	7.092140	-1.500864	-1.499336
H	5.163595	-1.262790	-0.534814
H	6.494260	-0.494849	0.335508
C	6.261574	-0.378349	-3.613801
H	4.289989	-0.087142	-2.757999
H	5.074633	1.412670	-3.263417
C	6.590049	-1.716316	-2.934842
H	7.280193	-2.463699	-1.011230
H	8.056349	-0.972411	-1.527899
H	5.865445	-0.546529	-4.621787
H	7.187373	0.202609	-3.735966
H	7.338561	-2.263731	-3.519523
H	5.687835	-2.342531	-2.912292
C	-0.304473	-2.637032	0.865854
N	-0.430792	-1.654875	-0.017818
C	-1.629705	-1.940986	-0.810678
H	-2.208530	-1.028036	-0.977533
O	-1.358313	-3.503800	0.922217
C	0.856796	-2.793132	1.671103
C	1.074856	-3.792155	2.700010
C	0.126770	-4.767731	3.087885
C	2.342408	-3.780334	3.373852
C	2.998582	-1.888075	2.006329
C	0.410474	-5.687986	4.090128
H	-0.834015	-4.796477	2.593052
C	2.600901	-4.728950	4.385249
C	3.309539	-2.795629	2.993398
H	3.723572	-1.138321	1.697428
C	1.650486	-5.673804	4.744095
H	-0.339575	-6.424956	4.364633
H	3.567069	-4.704814	4.883903
H	4.279251	-2.770611	3.480647
H	1.866535	-6.396948	5.525842
N	1.822765	-1.852741	1.354189
Ni	1.160197	-0.409356	-0.014379
C	-2.391244	-2.998074	0.035025
H	-3.188751	-2.582068	0.657262

C	0.330236	1.331695	-1.036437
H	0.470989	0.390061	-1.607005
C	0.955707	2.456516	-1.867761
H	1.994461	2.233106	-2.122690
H	0.405868	2.565651	-2.810036
H	0.913671	3.423700	-1.358794
C	-1.064549	1.529708	-0.785053
C	-2.249762	1.753554	-0.568838
Si	-3.966922	2.170319	-0.102880
C	-4.038560	4.004897	0.363757
C	-4.370985	4.436975	1.659848
C	-3.754067	4.991750	-0.600112
C	-4.421962	5.795872	1.980458
H	-4.593591	3.704075	2.430274
C	-3.802241	6.349840	-0.285770
H	-3.483018	4.699416	-1.612483
C	-4.138576	6.755334	1.008089
H	-4.682325	6.103714	2.989696
H	-3.578717	7.091497	-1.048131
H	-4.178373	7.812704	1.255449
C	-4.486609	1.089292	1.353698
C	-5.791596	1.164929	1.878342
C	-3.593710	0.179633	1.948645
C	-6.188818	0.367389	2.952937
H	-6.511608	1.859171	1.449304
C	-3.987000	-0.622592	3.023174
H	-2.580686	0.092746	1.564883
C	-5.285472	-0.529892	3.526931
H	-7.200916	0.445158	3.341037
H	-3.278483	-1.318737	3.463866
H	-5.592465	-1.152771	4.362629
C	-5.150846	1.921738	-1.584421
H	-4.830906	2.618791	-2.368446
H	-6.139574	2.265931	-1.255949
C	-5.238574	0.518174	-2.131551
C	-4.343495	0.068886	-3.115858
C	-6.210586	-0.379970	-1.664539
C	-4.419845	-1.229720	-3.620754
H	-3.582105	0.747684	-3.491542
C	-6.292164	-1.678630	-2.169134
H	-6.912766	-0.055842	-0.900896
C	-5.397582	-2.109771	-3.150692
H	-3.713098	-1.555925	-4.377968
H	-7.060335	-2.351805	-1.797725
H	-5.461471	-3.118053	-3.549460
C	-1.360600	-2.674594	-2.120134
C	-0.563399	-2.273963	-3.191907
C	-2.040981	-3.897793	-2.163364
C	-0.449938	-3.106996	-4.308245
H	-0.027616	-1.329178	-3.158836
C	-1.926262	-4.732118	-3.275533
C	-1.127256	-4.330711	-4.349368
H	0.171604	-2.805658	-5.147133
H	-2.447849	-5.685635	-3.308092
H	-1.027925	-4.973965	-5.219432
C	-2.871158	-4.104744	-0.914996
H	-2.749468	-5.094994	-0.463943
H	-3.938377	-3.968316	-1.131226
H	1.401128	0.756436	1.597985
C	0.394192	2.609713	1.481259
H	-0.598924	2.169138	1.597008
H	0.267207	3.474333	0.817766
C	0.872927	3.098960	2.860274
H	0.131619	3.774179	3.299732
H	1.010583	2.260137	3.552298
H	1.820182	3.646369	2.804648

B3LYP-D3BJ/BSI SCF energy in solution: -3059.401104a.u.

M06/BSII SCF energy in solution: -3057.723589a.u.

M06/BSII free energy in solution: -3056.786015a.u.

C	3.614688	0.641664	-0.423637
O	2.993008	-0.396616	-0.742374
N	4.937501	0.765457	-0.660082
C	2.888970	1.798529	0.230356
H	3.373857	2.008072	1.191172
H	3.046268	2.699010	-0.369977
C	1.408470	1.539344	0.468359
C	5.654298	1.944479	-0.256710
C	6.183844	2.025004	1.033671
C	5.846095	2.984942	-1.168793
C	6.904455	3.157855	1.413764
H	6.023287	1.205720	1.727306
C	6.569553	4.114337	-0.783677
H	5.425828	2.904463	-2.166293
C	7.097972	4.202019	0.506387

H	7.313891	3.223591	2.417089	C	0.540345	1.195674	-1.468810
H	6.718143	4.924978	-1.490339	H	0.575278	0.190787	-1.943091
H	7.659198	5.082551	0.803805	C	1.379482	2.125875	-2.340709
C	5.731229	-0.309922	-1.318107	H	2.383410	1.723792	-2.492205
C	5.797136	-1.587887	-0.470212	H	0.913999	2.217183	-3.329150
C	5.262103	-0.590383	-2.752410	H	1.459375	3.132755	-1.923840
H	6.742820	0.103099	-1.377178	C	-0.819626	1.589239	-1.298551
C	6.696387	-2.631762	-1.146815	C	-1.973752	1.923373	-1.065513
H	4.787965	-1.990578	-0.349058	Si	-3.532395	2.368549	-0.235605
H	6.178173	-1.341231	0.527566	C	-3.337586	4.120103	0.427953
C	6.169443	-1.637408	-3.413007	C	-2.901085	4.337277	1.747338
H	4.232210	-0.956606	-2.728307	C	-3.558863	5.243845	-0.387691
H	5.268625	0.344123	-3.325382	C	-2.686320	5.628464	2.232969
C	6.233617	-2.924135	-2.580043	H	-2.727312	3.488928	2.403383
H	6.704773	-3.551561	-0.551338	C	-3.349233	6.537108	0.094137
H	7.730950	-2.261159	-1.170208	H	-3.895417	5.114257	-1.413386
H	5.807350	-1.853173	-4.424581	C	-2.910507	6.731351	1.405922
H	7.182855	-1.225833	-3.521057	H	-2.349249	5.773343	3.255655
H	6.904724	-3.649810	-3.054083	H	-3.528171	7.392112	-0.551874
H	5.236465	-3.384152	-2.550170	H	-2.746707	7.737281	1.781880
C	-0.882855	-2.188932	0.971699	C	-3.754791	1.177930	1.202588
N	-0.819792	-1.371637	-0.062246	C	-5.032143	0.873122	1.704955
C	-2.061328	-1.526077	-0.826866	C	-2.641654	0.595393	1.834483
H	-2.489159	-0.549598	-1.056696	C	-5.192929	0.007988	2.789244
O	-2.058793	-2.852936	1.126911	H	-5.915256	1.310599	1.247509
C	0.217847	-2.380687	1.854351	C	-2.795459	-0.260246	2.926413
C	0.201184	-3.093792	3.112022	H	-1.646386	0.788302	1.451195
C	-0.951440	-3.678184	3.687301	C	-4.073168	-0.560662	3.401487
C	1.439293	-3.183056	3.835845	H	-6.189717	-0.222747	3.154815
C	2.502136	-1.876347	2.086012	H	-1.922973	-0.708146	3.391346
C	-0.889668	-4.334226	4.913201	H	-4.195288	-1.237942	4.241969
H	-1.893901	-3.609833	3.161795	C	-4.989100	2.268098	-1.442192
C	1.470071	-3.859836	5.072026	H	-4.849851	3.054804	-2.192758
C	2.604585	-2.564828	3.276359	H	-5.908284	2.512168	-0.898356
H	3.369321	-1.386839	1.650730	C	-5.094730	0.918567	-2.104109
C	0.322341	-4.431642	5.609420	C	-4.274845	0.590546	-3.196425
H	-1.792362	-4.773230	5.329219	C	-5.979279	-0.057583	-1.623487
H	2.415660	-3.922494	5.604935	C	-4.347321	-0.666446	-3.796025
H	3.554686	-2.629530	3.796818	H	-3.574676	1.329728	-3.575236
H	0.365954	-4.948159	6.564130	C	-6.054783	-1.316390	-2.223608
N	1.363954	-1.760085	1.382921	H	-6.619667	0.174511	-0.777726
Ni	0.982696	-0.448594	-0.198253	C	-5.240148	-1.626252	-3.313897
C	-2.971995	-2.389922	0.090961	H	-3.699456	-0.902446	-4.634552
H	-3.765303	-1.828038	0.584831	H	-6.755379	-2.052969	-1.839912

H	-5.290385	-2.606070	-3.777817
C	-1.896840	-2.367103	-2.075350
C	-1.116249	-2.093958	-3.197268
C	-2.671506	-3.530306	-2.009129
C	-1.112129	-3.002673	-4.259205
H	-0.527119	-1.183458	-3.250401
C	-2.668410	-4.438020	-3.068238
C	-1.883842	-4.168879	-4.193869
H	-0.510171	-2.801915	-5.140934
H	-3.270240	-5.341972	-3.023283
H	-1.874057	-4.869353	-5.024197
C	-3.489230	-3.575689	-0.738638
H	-3.387363	-4.516176	-0.187917
H	-4.553172	-3.440043	-0.961283
H	1.287305	0.841665	1.310079
C	0.635801	2.791503	0.849391
H	-0.419966	2.540252	0.956192
H	0.696391	3.549621	0.060310
C	1.119266	3.399974	2.173978
H	0.476672	4.240457	2.457283
H	1.081282	2.661080	2.983322

^{1}TS6-*RR*

B3LYP/BSI SCF energy: -3058.989612a.u.

M06/BSII SCF energy in solution:-3057.713307a.u.

M06/BSII free energy in solution:-3056.783212a.u.

B3LYP-D3(BJ)/BSII free energy in solution: -3059.102246 a.u.

C	3.708096	1.065944	-0.260335
O	3.110695	-0.024099	-0.362768
N	5.049696	1.155741	-0.450292
C	2.919416	2.318657	0.085509
H	3.456981	2.889065	0.851900
H	2.896646	2.977318	-0.795543
C	1.507675	1.983063	0.552531
C	5.733917	2.421400	-0.373194
C	6.393932	2.787462	0.805434
C	5.780292	3.263029	-1.489707
C	7.089735	3.995436	0.866898
H	6.353801	2.126218	1.665697
C	6.474814	4.471968	-1.421962
H	5.274848	2.964990	-2.403359
C	7.129732	4.839506	-0.245094
H	7.597917	4.277206	1.784195
H	6.506565	5.123489	-2.290120
H	7.670467	5.779743	-0.194701
C	5.885438	-0.043397	-0.773819
C	5.882183	-1.096690	0.348857
C	5.532652	-0.659931	-2.139616
H	6.902052	0.359274	-0.847069
C	6.832012	-2.255648	0.001847
H	4.866020	-1.476105	0.486794
H	6.186570	-0.626840	1.292168
C	6.485204	-1.820944	-2.470366
H	4.501096	-1.022670	-2.112357
H	5.590982	0.113392	-2.915582
C	6.488850	-2.880893	-1.358575
H	6.787054	-3.012626	0.792753
H	7.868412	-1.888046	-0.019383
H	6.196825	-2.270022	-3.427672
H	7.505092	-1.431857	-2.604146
H	7.200804	-3.679130	-1.598688
H	5.496958	-3.349154	-1.300987
C	-0.632288	-2.154721	0.904895
N	-0.430404	-1.414067	-0.181920
C	-1.359596	-1.901449	-1.204880
H	-1.792153	-1.064477	-1.761478
O	-1.709174	-2.992308	0.837465
C	0.206529	-2.086416	2.049659
C	0.049436	-2.824624	3.289856
C	-1.005758	-3.727092	3.562557
C	1.036185	-2.614289	4.311745
C	2.155368	-1.045967	2.841516
C	-1.091584	-4.386811	4.783718
H	-1.753830	-3.909202	2.803518
C	0.922446	-3.301466	5.538785
C	2.109655	-1.704146	4.050775
H	2.963279	-0.346615	2.626450
C	-0.126745	-4.176931	5.778627
H	-1.914770	-5.073680	4.961643
H	1.678789	-3.129333	6.301002
H	2.872834	-1.533040	4.803547
H	-0.198367	-4.696403	6.730356
N	1.248986	-1.197343	1.862667
Ni	1.052887	-0.093432	0.035732
C	-2.419082	-2.695911	-0.396202
H	-3.310472	-2.119686	-0.136018

C	0.484599	1.753129	-1.179233
C	-0.941580	1.752916	-0.962281
C	-2.146722	1.839752	-0.765944
Si	-3.918953	2.089892	-0.395492
C	-4.159943	3.881750	0.169993
C	-4.757730	4.207392	1.399971
C	-3.748629	4.943939	-0.658394
C	-4.942857	5.537508	1.785779
H	-5.081225	3.413335	2.067196
C	-3.930629	6.273562	-0.278687
H	-3.269452	4.731928	-1.612049
C	-4.530843	6.573233	0.946848
H	-5.406653	5.763359	2.742312
H	-3.604325	7.075431	-0.935818
H	-4.673954	7.608198	1.245547
C	-4.471281	0.890482	0.949416
C	-5.831682	0.756752	1.290354
C	-3.538445	0.110407	1.656790
C	-6.242769	-0.118514	2.296991
H	-6.585195	1.344272	0.769187
C	-3.944483	-0.771302	2.662271
H	-2.483026	0.184074	1.410314
C	-5.298027	-0.885324	2.983377
H	-7.297779	-0.204242	2.543590
H	-3.204861	-1.372357	3.183281
H	-5.616572	-1.570351	3.764389
C	-4.955027	1.862734	-1.988239
H	-4.676932	2.683771	-2.660058
H	-6.002558	2.037249	-1.712570
C	-4.809458	0.536639	-2.692390
C	-3.812598	0.341212	-3.662249
C	-5.659334	-0.540130	-2.395194
C	-3.673563	-0.883478	-4.316471
H	-3.143684	1.161873	-3.908144
C	-5.526035	-1.765184	-3.051563
H	-6.437034	-0.413708	-1.646576
C	-4.532447	-1.943387	-4.016702
H	-2.896289	-1.009253	-5.065168
H	-6.206293	-2.578570	-2.812961
H	-4.429016	-2.894190	-4.531225
C	-0.782040	-2.965173	-2.139304
C	0.352501	-2.898194	-2.948024
C	-1.550454	-4.136372	-2.102798
C	0.703591	-4.002645	-3.729073
H	0.972318	-2.007117	-2.960143
C	-1.199583	-5.240516	-2.879403
C	-0.069285	-5.167720	-3.697211
H	1.587344	-3.958425	-4.359945
H	-1.792402	-6.151382	-2.844066
H	0.215600	-6.022783	-4.304186
C	-2.724008	-3.990364	-1.159412
H	-2.844139	-4.837237	-0.475785
H	-3.664872	-3.876292	-1.712205
C	0.925279	1.035117	-2.475431
H	0.520925	0.026658	-2.554797
H	0.569116	1.610830	-3.342234
H	2.013802	0.972425	-2.545249
H	0.786511	2.796678	-1.317921
C	0.739876	3.186901	1.102317
H	0.779642	4.025331	0.392294
H	-0.315932	2.917085	1.197511
C	1.250978	3.659374	2.472778
H	2.293222	3.995837	2.437509
H	0.649427	4.500758	2.831727
H	1.181912	2.859586	3.217956
H	1.557071	1.262131	1.380980

B3LYP-D3BJ/BSI SCF energy in solution: -3059.400788a.u.

M06/BSII SCF energy in solution: -3057.722802a.u.

M06/BSII free energy in solution: -3056.779677a.u

C	3.682423	1.083681	0.079164
O	2.928417	0.089826	0.134042
N	5.029842	0.955517	0.106341
C	3.099109	2.487719	0.011923
H	3.715077	3.161361	0.615945
H	3.173794	2.865464	-1.015905
C	1.666868	2.504195	0.506062
C	5.884076	2.094983	-0.079059
C	6.557757	2.640513	1.017580
C	6.059032	2.633961	-1.355930
C	7.404164	3.733700	0.833411
H	6.406401	2.210803	2.002737
C	6.902161	3.732068	-1.533237
H	5.535137	2.191310	-2.197127
C	7.574765	4.282483	-0.440403

H	7.924391	4.160848	1.685258	C	0.626832	1.945074	-1.194177
H	7.035758	4.153240	-2.525009	C	-0.797778	1.734328	-1.171722
H	8.231070	5.135945	-0.580273	C	-1.999760	1.518974	-1.268545
C	5.699639	-0.364251	0.271832	Si	-3.730898	1.067788	-1.588216
C	5.298261	-1.075140	1.571472	C	-4.752450	2.646841	-1.689216
C	5.512541	-1.262825	-0.957093	C	-6.097661	2.666694	-1.282276
H	6.763119	-0.116891	0.347073	C	-4.204590	3.827756	-2.220807
C	6.092562	-2.379210	1.727697	C	-6.871848	3.821860	-1.408768
H	4.228673	-1.296732	1.546957	H	-6.543701	1.772952	-0.853560
H	5.479919	-0.406994	2.421302	C	-4.973018	4.985541	-2.347958
C	6.294199	-2.572927	-0.786690	H	-3.162002	3.844452	-2.529817
H	4.447774	-1.477530	-1.072867	C	-6.310184	4.983447	-1.942797
H	5.846487	-0.727563	-1.853520	H	-7.909480	3.817231	-1.086679
C	5.904388	-3.293255	0.510279	H	-4.530180	5.889110	-2.757993
H	5.779062	-2.892870	2.643404	H	-6.909421	5.884552	-2.038742
H	7.160436	-2.146181	1.844877	C	-4.428713	0.002176	-0.213606
H	6.120946	-3.221814	-1.652792	C	-5.206396	-1.139579	-0.468191
H	7.371091	-2.353575	-0.769535	C	-4.264472	0.408479	1.124145
H	6.497483	-4.207981	0.627061	C	-5.795081	-1.857570	0.576444
H	4.852349	-3.600582	0.449442	H	-5.362441	-1.472608	-1.489466
C	-1.035767	-1.455671	1.315714	C	-4.868854	-0.291307	2.167580
N	-0.216759	-1.191761	0.320241	H	-3.656247	1.279760	1.353112
C	-0.463333	-2.161791	-0.746980	C	-5.629572	-1.430819	1.894639
H	-0.740224	-1.633770	-1.661520	H	-6.384896	-2.744088	0.359827
O	-1.792703	-2.578058	1.170465	H	-4.731724	0.036183	3.192453
C	-1.184966	-0.577825	2.429689	H	-6.084721	-1.985307	2.710113
C	-1.974577	-0.827691	3.611294	C	-3.835029	0.208780	-3.287161
C	-2.621454	-2.051961	3.897006	H	-3.749921	1.018068	-4.022127
C	-2.117614	0.248274	4.551400	H	-4.851067	-0.190840	-3.387760
C	-0.646257	1.588073	3.160958	C	-2.810860	-0.855861	-3.576913
C	-3.406667	-2.202441	5.035522	C	-1.532427	-0.504531	-4.041040
H	-2.518954	-2.876699	3.205903	C	-3.094641	-2.218594	-3.401808
C	-2.923874	0.067781	5.693363	C	-0.574806	-1.478871	-4.323842
C	-1.430121	1.477112	4.288683	H	-1.292636	0.545041	-4.182916
H	-0.103872	2.507566	2.960029	C	-2.137339	-3.196464	-3.682290
C	-3.569748	-1.140394	5.935025	H	-4.078592	-2.518057	-3.052582
H	-3.898792	-3.153064	5.222171	C	-0.871557	-2.832239	-4.144234
H	-3.029542	0.896113	6.389580	H	0.406771	-1.179775	-4.680323
H	-1.516148	2.306245	4.983494	H	-2.384660	-4.245054	-3.542751
H	-4.188941	-1.261004	6.819476	H	-0.124386	-3.591005	-4.354551
N	-0.500857	0.615403	2.244981	C	0.667958	-3.134516	-0.988397
Ni	0.740384	0.562935	0.518482	C	1.948500	-2.857004	-1.463352
C	-1.621143	-3.045681	-0.195272	C	0.283464	-4.446042	-0.687154
H	-2.570756	-2.881927	-0.704607	C	2.848393	-3.911632	-1.638176

H	2.243892	-1.836064	-1.679116
C	1.185621	-5.498047	-0.851538
C	2.469720	-5.224133	-1.330709
H	3.846984	-3.713339	-2.014207
H	0.894119	-6.518561	-0.616925
H	3.179391	-6.035248	-1.467336
C	-1.159583	-4.512819	-0.237820
H	-1.279350	-4.984977	0.743053
H	-1.767006	-5.086775	-0.946640
C	1.312532	1.075131	-2.260118
H	1.040012	0.024029	-2.171806
H	1.001663	1.426462	-3.252108
H	2.398444	1.157659	-2.210786
H	0.823542	2.987882	-1.442887
C	1.061425	3.887166	0.703054
H	1.194476	4.489154	-0.205037
H	-0.018958	3.778799	0.852816
C	1.663035	4.648010	1.891830
H	2.731500	4.842678	1.750771
H	1.165440	5.615394	2.019011
H	1.547520	4.087445	2.825941
H	1.652705	2.009427	1.497092

^{1}TS6-*RS*

B3LYP/BSI SCF energy: -3058.980964a.u.

M06/BSII SCF energy in solution:-3057.705634a.u.

M06/BSII free energy in solution:-3056.775488a.u.

B3LYP-D3(BJ)/BSII free energy in solution: -3059.092262 a.u.

C	-3.223957	1.443719	0.273750
O	-2.996337	0.593814	1.159429
N	-4.206461	2.372433	0.416024
C	-2.386976	1.399543	-0.990648
H	-2.797307	0.570526	-1.581980
H	-2.509712	2.312677	-1.579469
C	-0.879367	1.137700	-0.736644
C	-4.597158	3.237335	-0.668265
C	-5.337104	2.728136	-1.740952
C	-4.283444	4.600207	-0.619400
C	-5.747844	3.578853	-2.768429
H	-5.581734	1.670647	-1.766375
C	-4.703374	5.447168	-1.645258
H	-3.706366	4.984999	0.215996
C	-5.434171	4.938348	-2.721476
H	-6.316716	3.178067	-3.601958
H	-4.453929	6.503312	-1.606193
H	-5.756987	5.599090	-3.520315
C	-5.043669	2.446831	1.654751
C	-5.950011	1.215306	1.832974
C	-4.221222	2.742249	2.921161
H	-5.693680	3.311235	1.479172
C	-6.865810	1.391508	3.056084
H	-5.324463	0.326600	1.958898
H	-6.550551	1.070263	0.926863
C	-5.150523	2.914827	4.134760
H	-3.526594	1.917374	3.100752
H	-3.622650	3.648364	2.766253
C	-6.058615	1.690860	4.328133
H	-7.474384	0.490354	3.191644
H	-7.568378	2.216911	2.870760
H	-4.549949	3.092202	5.034262
H	-5.773937	3.810021	3.995838
H	-6.734062	1.850853	5.176610
H	-5.440456	0.817725	4.578068
C	-0.552562	-3.077253	-0.629235
N	-0.075045	-2.201729	0.245460
C	1.281497	-2.636533	0.577200
H	1.957617	-1.779994	0.676977
O	0.360283	-3.990325	-1.087416
C	-1.908193	-3.067464	-1.057439
C	-2.539254	-3.998968	-1.974311
C	-1.862451	-5.033237	-2.661371
C	-3.950269	-3.854452	-2.196010
C	-3.948178	-1.959288	-0.680071
C	-2.539248	-5.885365	-3.526678
H	-0.799948	-5.161484	-2.508554
C	-4.608814	-4.736499	-3.077648
C	-4.647361	-2.810693	-1.506617
H	-4.458425	-1.158458	-0.150032
C	-3.917243	-5.741707	-3.738719
H	-1.989789	-6.670236	-4.039608
H	-5.678327	-4.613050	-3.231585
H	-5.718501	-2.694079	-1.638849
H	-4.441053	-6.412199	-4.414613
N	-2.623925	-2.041292	-0.455787
Ni	-1.409169	-0.697511	0.520368
C	1.661257	-3.575851	-0.596563

H	2.188773	-3.078945	-1.418545
C	-0.132994	1.144896	1.095245
C	1.242285	1.429382	0.751368
C	2.404679	1.673158	0.460251
Si	4.113890	2.200808	0.066193
C	4.184554	4.091947	0.046576
C	3.769812	4.813657	-1.089166
C	4.617431	4.829329	1.163634
C	3.783374	6.208899	-1.107717
H	3.440291	4.278453	-1.976148
C	4.635124	6.225562	1.150815
H	4.948444	4.313502	2.061263
C	4.216861	6.918634	0.014044
H	3.459824	6.741891	-1.997820
H	4.976897	6.770866	2.026457
H	4.231242	8.005071	0.000993
C	4.611498	1.536201	-1.628624
C	5.647824	2.145914	-2.361368
C	4.009618	0.389841	-2.177585
C	6.065289	1.632661	-3.590646
H	6.128958	3.041648	-1.975676
C	4.421437	-0.126574	-3.407433
H	3.207222	-0.103814	-1.636505
C	5.451248	0.494282	-4.116551
H	6.865201	2.122881	-4.139088
H	3.938076	-1.011541	-3.812606
H	5.771938	0.094832	-5.074832
C	5.305096	1.558177	1.415571
H	4.982234	1.982423	2.373690
H	6.291212	1.987683	1.198512
C	5.399071	0.054990	1.522901
C	4.579588	-0.657298	2.412636
C	6.301921	-0.671324	0.730631
C	4.663228	-2.046960	2.515101
H	3.874990	-0.113799	3.037200
C	6.388454	-2.060463	0.830217
H	6.945490	-0.141418	0.033143
C	5.570285	-2.755139	1.723308
H	4.020234	-2.575739	3.212181
H	7.101094	-2.599131	0.211307
H	5.641516	-3.835594	1.809593
C	1.387200	-3.566042	1.788459
C	0.935678	-3.361642	3.092401
C	2.029099	-4.763533	1.445642
C	1.149923	-4.353761	4.053682
H	0.407508	-2.452043	3.359792
C	2.239591	-5.756042	2.402383
C	1.801451	-5.543454	3.711986
H	0.799595	-4.203429	5.071155
H	2.730859	-6.688003	2.133519
H	1.957279	-6.310278	4.465738
C	2.421784	-4.772685	-0.015907
H	2.163512	-5.701733	-0.534414
H	3.501974	-4.617129	-0.136912
C	-0.157112	0.316554	2.417325
H	0.547547	-0.512553	2.389635
H	0.156282	0.992703	3.225126
H	-1.149539	-0.061203	2.689470
H	-0.662864	2.075301	1.312111
H	-0.405633	2.121695	-0.764874
C	-0.200304	0.324006	-1.845497
H	0.792975	0.024904	-1.500220
H	-0.757030	-0.595010	-2.048156
C	-0.045131	1.134244	-3.145564
H	-1.013896	1.433635	-3.561494
H	0.545824	2.041760	-2.978220
H	0.468168	0.539396	-3.908107

B3LYP-D3BJ/BSI SCF energy in solution: -3059.385914a.u.

M06/BSII SCF energy in solution: -3057.709571a.u.

M06/BSII free energy in solution: -3056.771485a.u

C	-3.513170	0.861750	0.336627
O	-3.077954	-0.182055	0.872937
N	-4.750179	1.327219	0.611478
C	-2.645493	1.586005	-0.668845
H	-2.808883	1.065361	-1.620556
H	-2.989017	2.612588	-0.807246
C	-1.136027	1.573346	-0.349868
C	-5.321910	2.420127	-0.125714
C	-5.753991	2.223321	-1.439710
C	-5.480715	3.661784	0.494802
C	-6.335004	3.281357	-2.140110
H	-5.628160	1.249926	-1.903079
C	-6.068765	4.713224	-0.208174
H	-5.137506	3.795379	1.515772

C	-6.494108	4.525285	-1.525752	H	3.488097	-2.159841	-0.556872
H	-6.665670	3.131400	-3.163263	C	-0.527895	1.237744	1.524828
H	-6.189378	5.679699	0.271499	C	0.823586	1.690179	1.336173
H	-6.948570	5.346405	-2.071532	C	1.975718	2.008871	1.084194
C	-5.655367	0.632178	1.570734	Si	3.661136	2.456093	0.557846
C	-6.089068	-0.747206	1.055821	C	3.739942	4.297831	0.191175
C	-5.080528	0.565268	2.991805	C	3.281718	4.786026	-1.046779
H	-6.544367	1.269105	1.606144	C	4.215239	5.226146	1.132961
C	-7.097809	-1.384402	2.021329	C	3.292652	6.151634	-1.331463
H	-5.206890	-1.387219	0.963979	H	2.920351	4.090267	-1.799348
H	-6.526491	-0.639412	0.056580	C	4.231442	6.593959	0.851386
C	-6.102703	-0.071748	3.943799	H	4.579389	4.884153	2.098080
H	-4.163941	-0.029995	2.984729	C	3.768550	7.058592	-0.381137
H	-4.816633	1.575688	3.325225	H	2.934463	6.508015	-2.293247
C	-6.538579	-1.456780	3.448144	H	4.605867	7.295353	1.591746
H	-7.368705	-2.384518	1.664618	H	3.781002	8.122228	-0.601751
H	-8.022171	-0.789780	2.025877	C	4.054596	1.510365	-1.017707
H	-5.674390	-0.142259	4.950009	C	5.114304	1.919794	-1.847471
H	-6.985149	0.579016	4.021350	C	3.316500	0.379394	-1.401122
H	-7.286525	-1.883372	4.126584	C	5.419738	1.225816	-3.019510
H	-5.673421	-2.133927	3.463007	H	5.700043	2.797851	-1.586040
C	0.609834	-2.335249	-1.060747	C	3.609259	-0.313372	-2.578050
N	0.586611	-1.693298	0.094089	H	2.497487	0.040003	-0.777623
C	1.757078	-2.134258	0.859264	C	4.663793	0.109872	-3.388848
H	2.230423	-1.290687	1.366769	H	6.240350	1.559327	-3.648615
O	1.766393	-3.009136	-1.328599	H	3.015364	-1.179461	-2.855092
C	-0.509477	-2.364187	-1.938335	H	4.894426	-0.425027	-4.305852
C	-0.551172	-2.935659	-3.267167	C	4.874277	2.001381	1.943332
C	0.551559	-3.536073	-3.917457	H	4.667482	2.644958	2.805377
C	-1.800513	-2.872866	-3.974221	H	5.886055	2.238821	1.595227
C	-2.773009	-1.736377	-2.061509	C	4.762510	0.550741	2.330024
C	0.435452	-4.051848	-5.204973	C	3.877939	0.142905	3.341776
H	1.498698	-3.600292	-3.399792	C	5.501079	-0.434864	1.658236
C	-1.887087	-3.407634	-5.276040	C	3.755951	-1.202710	3.690044
C	-2.923590	-2.263408	-3.327444	H	3.286287	0.891525	3.861598
H	-3.612382	-1.270003	-1.552130	C	5.382499	-1.781573	2.007709
C	-0.785107	-3.990659	-5.890198	H	6.179736	-0.140968	0.862188
H	1.301856	-4.506781	-5.677174	C	4.512265	-2.172252	3.027601
H	-2.840588	-3.353810	-5.795604	H	3.065105	-1.496570	4.474974
H	-3.882438	-2.219246	-3.833757	H	5.975626	-2.525561	1.483518
H	-0.871003	-4.396493	-6.894264	H	4.415675	-3.218941	3.296666
N	-1.621891	-1.756433	-1.371547	C	1.462459	-3.282161	1.818888
Ni	-1.124644	-0.625671	0.289318	C	0.556070	-3.324849	2.878740
C	2.676104	-2.795993	-0.207131	C	2.235735	-4.408725	1.509776

C	0.442529	-4.494955	3.634776
H	-0.063937	-2.468142	3.114970
C	2.122460	-5.577664	2.261929
C	1.222756	-5.615509	3.330432
H	-0.260992	-4.534921	4.461588
H	2.722955	-6.450158	2.017927
H	1.123304	-6.520994	3.922214
C	3.154355	-4.143418	0.342194
H	3.115227	-4.920951	-0.427029
H	4.196036	-4.062332	0.671215
C	-0.574826	0.171341	2.652798
H	0.242156	-0.541964	2.570770
H	-0.449725	0.702667	3.606488
H	-1.527506	-0.362281	2.705966
H	-1.189061	2.045017	1.841995
H	-0.883707	2.591676	-0.059074
C	-0.232173	1.258824	-1.543783
H	0.752211	0.964876	-1.181535
H	-0.629399	0.418981	-2.117381
C	-0.058387	2.482850	-2.454588
H	-1.015014	2.825116	-2.866594
H	0.388291	3.317685	-1.902476
H	0.601630	2.244382	-3.295974

3-*SS* **(4)**

B3LYP/BSI SCF energy: -1970.880527a.u.

M06/BSII SCF energy in solution:-1969.999607a.u.

M06/BSII free energy in solution:-1969.331348a.u.

C	-3.569309	0.206272	0.027304
O	-3.052119	1.147481	0.631188
N	-4.934925	0.009762	0.039035
C	-2.727362	-0.786838	-0.775586
H	-3.198422	-1.772580	-0.760612
H	-2.760627	-0.474166	-1.825957
C	-1.257910	-0.928740	-0.318248
C	-5.577061	-1.007380	-0.746747
C	-6.063384	-2.166720	-0.128721
C	-5.766297	-0.828121	-2.122273
C	-6.723636	-3.138278	-0.881526
H	-5.914665	-2.299352	0.938709
C	-6.421600	-1.805073	-2.873598
H	-5.399350	0.078521	-2.593903
C	-6.901840	-2.960976	-2.255418
H	-7.094579	-4.035722	-0.395079
H	-6.561271	-1.659366	-3.940805
H	-7.413418	-3.719417	-2.840500
C	-5.834691	0.934763	0.788563
C	-5.561962	0.945453	2.303847
C	-5.839940	2.358948	0.202029
H	-6.836507	0.514485	0.640149
C	-6.577307	1.842804	3.030668
H	-4.546383	1.310069	2.478653
H	-5.612605	-0.079761	2.690782
C	-6.848991	3.252273	0.942243
H	-4.832730	2.776847	0.287941
H	-6.086771	2.311216	-0.865813
C	-6.585685	3.267069	2.455513
H	-6.348371	1.865229	4.102594
H	-7.584432	1.410175	2.937576
H	-6.809143	4.270062	0.536600
H	-7.868983	2.884293	0.757454
H	-7.339727	3.878221	2.965896
H	-5.613111	3.740411	2.648406
C	-0.398575	0.364826	-0.513805
H	-0.704938	1.076599	0.260701
C	-0.604819	1.051998	-1.881837
H	-1.610970	1.473013	-1.950886
H	0.112258	1.867379	-2.006924
H	-0.455892	0.346645	-2.707179
C	1.026085	0.065302	-0.331038
C	2.218420	-0.165413	-0.215129
Si	4.015477	-0.461137	-0.075031
C	4.341048	-2.288901	0.292586
C	4.795143	-2.723464	1.550752
C	4.115801	-3.268843	-0.693245
C	5.016861	-4.077191	1.814077
H	4.980599	-1.995825	2.335856
C	4.335172	-4.622378	-0.436345
H	3.757584	-2.976839	-1.678021
C	4.788069	-5.029653	0.820565
H	5.367877	-4.386832	2.794903
H	4.153833	-5.358640	-1.214877
H	4.960904	-6.083155	1.023246
C	4.720742	0.619337	1.301715
C	6.098900	0.600570	1.593311
C	3.904164	1.479468	2.056056
C	6.638736	1.405998	2.596981

H	6.764366	-0.055720	1.035823
C	4.439149	2.287661	3.061633
H	2.838227	1.517251	1.849538
C	5.807342	2.252815	3.333812
H	7.705025	1.373345	2.804402
H	3.787570	2.945344	3.630652
H	6.225210	2.881675	4.115301
C	4.851758	-0.032551	-1.741591
H	4.536356	-0.786707	-2.472194
H	5.931283	-0.171538	-1.602463
C	4.558383	1.353552	-2.262082
C	3.487663	1.581176	-3.140557
C	5.334510	2.454867	-1.869059
C	3.204628	2.862740	-3.614045
H	2.873157	0.742527	-3.457596
C	5.053441	3.737663	-2.340726
H	6.166624	2.303902	-1.186326
C	3.987018	3.948509	-3.216327
H	2.374302	3.011515	-4.299412
H	5.671773	4.573397	-2.024259
H	3.769998	4.946339	-3.586791
H	-0.822206	-1.689717	-0.982518
C	-1.138001	-1.451443	1.128913
H	-0.074500	-1.480023	1.389964
H	-1.605539	-0.726763	1.805614
C	-1.736904	-2.843818	1.359356
H	-1.302394	-3.582999	0.676039
H	-1.537888	-3.184253	2.380803
H	-2.823328	-2.861035	1.220066

^{1}TS7-*R*

B3LYP/BSI SCF energy: -2280.188213a.u.

M06/BSII SCF energy in solution:-2279.258783a.u.

M06/BSII free energy in solution:-2278.691934a.u.

C	-3.055350	1.129117	0.243000
N	-3.242567	-0.030870	-0.285882
C	-4.307164	-0.711311	0.464327
H	-5.067543	-1.064196	-0.238503
C	-4.810439	0.381263	1.461084
H	-5.796919	0.787665	1.228076
O	-3.858963	1.480782	1.270088
C	-4.708659	-0.197111	2.885455
H	-5.710572	-0.353394	3.304154
H	-4.193324	0.505784	3.548779
C	-3.971729	-1.508720	2.708798
C	-3.528152	-2.388927	3.696959
C	-3.777560	-1.815381	1.358190
C	-2.889880	-3.571625	3.313145
H	-3.677053	-2.162885	4.749755
C	-3.146953	-2.997184	0.967047
C	-2.702091	-3.874423	1.958815
H	-2.540042	-4.264744	4.073031
H	-3.003601	-3.220140	-0.086703
H	-2.206862	-4.798836	1.676818
C	-1.995136	1.999053	-0.279446
C	-1.687511	3.317497	0.179004
C	-2.391191	3.999093	1.212024
C	-0.590486	3.989479	-0.455589
C	-0.285434	2.053983	-1.866919
C	-2.018445	5.271070	1.587598
H	-3.222935	3.511920	1.700775
C	-0.230676	5.296363	-0.038759
C	0.104072	3.313283	-1.488872
H	0.235412	1.512533	-2.645274
C	-0.931669	5.927528	0.963261
H	-2.567354	5.777220	2.376178
H	0.609890	5.782700	-0.524332
H	0.954745	3.783722	-1.970695
H	-0.654306	6.929249	1.277682
N	-1.318431	1.391474	-1.279238
Ni	-2.034666	-0.384513	-1.854714
C	2.089626	-0.540707	-1.194035
C	1.282050	-0.965925	-2.032179
Si	3.249355	0.093669	0.065008
C	2.521085	-0.196642	1.778647
C	1.257904	-0.792067	1.946172
C	3.238049	0.159591	2.937784
C	0.728336	-1.020473	3.218474
H	0.685757	-1.088428	1.071442
C	2.712273	-0.063154	4.211430
H	4.220509	0.619835	2.851438
C	1.454799	-0.654580	4.352709
H	-0.246899	-1.488817	3.320993
H	3.283408	0.220802	5.091318
H	1.045923	-0.832232	5.343789
C	3.533554	1.940222	-0.259372
C	3.249255	2.929783	0.697691

C	4.052276	2.361826	-1.499575
C	3.480069	4.282649	0.433274
H	2.840572	2.643485	1.662610
C	4.280457	3.711162	-1.772229
H	4.277190	1.627815	-2.270552
C	3.996428	4.676783	-0.802064
H	3.256340	5.026792	1.193001
H	4.684496	4.009527	-2.735994
H	4.182342	5.727607	-1.007839
C	4.939724	-0.783040	-0.114081
H	5.357441	-0.482092	-1.082541
H	5.601523	-0.356893	0.650703
C	4.896373	-2.287716	0.000119
C	5.042080	-2.922599	1.243011
C	4.689016	-3.090376	-1.132281
C	4.987717	-4.312643	1.350468
H	5.199445	-2.320356	2.134071
C	4.634321	-4.480376	-1.027552
H	4.572032	-2.619286	-2.104909
C	4.783910	-5.098691	0.215164
H	5.107248	-4.781386	2.323537
H	4.476548	-5.080811	-1.919360
H	4.744104	-6.181074	0.297261
C	0.375668	-1.424246	-2.963966
H	-0.205101	-2.309890	-2.720114
C	0.392197	-0.992977	-4.405952
H	1.037546	-1.661620	-4.995272
H	-0.612825	-1.055060	-4.831748
H	0.779600	0.022975	-4.530633
Br	-3.066418	-2.130745	-3.105674

1$^{\cdot}$

B3LYP/BSI SCF energy: -1178.549098a.u.

M06/BSII SCF energy in solution:-1178.052571a.u.

M06/BSII free energy in solution:-1177.748344a.u.

C	0.086116	-1.549236	0.868700
C	0.591422	-2.442386	1.567492
Si	-0.594504	-0.191285	-0.147488
C	-0.376914	1.438447	0.783534
C	0.833898	1.734579	1.439373
C	-1.400202	2.402834	0.826948
C	1.016942	2.948246	2.102749
H	1.640892	1.007137	1.436954
C	-1.220142	3.619095	1.489183
H	-2.353755	2.200599	0.346452
C	-0.010053	3.894430	2.127383
H	1.959548	3.154576	2.602541
H	-2.026072	4.347795	1.510923
H	0.130969	4.839062	2.645702
C	-2.418958	-0.533233	-0.491050
C	-3.106406	0.142468	-1.517645
C	-3.141017	-1.467935	0.273000
C	-4.458892	-0.098486	-1.766215
H	-2.584952	0.868458	-2.137747
C	-4.492973	-1.713994	0.027557
H	-2.635646	-2.014097	1.065016
C	-5.155344	-1.028521	-0.992251
H	-4.966905	0.435984	-2.564397
H	-5.028677	-2.441819	0.631031
H	-6.207401	-1.219672	-1.185132
C	0.337754	-0.150701	-1.819720
H	0.080998	-1.080378	-2.341379
H	-0.090288	0.668750	-2.410249
C	1.835540	0.004097	-1.720605
C	2.439419	1.270181	-1.765880
C	2.665278	-1.118054	-1.563552
C	3.823990	1.411337	-1.660025
H	1.817253	2.152852	-1.889132
C	4.049397	-0.979527	-1.458210
H	2.218250	-2.107972	-1.527754
C	4.636251	0.286931	-1.505124
H	4.267532	2.402432	-1.702903
H	4.671301	-1.863804	-1.346097
H	5.714306	0.395278	-1.427462
C	1.165248	-3.422624	2.330034
H	0.514544	-4.084358	2.899311
C	2.648164	-3.631194	2.433177
H	2.922809	-4.653943	2.141997
H	3.193895	-2.931465	1.796326
H	2.993338	-3.497940	3.467707

^{2}IM9 (LNi^{I}Br)

B3LYP/BSI SCF energy: -1101.63709a.u.

