Supporting Information

Mechanistic study on C(sp^2)–F bond activation by Ni^0(silyl)-ate complex: an outer-sphere pathway via Ni^0-mediated nucleophilic aromatic substitution

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Content

1. Benchmark calculations of functionals for geometry optimization

The crystal structure of a Ni[0] complex[1] is shown in Figure S1. Several functionals (See Table S1) have been tested for geometry optimization compared with the experimental results. The Ni–C1, Ni–C2, Ni–C3, Ni–C4, Ni–Si, and Ni–P distances were considered as parameters. As shown in Table S1, the RMSE of B3PW91-D3(BJ) and ωB97XD functional is almost the same, the MAE of B3PW91-D3(BJ) is the minimum. In this work, all geometry optimizations were performed by B3PW91-D3(BJ) functional because dispersion correction should be considered and the optimization by B3PW91-D3(BJ) functional reproduced other crystal structures well[2], in which the Stuttgart-Dresden-Bonn basis sets were employed for valence electrons of Ni atom with corresponding effective core potentials representing their core electrons and 6-31G(d) basis sets were employed for other atoms.
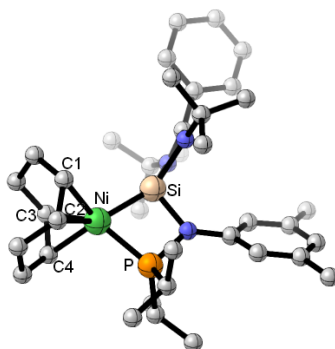

Figure S1. Crystal structure of Ni[0](silylene) complex. (distance [Å], hydrogen atoms are omitted for clarity).

Table S1. Benchmark of functionals for geometry optimization. Angstrom unit was used. Basis set: SDD for Ni, 6-31G(d) basis sets for other atoms.

	$R_{Ni–C1}$	$R_{Ni–C2}$	$R_{Ni–C3}$	$R_{Ni–C4}$	$R_{Ni–Si}$	$R_{Ni–P}$	RMSE	MAE
Experiment[1]	2.067	2.104	2.076	2.072	2.187	2.183		
B3LYP	2.123	2.161	2.132	2.108	2.215	2.235	0.049	0.048
B3LYP-D3(BJ)	2.104	2.142	2.109	2.081	2.183	2.195	0.026	0.022
B3PW91	2.088	2.120	2.103	2.082	2.199	2.207	0.019	0.018
B3PW91-D3(BJ)	2.067	2.099	2.081	2.057	2.161	2.169	0.014	0.011
M06	2.092	2.128	2.097	2.074	2.205	2.211	0.021	0.020
M062X	2.591	2.717	2.030	2.009	2.286	2.284	0.336	0.241
ωB97XD	2.090	2.120	2.090	2.066	2.189	2.194	0.014	0.012

(A) C(sp^3)-F activation

(B) C(sp^2)-F S$_N$Ar of Ni
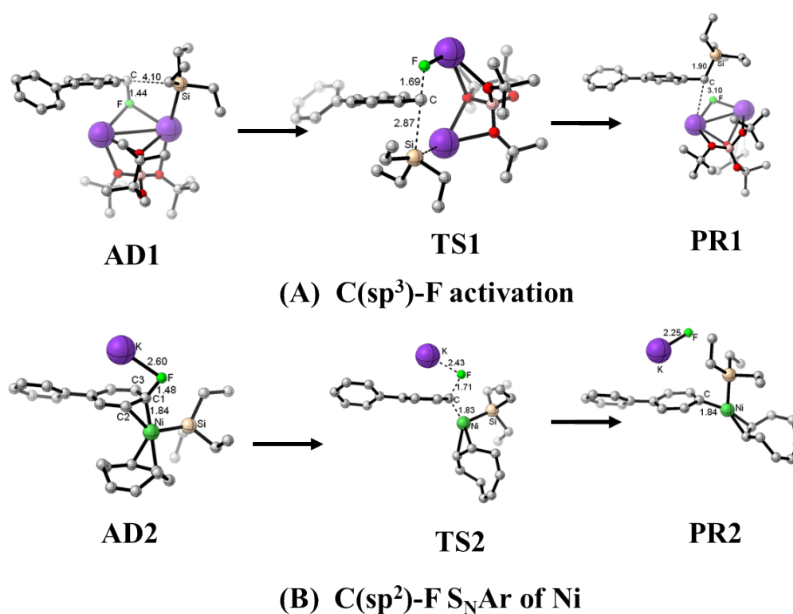
Figure S2. Important structures in the activation of C(sp^3)–F and the activation of C(sp^2) –F with the K$^+$[Ni^0(cod)$_2$(SiEt$_3$)]$^-$.

Table S2. Benchmark of functionals for potential energy change at B3PW91-D3(BJ)/BSII level.

	E_a1^a	ΔE_b1^b	E_c2^c	ΔE_d2^d	RMSE	MAE
B3LYP	16.5	-94.8	1.8	-26.2	2.5	2.1
B3LYP-D3(BJ)	10.0	-89.2	0.4	-29.2	6.6	6.1
B3PW91-D3(BJ)	9.4	-87.9	4.3	-27.8	6.5	5.4
M06	12.4	-89.5	6.1	-26.8	4.7	3.7
ωB97XD	16.3	-95.8	5.8	-29.0	2.4	1.8
DLPNO-CCSD(T)	19.5	-95.5	5.7	-25.4		

[a] E_a1 is the activation energy of nucleophilic substitution, which is the potential energy difference between TS1 and AD1;

[b] ΔE_b1 is the reaction energy, which is the potential energy difference between PR1 and TS1;

[c] E_a2 is the activation energy, which is the potential energy difference between TS2 and AD2;

[d] ΔE_d2 is the reaction energy, which is the potential energy difference between PR2 and TS2.

2. Plausible reactions and reaction energy

$\text{KOtBu} + \text{KOtBu} \longrightarrow$ [structure: K—OtBu / ButO—K]   **-21.7**   (eq 1)

$\text{KSiEt}_3 + \text{Ni(cod)}_2 \longrightarrow$ [structure E: η^2—cod, η^2—cod, Ni, Si(Et)(Et)(Et), K]   **-12.3**   (eq 2)

E

$\text{KSiEt}_3 + \text{Ni(cod)}_2 \longrightarrow$ [structure E-1: η^4—cod—Ni—Si(Et)(Et)(Et), K] $+$ cod   **4.2**   (eq 3)

E-1

$\text{KSiEt}_3 + \text{K(OtBu)}_2\text{Bpin} \longrightarrow$ [structure 1]   **-15.0**   (eq 4)

1
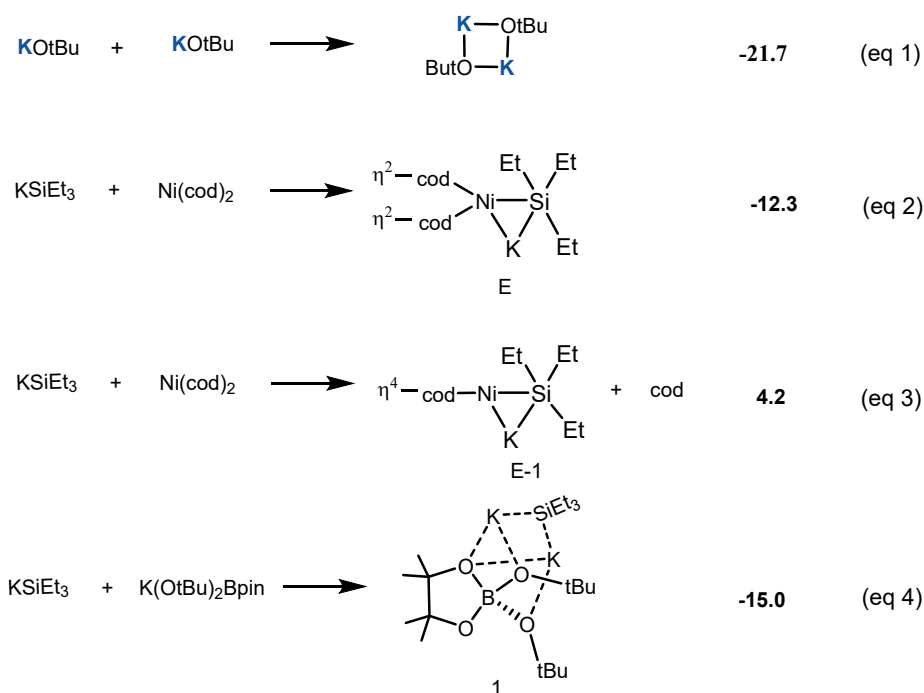
Scheme S1. Plausible conversion of substrates, base, and catalysts. The number on the right-hand side represents the Gibbs energy of reaction (ΔG° in kcal mol^{-1}).
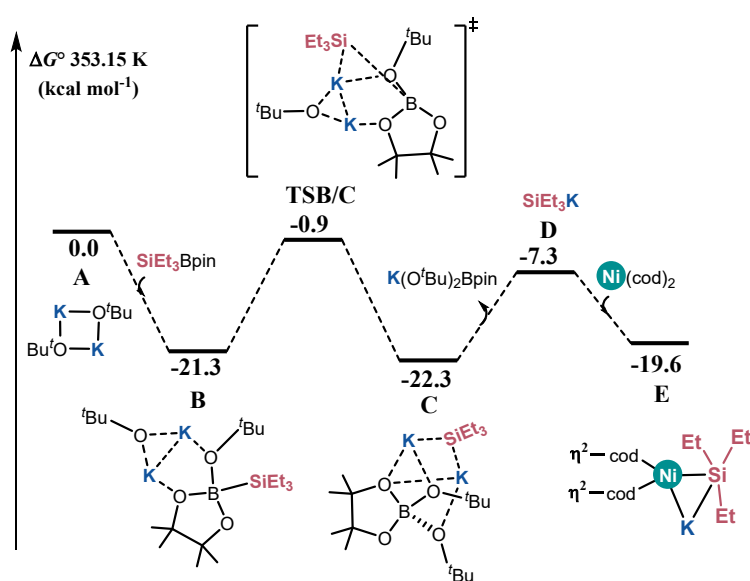
Figure S3. Gibbs energy profile for the generation of plausible reaction active species.
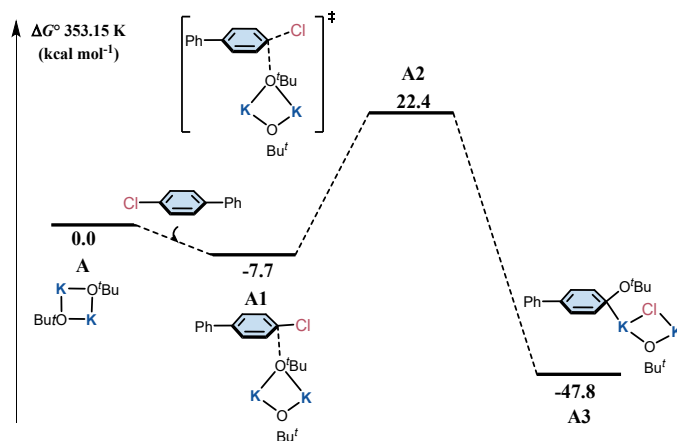
Figure S4. Gibbs energy profile of C(sp^2)–Cl catalyzed by the **A** complex.

The Gibbs free energy profile of C(sp^2)–Cl catalyzed by the **A** complex is shown in Figure S4. The $\Delta G^{\circ\ddagger}$ is 30.1 kcal mol^{-1}, which is higher than that to C(sp^2)–Cl borylation. It indicates that the tertiary butanol oxygen activate is not effective for the activation of C(sp^2)–Cl because such $\Delta G^{\circ\ddagger}$ is difficult to be overcome by the experimental temperature.
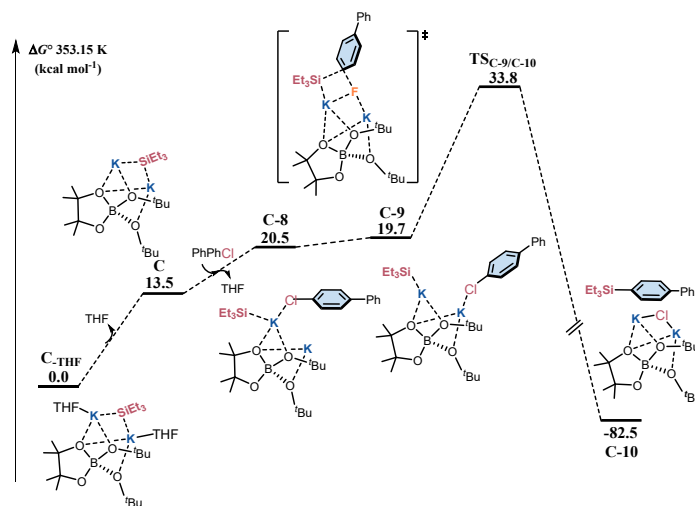
Figure S5. Gibbs energy profile in the full catalytic cycle of C(sp^2)–Cl silylation catalyzed by the **C** complex.

During the process where the silyl anion conducts a nucleophilic attack on the substituted carbon atom of the phenyl ring, it leads to the formation of a silyl

substitution product with $\Delta G^{o\ddagger}$ of 33.8 kcal mol^{-1} relative to $\mathbf{C_{-THF}}$ indicating that the activation of C(sp^2)–Cl bond is not activated by SiEt$_3$ as a nucleophilic reagent, as shown in Figure S5.

Scheme S2. Plausible Conversion of Substrates, Base, and Catalysts.