M06/BSII SCF energy in solution:-1101.19314a.u.

M06/BSII free energy in solution:-1100.957306a.u.

C	-0.632441	-0.777266	-0.676235

N	0.528396	-0.235881	-0.855033
C	1.454516	-1.288770	-1.300172
H	1.966888	-0.954916	-2.208163
O	-0.758937	-2.086182	-0.977240
C	-1.736591	0.036677	-0.160871
C	-3.083447	-0.389185	0.057005
C	-3.566008	-1.703697	-0.193448
C	-4.000296	0.592000	0.563913
C	-2.203004	2.208976	0.566369
C	-4.885473	-2.019601	0.049310
H	-2.889329	-2.454978	-0.576418
C	-5.350373	0.230402	0.801888
C	-3.517799	1.903487	0.810667
H	-1.798945	3.199701	0.744740
C	-5.786323	-1.051090	0.550031
H	-5.238788	-3.027495	-0.146872
H	-6.032400	0.983531	1.186210
H	-4.190120	2.664648	1.193700
H	-6.821539	-1.321835	0.734347
N	-1.317632	1.294927	0.088168
Ni	0.613213	1.671447	-0.281108
C	0.530163	-2.527404	-1.519095
H	0.350631	-2.778958	-2.566691
C	2.417811	-1.729328	-0.215224
C	3.397632	-0.963969	0.418011
C	2.204103	-3.066826	0.134217
C	4.169480	-1.562874	1.415941
H	3.547324	0.078899	0.152252
C	2.979863	-3.662638	1.129063
C	3.962399	-2.901974	1.767370
H	4.933991	-0.982921	1.924028
H	2.823762	-4.701666	1.407331
H	4.570686	-3.354085	2.545547
C	1.107635	-3.696400	-0.700262
H	1.504899	-4.468463	-1.370843
H	0.322845	-4.170215	-0.100888
Br	2.188720	3.370893	-0.081490

^{1}TS8-*S*

B3LYP/BSI SCF energy: -2280.183181a.u.

M06/BSII SCF energy in solution:-2279.253359a.u.

M06/BSII free energy in solution:-2278.686966a.u.

C	3.934406	0.386027	-0.565417
N	2.767635	0.505637	-1.110417
C	2.698561	1.826783	-1.753400
H	2.367923	1.697555	-2.788346
O	4.801640	1.408345	-0.730078
C	4.271890	-0.837294	0.158701
C	5.507753	-1.110769	0.828457
C	6.598764	-0.202006	0.908549
C	5.640731	-2.390096	1.463246
C	3.411112	-2.939376	0.710227
C	7.751313	-0.550706	1.581403
H	6.518854	0.767507	0.437661
C	6.838370	-2.715129	2.145151
C	4.551301	-3.297626	1.378292
H	2.573259	-3.621302	0.622554
C	7.877808	-1.812267	2.204610
H	8.573752	0.156565	1.632620
H	6.921290	-3.689149	2.619143
H	4.624112	-4.277235	1.840082
H	8.793823	-2.066961	2.728991
N	3.249471	-1.727194	0.109489
Ni	1.697159	-1.185611	-1.025537
C	4.151521	2.381286	-1.613523
H	4.726859	2.381746	-2.542104
C	-2.081023	-0.724550	0.906022
C	-1.148331	-1.534093	0.828116
Si	-3.555667	0.355838	0.956744
C	-4.123845	0.715845	-0.802721
C	-5.373746	1.314824	-1.056666
C	-3.304576	0.410921	-1.905134
C	-5.784464	1.609977	-2.357668
H	-6.044269	1.551665	-0.232630
C	-3.713498	0.703201	-3.208345
H	-2.342502	-0.071688	-1.755113
C	-4.951772	1.304992	-3.436843
H	-6.753055	2.072210	-2.529053
H	-3.061727	0.453239	-4.040752
H	-5.270624	1.530962	-4.450835
C	-3.106227	1.951178	1.874020
C	-2.177631	1.928159	2.931665
C	-3.713441	3.182445	1.564501
C	-1.874265	3.081644	3.656091
H	-1.674465	0.997747	3.183900
C	-3.414870	4.340103	2.287584
H	-4.419187	3.245056	0.740379

C	-2.494956	4.291266	3.336729
H	-1.150894	3.038200	4.465884
H	-3.897938	5.278854	2.029546
H	-2.261398	5.190434	3.900535
C	-4.936401	-0.519863	1.953375
H	-4.622859	-0.512795	3.003882
H	-5.825558	0.121357	1.895732
C	-5.261086	-1.925266	1.508017
C	-6.148738	-2.165727	0.447698
C	-4.664858	-3.030786	2.133721
C	-6.433633	-3.466253	0.030560
H	-6.616956	-1.325169	-0.057205
C	-4.949154	-4.332394	1.719376
H	-3.975213	-2.866425	2.958044
C	-5.835653	-4.556681	0.664614
H	-7.125197	-3.626741	-0.792059
H	-4.479964	-5.172562	2.224654
H	-6.059265	-5.569364	0.341484
C	-0.145670	-2.475704	0.727314
C	1.848547	2.819419	-0.985168
C	0.479853	2.748567	-0.725827
C	2.621240	3.883713	-0.508768
C	-0.111098	3.761823	0.032116
H	-0.111551	1.917503	-1.099314
C	2.028103	4.897279	0.244612
C	0.659422	4.826671	0.513876
H	-1.171985	3.720436	0.255537
H	2.619528	5.729012	0.619171
H	0.185210	5.604201	1.105766
C	4.066450	3.765398	-0.946063
H	4.333412	4.548800	-1.666441
H	4.780850	3.838968	-0.118968
Br	0.268655	-1.462134	-2.885353
C	-0.386261	-3.803079	0.056633
H	-0.921092	-4.485264	0.734404
H	-0.989956	-3.681159	-0.844891
H	0.552088	-4.289161	-0.227550
H	0.716110	-2.364018	1.381988

^{1}TS9-*SR*

B3LYP/BSI SCF energy: -3059.004764a.u.

M06/BSII SCF energy in solution:-3057.72064a.u.

M06/BSII free energy in solution:-3056.790711a.u.

B3LYP-D3(BJ)/BSII free energy in solution: -3059.116423 a.u.

C	3.430793	0.651046	-0.237262
O	2.707404	-0.081305	-0.949927
N	4.747509	0.799299	-0.536965
C	2.873942	1.352375	1.007887
H	2.965628	0.623395	1.822072
H	3.527081	2.194380	1.263038
C	1.455519	1.809147	0.863504
C	5.631758	1.595411	0.280681
C	6.199859	1.048504	1.435786
C	5.971788	2.891951	-0.120656
C	7.096390	1.803251	2.193745
H	5.932061	0.040405	1.736645
C	6.871291	3.640476	0.639113
H	5.523566	3.307832	-1.017653
C	7.434164	3.098334	1.796651
H	7.530639	1.377345	3.093220
H	7.128713	4.648425	0.327871
H	8.132269	3.683723	2.387316
C	5.399518	0.102353	-1.694294
C	5.366982	-1.431855	-1.571971
C	4.872134	0.581256	-3.056826
H	6.448117	0.411119	-1.621663
C	6.152505	-2.079639	-2.725050
H	4.329530	-1.776097	-1.592196
H	5.794884	-1.731346	-0.607541
C	5.658879	-0.080062	-4.201107
H	3.812184	0.330333	-3.139072
H	4.953466	1.673080	-3.119791
C	5.633724	-1.612148	-4.092976
H	6.088799	-3.170491	-2.642804
H	7.217542	-1.821822	-2.634320
H	5.246513	0.243436	-5.163589
H	6.702163	0.266714	-4.177239
H	6.230549	-2.058328	-4.897007
H	4.603671	-1.968670	-4.230926
C	-0.712647	-2.356746	0.973536
N	-0.722782	-1.745093	-0.204057
C	-2.023536	-2.012386	-0.826636
H	-2.423316	-1.110882	-1.296378
O	-1.897704	-2.893037	1.356763
C	0.487298	-2.455501	1.716481
C	0.683101	-3.129733	2.979972

C	-0.362633	-3.674233	3.760880
C	2.026443	-3.248760	3.463711
C	2.785580	-2.038886	1.497671
C	-0.094764	-4.305778	4.969085
H	-1.382525	-3.598452	3.407375
C	2.266257	-3.896505	4.691947
C	3.083262	-2.706270	2.661859
H	3.582006	-1.630771	0.885278
C	1.221337	-4.419905	5.440579
H	-0.916099	-4.715184	5.550754
H	3.291165	-3.980842	5.045228
H	4.115750	-2.821732	2.976149
H	1.422274	-4.916464	6.385705
N	1.533268	-1.854229	1.028038
Ni	0.879274	-0.767314	-0.572012
C	-2.894523	-2.494749	0.365029
H	-3.506443	-1.711399	0.818186
C	0.010798	0.237300	-2.072383
H	-0.432864	-0.586958	-2.646784
C	0.923275	1.045351	-3.007472
H	1.664741	0.389709	-3.472337
H	0.349096	1.524345	-3.812678
H	1.460937	1.832913	-2.473376
C	-1.057623	1.022092	-1.512949
C	-1.978210	1.675106	-1.028085
Si	-3.323916	2.588638	-0.224864
C	-2.846483	4.418797	-0.092562
C	-2.966127	5.147708	1.103815
C	-2.364608	5.100728	-1.226896
C	-2.626762	6.501667	1.165752
H	-3.322641	4.651274	2.002142
C	-2.023495	6.452531	-1.171322
H	-2.240428	4.564700	-2.165363
C	-2.155757	7.157506	0.027727
H	-2.727009	7.042262	2.103307
H	-1.653214	6.955646	-2.060785
H	-1.891034	8.210502	0.073929
C	-3.655231	1.865671	1.491541
C	-4.765515	2.265217	2.260329
C	-2.794292	0.900119	2.044392
C	-5.003011	1.728971	3.527563
H	-5.459414	3.007565	1.870650
C	-3.029259	0.354888	3.309491
H	-1.934990	0.565407	1.469751
C	-4.134411	0.770426	4.054169
H	-5.866181	2.055749	4.101565
H	-2.353000	-0.396847	3.707587
H	-4.319872	0.348681	5.038304
C	-4.918317	2.487435	-1.284316
H	-4.706335	3.024346	-2.216817
H	-5.696104	3.062975	-0.767247
C	-5.401639	1.089246	-1.578294
C	-4.909948	0.373448	-2.682692
C	-6.340633	0.456160	-0.748720
C	-5.346260	-0.924197	-2.952656
H	-4.179939	0.843538	-3.335984
C	-6.781326	-0.840903	-1.017103
H	-6.732063	0.988209	0.114275
C	-6.287653	-1.537779	-2.122133
H	-4.954543	-1.455219	-3.815813
H	-7.517948	-1.303449	-0.365373
H	-6.637882	-2.542790	-2.340225
C	-2.034187	-3.212052	-1.769304
C	-1.258811	-3.433713	-2.907382
C	-2.966487	-4.169695	-1.350103
C	-1.428859	-4.619099	-3.627318
H	-0.520538	-2.702887	-3.224278
C	-3.135717	-5.353669	-2.067698
C	-2.362733	-5.573570	-3.210473
H	-0.827922	-4.803129	-4.513610
H	-3.854537	-6.100945	-1.740569
H	-2.483465	-6.493764	-3.775451
C	-3.696169	-3.714587	-0.104679
H	-3.750003	-4.478906	0.677448
H	-4.723191	-3.407192	-0.338147
C	1.164767	3.139056	0.240248
H	1.900564	3.352006	-0.548801
H	0.183475	3.113837	-0.242107
C	1.183285	4.300140	1.262214
H	0.955292	5.250585	0.768552
H	0.432286	4.142272	2.042499
H	2.160386	4.394359	1.749896
H	0.697600	1.354785	1.493596

B3LYP-D3BJ/BSI SCF energy in solution: --3059.412126a.u.

M06/BSII SCF energy in solution: -3057.72064a.u.

M06/BSII free energy in solution: -3056.789367a.u

C	3.301677	0.215979	-0.319851
O	2.561115	-0.480025	-1.061640
N	4.628647	0.256105	-0.544093
C	2.723468	0.999041	0.853610
H	2.579531	0.282028	1.667184
H	3.463099	1.729017	1.199162
C	1.442396	1.679937	0.497198
C	5.512862	1.002159	0.312344
C	5.941278	0.446717	1.519613
C	5.965094	2.259531	-0.094552
C	6.821800	1.163282	2.331233
H	5.572983	-0.529385	1.818776
C	6.847771	2.968695	0.720100
H	5.614816	2.674905	-1.033928
C	7.275961	2.422392	1.932565
H	7.151382	0.737859	3.274106
H	7.196022	3.949071	0.409845
H	7.960409	2.978018	2.566206
C	5.281457	-0.498583	-1.654529
C	5.132475	-2.018387	-1.500549
C	4.831775	-0.005533	-3.035291
H	6.343338	-0.259335	-1.546176
C	5.896575	-2.741486	-2.618590
H	4.073437	-2.285564	-1.546007
H	5.510202	-2.322940	-0.517802
C	5.596064	-0.744480	-4.141832
H	3.760332	-0.181691	-3.146268
H	4.997444	1.075620	-3.106218
C	5.442771	-2.264533	-4.004152
H	5.754257	-3.823367	-2.519344
H	6.973202	-2.551915	-2.506412
H	5.237627	-0.409491	-5.121770
H	6.662254	-0.482658	-4.089329
H	6.014794	-2.776117	-4.786869
H	4.388248	-2.536114	-4.151617
C	-1.101659	-2.100242	1.009354
N	-1.057146	-1.589557	-0.213257
C	-2.412601	-1.657383	-0.774622
H	-2.676163	-0.718265	-1.261622
O	-2.334811	-2.410717	1.465427
C	0.092417	-2.316761	1.736456
C	0.221029	-2.881853	3.056946
C	-0.872132	-3.179945	3.902585
C	1.546538	-3.147313	3.534064
C	2.424198	-2.266742	1.445499
C	-0.667388	-3.714367	5.169472
H	-1.878042	-2.988410	3.554112
C	1.721325	-3.691705	4.821677
C	2.650964	-2.850506	2.669312
H	3.254611	-2.029186	0.791612
C	0.630296	-3.973007	5.634454
H	-1.523771	-3.933208	5.800910
H	2.731824	-3.889960	5.169565
H	3.663536	-3.078765	2.985133
H	0.782048	-4.392251	6.624841
N	1.197782	-1.951993	0.979508
Ni	0.676372	-0.909869	-0.685829
C	-3.302011	-1.955975	0.465005
H	-3.800134	-1.077405	0.875164
C	-0.019922	0.058199	-2.281734
H	-0.590879	-0.726101	-2.792424
C	1.017768	0.635311	-3.249521
H	1.651948	-0.163121	-3.643320
H	0.536252	1.131452	-4.104376
H	1.666031	1.367153	-2.763784
C	-0.935789	1.027094	-1.760896
C	-1.729302	1.822523	-1.268432
Si	-2.830145	2.840687	-0.261635
C	-2.049498	4.539481	-0.035556
C	-2.039400	5.194519	1.207460
C	-1.443315	5.186687	-1.128002
C	-1.452255	6.453621	1.354770
H	-2.486614	4.714172	2.073365
C	-0.854770	6.443732	-0.986589
H	-1.417232	4.694952	-2.097645
C	-0.859254	7.080528	0.257472
H	-1.453153	6.941570	2.325541
H	-0.389136	6.924440	-1.842537
H	-0.397997	8.057533	0.370876
C	-3.072092	2.021804	1.413533
C	-4.121483	2.398507	2.271408
C	-2.185491	1.024889	1.854975
C	-4.275916	1.803454	3.525167
H	-4.829576	3.163363	1.961598
C	-2.330844	0.429569	3.109839
H	-1.386492	0.698453	1.198758
C	-3.378968	0.817986	3.946302

H	-5.095195	2.105688	4.171747
H	-1.636738	-0.342107	3.427352
H	-3.498967	0.352861	4.920793
C	-4.510972	2.995248	-1.139450
H	-4.356539	3.599137	-2.040767
H	-5.200012	3.549293	-0.492620
C	-5.059605	1.638315	-1.486906
C	-4.657939	0.982330	-2.662275
C	-5.929538	0.963823	-0.616761
C	-5.114744	-0.301397	-2.961214
H	-3.977790	1.485413	-3.343120
C	-6.395879	-0.317047	-0.918732
H	-6.244087	1.449758	0.302405
C	-5.989376	-0.957154	-2.091712
H	-4.784295	-0.792590	-3.871929
H	-7.078370	-0.814433	-0.235126
H	-6.346242	-1.955321	-2.325769
C	-2.646833	-2.861151	-1.672581
C	-1.983218	-3.209710	-2.848178
C	-3.670550	-3.673168	-1.168262
C	-2.359684	-4.374029	-3.523231
H	-1.177902	-2.593151	-3.234042
C	-4.048326	-4.834600	-1.842098
C	-3.388384	-5.180792	-3.024362
H	-1.848452	-4.654990	-4.439467
H	-4.841604	-5.466075	-1.450686
H	-3.671965	-6.084196	-3.556738
C	-4.249819	-3.104391	0.105757
H	-4.305737	-3.834894	0.918693
H	-5.259785	-2.717089	-0.057546
C	1.510538	2.915112	-0.343422
H	2.303641	2.807860	-1.096460
H	0.571679	3.054267	-0.883262
C	1.791077	4.178267	0.497275
H	1.857632	5.063846	-0.143381
H	0.988355	4.349486	1.221187
H	2.734020	4.087983	1.048867

^{1}TS10-*SS*

B3LYP/BSI SCF energy: -3059.009223a.u.

M06/BSII SCF energy in solution:-3057.724327a.u.

M06/BSII free energy in solution:-3056.793015a.u.

B3LYP-D3(BJ)/BSII free energy in solution: -3059.119445 a.u.

C	3.183752	0.215079	-0.387572
O	2.555653	-0.812024	-0.738245
N	4.518515	0.296014	-0.621888
C	2.461132	1.392290	0.279899
H	3.201266	2.095503	0.673454
H	1.925523	1.904515	-0.529576
C	1.487789	0.993489	1.346632
C	5.283991	1.476003	-0.296143
C	6.039253	1.511430	0.880928
C	5.324340	2.553150	-1.187119
C	6.824144	2.628462	1.168851
H	5.999549	0.669971	1.565833
C	6.109296	3.668958	-0.892489
H	4.736726	2.514286	-2.099097
C	6.860277	3.708186	0.283736
H	7.404062	2.655541	2.086487
H	6.132465	4.506526	-1.583096
H	7.470095	4.577330	0.510963
C	5.291665	-0.795212	-1.302472
C	5.316811	-2.113388	-0.510197
C	4.862494	-1.020960	-2.762511
H	6.316285	-0.408179	-1.320104
C	6.248094	-3.128608	-1.194676
H	4.305114	-2.523514	-0.457212
H	5.650560	-1.921437	0.516858
C	5.787829	-2.046318	-3.440324
H	3.830408	-1.380450	-2.780977
H	4.887133	-0.068489	-3.304908
C	5.840899	-3.366490	-2.656502
H	6.236333	-4.071021	-0.635708
H	7.283006	-2.758499	-1.161259
H	5.447710	-2.223893	-4.466930
H	6.802423	-1.629358	-3.516730
H	6.538122	-4.063650	-3.135612
H	4.851464	-3.843347	-2.682344
C	-1.383615	-2.430849	0.765960
N	-1.162521	-1.798527	-0.380542
C	-2.435259	-1.736890	-1.104512
H	-2.584584	-0.747583	-1.545568
O	-2.685112	-2.719333	1.023348
C	-0.302678	-2.750816	1.620100
C	-0.354429	-3.458677	2.878991
C	-1.546343	-3.921952	3.482617

C	0.888527	-3.704334	3.547778
C	2.035519	-2.556999	1.736302
C	-1.514422	-4.594190	4.697796
H	-2.492738	-3.750263	2.986873
C	0.887990	-4.390267	4.779476
C	2.093798	-3.235217	2.931093
H	2.936396	-2.183046	1.264985
C	-0.296233	-4.831163	5.352284
H	-2.444109	-4.940266	5.141030
H	1.838515	-4.569531	5.276131
H	3.051706	-3.416439	3.408037
H	-0.279681	-5.358800	6.301803
N	0.888400	-2.291684	1.078827
Ni	0.628735	-1.173024	-0.576390
C	-3.483317	-2.054318	-0.003625
H	-3.930475	-1.168219	0.454478
C	0.134205	-0.026319	-2.148520
H	-0.574204	-0.669682	-2.682006
C	1.229256	0.390614	-3.143627
H	1.759932	-0.488888	-3.519900
H	0.803524	0.920504	-4.006864
H	1.971883	1.059047	-2.697893
C	-0.591584	1.078847	-1.584623
C	-1.222095	1.994658	-1.060808
Si	-2.246688	3.253546	-0.249867
C	-1.257495	4.851611	-0.007831
C	-0.915703	5.652985	-1.114171
C	-0.819446	5.273529	1.260344
C	-0.172420	6.824019	-0.962755
H	-1.228171	5.359151	-2.113894
C	-0.075565	6.445301	1.418977
H	-1.063636	4.680817	2.137438
C	0.248889	7.223975	0.307484
H	0.076267	7.425055	-1.833539
H	0.249317	6.749560	2.410566
H	0.825703	8.136957	0.429062
C	-2.853627	2.596734	1.416900
C	-2.567684	1.281676	1.826074
C	-3.640402	3.390163	2.273835
C	-3.042855	0.776953	3.039855
H	-1.968333	0.644680	1.181902
C	-4.116111	2.893695	3.489199
H	-3.881942	4.414638	1.997186
C	-3.817654	1.584614	3.874438
H	-2.809098	-0.244654	3.327602
H	-4.718261	3.527240	4.135239
H	-4.187630	1.196778	4.819693
C	-3.763231	3.665453	-1.347787
H	-3.388208	4.150394	-2.256811
H	-4.356964	4.418255	-0.814710
C	-4.616917	2.473770	-1.703246
C	-4.338323	1.700303	-2.842232
C	-5.697866	2.088913	-0.894262
C	-5.116313	0.587956	-3.166166
H	-3.503652	1.977777	-3.480314
C	-6.478837	0.977475	-1.215692
H	-5.929431	2.668849	-0.004717
C	-6.193304	0.221568	-2.354892
H	-4.884869	0.010187	-4.056916
H	-7.316547	0.707546	-0.578021
H	-6.808820	-0.635221	-2.614891
C	-2.648439	-2.859687	-2.116673
C	-1.856915	-3.213339	-3.209489
C	-3.809498	-3.585102	-1.820233
C	-2.242599	-4.292160	-4.009326
H	-0.942835	-2.670343	-3.430154
C	-4.194069	-4.663054	-2.617282
C	-3.405473	-5.012148	-3.716289
H	-1.631595	-4.577365	-4.861245
H	-5.091893	-5.230442	-2.384796
H	-3.693169	-5.851953	-4.342727
C	-4.508300	-3.025759	-0.599554
H	-4.801720	-3.789482	0.128098
H	-5.413931	-2.472757	-0.879031
C	1.916486	0.767124	2.763398
H	1.650915	-0.250021	3.088064
H	3.011249	0.828791	2.838843
C	1.278585	1.768425	3.749252
H	1.591782	1.558290	4.777967
H	1.562439	2.798649	3.509144
H	0.186406	1.705370	3.709774
H	0.430158	1.090669	1.129921

B3LYP-D3BJ/BSI SCF energy in solution: -3059.4194 a.u.

M06/BSII SCF energy in solution: -3057.735327a.u.

M06/BSII free energy in solution: -3056.791458a.u

C	2.889873	-0.481713	-0.566076
O	2.092803	-1.413218	-0.854220
N	4.217255	-0.693264	-0.635189
C	2.362823	0.893084	-0.180093
H	3.192979	1.572705	0.026651
H	1.847513	1.265768	-1.070092
C	1.406863	0.850792	0.966330
C	5.157273	0.307432	-0.202682
C	5.451898	0.434028	1.156397
C	5.785133	1.121890	-1.147018
C	6.367854	1.400106	1.574498
H	4.951012	-0.209043	1.872158
C	6.704159	2.082027	-0.722756
H	5.538318	1.010147	-2.197859
C	6.993458	2.224459	0.636567
H	6.591104	1.507759	2.631496
H	7.187096	2.723609	-1.453345
H	7.704122	2.976995	0.964145
C	4.803674	-1.976721	-1.121540
C	4.498985	-3.158064	-0.190922
C	4.427843	-2.281154	-2.577730
H	5.882975	-1.800856	-1.089687
C	5.227906	-4.417454	-0.679900
H	3.421465	-3.340461	-0.182870
H	4.803293	-2.906521	0.831617
C	5.153515	-3.546774	-3.055817
H	3.347099	-2.424444	-2.650495
H	4.689407	-1.423944	-3.208421
C	4.864475	-4.739645	-2.135246
H	4.980425	-5.262095	-0.027214
H	6.313426	-4.264654	-0.602191
H	4.853804	-3.775418	-4.084791
H	6.236450	-3.360645	-3.076210
H	5.415253	-5.623809	-2.476368
H	3.795812	-4.988875	-2.192012
C	-2.115913	-1.771933	0.761544
N	-1.755970	-1.427755	-0.468682
C	-2.972720	-1.147498	-1.233629
H	-2.860891	-0.230681	-1.816732
O	-3.443454	-1.675584	1.019094
C	-1.134987	-2.168064	1.699610
C	-1.335830	-2.543954	3.076685
C	-2.597456	-2.577630	3.713452
C	-0.174040	-2.893095	3.840469
C	1.192336	-2.484780	1.872505
C	-2.709702	-2.928093	5.053453
H	-3.484617	-2.331884	3.144908
C	-0.320948	-3.245771	5.197307
C	1.102684	-2.868742	3.189993
H	2.148466	-2.443710	1.365985
C	-1.570646	-3.260990	5.801961
H	-3.690023	-2.944954	5.521034
H	0.568097	-3.506313	5.765824
H	1.995830	-3.145945	3.739824
H	-1.666156	-3.533480	6.849034
N	0.129753	-2.118220	1.130373
Ni	0.129826	-1.318850	-0.731953
C	-4.063776	-1.017772	-0.137121
H	-4.282594	0.009327	0.155974
C	-0.078680	-0.384155	-2.498495
H	-0.938303	-0.875805	-2.963079
C	1.106113	-0.418666	-3.470646
H	1.387792	-1.452137	-3.693279
H	0.856206	0.071423	-4.422302
H	1.988724	0.085641	-3.069817
C	-0.450258	0.923307	-2.049143
C	-0.751061	2.010729	-1.563096
Si	-1.047123	3.480686	-0.549375
C	0.586762	4.396412	-0.378040
C	1.096003	5.169394	-1.436267
C	1.394995	4.222829	0.760143
C	2.368773	5.739210	-1.367021
H	0.499568	5.322456	-2.332725
C	2.671098	4.784703	0.832307
H	1.028359	3.634696	1.594929
C	3.161457	5.542044	-0.233785
H	2.743615	6.332100	-2.196724
H	3.281719	4.629201	1.717509
H	4.155249	5.977720	-0.181597
C	-1.687635	2.966919	1.141232
C	-2.153659	1.661522	1.363859
C	-1.784911	3.892396	2.195091
C	-2.701571	1.286255	2.591315
H	-2.066090	0.930869	0.568391
C	-2.325634	3.522657	3.428778
H	-1.430383	4.911603	2.058449

C	-2.786627	2.218240	3.627244
H	-3.048787	0.269112	2.740448
H	-2.386215	4.249715	4.234013
H	-3.204476	1.928484	4.587248
C	-2.406643	4.527178	-1.375078
H	-2.044536	4.905602	-2.336989
H	-2.626966	5.390456	-0.737637
C	-3.619773	3.653295	-1.555794
C	-3.767071	2.860698	-2.705519
C	-4.573938	3.521271	-0.534558
C	-4.835756	1.972564	-2.835202
H	-3.029612	2.937462	-3.499216
C	-5.645150	2.635799	-0.661936
H	-4.466503	4.110400	0.371653
C	-5.781932	1.856342	-1.813467
H	-4.929409	1.371229	-3.735335
H	-6.372992	2.554481	0.140665
H	-6.618346	1.171243	-1.916199
C	-3.454210	-2.324296	-2.067391
C	-2.767046	-3.028551	-3.055149
C	-4.751244	-2.700437	-1.696007
C	-3.397624	-4.106985	-3.682012
H	-1.752339	-2.755819	-3.327241
C	-5.380134	-3.777281	-2.319943
C	-4.696873	-4.477603	-3.318124
H	-2.872938	-4.664370	-4.452679
H	-6.384837	-4.073581	-2.030368
H	-5.174876	-5.320321	-3.809388
C	-5.290349	-1.802565	-0.605910
H	-5.759065	-2.346902	0.219414
H	-6.037317	-1.104369	-1.001569
C	1.906883	0.726218	2.364800
H	2.457438	-0.221117	2.489233
H	2.660906	1.510677	2.553173
C	0.800101	0.801809	3.416943
H	1.204461	0.676566	4.426924
H	0.282182	1.764983	3.375394
H	0.055517	0.019211	3.254257
H	0.360268	1.042454	0.779273

2$^{\cdot}$

B3LYP/BSI SCF energy: -792.226947a.u.

M06/BSII SCF energy in solution:-791.832224a.u.

M06/BSII free energy in solution:-791.50559a.u.

C	1.058450	-0.330485	-0.062187
O	1.241963	-1.541946	0.014498
N	-0.209349	0.214837	-0.099933
C	2.246841	0.660357	-0.124538
H	1.995229	1.485990	-0.798161
H	2.336362	1.106954	0.877287
C	3.531609	0.013184	-0.522535
C	-0.442208	1.630865	-0.044045
C	-0.832599	2.323017	-1.197812
C	-0.331711	2.321877	1.168942
C	-1.103182	3.690381	-1.138181
H	-0.914942	1.782101	-2.135783
C	-0.595641	3.691394	1.223829
H	-0.041937	1.778516	2.063352
C	-0.982850	4.377921	0.071654
H	-1.403279	4.219503	-2.038028
H	-0.504726	4.219545	2.168576
H	-1.190953	5.442859	0.115987
C	-1.417891	-0.658462	-0.056934
C	-1.502801	-1.628269	-1.249921
C	-1.562509	-1.398115	1.286353
H	-2.259075	0.040002	-0.142088
C	-2.806080	-2.442624	-1.198041
H	-0.639757	-2.298564	-1.222371
H	-1.444880	-1.059605	-2.186232
C	-2.862463	-2.217930	1.324582
H	-0.697616	-2.055111	1.417046
H	-1.549405	-0.669322	2.106190
C	-2.953482	-3.187959	0.137014
H	-2.831926	-3.149824	-2.035460
H	-3.666857	-1.771027	-1.332672
H	-2.927208	-2.765761	2.272162
H	-3.725942	-1.536951	1.300178
H	-3.904116	-3.734082	0.164547
H	-2.155744	-3.938669	0.221756
C	4.366660	-0.799980	0.413922
H	3.914396	-0.791081	1.413104
H	5.363486	-0.338783	0.524184
C	4.553553	-2.258650	-0.047662
H	5.030647	-2.298313	-1.033599
H	5.187626	-2.814147	0.652463
H	3.581747	-2.752071	-0.117333
H	3.796437	0.010417	-1.578200

^{2}IM10

B3LYP/BSI SCF energy: -2266.770899a.u.

M06/BSII SCF energy in solution:-2265.872124a.u.

M06/BSII free energy in solution:-2265.296051a.u.

C	-2.690044	0.276513	0.681387
N	-1.389423	0.309301	0.415166
C	-0.812553	1.407673	1.194961
H	0.151301	1.113759	1.614535
C	-1.892628	1.666342	2.281162
H	-1.711878	1.145324	3.226533
O	-3.093214	1.090185	1.689175
C	-2.053402	3.184179	2.433061
H	-1.514696	3.528793	3.325558
H	-3.105380	3.457260	2.565633
C	-1.435013	3.738635	1.167353
C	-1.486109	5.043888	0.678580
C	-0.730361	2.747746	0.472820
C	-0.822171	5.349768	-0.512278
H	-2.038263	5.813945	1.211633
C	-0.071291	3.051087	-0.717373
C	-0.118658	4.359174	-1.205751
H	-0.855817	6.362776	-0.903643
H	0.466845	2.283329	-1.262187
H	0.395685	4.605978	-2.130197
C	-3.547190	-0.552134	-0.074983
C	-4.969187	-0.739841	0.092671
C	-5.724210	-0.169171	1.143074
C	-5.647889	-1.554355	-0.869710
C	-3.519686	-1.941423	-1.979112
C	-7.092352	-0.388545	1.235620
H	-5.226302	0.446717	1.880312
C	-7.037044	-1.757609	-0.749825
C	-4.876575	-2.135954	-1.928289
H	-2.933227	-2.389855	-2.771566
C	-7.755870	-1.183290	0.288547
H	-7.650955	0.061869	2.051394
H	-7.538835	-2.376747	-1.489285
H	-5.364693	-2.736075	-2.688998
H	-8.826564	-1.348606	0.367948
N	-2.832787	-1.190114	-1.085331
Ni	-0.923670	-0.954348	-0.936232
C	1.200075	-0.884215	-1.022162
C	0.691849	-1.782725	-1.751724
Si	2.829134	-0.186990	-0.471554
C	2.703345	0.439520	1.304214
C	2.309054	-0.443674	2.330754
C	2.973442	1.774272	1.657658
C	2.192897	-0.010714	3.652349
H	2.084043	-1.480183	2.098055
C	2.858928	2.210976	2.979895
H	3.263876	2.488272	0.892860
C	2.468725	1.319263	3.979941
H	1.887363	-0.710938	4.424960
H	3.069390	3.248225	3.225774
H	2.378946	1.657666	5.008674
C	3.353416	1.177900	-1.669194
C	4.552867	1.887432	-1.461190
C	2.615013	1.474448	-2.829118
C	4.987186	2.860875	-2.362040
H	5.161378	1.683414	-0.582648
C	3.045298	2.447006	-3.734784
H	1.693120	0.935000	-3.029609
C	4.231306	3.144576	-3.501287
H	5.914447	3.395880	-2.176079
H	2.455678	2.656567	-4.623177
H	4.567475	3.901591	-4.204345
C	4.166849	-1.556993	-0.617979
H	4.155119	-1.868726	-1.669679
H	5.128540	-1.053167	-0.457839
C	4.051566	-2.756284	0.289081
C	4.714343	-2.792777	1.526114
C	3.276730	-3.869056	-0.076063
C	4.602053	-3.897256	2.371625
H	5.325870	-1.945922	1.826980
C	3.160605	-4.973900	0.768434
H	2.768411	-3.870446	-1.036478
C	3.821537	-4.992783	1.998286
H	5.129125	-3.902226	3.321867
H	2.558976	-5.824896	0.460597
H	3.735621	-5.854475	2.653884
C	-0.382052	-2.507043	-2.226103
C	-0.658085	-3.920652	-1.742518
H	-1.730351	-4.134647	-1.770465
H	-0.156522	-4.660554	-2.379685
H	-0.308844	-4.061106	-0.716676
H	-0.701086	-2.289272	-3.247239

^{1}TS11-*SS*

B3LYP/BSI SCF energy: -3313.06697a.u.

M06/BSII SCF energy in solution:-3311.779507a.u.

M06/BSII free energy in solution:-3310.860527a.u.

C	-0.081277	-2.423820	1.004621
N	0.308039	-1.224984	0.728885
C	0.919271	-0.664957	1.950269
H	1.902879	-0.255919	1.703838
C	0.993975	-1.880971	2.917769
H	1.987040	-2.322641	2.999933
O	0.160753	-2.886526	2.236129
C	0.362567	-1.459743	4.253697
H	1.142331	-1.355843	5.018095
H	-0.336304	-2.221478	4.614719
C	-0.299940	-0.130985	3.953432
C	-1.119884	0.633310	4.785051
C	0.018745	0.323992	2.668154
C	-1.620465	1.849856	4.314799
H	-1.371146	0.287479	5.784201
C	-0.487244	1.534413	2.192810
C	-1.310433	2.298151	3.025023
H	-2.261271	2.450728	4.953646
H	-0.268460	1.869211	1.183144
H	-1.723134	3.235522	2.664233
C	-0.798261	-3.228317	-0.006647
C	-1.159735	-4.604026	0.123727
C	-0.832391	-5.429270	1.237314
C	-1.892481	-5.183322	-0.967032
C	-1.761381	-3.065468	-2.115695
C	-1.226501	-6.747958	1.262905
H	-0.264675	-5.016409	2.058666
C	-2.287405	-6.545557	-0.901667
C	-2.190910	-4.370353	-2.084669
H	-1.961450	-2.421124	-2.963425
C	-1.962182	-7.311961	0.191925
H	-0.963946	-7.367297	2.114971
H	-2.843524	-6.968456	-1.733191
H	-2.750361	-4.779479	-2.920043
H	-2.261771	-8.354668	0.236175
N	-1.074083	-2.501900	-1.094707
Ni	-0.116443	-0.591002	-1.136079
C	-3.083775	0.905008	-1.100858
C	-2.158595	0.602586	-1.858295
Si	-4.503379	1.585395	-0.185850
C	-6.072795	1.366444	-1.220179
C	-7.252964	2.053348	-0.877058
C	-6.115007	0.507264	-2.331723
C	-8.429542	1.882953	-1.607547
H	-7.254928	2.741829	-0.034266
C	-7.289335	0.333529	-3.067361
H	-5.215013	-0.025992	-2.626000
C	-8.449615	1.019561	-2.705504
H	-9.327445	2.426055	-1.325022
H	-7.297869	-0.335398	-3.923943
H	-9.363753	0.886752	-3.277758
C	-4.173045	3.432876	0.095258
C	-4.574510	4.099361	1.267826
C	-3.525478	4.195400	-0.895176
C	-4.342776	5.466381	1.445496
H	-5.074733	3.551276	2.062363
C	-3.295976	5.561944	-0.726769
H	-3.191855	3.710139	-1.808737
C	-3.703041	6.201624	0.446888
H	-4.663792	5.955747	2.361264
H	-2.805620	6.129232	-1.513939
H	-3.525908	7.265349	0.580265
C	-4.756839	0.781828	1.529435
H	-3.924032	1.099164	2.166657
H	-5.664130	1.238494	1.948403
C	-4.886301	-0.722012	1.558102
C	-6.063789	-1.361940	1.138069
C	-3.831946	-1.521152	2.026218
C	-6.180865	-2.751568	1.182680
H	-6.896507	-0.764191	0.777987
C	-3.948985	-2.911549	2.076037
H	-2.918779	-1.043162	2.371264
C	-5.123904	-3.534501	1.651305
H	-7.104229	-3.222517	0.856049
H	-3.123807	-3.507380	2.456608
H	-5.217743	-4.615948	1.693436
C	-1.022358	0.304544	-2.674773
C	-0.437385	1.537506	-3.375228
H	0.477594	1.286595	-3.918085
H	-1.144834	1.957087	-4.103515
H	-0.203616	2.335771	-2.662990
H	-1.234539	-0.482865	-3.408067

C	3.275373	1.395938	-0.404773
O	3.840332	0.509804	0.280504
N	3.295508	2.688879	-0.003353
C	2.578467	1.031988	-1.713950
H	1.734991	1.710540	-1.870445
H	3.294772	1.292963	-2.509311
C	2.247814	-0.446657	-1.865509
H	1.842682	-1.021542	-1.026938
C	2.248423	-1.026776	-3.272380
H	1.459808	-0.579533	-3.894525
H	3.195081	-0.746931	-3.756863
C	2.107622	-2.552037	-3.329015
H	1.180973	-2.887047	-2.850555
H	2.094483	-2.899585	-4.367195
H	2.940609	-3.050675	-2.822388
C	2.687085	3.734789	-0.789951
C	1.445858	4.253337	-0.404936
C	3.356884	4.266951	-1.896135
C	0.866997	5.290723	-1.136820
H	0.941694	3.840067	0.463008
C	2.773471	5.304962	-2.625012
H	4.323666	3.863874	-2.181407
C	1.529932	5.816302	-2.248595
H	-0.103119	5.678212	-0.840256
H	3.293126	5.713133	-3.486636
H	1.079148	6.622573	-2.819478
C	4.072576	3.137772	1.198384
C	3.582353	2.511856	2.515526
C	5.590190	2.963851	1.008404
H	3.865407	4.212405	1.251594
C	4.352049	3.108411	3.706339
H	3.743358	1.431150	2.480770
H	2.505208	2.683173	2.629561
C	6.353398	3.541711	2.212481
H	5.820686	1.900745	0.891661
H	5.902638	3.466872	0.085829
C	5.868933	2.934477	3.537484
H	4.012644	2.635957	4.635385
H	4.116631	4.178711	3.798155
H	7.427198	3.367698	2.081594
H	6.215754	4.632441	2.243593
H	6.398980	3.393448	4.380344
H	6.114476	1.863883	3.556136
Zn	4.088957	-1.293043	-0.829047
Br	3.707745	-3.157447	0.659958
Br	6.014441	-0.931263	-2.213355

^{1}TS11-*SR*

B3LYP/BSI SCF energy: -3313.065323a.u.

M06/BSII SCF energy in solution:-3311.778779a.u.

M06/BSII free energy in solution:-3310.859a.u.

C	-0.042855	-1.313927	1.878919
N	0.183985	-1.738387	0.682154
C	0.473140	-3.185721	0.773887
H	-0.174507	-3.722534	0.077107
C	0.175110	-3.531051	2.261948
H	-0.764104	-4.062336	2.412184
O	-0.008416	-2.204998	2.875555
C	1.411661	-4.236678	2.841728
H	1.184092	-5.291506	3.037662
H	1.700789	-3.791328	3.799578
C	2.468271	-4.089492	1.766389
C	3.808631	-4.474799	1.817314
C	1.943613	-3.519032	0.600076
C	4.614527	-4.280098	0.692797
H	4.222512	-4.921218	2.717610
C	2.746217	-3.325315	-0.524668
C	4.088702	-3.708444	-0.472170
H	5.659363	-4.575523	0.721915
H	2.342701	-2.876303	-1.427165
H	4.727257	-3.554705	-1.336332
C	-0.276447	0.122831	2.135479
C	-0.675394	0.692381	3.383785
C	-1.006805	-0.056664	4.548422
C	-0.757855	2.124505	3.441853
C	-0.136643	2.203125	1.110842
C	-1.381665	0.589539	5.704976
H	-0.970233	-1.136037	4.515723
C	-1.139209	2.755885	4.654761
C	-0.459915	2.863094	2.272204
H	0.084427	2.737194	0.194241
C	-1.443903	2.003103	5.764338
H	-1.638430	0.006011	6.583632
H	-1.190942	3.840342	4.685999
H	-0.491484	3.948084	2.293354
H	-1.739456	2.489434	6.689074
N	-0.049227	0.853999	1.040024

Ni	0.181780	-0.306061	-0.744254	H	1.121461	-0.200690	-3.841295
C	3.301625	0.780676	-1.110316	H	0.367197	2.006139	-1.812982
C	2.160242	0.942952	-1.548017	C	-3.594362	0.876933	-1.019969
Si	5.080106	0.651275	-0.733318	O	-4.063743	0.069437	-0.184492
C	5.849284	2.379281	-0.815289	N	-3.946052	2.184798	-0.977967
C	7.219014	2.550275	-1.090015	C	-2.638032	0.393899	-2.106620
C	5.082739	3.532828	-0.569706	H	-3.255817	0.266435	-3.009516
C	7.802028	3.818499	-1.108696	H	-1.936237	1.197321	-2.349947
H	7.840029	1.684410	-1.307741	C	-1.974939	-0.941568	-1.810049
C	5.660359	4.803609	-0.587336	C	-3.511471	3.117089	-1.987897
H	4.019050	3.433231	-0.370469	C	-4.118627	3.124178	-3.247707
C	7.022825	4.949000	-0.855021	C	-2.522291	4.058702	-1.682633
H	8.861232	3.924888	-1.327386	C	-3.721093	4.060163	-4.204189
H	5.047224	5.680412	-0.395677	H	-4.894540	2.398493	-3.471109
H	7.473944	5.937458	-0.871997	C	-2.132732	4.995577	-2.640294
C	5.879771	-0.484159	-2.021954	H	-2.065488	4.045315	-0.697854
C	7.074859	-1.178377	-1.753803	C	-2.729506	4.995574	-3.903363
C	5.296976	-0.659891	-3.290648	H	-4.191182	4.059313	-5.182953
C	7.665591	-2.007998	-2.710045	H	-1.362219	5.722635	-2.401344
H	7.555521	-1.082026	-0.783093	H	-2.423869	5.723335	-4.648916
C	5.880972	-1.489012	-4.249925	C	-4.940365	2.705117	0.016197
H	4.368559	-0.146314	-3.525728	C	-6.350328	2.128740	-0.205427
C	7.068128	-2.165741	-3.961724	C	-4.476338	2.546705	1.474530
H	8.588303	-2.532611	-2.476539	H	-4.983254	3.778938	-0.198482
H	5.409067	-1.608471	-5.221609	C	-7.354049	2.770650	0.767551
H	7.523542	-2.812430	-4.706673	H	-6.324520	1.045837	-0.055488
C	5.425110	-0.129245	0.979015	H	-6.659629	2.306742	-1.242104
H	5.134465	-1.183403	0.911086	C	-5.490619	3.196690	2.430851
H	6.516423	-0.113545	1.103194	H	-4.374931	1.483903	1.708764
C	4.770376	0.515449	2.175456	H	-3.486837	3.003970	1.596039
C	5.253532	1.720037	2.712565	C	-6.901133	2.623446	2.228024
C	3.667819	-0.088937	2.799280	H	-8.341115	2.316842	0.625198
C	4.654778	2.299125	3.831910	H	-7.465024	3.838738	0.529363
H	6.110059	2.204202	2.251619	H	-5.162139	3.050709	3.466483
C	3.070511	0.485977	3.922640	H	-5.513859	4.283247	2.260450
H	3.290766	-1.030557	2.408080	H	-7.612330	3.121905	2.897240
C	3.559736	1.685388	4.443465	H	-6.901981	1.559876	2.502275
H	5.051402	3.228729	4.231562	Zn	-3.782748	-1.932582	-0.781304
H	2.229141	-0.011024	4.397945	Br	-3.359775	-3.288254	1.166797
H	3.099688	2.130559	5.321226	Br	-5.441387	-2.375164	-2.459026
C	0.829410	1.043181	-2.065020	C	-1.633292	-1.810622	-3.010855
C	0.732968	0.787680	-3.574171	H	-2.560530	-2.000724	-3.571280
H	-0.304006	0.843342	-3.916869	H	-0.981344	-1.272955	-3.713120
H	1.307413	1.528230	-4.147284	C	-0.984020	-3.157632	-2.683449

H	-0.835764	-3.745099	-3.594866
H	-0.001826	-3.027569	-2.214183
H	-1.609300	-3.750058	-2.006133
H	-1.638450	-1.191576	-0.799105

^{1}TS11-*RR*

B3LYP/BSI SCF energy: -3313.06558a.u.

M06/BSII SCF energy in solution:-3311.776347a.u.

M06/BSII free energy in solution:-3310.858084a.u.

C	-0.245602	-0.322161	2.244015
N	0.076917	-1.103807	1.269076
C	0.266230	-2.458897	1.832782
H	-0.309694	-3.176432	1.242679
C	-0.263421	-2.327827	3.289000
H	-1.261195	-2.743134	3.432654
O	-0.398284	-0.867964	3.456581
C	0.808597	-2.887076	4.234882
H	0.470467	-3.841806	4.655826
H	0.979016	-2.210602	5.079203
C	2.024820	-3.073858	3.352401
C	3.310775	-3.460402	3.730691
C	1.723189	-2.851629	2.002871
C	4.287566	-3.622913	2.745584
H	3.550734	-3.636962	4.775952
C	2.696954	-3.013807	1.017311
C	3.984380	-3.402986	1.396635
H	5.291865	-3.925479	3.028109
H	2.469018	-2.832638	-0.028325
H	4.751569	-3.531816	0.640025
C	-0.418016	1.126284	2.011087
C	-0.818604	2.087813	2.991184
C	-1.143112	1.783090	4.344174
C	-0.898014	3.455826	2.560499
C	-0.234502	2.744773	0.350371
C	-1.517948	2.784607	5.211460
H	-1.096272	0.759114	4.685222
C	-1.284703	4.461820	3.484489
C	-0.588364	3.754661	1.212684
H	0.001497	2.938309	-0.687663
C	-1.588524	4.132805	4.784436
H	-1.764765	2.536287	6.239068
H	-1.336763	5.491890	3.143933
H	-0.626629	4.781479	0.862208
H	-1.885183	4.904963	5.487768
N	-0.146309	1.449605	0.739578
Ni	0.226896	-0.199889	-0.530744
C	3.524590	0.227092	-1.288076
C	2.386724	0.280816	-1.758704
Si	5.288257	0.158366	-0.839296
C	6.209229	1.524274	-1.771430
C	7.587953	1.415127	-2.032680
C	5.553448	2.693798	-2.196363
C	8.286128	2.434965	-2.681477
H	8.124917	0.515735	-1.740193
C	6.246499	3.716271	-2.846795
H	4.486009	2.799748	-2.023073
C	7.615627	3.589976	-3.088797
H	9.349834	2.325326	-2.875351
H	5.717624	4.609919	-3.167807
H	8.156033	4.383804	-3.597414
C	5.974655	-1.538214	-1.325411
C	7.118549	-2.079812	-0.708290
C	5.355498	-2.302137	-2.332135
C	7.625305	-3.326960	-1.081592
H	7.624381	-1.529500	0.081755
C	5.855429	-3.550273	-2.708022
H	4.466417	-1.914750	-2.822670
C	6.992729	-4.065989	-2.083051
H	8.509872	-3.722089	-0.589122
H	5.356785	-4.121045	-3.486796
H	7.382612	-5.037772	-2.373065
C	5.561206	0.365435	1.044498
H	5.153773	-0.529916	1.527213
H	6.646842	0.345062	1.206969
C	4.973679	1.609715	1.662069
C	5.622428	2.850961	1.557643
C	3.757791	1.558671	2.361539
C	5.074991	3.999291	2.130509
H	6.567400	2.915215	1.025222
C	3.210446	2.705451	2.939575
H	3.246646	0.604588	2.462767
C	3.865491	3.933106	2.824838
H	5.599682	4.946626	2.039273
H	2.276548	2.636251	3.491297
H	3.444271	4.825236	3.279946
C	1.051511	0.362206	-2.265559
C	-3.634223	0.415137	-1.068374

O	-4.009424	-0.331385	-0.132676
N	-4.168063	1.650553	-1.217367
C	-2.572007	-0.063688	-2.054513
H	-3.108405	-0.352451	-2.970711
H	-1.948916	0.788969	-2.345427
C	-1.782481	-1.269808	-1.575834
C	-3.883454	2.455080	-2.379559
C	-4.448982	2.125253	-3.615734
C	-3.091095	3.601496	-2.255012
C	-4.204659	2.933152	-4.727638
H	-5.073104	1.240750	-3.699459
C	-2.856457	4.409052	-3.368436
H	-2.661006	3.846124	-1.288644
C	-3.410344	4.074716	-4.606533
H	-4.640963	2.670910	-5.686670
H	-2.238518	5.296731	-3.270103
H	-3.224375	4.702558	-5.472660
C	-5.241105	2.164523	-0.305459
C	-6.560034	1.384134	-0.449155
C	-4.787970	2.268424	1.160984
H	-5.418236	3.184400	-0.665512
C	-7.657098	2.015892	0.424352
H	-6.398511	0.343878	-0.152585
H	-6.868480	1.377920	-1.500970
C	-5.897358	2.900400	2.019133
H	-4.551895	1.270329	1.538728
H	-3.870902	2.867585	1.219521
C	-7.218204	2.126466	1.892002
H	-8.574829	1.422989	0.342902
H	-7.898948	3.018594	0.042554
H	-5.573465	2.937548	3.065732
H	-6.056953	3.942530	1.705334
H	-8.000551	2.613303	2.486135
H	-7.088058	1.118041	2.307656
Zn	-3.588311	-2.349788	-0.595183
Br	-3.256344	-3.638509	1.402252
Br	-5.100006	-2.908584	-2.377596
C	-1.253522	-2.218660	-2.634818
H	-2.102046	-2.654670	-3.182293
H	-0.684692	-1.665391	-3.399225
C	-0.379243	-3.352456	-2.092557
H	-0.065458	-4.022913	-2.898384
H	0.527935	-2.963408	-1.613349
H	-0.919177	-3.953056	-1.352227
H	-1.506196	-1.377109	-0.523884
H	0.839050	-0.483583	-2.930659
C	0.733845	1.685237	-2.974955
H	1.237782	1.749480	-3.948860
H	-0.339123	1.802490	-3.159510
H	1.078129	2.544387	-2.390215

^{1}TS11-*RS*

B3LYP/BSI SCF energy: -3313.067909a.u.

M06/BSII SCF energy in solution:-3311.777464a.u.

M06/BSII free energy in solution:-3310.856772a.u.

C	0.172664	-2.650433	1.085224
N	0.416204	-1.424486	0.764954
C	1.054530	-0.782626	1.932006
H	1.967885	-0.278606	1.606790
C	1.331011	-1.966445	2.901548
H	2.367875	-2.303040	2.905557
O	0.553456	-3.062592	2.300448
C	0.770987	-1.587567	4.281142
H	1.595652	-1.395079	4.978319
H	0.182875	-2.408338	4.705046
C	-0.041807	-0.335326	4.025308
C	-0.853143	0.365115	4.918958
C	0.119287	0.123235	2.712250
C	-1.501253	1.523354	4.483810
H	-0.982496	0.015873	5.939942
C	-0.534593	1.274421	2.271631
C	-1.346296	1.975913	3.167831
H	-2.135005	2.075650	5.171745
H	-0.436432	1.609536	1.243400
H	-1.866559	2.870198	2.837650
C	-0.512411	-3.546484	0.132974
C	-0.756164	-4.941177	0.330775
C	-0.359390	-5.682869	1.480716
C	-1.444620	-5.632055	-0.723396
C	-1.512383	-3.563045	-1.964338
C	-0.643027	-7.026820	1.572199
H	0.171723	-5.185980	2.279262
C	-1.722755	-7.018100	-0.591582
C	-1.816347	-4.900049	-1.873710
H	-1.770469	-2.981872	-2.838806
C	-1.330613	-7.701847	0.534318
H	-0.329997	-7.579305	2.452730

H	-2.245250	-7.524471	-1.397923	C	-1.028202	0.113800	-2.578432
H	-2.336391	-5.394749	-2.688002	C	3.009070	1.591001	-0.408389
H	-1.541890	-8.762535	0.630376	O	3.667935	0.744828	0.245615
N	-0.875327	-2.889213	-0.976259	N	2.953975	2.879170	-0.004031
Ni	-0.142232	-0.892248	-1.095937	C	2.274751	1.178496	-1.682701
C	-3.015701	0.949748	-1.015812	H	1.331951	1.737427	-1.742693
C	-2.094224	0.588272	-1.750608	H	2.876838	1.572637	-2.515597
Si	-4.461321	1.594564	-0.118333	C	2.138147	-0.321385	-1.887909
C	-5.990642	1.428970	-1.218080	H	1.901093	-0.997098	-1.060928
C	-7.149843	2.178100	-0.940442	C	2.184496	-0.815773	-3.323298
C	-6.028768	0.542886	-2.308719	H	1.382227	-0.354544	-3.919117
C	-8.303386	2.041813	-1.714035	H	3.119355	-0.461842	-3.782533
H	-7.151704	2.887996	-0.115889	C	2.110618	-2.337024	-3.480108
C	-7.179342	0.404190	-3.087613	H	1.172617	-2.734649	-3.077693
H	-5.144073	-0.038416	-2.553946	H	2.172585	-2.620462	-4.535695
C	-8.319960	1.151860	-2.790337	H	2.933356	-2.833067	-2.954101
H	-9.185392	2.632859	-1.482037	C	2.268502	3.883308	-0.782302
H	-7.184795	-0.285673	-3.927425	C	0.997630	4.315679	-0.390282
H	-9.215617	1.046175	-3.396531	C	2.898311	4.461302	-1.889229
C	-4.181390	3.430764	0.271261	C	0.350632	5.317709	-1.114196
C	-4.425775	3.983986	1.541483	H	0.522540	3.863605	0.474809
C	-3.746888	4.303940	-0.744421	C	2.246305	5.463319	-2.609983
C	-4.245692	5.348158	1.790381	H	3.888237	4.123020	-2.179718
H	-4.763718	3.347971	2.355707	C	0.974340	5.891291	-2.224718
C	-3.573130	5.668020	-0.505282	H	-0.641353	5.638790	-0.812106
H	-3.541446	3.910540	-1.737026	H	2.734801	5.908659	-3.471450
C	-3.820665	6.194106	0.765854	H	0.470119	6.670178	-2.789021
H	-4.442655	5.748913	2.781199	C	3.726735	3.379982	1.180376
H	-3.253295	6.322879	-1.311938	C	3.304358	2.722354	2.505273
H	-3.687074	7.255897	0.953810	C	5.248814	3.309991	0.962070
C	-4.759255	0.684493	1.536513	H	3.447436	4.437886	1.238496
H	-3.914993	0.912672	2.196806	C	4.053271	3.370378	3.682212
H	-5.648725	1.143640	1.988198	H	3.537755	1.654870	2.466643
C	-4.952183	-0.809497	1.438242	H	2.220517	2.819169	2.639187
C	-6.187961	-1.358145	1.059016	C	5.992086	3.940717	2.152090
C	-3.899676	-1.691055	1.729649	H	5.550550	2.265448	0.842852
C	-6.365521	-2.739311	0.974016	H	5.510046	3.830530	0.033459
H	-7.018570	-0.695163	0.832448	C	5.575203	3.301754	3.485186
C	-4.077007	-3.073557	1.649674	H	3.764426	2.875768	4.616831
H	-2.938290	-1.285683	2.034837	H	3.746156	4.421760	3.779596
C	-5.310597	-3.604962	1.269063	H	7.072685	3.841005	2.001052
H	-7.333140	-3.138935	0.682502	H	5.780422	5.019409	2.186711
H	-3.252540	-3.737362	1.896058	H	6.087988	3.795761	4.318862
H	-5.450721	-4.680783	1.212211	H	5.893921	2.250477	3.497441

Zn	4.150375	-0.950875	-0.935511
Br	4.069309	-2.912011	0.458453
Br	5.936322	-0.237808	-2.361189
C	-1.491107	-0.569434	-3.873088
H	-1.834436	0.164331	-4.614707
H	-0.680700	-1.144843	-4.332260
H	-2.334452	-1.241840	-3.688061
H	-0.324094	0.920923	-2.812724

^{1}TS12

B3LYP/BSI SCF energy: -1662.289278a.u.

M06/BSII SCF energy in solution:-1661.566852a.u.

M06/BSII free energy in solution:-1661.015397a.u.

C	-3.422109	1.529923	1.155778
C	-3.879068	1.250417	-0.290664
C	-3.883124	-1.327555	0.364753
C	-3.437692	-0.885509	1.773288
C	-3.936387	0.505488	2.168581
H	-2.325091	1.527564	1.186289
H	-3.742727	2.543959	1.422264
H	-3.779144	-1.643706	2.488048
H	-2.341724	-0.886291	1.814804
H	-5.031686	0.528170	2.225612
H	-3.569803	0.758095	3.169868
N	-3.692601	-0.204701	-0.615884
C	-3.006609	2.054207	-1.268270
H	-3.339570	1.904734	-2.296346
H	-3.075066	3.119360	-1.024238
H	-1.959938	1.745975	-1.194692
C	-5.360644	1.628892	-0.504426
H	-5.479617	2.715997	-0.449589
H	-5.684190	1.292412	-1.492704
H	-6.018378	1.181748	0.245469
C	-5.363195	-1.766098	0.345098
H	-5.678331	-1.938227	-0.687198
H	-5.483940	-2.697627	0.907881
H	-6.025374	-1.018383	0.789626
C	-3.002235	-2.497215	-0.103754
H	-3.061882	-3.311874	0.625371
H	-3.331968	-2.869177	-1.074636
H	-1.958183	-2.182493	-0.187812
O	-3.808942	-0.519084	-1.857225
C	0.899328	0.103367	-1.538361
C	0.047935	-0.220269	-2.383287
Si	2.089069	0.584538	-0.241417
C	1.337271	0.213188	1.455799
C	1.012448	-1.106635	1.829273
C	1.059242	1.240430	2.376372
C	0.444466	-1.386395	3.073213
H	1.205792	-1.927414	1.145050
C	0.486795	0.964618	3.620854
H	1.292647	2.269991	2.120197
C	0.179965	-0.350340	3.972843
H	0.209733	-2.413155	3.340789
H	0.283639	1.776359	4.314345
H	-0.261351	-0.568116	4.941733
C	2.460236	2.429381	-0.410153
C	3.444737	3.042056	0.389656
C	1.785860	3.233133	-1.346492
C	3.740154	4.400251	0.263435
H	3.989155	2.456275	1.127584
C	2.078420	4.592197	-1.477972
H	1.026413	2.786263	-1.982112
C	3.055857	5.178595	-0.672753
H	4.503468	4.850189	0.892540
H	1.544145	5.192392	-2.209579
H	3.285169	6.235851	-0.774261
C	3.736235	-0.356488	-0.501488
H	4.095792	-0.053334	-1.492744
H	4.453102	0.048964	0.223084
C	3.685094	-1.861191	-0.398807
C	4.106471	-2.522578	0.765070
C	3.205884	-2.640960	-1.464535
C	4.050297	-3.913885	0.864055
H	4.484975	-1.939469	1.600981
C	3.148505	-4.031347	-1.367760
H	2.874440	-2.149184	-2.374969
C	3.569629	-4.675485	-0.202155
H	4.386615	-4.401947	1.774890
H	2.777566	-4.613353	-2.207218
H	3.528420	-5.758438	-0.128419
C	-0.893698	-0.569277	-3.312764
H	-1.480539	0.224827	-3.768646
C	-1.226428	-1.981379	-3.689348
H	-1.159402	-2.126340	-4.775706
H	-0.561785	-2.697854	-3.201030
H	-2.260465	-2.201906	-3.396187

5

B3LYP/BSI SCF energy: -1662.324636a.u.

M06/BSII SCF energy in solution:-1661.611348a.u.

M06/BSII free energy in solution:-1661.048269a.u.

C	-4.915780	0.553475	-0.966003
C	-4.343888	-0.878551	-0.839442
C	-3.501414	-0.246984	1.521281
C	-4.099785	1.162404	1.311171
C	-5.306325	1.178370	0.372922
H	-4.155883	1.185976	-1.443475
H	-5.772362	0.517167	-1.649601
H	-4.360438	1.571684	2.294265
H	-3.318044	1.810698	0.895297
H	-6.150043	0.638457	0.819009
H	-5.650844	2.207982	0.219628
N	-3.224386	-0.818989	0.158910
C	-3.740121	-1.256777	-2.207557
H	-3.496451	-2.321217	-2.262344
H	-4.469033	-1.052238	-2.998971
H	-2.836815	-0.674517	-2.410101
C	-5.459488	-1.902271	-0.523742
H	-6.056364	-2.080124	-1.424798
H	-5.019343	-2.853138	-0.215306
H	-6.144556	-1.570255	0.257703
C	-4.420108	-1.114189	2.415605
H	-4.086305	-2.153816	2.405899
H	-4.366256	-0.751624	3.447505
H	-5.468992	-1.085930	2.116916
C	-2.155202	-0.087381	2.249583
H	-2.313781	0.436816	3.197895
H	-1.705441	-1.057595	2.471685
H	-1.449729	0.486362	1.646965
O	-2.729927	-2.159679	0.385250
C	0.423707	-0.597827	-0.342966
C	-0.477305	-1.415153	-0.274118
Si	1.697009	0.716108	-0.456878
C	2.488054	0.973933	1.237564
C	3.012480	-0.119492	1.955109
C	2.581014	2.248712	1.824862
C	3.611156	0.056461	3.202770
H	2.950007	-1.120793	1.538326
C	3.179808	2.428542	3.073767
H	2.174421	3.112547	1.306481
C	3.697537	1.332382	3.764456
H	4.008137	-0.802096	3.737650
H	3.237360	3.423199	3.507755
H	4.162034	1.469782	4.737218
C	0.854505	2.291989	-1.068212
C	1.611314	3.420269	-1.439646
C	-0.545380	2.373886	-1.186428
C	0.997771	4.585622	-1.902343
H	2.696853	3.396883	-1.367854
C	-1.162480	3.537707	-1.650450
H	-1.156762	1.515802	-0.918868
C	-0.393156	4.646080	-2.008050
H	1.603699	5.443121	-2.182378
H	-2.245353	3.578214	-1.734813
H	-0.873402	5.551179	-2.369783
C	2.996067	0.200901	-1.764264
H	2.453484	0.116716	-2.713825
H	3.689528	1.043234	-1.876713
C	3.758266	-1.069530	-1.477084
C	5.022438	-1.035722	-0.868507
C	3.214604	-2.323551	-1.800311
C	5.720561	-2.212537	-0.593146
H	5.464323	-0.076324	-0.611632
C	3.910423	-3.501067	-1.526149
H	2.236714	-2.371782	-2.271966
C	5.167630	-3.451657	-0.920065
H	6.700063	-2.159135	-0.125597
H	3.471565	-4.459313	-1.791344
H	5.711704	-4.367978	-0.709700
C	-1.489929	-2.476164	-0.277725
H	-1.699038	-2.711331	-1.330111
C	-0.988196	-3.747642	0.416387
H	-0.095761	-4.125833	-0.088560
H	-0.741024	-3.538624	1.459912
H	-1.768554	-4.512738	0.383943

^{2}TS13-*S*

B3LYP/BSI SCF energy: -2134.502729a.u.

M06/BSII SCF energy in solution:-2133.699458a.u.

M06/BSII free energy in solution:-2133.112699a.u.

C	-3.211883	-0.027702	0.319320
O	-2.831912	-0.255609	-0.856220

N	-4.421468	0.528353	0.554812
C	-2.289613	-0.416476	1.467589
H	-2.634814	0.022827	2.406172
H	-2.400841	-1.504302	1.573214
C	-0.792928	-0.080011	1.195758
Zn	-0.948523	-1.143877	-0.755535
Br	-1.205091	-3.513452	-0.548658
C	-4.935697	0.694061	1.891770
C	-4.941133	1.962840	2.481227
C	-5.479630	-0.398882	2.574228
C	-5.483243	2.133684	3.755514
H	-4.516510	2.803689	1.941411
C	-6.015978	-0.222548	3.850881
H	-5.475257	-1.377506	2.104256
C	-6.019915	1.042081	4.442203
H	-5.482687	3.118777	4.212409
H	-6.432713	-1.074118	4.380160
H	-6.439325	1.177109	5.434591
C	-5.350233	0.902144	-0.563052
C	-4.755634	1.966078	-1.502295
C	-5.868313	-0.326227	-1.332255
H	-6.204616	1.356642	-0.049382
C	-5.784607	2.374590	-2.570421
H	-3.861779	1.563630	-1.985686
H	-4.446356	2.840329	-0.916010
C	-6.884036	0.098280	-2.407150
H	-5.023454	-0.839648	-1.799914
H	-6.330888	-1.029297	-0.629258
C	-6.297469	1.156492	-3.352893
H	-5.332628	3.104978	-3.251049
H	-6.634522	2.880893	-2.089868
H	-7.207301	-0.783597	-2.971561
H	-7.783745	0.504786	-1.922588
H	-7.050241	1.467408	-4.086644
H	-5.466993	0.714744	-3.919906
C	3.495317	0.570280	0.854921
N	2.597992	-0.364315	0.656980
C	2.942606	-1.507902	1.516366
H	2.066637	-1.806683	2.102116
C	4.124496	-0.982272	2.389526
H	3.857176	-0.770422	3.428211
O	4.452271	0.300410	1.777066
C	5.291648	-1.976457	2.255930
H	5.438647	-2.517764	3.199115
H	6.226488	-1.446045	2.045067
C	4.863635	-2.909933	1.142891
C	5.603705	-3.928795	0.541719
C	3.542843	-2.672453	0.748272
C	5.004688	-4.702456	-0.454910
H	6.631151	-4.119411	0.841450
C	2.937090	-3.446282	-0.242073
C	3.680792	-4.464629	-0.842406
H	5.571240	-5.497149	-0.932226
H	1.908697	-3.269184	-0.542031
H	3.224914	-5.074913	-1.616236
C	3.465520	1.813383	0.113495
C	4.540756	2.764588	0.002104
C	5.780812	2.662582	0.683929
C	4.334462	3.885900	-0.868860
C	2.142905	3.015170	-1.412538
C	6.754721	3.632179	0.527104
H	5.959240	1.820828	1.338139
C	5.350826	4.858987	-1.005671
C	3.106502	3.974087	-1.588533
H	1.199843	3.049979	-1.948742
C	6.543269	4.738393	-0.318587
H	7.694138	3.536547	1.063790
H	5.177025	5.703684	-1.666821
H	2.933280	4.804799	-2.264926
H	7.317538	5.491475	-0.431818
N	2.284338	1.977800	-0.550337
Ni	0.971220	0.409474	-0.285611
Br	0.400208	-0.234462	-2.685058
H	-0.215053	-0.737178	1.854916
C	-0.517200	1.393238	1.603060
H	0.491537	1.730911	1.307631
H	-1.200601	2.058834	1.058452
C	-0.614529	1.676338	3.114965
H	-1.620979	1.500990	3.506776
H	0.077278	1.037117	3.674689
H	-0.357322	2.718931	3.331617

^{2}TS13-*R*

B3LYP/BSI SCF energy: -2134.517075a.u.

M06/BSII SCF energy in solution:-2133.710222a.u.

M06/BSII free energy in solution:-2133.125909a.u.

C	-2.866547	-0.116512	0.253989

O	-2.238906	-0.113351	-0.831310
N	-4.044745	0.547415	0.364123
C	-2.331285	-0.908354	1.436211
H	-2.766059	-0.528630	2.364644
H	-2.735618	-1.922866	1.299102
C	-0.785426	-1.001159	1.529791
H	-0.484314	-0.078243	2.067928
C	-0.367990	-2.198860	2.417407
H	-0.692385	-3.129680	1.936710
H	0.728880	-2.255431	2.458871
C	-0.893043	-2.158257	3.862728
H	-1.986400	-2.206927	3.903112
H	-0.509643	-3.005197	4.442986
H	-0.582929	-1.237133	4.372463
Zn	-0.654594	-1.529848	-0.729075
Br	-1.666401	-3.704913	-0.986782
C	-4.850789	0.472391	1.557806
C	-4.903091	1.566532	2.428068
C	-5.626540	-0.663311	1.813806
C	-5.721648	1.518845	3.556944
H	-4.297186	2.442859	2.218260
C	-6.440301	-0.707005	2.947033
H	-5.583117	-1.505410	1.130109
C	-6.489920	0.382199	3.818882
H	-5.755949	2.368031	4.233010
H	-7.036415	-1.592676	3.145352
H	-7.124672	0.345841	4.699157
C	-4.684623	1.221555	-0.811211
C	-3.838552	2.361331	-1.406115
C	-5.127758	0.215203	-1.888813
H	-5.588094	1.675592	-0.388765
C	-4.615384	3.069977	-2.529134
H	-2.908984	1.947958	-1.805924
H	-3.574272	3.073315	-0.613769
C	-5.887093	0.931896	-3.017177
H	-4.246025	-0.291741	-2.291650
H	-5.764442	-0.551876	-1.432643
C	-5.060531	2.079639	-3.616276
H	-3.992099	3.860110	-2.963960
H	-5.500120	3.568755	-2.107169
H	-6.155904	0.208157	-3.794670
H	-6.832582	1.334054	-2.624705
H	-5.638851	2.600850	-4.388241
H	-4.172519	1.665605	-4.112787
C	3.415289	1.061314	1.042883
N	2.926449	-0.129731	1.161540
C	4.009237	-1.010210	1.637193
H	3.649992	-1.587832	2.495272
C	5.162832	-0.022369	1.991317
H	5.302293	0.147549	3.061685
O	4.693941	1.248541	1.432220
C	6.435162	-0.508709	1.276781
H	7.148475	-0.906619	2.009596
H	6.933389	0.323030	0.767474
C	5.945005	-1.587184	0.333361
C	6.670334	-2.274318	-0.640223
C	4.595146	-1.886897	0.546364
C	6.026022	-3.256101	-1.396357
H	7.719396	-2.048631	-0.813150
C	3.947628	-2.866266	-0.206232
C	4.674468	-3.549804	-1.182634
H	6.578177	-3.793742	-2.161777
H	2.894081	-3.082218	-0.059109
H	4.182058	-4.306084	-1.785714
C	2.589515	2.147250	0.494229
C	3.006092	3.494546	0.254858
C	4.297401	4.010502	0.556233
C	2.036217	4.374513	-0.333863
C	0.456521	2.547294	-0.365379
C	4.601455	5.327136	0.288795
H	5.039887	3.360803	0.997755
C	2.386502	5.724739	-0.595967
C	0.753146	3.859249	-0.643545
H	-0.504819	2.105267	-0.602905
C	3.643495	6.192625	-0.290769
H	5.591144	5.706449	0.524796
H	1.643762	6.378582	-1.044062
H	0.009316	4.500215	-1.106131
H	3.905552	7.226463	-0.494830
N	1.354095	1.709753	0.208032
Ni	1.009624	-0.274549	0.622470
Br	1.044081	-0.816797	-2.349283

^{2}IM11-*S*

B3LYP/BSI SCF energy: -2134.519986a.u.

M06/BSII SCF energy in solution:-2133.709997a.u.

M06/BSII free energy in solution:-2133.124494a.u.

C	-2.896083	-0.219055	0.315304
O	-2.148637	0.084247	-0.649354
N	-4.188397	0.197262	0.298938
C	-2.373543	-1.076760	1.453183
H	-3.127483	-1.143118	2.244344
H	-2.287973	-2.078122	1.010343
C	-1.002605	-0.693530	2.056223
Zn	-0.346417	-0.876729	-0.910332
Br	-0.743921	-3.267011	-1.073310
C	-5.155431	-0.252856	1.269422
C	-5.654792	0.642672	2.221128
C	-5.648162	-1.561240	1.214484
C	-6.635127	0.225231	3.121870
H	-5.268756	1.656773	2.254181
C	-6.623271	-1.975313	2.122886
H	-5.259683	-2.246610	0.467618
C	-7.119282	-1.083888	3.076103
H	-7.016292	0.922197	3.862375
H	-6.996956	-2.993985	2.080933
H	-7.879920	-1.407537	3.780261
C	-4.744737	0.999282	-0.840765
C	-4.052606	2.361328	-1.021800
C	-4.799345	0.200746	-2.155837
H	-5.777664	1.199431	-0.535036
C	-4.754490	3.171558	-2.125306
H	-3.005773	2.201426	-1.291926
H	-4.070392	2.911124	-0.072442
C	-5.488801	1.025222	-3.256138
H	-3.782336	-0.055635	-2.464827
H	-5.339070	-0.739067	-1.989499
C	-4.810518	2.390111	-3.446873
H	-4.234246	4.126064	-2.266932
H	-5.777696	3.418905	-1.806332
H	-5.482068	0.460262	-4.194993
H	-6.545366	1.179708	-2.992056
H	-5.340877	2.973602	-4.208776
H	-3.788900	2.237339	-3.820195
C	3.476520	0.515035	1.215622
N	2.750867	-0.543260	1.334667
C	3.655419	-1.662879	1.665327
H	3.243219	-2.219240	2.512993
C	5.011846	-0.961204	1.977432
H	5.246976	-0.869693	3.040709
O	4.788373	0.406794	1.490743
C	6.106332	-1.663231	1.160057
H	6.735974	-2.268969	1.824377
H	6.764236	-0.930531	0.680822
C	5.338899	-2.523887	0.179096
C	5.838156	-3.256176	-0.897784
C	3.971102	-2.549454	0.473751
C	4.951012	-4.005053	-1.674776
H	6.898798	-3.241138	-1.135052
C	3.081765	-3.298734	-0.295500
C	3.583806	-4.025114	-1.377308
H	5.325944	-4.572134	-2.522029
H	2.016192	-3.306837	-0.087999
H	2.899181	-4.597281	-1.995425
C	2.868619	1.792326	0.785261
C	3.566093	3.003525	0.493081
C	4.972853	3.185483	0.618579
C	2.769189	4.107787	0.034926
C	0.810114	2.709253	0.208431
C	5.547121	4.397030	0.308658
H	5.587499	2.364070	0.958115
C	3.398561	5.343008	-0.275121
C	1.374411	3.923148	-0.104406
H	-0.249808	2.517921	0.092108
C	4.758769	5.484860	-0.141040
H	6.621234	4.521216	0.407522
H	2.784191	6.167870	-0.624010
H	0.753334	4.734312	-0.470611
H	5.235266	6.430294	-0.382238
N	1.545008	1.667847	0.661755
Ni	0.744717	-0.201586	1.228551
Br	0.862874	0.331222	-2.602136
H	-0.618732	-1.643659	2.468749
C	-1.171359	0.257167	3.268405
H	-1.866185	-0.202798	3.993991
H	-0.214018	0.345491	3.801728
C	-1.685708	1.667385	2.956365
H	-0.984126	2.217859	2.321865
H	-2.649395	1.639090	2.436275
H	-1.829836	2.246334	3.875909

^{2}IM11-*R*

B3LYP/BSI SCF energy: -2134.52159a.u.

M06/BSII SCF energy in solution:-2133.711264a.u.

M06/BSII free energy in solution:-2133.127219a.u.

C	-2.840391	-0.432802	0.071659
O	-2.068595	-0.201206	-0.892485
N	-4.070351	0.141141	0.084722
C	-2.418495	-1.373731	1.176039
H	-3.233881	-1.492445	1.892869
H	-2.285553	-2.345323	0.678776
C	-1.098258	-1.001409	1.888471
H	-1.312927	-0.117793	2.522192
C	-0.677874	-2.158929	2.832615
H	-0.501261	-3.061145	2.232566
H	0.285945	-1.916057	3.305530
C	-1.668728	-2.492846	3.964539
H	-2.622751	-2.866293	3.578843
H	-1.261511	-3.266786	4.625309
H	-1.880060	-1.608003	4.577484
Zn	-0.193929	-1.084017	-0.948925
Br	-0.425874	-3.479496	-1.236511
C	-4.999175	-0.047440	1.171893
C	-4.945289	0.787598	2.292494
C	-5.996923	-1.023328	1.074095
C	-5.879885	0.636493	3.318204
H	-4.169029	1.543886	2.355835
C	-6.930774	-1.167497	2.100521
H	-6.028011	-1.668546	0.201648
C	-6.873766	-0.339302	3.223600
H	-5.830641	1.282319	4.189889
H	-7.699795	-1.930323	2.023768
H	-7.600101	-0.455207	4.022418
C	-4.559131	0.992990	-1.047347
C	-3.762676	2.302298	-1.198418
C	-4.658984	0.226975	-2.378821
H	-5.577380	1.264489	-0.747512
C	-4.382088	3.185284	-2.295314
H	-2.727329	2.063315	-1.456892
H	-3.755721	2.836061	-0.239151
C	-5.273789	1.123364	-3.467015
H	-3.661711	-0.098655	-2.685361
H	-5.268622	-0.673591	-2.238256
C	-4.487070	2.432717	-3.630262
H	-3.783738	4.095979	-2.415470
H	-5.385077	3.510140	-1.981942
H	-5.305363	0.576139	-4.415819
H	-6.316624	1.357131	-3.206516
H	-4.962346	3.068919	-4.386198
H	-3.477597	2.204471	-3.997538
C	3.237436	0.842265	1.267907
N	2.699791	-0.323736	1.374065
C	3.789648	-1.296004	1.598523
H	3.532456	-1.926985	2.455391
C	5.040927	-0.397357	1.840238
H	5.349753	-0.315877	2.885220
O	4.565493	0.936656	1.452626
C	6.159339	-0.879682	0.903107
H	6.947472	-1.374026	1.485232
H	6.627164	-0.032219	0.390886
C	5.466651	-1.845551	-0.034547
C	5.992779	-2.475669	-1.162158
C	4.149797	-2.100574	0.363451
C	5.182863	-3.354865	-1.885004
H	7.014302	-2.282801	-1.479566
C	3.339446	-2.981486	-0.351211
C	3.865813	-3.604860	-1.484131
H	5.577801	-3.843926	-2.770863
H	2.309708	-3.168963	-0.064170
H	3.236101	-4.274588	-2.061032
C	2.405987	2.025641	0.958424
C	2.877185	3.354167	0.731273
C	4.241232	3.758253	0.794169
C	1.883014	4.341893	0.413777
C	0.191639	2.629397	0.580793
C	4.589212	5.068920	0.560071
H	5.002919	3.027627	1.025871
C	2.281484	5.684712	0.177609
C	0.529128	3.940221	0.341361
H	-0.830026	2.274316	0.514142
C	3.606605	6.041158	0.250044
H	5.633304	5.362542	0.610430
H	1.519528	6.420005	-0.063998
H	-0.238540	4.664396	0.087817
H	3.906261	7.068634	0.066884
N	1.115306	1.692954	0.893302
Ni	0.675811	-0.337079	1.250428
Br	1.089254	0.313660	-2.442707

^{2}IM12-*S*

B3LYP/BSI SCF energy: -1880.469266a.u.

M06/BSII SCF energy in solution:-1879.646729a.u.

M06/BSII free energy in solution:-1879.055884a.u.

C	-2.489103	0.055516	-0.322822
O	-1.508738	0.402734	0.380959
N	-3.754841	0.225544	0.139635
C	-2.246761	-0.560077	-1.692539
H	-2.272059	-1.652415	-1.550651
H	-3.092684	-0.334168	-2.355017
C	-0.864776	-0.151192	-2.230118
C	-4.893411	-0.276784	-0.586855
C	-5.207566	-1.638973	-0.544837
C	-5.719509	0.608562	-1.288258
C	-6.335660	-2.114944	-1.214813
H	-4.566290	-2.316791	0.010089
C	-6.849424	0.128999	-1.951030
H	-5.465462	1.663757	-1.317445
C	-7.158280	-1.232794	-1.917365
H	-6.572325	-3.174317	-1.183588
H	-7.484843	0.818761	-2.498547
H	-8.036422	-1.604304	-2.436927
C	-4.039857	0.847490	1.470161
C	-3.539208	-0.012005	2.645347
C	-3.545456	2.301129	1.570632
H	-5.134413	0.869530	1.520649
C	-3.939208	0.619506	3.989776
H	-2.450590	-0.099025	2.583195
H	-3.956592	-1.022892	2.561247
C	-3.951299	2.916694	2.920631
H	-2.457223	2.318138	1.466890
H	-3.962615	2.887323	0.742725
C	-3.448938	2.070654	4.100216
H	-3.538860	0.016134	4.812538
H	-5.033928	0.598927	4.092987
H	-3.562019	3.939033	2.989585
H	-5.046847	2.997162	2.973996
H	-3.778015	2.510301	5.049132
H	-2.350458	2.081887	4.111814
C	3.035248	-0.400012	-0.465915
N	2.237437	0.567920	-0.891012
C	3.063784	1.573630	-1.559697
H	2.644630	1.808706	-2.545297
O	4.352960	-0.255408	-0.787534
C	2.521036	-1.508018	0.263687
C	3.262469	-2.635078	0.783800
C	4.653668	-2.827299	0.609067
C	2.530966	-3.618158	1.527483
C	0.502905	-2.343391	1.149819
C	5.293116	-3.936286	1.144413
H	5.222950	-2.096893	0.050414
C	3.210175	-4.733772	2.060027
C	1.121120	-3.433219	1.704853
H	-0.565773	-2.182979	1.262440
C	4.573789	-4.896399	1.873836
H	6.362525	-4.058714	0.996127
H	2.640286	-5.469473	2.622238
H	0.548623	-4.157225	2.275835
H	5.083109	-5.760929	2.290178
N	1.155108	-1.392099	0.441103
Ni	0.318323	0.097519	-0.622432
C	4.473422	0.909221	-1.643054
H	4.735711	0.549592	-2.642455
C	-0.357202	-1.069471	-3.345121
H	-0.259481	-2.094087	-2.955969
H	0.660236	-0.761536	-3.620376
C	-1.215484	-1.106626	-4.624187
H	-1.316569	-0.103480	-5.056620
H	-0.772506	-1.755625	-5.389294
H	-2.226486	-1.480896	-4.424795
H	-0.953903	0.874854	-2.637099
C	3.301352	2.828909	-0.736554
C	2.355039	3.742229	-0.272429
C	4.659407	2.997416	-0.445876
C	2.781230	4.829430	0.493479
H	1.300323	3.607737	-0.497783
C	5.085219	4.083436	0.320152
C	4.138995	4.997775	0.788809
H	2.055420	5.547996	0.863653
H	6.138582	4.218223	0.552739
H	4.459283	5.845891	1.387505
C	5.500782	1.907119	-1.075815
H	6.166933	1.407859	-0.364410
H	6.131495	2.305931	-1.880524

^{2}IM12-*R*

B3LYP/BSI SCF energy: -1880.467834a.u.

M06/BSII SCF energy in solution:-1879.645247a.u.

M06/BSII free energy in solution:-1879.053945a.u.