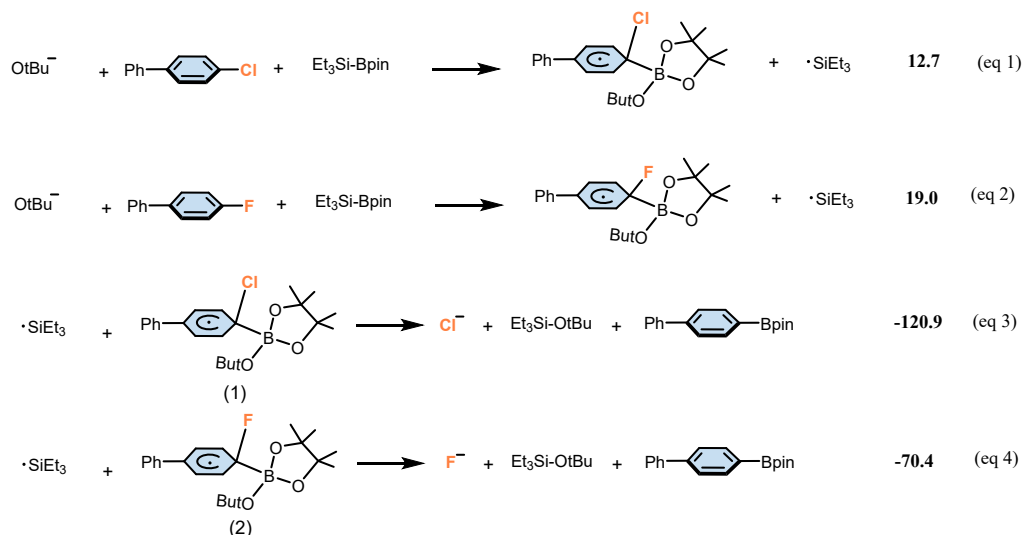The weaker but less polar C(sp^2)–Cl bond activation likely occurs through a homolytic manner (radical pathway) since KO^{t}Bu is also widely used as an initiator to facilitate the generation of a ·Bpin radical from Et$_3$SiBpin, which activates the C(sp^2)–X (X=Cl, Br, and I) bond leading to borylated products.[3] The activation of the C(sp^2)–Cl bond is relatively straightforward due to its low bond energy. In this study, we evaluated the energy change of the single-electron transfer (SET) process, initiated by the additional amount of KO^{t}Bu as a trigger. Results show that the $^-$O^{t}Bu anion could also react with Et$_3$SiBpin, generating a triethylsilyl radical ·SiEt$_3$ with ΔG^o of 12.7 kcal mol^{-1} as shown in Scheme S2. The C(sp^2)–Cl bond is thus activated by the attack of ·Bpin radical to form a radical complex, in which the single electron is distributed in the phenyl ring and chlorine. The subsequent single electron transfer from the aryl group to the chlorine proceeds rapidly. However, ΔG^o of C(sp^2)–F bond activated with the attack of ·Bpin radical is somewhat larger (19.0 kcal mol^{-1}), suggesting this SET process is slower than that of C(sp^2)–Cl bond activation. Importantly, the single electron is predominantly located in the phenyl ring, indicating that the generation of fluorine radical via a homolytic C(sp^2)–F bond activation is unlikely. Correspondingly,

the subsequent single electron transfer from the aryl group to the fluorine become markedly slower than the C(sp^2)–Cl. These results indicates that the low SET rate in the radical complex involve the ·Bpin and fluoride arenes plays a critical factor that borylation of C(sp^2)–F bond did not occur via a radical pathway. However, C(sp^2)–Cl bond activation also via unique carbanion-mediated mechanism involving the halogenophilic attack of a silyl nucleophile.[4] The detailed discussion of reactions is provided in the Figure S6.
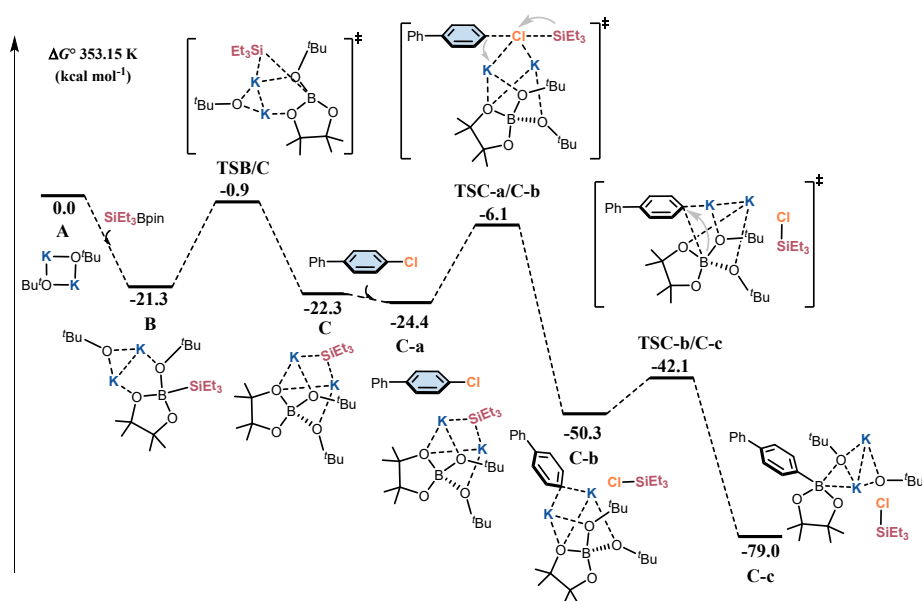
Figure S6. Gibbs energy profile in the full catalytic cycle of C(sp^2)–Cl borylation catalyzed by the **C** complex.

The most stable complex **C** combine with Ar-Cl to generate **C-a**, which rapidly consumed by the subsequent halogenophilic attack process, which proceeded via **TSC-a/C-b** with a very low energy barrier of 18.1 kcal/mol. Furthermore, significant cation−π interactions existed between the potassium cation and the phenyl group of the PhCH2CH2 moiety in the metastable intermediate **C-b**[5], which proceeds directly to the borylation reaction through **TSC-b/C-c**.

3. NBO charge changes along the IRC
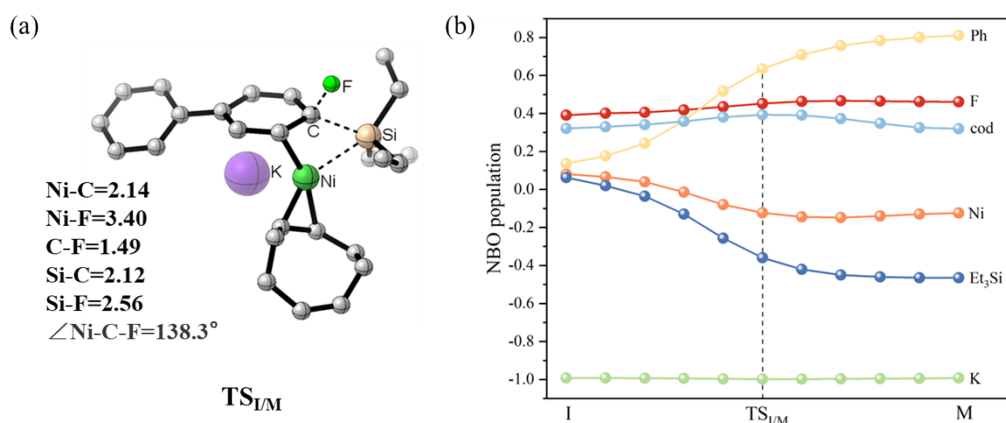
Figure S7. Main structure parameters in $TS_{I/M}$. (a) Main geometric parameters in $TS_{I/M}$. (b) NBO population of F, Ph, Et$_3$Si, cod, and Ni moieties changes along the IRC for $TS_{I/M}$.

We examined the geometric parameters of $\mathbf{TS_{I/M}}$ to elucidate the characteristic feature, as shown in Figure S7(a). In $\mathbf{TS_{I/M}}$, the Ni–F bond length (3.40 Å) is considerably longer compared to $\mathbf{TS_{I/L}}$ (2.06 Å), and the Ni–C (2.14 Å) is longer compared to $\mathbf{TS_{I/L}}$ (1.92 Å), while the C–F (1.56-1.71 Å) bond length are similar in both transition states. Additionally, the Ni–C–F angle (138.3°) in $\mathbf{TS_{I/M}}$ is notably greater than in $\mathbf{TS_{I/L}}$ (71.5°). The activation of the C(sp^2)–F bond in $\mathbf{TS_{I/L}}$ involves a homolytic mechanism characterized by a concerted oxidative addition, featuring a shorter Ni-F bond and a smaller Ni–C–F angle. Conversely, $\mathbf{TS_{I/M}}$ resembles a transition state typical of the S_NAr reaction, where the elongated Ni–F bond and increased Ni–C–F angle indicate a nucleophilic reaction process with SiEt$_3$ attacking and F anion departing from the bene-ring, leading to heterolytic C(sp^2)–F bond activation.

To analysis the electronic structure changes through the two transition states, we examined the variations in electron population along the IRC. During the I→$TS_{I/M}$→M transition, the electron population of F group increased from 0.45 e to 0.74 e and that of the Ph group increases from -0.02 e to 0.33 e. Correspondingly, the electron

population of the Ni atom decreased from 0.09 e to -0.10 e, and for Et_3Si, it reduced from 0.26 e to 0.06e. Note that in the equilibrium structure of PhF, the Natural Bond Orbital (NBO) population of F atom is 0.33 e greater than that of an isolated F atom.[6] This observation implies that Si attack on the benzene ring occurs through a S_NAr mechanism.

Table S3. NBO population change along IRC of $TS_{I/L}$ and $TS_{H/J}$.

Group	$TS_{I/L}$		$TS_{H/J}$	
	Charge transfer(e)	Total electronic change(e)	Charge transfer(e)	Total electronic change(e)
F	0.36 to 0.64	0.28	0.33 to 0.88	0.55
Ph	-0.05 to 0.45	0.50	0.48 to 0.41	0.07
Et_3Si	0.35 to 0.19	0.16	0.24 to -0.18	0.42
cod	0.18 to -0.05	0.23	0.01 to 0.03	0.02
Ni	0.14 to -0.25	0.39	-0.10 to -0.19	0.09
K	-0.97 to -0.97	0.00	-0.97 to -0.95	0.02

Table S4. NBO population change along IRC of $TS_{G/J}$ and $TS_{I/M}$.

Group	$TS_{G/J}$		$TS_{I/M}$	
	Charge transfer(e)	Total electronic change(e)	Charge transfer(e)	Total electronic change(e)
F	0.45 to 0.74	0.29	0.45 to 0.74	0.29
Ph	-0.02 to 0.33	0.35	-0.02 to 0.33	0.35
Et_3Si	0.26 to 0.06	0.20	0.26 to 0.06	0.20
cod	0.20 to -0.05	0.25	0.20 to -0.05	0.25
Ni	0.09 to -0.10	0.19	0.09 to -0.10	0.19
K	-0.97 to -0.99	0.02	-0.97 to -0.99	0.02

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TS$_{H/J}$–Na (Na replace K)   TS$_{G/J}$–Na (Na replace K)

0.0 kcal mol^{-1} 7.3 kcal mol^{-1}
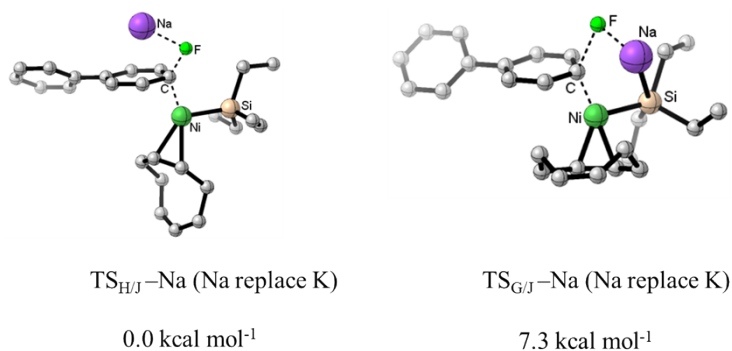
Figure S8. The ΔG of TS$_{G/J}$-Na (inner-sphere) and TS$_{H/J}$-Na (outer-sphere) transition state of C(sp^2)–F silylation where Na replaces K in the transition state.

To confirm radius effect, we conducted models with Na, and the results indicate that for smaller alkali metal ions, the inner-sphere transition state is more stable (7.3 kcal mol^{-1}) than the outer-sphere transition state.

Table S5. Orbital composition of the Ni–Si bond through NBO analysis in E, I, TS$_{I/L}$,

L, G, TS$_{G/J}$, H, TS$_{H/J}$ and J
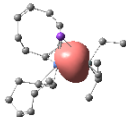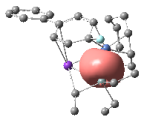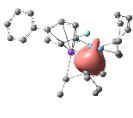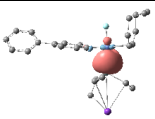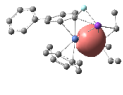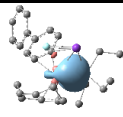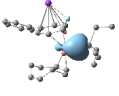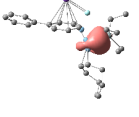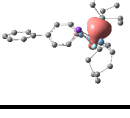
Type	Intermediate	Occupancy	Ni–Si orbital
Active species	E	Ni (s (39.08%) p (58.82%) d (2.09%)) Si (s (33.66%) p (66.27%) d (0.07%))	
Concerted OA	I	Ni (s (52.85%) p (45.48%) d (1.66%)) Si (s (33.51%) p (66.42%) d (0.07%))	
	TS$_{I/L}$	Ni (s (46.89%) p (22.56%) d (30.55%)) Si (s (28.34%) p (71.52%) d (0.14%))	
	L	Ni (s (39.56%) p (23.34%) d (37.08%)) Si (s (33.85%) p (66.05%) d (0.10%))	
Inner-sphere	G	Ni (s (47.11%) p (50.96%) d (1.92%)) Si (s (32.93%) p (67.00%) d (0.07%))	
	TS$_{G/J}$	Ni (s (40.21%) p (27.18%) d (32.60%)) Si (s (28.43%) p (71.40%) d (0.16%))	
Outer-sphere	H	Ni (s (42.81%) p (23.61%) d (33.56%)) Si (s (27.32%) p (72.49%) d (0.19%))	
	TS$_{H/J}$	Ni (s (53.68%) p (11.99%) d (34.31%)) Si (s (24.37%) p (75.37%) d (0.25%))	
	J	Ni (s (31.96%) p (23.80%) d (44.21%)) Si (s (5.03%) p (74.63%) d (0.34%))	

Table S6. NBO information of intermediate E.
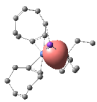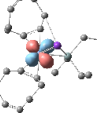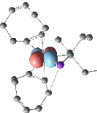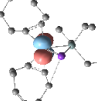
	Bond orbital	Atom/ Bond	Occupancy	orbital
E	BD	Ni–Si	Ni (s (39.08%) p (58.82%) d (2.09%)) Si (s (33.66%) p (66.27%) d (0.07%))	
	LP	Ni	1.99	
	LP	Ni	1.98	
	LP	Ni	1.97	
	LP	Ni	1.70	
	LP	Ni	1.59	

Table S7. The charge of Ni and Si in the intermediate **E**, Ni(cod)$_2$ and **C**.

		E	Ni(cod)$_2$	**C**
Hirshfeld charge	Ni	-0.20	-0.08	-
	Si	0.16	-	-0.02
NBO charge	Ni	-0.31	0.02	-
	Si	1.12	-	0.44

4. Full cycle of C(sp³)–F silylation catalyzed by Ni⁰(silyl)-ate complex.
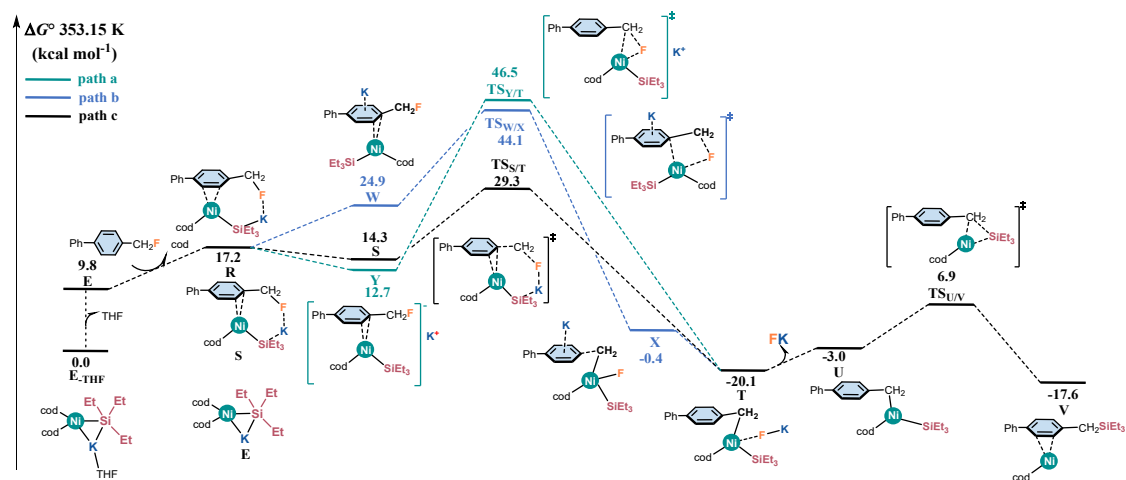
Figure S9. Gibbs energy profile in the full catalytic cycle of C(sp^3)–F silylation catalyzed by the K$^+$[Ni^0(cod)$_2$(SiEt$_3$)]$^-$ complex.

The activation of C(sp^3)–F bonds by the K$^+$[Ni^0(cod)$_2$(SiEt$_3$)]$^-$ complex potentially encompasses oxidative addition and nucleophilic substitution reactions, akin to those observed in C(sp^2)–F silylation, the Gibbs energy profile with geometry changes for this process is shown in Figure S9. ArCH$_2$F adds to **E**, forming the intermediate **R** with the free energy of 7.4 kcal mol^{-1}. In the presence of free K$^+$, intermediate **Y** is stabilized by 4.5 kcal mol^{-1} due to the Ni coordination with the carbon-carbon double bond. However, **Y** then undergoes fast oxidative addition of the C(sp^3)–F bond to Ni via a three-centered transition state, **TS$_{Y/T}$**, with the energy barrier of 46.5 kcal mol^{-1}, excluding this pathway. In pathway b and c, the internal nucleophilic aromatic substitution is assisted by K$^+$ complexation. Disruption of the FK interaction leads to K$^+$ interaction with the benzene ring and Ni coordinating to the carbon-carbon double bond, raising the energy of intermediate **W** by 7.7 kcal mol^{-1}. The nucleophilic attack of Ni, as shown by the blue line in path b, activates the C(sp^3)–F bond with an energy barrier of 44.1 kcal mol^{-1}. However, when K$^+$ interacts with F, the Ni nucleophilic attack activates C(sp^3)–F bond with the energy barrier is 29.3 kcal mol^{-1}, which is much lower than that of both pathway a and b, as shown by the blue line in pathway c. In other

words, the energy barrier for $C(sp^3)$–F bond activation in the presence of $Ni^0(cod)_2$ is 29.3 kcal mol-1, which exceeds the energy barrier for $C(sp^3)$–F activation in the absence of $Ni^0(cod)_2$ (23.6 kcal mol^{-1}). Therefore, it can be deduced that $C(sp^3)$–F bond activation is feasible with or without the presence of $Ni^0(cod)_2$.

5. AIMD simulations of $C(sp^3)$–F activation
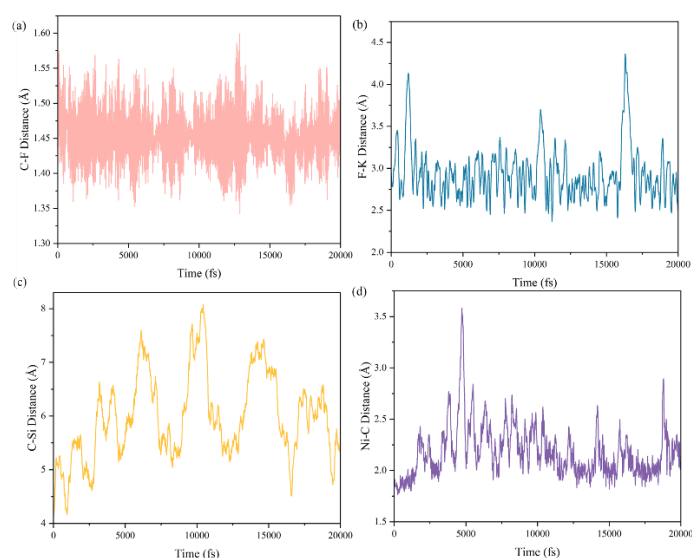
Figure S10. (a). The time-resolved evolution of $C(sp^3)$–F bond distances with time of $C(sp^3)$–F bond activation with $Et_3SiBpin$ and KO^tBu; (b). The time-resolved evolution of F–K bond distances with time of $C(sp^3)$–F bond activation with $Et_3SiBpin$ and KO^tBu; (c). The time-resolved evolution of C–Si bond distances with time of $C(sp^3)$–F bond activation with $Et_3SiBpin$ and KO^tBu; (d). The time-resolved evolution of Ni–C bond distances with time of outer-sphere Ni^0-mediated $C(sp^2)$–F bond activation.

To simulate dynamic effects of $C(sp^3)$–F bond activation using $Et_3SiBpin$ and KO^tBu with multiple non-covalent interactions, we conducted AIMD simulations. Figure S10 (a) illustrates the temporal evolution of $C(sp^3)$–F bond activation. The $C(sp^3)$–F bond remains inactive when its distance fluctuates between 1.35 and 1.55 Å, because the equilibrium distance of the $C(sp^3)$–F bond is 1.38 Å, which contradicts the results from DFT calculations. Notably, $K^+\cdots F$ interactions persist during the reaction, while $C\cdots Si$ interactions disappear, as shown in Figure S10 (b) and (c). This disruption

of synergistic effects among weak interactions means that even if the energy barrier of the reaction can be overcome, the reaction itself cannot occur, emphasize the importance of not overlooking the equilibrium of non-covalent interactions in such reactions. In contrast to the outer-sphere Ni^0-mediated $C(sp^2)$–F bond activation reaction with similar energy barriers, the presence of Ni···C interactions and continuous synergistic effects enables the reaction to proceed.

6. References

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7. Cartesian coordinates

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C-2, E(ωB97XD /BSII)= -3206.38633 au

F	-1.393674	-1.007137	2.010817
C	-2.773578	-0.691714	1.941275
H	-3.256855	-1.477022	1.356633
H	-3.138746	-0.708012	2.973390
C	-2.935328	0.649633	1.296991
C	-3.541130	0.773152	0.042537
C	-2.381667	1.789031	1.893635
C	-3.571845	2.001638	-0.612142
H	-3.968221	-0.101580	-0.437552
C	-2.394985	3.012468	1.230608
H	-1.894344	1.707541	2.862107
C	-2.976859	3.138161	-0.042347
H	-4.059373	2.077304	-1.580124
H	-1.913308	3.873212	1.686527
C	-2.940312	4.424804	-0.772289
C	-3.119332	5.642685	-0.100670
C	-2.711164	4.451420	-2.156286
C	-3.069032	6.850145	-0.791330
H	-3.326531	5.640123	0.966476
C	-2.659888	5.659099	-2.846619
H	-2.552682	3.518232	-2.692082
C	-2.837703	6.863250	-2.166372
H	-3.219186	7.783430	-0.254896
H	-2.474512	5.659400	-3.917637
H	-2.797868	7.806238	-2.704976
O	4.128197	-0.620864	0.798595
O	2.187919	-1.169942	-0.376843
C	4.394187	-0.348025	-0.563492
C	3.245735	-1.117385	-1.328600
C	4.345835	1.170921	-0.787389
H	5.078568	1.637708	-0.121498
H	4.593096	1.450138	-1.817968
H	3.362373	1.567796	-0.523946
C	5.799178	-0.845683	-0.890915
H	6.031282	-0.713550	-1.954327
H	6.530450	-0.276044	-0.307906
H	5.919242	-1.901398	-0.634922
C	2.761784	-0.405513	-2.593883
H	3.563638	-0.332394	-3.337636
H	1.935660	-0.966330	-3.045515
H	2.417551	0.612587	-2.383662
C	3.620729	-2.553076	-1.709880
H	3.981783	-3.108805	-0.843976
H	2.729485	-3.061818	-2.094613
H	4.387821	-2.587490	-2.491153
B	2.697071	-0.744292	0.984022
O	1.933612	0.514874	1.203867
C	2.004433	1.345499	2.354827
K	0.326557	-2.839349	0.569620
C	3.448412	1.634553	2.772227
C	1.217131	0.722226	3.514011
C	1.344788	2.668084	1.944828
H	3.977689	0.717997	3.027342
H	3.992936	2.112706	1.953512
H	3.463916	2.302600	3.642085
H	1.147022	1.415209	4.361906
H	0.208418	0.461447	3.179114
H	1.695426	-0.200623	3.844113
H	1.876888	3.106928	1.092203
H	0.298514	2.508217	1.659651
H	1.356222	3.393245	2.766743
O	2.314260	-1.714014	2.023408
C	3.156142	-2.614229	2.734356
C	2.219799	-3.394078	3.665088
C	4.195924	-1.871506	3.580441
C	3.880379	-3.585278	1.796811
H	1.646272	-2.700860	4.289335
H	1.507213	-4.004132	3.091994
H	2.780580	-4.073470	4.316439
H	4.801415	-2.581822	4.156319
H	4.856042	-1.292321	2.931517
H	3.704820	-1.194184	4.286420
H	3.168557	-4.121328	1.155596
H	4.571701	-3.028717	1.161901
H	4.444622	-4.332751	2.367007
K	-0.023983	0.484982	-0.605361
Si	-1.958559	-2.147285	-1.800407
C	-3.621417	-2.955873	-1.172401
C	-2.558550	-0.889485	-3.170138
C	-1.311333	-3.624769	-2.899663
H	-4.155204	-3.393716	-2.029168
H	-4.304470	-2.193864	-0.764262

C	-3.406355	-4.049625	-0.120354	O	0.553403	-1.201299	0.449122
H	-2.958662	0.010710	-2.677383	C	0.984731	-3.063500	-0.914666
H	-1.655906	-0.546354	-3.703308	C	-0.083604	-1.956436	-0.581935
C	-3.579426	-1.398281	-4.192682	C	2.007073	-2.607514	-1.966995
H	-1.046301	-4.471532	-2.245012	H	2.793099	-3.366232	-2.033157
H	-2.130054	-3.999445	-3.533844	H	1.561523	-2.484908	-2.960882
C	-0.107705	-3.274336	-3.776172	H	2.487803	-1.674071	-1.661117
H	-2.920718	-3.654053	0.785643	C	0.380993	-4.391928	-1.357830
H	-4.342310	-4.526218	0.204542	H	-0.209373	-4.274154	-2.274232
H	-2.759864	-4.848832	-0.507426	H	1.183140	-5.110442	-1.556556
H	-4.516204	-1.693486	-3.704839	H	-0.261003	-4.814010	-0.580991
H	-3.830648	-0.643694	-4.952767	C	-0.422767	-1.030043	-1.752200
H	-3.202716	-2.280279	-4.724382	H	-0.890035	-1.588666	-2.571015
H	0.269521	-4.130906	-4.352726	H	-1.133748	-0.265244	-1.418822
H	-0.357401	-2.484765	-4.496685	H	0.462821	-0.533782	-2.166602
H	0.726550	-2.895791	-3.170292	C	-1.403705	-2.515427	-0.046355
98				H	-1.235508	-3.215226	0.771206
				H	-2.012510	-1.687356	0.333225
C-3, E(ωB97XD /BSII)= -3206.38169 au				H	-1.978820	-3.027425	-0.825638
F	0.771809	2.378025	2.195314	B	1.691249	-2.008100	1.047811
C	-0.136915	3.431006	1.838314	O	2.850923	-1.099340	0.766795
H	-1.118277	3.127012	2.212317	C	4.209503	-1.306416	1.119439
H	0.223234	4.326311	2.352187	K	-0.459737	-0.267047	2.776893
C	-0.126547	3.565427	0.350644	C	4.701422	-2.685747	0.674166
C	-1.022273	2.805282	-0.411609	C	4.418339	-1.095327	2.622804
C	0.847793	4.327704	-0.308627	C	5.005080	-0.237420	0.355494
C	-0.925049	2.777965	-1.798862	H	4.130718	-3.479950	1.152463
H	-1.768478	2.201010	0.105379	H	4.575445	-2.797441	-0.406933
C	0.956822	4.285165	-1.697821	H	5.761993	-2.815077	0.921103
H	1.541029	4.936441	0.269451	H	5.478481	-1.178415	2.890818
C	0.086154	3.491305	-2.466647	H	4.063081	-0.097901	2.909681
H	-1.643074	2.195763	-2.370011	H	3.843504	-1.823134	3.193511
H	1.744442	4.847658	-2.193002	H	4.837767	-0.337523	-0.724797
C	0.249321	3.380394	-3.932937	H	4.708947	0.772766	0.674763
C	0.597856	4.493240	-4.711671	H	6.080794	-0.330639	0.540300
C	0.071241	2.143544	-4.571808	O	1.540885	-2.159075	2.498917
C	0.765487	4.372409	-6.088217	C	1.347433	-3.355353	3.251359
H	0.707936	5.465683	-4.238271	C	1.341689	-2.911488	4.718665
C	0.241455	2.023209	-5.947971	C	2.480200	-4.365353	3.036170
H	-0.185415	1.266014	-3.982691	C	0.017051	-4.035759	2.915233
C	0.590249	3.137010	-6.711011	H	2.264582	-2.372046	4.956285
H	1.024389	5.248051	-6.677649	H	0.494195	-2.244463	4.926943
H	0.105598	1.055816	-6.424390	H	1.254801	-3.771049	5.392271
H	0.721407	3.043617	-7.785659	H	2.320499	-5.253194	3.659502
O	1.653642	-3.258061	0.317510				