C	2.498099	-0.149524	-0.272148
O	1.491360	0.081075	0.442345
N	3.743535	0.114591	0.200118
C	2.310798	-0.731450	-1.665354
H	3.140549	-0.419801	-2.312454
H	2.424766	-1.822833	-1.557499
C	0.905066	-0.409230	-2.209753
H	0.932547	0.608026	-2.632704
C	0.463355	-1.377286	-3.313530
H	0.427703	-2.403687	-2.913846
H	-0.567933	-1.135075	-3.602063
C	1.333883	-1.379060	-4.584737
H	2.365344	-1.682301	-4.369850
H	0.942125	-2.066684	-5.344191
H	1.371979	-0.377591	-5.030103
C	4.923038	-0.246626	-0.544901
C	5.653912	0.740937	-1.214651
C	5.371870	-1.571128	-0.550511
C	6.824508	0.400656	-1.892867
H	5.294895	1.765559	-1.207519
C	6.540743	-1.907663	-1.235109
H	4.802355	-2.328647	-0.020833
C	7.268984	-0.923483	-1.905724
H	7.385675	1.169346	-2.415807
H	6.882769	-2.938349	-1.240709
H	8.178735	-1.186757	-2.436883
C	3.973572	0.709376	1.553477
C	3.343266	2.104355	1.711233
C	3.563178	-0.237583	2.695742
H	5.061162	0.834355	1.603931
C	3.699477	2.705540	3.081467
H	2.257548	2.020989	1.614988
H	3.695353	2.758250	0.903977
C	3.911971	0.378681	4.061601
H	2.486943	-0.423830	2.633239
H	4.072256	-1.201193	2.571599
C	3.287688	1.771826	4.229458
H	3.215361	3.682779	3.190318
H	4.782875	2.887432	3.133722
H	3.577068	-0.290262	4.862742
H	5.004499	0.457844	4.159352
H	3.580485	2.204051	5.193503
H	2.193203	1.678724	4.244890
C	-3.064267	0.004444	-0.575873
N	-2.158282	-0.962785	-0.579074
C	-2.859575	-2.238426	-0.728771
H	-2.406142	-2.821204	-1.539523
C	-4.334189	-1.825671	-1.030291
H	-4.625284	-1.955843	-2.076805
O	-4.353780	-0.402271	-0.755356
C	-5.248392	-2.590534	-0.054122
H	-5.827120	-3.354074	-0.589407
H	-5.969634	-1.908781	0.408743
C	-4.295811	-3.219661	0.940961
C	-4.603892	-3.920681	2.107770
C	-2.962653	-3.045651	0.554342
C	-3.565200	-4.446112	2.879758
H	-5.637516	-4.056127	2.416162
C	-1.924051	-3.571412	1.322261
C	-2.232198	-4.273612	2.489365
H	-3.793586	-4.992335	3.790688
H	-0.889112	-3.430901	1.021250
H	-1.433735	-4.687235	3.098913
C	-2.684539	1.365598	-0.412248
C	-3.552487	2.521846	-0.387939
C	-4.957634	2.471662	-0.549143
C	-2.939339	3.800779	-0.180575
C	-0.775993	2.709236	-0.083539
C	-5.722256	3.628628	-0.504890
H	-5.438943	1.516121	-0.707407
C	-3.744452	4.958562	-0.140270
C	-1.516730	3.861043	-0.022451
H	0.305365	2.726678	0.019792
C	-5.118682	4.879674	-0.299714
H	-6.799530	3.561392	-0.629606
H	-3.263503	5.920606	0.018707
H	-1.031085	4.817622	0.141874
H	-5.725392	5.780198	-0.265459
N	-1.315604	1.482229	-0.268504
Ni	-0.306702	-0.230837	-0.596763

^{2}TS14-*SS*

B3LYP/BSI SCF energy: -3072.424978a.u.

M06/BSII SCF energy in solution:-3071.114183a.u.

M06/BSII free energy in solution:-3070.191305a.u.

C	-2.522717	1.855745	-0.149106
O	-2.141696	0.771137	0.358842

N	-3.475669	2.602209	0.462326	H	-2.898489	-5.246074	-0.100273
C	-1.927303	2.313744	-1.468575	C	-4.958113	-4.331195	-3.273544
H	-2.685342	2.106952	-2.241703	C	-3.800813	-2.142600	-3.400023
H	-1.827647	3.406658	-1.463879	H	-2.678129	-0.304492	-3.332006
C	-0.627034	1.555344	-1.795897	C	-5.145608	-5.542670	-2.645867
C	-3.956654	3.828318	-0.126101	H	-4.547854	-6.822380	-1.004358
C	-4.971889	3.792483	-1.087069	H	-5.527279	-4.072373	-4.161773
C	-3.447853	5.057302	0.307509	H	-4.358884	-1.878717	-4.292576
C	-5.467172	4.983035	-1.621258	H	-5.868465	-6.253131	-3.035390
H	-5.365168	2.833839	-1.411449	N	-2.154902	-1.552484	-1.770584
C	-3.947940	6.244783	-0.227629	Ni	-0.789137	-0.235120	-0.886559
H	-2.658883	5.074201	1.053107	C	-0.229584	-3.818951	1.677375
C	-4.956599	6.209686	-1.192983	H	0.528379	-4.562810	1.425093
H	-6.252189	4.950891	-2.370881	C	1.242258	-1.459890	-2.375344
H	-3.546019	7.196482	0.106753	H	0.667795	-0.787227	-2.994404
H	-5.342164	7.134916	-1.610396	C	-0.231022	1.718490	-3.269937
C	-4.133009	2.182476	1.738987	H	-1.003669	1.267977	-3.914541
C	-4.929943	0.873120	1.596769	H	0.688116	1.158709	-3.472181
C	-3.157444	2.132332	2.926739	C	0.004939	3.167334	-3.735760
H	-4.853045	2.984353	1.937547	H	0.800109	3.637508	-3.145363
C	-5.670499	0.547183	2.904787	H	0.313601	3.195652	-4.786590
H	-4.240910	0.061707	1.346150	H	-0.894608	3.787067	-3.640361
H	-5.643512	0.966957	0.768849	H	0.174952	2.012355	-1.186714
C	-3.907574	1.799341	4.227534	C	1.061084	-2.944713	-2.541335
H	-2.392334	1.375306	2.735888	H	0.295817	-3.343266	-1.859410
H	-2.646032	3.098199	3.020098	H	0.758144	-3.170449	-3.564643
C	-4.708783	0.495007	4.101205	H	1.996254	-3.471122	-2.337120
H	-6.202119	-0.405626	2.798154	C	2.037381	-0.927184	-1.358621
H	-6.439089	1.311491	3.090582	C	2.773266	-0.500870	-0.463547
H	-3.190401	1.726085	5.052839	Si	4.100781	0.082163	0.650527
H	-4.591913	2.622733	4.478952	C	4.674446	-1.377006	1.715751
H	-5.266237	0.302619	5.025669	C	5.816741	-2.123485	1.373800
H	-4.011004	-0.343615	3.973376	C	3.948872	-1.782641	2.852940
C	-1.402581	-2.861624	-0.005004	C	6.218421	-3.226626	2.130392
N	-0.602497	-1.897060	0.314770	H	6.404490	-1.847087	0.502584
C	0.225105	-2.342384	1.447041	C	4.345268	-2.884471	3.613220
H	1.277921	-2.241898	1.161970	H	3.066565	-1.225870	3.158630
O	-1.316281	-3.999951	0.714967	C	5.482801	-3.609837	3.252774
C	-2.315194	-2.735333	-1.147429	H	7.105176	-3.785118	1.843218
C	-3.248938	-3.722933	-1.603267	H	3.770091	-3.172365	4.489593
C	-3.467619	-4.982011	-0.980099	H	5.795510	-4.466183	3.844216
C	-4.015623	-3.397655	-2.773649	C	3.424154	1.456834	1.760969
C	-2.880076	-1.267912	-2.876894	C	3.901324	1.653486	3.069821
C	-4.394788	-5.864849	-1.492975	C	2.456907	2.357895	1.275507

C	3.426402	2.697806	3.866937
H	4.647462	0.977880	3.479974
C	1.980041	3.404373	2.067318
H	2.077221	2.243876	0.263815
C	2.461742	3.574729	3.367576
H	3.809831	2.826337	4.875738
H	1.239423	4.091280	1.666015
H	2.093458	4.390215	3.984584
C	5.561166	0.722391	-0.400005
H	5.865286	-0.092469	-1.067758
H	6.399313	0.910109	0.283138
C	5.245426	1.963715	-1.203580
C	4.628224	1.868301	-2.461222
C	5.545358	3.238982	-0.700388
C	4.324735	3.018574	-3.191570
H	4.381707	0.895161	-2.878864
C	5.243744	4.388465	-1.432207
H	6.023876	3.330302	0.272062
C	4.630819	4.282851	-2.682162
H	3.852836	2.916646	-4.164697
H	5.491815	5.365671	-1.025714
H	4.399661	5.176282	-3.256019
C	-0.075647	-1.648877	2.760951
C	0.166647	-0.317301	3.100146
C	-0.626331	-2.538876	3.689501
C	-0.156319	0.118097	4.388105
H	0.609077	0.369339	2.385537
C	-0.957207	-2.099800	4.972392
C	-0.719413	-0.766263	5.315841
H	0.044485	1.147411	4.669415
H	-1.382205	-2.785685	5.700729
H	-0.962127	-0.416770	6.315439
C	-0.737188	-3.941191	3.128593
H	-1.761586	-4.329884	3.140504
H	-0.121975	-4.650357	3.694752
Br	2.907552	-1.144049	-4.566579

^{2}TS14-*SR*

B3LYP/BSI SCF energy: -3072.407402 a.u.

M06/BSII SCF energy in solution:-3071.089184a.u.

M06/BSII free energy in solution:-3070.169959a.u.

C	-2.348808	2.014984	-0.086827
O	-1.899751	1.041068	0.554396
N	-3.243063	2.874364	0.480494
C	-1.918329	2.235694	-1.527235
H	-2.773975	1.951575	-2.161242
H	-1.787614	3.311637	-1.706394
C	-0.683966	1.391660	-1.885829
C	-3.795521	3.981281	-0.259522
C	-4.929522	3.796429	-1.057560
C	-3.234472	5.257064	-0.133040
C	-5.492168	4.880630	-1.733141
H	-5.362565	2.804492	-1.144428
C	-3.800570	6.338317	-0.809164
H	-2.353505	5.391341	0.487082
C	-4.928945	6.152120	-1.610623
H	-6.370755	4.730958	-2.353775
H	-3.357847	7.325113	-0.711580
H	-5.367298	6.994603	-2.137143
C	-3.774606	2.679153	1.862843
C	-4.580678	1.375947	2.013845
C	-2.694214	2.806830	2.949876
H	-4.472806	3.513535	1.996561
C	-5.201049	1.284303	3.417977
H	-3.915248	0.525173	1.841472
H	-5.365418	1.341778	1.248223
C	-3.323971	2.711164	4.350089
H	-1.958450	2.008791	2.817232
H	-2.171470	3.764311	2.832410
C	-4.135873	1.417127	4.516269
H	-5.739542	0.335106	3.521363
H	-5.949445	2.081007	3.540204
H	-2.537950	2.769267	5.112164
H	-3.981280	3.577185	4.516361
H	-4.608126	1.391730	5.505612
H	-3.454123	0.557779	4.468562
C	-1.458562	-2.943618	0.050059
N	-0.674736	-1.959513	0.344323
C	0.221883	-2.418210	1.427891
H	1.255521	-2.220723	1.130329
O	-1.297492	-4.095854	0.722844
C	-2.433797	-2.811687	-1.044961
C	-3.367301	-3.811513	-1.468784
C	-3.509004	-5.094856	-0.870888
C	-4.217550	-3.475808	-2.575656
C	-3.131806	-1.322032	-2.694845
C	-4.444712	-5.986814	-1.348103

H	-2.871360	-5.367536	-0.042128
C	-5.168776	-4.419651	-3.040222
C	-4.071510	-2.199458	-3.175186
H	-2.981090	-0.345367	-3.140567
C	-5.281546	-5.652050	-2.438171
H	-4.538214	-6.963029	-0.882026
H	-5.803583	-4.151429	-3.880046
H	-4.697927	-1.921483	-4.017279
H	-6.010571	-6.371412	-2.798994
N	-2.323409	-1.615454	-1.645531
Ni	-0.883871	-0.315638	-0.859396
C	-0.094584	-3.938419	1.552564
H	0.665994	-4.582520	1.108169
C	1.326384	-1.809861	-2.084578
C	-0.372151	1.444907	-3.382633
H	-1.172805	0.947229	-3.954416
H	0.538714	0.867726	-3.567375
C	-0.155139	2.850706	-3.978246
H	0.656129	3.372142	-3.457911
H	0.119318	2.789924	-5.037948
H	-1.054357	3.473443	-3.909657
H	0.181495	1.814273	-1.345244
C	2.082346	-0.893356	-1.335861
C	2.831739	-0.133561	-0.724514
Si	4.131263	0.786557	0.176684
C	4.901759	-0.402686	1.429074
C	4.976246	-1.779349	1.137845
C	5.447534	0.044662	2.646322
C	5.584713	-2.668932	2.025426
H	4.543160	-2.170341	0.220078
C	6.058634	-0.843007	3.533759
H	5.385224	1.095995	2.915647
C	6.129890	-2.202327	3.223202
H	5.626739	-3.726321	1.778929
H	6.472238	-0.474754	4.469026
H	6.602714	-2.895096	3.914424
C	3.391557	2.289884	1.049536
C	4.214905	3.291801	1.598380
C	2.001527	2.433740	1.204329
C	3.675887	4.383013	2.282908
H	5.295872	3.227918	1.492100
C	1.455910	3.522798	1.887669
H	1.336469	1.689934	0.774854
C	2.292427	4.499246	2.430872
H	4.334256	5.141665	2.697610
H	0.377504	3.606940	1.992730
H	1.870620	5.347585	2.963180
C	5.469612	1.336545	-1.073860
H	5.990216	0.425073	-1.389436
H	6.205637	1.935159	-0.522011
C	4.951473	2.093359	-2.272395
C	4.655303	1.422919	-3.469547
C	4.731908	3.478856	-2.219678
C	4.159854	2.112403	-4.576689
H	4.820289	0.350275	-3.531132
C	4.235659	4.170638	-3.325237
H	4.952091	4.019284	-1.302877
C	3.946840	3.490760	-4.510010
H	3.944544	1.571648	-5.494398
H	4.078748	5.244154	-3.261147
H	3.564875	4.029269	-5.372579
C	-0.110457	-1.855354	2.797250
C	-0.046895	-0.528842	3.222773
C	-0.485912	-2.874486	3.680804
C	-0.376948	-0.229534	4.546803
H	0.255966	0.258771	2.540930
C	-0.822115	-2.572584	5.000943
C	-0.768081	-1.244136	5.428568
H	-0.320565	0.797303	4.896221
H	-1.112694	-3.359474	5.692301
H	-1.020813	-0.998027	6.456114
C	-0.405975	-4.238290	3.027226
H	-1.327635	-4.822804	3.120342
H	0.398448	-4.840667	3.466423
Br	2.537945	-4.061710	-1.478749
C	1.410081	-1.839166	-3.585291
H	0.747796	-1.075072	-4.009251
H	2.427044	-1.631776	-3.924812
H	1.101660	-2.816497	-3.959624
H	0.507421	-2.314419	-1.609285

^{2}TS14-*RS*

B3LYP/BSI SCF energy: -3072.4123 a.u.

M06/BSII SCF energy in solution:-3071.104142a.u.

M06/BSII free energy in solution:-3070.178444a.u.

C	2.816622	-1.638568	-0.405731
O	2.116764	-0.933944	0.367914

N	3.641470	-2.597622	0.076806	H	2.271817	5.516780	1.315344
C	2.750250	-1.360621	-1.896361	C	4.531598	5.755897	-1.843695
H	3.610742	-0.712898	-2.120308	C	3.811599	3.485568	-2.533767
H	2.918803	-2.277743	-2.472732	H	3.063091	1.515641	-2.958358
C	1.427877	-0.645116	-2.221930	C	4.474355	6.800380	-0.947122
C	4.468807	-3.380876	-0.809611	H	3.614294	7.529157	0.901482
C	5.722574	-2.903285	-1.203551	H	5.157995	5.817859	-2.729029
C	4.036837	-4.643381	-1.229586	H	4.428834	3.540587	-3.424749
C	6.537258	-3.684502	-2.024889	H	5.058470	7.699603	-1.118117
H	6.050666	-1.923973	-0.868512	N	2.277834	2.236526	-1.185560
C	4.855354	-5.420297	-2.050036	Ni	1.142163	0.561935	-0.691620
H	3.060215	-5.002651	-0.920233	C	-0.124474	3.269509	2.532621
C	6.105455	-4.942403	-2.449184	H	-0.996530	3.924396	2.499656
H	7.508639	-3.308885	-2.332431	C	-1.000143	1.779643	-2.094146
H	4.513852	-6.396830	-2.379836	H	-0.312607	1.227385	-2.715232
H	6.739879	-5.547839	-3.089417	C	-0.904814	3.278517	-2.022750
C	3.821828	-2.857575	1.538427	H	-0.400705	3.611119	-1.103755
C	4.447514	-1.663979	2.280739	H	-0.353281	3.663661	-2.881183
C	2.541417	-3.349403	2.233252	H	-1.902497	3.724008	-2.028776
H	4.546455	-3.679081	1.567671	C	-1.894267	1.078728	-1.282835
C	4.745323	-2.042303	3.741533	C	-2.722465	0.503545	-0.571044
H	3.754539	-0.818117	2.243408	Si	-4.149807	-0.291147	0.254532
H	5.369655	-1.357945	1.771843	C	-4.880078	0.933657	1.501363
C	2.845072	-3.725518	3.693991	C	-6.021485	1.694955	1.191692
H	1.785734	-2.559957	2.200792	C	-4.273980	1.149810	2.754689
H	2.138549	-4.214070	1.692151	C	-6.536112	2.632981	2.089571
C	3.489072	-2.558809	4.459157	H	-6.519656	1.561021	0.235294
H	5.158252	-1.175476	4.270372	C	-4.784152	2.085294	3.656554
H	5.523231	-2.819315	3.763731	H	-3.397059	0.572758	3.038406
H	1.920577	-4.041447	4.190866	C	-5.917782	2.830522	3.324762
H	3.521224	-4.592520	3.716171	H	-7.419237	3.207750	1.824153
H	3.740290	-2.871032	5.479972	H	-4.300930	2.227871	4.619821
H	2.761512	-1.742194	4.548415	H	-6.318289	3.557871	4.025780
C	1.240381	2.959218	0.759792	C	-3.570761	-1.852464	1.150949
N	0.636261	1.813038	0.808585	C	-4.169563	-2.279965	2.350123
C	-0.367220	1.868568	1.887355	C	-2.557591	-2.661490	0.600805
H	-1.355193	1.759724	1.424475	C	-3.769535	-3.460250	2.981240
O	0.885338	3.883926	1.678763	H	-4.953844	-1.681321	2.805969
C	2.193745	3.258851	-0.308388	C	-2.154781	-3.842469	1.227319
C	2.932744	4.477997	-0.469180	H	-2.080168	-2.367381	-0.329651
C	2.897671	5.573210	0.436280	C	-2.758592	-4.243621	2.421682
C	3.772316	4.578869	-1.629132	H	-4.247385	-3.767299	3.907843
C	3.065772	2.361361	-2.280302	H	-1.374789	-4.452563	0.779377
C	3.653317	6.702732	0.198161	H	-2.448359	-5.164491	2.908598

C	-5.457775	-0.724206	-1.068118
H	-5.706362	0.201682	-1.600111
H	-6.364528	-1.046431	-0.540483
C	-5.011041	-1.785017	-2.048844
C	-4.245761	-1.444582	-3.175705
C	-5.334936	-3.134928	-1.843219
C	-3.824245	-2.428571	-4.071706
H	-3.972627	-0.409325	-3.364476
C	-4.913641	-4.118460	-2.739436
H	-5.926497	-3.416145	-0.974934
C	-4.155855	-3.768950	-3.858928
H	-3.239958	-2.134496	-4.938949
H	-5.182555	-5.156979	-2.563767
H	-3.833246	-4.532447	-4.561824
C	-0.178912	0.894554	3.030126
C	-0.438278	-0.475974	3.036357
C	0.232319	1.554087	4.194321
C	-0.276771	-1.185903	4.229229
H	-0.781164	-0.982279	2.140065
C	0.402005	0.842255	5.382147
C	0.144436	-0.531346	5.392833
H	-0.500395	-2.248100	4.252300
H	0.713501	1.348206	6.292389
H	0.257655	-1.092569	6.316106
C	0.396764	3.042513	3.969846
H	1.443881	3.360955	4.038766
H	-0.164437	3.636095	4.699679
Br	-2.249888	1.713103	-4.576991
H	1.544148	-0.096030	-3.166530
C	0.257953	-1.635884	-2.372411
H	-0.688692	-1.088886	-2.431255
H	0.186287	-2.259746	-1.467915
C	0.339637	-2.551539	-3.608053
H	1.228175	-3.194109	-3.595876
H	-0.539596	-3.202157	-3.665274
H	0.369471	-1.955360	-4.526352

^{2}TS14-*RR*

B3LYP/BSI SCF energy: -3072.410073a.u.

M06/BSII SCF energy in solution:-3071.094747a.u.

M06/BSII free energy in solution:-3070.171663a.u.

C	3.194126	-1.452101	-0.611178
O	2.446345	-0.913861	0.233815
N	4.303094	-2.145498	-0.227643
C	2.888661	-1.296668	-2.095521
H	3.568095	-0.512419	-2.460053
H	3.192170	-2.203911	-2.634583
C	1.420550	-0.890622	-2.324173
C	5.203487	-2.719723	-1.196168
C	6.210844	-1.937296	-1.770666
C	5.109483	-4.078574	-1.517016
C	7.112337	-2.509971	-2.669392
H	6.280828	-0.885413	-1.510684
C	6.013722	-4.647367	-2.414567
H	4.323201	-4.676934	-1.067099
C	7.015556	-3.864593	-2.992635
H	7.890630	-1.897356	-3.114897
H	5.933157	-5.701230	-2.664013
H	7.717426	-4.308815	-3.692065
C	4.726219	-2.259940	1.200179
C	5.104972	-0.902537	1.819686
C	3.716596	-3.019492	2.076878
H	5.638833	-2.865662	1.154913
C	5.663475	-1.096534	3.239362
H	4.216925	-0.263965	1.849166
H	5.847690	-0.405211	1.183960
C	4.280017	-3.207943	3.496319
H	2.781826	-2.453723	2.114939
H	3.494405	-3.992482	1.621993
C	4.679384	-1.867028	4.132080
H	5.895045	-0.120467	3.681283
H	6.614068	-1.647138	3.186242
H	3.540127	-3.721673	4.121742
H	5.159857	-3.866567	3.455610
H	5.119380	-2.035220	5.122427
H	3.778763	-1.258526	4.284614
C	0.664728	2.803171	0.582549
N	0.285047	1.568012	0.633310
C	-0.641413	1.438394	1.775286
H	-1.555445	0.953759	1.427071
O	0.153454	3.650643	1.496501
C	1.570996	3.257517	-0.481765
C	2.042286	4.596072	-0.677867
C	1.722200	5.700194	0.159707
C	2.903199	4.820674	-1.804315
C	2.693160	2.482837	-2.370955
C	2.233910	6.951304	-0.109289

H	1.069803	5.551809	1.008149
C	3.410964	6.121590	-2.050278
C	3.213724	3.722632	-2.646205
H	2.891122	1.625916	-3.005318
C	3.083327	7.168264	-1.218704
H	1.977455	7.783766	0.538956
H	4.058841	6.275189	-2.908652
H	3.855404	3.866521	-3.510057
H	3.472922	8.162983	-1.413372
N	1.891668	2.244104	-1.304192
Ni	1.017695	0.380204	-0.836637
C	-0.869242	2.906468	2.238942
H	-1.832001	3.323210	1.938725
C	-1.344855	1.311293	-2.205672
C	-2.040493	0.435902	-1.349018
C	-2.735610	-0.312430	-0.665862
Si	-4.015576	-1.094097	0.381357
C	-4.279193	0.054611	1.866218
C	-4.579147	1.413741	1.636333
C	-4.190448	-0.381814	3.199661
C	-4.793344	2.294647	2.697972
H	-4.629148	1.797078	0.619205
C	-4.401436	0.497830	4.264973
H	-3.948815	-1.419451	3.412892
C	-4.706727	1.836773	4.016431
H	-5.031428	3.335441	2.494889
H	-4.326832	0.136506	5.287174
H	-4.879859	2.520007	4.843899
C	-3.467324	-2.811109	0.936078
C	-4.322822	-3.630487	1.698543
C	-2.201642	-3.321923	0.599217
C	-3.928418	-4.903255	2.114186
H	-5.313146	-3.274595	1.975732
C	-1.803361	-4.595977	1.009961
H	-1.524609	-2.719813	-0.000228
C	-2.664888	-5.388436	1.769730
H	-4.606089	-5.516127	2.702465
H	-0.822121	-4.971258	0.731428
H	-2.356537	-6.380271	2.089104
C	-5.652161	-1.184098	-0.598661
H	-6.003850	-0.152555	-0.715817
H	-6.384243	-1.690772	0.043289
C	-5.558724	-1.866007	-1.942258
C	-5.294094	-1.124852	-3.104923
C	-5.717950	-3.255104	-2.062591
C	-5.197750	-1.752691	-4.347277
H	-5.168313	-0.047505	-3.033872
C	-5.620789	-3.884212	-3.304505
H	-5.922647	-3.847726	-1.174446
C	-5.360233	-3.135529	-4.453430
H	-5.000552	-1.157299	-5.234772
H	-5.752536	-4.960819	-3.373499
H	-5.288708	-3.623582	-5.421392
C	-0.056405	0.750041	2.993370
C	0.371999	-0.571522	3.110870
C	-0.025915	1.615722	4.093012
C	0.840185	-1.018855	4.348798
H	0.342857	-1.240055	2.256436
C	0.451314	1.169737	5.325870
C	0.884960	-0.152362	5.447446
H	1.165635	-2.048909	4.461381
H	0.476803	1.836085	6.184337
H	1.251497	-0.513638	6.404250
C	-0.616521	2.968150	3.753976
H	0.035488	3.810373	4.009392
H	-1.566254	3.122219	4.280240
Br	-2.987683	3.287446	-2.219788
H	1.352717	-0.403441	-3.306922
C	0.483060	-2.112280	-2.307959
H	-0.560855	-1.777455	-2.308032
H	0.614485	-2.659492	-1.361333
C	0.662771	-3.101634	-3.476213
H	1.670162	-3.532689	-3.507263
H	-0.046712	-3.934083	-3.403297
H	0.490734	-2.602615	-4.437097
H	-0.665365	2.025841	-1.779201
C	-1.272559	1.009217	-3.679838
H	-0.868079	1.864698	-4.223232
H	-0.634753	0.136722	-3.857769
H	-2.267473	0.782301	-4.068772

^{2}IM13-*SS*$^{+}$

B3LYP/BSI SCF energy: -3058.88311a.u.

M06/BSII SCF energy in solution:-3057.612753a.u.

M06/BSII free energy in solution:-3056.680277a.u.

C	-3.424142	-1.215773	-0.521529
O	-2.681712	-0.204383	-0.642403

N	-4.765600	-1.115994	-0.571214	H	0.036386	3.003851	3.563561
C	-2.762186	-2.564396	-0.284939	C	-1.001372	0.081152	5.925838
H	-2.779884	-2.746097	0.796749	C	-1.157113	-1.433206	3.974115
H	-3.358304	-3.371983	-0.722964	H	-1.256565	-2.583464	2.171903
C	-1.335792	-2.557420	-0.858947	C	-0.742829	1.332133	6.431749
C	-5.608116	-2.275708	-0.381233	H	-0.177796	3.373176	5.973843
C	-5.952270	-2.682958	0.911123	H	-1.294039	-0.735201	6.579166
C	-6.119919	-2.951518	-1.493777	H	-1.432701	-2.263755	4.616262
C	-6.802028	-3.776219	1.089180	H	-0.827192	1.518666	7.497736
H	-5.559104	-2.141820	1.766560	N	-0.710893	-0.627448	1.758747
C	-6.969265	-4.043098	-1.308682	Ni	-0.676001	-0.710198	-0.488315
H	-5.849014	-2.622945	-2.492566	C	1.234649	3.220767	0.296409
C	-7.310270	-4.456683	-0.018821	H	2.317034	3.109682	0.374631
H	-7.069377	-4.092304	2.092807	C	0.255263	-0.693588	-2.286800
H	-7.364139	-4.569366	-2.172132	H	0.019768	0.346949	-2.528895
H	-7.972083	-5.305530	0.121725	C	-0.394793	-3.653099	-0.368408
C	-5.475480	0.193183	-0.755831	H	-0.240372	-3.588367	0.716149
C	-5.267912	1.148785	0.431690	H	0.592755	-3.490172	-0.816793
C	-5.156089	0.869373	-2.099437	C	-0.866931	-5.079110	-0.715762
H	-6.533053	-0.089971	-0.772740	H	-1.004405	-5.195735	-1.796217
C	-6.117758	2.418767	0.248924	H	-0.128417	-5.818977	-0.391823
H	-4.207981	1.414257	0.496554	H	-1.817111	-5.324689	-0.229525
H	-5.540178	0.640175	1.364467	H	-1.431777	-2.628395	-1.940452
C	-6.012052	2.137302	-2.269469	C	-0.051811	-1.581577	-3.489136
H	-4.094952	1.132432	-2.127730	H	-1.103271	-1.501504	-3.782209
H	-5.345965	0.166997	-2.919925	H	0.553913	-1.260062	-4.345631
C	-5.825768	3.106825	-1.092593	H	0.185655	-2.632223	-3.305282
H	-5.932865	3.106888	1.081315	C	1.587004	-0.820547	-1.768391
H	-7.182924	2.152514	0.296921	C	2.712926	-0.938544	-1.294513
H	-5.754536	2.628214	-3.214824	Si	4.474826	-1.072189	-0.778670
H	-7.071716	1.856240	-2.346686	C	5.071611	-2.845521	-1.000291
H	-6.477776	3.978729	-1.216885	C	5.038848	-3.760324	0.069194
H	-4.793670	3.482118	-1.093012	C	5.535010	-3.309355	-2.245996
C	0.067619	1.508317	1.204124	C	5.450939	-5.083297	-0.098437
N	-0.014818	1.213697	-0.045866	H	4.697051	-3.434050	1.047845
C	0.570517	2.344888	-0.804450	C	5.948932	-4.630735	-2.418066
H	1.296198	1.957508	-1.524214	H	5.577057	-2.636257	-3.098651
O	0.674910	2.653110	1.537288	C	5.907473	-5.520636	-1.343031
C	-0.408644	0.577898	2.254913	H	5.420987	-5.770577	0.742479
C	-0.499667	0.898335	3.645923	H	6.306685	-4.964419	-3.387943
C	-0.248257	2.184638	4.206754	H	6.232860	-6.548654	-1.474134
C	-0.892827	-0.163663	4.531449	C	4.634325	-0.534508	1.021878
C	-1.064993	-1.616343	2.615097	C	5.836379	-0.747857	1.723842
C	-0.369610	2.387121	5.562598	C	3.602183	0.149226	1.687097

C	5.999224	-0.294003	3.033925
H	6.655274	-1.283044	1.248607
C	3.759040	0.607862	2.996524
H	2.664929	0.322609	1.166283
C	4.960186	0.386602	3.672483
H	6.934890	-0.471955	3.556251
H	2.947755	1.139673	3.486720
H	5.087481	0.741457	4.691281
C	5.489193	0.099860	-1.899551
H	5.455737	-0.296523	-2.920597
H	6.532807	0.023358	-1.570093
C	5.036710	1.539985	-1.888925
C	4.165078	2.030034	-2.875228
C	5.473118	2.428967	-0.892976
C	3.753892	3.364669	-2.876378
H	3.825144	1.362393	-3.662847
C	5.065289	3.764254	-0.891342
H	6.150685	2.074133	-0.121245
C	4.204787	4.240030	-1.884495
H	3.099697	3.725916	-3.665352
H	5.436508	4.437448	-0.123400
H	3.911977	5.286242	-1.902212
C	-0.460997	3.267115	-1.433635
C	-1.406239	2.971779	-2.416593
C	-0.356646	4.561424	-0.909754
C	-2.250680	3.988175	-2.869445
H	-1.495104	1.969486	-2.824232
C	-1.203407	5.574835	-1.359703
C	-2.151422	5.280943	-2.341928
H	-2.985717	3.775299	-3.639743
H	-1.124609	6.581454	-0.958409
H	-2.812620	6.062656	-2.703571
C	0.770280	4.668199	0.094536
H	0.474075	5.126227	1.043952
H	1.600818	5.263331	-0.302626

^{2}IM13-*SR*$^{+}$

B3LYP/BSI SCF energy: -3058.881636a.u.

M06/BSII SCF energy in solution:-3057.613728a.u.

M06/BSII free energy in solution:-3056.679768a.u.

C	3.578691	1.001166	-0.801359
O	2.693245	0.104542	-0.832946
N	4.890534	0.706441	-0.747043
C	3.128739	2.452131	-0.776458
H	3.224811	2.803301	0.258637
H	3.816009	3.078756	-1.355324
C	1.693209	2.576041	-1.304537
C	5.886041	1.755654	-0.709443
C	6.303147	2.277169	0.518823
C	6.468098	2.202134	-1.900140
C	7.298137	3.255790	0.552833
H	5.852633	1.913069	1.437352
C	7.460995	3.181978	-1.859083
H	6.140472	1.783568	-2.846935
C	7.876308	3.709426	-0.634322
H	7.622559	3.660617	1.506512
H	7.910884	3.530408	-2.783528
H	8.650502	4.469721	-0.605379
C	5.414270	-0.695244	-0.644226
C	4.993303	-1.388895	0.662560
C	5.098986	-1.560046	-1.875207
H	6.499987	-0.557508	-0.609686
C	5.691133	-2.754441	0.784184
H	3.906497	-1.520698	0.666021
H	5.253047	-0.752596	1.517405
C	5.797815	-2.925852	-1.746895
H	4.016678	-1.699126	-1.949948
H	5.431058	-1.045056	-2.784502
C	5.417834	-3.640198	-0.440577
H	5.360402	-3.256025	1.700466
H	6.774155	-2.599419	0.888479
H	5.543884	-3.549436	-2.611575
H	6.886800	-2.781656	-1.780722
H	5.971065	-4.582118	-0.353746
H	4.352163	-3.901839	-0.468097
C	-0.139125	-0.949962	1.349945
N	-0.038018	-0.857621	0.068322
C	-0.731920	-2.039203	-0.501688
H	-1.382924	-1.715380	-1.315868
O	-0.864054	-1.956650	1.846802
C	0.463376	0.055059	2.259621
C	0.527509	-0.066059	3.684344
C	0.101806	-1.204568	4.429429
C	1.082019	1.048143	4.404884
C	1.426743	2.165698	2.297494
C	0.216084	-1.220058	5.800986
H	-0.310746	-2.058502	3.913710

C	1.178024	0.998469	5.820610
C	1.515847	2.172024	3.668692
H	1.746490	3.019272	1.715638
C	0.752417	-0.114034	6.505521
H	-0.109403	-2.096096	6.353113
H	1.595220	1.851634	6.346906
H	1.918751	3.038430	4.183603
H	0.827931	-0.151531	7.587725
N	0.922626	1.121359	1.596230
Ni	0.782062	0.911304	-0.649514
C	-1.526955	-2.611766	0.702492
H	-2.573908	-2.308433	0.747864
C	-0.342236	1.088389	-2.335278
C	0.980263	3.883486	-0.968709
H	0.903163	4.017218	0.117823
H	-0.052868	3.832790	-1.332865
C	1.650636	5.132205	-1.574708
H	1.722882	5.049188	-2.664615
H	1.068439	6.030353	-1.346641
H	2.661520	5.285893	-1.182682
H	1.740404	2.457578	-2.391060
C	-1.668896	0.993828	-1.792290
C	-2.798248	0.949794	-1.315315
Si	-4.566511	0.939471	-0.804053
C	-5.275568	2.666606	-1.060605
C	-6.001785	3.328646	-0.054672
C	-5.111953	3.322669	-2.296229
C	-6.548769	4.594761	-0.274953
H	-6.141860	2.854228	0.912772
C	-5.656157	4.586895	-2.520005
H	-4.545877	2.845336	-3.093316
C	-6.377436	5.225132	-1.507802
H	-7.107017	5.087924	0.515816
H	-5.518993	5.074637	-3.481039
H	-6.802810	6.209598	-1.680565
C	-4.700151	0.416373	1.003511
C	-5.928239	-0.019613	1.537904
C	-3.597956	0.481551	1.874597
C	-6.049824	-0.378243	2.881552
H	-6.809177	-0.077504	0.902801
C	-3.711889	0.120917	3.219137
H	-2.640856	0.829890	1.494309
C	-4.938941	-0.311534	3.724719
H	-7.009118	-0.708731	3.269431
H	-2.845584	0.177856	3.872549
H	-5.031349	-0.591385	4.770218
C	-5.497240	-0.290253	-1.933983
H	-5.514242	0.159425	-2.933734
H	-6.540342	-0.308607	-1.594722
C	-4.935694	-1.689678	-1.997367
C	-3.999057	-2.044580	-2.982623
C	-5.333221	-2.676590	-1.080855
C	-3.483581	-3.339931	-3.055302
H	-3.688889	-1.300571	-3.711716
C	-4.822794	-3.974748	-1.153256
H	-6.063952	-2.431200	-0.315312
C	-3.894948	-4.313599	-2.141333
H	-2.775379	-3.595000	-3.838854
H	-5.167656	-4.726688	-0.448462
H	-3.512466	-5.327681	-2.212309
C	0.194058	-3.182434	-0.893706
C	1.227491	-3.189406	-1.831339
C	-0.133610	-4.347759	-0.188137
C	1.920946	-4.379730	-2.065116
H	1.498306	-2.287485	-2.368634
C	0.565183	-5.533128	-0.416555
C	1.592687	-5.544223	-1.361959
H	2.719251	-4.401639	-2.800894
H	0.311308	-6.438707	0.127604
H	2.139356	-6.462629	-1.553865
C	-1.307923	-4.125962	0.738638
H	-1.140974	-4.482527	1.760272
H	-2.208322	-4.625591	0.363243
H	-0.195607	2.094760	-2.728615
C	0.042466	0.058382	-3.397836
H	-0.124767	-0.967821	-3.068973
H	-0.554952	0.211728	-4.305913
H	1.096441	0.165838	-3.672108

^{2}IM13-*RR*$^{+}$

B3LYP/BSI SCF energy: -3058.886191a.u.

M06/BSII SCF energy in solution:-3057.620713a.u.

M06/BSII free energy in solution:-3056.686349a.u.

C	-3.604866	-1.331032	-0.065642
O	-2.840097	-0.328670	-0.101276
N	-4.933557	-1.213832	-0.250096
C	-2.982965	-2.686301	0.227036

H	-3.702969	-3.350353	0.719880	C	-1.206430	0.628671	4.686836
H	-2.739981	-3.171691	-0.727844	H	-1.847338	-1.052756	3.530862
C	-1.728779	-2.485384	1.076831	C	0.283393	3.857207	5.784220
C	-5.773540	-2.385499	-0.354433	H	1.354284	5.261794	4.529550
C	-6.620433	-2.729014	0.704845	H	-0.814292	2.298987	6.767367
C	-5.775870	-3.139489	-1.531594	H	-1.642528	0.260667	5.610084
C	-7.462274	-3.834946	0.585754	H	0.386903	4.465192	6.677468
H	-6.613243	-2.133974	1.613096	N	-0.799013	0.295054	2.348763
C	-6.617039	-4.248246	-1.642052	Ni	-0.877624	-0.806460	0.393112
H	-5.127648	-2.853160	-2.354307	C	1.670611	2.639140	-0.684821
C	-7.460059	-4.596482	-0.585551	H	2.693099	2.261794	-0.636760
H	-8.117683	-4.102702	1.408666	C	-0.176055	-1.906345	-1.145655
H	-6.617474	-4.833608	-2.556283	C	1.241002	-1.742527	-0.963028
H	-8.115924	-5.456757	-0.674951	C	2.446074	-1.595658	-0.788901
C	-5.614270	0.110550	-0.435266	Si	4.279908	-1.499007	-0.668626
C	-5.402886	1.066037	0.751488	C	4.936431	-3.171921	-0.102215
C	-5.263323	0.773903	-1.777458	C	5.899531	-3.283916	0.916675
H	-6.677173	-0.150746	-0.462719	C	4.492868	-4.356013	-0.722860
C	-6.220920	2.353700	0.548640	C	6.404063	-4.529050	1.298303
H	-4.340379	1.311433	0.835054	H	6.259106	-2.391972	1.422526
H	-5.700602	0.567489	1.682150	C	4.993666	-5.601176	-0.344043
C	-6.079845	2.064565	-1.965361	H	3.740901	-4.308496	-1.507679
H	-4.194576	1.007538	-1.788557	C	5.952497	-5.689163	0.668314
H	-5.461571	0.073105	-2.597154	H	7.147544	-4.592362	2.087837
C	-5.884780	3.031364	-0.788180	H	4.637994	-6.501883	-0.836528
H	-6.036572	3.039195	1.383231	H	6.344326	-6.658071	0.964306
H	-7.293155	2.114054	0.574464	C	4.758305	-0.138725	0.549168
H	-5.794936	2.545322	-2.908031	C	6.056118	0.408596	0.547566
H	-7.145322	1.811945	-2.057837	C	3.853076	0.337606	1.514981
H	-6.506841	3.922788	-0.925274	C	6.432379	1.390269	1.466170
H	-4.841190	3.374509	-0.771270	H	6.792387	0.064405	-0.175027
C	0.367440	1.735754	0.926240	C	4.222196	1.321487	2.435045
N	0.029411	1.010347	-0.086392	H	2.848324	-0.076228	1.552121
C	0.633453	1.652723	-1.281531	C	5.513397	1.851231	2.410747
H	1.095787	0.892697	-1.913640	H	7.440638	1.793857	1.445094
O	1.209792	2.749601	0.713119	H	3.504703	1.673645	3.171270
C	-0.135323	1.454579	2.291516	H	5.804441	2.615020	3.126162
C	0.045268	2.309457	3.425135	C	4.963435	-1.120382	-2.413614
C	0.724512	3.563066	3.408541	H	4.776902	-2.017005	-3.016372
C	-0.519779	1.861521	4.669366	H	6.053759	-1.042679	-2.320910
C	-1.322884	-0.105250	3.530972	C	4.402254	0.100203	-3.101224
C	0.835446	4.308823	4.560013	C	3.267701	0.004468	-3.924624
H	1.153291	3.928143	2.487812	C	4.998122	1.362083	-2.946609
C	-0.382284	2.656635	5.837674	C	2.751751	1.126209	-4.575896

H	2.799341	-0.965209	-4.071542
C	4.487830	2.485704	-3.600870
H	5.883078	1.462114	-2.324329
C	3.361140	2.373884	-4.419161
H	1.885103	1.022599	-5.223059
H	4.984924	3.445208	-3.485589
H	2.974093	3.242268	-4.944226
C	-0.328431	2.565780	-2.031180
C	-1.553605	2.251802	-2.620383
C	0.173089	3.872850	-2.086751
C	-2.267863	3.258791	-3.274499
H	-1.955191	1.246343	-2.564095
C	-0.542359	4.877559	-2.737709
C	-1.765812	4.563268	-3.333104
H	-3.219972	3.026268	-3.742082
H	-0.155435	5.891900	-2.782627
H	-2.331421	5.336837	-3.843819
C	1.521077	3.978126	-1.409373
H	1.606120	4.821610	-0.716762
H	2.328591	4.076805	-2.144107
H	-0.445586	-2.948768	-0.987027
C	-0.731021	-1.438645	-2.493986
H	-0.470696	-0.406318	-2.725351
H	-0.329269	-2.066395	-3.299991
H	-1.820667	-1.527666	-2.517910
H	-2.039011	-2.047530	2.032170
C	-0.947459	-3.760767	1.363802
H	-1.628186	-4.465823	1.868427
H	-0.659573	-4.265048	0.432531
C	0.294147	-3.554200	2.238529
H	1.038462	-2.933393	1.730334
H	0.035934	-3.070572	3.187883
H	0.768973	-4.510711	2.475282

^{2}IM13-*RS*$^{+}$

B3LYP/BSI SCF energy: -3058.883765a.u.

M06/BSII SCF energy in solution:-3057.616368a.u.

M06/BSII free energy in solution:-3056.68276a.u.

C	-3.482277	-1.390798	0.015063
O	-2.831878	-0.315038	-0.090620
N	-4.812919	-1.424215	-0.187706
C	-2.731574	-2.663824	0.377570
H	-3.341823	-3.288504	1.042333
H	-2.604442	-3.255721	-0.534340
C	-1.386126	-2.325375	1.016083
C	-5.540922	-2.672526	-0.139443
C	-6.270839	-3.005953	1.006321
C	-5.557263	-3.514556	-1.255282
C	-7.009363	-4.189421	1.035777
H	-6.255048	-2.341442	1.864969
C	-6.295783	-4.698633	-1.218170
H	-4.999051	-3.239059	-2.144999
C	-7.021265	-5.036918	-0.074477
H	-7.574303	-4.448848	1.925735
H	-6.307468	-5.352435	-2.084712
H	-7.596788	-5.956918	-0.048943
C	-5.610647	-0.203121	-0.538261
C	-5.571179	0.879384	0.554333
C	-5.247871	0.364562	-1.921617
H	-6.638306	-0.576986	-0.593885
C	-6.501316	2.046741	0.180732
H	-4.545858	1.243365	0.667023
H	-5.874063	0.443816	1.514351
C	-6.179431	1.534717	-2.280724
H	-4.209271	0.709388	-1.906614
H	-5.324672	-0.428625	-2.674970
C	-6.157322	2.625855	-1.199984
H	-6.437428	2.824931	0.949399
H	-7.543523	1.697967	0.178805
H	-5.887334	1.950774	-3.251595
H	-7.205896	1.161198	-2.401229
H	-6.858436	3.427328	-1.457865
H	-5.157388	3.080101	-1.165739
C	0.277861	2.068049	0.827852
N	0.013229	1.302214	-0.175298
C	0.619748	1.931462	-1.374120
H	1.190603	1.185503	-1.932405
O	1.056264	3.131468	0.611292
C	-0.249017	1.775399	2.181357
C	-0.150569	2.651084	3.308444
C	0.484925	3.927412	3.303647
C	-0.751326	2.197257	4.533707
C	-1.424481	0.184409	3.390646
C	0.523085	4.689068	4.449255
H	0.939219	4.297022	2.396931
C	-0.691269	3.010790	5.696086
C	-1.394757	0.941363	4.537678

H	-1.913937	-0.782021	3.380092
C	-0.064608	4.232584	5.655050
H	1.011559	5.658207	4.428786
H	-1.149210	2.649132	6.611718
H	-1.864094	0.572580	5.444160
H	-0.018933	4.853690	6.544082
N	-0.856629	0.584771	2.229874
Ni	-0.818303	-0.559392	0.285032
C	1.521673	3.052836	-0.786729
H	2.583553	2.807578	-0.739726
C	-0.151894	-1.348694	-1.447466
C	1.249594	-1.459987	-1.158889
C	2.445041	-1.513159	-0.892428
Si	4.260976	-1.589856	-0.613085
C	4.759539	-3.354717	-0.182292
C	5.138755	-3.716678	1.123317
C	4.742882	-4.363392	-1.165122
C	5.488604	-5.032210	1.435051
H	5.167640	-2.963397	1.905708
C	5.091269	-5.678589	-0.858140
H	4.452381	-4.126332	-2.186185
C	5.465954	-6.015045	0.444696
H	5.781821	-5.288151	2.449347
H	5.074251	-6.439198	-1.633567
H	5.741282	-7.037963	0.685022
C	4.711080	-0.394740	0.775778
C	6.054857	-0.241214	1.169759
C	3.746168	0.390895	1.429656
C	6.418035	0.659324	2.172440
H	6.833111	-0.835792	0.696006
C	4.103268	1.295640	2.432163
H	2.701450	0.287786	1.148126
C	5.441276	1.431703	2.804861
H	7.460703	0.757669	2.460628
H	3.339716	1.894578	2.921779
H	5.722907	2.133396	3.584768
C	5.129848	-1.060538	-2.231970
H	4.967888	-1.853543	-2.970975
H	6.206518	-1.052617	-2.021463
C	4.692191	0.270974	-2.792027
C	3.683381	0.346238	-3.766536
C	5.278709	1.470083	-2.355712
C	3.284054	1.573692	-4.298691
H	3.223382	-0.570430	-4.126574
C	4.884162	2.699557	-2.887604
H	6.064337	1.437432	-1.605892
C	3.886242	2.757606	-3.864183
H	2.517918	1.603605	-5.068642
H	5.373278	3.610471	-2.553029
H	3.599750	3.709951	-4.301618
C	-0.388039	2.684927	-2.226762
C	-1.506844	2.185054	-2.894161
C	-0.066178	4.045857	-2.292131
C	-2.304701	3.065415	-3.628435
H	-1.765130	1.131739	-2.841086
C	-0.864570	4.924362	-3.025085
C	-1.986066	4.426637	-3.691780
H	-3.176491	2.690734	-4.156371
H	-0.618671	5.981224	-3.080636
H	-2.614251	5.100757	-4.266247
C	1.208321	4.353201	-1.536261
H	1.120255	5.198321	-0.845811
H	2.031847	4.581912	-2.222437
H	-1.582504	-1.933984	2.020450
C	-0.406515	-3.484376	1.154113
H	-0.961698	-4.373503	1.496138
H	0.021151	-3.761317	0.185118
C	0.730419	-3.200614	2.142292
H	1.326564	-2.339745	1.824446
H	0.340707	-2.994552	3.146226
H	1.407752	-4.056016	2.217612
C	-0.766347	-2.521574	-2.205625
H	-0.263444	-2.630629	-3.174981
H	-0.661373	-3.474706	-1.684678
H	-1.825312	-2.340258	-2.410103
H	-0.350888	-0.434233	-2.015342

^{2}IM14-*SS*

B3LYP/BSI SCF energy: -3072.466336a.u.

M06/BSII SCF energy in solution:-3071.159639a.u.

M06/BSII free energy in solution:-3070.230454a.u.

C	3.292265	1.179746	0.011947
O	2.999467	0.472753	-0.970650
N	4.417676	1.947810	0.018086
C	2.380187	1.151490	1.224444
H	2.770327	0.384794	1.909795
H	2.439503	2.098671	1.773024

C	0.938912	0.823921	0.816260	C	3.104447	-5.966252	3.649210
C	4.825956	2.681321	1.187039	H	1.089670	-6.623940	4.101039
C	5.425646	2.016487	2.262146	H	4.964242	-5.103005	3.018946
C	4.673059	4.072249	1.227812	H	5.128031	-3.173907	1.449635
C	5.856022	2.737157	3.377257	H	3.570926	-6.734124	4.259209
H	5.551668	0.939073	2.216917	N	2.064771	-2.064601	0.599653
C	5.111811	4.789424	2.341102	Ni	1.068717	-0.626912	-0.648299
H	4.204823	4.580546	0.390509	C	-2.379020	-2.916723	1.127025
C	5.701460	4.123893	3.418282	H	-2.766791	-2.265103	1.914590
H	6.317210	2.214725	4.210235	C	-0.137052	0.529554	-1.848157
H	4.987449	5.867894	2.368714	H	-0.412044	-0.309155	-2.493704
H	6.039423	4.683953	4.285018	C	0.057448	0.446629	1.998801
C	5.335302	2.007723	-1.163340	H	0.450403	-0.451995	2.496175
C	6.014113	0.657674	-1.459335	H	-0.938922	0.197000	1.621378
C	4.660952	2.590453	-2.417406	C	-0.098691	1.560152	3.053628
H	6.118348	2.708593	-0.851506	H	-0.473894	2.480360	2.592838
C	7.024524	0.802248	-2.610133	H	-0.812900	1.265144	3.829798
H	5.248271	-0.074081	-1.732389	H	0.850673	1.794401	3.547787
H	6.518122	0.296161	-0.553784	H	0.510752	1.694367	0.315701
C	5.677818	2.724865	-3.563501	C	0.676805	1.561561	-2.631585
H	3.842629	1.933303	-2.722501	H	1.515438	1.068827	-3.126500
H	4.224361	3.568030	-2.178444	H	0.054509	2.048116	-3.394944
C	6.363431	1.384607	-3.868302	H	1.066710	2.347991	-1.977689
H	7.470744	-0.174292	-2.830381	C	-1.298892	1.081828	-1.218772
H	7.849083	1.458665	-2.295065	C	-2.290048	1.595267	-0.704035
H	5.172327	3.107576	-4.457447	Si	-3.743047	2.573792	-0.199264
H	6.440844	3.470043	-3.293880	C	-3.375273	4.414607	-0.449094
H	7.108365	1.511748	-4.662761	C	-2.626388	5.132763	0.502896
H	5.616346	0.673568	-4.245231	C	-3.798801	5.106378	-1.598162
C	-0.132470	-2.775513	0.930370	C	-2.312826	6.479533	0.315462
N	-0.504738	-2.003555	-0.023692	H	-2.289470	4.634964	1.408876
C	-1.958817	-2.189479	-0.178340	C	-3.489995	6.454579	-1.791362
H	-2.440613	-1.219778	-0.326491	H	-4.377939	4.591491	-2.360185
O	-1.093826	-3.437392	1.615710	C	-2.745092	7.144320	-0.834029
C	1.301562	-2.948547	1.246548	H	-1.734274	7.010785	1.066694
C	1.846482	-3.985594	2.071664	H	-3.831056	6.965097	-2.688024
C	1.074441	-4.942037	2.790319	H	-2.503933	8.193555	-0.981618
C	3.276542	-4.056609	2.162923	C	-4.174760	2.283076	1.619883
C	3.414840	-2.166826	0.669370	C	-4.892853	3.248377	2.351199
C	1.693338	-5.902688	3.558449	C	-3.854289	1.080201	2.273563
H	-0.003587	-4.907397	2.730439	C	-5.271341	3.023569	3.676298
C	3.880155	-5.061507	2.963874	H	-5.151123	4.196300	1.885452
C	4.043806	-3.123352	1.426585	C	-4.227876	0.848864	3.598741
H	3.962363	-1.456824	0.063534	H	-3.299029	0.315639	1.737356

C	-4.937864	1.822127	4.304111
H	-5.821643	3.787309	4.219438
H	-3.964895	-0.088804	4.081797
H	-5.228020	1.646336	5.336458
C	-5.244937	2.096997	-1.287646
H	-4.972871	2.297426	-2.330666
H	-6.059772	2.786347	-1.033642
C	-5.702975	0.666742	-1.138989
C	-5.173989	-0.348530	-1.952123
C	-6.659688	0.309841	-0.175200
C	-5.590828	-1.673643	-1.814007
H	-4.431555	-0.094222	-2.703909
C	-7.078622	-1.013647	-0.033803
H	-7.080936	1.079151	0.466761
C	-6.546898	-2.011992	-0.853113
H	-5.169930	-2.439304	-2.458769
H	-7.826982	-1.262664	0.714069
H	-6.881314	-3.041007	-0.753447
C	-2.322484	-3.191764	-1.265340
C	-1.984626	-3.161856	-2.617669
C	-3.090127	-4.237863	-0.739751
C	-2.448748	-4.185882	-3.447112
H	-1.336768	-2.386727	-3.011969
C	-3.552376	-5.259246	-1.569229
C	-3.231457	-5.223840	-2.928654
H	-2.185896	-4.181505	-4.500692
H	-4.148748	-6.074012	-1.166336
H	-3.581593	-6.015134	-3.585638
C	-3.329656	-4.055381	0.743021
H	-3.140315	-4.954839	1.338313
H	-4.363327	-3.744270	0.942256
Br	1.753905	-2.126588	-2.640118

^{2}IM14-*RS*

B3LYP/BSI SCF energy: -3072.465832a.u.

M06/BSII SCF energy in solution:-3071.156541a.u.

M06/BSII free energy in solution:-3070.228616a.u.

C	2.974486	-1.596762	0.057605
O	3.166079	-0.491920	0.601142
N	3.836072	-2.636706	0.238102
C	1.757448	-1.783068	-0.835438
H	2.024134	-2.411293	-1.695947
H	0.991899	-2.343280	-0.283918
C	1.230607	-0.419378	-1.259755
C	3.568824	-3.934618	-0.325972
C	4.237818	-4.344406	-1.485482
C	2.679220	-4.807809	0.308880
C	4.010580	-5.617071	-2.009738
H	4.925927	-3.659588	-1.971799
C	2.450924	-6.079157	-0.221781
H	2.173606	-4.488062	1.214703
C	3.115654	-6.485768	-1.380552
H	4.529873	-5.928217	-2.911357
H	1.758590	-6.752095	0.275382
H	2.940153	-7.476247	-1.789742
C	5.063841	-2.515819	1.083293
C	6.071185	-1.492182	0.530502
C	4.748353	-2.254765	2.567452
H	5.529556	-3.505552	1.012483
C	7.358419	-1.492907	1.372128
H	5.614988	-0.498759	0.554854
H	6.298199	-1.726049	-0.517067
C	6.041582	-2.251044	3.400130
H	4.239753	-1.291234	2.661114
H	4.061287	-3.025980	2.935443
C	7.059988	-1.237534	2.857317
H	8.052284	-0.737493	0.984895
H	7.864579	-2.463497	1.265339
H	5.802359	-2.028479	4.446028
H	6.489443	-3.255688	3.388856
H	7.986678	-1.280161	3.441806
H	6.657508	-0.222683	2.976907
C	0.238489	3.070013	-1.111573
N	-0.226413	2.227063	-0.263350
C	-1.696449	2.343216	-0.300315
H	-2.138507	1.344132	-0.328958
O	-0.646264	3.757079	-1.868694
C	1.695988	3.253146	-1.279620
C	2.326379	4.347955	-1.952065
C	1.633867	5.420726	-2.580754
C	3.761163	4.355110	-1.967684
C	3.741335	2.307611	-0.689226
C	2.332691	6.433811	-3.197884
H	0.553222	5.433915	-2.569878
C	4.447690	5.414917	-2.617063
C	4.448915	3.302089	-1.317683
H	4.216076	1.493117	-0.156691

C	3.748214	6.433163	-3.220521
H	1.790719	7.246563	-3.671972
H	5.533928	5.407627	-2.620483
H	5.534366	3.290352	-1.305232
H	4.278878	7.242898	-3.712556
N	2.386857	2.283328	-0.681846
Ni	1.289029	0.806833	0.395355
C	-1.969436	3.187484	-1.577890
H	-2.256174	2.605091	-2.456685
C	0.063329	-0.364371	1.594513
H	-0.254591	0.528339	2.140422
C	0.847170	-1.281063	2.542761
H	1.695271	-0.741128	2.965585
H	0.203783	-1.619275	3.366704
H	1.212953	-2.180913	2.038117
C	-1.072633	-0.999892	1.006945
C	-2.060107	-1.560245	0.535707
Si	-3.562891	-2.309600	-0.166373
C	-3.106965	-3.870972	-1.134241
C	-4.096015	-4.632460	-1.787008
C	-1.782809	-4.339932	-1.192168
C	-3.775823	-5.804945	-2.473594
H	-5.134107	-4.306806	-1.767096
C	-1.455242	-5.513765	-1.874631
H	-0.999460	-3.778904	-0.690829
C	-2.452146	-6.248032	-2.518887
H	-4.557662	-6.372626	-2.971099
H	-0.422495	-5.851679	-1.901804
H	-2.200991	-7.160797	-3.052470
C	-4.393253	-1.042041	-1.306882
C	-4.904467	0.162914	-0.782892
C	-4.493461	-1.242033	-2.695925
C	-5.497232	1.119107	-1.610417
H	-4.845461	0.359367	0.283446
C	-5.081128	-0.285888	-3.528332
H	-4.106914	-2.156380	-3.137103
C	-5.586854	0.896881	-2.987098
H	-5.898220	2.031797	-1.176883
H	-5.145497	-0.466767	-4.598101
H	-6.051755	1.638156	-3.631819
C	-4.746934	-2.869997	1.231798
H	-4.181521	-3.612577	1.809084
H	-5.570448	-3.414661	0.753743
C	-5.290905	-1.800026	2.146158
C	-4.498264	-1.252796	3.168620
C	-6.600840	-1.318714	1.997372
C	-4.997677	-0.257975	4.009288
H	-3.480919	-1.610468	3.300236
C	-7.102912	-0.323496	2.837795
H	-7.233727	-1.732037	1.215711
C	-6.302734	0.212853	3.847600
H	-4.365714	0.148541	4.794173
H	-8.122120	0.029377	2.704244
H	-6.691900	0.986075	4.503758
C	-2.265620	3.202802	0.819655
C	-2.150733	3.018127	2.197062
C	-2.969600	4.296391	0.301241
C	-2.756470	3.940515	3.052729
H	-1.581156	2.189250	2.602024
C	-3.576433	5.215287	1.157289
C	-3.466147	5.030305	2.537081
H	-2.666312	3.813863	4.127356
H	-4.122776	6.066669	0.759168
H	-3.929405	5.741718	3.214975
C	-2.973515	4.287091	-1.212107
H	-2.692503	5.246127	-1.660188
H	-3.961707	4.023981	-1.610022
H	2.027502	0.107819	-1.797658
C	-0.025402	-0.434864	-2.115495
H	-0.246098	0.592831	-2.427236
H	-0.881380	-0.775651	-1.525361
C	0.074419	-1.303032	-3.386706
H	-0.823302	-1.180804	-4.002618
H	0.940673	-1.023751	-3.999207
H	0.159625	-2.368060	-3.148418
Br	1.961323	2.206568	2.467479

^{2}IM14-*RR*

B3LYP/BSI SCF energy: -3072.46179a.u.

M06/BSII SCF energy in solution:-3071.15157a.u.

M06/BSII free energy in solution:-3070.221568a.u.

C	3.580057	-1.276865	-0.057879
O	3.263696	-0.351561	0.712758
N	4.688429	-2.036658	0.166784
C	2.710855	-1.583015	-1.269872
H	3.357655	-1.737860	-2.143519
H	2.234595	-2.558811	-1.103256

C	1.660007	-0.501149	-1.527929	C	3.348027	6.694111	-2.685324
C	5.023432	-3.145268	-0.690229	H	1.410588	7.203173	-3.511717
C	5.968760	-2.980881	-1.709007	H	5.124756	5.935212	-1.753631
C	4.444785	-4.400677	-0.473271	H	5.216630	3.793074	-0.494804
C	6.325815	-4.065812	-2.510690	H	3.825321	7.597458	-3.053528
H	6.414138	-2.003395	-1.867777	N	2.221320	2.261969	-0.527215
C	4.803186	-5.482523	-1.279075	Ni	1.230445	0.495286	0.225688
H	3.718849	-4.521294	0.325138	C	-2.059079	2.718874	-2.034390
C	5.743032	-5.317007	-2.298174	H	-2.184708	2.232684	-3.005740
H	7.057628	-3.932557	-3.301933	C	0.349055	-1.254529	0.917884
H	4.349385	-6.454126	-1.107816	C	-1.027568	-1.407248	0.539214
H	6.021248	-6.159832	-2.923786	C	-2.201826	-1.623099	0.250864
C	5.566707	-1.834283	1.361234	Si	-3.879914	-2.214504	-0.145154
C	6.268563	-0.465116	1.369740	C	-3.734239	-3.735817	-1.266935
C	4.841740	-2.103374	2.691941	C	-4.887198	-4.401170	-1.728382
H	6.343240	-2.599230	1.246252	C	-2.486214	-4.272220	-1.628258
C	7.250614	-0.371765	2.550090	C	-4.798042	-5.548173	-2.518514
H	5.512860	0.319877	1.460003	H	-5.873463	-4.016847	-1.476323
H	6.794810	-0.314384	0.418890	C	-2.389873	-5.419755	-2.418739
C	5.825437	-2.000271	3.870193	H	-1.580274	-3.784483	-1.279378
H	4.036922	-1.373250	2.814162	C	-3.546047	-6.060270	-2.866281
H	4.383409	-3.099413	2.665559	H	-5.703212	-6.041778	-2.862261
C	6.546495	-0.644044	3.887976	H	-1.412354	-5.813478	-2.685145
H	7.721523	0.618077	2.559646	H	-3.473565	-6.953200	-3.481381
H	8.061596	-1.101386	2.410227	C	-4.902844	-0.885511	-1.027691
H	5.286574	-2.157693	4.811236	C	-5.385234	0.244863	-0.338354
H	6.570311	-2.806450	3.798159	C	-5.202001	-0.988310	-2.400266
H	7.271111	-0.611393	4.710105	C	-6.143067	1.221013	-0.989473
H	5.814459	0.151739	4.080288	H	-5.169018	0.373338	0.717288
C	0.084039	2.740717	-1.316442	C	-5.955378	-0.012525	-3.056206
N	-0.375781	1.742905	-0.652051	H	-4.846869	-1.845564	-2.965007
C	-1.841023	1.750329	-0.839786	C	-6.431739	1.093979	-2.350266
H	-2.193058	0.732468	-1.015751	H	-6.501944	2.081041	-0.431308
O	-0.780542	3.436995	-2.088721	H	-6.174010	-0.119150	-4.115615
C	1.503479	3.143038	-1.222071	H	-7.026948	1.850076	-2.855925
C	2.062434	4.356527	-1.743063	C	-4.746750	-2.828204	1.449101
C	1.343198	5.333819	-2.488289	H	-4.132571	-3.669908	1.793572
C	3.453361	4.591432	-1.478846	H	-5.706074	-3.259362	1.136720
C	3.528816	2.505002	-0.269846	C	-4.959181	-1.849605	2.578555
C	1.975187	6.468747	-2.945155	C	-3.902212	-1.493420	3.432395
H	0.294422	5.178589	-2.693975	C	-6.219931	-1.280429	2.816448
C	4.071756	5.773200	-1.965876	C	-4.100437	-0.602006	4.486992
C	4.167693	3.631632	-0.723636	H	-2.917318	-1.920036	3.265210
H	4.024537	1.752164	0.328029	C	-6.420299	-0.385572	3.869105

H	-7.054001	-1.547718	2.171961
C	-5.360919	-0.042709	4.710536
H	-3.267985	-0.347212	5.137411
H	-7.407502	0.037751	4.034588
H	-5.516184	0.647443	5.534988
C	-2.584959	2.429341	0.300619
C	-2.591440	2.084342	1.651286
C	-3.329831	3.518150	-0.167498
C	-3.364894	2.844092	2.532048
H	-1.993280	1.256672	2.012574
C	-4.097180	4.278625	0.714538
C	-4.110986	3.933210	2.068242
H	-3.383015	2.585197	3.585796
H	-4.674383	5.128067	0.357499
H	-4.702709	4.518045	2.767150
C	-3.202076	3.671679	-1.666815
H	-2.988267	4.694753	-1.993997
H	-4.120151	3.350810	-2.175353
C	0.553494	-1.437750	2.432444
H	-0.034678	-0.724790	3.009555
H	0.258111	-2.456986	2.723743
H	1.600125	-1.287910	2.702127
H	0.917775	-2.026290	0.395177
C	0.499770	-0.992932	-2.384776
H	-0.002090	-1.837009	-1.898078
H	-0.253812	-0.202203	-2.459793
C	0.908819	-1.410732	-3.811541
H	1.607333	-2.254741	-3.806832
H	0.032183	-1.714709	-4.394305
H	1.393421	-0.583317	-4.343707
H	2.140394	0.347542	-2.027390
Br	1.177257	1.845441	2.401953

^{2}IM14-*SR*

B3LYP/BSI SCF energy: -3072.461404a.u.

M06/BSII SCF energy in solution:-3071.151279a.u.

M06/BSII free energy in solution:-3070.22001.u.

C	3.446037	0.960782	-0.076008
O	3.065716	0.257070	-1.031363
N	4.616202	1.654722	-0.138154
C	2.584807	1.021104	1.173440
H	2.933865	0.230343	1.852944
H	2.749096	1.964576	1.706328
C	1.103559	0.822935	0.827732
C	5.129978	2.376757	0.995529
C	5.715611	1.688301	2.063507
C	5.091338	3.776097	1.007995
C	6.244405	2.395291	3.144505
H	5.753274	0.603494	2.039872
C	5.628876	4.478753	2.086546
H	4.633474	4.303083	0.176505
C	6.203594	3.790502	3.157508
H	6.693720	1.854930	3.972482
H	5.592526	5.564081	2.092593
H	6.618201	4.339548	3.997571
C	5.470459	1.637250	-1.367889
C	6.050452	0.242774	-1.668164
C	4.762975	2.235306	-2.596769
H	6.308520	2.296460	-1.114181
C	7.001460	0.302557	-2.875503
H	5.228358	-0.447375	-1.879347
H	6.582234	-0.128932	-0.783017
C	5.720847	2.284751	-3.799051
H	3.891956	1.621881	-2.842814
H	4.399714	3.242380	-2.356728
C	6.307849	0.899638	-4.109030
H	7.375203	-0.703517	-3.097272
H	7.880369	0.913554	-2.621511
H	5.190345	2.679420	-4.673117
H	6.540597	2.987578	-3.588640
H	7.014572	0.966784	-4.944637
H	5.500810	0.227764	-4.430314
C	-0.398491	-2.546204	1.008701
N	-0.668522	-1.800801	-0.000594
C	-2.130187	-1.851630	-0.178579
H	-2.506169	-0.855261	-0.421409
O	-1.435940	-3.050704	1.714471
C	1.002547	-2.858425	1.358924
C	1.422393	-3.897673	2.251474
C	0.542248	-4.717931	3.012290
C	2.834791	-4.119960	2.368259
C	3.194646	-2.351693	0.766571
C	1.043763	-5.694282	3.843956
H	-0.524713	-4.567212	2.933783
C	3.315752	-5.136020	3.234980
C	3.707443	-3.321823	1.590379
H	3.821371	-1.746514	0.124393

C	2.438057	-5.907859	3.959293
H	0.359017	-6.310923	4.418328
H	4.387956	-5.294045	3.309000
H	4.779203	-3.489388	1.633659
H	2.811127	-6.685416	4.619283
N	1.864420	-2.107427	0.670893
Ni	1.053978	-0.644039	-0.662183
C	-2.646925	-2.412893	1.171382
H	-2.953705	-1.656694	1.898385
C	0.171143	0.815819	-1.856273
C	-1.022581	1.349537	-1.264140
C	-2.053464	1.816680	-0.784301
Si	-3.480215	2.741335	-0.129098
C	-3.057466	4.587413	-0.128180
C	-1.846624	5.068205	-0.656234
C	-3.976215	5.533943	0.366264
C	-1.563042	6.435445	-0.690609
H	-1.121362	4.360149	-1.047800
C	-3.698164	6.901133	0.335525
H	-4.922101	5.202985	0.790555
C	-2.488312	7.354911	-0.194786
H	-0.620419	6.782486	-1.105832
H	-4.423376	7.611345	0.723848
H	-2.269739	8.419072	-0.221402
C	-3.870939	2.191826	1.644776
C	-3.468439	2.972246	2.744410
C	-4.534550	0.978757	1.918829
C	-3.711786	2.563069	4.057997
H	-2.960649	3.917418	2.574595
C	-4.784446	0.567622	3.229933
H	-4.874109	0.351217	1.100538
C	-4.371122	1.358588	4.304570
H	-3.389551	3.187721	4.886942
H	-5.310226	-0.366253	3.412555
H	-4.566234	1.039979	5.325017
C	-4.994856	2.542091	-1.284979
H	-4.645193	2.885766	-2.267053
H	-5.739791	3.275421	-0.952959
C	-5.629208	1.177732	-1.406091
C	-5.002025	0.147969	-2.127585
C	-6.864129	0.899728	-0.799106
C	-5.584491	-1.116126	-2.231889
H	-4.047933	0.343022	-2.609637
C	-7.449568	-0.363758	-0.900674
H	-7.371331	1.684105	-0.242471
C	-6.811063	-1.378482	-1.615717
H	-5.078468	-1.895559	-2.793479
H	-8.408559	-0.551607	-0.424762
H	-7.266126	-2.361175	-1.700787
C	-2.571197	-2.911613	-1.180420
C	-2.180772	-3.063604	-2.510235
C	-3.470716	-3.807721	-0.590152
C	-2.731084	-4.110083	-3.255213
H	-1.426867	-2.416287	-2.943440
C	-4.018663	-4.851485	-1.334979
C	-3.648475	-4.993426	-2.674788
H	-2.429256	-4.246663	-4.289403
H	-4.716390	-5.550440	-0.880522
H	-4.063924	-5.805057	-3.265643
C	-3.723509	-3.457163	0.859970
H	-3.663085	-4.313027	1.540465
H	-4.715531	-3.006092	0.993769
C	-0.044347	0.398138	-3.317953
H	-0.791828	-0.392557	-3.408902
H	-0.399645	1.260607	-3.900910
H	0.881570	0.027136	-3.756275
H	0.973909	1.556991	-1.799927
H	0.738287	1.726932	0.337716
C	0.225546	0.546261	2.040094
H	-0.808479	0.425506	1.700557
H	0.520474	-0.393961	2.525678
C	0.248031	1.667516	3.099264
H	1.235693	1.776532	3.560832
H	-0.023128	2.631328	2.654634
H	-0.472171	1.459259	3.897581
Br	1.629510	-2.407552	-2.462098

^{2}TS15-*SS*

B3LYP/BSI SCF energy: -3072.430234a.u.

M06/BSII SCF energy in solution:-3071.128381a.u.

M06/BSII free energy in solution:-3070.202128a.u.

C	-3.182724	-1.548447	0.216508
O	-3.041644	-0.730377	-0.711604
N	-4.108552	-2.540778	0.148921
C	-2.342729	-1.352484	1.463315
H	-2.795023	-0.484883	1.964069
H	-2.432435	-2.201179	2.147164

C	-0.855775	-1.051004	1.188400	C	-4.364804	6.518080	2.145978
C	-4.243283	-3.537369	1.180728	H	-2.487686	7.552072	2.458204
C	-5.232752	-3.400260	2.160468	H	-6.048598	5.255403	1.724737
C	-3.422787	-4.671152	1.171139	H	-5.855113	2.948789	0.808044
C	-5.392182	-4.388930	3.132305	H	-4.969394	7.357154	2.477383
H	-5.866711	-2.518823	2.157749	N	-2.621466	2.069185	0.444398
C	-3.583250	-5.654575	2.148380	Ni	-1.381553	0.621619	-0.449998
H	-2.663199	-4.770684	0.401852	C	1.620573	3.560811	1.103276
C	-4.567498	-5.515814	3.129075	H	1.951235	3.236617	2.093447
H	-6.158705	-4.276484	3.893317	C	0.076478	-1.097395	-0.758996
H	-2.940829	-6.530083	2.140405	H	-0.042101	-0.344714	-1.555176
H	-4.691733	-6.283035	3.887381	C	-0.214026	-0.186078	2.270532
C	-5.022459	-2.683119	-1.032037	H	-0.803779	0.723046	2.428555
C	-5.955322	-1.472830	-1.217147	H	0.779066	0.126224	1.935810
C	-4.275539	-3.020410	-2.334722	C	-0.056698	-0.930571	3.611101
H	-5.647211	-3.545435	-0.773381	H	0.550733	-1.834766	3.488961
C	-6.949838	-1.732473	-2.361917	H	0.437842	-0.292473	4.352199
H	-5.351961	-0.591247	-1.450869	H	-1.021952	-1.232597	4.032477
H	-6.493739	-1.275258	-0.281352	H	-0.336816	-2.009722	1.192321
C	-5.276107	-3.274050	-3.475606	C	-0.390377	-2.445847	-1.304231
H	-3.621529	-2.184605	-2.598446	H	-1.379520	-2.350738	-1.752083
H	-3.644697	-3.904069	-2.179288	H	0.299224	-2.788356	-2.084089
C	-6.222026	-2.079585	-3.669225	H	-0.410142	-3.222181	-0.530169
H	-7.586199	-0.850914	-2.500470	C	1.425909	-1.095111	-0.290374
H	-7.618905	-2.560692	-2.085824	C	2.582718	-1.138032	0.113057
H	-4.727753	-3.480212	-4.401506	Si	4.326306	-1.180047	0.647522
H	-5.867161	-4.175033	-3.254047	C	4.690619	0.386156	1.655523
H	-6.949516	-2.296670	-4.460207	C	5.531546	1.402978	1.169122
H	-5.640824	-1.209490	-4.002011	C	4.104418	0.575807	2.922585
C	-0.561796	3.112137	0.721249	C	5.781489	2.558071	1.915400
N	-0.002883	2.127248	0.102644	H	6.000431	1.291646	0.195662
C	1.447868	2.412350	0.073089	C	4.348240	1.727415	3.672810
H	1.999276	1.506816	0.333319	H	3.443918	-0.184202	3.334445
O	0.248732	4.053454	1.257538	C	5.190890	2.722720	3.169542
C	-2.022046	3.202595	0.847047	H	6.440964	3.325408	1.518729
C	-2.753286	4.353650	1.291794	H	3.889022	1.845735	4.650783
C	-2.165154	5.577087	1.718040	H	5.389094	3.616817	3.754497
C	-4.184529	4.252231	1.294206	C	5.457322	-1.258677	-0.859464
C	-3.977408	2.011094	0.419266	C	6.849934	-1.406951	-0.705552
C	-2.955819	6.626863	2.135255	C	4.947970	-1.173154	-2.166750
H	-1.089597	5.678572	1.714370	C	7.698585	-1.467989	-1.811610
C	-4.966327	5.351056	1.730778	H	7.284771	-1.471838	0.290041
C	-4.774110	3.045822	0.837060	C	5.793109	-1.232655	-3.276980
H	-4.388985	1.088112	0.030691	H	3.877760	-1.061107	-2.315412

C	7.169380	-1.381095	-3.101550
H	8.769750	-1.582210	-1.668317
H	5.375677	-1.164048	-4.277738
H	7.827865	-1.428413	-3.964591
C	4.624887	-2.689412	1.783782
H	4.106709	-2.497515	2.730737
H	5.696689	-2.704448	2.019324
C	4.189149	-4.016403	1.210737
C	2.923340	-4.545447	1.505256
C	5.027490	-4.748531	0.355403
C	2.510088	-5.765540	0.969323
H	2.258848	-3.994779	2.166734
C	4.615969	-5.967968	-0.183252
H	6.010813	-4.356816	0.109250
C	3.354928	-6.483535	0.121311
H	1.527629	-6.157801	1.219024
H	5.284358	-6.517021	-0.840948
H	3.036051	-7.434785	-0.295092
C	1.945008	3.025990	-1.228534
C	1.874352	2.500007	-2.518091
C	2.543448	4.270197	-0.994666
C	2.417885	3.235497	-3.573682
H	1.366681	1.561891	-2.711126
C	3.086377	5.002366	-2.050247
C	3.021465	4.476121	-3.342294
H	2.355756	2.844352	-4.584758
H	3.549127	5.970163	-1.873271
H	3.435254	5.038588	-4.174768
C	2.524175	4.628562	0.475188
H	2.146635	5.636505	0.678675
H	3.526001	4.562496	0.917889
Br	-1.665324	1.280212	-2.941842

^{2}TS15-*RR*

B3LYP/BSI SCF energy: -3072.421594a.u.

M06/BSII SCF energy in solution:-3071.126583a.u.

M06/BSII free energy in solution:-3070.200592a.u.

C	4.045499	0.965929	0.418704
O	4.041703	-0.144109	-0.111893
N	4.969709	1.929813	0.083780
C	3.010664	1.326020	1.488130
H	3.498551	1.167365	2.461447
H	2.780767	2.396613	1.460989
C	1.745934	0.469797	1.461216
C	5.110066	3.150764	0.827781
C	5.687655	3.139741	2.103243
C	4.717509	4.368964	0.258247
C	5.853060	4.332556	2.809049
H	6.009939	2.195280	2.531493
C	4.893282	5.560140	0.962888
H	4.272376	4.372626	-0.731982
C	5.457525	5.544562	2.240637
H	6.299492	4.314368	3.799039
H	4.584023	6.499952	0.514966
H	5.590535	6.472573	2.788669
C	5.973584	1.688718	-0.995966
C	6.990880	0.592440	-0.626969
C	5.328677	1.430449	-2.369369
H	6.522579	2.635289	-1.064968
C	8.059013	0.450095	-1.723753
H	6.455226	-0.352549	-0.497850
H	7.460920	0.838565	0.333369
C	6.408091	1.287141	-3.454737
H	4.722453	0.522412	-2.321489
H	4.650486	2.255915	-2.616261
C	7.426044	0.192586	-3.099536
H	8.751561	-0.358820	-1.462181
H	8.660311	1.369894	-1.769901
H	5.932031	1.069370	-4.417373
H	6.937390	2.243711	-3.577356
H	8.204506	0.132789	-3.869562
H	6.918780	-0.782012	-3.088593
C	-0.124560	-2.879718	1.289841
N	-0.556939	-1.744276	0.853302
C	-1.999430	-1.702904	1.178050
H	-2.291376	-0.694775	1.477848
O	-0.965296	-3.605300	2.057480
C	1.196371	-3.422899	0.901703
C	1.730563	-4.692412	1.299450
C	1.129862	-5.586406	2.231164
C	2.980281	-5.069889	0.699889
C	2.997562	-2.970560	-0.495642
C	1.735108	-6.783506	2.540743
H	0.191674	-5.318313	2.694961
C	3.570832	-6.317420	1.039201
C	3.590500	-4.180550	-0.215756
H	3.435279	-2.246079	-1.170103

C	2.962136	-7.157132	1.940511
H	1.263820	-7.452451	3.254761
H	4.513306	-6.590248	0.572867
H	4.528146	-4.453777	-0.690509
H	3.419368	-8.108359	2.196613
N	1.822895	-2.604820	0.061053
Ni	0.748844	-0.530273	-0.228516
C	-2.157204	-2.776663	2.281630
H	-2.095793	-2.406539	3.309377
C	0.592243	1.654922	0.214488
C	-0.846637	1.569083	0.120245
C	-2.068180	1.682923	0.081459
Si	-3.813686	2.239241	0.048063
C	-3.941496	3.783587	1.142664
C	-5.201094	4.263029	1.551269
C	-2.808998	4.527571	1.517369
C	-5.324624	5.435731	2.297871
H	-6.100620	3.708219	1.294001
C	-2.925601	5.701220	2.265270
H	-1.823222	4.179623	1.220384
C	-4.184821	6.158479	2.656704
H	-6.308297	5.783820	2.601844
H	-2.034106	6.257333	2.543606
H	-4.278310	7.071046	3.239279
C	-4.987491	0.934582	0.752373
C	-5.733480	0.065724	-0.065116
C	-5.135533	0.808305	2.148066
C	-6.591074	-0.888228	0.487168
H	-5.640180	0.123166	-1.144825
C	-5.987381	-0.147439	2.704763
H	-4.591675	1.477363	2.810494
C	-6.719731	-0.997769	1.872649
H	-7.151672	-1.549919	-0.166563
H	-6.089508	-0.219449	3.784664
H	-7.391109	-1.736773	2.302234
C	-4.282539	2.810953	-1.714646
H	-3.611785	3.660321	-1.902955
H	-5.288880	3.242311	-1.638880
C	-4.217433	1.845783	-2.877676
C	-2.989387	1.338207	-3.332217
C	-5.383439	1.460821	-3.557910
C	-2.928411	0.475861	-4.427318
H	-2.070222	1.610412	-2.822904
C	-5.326820	0.598156	-4.654866
H	-6.344661	1.852011	-3.231553
C	-4.098194	0.103433	-5.095783
H	-1.962531	0.092569	-4.743337
H	-6.243827	0.320806	-5.168377
H	-4.050739	-0.562015	-5.953390
C	-2.860686	-2.255580	0.048448
C	-2.905756	-1.845069	-1.282598
C	-3.645813	-3.323415	0.500789
C	-3.765372	-2.514141	-2.158432
H	-2.270720	-1.043621	-1.642735
C	-4.500146	-3.990800	-0.375064
C	-4.556403	-3.576685	-1.708714
H	-3.812538	-2.200586	-3.196227
H	-5.107299	-4.824369	-0.030748
H	-5.213838	-4.091281	-2.404359
C	-3.424560	-3.578344	1.975273
H	-3.302831	-4.635228	2.234518
H	-4.255610	-3.186902	2.576672
C	1.244567	2.292732	-1.025576
H	0.980029	1.766243	-1.941437
H	0.911925	3.336578	-1.099670
H	2.333099	2.297506	-0.943194
H	0.773784	2.328449	1.055226
C	0.945409	0.574356	2.763184
H	0.903696	1.622635	3.090218
H	-0.090719	0.273261	2.583094
C	1.519134	-0.283510	3.901989
H	2.555237	-0.016865	4.137655
H	0.932646	-0.155390	4.818301
H	1.505547	-1.347328	3.641190
H	2.071171	-0.564418	1.305124
Br	0.666741	-0.800849	-2.698587

^{2}TS15-*RS*

B3LYP/BSI SCF energy: -3072.4296a.u.

M06/BSII SCF energy in solution:-3071.124566a.u.

M06/BSII free energy in solution:-3070.197712a.u.

C	3.450203	1.498696	0.096886
O	3.217352	0.443582	-0.519190
N	4.522779	2.274986	-0.218759
C	2.514799	1.958752	1.202821
H	3.080490	1.952309	2.146001
H	2.258208	3.009995	1.040742

C	1.268460	1.095737	1.349145	C	3.655457	-6.543989	3.053956
C	4.859750	3.438327	0.559984	H	1.679059	-7.185349	3.665780
C	5.585632	3.299366	1.748092	H	5.467635	-5.660978	2.318446
C	4.504687	4.713834	0.106148	H	5.555982	-3.502000	1.088078
C	5.943699	4.430039	2.484071	H	4.149609	-7.418285	3.467304
H	5.868143	2.306520	2.085225	N	2.480332	-2.158619	0.803047
C	4.869359	5.841706	0.842524	Ni	1.357240	-0.592405	-0.203470
H	3.943140	4.813223	-0.817729	C	-1.876723	-2.843709	1.923988
C	5.586542	5.702023	2.032741	H	-2.088406	-2.317883	2.859496
H	6.505900	4.316014	3.406164	C	0.157495	1.332185	-0.601871
H	4.589833	6.829005	0.487062	H	0.263732	0.575310	-1.395235
H	5.867478	6.581157	2.604831	C	0.717562	2.653300	-1.135273
C	5.412700	1.965455	-1.383411	H	1.746212	2.539343	-1.481223
C	6.246458	0.688012	-1.181716	H	0.124078	2.973851	-1.999964
C	4.661506	1.941699	-2.726639	H	0.667429	3.459810	-0.397304
H	6.109623	2.811169	-1.407073	C	-1.221891	1.444105	-0.251338
C	7.232196	0.501025	-2.347896	C	-2.412938	1.635130	-0.021351
H	5.570072	-0.170017	-1.135042	Si	-4.182568	2.059874	0.149613
H	6.785312	0.744491	-0.227624	C	-4.357628	3.536904	1.320291
C	5.653145	1.751331	-3.887350	C	-5.595494	4.193264	1.468085
H	3.932586	1.126269	-2.726012	C	-3.267295	4.032841	2.056154
H	4.107992	2.880643	-2.853172	C	-5.739334	5.292232	2.316400
C	6.503692	0.485847	-3.700286	H	-6.466056	3.843666	0.916971
H	7.797376	-0.427540	-2.206119	C	-3.404043	5.132899	2.905612
H	7.968244	1.318177	-2.338294	H	-2.298283	3.552460	1.955970
H	5.100957	1.701808	-4.832165	C	-4.641168	5.764983	3.038071
H	6.315148	2.627394	-3.955482	H	-6.705521	5.780335	2.412484
H	7.227943	0.391746	-4.518050	H	-2.544814	5.497228	3.462745
H	5.851684	-0.395995	-3.751168	H	-4.749859	6.621686	3.697635
C	0.316424	-2.778706	1.378666	C	-5.162643	0.585747	0.816416
N	-0.145096	-1.823140	0.641633	C	-5.202727	-0.630670	0.106220
C	-1.620004	-1.924801	0.701157	C	-5.889246	0.665805	2.019427
H	-2.054481	-0.927609	0.792761	C	-5.944531	-1.717270	0.575280
O	-0.576548	-3.498085	2.095022	H	-4.652335	-0.738049	-0.823358
C	1.751428	-3.096845	1.422332	C	-6.629944	-0.419268	2.493103
C	2.328672	-4.281050	1.990965	H	-5.878691	1.587266	2.594747
C	1.600326	-5.311683	2.648465	C	-6.660784	-1.613130	1.770184
C	3.752120	-4.424804	1.873255	H	-5.957741	-2.641724	0.005206
C	3.818534	-2.325974	0.681422	H	-7.183175	-0.331344	3.424524
C	2.252590	-6.410203	3.166166	H	-7.242287	-2.456456	2.133734
H	0.527521	-5.226877	2.742001	C	-4.858666	2.626594	-1.551411
C	4.389696	-5.568799	2.418201	H	-4.265193	3.507968	-1.825005
C	4.479670	-3.412132	1.199268	H	-5.882110	2.984197	-1.383396
H	4.331396	-1.539369	0.142417	C	-4.839462	1.613337	-2.669740

C	-3.663455	1.361276	-3.394923
C	-5.993836	0.892844	-3.013271
C	-3.641199	0.421029	-4.425285
H	-2.758087	1.907530	-3.145892
C	-5.974977	-0.048151	-4.044086
H	-6.916853	1.074747	-2.468132
C	-4.798018	-0.289178	-4.754450
H	-2.718750	0.246069	-4.972050
H	-6.883227	-0.590369	-4.293429
H	-4.782774	-1.018286	-5.559526
C	-2.224279	-2.711952	-0.454782
C	-2.125861	-2.454567	-1.821755
C	-2.955337	-3.808934	0.018964
C	-2.778990	-3.310484	-2.712366
H	-1.525247	-1.632168	-2.193442
C	-3.603008	-4.663683	-0.872783
C	-3.511909	-4.405609	-2.243150
H	-2.707204	-3.124301	-3.779298
H	-4.165816	-5.520468	-0.510314
H	-4.008622	-5.065066	-2.949548
C	-2.947279	-3.866291	1.530487
H	-2.720597	-4.857155	1.938168
H	-3.915660	-3.556664	1.943874
H	1.547786	0.123934	1.769515
C	0.220730	1.702731	2.266078
H	-0.694106	1.104990	2.218278
H	-0.057331	2.704089	1.913462
C	0.671945	1.794126	3.736010
H	-0.136576	2.186906	4.362051
H	0.946803	0.807909	4.128332
H	1.535771	2.455374	3.864329
Br	1.450872	-1.465597	-2.627435

^{2}TS15-*SR*

B3LYP/BSI SCF energy: -3072.410963a.u.