H	2.508722	-4.674483	1.989231	H	-5.831063	5.705602	1.545110
H	3.448215	-3.933837	3.308735	C	-5.880873	3.709732	-0.308960
H	-0.827442	-3.346638	3.039579	C	-7.112246	4.346040	-0.535719
H	0.037117	-4.385518	1.881546	C	-5.243098	3.099463	-1.401295
H	-0.157480	-4.894662	3.573831	C	-7.681855	4.373130	-1.805220
K	1.828294	1.019963	-0.226637	H	-7.639173	4.796688	0.301613
Si	-3.392881	0.936988	1.808096	C	-5.815021	3.121734	-2.669887
C	-4.079963	2.709593	2.227137	H	-4.273553	2.628289	-1.257364
C	-4.084923	0.674383	-0.007146	C	-7.037330	3.759933	-2.879316
C	-4.570552	-0.205960	2.853826	H	-8.639750	4.865586	-1.953863
H	-5.160038	2.759012	2.020590	H	-5.297820	2.649217	-3.501541
H	-3.614775	3.438488	1.542522	H	-7.483117	3.779456	-3.870361
C	-3.832587	3.140266	3.675714	O	-1.697703	-2.042594	5.264152
H	-3.668275	1.466467	-0.651461	O	-2.780428	-0.460018	3.918583
H	-3.674308	-0.264804	-0.407810	C	-1.166145	-2.173025	3.964588
C	-5.608259	0.662898	-0.172166	C	-2.228393	-1.443850	3.053663
H	-4.372375	-0.029165	3.921990	C	0.217420	-1.504101	3.941623
H	-5.619656	0.086948	2.692338	H	0.842101	-1.990882	4.696655
C	-4.408065	-1.698411	2.549458	H	0.720119	-1.583568	2.971080
H	-2.764313	3.086207	3.936892	H	0.139080	-0.454095	4.237051
H	-4.168999	4.166560	3.883418	C	-0.993815	-3.655365	3.645202
H	-4.356628	2.479421	4.377801	H	-0.633091	-3.802857	2.620224
H	-6.058857	1.589950	0.202383	H	-0.262708	-4.094099	4.331966
H	-5.918552	0.550224	-1.221973	H	-1.932543	-4.201122	3.767091
H	-6.062493	-0.162715	0.388701	C	-1.633018	-0.770864	1.814806
H	-5.075119	-2.334105	3.149443	H	-1.225530	-1.514896	1.121325
H	-4.614473	-1.915419	1.493163	H	-2.410684	-0.206754	1.286202
H	-3.379825	-2.041688	2.740615	H	-0.815176	-0.084631	2.056290

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TS$_{C-3/C-4}$, E(ωB97XD /BSII)= -3206.355735au

				C	-3.357012	-2.362394	2.572066
				H	-3.826761	-2.876495	3.409429
				H	-4.118955	-1.749836	2.073312
F	-2.054189	4.025864	4.700190	H	-3.010085	-3.112004	1.852751
C	-3.645794	3.568626	5.041839	B	-2.468580	-0.816162	5.369704
H	-3.418622	2.616922	5.506754	O	-1.766025	0.420164	5.795246
H	-3.873438	4.373130	5.725363	C	-1.288745	0.736581	7.101361
C	-4.268741	3.582994	3.711035	K	-5.311583	0.363372	4.655783
C	-4.093379	2.508333	2.808521	C	-0.382399	-0.375895	7.632261
C	-4.857309	4.753063	3.189582	C	-2.449282	1.027231	8.058629
C	-4.607245	2.548790	1.518178	C	-0.456313	2.017066	6.945544
H	-3.589754	1.596944	3.130680	H	-0.922589	-1.315934	7.733036
C	-5.371236	4.788742	1.906002	H	0.444487	-0.546709	6.934584
H	-4.928241	5.631778	3.824376	H	0.033666	-0.102784	8.609284
C	-5.286618	3.679565	1.040610	H	-2.073119	1.345350	9.038225
H	-4.503077	1.674796	0.877511	H	-3.082147	1.826213	7.656628

Atom	X	Y	Z	Atom	X	Y	Z
H	-3.076240	0.147045	8.187217	C	-1.446039	1.453895	0.780774
H	0.428290	1.824072	6.319906	H	-1.739957	0.581495	1.377058
H	-1.047678	2.824170	6.497233	H	-0.362842	1.423308	0.596210
H	-0.089089	2.366367	7.916470	C	-2.156893	1.466256	-0.539178
O	-3.692844	-0.997690	6.168041	C	-3.446400	0.938733	-0.695670
C	-4.166804	-2.160067	6.848065	C	-1.537962	2.028391	-1.670273
C	-5.416501	-1.703824	7.610703	H	-3.954530	0.511280	0.166708
C	-3.145744	-2.712603	7.847667	C	-4.089789	0.960700	-1.928971
C	-4.546233	-3.273718	5.867810	H	-3.954530	0.511280	0.166708
H	-5.178248	-0.864821	8.271772	C	-2.182694	2.044833	-2.903725
H	-6.208344	-1.377193	6.922422	H	-0.519031	2.398378	-1.564869
H	-5.829293	-2.518873	8.215175	C	-3.471428	1.511783	-3.061097
H	-3.560322	-3.584965	8.366557	H	-5.099181	0.564649	-2.012428
H	-2.236756	-3.015923	7.324561	H	-1.666112	2.455628	-3.768862
H	-2.892232	-1.963099	8.602929	C	-4.150149	1.523908	-4.375610
H	-5.276288	-2.916554	5.129928	C	-4.043588	2.630748	-5.231488
H	-3.653064	-3.621517	5.345659	C	-4.916119	0.428437	-4.802636
H	-4.997256	-4.121527	6.396535	C	-4.677629	2.641023	-6.470806
K	-1.045969	1.987471	3.786538	H	-3.479142	3.501438	-4.907082
Si	-6.313427	3.150137	6.017313	C	-5.553430	0.439162	-6.040384
C	-7.847645	2.374874	5.095081	H	-4.991479	-0.449208	-4.165162
C	-6.460747	2.476499	7.826553	C	-5.436237	1.545355	-6.881219
C	-6.858851	4.993660	6.131100	H	-4.587435	3.513007	-7.113976
H	-8.752421	2.727264	5.613440	H	-6.136316	-0.423791	-6.353036
H	-7.882880	1.276423	5.217337	H	-5.932751	1.553780	-7.848086
C	-7.948690	2.745678	3.609428	O	3.173148	-3.336241	0.907847
H	-6.273462	1.391486	7.815218	O	3.024524	-1.259818	-0.149470
H	-5.624553	2.898156	8.403507	C	4.498162	-2.904567	0.673780
C	-7.782711	2.760101	8.549520	C	4.329210	-1.761449	-0.401425
H	-6.866844	5.423187	5.119621	C	5.093900	-2.395956	1.995292
H	-7.908724	5.009110	6.462124	H	5.040296	-3.207803	2.727387
C	-6.021382	5.874030	7.063401	H	6.142167	-2.091576	1.895454
H	-7.063657	2.442350	3.033844	H	4.503061	-1.564370	2.388007
H	-8.828920	2.303222	3.123067	C	5.319910	-4.095485	0.189516
H	-8.018161	3.832191	3.486506	H	6.342796	-3.796063	-0.068295
H	-8.633269	2.313773	8.019635	H	5.373750	-4.847403	0.983759
H	-7.791147	2.361211	9.573959	H	4.862045	-4.566687	-0.683964
H	-7.975387	3.837465	8.618277	C	5.349478	-0.628119	-0.266671
H	-6.419017	6.895270	7.137308	H	6.369283	-0.989591	-0.441470
H	-5.989086	5.463203	8.080252	H	5.138408	0.151838	-1.008809
H	-4.981782	5.962508	6.722140	H	5.332215	-0.174991	0.730056
98				C	4.382764	-2.264714	-1.848037
C-4, E(ωB97XD /BSII)= -3206.50838 au				H	3.676906	-3.079849	-2.006485
F	1.342556	1.738329	-0.544942	H	4.106124	-1.439670	-2.516367
				H	5.383203	-2.607402	-2.134265

B	2.269306	-2.211728	0.756378	H	0.831170	3.639433	0.255586
O	2.043696	-1.355017	1.955293	H	0.822942	5.414034	0.238696
C	1.342870	-1.720941	3.134537	H	0.943612	4.559474	1.777855
K	0.791795	-0.445648	-1.451327	H	-3.663356	5.337147	2.619366
C	1.868972	-3.033862	3.720078	H	-5.078572	4.444721	3.184803
C	-0.165418	-1.800607	2.875098	H	-3.533713	4.278108	4.026347
C	1.608149	-0.591012	4.139161	H	-0.878340	1.617667	5.323711
H	1.758237	-3.851825	3.008793	H	-2.482284	1.957322	4.662156
H	2.933881	-2.943378	3.954437	H	-1.451326	0.739003	3.906491
H	1.327469	-3.288431	4.639206	95			
H	-0.720324	-1.927957	3.812604	C-5, E(ωB97XD /BSII)= -3167.077033 au			
H	-0.497713	-0.876878	2.391209	C	-3.658090	1.754078	-1.177250
H	-0.402396	-2.623777	2.202737	C	-3.190426	2.923666	-0.589509
H	2.687256	-0.473293	4.300634	C	-3.717450	0.556961	-0.471845
H	1.191824	0.358459	3.776576	C	-2.793277	2.892264	0.744706
H	1.139113	-0.797522	5.107294	H	-3.161522	3.841153	-1.168906
O	0.964412	-2.579672	0.188803	C	-3.298501	0.543275	0.858000
C	0.540595	-3.848127	-0.298394	H	-4.060348	-0.345662	-0.968209
C	-0.917532	-3.649270	-0.729055	C	-2.835080	1.706702	1.498258
C	0.601981	-4.931028	0.785461	H	-2.461942	3.815200	1.210799
C	1.374850	-4.303302	-1.499577	H	-3.304025	-0.402883	1.389671
H	-1.508420	-3.257524	0.105449	C	-2.393654	1.675659	2.912144
H	-0.992224	-2.936118	-1.561322	C	-1.392502	2.541484	3.378729
H	-1.364856	-4.591696	-1.063927	C	-2.942965	0.755648	3.817828
H	0.231572	-5.885558	0.392528	C	-0.940114	2.473386	4.692444
H	1.632798	-5.064354	1.119443	H	-0.927668	3.248492	2.699151
H	-0.017673	-4.657814	1.645188	C	-2.489928	0.685315	5.131785
H	1.378510	-3.538632	-2.286900	H	-3.747762	0.098990	3.498896
H	2.402604	-4.484991	-1.180102	C	-1.481635	1.539986	5.574723
H	0.970175	-5.226582	-1.930880	H	-0.150242	3.143223	5.022073
K	2.727273	1.106105	1.283437	H	-2.932538	-0.036277	5.813501
Si	-1.755129	3.017624	1.818277	H	-1.124230	1.481938	6.599304
C	-1.060999	4.522478	0.909118	F	-4.025647	1.774549	-2.470796
C	-3.614557	3.207981	2.119131	O	3.112911	0.589876	1.103129
C	-0.854040	2.800965	3.477048	O	1.369330	-0.750598	0.325268
H	-1.409650	5.432830	1.417467	C	2.901576	-0.406496	2.084890
H	-1.514505	4.542268	-0.091878	C	1.481745	-0.995045	1.724079
C	0.469950	4.529920	0.785966	C	4.026550	-1.446132	1.975423
H	-4.106868	3.312454	1.142533	H	4.982797	-0.928824	2.102818
H	-3.990472	2.264394	2.540543	H	3.954248	-2.228660	2.739339
C	-3.993655	4.377656	3.035162	H	4.032374	-1.901216	0.981302
H	0.201830	2.575390	3.264836	C	2.962894	0.246490	3.462808
H	-0.845740	3.770080	3.996268	H	3.964206	0.658823	3.625777
C	-1.446274	1.722032	4.390700	H	2.243682	1.065088	3.550078

H	2.758155	-0.481857	4.256421	H	-1.129985	-4.522444	-0.327306
C	1.344026	-2.494480	1.998050	H	-2.738932	-4.718984	-0.997290
H	1.441283	-2.708080	3.068573	C	-2.573084	-3.115997	0.445075
H	0.355078	-2.843070	1.677332	H	-3.530378	-3.459061	-3.591681
H	2.109006	-3.083580	1.480425	H	-3.925908	-2.386994	-2.267471
C	0.323242	-0.283405	2.421295	C	-3.241656	-1.362627	-4.043499
H	0.364573	0.790555	2.251777	H	0.018367	-4.905780	-2.874270
H	-0.622084	-0.649175	2.004858	H	-1.605063	-5.129386	-3.479855
H	0.297652	-0.457252	3.501912	C	-0.348835	-3.947639	-4.783245
B	2.455486	0.200798	-0.126910	H	-2.849227	-3.713625	1.325749
O	3.218505	-0.667888	-1.071063	H	-1.850895	-2.356742	0.777310
C	4.353052	-0.292359	-1.838974	H	-3.477621	-2.580185	0.126050
K	-0.488031	0.200368	-1.366434	H	-3.066400	-0.409397	-3.526929
C	4.938039	-1.603293	-2.382171	H	-2.473899	-1.448274	-4.823244
C	5.415205	0.394853	-0.977306	H	-4.213345	-1.270196	-4.549656
C	3.941098	0.595236	-3.019131	H	0.041083	-4.782486	-5.382709
H	5.847816	-1.423704	-2.965534	H	-1.179050	-3.504326	-5.346725
H	5.190253	-2.277308	-1.554161	H	0.437448	-3.178880	-4.735198
H	4.221178	-2.106254	-3.046743	95			
H	5.721378	-0.264045	-0.159630	C-6, E(ωB97XD /BSII)= -3167.080564 au			
H	6.297227	0.642028	-1.580203	C	-3.305646	-1.398461	2.593579
H	5.027992	1.310349	-0.532343	C	-3.867740	-1.128301	1.351763
H	3.512356	1.530993	-2.661402	C	-2.461155	-0.492080	3.225084
H	4.798543	0.812822	-3.667342	C	-3.574944	0.083969	0.731476
H	3.174662	0.086680	-3.617143	H	-4.512637	-1.861701	0.879670
O	1.902859	1.339733	-0.880087	C	-2.180093	0.717143	2.591215
C	1.853027	2.707996	-0.488137	H	-2.025410	-0.741528	4.186788
C	1.165883	3.439554	-1.647831	C	-2.730552	1.033681	1.336576
C	3.253203	3.294536	-0.281833	H	-4.021342	0.292318	-0.235231
C	1.034061	2.902435	0.790638	H	-1.488749	1.403785	3.069523
H	1.692918	3.240948	-2.586896	C	-2.403940	2.307606	0.653936
H	0.123378	3.111569	-1.762499	C	-2.117401	3.474831	1.378458
H	1.149286	4.521980	-1.478281	C	-2.367624	2.376022	-0.749084
H	3.759857	2.767550	0.529164	C	-1.784089	4.659724	0.727873
H	3.849680	3.203456	-1.195144	H	-2.171391	3.462435	2.463614
H	3.188345	4.358731	-0.024619	C	-2.042533	3.565080	-1.400437
H	0.033560	2.468099	0.680536	H	-2.564383	1.482016	-1.334028
H	1.536887	2.417748	1.628846	C	-1.741963	4.712052	-0.665114
H	0.912869	3.969342	1.016678	H	-1.564529	5.548618	1.313153
K	1.707655	-2.786610	-1.413181	H	-2.036181	3.592302	-2.488398
Si	-1.464612	-2.920693	-2.261610	H	-1.487430	5.639253	-1.171545
C	-2.001481	-3.956961	-0.698661	O	3.934890	-0.454414	0.736020
C	-3.192439	-2.547509	-3.073808	O	2.059642	-0.981884	-0.550063
C	-0.806532	-4.376118	-3.386422	C	4.408615	-0.845266	-0.538789

Atom	x	y	z	Atom	x	y	z
C	3.179333	-1.599193	-1.176210	H	2.018328	-3.225994	2.212911
C	4.805410	0.412585	-1.325290	H	3.664312	-2.559174	2.083458
H	5.560255	0.953684	-0.746189	H	3.060141	-3.157559	3.645648
H	5.228623	0.177792	-2.308482	K	0.623012	0.948209	-1.894978
H	3.946659	1.078716	-1.443444	Si	-1.934789	-1.215545	-2.525683
C	5.643270	-1.721109	-0.351171	C	-3.219862	-2.594139	-2.022957
H	6.008861	-2.104429	-1.311163	C	-3.104099	0.001899	-3.511868
H	6.442817	-1.130662	0.108339	C	-1.000842	-2.120465	-3.981178
H	5.434068	-2.568075	0.307232	H	-3.604899	-3.056499	-2.944007
C	3.070450	-1.443191	-2.693439	H	-4.087544	-2.106913	-1.552113
H	3.938291	-1.883561	-3.197695	C	-2.701394	-3.703450	-1.102980
H	2.173222	-1.956161	-3.057480	H	-3.814921	0.445739	-2.795805
H	3.016017	-0.393235	-2.999636	H	-2.504920	0.853002	-3.877930
C	3.144564	-3.098610	-0.863355	C	-3.895526	-0.591940	-4.681920
H	3.224089	-3.281312	0.207866	H	-0.328794	-2.881040	-3.554730
H	2.187592	-3.506997	-1.211019	H	-1.731319	-2.676443	-4.589033
H	3.945608	-3.646479	-1.371462	C	-0.197290	-1.198516	-4.902738
B	2.514895	-0.186079	0.657191	H	-2.498455	-3.325005	-0.089111
O	2.092945	1.189547	0.263660	H	-3.419023	-4.526578	-0.977981
C	2.257595	2.376905	1.027499	H	-1.772018	-4.147221	-1.487535
K	-0.298037	-1.604128	0.483146	H	-4.553235	-1.401784	-4.345223
C	3.699461	2.539607	1.513560	H	-4.528668	0.154625	-5.183039
C	1.270608	2.408562	2.198480	H	-3.229171	-1.016077	-5.442643
C	1.921493	3.532492	0.075119	H	0.295694	-1.738558	-5.723264
H	3.997249	1.707455	2.150463	H	-0.836272	-0.430646	-5.357901
H	4.384728	2.562793	0.661148	H	0.604181	-0.672633	-4.361449
H	3.809349	3.473521	2.077840	F	-3.558189	-2.579175	3.186228
H	1.318766	3.367413	2.729017	95			
H	0.255740	2.278883	1.811318	TS$_{C-6/C-7}$, E(ωB97XD /BSII)=			
H	1.472522	1.597109	2.896468	-3167.044214 au			
H	2.576314	3.499903	-0.805297	C	-3.768290	1.274744	3.412492
H	0.872986	3.483531	-0.247225	C	-4.521968	2.213846	4.130272
H	2.060722	4.503357	0.563648	C	-3.939084	1.161288	2.021933
O	1.772032	-0.572937	1.867926	C	-5.562411	2.870877	3.495498
C	2.265207	-1.223118	3.034954	H	-4.314144	2.369522	5.183201
C	1.064067	-1.316196	3.982161	C	-4.990843	1.826411	1.406439
C	3.381180	-0.420836	3.713835	H	-3.331090	0.453798	1.466918
C	2.784195	-2.629832	2.725059	C	-5.839618	2.685557	2.125777
H	0.647908	-0.319115	4.161369	H	-6.168137	3.567816	4.068883
H	0.270668	-1.941272	3.552051	H	-5.181911	1.640592	0.352168
H	1.349427	-1.756301	4.944102	C	-6.979786	3.360016	1.480233
H	3.708332	-0.924556	4.631340	C	-8.195345	3.525576	2.164732
H	4.235293	-0.328374	3.040203	C	-6.891408	3.848171	0.166214
H	3.032220	0.580396	3.985067	C	-9.275981	4.161610	1.561523

H	-8.300303	3.117842	3.167059	H	-1.719948	-0.123701	-1.980415
C	-7.974445	4.478174	-0.439478	H	-2.755165	0.020873	-0.558867
H	-5.953599	3.753111	-0.376582	H	-1.425159	1.172154	-0.823991
C	-9.172299	4.641383	0.255932	H	-0.776257	-2.950659	0.299966
H	########	4.269401	2.108905	H	-2.382873	-2.200923	0.307580
H	-7.879365	4.852709	-1.455913	H	-1.581319	-2.555985	-1.228940
H	########	5.134684	-0.216269	H	1.885735	-2.280646	5.070196
F	-2.481590	1.010948	3.916832	H	0.456379	-3.271790	4.715272
K	-1.110940	2.222423	1.846734	H	2.064858	-3.993257	4.624703
O	1.050822	0.857287	2.081833	H	3.594666	-3.497328	2.709739
B	0.760347	-0.553205	1.679846	H	3.180475	-2.229652	1.534804
C	2.264789	1.363569	2.618820	H	3.585785	-1.801418	3.215279
O	1.448221	-1.059594	0.511466	H	-0.089322	-3.886666	2.297983
O	-0.691201	-0.420547	1.223340	H	1.086920	-3.486306	1.021949
O	0.898168	-1.432099	2.849531	H	1.467644	-4.723609	2.240767
C	3.464864	0.983164	1.748413	Si	-4.954337	-1.356060	3.950402
C	2.453369	0.906024	4.068850	C	-6.654557	-0.462433	4.097283
C	2.122819	2.893069	2.603182	C	-4.962417	-2.109867	2.143735
C	0.697566	-0.763492	-0.647591	C	-5.252596	-2.957471	5.019306
C	-0.792847	-0.819938	-0.144277	H	-7.456925	-1.162536	3.821069
K	-1.678972	-1.556439	3.581032	H	-6.688202	0.345082	3.354186
C	1.603923	-2.670400	2.951713	C	-6.942388	0.104567	5.490618
H	3.572326	-0.097578	1.676786	H	-4.526434	-1.395111	1.429551
H	3.328205	1.366678	0.732682	H	-4.281132	-2.978534	2.148211
H	4.389358	1.403617	2.161617	C	-6.324979	-2.557423	1.602432
H	3.342612	1.366908	4.515158	H	-5.547708	-2.639929	6.029202
H	1.577163	1.190306	4.664007	H	-6.121428	-3.494903	4.606787
H	2.546339	-0.177408	4.120616	C	-4.069098	-3.921775	5.127087
H	1.940587	3.249740	1.580713	H	-6.139921	0.772102	5.827448
H	1.298956	3.217810	3.255541	H	-7.880862	0.676867	5.523096
H	3.031756	3.381670	2.970075	H	-7.027050	-0.695106	6.237097
C	1.104075	0.629479	-1.153952	H	-6.999173	-1.701255	1.485057
C	1.026797	-1.794261	-1.722436	H	-6.246979	-3.051367	0.622665
C	-1.723267	0.121705	-0.912440	H	-6.815043	-3.262735	2.285004
C	-1.411081	-2.219917	-0.200310	H	-4.306654	-4.830408	5.698279
C	1.498292	-3.077027	4.426445	H	-3.726364	-4.257893	4.136762
C	3.084340	-2.535911	2.578105	H	-3.215462	-3.447384	5.636242
C	0.977212	-3.757711	2.073334	95			
H	2.183045	0.623323	-1.336586	C-7, E(ωB97XD /BSII)= -3167.190037 au			
H	0.598738	0.907502	-2.085540	C	-3.133824	-1.070152	-2.193275
H	0.913472	1.388259	-0.389868	C	-3.460000	-1.572108	-0.919596
H	0.413399	-1.644995	-2.618851	C	-3.195342	0.322410	-2.370042
H	2.079393	-1.700040	-2.008899	C	-3.743628	-0.715072	0.145464
H	0.870360	-2.812306	-1.357355	H	-3.455834	-2.646150	-0.740346

C	-3.453785	1.183132	-1.310397	H	2.370193	-3.929544	2.027700
H	-2.969056	0.756454	-3.341291	C	5.217133	1.476064	0.247498
C	-3.686188	0.679572	-0.022652	C	5.838204	-0.933627	0.135148
H	-3.937358	-1.125334	1.134876	H	4.886206	0.525957	-2.681656
H	-3.405444	2.255255	-1.463134	H	3.145331	0.620697	-2.987105
C	-3.711304	1.594848	1.141447	H	3.949799	1.820811	-1.945588
C	-4.615735	1.431045	2.198417	H	3.415592	-2.301224	-0.752277
C	-2.749861	2.619263	1.212109	H	2.717915	-1.660163	-2.241833
C	-4.568824	2.275663	3.305147	H	4.476978	-1.872924	-2.108383
H	-5.370467	0.649726	2.141856	H	3.411950	0.884210	3.660654
C	-2.705465	3.454584	2.326262	H	4.189036	2.298352	2.955617
H	-2.013122	2.704460	0.409017	H	3.224968	2.468373	4.444070
C	-3.612609	3.289163	3.373247	H	0.666978	2.311818	4.316993
H	-5.282765	2.144798	4.114674	H	-0.109229	2.001358	2.753250
H	-1.946258	4.231389	2.383030	H	0.801583	0.709035	3.550574
H	-3.573396	3.943860	4.240279	H	2.838340	4.081376	1.812017
F	-0.686647	2.075227	-1.108011	H	1.050990	3.970450	1.784789
K	-0.347381	-0.064605	0.022844	H	1.898438	4.305413	3.299879
K	1.538704	2.791576	-0.951325	H	5.793225	1.562798	1.174147
O	1.537843	-0.657649	1.743819	H	5.874437	1.731286	-0.591742
O	2.392767	0.172702	-0.438269	H	4.398342	2.198403	0.309877
O	2.149017	1.619197	1.352067	H	6.435669	-0.814838	-0.776672
B	2.522654	0.198927	1.072254	H	6.488008	-0.748341	0.996924
C	1.732121	-1.887447	2.429279	H	5.492977	-1.968805	0.194295
C	3.643817	-0.153142	-1.025065	Si	-2.345445	-2.120172	-3.542274
C	2.048304	2.228212	2.631855	C	-0.473765	-1.781338	-3.486692
O	3.891987	-0.205614	1.315348	C	-2.666287	-3.956782	-3.211981
C	0.330649	-2.331795	2.865690	C	-3.032840	-1.624009	-5.233203
C	2.615664	-1.702684	3.667501	H	0.004432	-2.418606	-4.244955
C	2.344001	-2.956464	1.522717	H	-0.090357	-2.148502	-2.521888
C	4.667045	0.043550	0.161311	C	-0.051228	-0.320148	-3.705636
C	3.919170	0.761836	-2.223079	H	-2.191437	-4.232557	-2.259499
C	3.572642	-1.587540	-1.559073	H	-3.745474	-4.099340	-3.062004
C	3.292608	1.951996	3.478906	C	-2.166129	-4.882749	-4.328263
C	0.775753	1.782107	3.362661	H	-2.809707	-0.562811	-5.409502
C	1.954505	3.737016	2.364868	H	-2.477668	-2.174212	-6.006065
H	-0.149814	-1.547250	3.460778	C	-4.538799	-1.874059	-5.377406
H	-0.302223	-2.539079	1.991975	H	-0.457062	0.370077	-2.954676
H	0.373327	-3.246708	3.467125	H	1.041646	-0.222476	-3.678391
H	2.725776	-2.650670	4.207985	H	-0.382272	0.041747	-4.687068
H	3.605162	-1.352145	3.365805	H	-1.085751	-4.778456	-4.485731
H	2.172359	-0.971380	4.351437	H	-2.361101	-5.937453	-4.098849
H	1.754301	-3.060583	0.604373	H	-2.657928	-4.660106	-5.282761
H	3.364000	-2.670886	1.259275	H	-4.912251	-1.562317	-6.360561