M06/BSII SCF energy in solution:-3071.102772a.u.

M06/BSII free energy in solution:-3070.175263a.u.

C	3.210109	1.467107	-0.031392
O	3.065145	0.514235	-0.822914
N	4.216503	2.361100	-0.198108
C	2.263245	1.569219	1.150126
H	2.573500	0.773051	1.839267
H	2.389473	2.520989	1.675699
C	0.790105	1.372353	0.779652
C	4.443681	3.446117	0.722540
C	5.233462	3.245895	1.859947
C	3.925699	4.716335	0.446531
C	5.493563	4.311235	2.723153
H	5.636691	2.258254	2.061432
C	4.189822	5.778419	1.312330
H	3.317509	4.861932	-0.440927
C	4.972825	5.577843	2.451125
H	6.103880	4.150617	3.606846
H	3.782480	6.761694	1.096874
H	5.176554	6.405626	3.123632
C	5.195651	2.232108	-1.329048
C	6.032872	0.943048	-1.241543
C	4.534341	2.393788	-2.709332
H	5.873503	3.080899	-1.183971
C	7.083022	0.903886	-2.364712
H	5.369952	0.077957	-1.331028
H	6.523097	0.892222	-0.260822
C	5.594545	2.342713	-3.822980
H	3.808858	1.589343	-2.855477
H	3.989295	3.345555	-2.744934
C	6.429646	1.055978	-3.746168
H	7.641322	-0.037234	-2.307555
H	7.814611	1.712001	-2.215972
H	5.101289	2.421282	-4.798441
H	6.260426	3.214428	-3.738691
H	7.196562	1.056436	-4.529622
H	5.780847	0.190825	-3.935601
C	0.086083	-2.659491	1.097654
N	-0.141166	-1.930913	0.047806
C	-1.542828	-2.169523	-0.337238
H	-2.014427	-1.228483	-0.633973
O	-0.977267	-3.305076	1.633243
C	1.426948	-2.764688	1.662048
C	1.859078	-3.720682	2.641670
C	1.013427	-4.673583	3.270493
C	3.249245	-3.705803	2.996790
C	3.586615	-1.910085	1.413650
C	1.519832	-5.551006	4.208929
H	-0.035242	-4.705615	3.010657
C	3.734390	-4.619966	3.962365
C	4.103678	-2.774894	2.343470
H	4.214072	-1.212659	0.869523

C	2.885881	-5.527872	4.561324
H	0.856103	-6.270018	4.680234
H	4.790244	-4.596283	4.218071
H	5.164200	-2.759456	2.574829
H	3.266798	-6.226827	5.300107
N	2.269213	-1.871242	1.095086
Ni	1.474491	-0.799084	-0.511730
C	-2.164021	-2.796009	0.937510
H	-2.643406	-2.080455	1.611768
C	0.112566	1.282094	-1.390155
C	-1.234234	1.582159	-1.029975
C	-2.392759	1.825217	-0.704681
Si	-4.073470	2.335745	-0.198266
C	-4.123749	4.225349	-0.117836
C	-3.014776	5.014051	-0.470213
C	-5.305150	4.891545	0.262955
C	-3.079968	6.408928	-0.444154
H	-2.091399	4.526754	-0.771322
C	-5.375961	6.284867	0.291941
H	-6.184634	4.318306	0.549484
C	-4.260911	7.047336	-0.063050
H	-2.209390	6.997106	-0.722367
H	-6.298809	6.775099	0.590079
H	-4.313642	8.132468	-0.042883
C	-4.461307	1.615876	1.510634
C	-4.398973	2.423124	2.661676
C	-4.766213	0.251071	1.687970
C	-4.625067	1.894330	3.934784
H	-4.172014	3.481056	2.564527
C	-4.997158	-0.280424	2.958190
H	-4.836342	-0.404412	0.825342
C	-4.924076	0.540054	4.086372
H	-4.569817	2.541118	4.806356
H	-5.241094	-1.334062	3.067254
H	-5.103157	0.126556	5.075139
C	-5.354537	1.810941	-1.519123
H	-5.027020	2.301357	-2.444793
H	-6.302348	2.287871	-1.240904
C	-5.565567	0.335017	-1.756184
C	-4.625963	-0.424303	-2.473687
C	-6.705375	-0.319556	-1.263978
C	-4.815376	-1.790601	-2.685471
H	-3.739695	0.064322	-2.869366
C	-6.897798	-1.686842	-1.472619
H	-7.449857	0.249951	-0.712869
C	-5.952194	-2.429174	-2.182138
H	-4.074502	-2.357710	-3.240758
H	-7.791335	-2.169039	-1.084871
H	-6.098747	-3.492123	-2.349862
C	-1.730768	-3.267365	-1.380814
C	-1.164370	-3.371041	-2.651295
C	-2.600383	-4.256917	-0.904453
C	-1.504510	-4.465238	-3.451794
H	-0.429513	-2.652239	-2.996506
C	-2.937118	-5.348674	-1.703842
C	-2.389034	-5.443787	-2.985400
H	-1.060699	-4.562973	-4.438080
H	-3.608403	-6.119823	-1.334098
H	-2.638442	-6.291681	-3.617370
C	-3.074924	-3.945001	0.497620
H	-3.010111	-4.793949	1.186265
H	-4.118807	-3.604402	0.497479
C	0.207876	0.480018	-2.699428
H	-0.374466	-0.441444	-2.670510
H	-0.207433	1.103120	-3.507718
H	1.234026	0.223051	-2.962662
H	0.729386	2.176466	-1.471954
H	0.367678	2.345950	0.541248
C	-0.070534	0.734005	1.852028
H	-1.041291	0.472376	1.419286
H	0.389778	-0.186927	2.220508
C	-0.316946	1.685072	3.042777
H	0.615280	1.948135	3.555431
H	-0.795011	2.613563	2.712906
H	-0.979728	1.214018	3.776345
Br	2.465354	-2.294382	-2.341885

^{2}TS16-*SS*

B3LYP/BSI SCF energy: -3072.435817a.u.

M06/BSII SCF energy in solution:-3071.130418a.u.

M06/BSII free energy in solution:-3070.204639a.u.

C	3.144450	0.362866	0.005432
O	2.552412	-0.697400	-0.273344
N	4.479314	0.480569	-0.229881
C	2.387998	1.551553	0.621371
H	3.104935	2.250513	1.064306
H	1.901134	2.072381	-0.212194

C	1.360136	1.142486	1.626784	C	-0.834594	-4.842085	5.423754
C	5.184575	1.721629	-0.034570	H	-2.985515	-4.637875	5.254626
C	6.067000	1.856324	1.043480	H	1.307678	-4.890277	5.325054
C	5.037901	2.768989	-0.950537	H	2.628617	-3.843810	3.485546
C	6.791246	3.037175	1.207583	H	-0.888000	-5.409622	6.348057
H	6.174107	1.036891	1.747719	N	0.595478	-2.338047	1.268693
C	5.759405	3.951200	-0.777530	Ni	0.554139	-1.274687	-0.567311
H	4.358648	2.653030	-1.789304	C	-3.749145	-1.464163	0.290397
C	6.637562	4.086943	0.298941	H	-4.033587	-0.506241	0.730297
H	7.471953	3.138319	2.047719	C	0.164928	0.000192	-2.094848
H	5.636942	4.763252	-1.487924	H	-0.551384	-0.616454	-2.649730
H	7.200284	5.006380	0.429797	C	1.342476	0.351898	-3.011278
C	5.281961	-0.626514	-0.854056	H	1.818780	-0.565363	-3.363952
C	5.312571	-1.914791	-0.014840	H	1.012165	0.929785	-3.885989
C	4.870938	-0.918896	-2.307220	H	2.098038	0.952723	-2.495982
H	6.300678	-0.222793	-0.869256	C	-0.502971	1.127478	-1.522049
C	6.277880	-2.933617	-0.645817	C	-1.081657	2.080117	-0.995890
H	4.308805	-2.344971	0.011683	Si	-1.988598	3.511960	-0.356179
H	5.613916	-1.682345	1.014928	C	-0.841227	5.014106	-0.224335
C	5.830991	-1.944038	-2.935019	C	-0.391348	5.670366	-1.386271
H	3.852708	-1.317183	-2.319658	C	-0.387995	5.502270	1.014415
H	4.876948	0.012934	-2.885746	C	0.470015	6.765681	-1.315967
C	5.894622	-3.233709	-2.103233	H	-0.710822	5.320203	-2.365211
H	6.275186	-3.855324	-0.052300	C	0.474996	6.597943	1.091769
H	7.304760	-2.540291	-0.608081	H	-0.714392	5.022596	1.932941
H	5.504827	-2.167737	-3.956754	C	0.905105	7.233142	-0.073761
H	6.838226	-1.507833	-3.014381	H	0.800343	7.255048	-2.228437
H	6.612302	-3.935322	-2.545051	H	0.809703	6.955579	2.062038
H	4.911494	-3.720905	-2.125081	H	1.574101	8.087555	-0.015770
C	-1.689873	-2.121745	0.954294	C	-2.728981	3.120390	1.343073
N	-1.427772	-1.612538	-0.200309	C	-2.615414	1.839984	1.912297
C	-2.721440	-1.371410	-0.868187	C	-3.450360	4.090047	2.065388
H	-2.708493	-0.394410	-1.356219	C	-3.196383	1.535033	3.146388
O	-2.982277	-2.184102	1.327397	H	-2.062967	1.073609	1.375520
C	-0.595401	-2.623603	1.804196	C	-4.030683	3.795003	3.300841
C	-0.744355	-3.364794	3.018072	H	-3.557215	5.096410	1.665540
C	-1.990818	-3.683527	3.626920	C	-3.905880	2.514334	3.843929
C	0.463358	-3.814278	3.649898	H	-3.096585	0.534367	3.559316
C	1.725112	-2.780836	1.867979	H	-4.579524	4.563069	3.839282
C	-2.027552	-4.402339	4.800861	H	-4.358377	2.282274	4.804170
H	-2.909203	-3.356394	3.160071	C	-3.419574	3.972349	-1.546226
C	0.385729	-4.554531	4.858956	H	-2.966541	4.304177	-2.487876
C	1.700733	-3.504350	3.035745	H	-3.929248	4.845754	-1.120838
H	2.645081	-2.527223	1.358634	C	-4.405884	2.860737	-1.805228

C	-4.200509	1.941082	-2.847408
C	-5.545935	2.701228	-1.001420
C	-5.106003	0.905602	-3.084068
H	-3.323342	2.044834	-3.480293
C	-6.454728	1.667906	-1.236139
H	-5.724007	3.398059	-0.186602
C	-6.240583	0.765101	-2.280247
H	-4.928507	0.211750	-3.901045
H	-7.336505	1.575220	-0.607416
H	-6.954409	-0.030386	-2.475429
C	-3.139620	-2.503739	-1.797214
C	-2.445347	-3.037185	-2.883081
C	-4.384082	-3.021104	-1.415380
C	-3.029606	-4.083339	-3.601485
H	-1.449265	-2.690015	-3.137266
C	-4.965390	-4.063382	-2.136420
C	-4.281939	-4.588395	-3.235976
H	-2.495083	-4.517079	-4.441211
H	-5.930346	-4.469616	-1.843625
H	-4.720337	-5.405263	-3.802545
C	-4.931824	-2.303340	-0.200880
H	-5.299457	-2.975179	0.581874
H	-5.756452	-1.630857	-0.468481
C	1.710034	0.851624	3.052619
H	1.320597	-0.135375	3.345138
H	2.800608	0.795290	3.169428
C	1.145875	1.900123	4.036904
H	1.401479	1.644785	5.071401
H	1.547036	2.896062	3.822648
H	0.055382	1.957294	3.960136
H	0.316367	1.173181	1.334988
Br	1.316486	-3.359727	-1.951091

^{1}TS17

B3LYP/BSI SCF energy: -1275.962425a.u.

M06/BSII SCF energy in solution:-1275.345525a.u.

M06/BSII free energy in solution:-1274.771469a.u.

C	6.074791	-0.375057	0.091319
C	4.692601	-0.973049	0.434328
C	3.634172	1.135087	-0.762935
C	5.078431	1.610157	-1.032735
C	6.080468	0.465377	-1.185272
H	6.398040	0.259796	0.926780
H	6.795134	-1.198710	0.025568
H	5.066282	2.247644	-1.924561
H	5.399189	2.244527	-0.195986
H	5.838449	-0.150901	-2.059515
H	7.084229	0.868309	-1.363473
N	3.640487	0.084808	0.303967
C	4.704502	-1.432681	1.902255
H	3.764956	-1.912990	2.176058
H	5.522669	-2.143907	2.055515
H	4.856896	-0.579157	2.569288
C	4.370152	-2.180239	-0.472821
H	5.047978	-3.009681	-0.244531
H	3.346461	-2.516645	-0.297495
H	4.477594	-1.945509	-1.534998
C	2.980387	0.599064	-2.055601
H	2.012299	0.149743	-1.826565
H	2.820557	1.420537	-2.762261
H	3.596241	-0.153759	-2.554049
C	2.811632	2.323141	-0.234701
H	2.859121	3.147881	-0.953538
H	1.767635	2.049855	-0.080651
H	3.214518	2.672607	0.720461
O	2.491258	-0.178094	0.857214
C	-1.731503	-0.768216	-0.103765
O	-2.049748	-1.915892	-0.407146
N	-2.673422	0.231646	0.041031
C	-0.260901	-0.369475	0.133044
H	0.006035	0.397947	-0.601480
H	-0.179715	0.127197	1.108879
C	0.686523	-1.522939	0.070088
C	-2.317199	1.584047	0.369481
C	-1.956886	2.486191	-0.639178
C	-2.374383	2.023433	1.697981
C	-1.648162	3.809567	-0.320383
H	-1.920992	2.141387	-1.668309
C	-2.069675	3.348121	2.013476
H	-2.653081	1.318831	2.475715
C	-1.704139	4.243019	1.005760
H	-1.367403	4.501991	-1.108784
H	-2.113668	3.679319	3.046954
H	-1.464199	5.273023	1.252675
C	-4.124272	-0.045575	-0.161550
C	-4.452462	-0.456424	-1.609383
C	-4.686177	-1.055652	0.856335

H	-4.613415	0.917836	0.026747
C	-5.965576	-0.656977	-1.794628
H	-3.919428	-1.383438	-1.838718
H	-4.083456	0.313848	-2.297909
C	-6.198227	-1.250242	0.657037
H	-4.163358	-2.007714	0.730527
H	-4.479167	-0.700413	1.873386
C	-6.528245	-1.667472	-0.783902
H	-6.171819	-0.986366	-2.819966
H	-6.483210	0.305374	-1.668155
H	-6.571538	-1.997982	1.366812
H	-6.723805	-0.312199	0.889340
H	-7.612817	-1.768965	-0.911395
H	-6.093090	-2.656686	-0.981796
C	0.668495	-2.592385	1.121972
H	-0.080171	-2.343800	1.884760
H	1.634397	-2.604532	1.647611
C	0.379282	-3.996168	0.561798
H	1.133191	-4.285592	-0.180181
H	0.393959	-4.748356	1.358677
H	-0.599267	-4.012932	0.076799
H	1.094462	-1.788644	-0.901887

6

B3LYP/BSI SCF energy: -1276.011356a.u.

M06/BSII SCF energy in solution:-1275.400589a.u.

M06/BSII free energy in solution:-1274.815987a.u.

C	-5.737171	-0.518659	-0.042604
C	-4.413872	-0.263248	-0.810388
C	-3.259574	0.033120	1.528109
C	-4.648778	-0.245131	2.163086
C	-5.535541	-1.162718	1.326169
H	-6.243300	0.444270	0.100469
H	-6.387448	-1.130403	-0.678316
H	-4.485819	-0.656208	3.165942
H	-5.167257	0.713575	2.289875
H	-5.090620	-2.160895	1.231100
H	-6.503425	-1.304456	1.822101
N	-3.488695	0.429291	0.117514
C	-4.750513	0.705534	-1.961916
H	-3.891109	0.907895	-2.600061
H	-5.545548	0.277849	-2.582395
H	-5.097068	1.659363	-1.555140
C	-3.915061	-1.608505	-1.404405
H	-4.689580	-2.034227	-2.052741
H	-3.019593	-1.483975	-2.014891
H	-3.691375	-2.346479	-0.630454
C	-2.347249	-1.200163	1.761840
H	-1.346615	-1.080718	1.344483
H	-2.233188	-1.370169	2.839040
H	-2.771757	-2.111727	1.333317
C	-2.678250	1.247332	2.280612
H	-2.679862	1.047002	3.357477
H	-1.654082	1.475791	1.985524
H	-3.287139	2.134153	2.086152
O	-2.381427	1.068273	-0.514771
C	1.107218	-0.290223	-0.134127
O	0.809678	-1.485458	-0.123692
N	2.415070	0.131939	-0.024127
C	0.021390	0.781444	-0.247723
H	-0.258769	1.053936	0.773165
H	0.402443	1.696947	-0.708033
C	-1.236958	0.285434	-0.987947
C	2.769188	1.515970	0.129811
C	2.515462	2.186788	1.332311
C	3.421204	2.189190	-0.911163
C	2.894279	3.521452	1.484350
H	2.023043	1.657194	2.142150
C	3.807475	3.520118	-0.752101
H	3.615908	1.663903	-1.841363
C	3.542099	4.190221	0.444344
H	2.688505	4.035429	2.418719
H	4.309671	4.035468	-1.565655
H	3.839114	5.227725	0.565152
C	3.525691	-0.854507	0.119722
C	3.451544	-1.634173	1.446156
C	3.657448	-1.801382	-1.086976
H	4.431415	-0.237513	0.150687
C	4.663618	-2.567122	1.601987
H	2.524380	-2.214542	1.458651
H	3.408137	-0.925701	2.282519
C	4.873743	-2.727004	-0.917651
H	2.743514	-2.394613	-1.173996
H	3.753111	-1.210743	-2.006436
C	4.806354	-3.513374	0.400313
H	4.571758	-3.140471	2.531989
H	5.579372	-1.965403	1.697657

H	4.935207	-3.413898	-1.769928
H	5.796867	-2.129054	-0.933889
H	5.698538	-4.140691	0.514486
H	3.943787	-4.193170	0.371353
C	-1.116225	0.514390	-2.502853
H	-1.102366	1.598462	-2.675850
H	-2.021901	0.139767	-2.987915
C	0.102831	-0.140977	-3.164872
H	0.132608	-1.217743	-2.971756
H	0.072145	0.008789	-4.249064
H	1.046086	0.283172	-2.805607
H	-1.380543	-0.771860	-0.769041

^{2}TS18-*SS*

B3LYP/BSI SCF energy: -3072.456878 a.u.

M06/BSII SCF energy in solution:-3071.14056 a.u.

M06/BSII free energy in solution:-3070.216602 a.u.

C	3.410297	1.286853	-0.177765
O	3.079034	0.483966	-1.076485
N	4.487337	2.103750	-0.343921
C	2.612376	1.326668	1.113153
H	3.138874	0.670141	1.825113
H	2.667752	2.329948	1.553947
C	1.180124	0.813970	0.895855
C	4.953760	2.961213	0.714711
C	5.698087	2.432164	1.774449
C	4.714438	4.338933	0.653055
C	6.186927	3.274729	2.773966
H	5.887854	1.363780	1.809613
C	5.210574	5.178412	1.650730
H	4.135568	4.741008	-0.172820
C	5.945545	4.648295	2.713578
H	6.760293	2.857398	3.596511
H	5.018631	6.246107	1.599614
H	6.328593	5.303085	3.490550
C	5.312857	2.085698	-1.592547
C	6.056108	0.752019	-1.792555
C	4.518866	2.483049	-2.848979
H	6.067774	2.861183	-1.419117
C	6.975156	0.823250	-3.023651
H	5.319563	-0.045243	-1.930002
H	6.640392	0.520388	-0.892880
C	5.446395	2.549205	-4.073840
H	3.731485	1.744844	-3.020195
H	4.032527	3.452497	-2.684350
C	6.194725	1.224328	-4.284431
H	7.467416	-0.145014	-3.170830
H	7.775592	1.555752	-2.842855
H	4.859209	2.801617	-4.964121
H	6.176479	3.361388	-3.940862
H	6.875004	1.304827	-5.140553
H	5.470928	0.435071	-4.527273
C	0.223971	-2.761634	1.097765
N	-0.232561	-1.963822	0.199375
C	-1.705091	-2.035044	0.269304
H	-2.120547	-1.024437	0.236987
O	-0.667244	-3.366867	1.914141
C	1.675309	-2.993961	1.244529
C	2.282715	-4.024506	2.032882
C	1.570937	-4.953348	2.843167
C	3.713736	-4.119986	1.980102
C	3.737401	-2.252954	0.451396
C	2.247764	-5.912795	3.562831
H	0.492950	-4.897975	2.890630
C	4.377204	-5.122876	2.734613
C	4.422277	-3.208691	1.159680
H	4.232079	-1.545964	-0.203381
C	3.659337	-6.001169	3.511882
H	1.689943	-6.613482	4.176799
H	5.460594	-5.183293	2.682549
H	5.503308	-3.274702	1.084415
H	4.172229	-6.766916	4.086282
N	2.388409	-2.141008	0.505911
Ni	1.306651	-0.667765	-0.553516
C	-1.978922	-2.782992	1.605529
H	-2.236722	-2.135094	2.446398
C	-0.481488	0.982324	-2.114846
H	-0.473001	-0.015368	-2.547014
C	0.500596	0.442207	2.215003
H	0.997467	-0.436890	2.656995
H	-0.531200	0.135667	2.004514
C	0.452308	1.549850	3.286054
H	-0.066299	2.438677	2.909589
H	-0.080794	1.211181	4.182728
H	1.455515	1.858337	3.601321
H	0.598711	1.615149	0.420741
C	0.465800	1.991436	-2.703716

H	1.375151	1.494928	-3.046440
H	0.006158	2.491503	-3.569636
H	0.727843	2.771457	-1.981395
C	-1.547898	1.363925	-1.324861
C	-2.500305	1.733467	-0.624177
Si	-3.943483	2.336428	0.315124
C	-3.406602	3.762609	1.433943
C	-4.345813	4.431338	2.243191
C	-2.079469	4.226696	1.454410
C	-3.974823	5.512387	3.044286
H	-5.383648	4.104236	2.256221
C	-1.703351	5.310332	2.251643
H	-1.333985	3.733794	0.836519
C	-2.650184	5.954555	3.049250
H	-4.717837	6.010186	3.661594
H	-0.671200	5.650391	2.249915
H	-2.359139	6.797144	3.670580
C	-4.669620	0.918510	1.337772
C	-5.243264	-0.203135	0.705326
C	-4.650276	0.936886	2.744836
C	-5.788732	-1.251737	1.448682
H	-5.270602	-0.261674	-0.378408
C	-5.188529	-0.113533	3.492290
H	-4.210566	1.782613	3.265647
C	-5.764201	-1.208483	2.845333
H	-6.236638	-2.098503	0.935547
H	-5.162753	-0.073458	4.578043
H	-6.194729	-2.020984	3.424860
C	-5.239346	3.060743	-0.896480
H	-4.711735	3.849977	-1.447064
H	-5.994450	3.568290	-0.283413
C	-5.904502	2.104278	-1.855757
C	-5.222249	1.621139	-2.984689
C	-7.219777	1.664744	-1.641199
C	-5.833425	0.727708	-3.864553
H	-4.202394	1.946904	-3.169886
C	-7.834170	0.772224	-2.521385
H	-7.767853	2.029371	-0.775744
C	-7.142905	0.298021	-3.637141
H	-5.284894	0.367723	-4.730651
H	-8.855171	0.450051	-2.334853
H	-7.619256	-0.395697	-4.323948
C	-2.317790	-2.951273	-0.780892
C	-2.218808	-2.863781	-2.169103
C	-3.043680	-3.985713	-0.178007
C	-2.869034	-3.821266	-2.950447
H	-1.615624	-2.093941	-2.636924
C	-3.693923	-4.939887	-0.960729
C	-3.604100	-4.850102	-2.351550
H	-2.791681	-3.771136	-4.032434
H	-4.257099	-5.746286	-0.497494
H	-4.101530	-5.589936	-2.972584
C	-3.014852	-3.879887	1.331092
H	-2.742080	-4.815018	1.831929
H	-3.987307	-3.568843	1.730968
Br	1.522572	-1.888887	-2.802343

^{2}TS19-*RR*

B3LYP/BSI SCF energy: -3072.448365 a.u.

M06/BSII SCF energy in solution:-3071.13238 a.u.

M06/BSII free energy in solution:-3070.207931 a.u.

C	3.595924	1.237510	0.025890
O	3.014657	0.726896	-0.955831
N	4.640976	2.090444	-0.158529
C	3.147135	0.868109	1.434462
H	3.803398	0.042622	1.744829
H	3.373168	1.691142	2.123335
C	1.673510	0.417305	1.466728
C	5.399709	2.607723	0.950621
C	6.368917	1.813084	1.572077
C	5.210194	3.929123	1.371073
C	7.134114	2.333218	2.616960
H	6.516435	0.792383	1.232796
C	5.981373	4.447079	2.411890
H	4.454617	4.538286	0.884513
C	6.942843	3.650464	3.037864
H	7.882218	1.709920	3.097909
H	5.827132	5.471822	2.736701
H	7.540096	4.054962	3.849532
C	5.122057	2.469326	-1.524276
C	5.701333	1.274699	-2.304228
C	4.062348	3.225005	-2.345139
H	5.945190	3.166325	-1.329035
C	6.278205	1.738734	-3.652311
H	4.907611	0.541587	-2.475668
H	6.481137	0.790321	-1.702976
C	4.645881	3.676625	-3.694736

H	3.205114	2.567754	-2.511979	C	-3.609425	5.743831	3.453156
H	3.707009	4.091923	-1.774296	H	-5.765051	5.823804	3.469523
C	5.228537	2.493222	-4.481946	H	-1.490052	5.421393	3.224439
H	6.653327	0.872143	-4.208585	H	-3.492253	6.573564	4.144963
H	7.142883	2.395573	-3.476590	C	-4.939331	0.679789	1.307464
H	3.867951	4.179875	-4.280283	C	-5.210198	-0.513045	0.607690
H	5.436429	4.421723	-3.521778	C	-5.307966	0.740211	2.664898
H	5.669969	2.844769	-5.422004	C	-5.834988	-1.592869	1.235556
H	4.417827	1.803195	-4.751513	H	-4.932263	-0.608235	-0.437320
C	0.395765	-2.828187	1.088133	C	-5.928847	-0.339074	3.297268
N	-0.137315	-1.851981	0.443820	H	-5.109001	1.641794	3.237110
C	-1.586450	-1.901303	0.706682	C	-6.197429	-1.507523	2.582096
H	-1.958702	-0.894916	0.914379	H	-6.033816	-2.498446	0.669669
O	-0.406743	-3.556267	1.898372	H	-6.204228	-0.265896	4.346105
C	1.830766	-3.147789	0.941008	H	-6.688806	-2.345535	3.069794
C	2.483753	-4.323440	1.437112	C	-5.238022	2.793027	-0.995251
C	1.855269	-5.337027	2.213624	H	-4.712055	3.664358	-1.404585
C	3.872424	-4.477398	1.108283	H	-6.160596	3.174742	-0.540627
C	3.775628	-2.387272	-0.093279	C	-5.567871	1.813750	-2.095061
C	2.570766	-6.434074	2.639805	C	-4.653006	1.554267	-3.128457
H	0.809873	-5.238347	2.467995	C	-6.795851	1.134335	-2.114751
C	4.577303	-5.622223	1.563938	C	-4.954766	0.646750	-4.144058
C	4.497197	-3.478653	0.321635	H	-3.696876	2.070084	-3.133784
H	4.201168	-1.608756	-0.715804	C	-7.100508	0.226388	-3.130188
C	3.940194	-6.581602	2.315454	H	-7.521426	1.323282	-1.327310
H	2.075964	-7.198304	3.231617	C	-6.180547	-0.022516	-4.149803
H	5.626943	-5.725601	1.303763	H	-4.231709	0.466338	-4.934919
H	5.540147	-3.584818	0.039397	H	-8.060167	-0.283547	-3.125053
H	4.484433	-7.455992	2.659860	H	-6.417587	-0.725835	-4.942944
N	2.470289	-2.221741	0.225539	C	-2.366194	-2.590569	-0.402790
Ni	1.330482	-0.527350	-0.371524	C	-2.442858	-2.234043	-1.748348
C	-1.713730	-2.887615	1.902252	C	-3.048966	-3.709743	0.087291
H	-1.816480	-2.412222	2.881201	C	-3.231054	-3.010107	-2.601278
C	-0.101687	1.621972	-1.312062	H	-1.874824	-1.393625	-2.130186
C	-1.358692	1.639211	-0.724225	C	-3.831819	-4.485790	-0.767845
C	-2.495300	1.709393	-0.238666	C	-3.921092	-4.126272	-2.115134
Si	-4.136041	2.154552	0.435181	H	-3.300419	-2.747258	-3.652243
C	-3.913606	3.585541	1.653266	H	-4.361311	-5.359515	-0.395841
C	-5.032373	4.257268	2.184085	H	-4.525530	-4.723230	-2.792468
C	-2.638868	4.030662	2.046608	C	-2.836340	-3.880002	1.575677
C	-4.885672	5.322441	3.074163	H	-2.564907	-4.898663	1.872178
H	-6.037217	3.946476	1.905477	H	-3.738203	-3.604676	2.136952
C	-2.486298	5.096243	2.936478	Br	1.222287	-1.546076	-2.721002
H	-1.756310	3.540069	1.646302	C	0.036281	1.701515	-2.810375

H	-0.692855	1.067210	-3.318413
H	-0.127163	2.740248	-3.139699
H	1.029796	1.384603	-3.127940
H	0.724585	1.992407	-0.715201
H	1.589366	-0.419089	2.173607
C	0.738983	1.530159	1.956650
H	0.901099	2.449134	1.371949
H	-0.303349	1.246425	1.772465
C	0.878856	1.880461	3.450908
H	0.666440	1.004372	4.075244
H	1.888991	2.223409	3.703445
H	0.179852	2.673263	3.743851

^{2}TS20-*RS*

B3LYP/BSI SCF energy: -3072.454956 a.u.

M06/BSII SCF energy in solution:-3071.139457a.u.

M06/BSII free energy in solution:-3070.216504 a.u.

C	-2.949954	1.724478	0.038417
O	-3.164983	0.649226	0.638827
N	-3.777507	2.792420	0.207977
C	-1.753896	1.836729	-0.891246
H	-2.015998	2.479430	-1.743164
H	-0.963458	2.379061	-0.351515
C	-1.261126	0.441207	-1.287212
C	-3.487497	4.064866	-0.401834
C	-4.168664	4.457595	-1.559800
C	-2.565043	4.934017	0.190068
C	-3.918940	5.707697	-2.126455
H	-4.882423	3.776240	-2.012759
C	-2.314698	6.182713	-0.382297
H	-2.051266	4.628117	1.096070
C	-2.990285	6.571287	-1.540793
H	-4.447016	6.005045	-3.027644
H	-1.596888	6.852557	0.082070
H	-2.796698	7.543699	-1.983775
C	-4.973451	2.743243	1.103823
C	-6.030730	1.726700	0.637701
C	-4.608344	2.537757	2.585465
H	-5.415227	3.741720	1.006716
C	-7.284596	1.807710	1.524343
H	-5.603334	0.721745	0.692850
H	-6.289355	1.919092	-0.410998
C	-5.867775	2.613913	3.465108
H	-4.127065	1.562598	2.704026
H	-3.885096	3.302772	2.892981
C	-6.938872	1.612021	3.008418
H	-8.014890	1.057483	1.198871
H	-7.765456	2.787763	1.389788
H	-5.595529	2.429893	4.510480
H	-6.283166	3.631760	3.424840
H	-7.840838	1.714481	3.623434
H	-6.565630	0.590774	3.162369
C	-0.564527	-3.085052	-1.043532
N	-0.092720	-2.265642	-0.172159
C	1.368594	-2.453750	-0.154232
H	1.864503	-1.479653	-0.135373
O	0.320162	-3.801699	-1.773709
C	-2.021436	-3.208282	-1.257349
C	-2.676788	-4.235212	-2.008569
C	-2.010571	-5.289558	-2.693903
C	-4.110918	-4.188365	-2.049489
C	-4.044475	-2.213611	-0.662870
C	-2.732729	-6.235671	-3.386231
H	-0.931260	-5.340184	-2.667096
C	-4.821429	-5.181136	-2.774573
C	-4.775393	-3.150149	-1.351826
H	-4.501244	-1.405664	-0.103811
C	-4.146694	-6.183663	-3.430598
H	-2.210569	-7.034510	-3.904208
H	-5.906475	-5.133909	-2.796678
H	-5.859882	-3.101742	-1.356959
H	-4.696097	-6.940811	-3.982184
N	-2.692199	-2.243138	-0.626845
Ni	-1.539321	-0.781456	0.364758
C	1.652293	-3.274547	-1.442860
H	1.974861	-2.680899	-2.301533
C	0.320183	0.777609	2.017553
H	0.234810	-0.261830	2.324018
C	-0.561980	1.762430	2.735453
H	-1.518112	1.296413	2.981142
H	-0.093099	2.079622	3.679232
H	-0.731159	2.667781	2.142860
C	1.435206	1.173680	1.308710
C	2.437924	1.545616	0.682445
Si	3.925545	2.105237	-0.213738
C	3.488810	3.640035	-1.227963
C	4.477947	4.329629	-1.955916

C	2.180803	4.155246	-1.256690
C	4.173005	5.480048	-2.685244
H	5.503447	3.965717	-1.960895
C	1.869541	5.307245	-1.982116
H	1.397581	3.647530	-0.701194
C	2.865840	5.971585	-2.699067
H	4.953931	5.993004	-3.240187
H	0.849539	5.682695	-1.986566
H	2.626822	6.867606	-3.265471
C	4.529233	0.702481	-1.331137
C	4.954867	-0.522437	-0.778339
C	4.546928	0.828790	-2.732310
C	5.387603	-1.570821	-1.592788
H	4.955542	-0.661906	0.298676
C	4.973442	-0.220128	-3.550673
H	4.221729	1.757191	-3.193359
C	5.397043	-1.422354	-2.982384
H	5.727840	-2.498745	-1.140241
H	4.976562	-0.096611	-4.630361
H	5.737148	-2.236635	-3.616811
C	5.272308	2.633787	1.043275
H	4.813095	3.425442	1.648647
H	6.074476	3.112521	0.468262
C	5.839393	1.552402	1.929852
C	5.118763	1.074259	3.036701
C	7.096690	0.987371	1.666769
C	5.636362	0.065004	3.848736
H	4.142570	1.496656	3.258386
C	7.617474	-0.021611	2.478824
H	7.673490	1.344876	0.817173
C	6.888691	-0.488931	3.573458
H	5.059828	-0.288306	4.699254
H	8.595225	-0.440244	2.255739
H	7.292309	-1.273464	4.207046
C	1.841620	-3.377930	0.960231
C	1.638051	-3.252707	2.334069
C	2.540570	-4.471835	0.435336
C	2.165998	-4.229165	3.181838
H	1.043097	-2.440450	2.737642
C	3.068969	-5.444077	1.284232
C	2.881181	-5.313566	2.662142
H	2.007128	-4.150035	4.253168
H	3.611278	-6.296025	0.881760
H	3.283068	-6.066638	3.334282
C	2.616637	-4.407420	-1.074999
H	2.338890	-5.343816	-1.570452
H	3.625678	-4.147717	-1.418909
H	-2.016467	0.000417	-1.958319
C	0.072614	0.470934	-2.032019
H	0.349832	-0.556568	-2.302270
H	0.866062	0.834075	-1.366416
C	0.094022	1.311341	-3.324291
H	1.057672	1.217731	-3.838931
H	-0.690050	0.986554	-4.019929
H	-0.061102	2.376926	-3.123568
Br	-2.053458	-1.774159	2.681341

^{2}TS21-*RS*

B3LYP/BSI SCF energy: -3072.430722 a.u.

M06/BSII SCF energy in solution:-3071.12796 a.u.

M06/BSII free energy in solution:-3070.202423 a.u.

C	3.296917	0.963294	0.128798
O	2.658047	0.358604	-0.750146
N	4.567608	1.390433	-0.110533
C	2.700850	1.183285	1.529093
H	2.951506	0.283926	2.104922
H	3.219472	2.016098	2.017970
C	1.223898	1.419874	1.516097
C	5.325724	2.139045	0.859929
C	6.188400	1.473625	1.737535
C	5.250269	3.536628	0.882886
C	6.962776	2.202852	2.641034
H	6.246283	0.389950	1.705955
C	6.024332	4.261262	1.790220
H	4.581599	4.043651	0.194153
C	6.881010	3.596393	2.670113
H	7.629088	1.681589	3.322014
H	5.958151	5.345027	1.807737
H	7.483198	4.162142	3.374668
C	5.264372	1.130702	-1.415745
C	5.426617	-0.367640	-1.727190
C	4.626769	1.896089	-2.587420
H	6.267167	1.543889	-1.257478
C	6.244326	-0.559471	-3.016048
H	4.444248	-0.831719	-1.853821
H	5.929245	-0.861484	-0.884627
C	5.436917	1.681736	-3.877589

H	3.603008	1.542802	-2.729036	C	-2.494495	5.036166	-1.508768
H	4.576784	2.964739	-2.343025	C	-2.914999	6.784725	0.617976
C	5.606692	0.188690	-4.195927	H	-3.633200	5.073025	1.693899
H	6.318824	-1.629148	-3.240018	C	-2.177054	6.387721	-1.645940
H	7.271552	-0.195103	-2.863944	H	-2.305132	4.362353	-2.341216
H	4.941939	2.197689	-4.708429	C	-2.388808	7.266755	-0.581129
H	6.428650	2.145698	-3.769502	H	-3.076127	7.461502	1.453085
H	6.216557	0.062411	-5.098392	H	-1.761024	6.754489	-2.580607
H	4.625284	-0.253740	-4.409561	H	-2.141032	8.319757	-0.684871
C	-0.589094	-2.423925	1.122950	C	-3.820608	2.206182	1.603695
N	-0.786265	-1.762965	0.033688	C	-4.951952	2.669719	2.301578
C	-2.221060	-1.899167	-0.289855	C	-2.931154	1.365088	2.296866
H	-2.613243	-0.943705	-0.642215	C	-5.182508	2.317296	3.633285
O	-1.670140	-2.909665	1.760769	H	-5.669649	3.318411	1.803583
C	0.784723	-2.683020	1.590154	C	-3.155952	1.006784	3.628875
C	1.157868	-3.573935	2.646339	H	-2.053347	0.987152	1.779268
C	0.241326	-4.248325	3.501103	C	-4.283315	1.483545	4.300605
C	2.563308	-3.786761	2.843238	H	-6.063453	2.690970	4.148411
C	3.000065	-2.285076	1.002714	H	-2.451415	0.357497	4.142760
C	0.702429	-5.080020	4.497365	H	-4.460678	1.207130	5.336365
H	-0.820497	-4.100736	3.363779	C	-5.096040	2.438480	-1.219649
C	3.001178	-4.654575	3.877487	H	-4.889597	2.837882	-2.219832
C	3.471476	-3.128741	1.978537	H	-5.869056	3.084220	-0.784659
H	3.656477	-1.789690	0.298938	C	-5.586102	1.014705	-1.309541
C	2.089299	-5.287642	4.689462	C	-5.088137	0.140690	-2.290691
H	-0.008370	-5.585622	5.143991	C	-6.539854	0.516821	-0.407998
H	4.067870	-4.809689	4.011959	C	-5.531000	-1.180084	-2.371495
H	4.538406	-3.301144	2.080993	H	-4.347754	0.503669	-2.998432
H	2.429836	-5.950508	5.479342	C	-6.987002	-0.803393	-0.486813
N	1.678302	-2.042268	0.830567	H	-6.939653	1.173139	0.360622
Ni	0.868594	-0.803882	-0.703767	C	-6.485506	-1.658895	-1.469980
C	-2.847733	-2.378918	1.043303	H	-5.128721	-1.836771	-3.137348
H	-3.258939	-1.585687	1.671891	H	-7.735756	-1.159588	0.216156
C	-0.156499	0.339894	-2.023937	H	-6.836607	-2.684467	-1.539942
H	-0.578644	-0.480792	-2.615832	C	-2.509373	-3.053048	-1.242378
C	0.743472	1.204371	-2.916564	C	-1.985683	-3.281167	-2.514517
H	1.525428	0.580955	-3.356114	C	-3.418485	-3.950456	-0.667817
H	0.171574	1.667777	-3.732990	C	-2.405691	-4.413183	-3.217990
H	1.217907	2.007707	-2.346149	H	-1.231026	-2.625757	-2.936182
C	-1.216355	1.074711	-1.403265	C	-3.837347	-5.077995	-1.373110
C	-2.137165	1.704361	-0.881595	C	-3.328518	-5.301409	-2.655127
Si	-3.494241	2.692806	-0.198469	H	-1.997146	-4.610193	-4.204555
C	-3.034908	4.528316	-0.311448	H	-4.541636	-5.778474	-0.931255
C	-3.232919	5.430371	0.748962	H	-3.641639	-6.179393	-3.213340

C	-3.836223	-3.500551	0.715179
H	-3.809491	-4.294236	1.469159
H	-4.852905	-3.087665	0.708185
C	0.683773	2.772077	1.174790
H	1.396300	3.304818	0.530389
H	-0.237462	2.665904	0.591832
C	0.386451	3.636693	2.421705
H	-0.018565	4.610103	2.125920
H	-0.353782	3.149184	3.064528
H	1.289886	3.808284	3.017971
H	0.582973	0.728956	2.056728
Br	1.850062	-2.481913	-2.480711

^{2}TS22-*SS*

B3LYP/BSI SCF energy: -3072.435817 a.u.