H	-4.781780	-2.937073	-5.257715	H	-1.425760	0.373516	-2.637904
H	-5.105291	-1.322784	-4.617507	C	-0.131845	1.969882	1.733208
30				H	-0.865418	1.572310	2.448594

A, E(ωB97XD /BSII)= -1666.105675 au

C	-0.753923	1.247181	3.023867	H	0.852127	1.815840	2.196914
C	-0.581663	2.093229	4.303595	C	-0.377776	3.466482	1.506124
H	0.117299	1.590044	4.984565	H	-1.365670	3.650686	1.066381
H	-0.146094	3.066789	4.043450	H	-0.326875	4.034903	2.443617
H	-1.523257	2.268187	4.842181	H	0.366647	3.895219	0.824185
C	-1.378372	-0.113588	3.415108	C	1.034533	1.643746	-1.110495
H	-2.366810	-0.022040	3.885318	H	1.001899	1.032755	-2.023202
H	-1.478538	-0.739229	2.518744	H	0.687935	2.643850	-1.408365
H	-0.720666	-0.634815	4.126242	C	2.471613	1.715013	-0.579541
C	-1.751346	1.971232	2.088098	H	3.169073	2.094022	-1.337544
H	-1.363050	2.967165	1.828960	H	2.542426	2.380435	0.289710
H	-1.865316	1.394943	1.160747	H	2.825310	0.728072	-0.259932
H	-2.745694	2.109428	2.533788	B	0.351148	-0.978553	0.557387
O	0.456399	1.066450	2.400861	O	-0.463493	-2.077832	0.421406
K	2.245289	-0.654332	2.572559	O	1.613151	-1.310672	0.992442
C	4.649302	0.339678	0.095241	C	0.373753	-3.256392	0.558240
C	4.438947	0.545343	-1.423237	C	1.584547	-2.708450	1.382184
H	3.639257	-0.119966	-1.772186	C	-0.427249	-4.351325	1.243459
H	4.128533	1.581937	-1.620635	H	-1.250278	-4.668771	0.595456
H	5.340397	0.350303	-2.019926	H	0.206535	-5.222540	1.444057
C	5.167889	-1.102939	0.309437	H	-0.856028	-4.003767	2.186001
H	6.097331	-1.318128	-0.234748	C	0.756206	-3.680773	-0.859301
H	5.360887	-1.272133	1.378629	H	1.335385	-4.609979	-0.861438
H	4.404550	-1.819652	-0.022392	H	-0.157841	-3.838798	-1.439636
C	5.737722	1.321610	0.580827	H	1.341249	-2.899723	-1.355398
H	5.405035	2.354965	0.412080	C	1.344745	-2.733359	2.891357
H	5.888179	1.194432	1.660280	H	1.375404	-3.753085	3.288653
H	6.704260	1.187543	0.075794	H	2.124610	-2.144043	3.382883
O	3.476504	0.544574	0.779411	H	0.376446	-2.287479	3.140221
K	1.700069	2.282408	0.624445	C	2.928201	-3.336140	1.047503
43				H	3.194202	-3.178113	-0.000065

Et₃SiBpin, E(ωB97XD/BSII)= -1666.105675 au

				H	3.710239	-2.884362	1.665849
Si	-0.201874	0.924929	0.144995	H	2.912313	-4.413317	1.248714
C	-1.950116	0.955763	-0.594694	73			
H	-2.214864	1.993665	-0.842485				

B, E(ωB97XD/BSII)= -2604.579078 au

H	-2.659468	0.638811	0.182496	Si	-1.059843	-0.937631	2.193061
C	-2.100229	0.060031	-1.831345	C	-2.456499	-2.245087	2.284420
H	-1.863676	-0.982028	-1.588230	H	-3.034014	-2.064885	3.203160
H	-3.121109	0.086466	-2.233509	H	-1.975018	-3.224059	2.425508
				C	-3.398866	-2.319903	1.080208
				H	-2.835191	-2.537871	0.167333

H	-4.162855	-3.099382	1.205512	H	-2.437774	-0.602946	-0.980542
H	-3.926465	-1.371631	0.921493	H	-2.674894	0.805556	0.073770
C	0.101244	-1.433544	3.659210	C	-0.544175	0.472526	-2.630951
H	0.699656	-2.300354	3.334512	H	0.465472	0.822776	-2.880475
H	0.792094	-0.590590	3.825623	H	-0.560029	-0.618842	-2.663446
C	-0.590602	-1.766092	4.984303	H	-1.233600	0.862565	-3.389950
H	-1.257147	-2.628702	4.875661	O	-0.001647	0.474100	-0.266031
H	0.123286	-2.002312	5.786289	K	3.153463	-1.187107	2.800095
H	-1.202784	-0.926451	5.333433	C	4.920930	1.877181	2.762880
C	-1.800394	0.727837	2.790415	C	5.396684	1.356371	4.139669
H	-2.654020	0.999260	2.155470	H	4.543687	1.303179	4.829819
H	-2.220452	0.586544	3.796826	H	5.820896	0.347378	4.030533
C	-0.789183	1.878621	2.804517	H	6.166316	1.989217	4.600797
H	-1.227182	2.824977	3.149740	C	4.379330	3.311144	2.962357
H	0.063597	1.662737	3.462793	H	5.109995	3.990814	3.420569
H	-0.398244	2.041679	1.793937	H	4.091384	3.744101	1.992992
B	-0.008835	-0.884788	0.360746	H	3.486616	3.279868	3.599335
O	-0.453814	-1.908736	-0.589068	C	6.140234	1.935178	1.819303
O	1.444725	-1.262971	0.643220	H	6.531345	0.921924	1.663024
C	0.490893	-2.952636	-0.659444	H	5.833297	2.326983	0.840139
C	1.839316	-2.231384	-0.334262	H	6.953914	2.567320	2.199844
C	0.142170	-4.017829	0.390601	O	3.946501	1.056866	2.237801
H	-0.905114	-4.303632	0.256485	K	2.249649	1.547799	0.462612
H	0.762043	-4.917784	0.300476	73			
H	0.248538	-3.615216	1.402459	TSB/C, E(ωB97XD/BSII)= -2604.579078			
C	0.431365	-3.577876	-2.049602	au			
H	1.210022	-4.339161	-2.181438	Si	-1.664819	-0.954050	3.078179
H	-0.542286	-4.058732	-2.190029	C	-2.800701	-2.510071	2.847938
H	0.544128	-2.820168	-2.829032	H	-3.555951	-2.535931	3.648760
C	2.901978	-3.162507	0.248649	H	-2.188940	-3.415226	2.988343
H	3.108326	-3.991365	-0.437493	C	-3.504222	-2.580579	1.489582
H	3.852660	-2.629391	0.391853	H	-2.780990	-2.534949	0.667650
H	2.581695	-3.599045	1.201182	H	-4.096621	-3.499056	1.367908
C	2.435290	-1.512785	-1.548572	H	-4.192048	-1.735967	1.355876
H	1.690102	-0.860080	-2.004186	C	-1.170865	-1.169515	4.980995
H	3.288151	-0.902944	-1.221947	H	-0.715509	-2.173713	5.082775
H	2.805350	-2.212961	-2.305842	H	-0.381117	-0.446522	5.247132
C	-0.942596	0.945088	-1.227384	C	-2.292093	-1.062932	6.019319
C	-0.886232	2.476041	-1.171976	H	-3.114232	-1.752108	5.793517
H	-1.166895	2.837263	-0.176835	H	-1.943731	-1.288653	7.037608
H	0.125064	2.838327	-1.405944	H	-2.715748	-0.052184	6.040850
H	-1.567481	2.923543	-1.904368	C	-3.024536	0.434562	3.225181
C	-2.369852	0.484300	-0.925523	H	-3.576896	0.511825	2.278741
H	-3.070829	0.914210	-1.650840	H	-3.766983	0.091799	3.960803

C	-2.528740	1.825397	3.628151	H	4.048763	0.731548	6.955550
H	-3.346693	2.526959	3.843551	C	2.265712	2.429771	5.690333
H	-1.894655	1.788523	4.525438	H	2.799112	2.925914	6.512353
H	-1.938608	2.288619	2.822044	H	2.026201	3.198178	4.940596
B	0.015242	-0.867953	0.299266	H	1.321365	2.029250	6.079802
O	-0.513416	-1.893940	-0.465524	C	4.374270	1.875367	4.444038
O	1.281820	-1.216658	0.826362	H	4.953952	1.074382	3.968617
C	0.380737	-3.017941	-0.370682	H	4.126005	2.611510	3.667571
C	1.731749	-2.322869	0.007067	H	5.008393	2.368527	5.193518
C	-0.143606	-3.947060	0.721374	O	2.336883	0.672280	4.051492
H	-1.163349	-4.250023	0.470633	K	0.748762	1.554319	2.356093
H	0.470589	-4.848742	0.819417	73			
H	-0.195866	-3.421437	1.679438	C, E(ωB97XD/BSII)= -2604.58237 au			
C	0.394693	-3.733045	-1.713391	K	-0.469295	-0.870709	0.473893
H	1.136905	-4.539402	-1.716090	K	1.614816	0.730771	-2.039552
H	-0.588793	-4.173559	-1.903843	O	1.656840	-0.934883	1.997468
H	0.619384	-3.044525	-2.531536	O	2.046638	-1.480814	-0.395022
C	2.698658	-3.192752	0.795983	O	2.566547	0.622055	0.418480
H	3.039248	-4.034284	0.183441	B	2.578520	-0.807915	0.856622
H	3.580176	-2.608286	1.083355	C	1.815341	-1.691363	3.194212
H	2.240329	-3.614122	1.695833	C	3.013168	-2.399696	-0.894545
C	2.455241	-1.722044	-1.199880	C	2.948779	1.745898	1.202107
H	1.773692	-1.110280	-1.798377	O	3.857698	-1.439915	1.083350
H	3.261358	-1.075149	-0.839564	C	0.529758	-1.452995	3.995108
H	2.888914	-2.494679	-1.843236	C	3.016348	-1.207521	4.012997
C	-1.232177	0.954244	-0.872933	C	1.967950	-3.186264	2.909138
C	-1.333459	2.453027	-0.596590	C	4.331652	-1.993495	-0.128170
H	-1.744845	2.629718	0.403930	C	3.126847	-2.270750	-2.416353
H	-0.346820	2.926772	-0.670637	C	2.530491	-3.821735	-0.594254
H	-1.996026	2.935824	-1.322135	C	4.296919	1.519258	1.889533
C	-2.596760	0.294491	-0.698319	C	1.859595	2.092973	2.223763
H	-3.330542	0.778391	-1.353015	C	3.090708	2.913677	0.216630
H	-2.555143	-0.767500	-0.944867	H	0.371460	-0.380355	4.152064
H	-2.929722	0.391990	0.337032	H	-0.343340	-1.859174	3.465269
C	-0.669037	0.704032	-2.271968	H	0.574698	-1.943406	4.973614
H	0.321767	1.161669	-2.371016	H	3.095300	-1.773808	4.948702
H	-0.583669	-0.370326	-2.455817	H	3.935582	-1.346548	3.440103
H	-1.328334	1.134689	-3.033812	H	2.910606	-0.147805	4.266838
O	-0.281529	0.461510	0.099749	H	1.140832	-3.546899	2.286066
K	1.575387	-1.625690	3.642409	H	2.909199	-3.363845	2.386150
C	3.075952	1.287726	5.035244	H	1.969111	-3.763097	3.841540
C	3.458466	0.281453	6.146236	C	5.148633	-0.920376	-0.864093
H	2.547242	-0.144144	6.588421	C	5.245173	-3.171415	0.195554
H	4.052482	-0.537158	5.715061	H	3.876722	-2.966040	-2.810239

H	2.167270	-2.511637	-2.887501		-1477.44735 au		
H	3.431268	-1.267123	-2.732436	O	-3.550360	-1.135736	0.227409
H	2.449219	-3.993137	0.477935	O	-1.759966	-2.608020	0.284167
H	1.535026	-3.950819	-1.035097	C	-4.104567	-2.371729	0.641798
H	3.192209	-4.583271	-1.021250	C	-2.901584	-3.417999	0.500599
H	4.252217	0.674258	2.575127	C	-4.611280	-2.219961	2.082918
H	5.066807	1.297564	1.144623	H	-5.364914	-1.425237	2.101519
H	4.596104	2.412514	2.450710	H	-5.074890	-3.137101	2.463649
H	2.114814	3.004141	2.777843	H	-3.795685	-1.924223	2.744937
H	0.906312	2.262795	1.706930	C	-5.301581	-2.670215	-0.259970
H	1.721774	1.271565	2.926588	H	-5.782401	-3.618314	0.007308
H	3.841924	2.677201	-0.548159	H	-6.038944	-1.868501	-0.146329
H	2.130964	3.130489	-0.272699	H	-5.014989	-2.708137	-1.313836
H	3.408044	3.829509	0.727061	C	-2.665289	-4.262559	1.757226
H	5.957797	-0.596209	-0.202224	H	-3.526010	-4.895663	2.002379
H	5.592865	-1.288458	-1.795764	H	-1.804577	-4.922111	1.587370
H	4.532265	-0.040804	-1.070777	H	-2.439371	-3.623293	2.614209
H	5.590801	-3.669389	-0.718062	C	-3.031854	-4.357619	-0.701356
H	6.123022	-2.813045	0.743192	H	-3.143534	-3.799354	-1.632946
H	4.737676	-3.907515	0.823882	H	-2.115443	-4.954389	-0.782250
Si	-1.656335	0.365183	-2.410883	H	-3.878209	-5.045915	-0.598663
C	-2.088040	-1.447279	-2.988254	B	-2.128524	-1.169251	0.463106
C	-3.403996	1.151030	-2.108760	O	-1.671801	-0.858016	1.855048
C	-1.133110	1.147792	-4.125238	C	-1.781831	0.420390	2.468221
H	-2.713944	-1.414577	-3.893114	K	0.569541	-1.813454	0.819190
H	-2.709988	-1.931266	-2.217067	C	-3.044268	1.173656	2.040990
C	-0.856317	-2.315748	-3.267351	C	-0.548020	1.274224	2.130445
H	-3.848581	0.635201	-1.242252	C	-1.822159	0.154262	3.975534
H	-3.256540	2.189292	-1.776084	H	-3.021528	1.388514	0.970828
C	-4.392232	1.121692	-3.279193	H	-3.934469	0.573824	2.238820
H	-0.211810	0.666251	-4.498985	H	-3.120754	2.120542	2.589431
H	-1.899858	0.887791	-4.870699	H	-0.594637	2.256355	2.615889
C	-0.952193	2.668515	-4.104787	H	0.370063	0.781932	2.487659
H	-0.214344	-2.413144	-2.378920	H	-0.483713	1.413207	1.048103
H	-1.110201	-3.334199	-3.594368	H	-2.713319	-0.427121	4.233815
H	-0.232373	-1.875128	-4.057938	H	-0.941095	-0.424441	4.280113
H	-4.583197	0.095863	-3.617067	H	-1.837756	1.088921	4.548597
H	-5.363812	1.565425	-3.018128	O	-1.308599	-0.325325	-0.415459
H	-4.006506	1.677659	-4.142623	C	-1.606679	-0.037878	-1.775492
H	-0.632540	3.077060	-5.073600	C	-0.300478	0.491091	-2.374519
H	-1.890124	3.167709	-3.832878	C	-2.687160	1.046470	-1.839889
H	-0.211855	2.991167	-3.354624	C	-2.063987	-1.279607	-2.544731
50				H	0.067954	1.336679	-1.782237
K(OᵗBu)₂Bpin, E(ωB97XD/BSII) =				H	0.468341	-0.293828	-2.375953

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K(O^{t}Bu)$_2$Bpin, E(ωB97XD/BSII) = −1477.44735 au

H	-0.439684	0.825535	-3.408697	H	-2.342188	-0.184726	-0.317376
H	-2.920466	1.313768	-2.877970	H	-0.522001	1.056441	1.687714
H	-3.594789	0.682978	-1.351527	H	2.363866	2.061727	-0.299780
H	-2.344964	1.948245	-1.319145	H	-0.274101	-1.965356	1.553243
H	-1.341095	-2.093580	-2.427545	H	2.549532	-0.173270	-1.022197
H	-3.024491	-1.620448	-2.154908	H	1.691590	-1.996697	0.198706
H	-2.173375	-1.052334	-3.612066	C	-0.872257	1.135225	-1.047773
23				H	-1.532067	1.376901	-1.881217

D, E(ωB97XD/BSII) = -1127.102983 au

				C	0.275921	2.097975	-0.855820
C	-1.880348	0.986291	-0.576338	H	0.634153	2.382049	-1.853841
H	-1.987396	2.039691	-0.877960	H	-0.068026	3.030941	-0.379396
H	-2.648451	0.809743	0.191059	Ni	-0.004559	-0.745717	-1.424407
C	-2.146169	0.090682	-1.788518	C	1.086389	-1.013702	-3.223890
H	-2.091610	-0.973923	-1.516793	C	-1.417933	-2.235199	-1.954927
H	-3.136699	0.261976	-2.233401	C	-0.260548	-2.835181	-1.481814
H	-1.402430	0.257240	-2.578735	C	-0.038048	-0.239811	-3.467661
C	-0.151333	1.955773	1.747068	H	2.025176	-0.476388	-3.104131
H	-0.905830	1.587853	2.458581	C	1.221166	-2.495266	-3.528543
H	0.812297	1.862225	2.269300	C	-1.802941	-2.080798	-3.416121
C	-0.418769	3.431090	1.427206	H	-2.241304	-2.155212	-1.247739
H	-1.385099	3.563128	0.925605	C	0.877870	-3.376172	-2.315415
H	-0.431150	4.058037	2.330605	H	-0.284189	-3.201530	-0.455225
H	0.349530	3.840227	0.759669	H	0.117183	0.835833	-3.550853
C	1.035204	1.611887	-1.046884	C	-1.363856	-0.726938	-4.002354
H	0.999597	1.046536	-1.989670	H	2.250631	-2.704884	-3.843011
H	0.627373	2.607873	-1.280512	H	0.592563	-2.756645	-4.385865
C	2.486793	1.751145	-0.584442	H	-1.384841	-2.907233	-4.000074
H	3.128214	2.231521	-1.336713	H	-2.891375	-2.174839	-3.511201
H	2.556012	2.349960	0.332882	H	0.673519	-4.411011	-2.636278
H	2.929294	0.769763	-0.357387	H	1.761004	-3.428814	-1.665793
Si	-0.137382	0.751875	0.230704	H	-2.118461	0.025675	-3.740197
K	0.690420	-2.305824	0.716792	H	-1.349395	-0.773108	-5.103833
41				64			

Ni(cod)₂, E(ωB97XD/BSII) = -794.9880765 au

E, E(ωB97XD/BSII) = -1922.12016 au

				Ni	0.602517	-0.527059	-1.867092
C	-1.355484	0.228194	-0.116146	Si	0.292209	0.586041	0.116348
C	-0.877808	0.089236	1.318833	C	2.088028	0.593826	0.810009
C	1.453029	1.496252	-0.068932	C	-0.183821	2.476230	0.164736
C	0.212427	-0.984342	1.475368	C	-0.748243	-0.122907	1.587167
C	1.682243	0.031275	-0.397262	K	-2.177352	0.577192	-1.999949
C	1.167280	-1.047083	0.306008	H	2.078986	1.004423	1.830835
H	-1.731110	-0.172400	1.956041	H	2.674279	1.298894	0.202528
H	0.759921	-0.841163	2.421607	C	2.782163	-0.772283	0.811749
H	1.297881	1.616659	1.008118	H	0.501503	2.986319	-0.526968

H	-1.192149	2.652227	-0.256069		H	0.581350	-2.402202	-0.127209
C	-0.114625	3.154103	1.537082		C	-1.421246	-2.619180	-0.958050
H	-0.539858	-1.197522	1.679098		H	0.634889	-2.863641	-4.387029
H	-0.374020	0.333254	2.515411		H	-0.872526	-2.963755	-3.516834
C	-2.262097	0.099901	1.511270		H	-2.144240	-4.176120	-2.302748
H	2.841995	-1.181110	-0.204847		H	-2.660774	-4.383970	-0.643383
H	3.803534	-0.720245	1.213212		H	-0.224506	-5.234345	-4.063840
H	2.230535	-1.501939	1.418535		H	1.451652	-4.926194	-3.669207
H	0.886055	3.054651	1.973158		H	-1.756319	-2.363546	0.052599
H	-0.343273	4.228207	1.486922		H	-2.038666	-2.016995	-1.644607
H	-0.819047	2.703124	2.246492		77			
H	-2.794038	-0.265549	2.400430		E-THF, E(ωB97XD/BSII) =			
H	-2.509536	1.166604	1.411218		-2154.5763014au			
H	-2.710160	-0.433909	0.657541		Ni	0.408793	-0.389650	-1.798458
C	-0.005079	0.901643	-6.247150		Si	0.483627	0.665761	0.239112
C	1.278369	1.140286	-2.712911		C	2.345279	0.458700	0.694495
C	1.832283	-0.009132	-3.338002		C	0.217414	2.591434	0.394966
C	0.286245	2.181235	-5.973991		C	-0.422325	0.016451	1.821900
H	-0.462370	0.708894	-7.218625		K	-2.250689	0.992754	-1.605065
C	0.274829	-0.333938	-5.421668		H	2.517422	0.842560	1.711121
C	0.318508	2.083851	-3.414377		H	2.928552	1.103378	0.020490
H	1.936988	1.674557	-2.023439		C	2.863235	-0.979739	0.592474
C	1.676750	-0.424923	-4.783687		H	0.844645	3.064532	-0.374490
H	2.815237	-0.302183	-2.952675		H	-0.819062	2.874141	0.129392
H	0.056750	2.912408	-6.750225		C	0.543805	3.208758	1.759062
C	0.868730	2.747147	-4.703435		H	-0.295177	-1.073456	1.874567
H	0.137176	-1.197501	-6.083411		H	0.098487	0.419059	2.703431
H	-0.470187	-0.474854	-4.621001		C	-1.909579	0.366660	1.928451
H	-0.602924	1.571221	-3.722086		H	2.749423	-1.363274	-0.429647
H	0.020784	2.864665	-2.703314		H	3.924263	-1.063171	0.866193
H	2.018858	-1.463502	-4.859045		H	2.302461	-1.655251	1.251715
H	2.373761	0.156471	-5.409157		H	1.580131	2.998107	2.047192
H	1.963924	2.657360	-4.711026		H	0.418610	4.301105	1.766886
H	0.659724	3.824156	-4.683819		H	-0.097653	2.801381	2.550095
C	0.799407	-2.461437	-2.261230		H	-2.365497	0.024373	2.868043
C	-0.687751	-5.095229	-1.066038		H	-2.070863	1.453111	1.876041
C	0.262433	-5.355215	-1.970956		H	-2.493760	-0.101602	1.121417
C	0.052120	-2.253938	-1.069842		C	0.544461	1.472110	-6.216287
H	1.864449	-2.680392	-2.131402		C	1.173664	1.224636	-2.676499
C	0.197128	-3.190573	-3.438345		C	1.602565	0.037118	-3.329167
C	-1.799042	-4.106332	-1.264272		C	0.796208	2.683679	-5.704112
H	-0.648919	-5.615621	-0.109242		H	0.668675	1.386611	-7.296893
C	0.425717	-4.722927	-3.335008		C	0.220410	0.165461	-5.530635
H	1.016766	-6.097274	-1.707978		C	0.187884	2.243252	-3.219548

H	1.912681	1.708073	-2.031673	H	-5.839023	-0.938384	-2.754882
C	1.412131	-0.422180	-4.755886	O	-3.914682	-0.340170	-3.258677
H	2.556469	-0.340856	-2.940239	22			
H	1.087065	3.453812	-6.421976	ArF, E(ωB97XD/BSII) = -562.4747319 au			
C	0.734148	3.192876	-4.293084	C	-1.509996	0.971856	-0.017625
H	-0.083677	-0.550345	-6.304906	C	-0.173796	1.027613	-0.439836
H	-0.633175	0.243960	-4.848727	C	0.515049	2.237022	-0.472832
H	-0.710183	1.763872	-3.632031	C	-0.117553	3.416012	-0.080820
H	-0.140541	2.863822	-2.373390	C	-1.445491	3.374822	0.342599
H	1.340263	-1.517625	-4.758744	C	-2.134659	2.165757	0.372217
H	2.325574	-0.188245	-5.325958	C	-2.242614	-0.314061	0.016524
H	1.738147	3.529518	-3.990321	C	-2.091853	-1.257895	-1.010267
H	0.119851	4.108295	-4.304662	C	-2.776188	-2.469118	-0.985466
C	0.154793	-2.250002	-2.397908	C	-3.623783	-2.735376	0.081412
C	-1.417819	-4.807876	-1.251244	C	-3.801538	-1.827883	1.117305
C	-0.826745	-5.014386	-2.433211	C	-3.107580	-0.622915	1.077221
C	-0.233935	-2.106179	-1.037260	H	0.335689	0.108560	-0.718832
H	1.143457	-2.678112	-2.590795	H	1.552832	2.256530	-0.796030
C	-0.867233	-2.614072	-3.447247	H	0.420138	4.360223	-0.105130
C	-2.348279	-3.666549	-0.964324	H	-1.950659	4.289805	0.641700
H	-1.202001	-5.495041	-0.433405	H	-3.178481	2.146962	0.675750
C	-0.949633	-4.149525	-3.667664	H	-1.448028	-1.029637	-1.855467
H	-0.168908	-5.878537	-2.526751	H	-2.671756	-3.199803	-1.781093
H	0.498802	-2.429906	-0.295118	H	-4.464640	-2.077617	1.939328
C	-1.660974	-2.324764	-0.548720	H	-3.219354	0.081262	1.897278
H	-0.637112	-2.157913	-4.417665	F	-4.289471	-3.903190	0.112996
H	-1.844561	-2.212084	-3.156968	20			
H	-2.951187	-3.490064	-1.862912	cod, E(ωB97XD/BSII) = -311.9957903 au			
H	-3.060433	-3.952579	-0.178892	C	0.639700	-2.435459	-2.373398
H	-1.881245	-4.392271	-4.207226	C	-0.954015	-5.196201	-1.242371
H	-0.138778	-4.431356	-4.351804	C	0.072993	-5.525091	-2.034022
H	-1.655443	-2.249666	0.542787	C	0.018927	-2.190398	-1.214085
H	-2.339757	-1.530103	-0.888308	H	1.586924	-1.918674	-2.533060
C	-4.819267	-2.373963	-4.036836	C	0.234981	-3.367653	-3.487909
C	-4.619857	-1.447320	-5.238653	C	-1.861669	-3.993609	-1.314789
C	-3.654465	-0.406656	-4.677045	H	-1.152970	-5.866832	-0.405455
C	-4.838551	-1.376344	-2.887053	C	0.643363	-4.829940	-3.239791
H	-5.734347	-2.970602	-4.092109	H	0.598073	-6.448700	-1.783236
H	-3.967536	-3.055521	-3.933843	H	0.505922	-1.475311	-0.548422
H	-5.570531	-0.981134	-5.523539	C	-1.265128	-2.738571	-0.654247
H	-4.212365	-1.957332	-6.116100	H	0.726875	-3.039526	-4.412325
H	-2.612107	-0.710697	-4.821968	H	-0.836883	-3.307267	-3.691089
H	-3.794239	0.592255	-5.105443	H	-2.153574	-3.772444	-2.344377
H	-4.512151	-1.801625	-1.932492	H	-2.796098	-4.230375	-0.790464