M06/BSII SCF energy in solution:-3071.13042 a.u.

M06/BSII free energy in solution:-3070.204639 a.u.

C	3.144450	0.362866	0.005432
O	2.552412	-0.697400	-0.273344
N	4.479314	0.480569	-0.229881
C	2.387998	1.551553	0.621371
H	3.104935	2.250513	1.064306
H	1.901134	2.072381	-0.212194
C	1.360136	1.142486	1.626784
C	5.184575	1.721629	-0.034570
C	6.067000	1.856324	1.043480
C	5.037901	2.768989	-0.950537
C	6.791246	3.037175	1.207583
H	6.174107	1.036891	1.747719
C	5.759405	3.951200	-0.777530
H	4.358648	2.653030	-1.789304
C	6.637562	4.086943	0.298941
H	7.471953	3.138319	2.047719
H	5.636942	4.763252	-1.487924
H	7.200284	5.006380	0.429797
C	5.281961	-0.626514	-0.854056
C	5.312571	-1.914791	-0.014840
C	4.870938	-0.918896	-2.307220
H	6.300678	-0.222793	-0.869256
C	6.277880	-2.933617	-0.645817
H	4.308805	-2.344971	0.011683
H	5.613916	-1.682345	1.014928
C	5.830991	-1.944038	-2.935019
H	3.852708	-1.317183	-2.319658
H	4.876948	0.012934	-2.885746
C	5.894622	-3.233709	-2.103233
H	6.275186	-3.855324	-0.052300
H	7.304760	-2.540291	-0.608081
H	5.504827	-2.167737	-3.956754
H	6.838226	-1.507833	-3.014381
H	6.612302	-3.935322	-2.545051
H	4.911494	-3.720905	-2.125081
C	-1.689873	-2.121745	0.954294
N	-1.427772	-1.612538	-0.200309
C	-2.721440	-1.371410	-0.868187
H	-2.708493	-0.394410	-1.356219
O	-2.982277	-2.184102	1.327397
C	-0.595401	-2.623603	1.804196
C	-0.744355	-3.364794	3.018072
C	-1.990818	-3.683527	3.626920
C	0.463358	-3.814278	3.649898
C	1.725112	-2.780836	1.867979
C	-2.027552	-4.402339	4.800861
H	-2.909203	-3.356394	3.160071
C	0.385729	-4.554531	4.858956
C	1.700733	-3.504350	3.035745
H	2.645081	-2.527223	1.358634
C	-0.834594	-4.842085	5.423754
H	-2.985515	-4.637875	5.254626
H	1.307678	-4.890277	5.325054
H	2.628617	-3.843810	3.485546
H	-0.888000	-5.409622	6.348057
N	0.595478	-2.338047	1.268693
Ni	0.554139	-1.274687	-0.567311
C	-3.749145	-1.464163	0.290397
H	-4.033587	-0.506241	0.730297
C	0.164928	0.000192	-2.094848
H	-0.551384	-0.616454	-2.649730
C	1.342476	0.351898	-3.011278
H	1.818780	-0.565363	-3.363952
H	1.012165	0.929785	-3.885989
H	2.098038	0.952723	-2.495982
C	-0.502971	1.127478	-1.522049
C	-1.081657	2.080117	-0.995890
Si	-1.988598	3.511960	-0.356179
C	-0.841227	5.014106	-0.224335
C	-0.391348	5.670366	-1.386271

C	-0.387995	5.502270	1.014415
C	0.470015	6.765681	-1.315967
H	-0.710822	5.320203	-2.365211
C	0.474996	6.597943	1.091769
H	-0.714392	5.022596	1.932941
C	0.905105	7.233142	-0.073761
H	0.800343	7.255048	-2.228437
H	0.809703	6.955579	2.062038
H	1.574101	8.087555	-0.015770
C	-2.728981	3.120390	1.343073
C	-2.615414	1.839984	1.912297
C	-3.450360	4.090047	2.065388
C	-3.196383	1.535033	3.146388
H	-2.062967	1.073609	1.375520
C	-4.030683	3.795003	3.300841
H	-3.557215	5.096410	1.665540
C	-3.905880	2.514334	3.843929
H	-3.096585	0.534367	3.559316
H	-4.579524	4.563069	3.839282
H	-4.358377	2.282274	4.804170
C	-3.419574	3.972349	-1.546226
H	-2.966541	4.304177	-2.487876
H	-3.929248	4.845754	-1.120838
C	-4.405884	2.860737	-1.805228
C	-4.200509	1.941082	-2.847408
C	-5.545935	2.701228	-1.001420
C	-5.106003	0.905602	-3.084068
H	-3.323342	2.044834	-3.480293
C	-6.454728	1.667906	-1.236139
H	-5.724007	3.398059	-0.186602
C	-6.240583	0.765101	-2.280247
H	-4.928507	0.211750	-3.901045
H	-7.336505	1.575220	-0.607416
H	-6.954409	-0.030386	-2.475429
C	-3.139620	-2.503739	-1.797214
C	-2.445347	-3.037185	-2.883081
C	-4.384082	-3.021104	-1.415380
C	-3.029606	-4.083339	-3.601485
H	-1.449265	-2.690015	-3.137266
C	-4.965390	-4.063382	-2.136420
C	-4.281939	-4.588395	-3.235976
H	-2.495083	-4.517079	-4.441211
H	-5.930346	-4.469616	-1.843625
H	-4.720337	-5.405263	-3.802545
C	-4.931824	-2.303340	-0.200880
H	-5.299457	-2.975179	0.581874
H	-5.756452	-1.630857	-0.468481
C	1.710034	0.851624	3.052619
H	1.320597	-0.135375	3.345138
H	2.800608	0.795290	3.169428
C	1.145875	1.900123	4.036904
H	1.401479	1.644785	5.071401
H	1.547036	2.896062	3.822648
H	0.055382	1.957294	3.960136
H	0.316367	1.173181	1.334988
Br	1.316486	-3.359727	-1.951091

^{2}IM15-S^{+}

B3LYP/BSI SCF energy: -2280.009625a.u.

M06/BSII SCF energy in solution:-2279.109263a.u.

M06/BSII free energy in solution:-2278.539611a.u

C	2.971442	0.740796	-0.361048
N	1.748434	0.490229	-0.024050
C	1.115852	1.763581	0.381461
H	0.147056	1.868047	-0.113396
O	3.350625	2.015388	-0.381423
C	3.901294	-0.370689	-0.676111
C	5.259982	-0.247371	-1.082475
C	5.939741	0.987418	-1.287070
C	5.980111	-1.477143	-1.300222
C	3.988064	-2.710144	-0.705504
C	7.256579	0.991763	-1.684475
H	5.417848	1.920415	-1.129467
C	7.339631	-1.428793	-1.707685
C	5.308522	-2.703116	-1.095390
H	3.438282	-3.626156	-0.520264
C	7.963820	-0.219240	-1.895875
H	7.765078	1.938076	-1.838973
H	7.872184	-2.361351	-1.866204
H	5.833636	-3.641509	-1.240896
H	9.002860	-0.184965	-2.207585
N	3.303085	-1.559253	-0.510231
Ni	1.347594	-1.466682	0.122582
C	2.157737	2.834000	-0.057747
H	1.907751	3.367941	-0.975666
C	-1.793509	-0.379682	-0.887464
C	-0.856502	-1.087537	-1.274567

Si	-3.217535	0.728122	-0.408590
C	-4.549338	0.444499	-1.698555
C	-5.220674	1.531432	-2.289751
C	-4.935064	-0.859819	-2.068000
C	-6.247004	1.323080	-3.212526
H	-4.943427	2.549450	-2.030279
C	-5.957816	-1.067311	-2.993079
H	-4.439714	-1.720443	-1.627556
C	-6.615184	0.023776	-3.566065
H	-6.757450	2.173745	-3.654510
H	-6.242775	-2.079293	-3.265433
H	-7.411952	-0.138559	-4.286083
C	-2.525987	2.484565	-0.478880
C	-2.458671	3.299963	0.665927
C	-2.027980	3.008594	-1.690040
C	-1.915254	4.586260	0.607148
H	-2.834578	2.937276	1.618437
C	-1.484569	4.292435	-1.753586
H	-2.075787	2.411873	-2.597946
C	-1.426719	5.083825	-0.602009
H	-1.882786	5.200067	1.502584
H	-1.121154	4.681404	-2.700772
H	-1.016879	6.088740	-0.652043
C	-3.744997	0.274176	1.360896
H	-2.890702	0.448165	2.026586
H	-4.518300	0.997007	1.650324
C	-4.263250	-1.138954	1.517734
C	-5.632848	-1.417838	1.395119
C	-3.385470	-2.202907	1.776586
C	-6.111809	-2.721607	1.530445
H	-6.329459	-0.606637	1.200105
C	-3.863027	-3.507132	1.910523
H	-2.320257	-2.014556	1.885487
C	-5.228650	-3.771734	1.787161
H	-7.176889	-2.914455	1.440347
H	-3.165979	-4.313807	2.118657
H	-5.601578	-4.785594	1.897015
C	0.217871	-1.865088	-1.701352
C	1.011415	-1.468849	-2.923814
H	1.953414	-2.017884	-2.982040
H	0.425694	-1.729236	-3.816684
H	1.207217	-0.395138	-2.958145
H	0.128346	-2.935334	-1.510113
C	1.043015	1.918882	1.888838
C	0.355829	1.120138	2.803982
C	1.806675	3.011291	2.314769
C	0.445459	1.428217	4.163437
H	-0.230152	0.265433	2.476632
C	1.889939	3.320570	3.672427
C	1.206896	2.521372	4.592549
H	-0.076624	0.814470	4.890733
H	2.478266	4.167639	4.013845
H	1.268815	2.749687	5.652122
C	2.429748	3.746040	1.146150
H	1.948193	4.717627	0.982660
H	3.501442	3.936609	1.262586
Br	0.737595	-3.316732	1.408688

[2]IM16-*R*

B3LYP/BSI SCF energy: -1880.467717a.u.

M06/BSII SCF energy in solution:-1879.646218a.u.

M06/BSII free energy in solution:-1879.053996a.u

C	2.450081	-0.028593	-0.333208
O	1.463934	-0.296369	0.396798
N	3.707643	-0.073894	0.176991
C	2.219936	0.373377	-1.785977
H	2.228122	1.472706	-1.797615
H	3.084329	0.070872	-2.392269
C	0.859564	-0.138597	-2.290769
C	4.850944	0.328385	-0.603182
C	5.140789	1.685552	-0.776951
C	5.707142	-0.641604	-1.135995
C	6.275842	2.069501	-1.492615
H	4.475279	2.431220	-0.352922
C	6.843711	-0.252937	-1.845577
H	5.471835	-1.692533	-0.998478
C	7.129075	1.102284	-2.026689
H	6.493848	3.124582	-1.628897
H	7.502641	-1.009358	-2.261439
H	8.012441	1.402815	-2.582061
C	3.978570	-0.444480	1.600594
C	3.411019	0.582080	2.597790
C	3.539621	-1.879125	1.944048
H	5.071215	-0.409183	1.677884
C	3.804774	0.214163	4.038219
H	2.321504	0.604876	2.503039
H	3.785339	1.581561	2.344703

C	3.940174	-2.231181	3.386603
H	2.455461	-1.960267	1.827797
H	3.998455	-2.581392	1.237389
C	3.374436	-1.217265	4.392412
H	3.358544	0.931981	4.735994
H	4.894684	0.303329	4.154733
H	3.594647	-3.243132	3.627401
H	5.036730	-2.248964	3.469174
H	3.698966	-1.469947	5.408704
H	2.277409	-1.276879	4.387702
C	-3.050911	0.402675	-0.590348
N	-2.267157	-0.637046	-0.837896
C	-3.112019	-1.738085	-1.302630
H	-2.703795	-2.159278	-2.229124
O	-4.372537	0.218334	-0.873156
C	-2.520185	1.618837	-0.078173
C	-3.248056	2.827242	0.240394
C	-4.639777	2.997412	0.048483
C	-2.501726	3.919227	0.792732
C	-0.486897	2.580443	0.625653
C	-5.266369	4.187825	0.388682
H	-5.219726	2.185100	-0.367918
C	-3.167949	5.116237	1.128993
C	-1.091276	3.756677	0.985739
H	0.582087	2.433811	0.754440
C	-4.532722	5.254512	0.931971
H	-6.336664	4.291084	0.232516
H	-2.587246	5.934232	1.548282
H	-0.507542	4.565210	1.414062
H	-5.031873	6.182371	1.196762
N	-1.153516	1.524756	0.103555
Ni	-0.343562	-0.155571	-0.664254
C	-4.513108	-1.080458	-1.502032
H	-4.775081	-0.905261	-2.549732
C	-3.361096	-2.815087	-0.259886
C	-2.423983	-3.639519	0.362289
C	-4.720059	-2.910661	0.058325
C	-2.860550	-4.563120	1.314430
H	-1.368526	-3.561337	0.115053
C	-5.156148	-3.832931	1.010709
C	-4.219203	-4.658007	1.637060
H	-2.142183	-5.210974	1.808778
H	-6.210177	-3.909917	1.265511
H	-4.547401	-5.378711	2.380831
C	-5.550556	-1.943823	-0.759585
H	-6.207542	-1.313928	-0.150682
H	-6.189822	-2.475275	-1.476092
H	0.476631	0.562862	-3.042441
C	0.950528	-1.539851	-2.925461
H	-0.063843	-1.916695	-3.117427
H	1.398242	-2.250931	-2.212135
C	1.736431	-1.615298	-4.248924
H	2.777355	-1.294668	-4.126996
H	1.754754	-2.635664	-4.650954
H	1.280403	-0.965587	-5.004904

^{2}IM16-*S*

B3LYP/BSI SCF energy:-1880.469266a.u.

M06/BSII SCF energy in solution:-1879.646729a.u.

M06/BSII free energy in solution:-1879.055884a.u

C	-2.489103	0.055516	-0.322822
O	-1.508738	0.402734	0.380959
N	-3.754841	0.225544	0.139635
C	-2.246761	-0.560077	-1.692539
H	-2.272059	-1.652415	-1.550651
H	-3.092684	-0.334168	-2.355017
C	-0.864776	-0.151192	-2.230118
C	-4.893411	-0.276784	-0.586855
C	-5.207566	-1.638973	-0.544837
C	-5.719509	0.608562	-1.288258
C	-6.335660	-2.114944	-1.214813
H	-4.566290	-2.316791	0.010089
C	-6.849424	0.128999	-1.951030
H	-5.465462	1.663757	-1.317445
C	-7.158280	-1.232794	-1.917365
H	-6.572325	-3.174317	-1.183588
H	-7.484843	0.818761	-2.498547
H	-8.036422	-1.604304	-2.436927
C	-4.039857	0.847490	1.470161
C	-3.539208	-0.012005	2.645347
C	-3.545456	2.301129	1.570632
H	-5.134413	0.869530	1.520649
C	-3.939208	0.619506	3.989776
H	-2.450590	-0.099025	2.583195
H	-3.956592	-1.022892	2.561247
C	-3.951299	2.916694	2.920631
H	-2.457223	2.318138	1.466890

H	-3.962615	2.887323	0.742725
C	-3.448938	2.070654	4.100216
H	-3.538860	0.016134	4.812538
H	-5.033928	0.598927	4.092987
H	-3.562019	3.939033	2.989585
H	-5.046847	2.997162	2.973996
H	-3.778015	2.510301	5.049132
H	-2.350458	2.081887	4.111814
C	3.035248	-0.400012	-0.465915
N	2.237437	0.567920	-0.891012
C	3.063784	1.573630	-1.559697
H	2.644630	1.808706	-2.545297
O	4.352960	-0.255408	-0.787534
C	2.521036	-1.508018	0.263687
C	3.262469	-2.635078	0.783800
C	4.653668	-2.827299	0.609067
C	2.530966	-3.618158	1.527483
C	0.502905	-2.343391	1.149819
C	5.293116	-3.936286	1.144413
H	5.222950	-2.096893	0.050414
C	3.210175	-4.733772	2.060027
C	1.121120	-3.433219	1.704853
H	-0.565773	-2.182979	1.262440
C	4.573789	-4.896399	1.873836
H	6.362525	-4.058714	0.996127
H	2.640286	-5.469473	2.622238
H	0.548623	-4.157225	2.275835
H	5.083109	-5.760929	2.290178
N	1.155108	-1.392099	0.441103
Ni	0.318323	0.097519	-0.622432
C	4.473422	0.909221	-1.643054
H	4.735711	0.549592	-2.642455
C	-0.357202	-1.069471	-3.345121
H	-0.259481	-2.094087	-2.955969
H	0.660236	-0.761536	-3.620376
C	-1.215484	-1.106626	-4.624187
H	-1.316569	-0.103480	-5.056620
H	-0.772506	-1.755625	-5.389294
H	-2.226486	-1.480896	-4.424795
H	-0.953903	0.874854	-2.637099
C	3.301352	2.828909	-0.736554
C	2.355039	3.742229	-0.272429
C	4.659407	2.997416	-0.445876
C	2.781230	4.829430	0.493479
H	1.300323	3.607737	-0.497783
C	5.085219	4.083436	0.320152
C	4.138995	4.997775	0.788809
H	2.055420	5.547996	0.863653
H	6.138582	4.218223	0.552739
H	4.459283	5.845891	1.387505
C	5.500782	1.907119	-1.075815
H	6.166933	1.407859	-0.364410
H	6.131495	2.305931	-1.880524

^{1}TS23-*RR*

B3LYP/BSI SCF energy: -3059.019561a.u.

M06/BSII SCF energy in solution:-3057.724782a.u.

M06/BSII free energy in solution:-3056.793971a.u

C	4.032981	0.648032	-0.394218
O	2.890168	0.128287	-0.266750
N	5.096760	-0.078591	-0.810771
C	4.162620	2.113963	-0.055549
H	4.400095	2.163207	1.016523
H	5.012351	2.571654	-0.574528
C	2.803484	2.798893	-0.320819
C	6.418426	0.500362	-0.819766
C	7.129767	0.642812	0.375458
C	7.007464	0.869717	-2.033913
C	8.422726	1.168499	0.356395
H	6.666920	0.344135	1.310984
C	8.302035	1.388912	-2.047717
H	6.444748	0.758107	-2.955653
C	9.010649	1.541008	-0.853539
H	8.970285	1.282278	1.287167
H	8.754237	1.680017	-2.991042
H	10.017125	1.948154	-0.866700
C	5.015931	-1.521357	-1.204110
C	4.707110	-2.447792	-0.016784
C	4.065992	-1.776614	-2.384836
H	6.031635	-1.750873	-1.544631
C	4.767725	-3.921397	-0.452396
H	3.710000	-2.217622	0.367672
H	5.422286	-2.260215	0.793240
C	4.131776	-3.252262	-2.814198
H	3.046015	-1.519629	-2.090065
H	4.335404	-1.122702	-3.223039
C	3.832900	-4.196203	-1.639715

H	4.509910	-4.564964	0.396191
H	5.798859	-4.177192	-0.736030
H	3.426434	-3.426449	-3.634604
H	5.132442	-3.475439	-3.211833
H	3.922621	-5.240741	-1.959797
H	2.791735	-4.053718	-1.317884
C	-0.679678	0.691281	1.776569
N	0.369786	0.136780	1.223383
C	0.288086	-1.301209	1.490410
H	0.521545	-1.871747	0.586642
O	-1.556513	-0.147912	2.377450
C	-0.854169	2.111242	1.695959
C	-1.885748	2.890279	2.325961
C	-2.832259	2.363888	3.241386
C	-1.932275	4.290733	2.029649
C	0.034951	4.007814	0.641710
C	-3.787833	3.184551	3.818578
H	-2.799855	1.311926	3.491194
C	-2.926244	5.097356	2.625565
C	-0.948203	4.820943	1.142864
H	0.804116	4.406950	-0.005883
C	-3.844943	4.555402	3.506926
H	-4.496430	2.763445	4.526406
H	-2.952099	6.156587	2.383378
H	-0.960746	5.875050	0.885370
H	-4.602927	5.185875	3.962500
N	0.121304	2.681254	0.912116
Ni	1.482133	1.442689	0.241490
C	-1.177449	-1.499982	1.967681
H	-1.869999	-1.801297	1.179188
C	-0.072907	1.048186	-1.999467
C	-1.317184	0.565949	-1.642565
C	-2.422070	0.079828	-1.343469
Si	-4.061979	-0.639434	-1.640571
C	-4.968363	0.347640	-2.987288
C	-6.366694	0.499778	-2.996463
C	-4.242776	0.925454	-4.046033
C	-7.015294	1.187417	-4.024695
H	-6.959424	0.087253	-2.184300
C	-4.885182	1.612542	-5.076789
H	-3.158230	0.849573	-4.053061
C	-6.275593	1.743439	-5.069375
H	-8.096928	1.293852	-4.006435
H	-4.301457	2.051703	-5.881800
H	-6.778199	2.281236	-5.868987
C	-5.140059	-0.699636	-0.089685
C	-6.269313	-1.538734	-0.016527
C	-4.874248	0.130719	1.012823
C	-7.099970	-1.547964	1.105613
H	-6.511651	-2.197342	-0.847963
C	-5.704378	0.129962	2.135909
H	-4.006384	0.783052	0.995478
C	-6.818007	-0.709664	2.186068
H	-7.964694	-2.205847	1.136074
H	-5.479693	0.790746	2.967913
H	-7.463359	-0.711235	3.060572
C	-3.834941	-2.422860	-2.321638
H	-3.412147	-2.310732	-3.326595
H	-4.836787	-2.849661	-2.457579
C	-2.976598	-3.346127	-1.495606
C	-1.609879	-3.505347	-1.779104
C	-3.510921	-4.073460	-0.418845
C	-0.809605	-4.362559	-1.022603
H	-1.175477	-2.955378	-2.609586
C	-2.712899	-4.931219	0.340533
H	-4.564503	-3.967557	-0.176053
C	-1.356398	-5.081703	0.043110
H	0.241014	-4.480908	-1.276151
H	-3.156170	-5.491238	1.159952
H	-0.736931	-5.757951	0.625514
C	1.105193	-1.753088	2.694923
C	2.466343	-1.573141	2.936347
C	0.291344	-2.389206	3.640960
C	3.014991	-2.059009	4.126335
H	3.081338	-1.045854	2.214773
C	0.839551	-2.873825	4.828668
C	2.207010	-2.709900	5.064761
H	4.074106	-1.924243	4.328911
H	0.211484	-3.364212	5.568266
H	2.643249	-3.080101	5.988443
C	-1.149275	-2.440201	3.177098
H	-1.867429	-2.127210	3.941876
H	-1.434454	-3.450188	2.857520
C	0.808066	0.196774	-2.886467
H	0.776005	-0.853237	-2.578889
H	0.484367	0.234754	-3.939476
H	1.849457	0.525681	-2.856101
H	0.036018	2.126099	-2.082376

C	2.687877	3.313887	-1.763801
H	2.873861	2.493181	-2.470926
H	1.655493	3.631784	-1.956881
C	3.617620	4.491175	-2.112808
H	4.676227	4.231137	-1.999649
H	3.472270	4.819287	-3.148569
H	3.421907	5.350605	-1.460709
H	2.726635	3.651998	0.364754

^{1}TS24-*SR*

B3LYP/BSI SCF energy: -3059.012357a.u.

M06/BSII SCF energy in solution:-3057.726353a.u.

M06/BSII free energy in solution:-3056.792429a.u

C	3.937869	0.807072	0.196053
O	2.962530	0.017012	0.255780
N	5.003896	0.557956	-0.607969
C	3.894459	2.047080	1.054794
H	4.500366	1.829688	1.945532
H	4.404503	2.877094	0.553803
C	2.431858	2.393157	1.442841
C	6.169836	1.405204	-0.562987
C	7.095805	1.273982	0.476798
C	6.399814	2.326674	-1.590903
C	8.241850	2.070803	0.493258
H	6.913824	0.550663	1.265863
C	7.549096	3.117076	-1.572300
H	5.673408	2.423936	-2.392031
C	8.470663	2.992026	-0.530107
H	8.956456	1.967605	1.304383
H	7.721118	3.834007	-2.369532
H	9.363285	3.610113	-0.516298
C	5.089607	-0.619806	-1.525950
C	5.232189	-1.952907	-0.773192
C	3.956848	-0.669900	-2.565190
H	6.024084	-0.451767	-2.073105
C	5.448875	-3.113051	-1.759258
H	4.326052	-2.133057	-0.189285
H	6.070465	-1.889110	-0.068831
C	4.184870	-1.833077	-3.545575
H	2.999573	-0.795768	-2.052911
H	3.910072	0.282655	-3.105976
C	4.330386	-3.173998	-2.810508
H	5.507858	-4.057876	-1.207224
H	6.416225	-2.986623	-2.266568
H	3.356104	-1.876217	-4.261488
H	5.093767	-1.643276	-4.134777
H	4.527149	-3.979898	-3.527131
H	3.381851	-3.420252	-2.313222
C	-0.791173	-0.818640	1.808027
N	0.329839	-0.886878	1.147729
C	0.371869	-2.204275	0.507830
H	0.719939	-2.114258	-0.525420
O	-1.628716	-1.873372	1.694721
C	-1.056802	0.359303	2.590162
C	-2.176705	0.560650	3.467119
C	-3.179387	-0.413862	3.713899
C	-2.253333	1.804082	4.168958
C	-0.179131	2.460509	3.105878
C	-4.196456	-0.160358	4.616416
H	-3.139420	-1.362048	3.196041
C	-3.315811	2.040301	5.070475
C	-1.222448	2.757383	3.937507
H	0.615922	3.174760	2.957189
C	-4.274796	1.072674	5.295619
H	-4.942556	-0.926715	4.806539
H	-3.358260	2.994245	5.589242
H	-1.243913	3.714422	4.449397
H	-5.084171	1.256405	5.995998
N	-0.043337	1.269285	2.453447
Ni	1.300525	0.823998	1.097879
C	-1.093308	-2.709480	0.615494
H	-1.704627	-2.521798	-0.268379
C	0.486004	1.019030	-1.075123
H	0.959156	0.070514	-1.339297
C	1.036245	2.176609	-1.901772
H	2.124783	2.253028	-1.806187
H	0.818457	2.054189	-2.974948
H	0.605128	3.133776	-1.595905
C	-0.907982	0.910837	-1.025927
C	-2.144246	0.804133	-0.951941
Si	-3.725880	0.662831	-1.828609
C	-4.272909	2.388151	-2.406834
C	-5.623284	2.687716	-2.665050
C	-3.325447	3.402440	-2.636337
C	-6.011010	3.940592	-3.144199
H	-6.388297	1.938446	-2.476958
C	-3.706763	4.657359	-3.114469

H	-2.277591	3.207264	-2.423982
C	-5.051880	4.928927	-3.372172
H	-7.061424	4.147058	-3.333177
H	-2.955144	5.425044	-3.280689
H	-5.351517	5.906075	-3.742016
C	-5.114892	-0.093991	-0.790137
C	-6.250307	-0.675397	-1.387685
C	-5.081980	-0.032903	0.613766
C	-7.308507	-1.168792	-0.621824
H	-6.318858	-0.745476	-2.471033
C	-6.138317	-0.520575	1.386019
H	-4.217171	0.401690	1.107088
C	-7.254384	-1.089769	0.770709
H	-8.172289	-1.612107	-1.110668
H	-6.086018	-0.453019	2.468642
H	-8.076533	-1.469863	1.371537
C	-3.506201	-0.400603	-3.421918
H	-2.918310	0.219458	-4.108356
H	-4.492550	-0.521094	-3.887219
C	-2.841775	-1.740395	-3.240514
C	-1.452883	-1.881753	-3.402582
C	-3.580308	-2.887617	-2.904754
C	-0.829189	-3.121021	-3.251959
H	-0.859454	-1.007894	-3.657266
C	-2.959567	-4.128635	-2.750706
H	-4.654910	-2.806474	-2.767269
C	-1.579494	-4.254429	-2.926857
H	0.244488	-3.204530	-3.402492
H	-3.558669	-5.000839	-2.502158
H	-1.097593	-5.223058	-2.825483
C	1.154707	-3.239944	1.303127
C	2.470352	-3.166388	1.758048
C	0.353761	-4.348966	1.601854
C	2.991956	-4.235258	2.491868
H	3.062523	-2.278192	1.564039
C	0.876110	-5.415388	2.334038
C	2.201673	-5.355462	2.772044
H	4.014788	-4.192825	2.856035
H	0.259015	-6.277977	2.572700
H	2.617143	-6.178808	3.346478
C	-1.044224	-4.179959	1.045020
H	-1.834026	-4.410936	1.767204
H	-1.211637	-4.817389	0.167851
H	2.401421	2.450695	2.538190
C	2.011372	3.758001	0.874879
H	0.920423	3.862322	0.904049
H	2.280204	3.814389	-0.184650
C	2.642952	4.956781	1.606230
H	3.738411	4.919631	1.575937
H	2.333684	5.908004	1.158040
H	2.350848	4.977009	2.663630

^{1}TS25-*SR*

B3LYP/BSI SCF energy: -3059.017539a.u.

M06/BSII SCF energy in solution:-3057.721457a.u.

M06/BSII free energy in solution:-3056.796295a.u

C	-3.514686	1.075274	0.182079
O	-2.990424	0.281669	0.999967
N	-4.636398	1.765998	0.518585
C	-2.905987	1.241979	-1.203945
H	-3.493156	0.587946	-1.867438
H	-3.090113	2.260800	-1.567307
C	-1.431785	0.804592	-1.240222
C	-5.309401	2.616525	-0.431541
C	-6.151505	2.060789	-1.400105
C	-5.165231	4.005749	-0.346324
C	-6.834838	2.892124	-2.288845
H	-6.263102	0.982275	-1.454487
C	-5.854306	4.832824	-1.233666
H	-4.506942	4.427744	0.406924
C	-6.688165	4.277945	-2.207053
H	-7.482999	2.455492	-3.042802
H	-5.734794	5.910136	-1.167579
H	-7.220820	4.923289	-2.899058
C	-5.299728	1.613075	1.850508
C	-5.872693	0.200607	2.067150
C	-4.407756	2.056099	3.023734
H	-6.146352	2.307374	1.803187
C	-6.630678	0.120954	3.402934
H	-5.051914	-0.522624	2.059971
H	-6.541635	-0.052342	1.235570
C	-5.177086	1.966535	4.352520
H	-3.523739	1.414038	3.062712
H	-4.060383	3.082267	2.852330
C	-5.747113	0.558519	4.580615
H	-6.996574	-0.900517	3.557474
H	-7.519794	0.766595	3.359294

H	-4.515969	2.250856	5.179365	C	5.289615	1.697836	-2.419840
H	-6.001327	2.694489	4.350174	C	3.115178	0.682738	-2.205526
H	-6.318875	0.527894	5.515538	C	5.500513	1.005363	-3.613324
H	-4.918324	-0.153732	4.694969	H	6.069254	2.365893	-2.059231
C	0.047829	-2.931662	-0.613311	C	3.320877	-0.012383	-3.399950
N	0.266376	-1.921537	0.225119	H	2.179761	0.551060	-1.668693
C	1.663278	-2.033168	0.656591	C	4.514988	0.146581	-4.105018
H	2.127219	-1.045399	0.730425	H	6.431389	1.135599	-4.158700
O	1.154332	-3.651394	-0.955186	H	2.545819	-0.672197	-3.780559
C	-1.252716	-3.201698	-1.116215	H	4.676514	-0.393380	-5.033959
C	-1.644454	-4.275222	-2.004311	C	5.279794	2.205664	1.126797
C	-0.748679	-5.216240	-2.564436	H	5.079612	2.810403	2.019726
C	-3.036644	-4.388965	-2.325169	H	6.171607	2.640245	0.658403
C	-3.471321	-2.431498	-0.961467	C	5.535096	0.768074	1.509288
C	-1.205473	-6.224273	-3.401842	C	4.828700	0.162494	2.561134
H	0.305200	-5.146292	-2.331544	C	6.477791	-0.006043	0.815771
C	-3.469979	-5.426204	-3.177491	C	5.058985	-1.168326	2.911186
C	-3.947956	-3.436224	-1.764692	H	4.093149	0.743964	3.110840
H	-4.141402	-1.693149	-0.530057	C	6.714086	-1.336414	1.165305
C	-2.570268	-6.334606	-3.712198	H	7.034683	0.440627	-0.003782
H	-0.496616	-6.935185	-3.817422	C	6.006394	-1.923737	2.215702
H	-4.529595	-5.499940	-3.409870	H	4.496632	-1.617895	3.724222
H	-5.009742	-3.513955	-1.976345	H	7.456882	-1.911586	0.618843
H	-2.919283	-7.128168	-4.367006	H	6.189921	-2.957436	2.493832
N	-2.168614	-2.288380	-0.631618	C	1.859475	-2.849978	1.932182
Ni	-1.256382	-0.645638	0.163189	C	1.270397	-2.667053	3.181866
C	2.309265	-2.939737	-0.422514	C	2.749614	-3.909698	1.716695
H	2.775928	-2.394974	-1.249054	C	1.596697	-3.539765	4.223997
C	-0.045783	1.391691	1.798796	H	0.551951	-1.869895	3.339460
C	1.171878	1.679259	1.215942	C	3.073031	-4.783642	2.754227
C	2.264038	1.943960	0.695397	C	2.496203	-4.590186	4.012457
Si	3.825932	2.495910	-0.080607	H	1.141521	-3.407867	5.201779
C	3.717176	4.355717	-0.413091	H	3.756997	-5.612171	2.587154
C	3.705072	4.879760	-1.717926	H	2.738011	-5.266864	4.827421
C	3.640461	5.266537	0.658286	C	3.251508	-3.915438	0.289354
C	3.623596	6.255708	-1.944903	H	3.235469	-4.904130	-0.180623
H	3.760152	4.206524	-2.568774	H	4.280820	-3.538233	0.234379
C	3.559352	6.641336	0.437529	C	-0.170427	0.876184	3.206405
H	3.636089	4.900532	1.682750	H	0.739600	0.368288	3.532767
C	3.551687	7.139306	-0.867635	H	-0.356309	1.706035	3.905127
H	3.615639	6.636005	-2.962882	H	-1.017845	0.188445	3.299939
H	3.501764	7.323825	1.281291	H	-0.934016	1.818148	1.345750
H	3.488977	8.209959	-1.042358	H	-0.801475	1.651791	-0.933549
C	4.093910	1.551192	-1.690573	C	-0.994024	0.353347	-2.636266

H	0.028232	-0.043339	-2.579986
H	-1.620051	-0.489720	-2.961729
C	-1.025310	1.447100	-3.721129
H	-2.037916	1.839030	-3.872832
H	-0.383057	2.291496	-3.443921
H	-0.674791	1.064600	-4.687254

^{1}TS26-*SS*

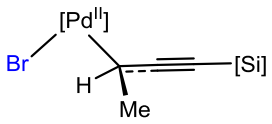
B3LYP/BSI SCF energy: -3059.018661a.u.

M06/BSII SCF energy in solution:-3057.721423a.u.

M06/BSII free energy in solution:-3056.79632a.u

C	3.589830	1.034594	-0.218709
O	3.024910	0.080519	-0.805077
N	4.827916	1.440182	-0.607317
C	2.897832	1.717645	0.952462
H	3.372589	1.315548	1.861086
H	3.150504	2.785959	0.953148
C	1.389059	1.413691	0.982833
C	5.531718	2.482500	0.097695
C	6.218165	2.191807	1.281135
C	5.578165	3.775135	-0.435827
C	6.936494	3.194271	1.934541
H	6.183544	1.184229	1.684003
C	6.300967	4.773026	0.218551
H	5.040930	3.991171	-1.354282
C	6.979549	4.485115	1.404831
H	7.463661	2.964521	2.855705
H	6.329823	5.776109	-0.196508
H	7.539249	5.263879	1.914083
C	5.587291	0.758055	-1.700786
C	5.959812	-0.692961	-1.345161
C	4.893652	0.849869	-3.071094
H	6.519238	1.330797	-1.768484
C	6.830702	-1.315705	-2.449329
H	5.043230	-1.276577	-1.217760
H	6.494135	-0.707953	-0.387512
C	5.776319	0.224073	-4.164305
H	3.935793	0.324773	-3.022667
H	4.682188	1.900409	-3.305280
C	6.150926	-1.226240	-3.823680
H	7.051069	-2.359527	-2.198404
H	7.798271	-0.794526	-2.490354
H	5.255581	0.269080	-5.127838
H	6.694647	0.818076	-4.279471
H	6.806810	-1.640193	-4.598577
H	5.241684	-1.843066	-3.818234
C	-0.319105	-2.605716	0.840526
N	-0.315274	-1.697493	-0.133903
C	-1.474909	-1.989323	-0.984774
H	-1.974451	-1.064185	-1.286230
O	-1.423319	-3.402999	0.886697
C	0.758806	-2.708386	1.758240
C	0.866812	-3.617657	2.880254
C	-0.138766	-4.535444	3.265640
C	2.078498	-3.579537	3.644579
C	2.881075	-1.801980	2.205222
C	0.043685	-5.378886	4.352493
H	-1.059271	-4.579599	2.699789
C	2.234759	-4.451409	4.743168
C	3.096180	-2.647228	3.265166
H	3.637165	-1.080015	1.910361
C	1.233516	-5.341250	5.097033
H	-0.744110	-6.075563	4.625581
H	3.160618	-4.410304	5.311684
H	4.029322	-2.608896	3.818096
H	1.368482	-6.006177	5.945541
N	1.757704	-1.803846	1.456767
Ni	1.166265	-0.386573	0.086865
C	-2.370302	-2.891881	-0.094449
H	-3.150515	-2.352314	0.449426
C	-0.116786	1.218036	-2.113173
H	0.006633	0.196474	-2.463700
C	0.804719	1.496300	2.397168
H	1.306362	0.764163	3.046431
H	-0.249656	1.193625	2.366421
C	0.883946	2.885793	3.058264
H	0.363952	3.636873	2.451633
H	0.422984	2.883601	4.053299
H	1.921302	3.220256	3.179248
H	0.873875	2.152898	0.355146
C	0.877634	2.247322	-2.571637
H	1.887327	1.829961	-2.586360
H	0.645936	2.587028	-3.592505
H	0.865644	3.128520	-1.924125
C	-1.317409	1.559708	-1.528883
C	-2.391680	1.873351	-0.999303
Si	-3.972137	2.331003	-0.204793

C	-3.954538	4.176635	0.204137
C	-3.952243	4.643734	1.530382
C	-3.934396	5.135096	-0.827378
C	-3.933237	6.010942	1.816077
H	-3.965009	3.932371	2.351295
C	-3.914982	6.501513	-0.547890
H	-3.925977	4.814268	-1.866912
C	-3.915462	6.942428	0.777572
H	-3.930777	6.347146	2.849441
H	-3.899310	7.221629	-1.361651
H	-3.900861	8.006322	0.998199
C	-4.206631	1.296423	1.354351
C	-5.390396	1.394767	2.111236
C	-3.220592	0.395449	1.795119
C	-5.581846	0.625794	3.260457
H	-6.175897	2.084559	1.808470
C	-3.408351	-0.378664	2.943476
H	-2.294872	0.295723	1.235399
C	-4.589954	-0.264603	3.677715
H	-6.503020	0.721190	3.829115
H	-2.631327	-1.068470	3.261225
H	-4.737195	-0.865063	4.571196
C	-5.405937	2.010140	-1.432391
H	-5.270162	2.696353	-2.276901
H	-6.329705	2.321236	-0.928896
C	-5.525874	0.588283	-1.923159
C	-4.811006	0.150197	-3.049923
C	-6.343734	-0.339197	-1.259155
C	-4.917928	-1.164771	-3.504095
H	-4.168930	0.850774	-3.577354
C	-6.455024	-1.654655	-1.711900
H	-6.900940	-0.024378	-0.380821
C	-5.744647	-2.073643	-2.838956
H	-4.359064	-1.478782	-4.381260
H	-7.104584	-2.350116	-1.187067
H	-5.840256	-3.093280	-3.201447
C	-1.167985	-2.888157	-2.179504
C	-0.229758	-2.699733	-3.193484
C	-1.970388	-4.036121	-2.162076
C	-0.109836	-3.661457	-4.200058
H	0.418894	-1.828290	-3.194895
C	-1.850351	-4.997631	-3.165302
C	-0.917790	-4.803120	-4.187356
H	0.620040	-3.525406	-4.993275
H	-2.467006	-5.892923	-3.149844
H	-0.813253	-5.547330	-4.972029
C	-2.903566	-4.031684	-0.970451
H	-2.920833	-4.979956	-0.423360
H	-3.933369	-3.806598	-1.274774



B3LYP/BSI SCF energy: -2237.178891a.u.

M06/BSII SCF energy in solution:-2236.215765a.u.

M06/BSII free energy in solution:-2235.642316a.u.

C	2.908036	1.063294	-0.272048
N	1.762484	0.460325	-0.270149
C	0.735169	1.492540	-0.018652
H	-0.138549	1.308538	-0.644408
O	2.890162	2.407049	-0.227669
C	4.177381	0.312281	-0.244523
C	5.485634	0.877045	-0.369692
C	5.760428	2.254147	-0.606887
C	6.592155	-0.031827	-0.257160
C	5.021192	-1.845734	0.031665
C	7.059455	2.696316	-0.713594
H	4.940910	2.951957	-0.701055
C	7.919389	0.463045	-0.367442
C	6.320904	-1.403526	-0.047412
H	4.758784	-2.889698	0.166721
C	8.148847	1.799421	-0.590316
H	7.252641	3.749197	-0.895457
H	8.745189	-0.236553	-0.276585
H	7.139641	-2.110441	0.044654
H	9.165037	2.172338	-0.675915
N	3.969635	-0.997073	-0.059779
C	1.478248	2.817825	-0.317414
H	1.331005	3.215845	-1.324376
C	-2.032252	-0.439771	-0.498462
C	-1.098710	-1.207892	-0.706107
Si	-3.478213	0.646649	-0.254286
C	-4.832124	0.157168	-1.474765
C	-5.847864	1.068806	-1.820157
C	-4.888586	-1.131930	-2.033708
C	-6.882497	0.706429	-2.683913

H	-5.827581	2.080320	-1.420287
C	-5.919885	-1.498144	-2.900566
H	-4.113420	-1.853647	-1.791540
C	-6.919646	-0.579993	-3.226157
H	-7.654854	1.427602	-2.937928
H	-5.941871	-2.499465	-3.322043
H	-7.722118	-0.863692	-3.901767
C	-2.979457	2.445610	-0.605436
C	-2.970284	3.439019	0.389696
C	-2.600433	2.827019	-1.908372
C	-2.604937	4.757308	0.099742
H	-3.252587	3.190296	1.408979
C	-2.226979	4.138854	-2.203922
H	-2.606234	2.089280	-2.707514
C	-2.231003	5.109910	-1.198207
H	-2.618460	5.507508	0.886066
H	-1.945042	4.407056	-3.218723
H	-1.953751	6.135338	-1.427905
C	-4.097620	0.517786	1.547244
H	-3.275983	0.832711	2.201565
H	-4.903973	1.251685	1.670819
C	-4.581561	-0.859508	1.936311
C	-5.921402	-1.233231	1.749800
C	-3.699454	-1.808947	2.474694
C	-6.365312	-2.510565	2.093497
H	-6.621859	-0.515093	1.331052
C	-4.140342	-3.087406	2.818105
H	-2.657601	-1.540484	2.626690
C	-5.476655	-3.444404	2.629031
H	-7.408466	-2.775134	1.942675
H	-3.437929	-3.803892	3.235185
H	-5.821677	-4.438752	2.897608
C	-0.057643	-2.148444	-1.020594
C	0.076026	-2.378727	-2.538102
H	0.820026	-3.151896	-2.739615
H	-0.884815	-2.704445	-2.959571
H	0.371231	-1.462270	-3.059341
H	-0.261467	-3.093122	-0.508798
C	0.387449	1.616807	1.458221
C	-0.094964	0.631728	2.320776
C	0.638438	2.915051	1.919200
C	-0.329855	0.967032	3.657637
H	-0.277652	-0.373772	1.958173
C	0.398900	3.247963	3.252037
C	-0.087005	2.265838	4.118831
H	-0.699389	0.211058	4.344249
H	0.592923	4.253688	3.615720
H	-0.272204	2.510776	5.160806
C	1.142181	3.805046	0.804115
H	0.357115	4.489244	0.458996
H	2.012018	4.411667	1.076430
Br	2.321014	-4.103990	-0.159702
Pd	1.844438	-1.641213	-0.332503

[Pd^{I}]—Br

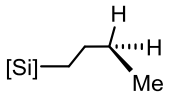
B3LYP/BSI SCF energy: -1058.577689a.u.

M06/BSII SCF energy in solution:-1058.096845a.u.

M06/BSII free energy in solution:-1057.86117a.u.

C	0.862684	0.730244	-0.645194
N	-0.353553	0.331758	-0.770339
C	-1.162416	1.464108	-1.250125
H	-1.732399	1.142298	-2.126878
O	1.139623	1.999093	-1.014972
C	1.904188	-0.172766	-0.111813
C	3.293106	0.144265	0.028518
C	3.883491	1.388136	-0.335587
C	4.142079	-0.877134	0.575222
C	2.216660	-2.320380	0.750363
C	5.233388	1.596941	-0.161500
H	3.264407	2.169852	-0.751011
C	5.528906	-0.625074	0.741625
C	3.561781	-2.117543	0.932173
H	1.737298	-3.257347	1.010100
C	6.065327	0.588324	0.380809
H	5.666726	2.551257	-0.445091
H	6.154971	-1.409236	1.157305
H	4.179561	-2.907299	1.347869
H	7.126900	0.776578	0.509208
N	1.398009	-1.365897	0.237684
C	-0.102768	2.570217	-1.550505
H	0.079230	2.748841	-2.612441
C	-2.037305	2.067815	-0.168823
C	-3.089496	1.457924	0.515353
C	-1.652481	3.383363	0.111087
C	-3.756703	2.194153	1.497052
H	-3.372538	0.430795	0.300990

C	-2.324819	4.115467	1.090294
C	-3.377496	3.511230	1.781815
H	-4.575725	1.737431	2.044490
H	-2.036392	5.139127	1.314820
H	-3.906990	4.069926	2.548431
C	-0.511492	3.836420	-0.776379
H	-0.831035	4.618923	-1.475855
H	0.341106	4.239069	-0.218924
Br	-3.060792	-2.575330	-0.220124
Pd	-0.727291	-1.701776	-0.075579



B3LYP/BSI SCF energy: -1142.345156a.u.

M06/BSII SCF energy in solution:-1141.861166a.u.

M06/BSII free energy in solution:-1141.51922a.u.

Si	-0.503934	-0.318068	0.108436
C	-0.379605	1.573304	0.034983
C	0.847005	2.239769	0.237174
C	-1.508943	2.367877	-0.239733
C	0.938783	3.630849	0.170016
H	1.747717	1.668971	0.441341
C	-1.422303	3.760285	-0.307017
H	-2.472235	1.893237	-0.402957
C	-0.197474	4.395744	-0.101394
H	1.897373	4.117279	0.330104
H	-2.311806	4.347247	-0.520098
H	-0.127595	5.478955	-0.152549
C	-2.306761	-0.827459	-0.202972
C	-2.727290	-1.396992	-1.419261
C	-3.286891	-0.640896	0.792108
C	-4.057661	-1.764762	-1.633659
H	-2.010307	-1.560999	-2.219174
C	-4.618600	-1.003219	0.585269
H	-3.011759	-0.200519	1.747892
C	-5.007406	-1.568898	-0.630634
H	-4.351086	-2.204174	-2.583285
H	-5.351317	-0.846477	1.372368
H	-6.042766	-1.854885	-0.794250
C	0.544698	-1.119280	-1.288010
H	0.230429	-2.169741	-1.337470
H	0.232045	-0.657189	-2.232302
C	2.047029	-1.046656	-1.156766
C	2.774800	0.022049	-1.704709
C	2.761471	-2.051821	-0.484539
C	4.162978	0.089515	-1.575661
H	2.245307	0.806767	-2.238548
C	4.149279	-1.987040	-0.353862
H	2.222032	-2.898636	-0.066643
C	4.857615	-0.913509	-0.897289
H	4.702660	0.925619	-2.012278
H	4.677881	-2.780325	0.167831
H	5.938228	-0.863542	-0.800063
C	1.225685	-0.405412	2.526743
H	2.114759	-0.516247	1.894791
H	1.079719	0.672422	2.665677
C	-0.004361	-1.001616	1.815462
H	0.131202	-2.087188	1.696776
H	-0.878488	-0.895695	2.473319
C	1.493180	-1.057873	3.888452
H	1.681871	-2.132559	3.782544
H	2.365309	-0.613889	4.380911
H	0.634552	-0.939232	4.559756

^{1}LNi^{0}

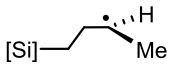
B3LYP/BSI SCF energy: -1088.146756 a.u.

M06/BSII SCF energy in solution: -1087.73277 a.u.

M06/BSII free energy in solution:-1087.493675 a.u.

C	0.152725	-0.075914	0.691201
N	-0.817810	0.801101	0.944163
C	-2.022094	0.062837	1.318565
H	-2.470411	0.501807	2.218266
C	-1.499641	-1.386645	1.552516
H	-1.375332	-1.649168	2.607322
O	-0.178591	-1.371059	0.954128
C	-2.427702	-2.350889	0.792290
H	-3.065326	-2.899938	1.496921
H	-1.842510	-3.094951	0.242160
C	-3.250658	-1.448410	-0.102659
C	-4.144245	-1.812359	-1.110751
C	-3.047624	-0.099139	0.207147
C	-4.834329	-0.813171	-1.801004
H	-4.302807	-2.858614	-1.359452
C	-3.740758	0.899210	-0.476533
C	-4.635832	0.535730	-1.484951

H	-5.530835	-1.084926	-2.589099
H	-3.586061	1.947434	-0.232554
H	-5.180488	1.303021	-2.027689
C	1.429897	0.303194	0.184996
C	2.558079	-0.574234	-0.062316
C	2.550756	-1.971468	0.161123
C	3.763789	0.019083	-0.565159
C	2.677480	2.186109	-0.536023
C	3.674142	-2.745545	-0.097525
H	1.655663	-2.443954	0.539585
C	4.887406	-0.794433	-0.819502
C	3.794080	1.432348	-0.794585
H	2.678792	3.259528	-0.706543
C	4.849983	-2.160823	-0.590367
H	3.636256	-3.815866	0.085340
H	5.791003	-0.325426	-1.200809
H	4.695869	1.902322	-1.172173
H	5.724415	-2.773365	-0.790801
N	1.520987	1.670227	-0.065231
Ni	-0.169088	2.516729	0.368043

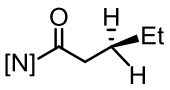


B3LYP/BSI SCF energy: -1141.671322a.u.

M06/BSII SCF energy in solution:-1141.190057a.u.

M06/BSII free energy in solution:-1140.864516a.u.

Si	-0.501710	-0.325044	0.136100
C	-0.350975	1.562374	0.025739
C	0.885462	2.215054	0.212820
C	-1.470155	2.367602	-0.259118
C	0.996154	3.603424	0.121973
H	1.779422	1.635540	0.422683
C	-1.364524	3.757324	-0.350062
H	-2.440324	1.903569	-0.411627
C	-0.130417	4.379174	-0.158734
H	1.961905	4.079157	0.270638
H	-2.246488	4.352879	-0.570426
H	-0.045846	5.460294	-0.228322
C	-2.306566	-0.820707	-0.182179
C	-2.720762	-1.417501	-1.387526
C	-3.294981	-0.595860	0.796764
C	-4.053187	-1.774829	-1.606757
H	-1.997391	-1.611795	-2.174831
C	-4.628748	-0.947337	0.584667
H	-3.024850	-0.133864	1.743686
C	-5.011262	-1.540602	-0.620016
H	-4.341708	-2.236076	-2.547472
H	-5.367877	-0.760755	1.359135
H	-6.048243	-1.818314	-0.787525
C	0.553142	-1.170263	-1.228750
H	0.236869	-2.221189	-1.247551
H	0.245775	-0.736930	-2.188276
C	2.055162	-1.096089	-1.093442
C	2.788879	-0.057590	-1.689134
C	2.762960	-2.069629	-0.369532
C	4.176794	0.011335	-1.557497
H	2.264228	0.702174	-2.262431
C	4.150453	-2.003369	-0.236129
H	2.218680	-2.893346	0.086363
C	4.864847	-0.960013	-0.828213
H	4.721362	0.823424	-2.031727
H	4.673863	-2.771832	0.326254
H	5.945204	-0.909078	-0.728800
C	1.193105	-0.371773	2.582140
H	2.087813	-0.512966	1.949912
H	1.076671	0.716422	2.671437
C	-0.035591	-0.974175	1.866380
H	0.093458	-2.063051	1.778260
H	-0.914020	-0.842569	2.511718
C	1.432965	-0.960958	3.932494
H	2.017776	-0.430303	4.677417
H	1.171133	-1.994327	4.140769



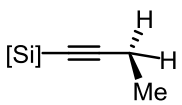
B3LYP/BSI SCF energy: -792.895972a.u.

M06/BSII SCF energy in solution:-792.497868a.u.

M06/BSII free energy in solution:-792.155236a.u.

C	0.831569	-0.599964	-0.446709
O	0.692739	-1.808439	-0.624441
N	-0.231850	0.210941	-0.103089
C	2.198130	0.076235	-0.602921
H	2.369457	0.762669	0.234631
H	2.157633	0.713061	-1.495860

C	3.347665	-0.929898	-0.725414
H	3.090050	-1.668173	-1.492444
C	3.680548	-1.657209	0.584082
H	2.789213	-2.194415	0.925562
H	3.921378	-0.915662	1.359367
C	4.847300	-2.638720	0.437876
H	4.619013	-3.414200	-0.301956
H	5.069900	-3.140186	1.385665
H	5.760512	-2.127882	0.109956
C	-0.101420	1.636071	0.023170
C	0.012534	2.221196	1.290596
C	-0.132574	2.454267	-1.112830
C	0.099684	3.608009	1.418245
H	0.037368	1.581120	2.167392
C	-0.039849	3.840818	-0.982590
H	-0.230231	1.995667	-2.092342
C	0.075849	4.420203	0.282392
H	0.190223	4.053360	2.404782
H	-0.062341	4.467680	-1.869346
H	0.146234	5.499264	0.382930
C	-1.601206	-0.352329	0.068714
C	-1.688143	-1.377530	1.214479
C	-2.175888	-0.919053	-1.243208
H	-2.215850	0.510342	0.352758
C	-3.134926	-1.863450	1.402493
H	-1.034258	-2.222256	0.981515
H	-1.315898	-0.921459	2.140224
C	-3.618189	-1.412686	-1.043191
H	-1.537913	-1.742802	-1.575897
H	-2.143523	-0.144041	-2.018909
C	-3.711828	-2.435605	0.098899
H	-3.171467	-2.615497	2.199479
H	-3.764020	-1.025427	1.737221
H	-3.993254	-1.847174	-1.977429
H	-4.270927	-0.557116	-0.815336
H	-4.753526	-2.744620	0.247621
H	-3.151104	-3.338890	-0.178030
H	4.238837	-0.394568	-1.078916



B3LYP/BSI SCF energy: -1179.193952a.u.

M06/BSII SCF energy in solution:-1178.696819a.u.

M06/BSII free energy in solution:-1178.37642a.u.

C	0.042830	1.629752	0.708752
C	0.482902	2.591847	1.313855
Si	-0.597673	0.172923	-0.196327
C	-0.308971	-1.372073	0.850303
C	0.899986	-1.549595	1.550385
C	-1.272029	-2.394131	0.934642
C	1.139456	-2.704098	2.296382
H	1.660362	-0.774127	1.517994
C	-1.035861	-3.551507	1.679492
H	-2.223978	-2.282814	0.422084
C	0.171835	-3.709107	2.360856
H	2.079664	-2.818623	2.829162
H	-1.796463	-4.325953	1.731933
H	0.356553	-4.607705	2.943367
C	-2.438974	0.421968	-0.533946
C	-3.116637	-0.340710	-1.504526
C	-3.184858	1.372782	0.186243
C	-4.481703	-0.167558	-1.741021
H	-2.577699	-1.082347	-2.090194
C	-4.549549	1.550944	-0.046908
H	-2.687273	1.985449	0.933206
C	-5.201479	0.779899	-1.010747
H	-4.981461	-0.768526	-2.495970
H	-5.103444	2.292855	0.522084
H	-6.263455	0.918129	-1.194349
C	0.310737	0.037831	-1.875521
H	0.032906	0.927166	-2.453775
H	-0.110640	-0.824711	-2.406477
C	1.812076	-0.087119	-1.786716
C	2.434014	-1.344015	-1.728762
C	2.626993	1.055389	-1.742605
C	3.821882	-1.456175	-1.634107
H	1.823234	-2.242540	-1.761184
C	4.014480	0.945903	-1.648128
H	2.164787	2.038010	-1.785735
C	4.619485	-0.311424	-1.593259
H	4.279630	-2.440991	-1.595577
H	4.624494	1.845090	-1.623087
H	5.700133	-0.397828	-1.524234
C	1.040448	3.729759	2.043819
H	1.091490	4.597438	1.372754
C	2.437391	3.441463	2.627173

H	3.142481	3.178405	1.834043
H	2.398379	2.608401	3.334269
H	2.818262	4.322744	3.152195
H	0.352753	4.011404	2.852148

^{1}TS6A-*SS*

B3LYP/BSI SCF energy: -3058.990827a.u.

M06/BSII SCF energy in solution: -3057.71466a.u.

M06/BSII free energy in solution: -3056.785513a.u.

C	2.821786	1.553048	-0.424507
O	2.643779	0.648886	-1.262845
N	3.858625	2.428423	-0.532668
C	1.900098	1.626663	0.781014
H	2.334692	0.937535	1.516456
H	1.928276	2.620545	1.234979
C	0.435729	1.198497	0.524447
C	4.081452	3.479010	0.430326
C	4.934987	3.262116	1.517421
C	3.494462	4.735338	0.242255
C	5.189043	4.297040	2.418912
H	5.392879	2.286769	1.651050
C	3.749346	5.765406	1.148527
H	2.838695	4.893559	-0.608472
C	4.596365	5.548053	2.237383
H	5.849085	4.124121	3.263694
H	3.287301	6.737148	1.002230
H	4.794024	6.350783	2.941315
C	4.860696	2.337771	-1.641780
C	5.665153	1.026377	-1.618808
C	4.251225	2.603218	-3.029691
H	5.558400	3.155391	-1.428810
C	6.760047	1.047616	-2.698708
H	4.984067	0.189737	-1.797551
H	6.108342	0.880669	-0.626752
C	5.351404	2.616502	-4.105426
H	3.522164	1.819502	-3.255034
H	3.715730	3.560171	-3.019849
C	6.171796	1.318040	-4.091669
H	7.303213	0.095720	-2.690079
H	7.496656	1.827967	-2.458818
H	4.898611	2.772970	-5.091160
H	6.021851	3.470691	-3.932267
H	6.972529	1.368544	-4.838644
H	5.524608	0.478469	-4.380529
C	1.630979	-3.260621	-0.070762
N	2.261709	-2.098627	-0.176128
C	3.701664	-2.379651	-0.119112
H	4.217028	-1.848530	-0.927473
O	2.443950	-4.355829	0.051251
C	0.221031	-3.384530	-0.173049
C	-0.542973	-4.604285	0.010065
C	-0.004053	-5.830656	0.466697
C	-1.946876	-4.554675	-0.276132
C	-1.703966	-2.197926	-0.796681
C	-0.803134	-6.958193	0.610148
H	1.048060	-5.891797	0.706509
C	-2.732464	-5.716446	-0.123637
C	-2.506669	-3.311596	-0.708743
H	-2.132446	-1.251242	-1.106035
C	-2.172476	-6.908368	0.311253
H	-0.357741	-7.885485	0.960716
H	-3.793798	-5.657315	-0.352526
H	-3.557801	-3.244831	-0.968697
H	-2.790719	-7.794880	0.423762
N	-0.380427	-2.186232	-0.530095
Ni	0.971624	-0.593563	-0.665851
C	3.784875	-3.928181	-0.268568
H	4.008064	-4.262604	-1.287824
C	-0.365611	0.984591	-1.364287
H	-0.260104	0.085080	-2.005510
C	-0.187333	0.403752	1.681217
H	0.426377	-0.471525	1.920302
H	-1.164282	0.026941	1.367525
C	-0.377990	1.262310	2.945692
H	-1.025261	2.123251	2.743562
H	-0.847936	0.672387	3.739050
H	0.573970	1.640571	3.335960
H	-0.136189	2.124262	0.444084
C	0.158447	2.200869	-2.138237
H	1.145743	2.003320	-2.553959
H	-0.522437	2.435912	-2.963586
H	0.211036	3.092001	-1.501655
C	-1.746299	1.151893	-0.992819
C	-2.901961	1.380151	-0.661325
Si	-4.622463	1.722234	-0.133418
C	-4.784074	3.569747	0.244079
C	-3.652681	4.367084	0.493925

C	-6.045243	4.193836	0.300190
C	-3.773052	5.725149	0.793459
H	-2.664419	3.917579	0.445356
C	-6.172525	5.551422	0.600775
H	-6.947660	3.618459	0.105978
C	-5.034450	6.320524	0.849147
H	-2.882771	6.319397	0.982205
H	-7.157856	6.008187	0.637924
H	-5.130405	7.377586	1.081743
C	-5.009713	0.695414	1.402553
C	-5.801057	1.210963	2.445764
C	-4.533097	-0.623878	1.529438
C	-6.111850	0.439148	3.567131
H	-6.170029	2.231921	2.390998
C	-4.839008	-1.397007	2.650447
H	-3.909576	-1.057762	0.753316
C	-5.631001	-0.867189	3.671219
H	-6.722507	0.860272	4.361484
H	-4.455420	-2.410839	2.724135
H	-5.868130	-1.467765	4.545358
C	-5.827026	1.320419	-1.564529
H	-5.583166	2.011147	-2.380600
H	-6.834051	1.587557	-1.220677
C	-5.810624	-0.105586	-2.057508
C	-4.951842	-0.498383	-3.096409
C	-6.645854	-1.078552	-1.487134
C	-4.932871	-1.816035	-3.554610
H	-4.296495	0.239675	-3.551748
C	-6.630351	-2.397030	-1.944648
H	-7.317340	-0.797851	-0.679787
C	-5.774333	-2.772430	-2.981962
H	-4.261540	-2.095384	-4.361866
H	-7.291458	-3.130536	-1.491046
H	-5.763582	-3.797200	-3.341647
C	4.393141	-2.129342	1.220048
C	4.530145	-0.932778	1.923311
C	4.963156	-3.304131	1.727491
C	5.207656	-0.922342	3.145152
H	4.118909	-0.013606	1.523818
C	5.638544	-3.298411	2.948458
C	5.754533	-2.102240	3.659726
H	5.307310	0.006231	3.701151
H	6.072106	-4.213975	3.343052
H	6.274955	-2.087172	4.613209
C	4.775706	-4.463117	0.774558
H	4.386690	-5.367670	1.253345
H	5.725537	-4.735297	0.296079

^{1}TS6B-*SS*

B3LYP/BSI SCF energy: -3058.98938a.u.

M06/BSII SCF energy in solution: -3057.71613a.u.

M06/BSII free energy in solution: -3056.78639a.u.

C	-3.543159	0.842173	0.365616
O	-3.113684	-0.080701	1.086291
N	-4.718012	1.458043	0.675221
C	-2.739026	1.186018	-0.873101
H	-2.998895	0.401607	-1.597033
H	-3.038571	2.138762	-1.311603
C	-1.202105	1.169951	-0.660119
C	-5.419374	0.972573	1.846210
C	-5.298951	1.653436	3.059911
C	-6.250158	-0.146070	1.747742
C	-6.015384	1.215821	4.175085
H	-4.641934	2.515068	3.128638
C	-6.960842	-0.582121	2.865975
H	-6.328156	-0.673164	0.802124
C	-6.846677	0.098639	4.079935
H	-5.918463	1.745516	5.118149
H	-7.601113	-1.455661	2.788325
H	-7.400515	-0.243058	4.949204
C	-5.399571	2.561829	-0.065199
C	-4.657589	3.911042	-0.005683
C	-5.834427	2.187249	-1.495146
H	-6.324121	2.700684	0.504709
C	-5.509705	5.022355	-0.643405
H	-3.696102	3.850588	-0.528348
H	-4.432050	4.153917	1.038776
C	-6.675721	3.317253	-2.114125
H	-4.961748	2.002931	-2.130293
H	-6.407899	1.253763	-1.465270
C	-5.934030	4.661750	-2.074890
H	-4.951763	5.965373	-0.633491
H	-6.407587	5.185657	-0.030748
H	-6.941294	3.054959	-3.144273
H	-7.622100	3.409269	-1.562671
H	-6.565743	5.454182	-2.492162
H	-5.042304	4.604173	-2.714946

C	0.128438	-2.983100	-0.727655	C	2.969325	6.201102	-1.592338
N	0.387682	-1.978044	0.094342	H	3.046867	4.166433	-2.269158
C	1.748459	-2.170263	0.599422	C	3.507984	6.571223	0.731675
H	2.292946	-1.221091	0.616622	H	3.994370	4.831071	1.881298
O	1.193347	-3.793738	-1.006867	C	3.138079	7.074923	-0.516528
C	-1.172336	-3.221634	-1.251944	H	2.685616	6.586944	-2.567911
C	-1.557231	-4.270060	-2.176940	H	3.644795	7.245741	1.572691
C	-0.656760	-5.177595	-2.782390	H	2.985523	8.142393	-0.650792
C	-2.950049	-4.385585	-2.503559	C	4.385840	1.671767	-1.547033
C	-3.397978	-2.489528	-1.057494	C	5.473085	2.251415	-2.229240
C	-1.104646	-6.155315	-3.663034	C	3.820317	0.504971	-2.090419
H	0.397496	-5.107593	-2.553452	C	5.976914	1.687729	-3.402307
C	-3.373747	-5.389778	-3.398187	H	5.928551	3.163319	-1.848749
C	-3.870171	-3.468479	-1.901219	C	4.317593	-0.061317	-3.266335
H	-4.081593	-1.790502	-0.582962	H	2.978599	0.034288	-1.589979
C	-2.466792	-6.267859	-3.974400	C	5.398556	0.528252	-3.923439
H	-0.387299	-6.837605	-4.111290	H	6.815907	2.154404	-3.911496
H	-4.433493	-5.463558	-3.630990	H	3.859534	-0.960360	-3.670030
H	-4.931993	-3.548320	-2.112113	H	5.786465	0.089100	-4.838498
H	-2.810570	-7.036091	-4.661674	C	5.030321	2.153146	1.471907
N	-2.099770	-2.326187	-0.738072	H	4.600897	2.573779	2.389264
Ni	-1.250701	-0.801763	0.347723	H	5.911511	2.761356	1.232574
C	2.363122	-3.211714	-0.376831	C	5.432435	0.715268	1.698023
H	2.984148	-2.775099	-1.166009	C	4.704409	-0.111196	2.567967
C	-0.320860	0.973544	1.171873	C	6.540083	0.164340	1.034733
H	-0.322469	0.032306	1.764228	C	5.073925	-1.441282	2.776158
C	-0.429651	0.697714	-1.899111	H	3.841517	0.293759	3.090319
H	-0.806721	-0.272494	-2.238385	C	6.912501	-1.164362	1.239822
H	0.617803	0.552717	-1.622821	H	7.116102	0.785135	0.353309
C	-0.493012	1.712275	-3.056065	C	6.182190	-1.973135	2.113067
H	-0.090824	2.685239	-2.750855	H	4.494987	-2.059820	3.455079
H	0.098368	1.358971	-3.907089	H	7.777897	-1.565859	0.719302
H	-1.517724	1.868288	-3.413042	H	6.476583	-3.005257	2.281404
H	-0.909092	2.209557	-0.493983	C	1.826671	-2.873121	1.949699
C	-1.008468	2.053194	2.016629	C	1.272622	-2.475430	3.166015
H	-1.984297	1.709853	2.362211	C	2.567606	-4.057821	1.861811
H	-0.398417	2.281296	2.897645	C	1.466336	-3.272805	4.297026
H	-1.130963	2.988594	1.459034	H	0.689140	-1.561528	3.235189
C	1.029362	1.322106	0.826418	C	2.757986	-4.857642	2.988936
C	2.151968	1.701671	0.518002	C	2.204419	-4.458689	4.208570
Si	3.767244	2.433689	0.064383	H	1.037188	-2.973941	5.249384
C	3.541306	4.299132	-0.168594	H	3.326961	-5.781765	2.922419
C	3.170680	4.830883	-1.417971	H	2.344112	-5.074766	5.092557
C	3.706073	5.199477	0.899944	C	3.104001	-4.264774	0.461430

H	2.933683	-5.272633	0.069077
H	4.184727	-4.075581	0.425745

^{1}TS6C-*SS*

B3LYP/BSI SCF energy: -3058.997151a.u.

M06/BSII SCF energy in solution: -3057.72122a.u.

M06/BSII free energy in solution: -3056.790571a.u.

C	3.384937	-1.362817	0.070180
O	2.980159	-0.604111	0.973911
N	4.466851	-2.165947	0.249666
C	2.676165	-1.337803	-1.273152
H	3.130422	-0.495632	-1.814029
H	2.897793	-2.240106	-1.849386
C	1.144137	-1.105746	-1.202546
C	5.000890	-2.974346	-0.818288
C	5.829371	-2.400549	-1.788638
C	4.733655	-4.347624	-0.850060
C	6.376360	-3.197853	-2.795315
H	6.036850	-1.335533	-1.751747
C	5.286769	-5.140571	-1.855950
H	4.088870	-4.782210	-0.092286
C	6.107061	-4.567220	-2.830264
H	7.014504	-2.747736	-3.549803
H	5.073156	-6.204977	-1.880297
H	6.534467	-5.185643	-3.613747
C	5.246885	-2.170001	1.528701
C	5.968595	-0.834401	1.783734
C	4.416094	-2.610171	2.746779
H	6.014343	-2.934253	1.362825
C	6.843977	-0.924021	3.045081
H	5.223274	-0.042495	1.903649
H	6.583897	-0.578937	0.912492
C	5.304389	-2.695435	3.999782
H	3.612321	-1.887793	2.912304
H	3.950296	-3.581991	2.542145
C	6.027807	-1.367241	4.268380
H	7.318214	0.046089	3.231567
H	7.659395	-1.641913	2.874829
H	4.692753	-2.980386	4.863437
H	6.049215	-3.493928	3.869077
H	6.679543	-1.461257	5.144799
H	5.286231	-0.593070	4.508277
C	0.386137	3.103143	-0.383647
N	-0.124187	1.976425	0.088005
C	-1.545421	2.217433	0.348626
H	-2.148480	1.381173	-0.015859
O	-0.518833	4.102339	-0.608606
C	1.778177	3.267697	-0.627262
C	2.432749	4.449003	-1.156933
C	1.761626	5.623008	-1.573064
C	3.863206	4.418111	-1.270160
C	3.837714	2.161974	-0.378221
C	2.462795	6.712984	-2.075580
H	0.684445	5.671210	-1.498488
C	4.546232	5.540510	-1.781590
C	4.554502	3.235928	-0.852172
H	4.347554	1.262078	-0.047047
C	3.859946	6.678200	-2.181937
H	1.916667	7.599470	-2.386883
H	5.630303	5.497717	-1.857185
H	5.637726	3.192621	-0.908044
H	4.401947	7.534503	-2.573920
N	2.494829	2.133959	-0.270409
Ni	1.310448	0.539194	0.255203
C	-1.841568	3.549487	-0.395392
H	-2.307435	3.418381	-1.377510
C	0.091724	-1.214804	0.546739
H	0.146131	-0.455988	1.359508
C	0.609934	-0.229307	-2.345074
H	1.167485	0.711226	-2.397628
H	-0.429049	0.035405	-2.127822
C	0.669849	-0.942554	-3.708822
H	0.074332	-1.862619	-3.702425
H	0.276235	-0.293442	-4.498606
H	1.695763	-1.208189	-3.987998
H	0.682087	-2.087236	-1.330279
C	0.535076	-2.559952	1.136144
H	1.509954	-2.474952	1.615903
H	-0.188337	-2.886847	1.890957
H	0.580038	-3.341937	0.369530
C	-1.255096	-1.270575	0.046494
C	-2.398016	-1.405893	-0.370718
Si	-4.144543	-1.675420	-0.848612
C	-4.262827	-1.962362	-2.713246
C	-3.300567	-1.430122	-3.590853
C	-5.323730	-2.696047	-3.277513
C	-3.393915	-1.616690	-4.970869

H	-2.463477	-0.866709	-3.188280
C	-5.422921	-2.886042	-4.657513
H	-6.087311	-3.131820	-2.637335
C	-4.456827	-2.345624	-5.507659
H	-2.636222	-1.195543	-5.626119
H	-6.251529	-3.457332	-5.067336
H	-4.530912	-2.493397	-6.581563
C	-5.161096	-0.161327	-0.355103
C	-6.206735	0.311514	-1.169533
C	-4.909760	0.518015	0.852382
C	-6.974484	1.415113	-0.792375
H	-6.418207	-0.180062	-2.115692
C	-5.671154	1.625572	1.231355
H	-4.104355	0.188031	1.502135
C	-6.706739	2.074870	0.408730
H	-7.775312	1.763935	-1.438982
H	-5.449052	2.138130	2.162988
H	-7.300680	2.936721	0.701286
C	-4.787153	-3.251290	0.030599
H	-4.250126	-4.099328	-0.410618
H	-5.841805	-3.368090	-0.248545
C	-4.644296	-3.260692	1.532561
C	-3.508506	-3.815183	2.143448
C	-5.634190	-2.707243	2.359580
C	-3.366700	-3.818320	3.531492
H	-2.732905	-4.254230	1.521187
C	-5.494016	-2.707577	3.748092
H	-6.523894	-2.274666	1.909625
C	-4.359081	-3.262691	4.341510
H	-2.482079	-4.261821	3.981150
H	-6.276198	-2.275829	4.366604
H	-4.251596	-3.267237	5.422404
C	-1.882312	2.544640	1.798456
C	-1.665983	1.766250	2.935682
C	-2.486649	3.803124	1.906204
C	-2.055586	2.258790	4.183937
H	-1.197659	0.789355	2.855756
C	-2.871859	4.298169	3.152555
C	-2.653552	3.519180	4.292063
H	-1.891257	1.660697	5.075913
H	-3.333323	5.278813	3.240036
H	-2.947398	3.895478	5.268075
C	-2.658865	4.446844	0.546924
H	-2.308816	5.483478	0.504646
H	-3.713714	4.445391	0.243383

^{1}TS6D-*SS*

B3LYP/BSI SCF energy: -3058.99729a.u.

M06/BSII SCF energy in solution: -3057.71996a.u.

M06/BSII free energy in solution: -3056.791272a.u.

C	3.241925	-1.445430	0.207542
O	2.900872	-0.646927	1.103225
N	4.286341	-2.298952	0.378039
C	2.496138	-1.419130	-1.115919
H	2.980490	-0.623347	-1.698870
H	2.648219	-2.351548	-1.666824
C	0.982267	-1.097600	-1.009100
C	4.766517	-3.136475	-0.692672
C	5.578347	-2.597475	-1.696461
C	4.465906	-4.503206	-0.694717
C	6.075545	-3.422705	-2.706424
H	5.812364	-1.537427	-1.682166
C	4.969998	-5.324360	-1.703757
H	3.833929	-4.910387	0.088656
C	5.773675	-4.785692	-2.711190
H	6.701065	-2.999477	-3.486609
H	4.731016	-6.383647	-1.704676
H	6.162916	-5.426110	-3.496898
C	5.089933	-2.322301	1.642093
C	5.879823	-1.019794	1.864974
C	4.260495	-2.705619	2.879899
H	5.816818	-3.124826	1.473827
C	6.770170	-1.132815	3.113903
H	5.175664	-0.190967	1.983769
H	6.492538	-0.807895	0.980337
C	5.164513	-2.815242	4.119538
H	3.493968	-1.944294	3.048126
H	3.746002	-3.656948	2.696716
C	5.953995	-1.518958	4.356314
H	7.292212	-0.183463	3.278267
H	7.548601	-1.890414	2.942275
H	4.554810	-3.058803	4.997118
H	5.868862	-3.649653	3.988720
H	6.614524	-1.630472	5.224058
H	5.253313	-0.707309	4.595318
C	0.527877	3.170392	-0.356915
N	-0.036452	2.111964	0.202316

C	-1.427800	2.465939	0.497339	C	-4.442409	2.359447	-3.095743
H	-2.096979	1.650881	0.209110	H	-3.476917	0.449345	-3.139183
O	-0.316602	4.212706	-0.614268	C	-5.302434	3.214440	-2.401148
C	1.918183	3.224505	-0.656903	H	-6.536696	3.455006	-0.649446
C	2.629581	4.326914	-1.275346	H	-4.001349	2.676871	-4.036748
C	2.022829	5.518929	-1.736864	H	-5.533184	4.198164	-2.800701
C	4.050025	4.193000	-1.432800	C	-5.406423	-1.485981	0.771266
C	3.908171	1.998414	-0.407977	C	-6.801586	-1.564011	0.589902
C	2.775696	6.528738	-2.324984	C	-4.897678	-1.751117	2.054228
H	0.954732	5.644500	-1.629155	C	-7.652523	-1.892520	1.646033
C	4.786418	5.235539	-2.031510	H	-7.236359	-1.359588	-0.386657
C	4.676695	2.992704	-0.967165	C	-5.744708	-2.080498	3.114589
H	4.370785	1.087543	-0.039133	H	-3.825570	-1.699516	2.222103
C	4.162584	6.393047	-2.475224	C	-7.123448	-2.152363	2.912501
H	2.278310	7.431707	-2.668986	H	-8.725550	-1.944530	1.482375
H	5.861831	5.114930	-2.139648	H	-5.327796	-2.280752	4.097890
H	5.752226	2.873514	-1.053437	H	-7.783765	-2.408103	3.736653
H	4.745208	7.187130	-2.934210	C	-4.491249	-2.342420	-2.079017
N	2.570766	2.066309	-0.257697	H	-3.957716	-1.966568	-2.959758
Ni	1.297707	0.584954	0.382657	H	-5.556796	-2.344102	-2.341965
C	-1.665227	3.763741	-0.322629	C	-4.026583	-3.738734	-1.741689
H	-2.175073	3.600476	-1.276785	C	-2.752862	-4.186573	-2.123885
C	-0.027875	-1.075906	0.766904	C	-4.847875	-4.621291	-1.022023
H	0.114614	-0.302211	1.554910	C	-2.314427	-5.471527	-1.801425
C	0.461203	-0.237562	-2.169993	H	-2.103618	-3.522222	-2.688870
H	1.056679	0.675596	-2.269019	C	-4.411572	-5.905950	-0.697367
H	-0.561842	0.075050	-1.942164	H	-5.837816	-4.296005	-0.713787
C	0.460078	-0.999176	-3.508741	C	-3.141818	-6.337908	-1.085036
H	-0.152318	-1.906871	-3.448347	H	-1.326833	-5.797898	-2.117035
H	0.051419	-0.371806	-4.308086	H	-5.067523	-6.571425	-0.142677
H	1.469217	-1.298903	-3.813229	H	-2.803485	-7.339802	-0.836408
H	0.463424	-2.055634	-1.085543	C	-1.679001	2.909047	1.933581
C	0.323756	-2.437494	1.379173	C	-1.454089	2.197747	3.111670
H	1.326605	-2.427045	1.806250	C	-2.196980	4.209057	1.978778
H	-0.382403	-2.677688	2.181554	C	-1.746689	2.799434	4.338030
H	0.254569	-3.242391	0.639428	H	-1.049527	1.189879	3.079063
C	-1.384192	-1.026102	0.297491	C	-2.488075	4.811650	3.202837
C	-2.537110	-1.051083	-0.112754	C	-2.259923	4.100200	4.383381
Si	-4.275177	-1.059408	-0.677310	H	-1.572377	2.255618	5.262451
C	-4.710209	0.649893	-1.367156	H	-2.883497	5.823787	3.241456
C	-5.570866	1.528961	-0.685335	H	-2.480047	4.560602	5.342639
C	-4.152738	1.094537	-2.582076	C	-2.386430	4.771286	0.585758
C	-5.865548	2.796507	-1.194355	H	-1.976409	5.778922	0.460167
H	-6.019381	1.221001	0.254867	H	-3.450112	4.816763	0.318047

^{1}TS6E-*SS*

B3LYP/BSI SCF energy: -3058.980357a.u.

M06/BSII SCF energy in solution: -3057.70991a.u.

M06/BSII free energy in solution: -3056.77987a.u.

C	0.460870	-2.289513	0.631867
N	0.422321	-1.004866	0.782237
C	1.070936	-0.714192	2.089163
H	1.788045	0.095807	1.949722
C	1.757721	-2.046469	2.476447
H	2.823185	-2.072380	2.243384
O	1.107893	-3.003504	1.588687
C	1.415729	-2.344424	3.943679
H	2.288041	-2.141985	4.578690
H	1.161490	-3.400423	4.084475
C	0.278352	-1.394382	4.254897
C	-0.516247	-1.342178	5.400348
C	0.094483	-0.463630	3.224563
C	-1.493585	-0.349039	5.503493
H	-0.379608	-2.063112	6.202669
C	-0.875368	0.532673	3.328486
C	-1.671463	0.583998	4.475700
H	-2.120466	-0.301006	6.389750
H	-1.021341	1.244916	2.523782
H	-2.434139	1.351827	4.562462
C	-0.106873	-3.044378	-0.509146
C	-0.599525	-4.392510	-0.390645
C	-0.675926	-5.131229	0.822756
C	-1.076987	-5.010829	-1.593122
C	-0.592928	-2.963041	-2.766053
C	-1.175354	-6.414878	0.833036
H	-0.333330	-4.677208	1.741845
C	-1.574676	-6.340132	-1.549074
C	-1.052278	-4.258293	-2.793422
H	-0.574352	-2.353688	-3.665566
C	-1.621907	-7.029768	-0.360450
H	-1.228258	-6.962107	1.769577
H	-1.927279	-6.795530	-2.470379
H	-1.401447	-4.704040	-3.720502
H	-2.008934	-8.044176	-0.332368
N	-0.119804	-2.365139	-1.647963
Ni	-0.111269	0.417450	-0.410971
C	-1.911798	1.291503	-0.464223
C	-1.069944	1.810283	-1.276026
Si	-3.637231	1.498335	0.156550
C	-4.744684	2.288419	-1.164248
C	-5.523247	3.427219	-0.889496
C	-4.807868	1.754758	-2.466728
C	-6.333652	4.008206	-1.868141
H	-5.493557	3.872133	0.101283
C	-5.615411	2.330971	-3.447347
H	-4.221504	0.875544	-2.718496
C	-6.381613	3.460654	-3.150231
H	-6.923868	4.889187	-1.628895
H	-5.647733	1.897966	-4.443780
H	-7.010032	3.911043	-3.914207
C	-3.604913	2.653186	1.667357
C	-4.627428	2.643952	2.634780
C	-2.569264	3.592142	1.831293
C	-4.618241	3.528423	3.716457
H	-5.452620	1.941237	2.548141
C	-2.551423	4.478152	2.910587
H	-1.763775	3.622341	1.102066
C	-3.576801	4.447807	3.857881
H	-5.422502	3.499536	4.447079
H	-1.737540	5.191371	3.012814
H	-3.565566	5.135759	4.699025
C	-4.330917	-0.195511	0.720692
H	-3.503476	-0.696711	1.237944
H	-5.106144	-0.013121	1.473513
C	-4.887386	-1.069840	-0.376358
C	-6.269873	-1.142263	-0.605955
C	-4.040745	-1.814138	-1.213990
C	-6.792389	-1.928491	-1.633394
H	-6.944317	-0.572898	0.029240
C	-4.561200	-2.600300	-2.243112
H	-2.966512	-1.769041	-1.058471
C	-5.939381	-2.662262	-2.458965
H	-7.867594	-1.967092	-1.787442
H	-3.883550	-3.167785	-2.874840
H	-6.343568	-3.276546	-3.258867
C	0.181137	2.038274	-1.899641
C	0.750789	3.442325	-1.690234
H	1.722442	3.569044	-2.173304
H	0.064318	4.176449	-2.126215
H	0.854148	3.676467	-0.627315
H	0.171814	1.765554	-2.954389

C	3.963750	0.635268	-0.139556
O	3.766481	-0.452817	0.410006
N	5.239333	1.042283	-0.477280
C	2.781119	1.532769	-0.516546
H	2.256686	1.769349	0.416535
H	3.122919	2.478124	-0.935255
C	1.832716	0.814167	-1.495434
H	1.735761	-0.231028	-1.189061
C	2.382004	0.789923	-2.928060
H	2.323914	1.784845	-3.393873
H	3.457143	0.558797	-2.878738
C	1.720052	-0.244718	-3.844104
H	0.641036	-0.077821	-3.931997
H	2.148480	-0.207354	-4.851708
H	1.858331	-1.255084	-3.448198
C	5.550647	2.387481	-0.873423
C	5.475149	3.434883	0.053216
C	5.988637	2.651492	-2.177312
C	5.813597	4.734410	-0.327050
H	5.147923	3.222814	1.066606
C	6.338134	3.949442	-2.550132
H	6.043561	1.837270	-2.893425
C	6.248298	4.994570	-1.627855
H	5.745240	5.541161	0.396916
H	6.672567	4.145399	-3.564745
H	6.515906	6.005193	-1.921477
C	6.407595	0.136109	-0.268575
C	6.713266	-0.110896	1.220703
C	6.289986	-1.182735	-1.052948
H	7.255600	0.689423	-0.688607
C	7.976870	-0.972778	1.383672
H	5.853159	-0.611968	1.673882
H	6.840552	0.851924	1.730668
C	7.560389	-2.031820	-0.880176
H	5.418688	-1.735675	-0.692828
H	6.120231	-0.961738	-2.113884
C	7.867949	-2.290759	0.602304
H	8.154818	-1.171370	2.447226
H	8.851276	-0.411634	1.022886
H	7.446177	-2.980024	-1.418418
H	8.415242	-1.514557	-1.340085
H	8.794343	-2.868815	0.703084
H	7.065503	-2.903614	1.035837