H	0.401738	-5.423685	-4.136278	C	-0.499387	-4.306089	-2.784002
H	1.739716	-4.872505	-3.157657	H	-0.656154	-3.547649	-0.772936
H	-1.094008	-2.958223	0.410146	C	0.171524	-4.221134	-4.003797
H	-2.022944	-1.938422	-0.661792	H	1.775277	-3.265633	-5.082795
66				H	-1.341373	-4.984786	-2.670942
F, E(ωB97XD/BSII) = -2172.588817 au				H	-0.138161	-4.837235	-4.844057
Ni	-0.154132	0.579539	-0.536455	Si	-1.719713	0.442623	1.181429
K	0.356266	2.795367	1.790351	C	-3.430034	1.339703	1.054289
H	1.299215	-3.321704	0.740495	C	-2.095411	-1.432388	0.937693
C	1.464896	-2.260060	0.577125	C	-1.560233	0.577537	3.141156
C	1.774217	0.506981	0.203323	H	-4.142829	0.824283	1.714368
C	2.004186	-0.120749	1.458637	H	-3.833311	1.228279	0.039567
C	1.856528	-1.451651	1.683580	C	-3.399004	2.824100	1.436180
H	2.263068	1.473431	0.048855	H	-2.235564	-1.596158	-0.140526
H	1.990817	-1.869949	2.674164	H	-1.165910	-1.962160	1.186017
C	-0.580409	0.407035	-2.529396	C	-3.272364	-2.022638	1.719392
C	0.355312	0.971253	-3.585172	H	-1.427042	1.620110	3.488300
C	-1.039494	3.587058	-1.704703	H	-2.573746	0.330349	3.492154
C	1.198382	2.223938	-3.236455	C	-0.560809	-0.323704	3.872393
C	-0.420091	4.128488	-2.959917	H	-2.673050	3.383251	0.825771
C	0.558291	3.521859	-3.638598	H	-4.368723	3.322254	1.298925
H	-0.220849	1.181363	-4.499990	H	-3.124640	2.959268	2.492000
H	1.391572	2.212376	-2.154698	H	-4.219343	-1.541664	1.446561
H	-0.264809	3.154405	-1.050875	H	-3.390888	-3.099713	1.534604
H	-0.855424	5.041367	-3.367200	H	-3.143694	-1.893741	2.801575
H	-0.714948	-0.669431	-2.665912	H	-0.721788	-0.318318	4.959777
H	1.042331	0.160360	-3.857852	H	-0.649188	-1.361546	3.532451
H	-1.511574	4.409527	-1.150429	H	0.475948	-0.023453	3.696445
H	2.175016	2.143771	-3.729681	66			
H	0.891822	3.962875	-4.578258	G, E(ωB97XD/BSII) = -2172.590058 au			
C	-1.634302	1.032568	-1.839566	Ni	-0.115348	0.459144	0.009280
H	-2.477780	0.373222	-1.617174	K	0.799614	2.246443	2.407569
C	-2.089074	2.477579	-1.958360	H	0.285745	-3.947902	0.298014
H	-2.517520	2.631191	-2.961302	C	0.716339	-2.960394	0.151184
H	-2.914621	2.618181	-1.256645	C	1.731122	-0.376248	-0.277111
F	2.335829	0.725716	2.491857	C	1.101447	-0.698811	0.978557
C	1.342559	-1.747241	-0.696838	C	0.665283	-2.056210	1.172773
C	1.575254	-0.339897	-0.939467	H	2.434313	0.454861	-0.310923
H	1.971348	-0.042526	-1.904826	H	0.246822	-2.332840	2.132910
C	0.965864	-2.615052	-1.832567	C	-0.294792	0.828968	-1.968614
C	1.632181	-2.539564	-3.064816	C	0.832082	1.403656	-2.809290
C	-0.107383	-3.510272	-1.710110	C	-0.452178	3.890251	-0.698256
C	1.240991	-3.335327	-4.138316	C	1.752879	2.485984	-2.195152
H	2.476280	-1.863519	-3.176279	C	0.339472	4.518363	-1.807124

C	1.311706	3.892376	-2.475908	H	-3.637937	3.850514	2.141847
H	0.407334	1.801163	-3.744832	H	-2.561356	3.042581	3.277691
H	1.802629	2.308904	-1.113057	H	-4.616196	-0.907132	2.148645
H	0.202839	3.270421	-0.066796	H	-4.328388	-2.570429	1.628597
H	0.043748	5.521723	-2.113457	H	-3.462586	-1.916505	3.022277
H	-0.541978	-0.187526	-2.295190	H	-0.796447	-0.867902	5.256022
H	1.460190	0.557101	-3.105577	H	-1.174601	-1.837412	3.831214
H	-0.869375	4.680030	-0.060456	H	0.278289	-0.840022	3.847858
H	2.769634	2.345023	-2.581517	66			
H	1.788606	4.403261	-3.312376	H, E(ωB97XD/BSII) = -2172.586534 au			
C	-1.332969	1.481932	-1.285618	Ni	-0.659838	0.507399	0.198378
H	-2.271380	0.921831	-1.249814	C	1.873290	-2.275539	0.356184
C	-1.597288	2.974455	-1.188362	C	0.779654	0.268922	1.319625
H	-1.925063	3.332809	-2.176630	C	0.636673	-0.985092	2.053184
H	-2.453498	3.112377	-0.524367	C	1.138394	-2.177133	1.582411
F	1.732230	-0.131331	2.145660	H	0.979109	-3.077586	2.173021
C	1.325343	-2.649970	-1.109691	C	-1.506828	-0.356517	-1.423414
C	1.872026	-1.396075	-1.265428	C	-0.613395	-0.941530	-2.502865
H	2.461542	-1.177423	-2.152468	C	-0.815753	2.621261	-2.611193
C	1.409791	-3.659096	-2.182521	C	0.389699	-0.068362	-3.268475
C	1.266833	-3.284275	-3.528989	C	-0.741996	2.041969	-3.993202
C	1.634900	-5.016000	-1.898161	C	-0.233153	0.842863	-4.284224
C	1.360617	-4.224581	-4.551178	H	-1.276840	-1.426966	-3.237956
H	1.052415	-2.244885	-3.766960	H	0.967121	0.510519	-2.540997
C	1.720589	-5.958481	-2.919351	H	0.040415	2.317579	-1.993863
H	1.771513	-5.329037	-0.865981	H	-1.215376	2.623402	-4.785286
C	1.586619	-5.568195	-4.251930	H	-2.003246	-1.187212	-0.905632
H	1.240595	-3.909248	-5.585050	H	-0.054168	-1.755746	-2.023547
H	1.902752	-7.002070	-2.673540	H	-0.787280	3.716691	-2.670314
H	1.652889	-6.304595	-5.048767	H	1.099951	-0.739432	-3.769448
Si	-1.793106	0.422039	1.615385	H	-0.298628	0.472847	-5.307635
C	-3.199671	1.749036	1.635937	C	-2.157425	0.858965	-1.201729
C	-2.712128	-1.186431	1.101195	H	-3.087924	0.764096	-0.642095
C	-1.579115	0.281719	3.558497	C	-2.105481	2.205458	-1.888229
H	-4.033191	1.340802	2.226133	H	-2.943261	2.252994	-2.603392
H	-3.593108	1.867639	0.617962	H	-2.329892	2.953515	-1.121963
C	-2.823004	3.117114	2.213022	C	1.988236	-1.106309	-0.399910
H	-3.110941	-0.996307	0.093089	C	1.416102	0.115847	0.006938
H	-1.965863	-1.979069	0.966416	H	1.659074	1.018500	-0.554984
C	-3.837584	-1.669346	2.021428	K	3.518653	-0.299139	2.117405
H	-1.213501	1.234732	3.985444	H	0.100844	-0.962238	2.998849
H	-2.612440	0.221712	3.933192	F	1.453508	1.287304	2.149451
C	-0.771058	-0.871320	4.157378	H	2.492299	-1.145045	-1.364531
H	-1.964026	3.557750	1.685410	C	2.461376	-3.551896	-0.086958

C	3.673366	-3.586403	-0.802099	H	-2.230255	3.454348	3.260046
C	1.842672	-4.783425	0.195088	H	0.754428	3.108597	-1.527528
C	4.234767	-4.788855	-1.222323	H	2.149897	3.034959	0.327098
H	4.187507	-2.653248	-1.025425	H	-3.094269	1.634142	1.954309
C	2.409546	-5.987186	-0.214150	H	1.786554	2.466119	2.513926
H	0.887159	-4.793379	0.713075	H	0.114912	3.867704	3.513917
C	3.609217	-5.999996	-0.926265	C	-1.099722	2.500595	-0.763315
H	5.171747	-4.780291	-1.774667	H	-1.464526	2.711338	-1.772219
H	1.901486	-6.921743	0.011874	C	-2.249617	2.615922	0.220115
H	4.048737	-6.940160	-1.248556	H	-2.477404	3.685352	0.354144
Si	-1.867706	1.383682	1.923367	H	-3.128605	2.184822	-0.264361
C	-3.003013	-0.038636	2.556307	Si	-1.720447	-0.383209	-2.087199
C	-0.979992	1.989484	3.522984	C	-1.451053	-0.162317	-3.976408
C	-3.040567	2.846668	1.501913	C	-1.891017	-2.318059	-1.833896
H	-3.550095	0.342177	3.431785	C	-3.570537	0.139253	-1.885583
H	-2.355294	-0.844100	2.932589	H	-2.314455	-0.580067	-4.514295
C	-3.999177	-0.618988	1.550759	H	-0.573049	-0.744836	-4.279243
H	-0.362240	1.170032	3.913457	C	-1.246388	1.302627	-4.376727
H	-0.262058	2.767181	3.234779	H	-0.900602	-2.775541	-1.697942
C	-1.900859	2.511703	4.631390	H	-2.453713	-2.513986	-0.901779
H	-3.626824	2.611368	0.604102	C	-2.622800	-3.048748	-2.965357
H	-3.775204	2.941718	2.315600	H	-3.637959	1.228192	-2.012332
C	-2.302729	4.177420	1.315646	H	-4.132877	-0.283517	-2.731392
H	-3.480656	-1.085143	0.704428	C	-4.253891	-0.280691	-0.581120
H	-4.643452	-1.388008	1.999285	H	-0.360100	1.716369	-3.880686
H	-4.659323	0.157791	1.143496	H	-1.108333	1.423152	-5.459952
H	-2.603513	1.742470	4.974549	H	-2.105330	1.923055	-4.087714
H	-1.334914	2.846814	5.512592	H	-2.071627	-2.961077	-3.907953
H	-2.500872	3.365015	4.292851	H	-2.752834	-4.120329	-2.757480
H	-2.970301	4.987168	0.990196	H	-3.619782	-2.624040	-3.134060
H	-1.828429	4.501140	2.250173	H	-5.257601	0.151257	-0.466182
H	-1.499581	4.089396	0.571633	H	-4.371191	-1.371025	-0.527892
66				H	-3.677808	0.031332	0.302616
I, E(ωB97XD/BSII) = -2172.5896425 au				Ni	0.001939	0.812166	-1.081374
K	-0.828091	-1.436394	0.957039	C	1.384414	-0.388442	-1.889730
C	0.273200	2.765800	-0.603754	F	1.480667	-0.032453	-3.219651
C	1.096576	3.189510	0.597095	C	1.994264	0.527055	-0.951690
C	-2.108853	1.977429	1.615483	C	1.498928	-1.798699	-1.650237
C	0.847092	2.484792	1.946644	C	2.358028	-0.009291	0.317371
C	-1.523624	2.898241	2.644245	H	2.506752	1.413948	-1.317449
C	-0.215838	3.128929	2.783866	C	1.855440	-2.265246	-0.415001
H	0.989074	4.276179	0.743226	C	2.229351	-1.355551	0.638336
H	0.594580	1.439970	1.723938	H	2.823081	0.659929	1.036829
H	-1.477782	1.085233	1.496126	H	1.271885	-2.471972	-2.471670

H	1.870701	-3.337274	-0.232687	H	-2.381624	-3.085659	0.651239
C	2.495804	-1.850259	2.005903	C	-2.342159	-3.905081	-1.322302
C	2.214393	-1.046547	3.129442	H	-4.024891	0.287196	-0.866512
C	2.988476	-3.146988	2.244398	H	-4.201233	-1.241158	-1.691055
C	2.419755	-1.514739	4.425261	C	-4.561718	-1.356369	0.427304
H	1.825460	-0.041638	2.983223	H	-0.678338	0.974719	-2.858220
C	3.188154	-3.615690	3.539998	H	-1.298347	0.312268	-4.378826
H	3.250185	-3.783795	1.403817	H	-2.422605	0.851164	-3.123829
C	2.903014	-2.805413	4.639856	H	-1.734914	-3.881642	-2.233358
H	2.193660	-0.868398	5.270125	H	-2.352218	-4.942703	-0.961038
H	3.581151	-4.618236	3.691114	H	-3.368905	-3.647444	-1.610176
H	3.060307	-3.173660	5.650030	H	-5.619967	-1.063286	0.429675
66				H	-4.532039	-2.452548	0.435736
TSI/L, E(ωB97XD/BSII) = -2172.550352				H	-4.143917	-1.013564	1.387098
au				Ni	-0.500810	0.589821	-0.031315
K	-1.014045	-1.656983	2.425856	C	1.019513	-0.535626	0.306670
C	-0.823155	2.618609	-0.166367	F	1.443500	0.579659	-0.696629
C	0.273890	3.407427	0.520535	C	1.496403	-0.167930	1.617139
C	-2.156637	2.065853	2.822673	C	1.387065	-1.855079	-0.124096
C	0.413908	3.407949	2.047766	C	1.942370	-1.128232	2.513840
C	-1.828418	3.494899	3.144594	H	1.500517	0.880559	1.891855
C	-0.699290	4.101914	2.772767	C	1.812062	-2.794335	0.788976
H	0.172471	4.451331	0.182702	C	2.028824	-2.493339	2.164270
H	0.491553	2.372028	2.394402	H	2.213865	-0.810751	3.520060
H	-1.246458	1.447014	2.808490	H	1.229493	-2.123976	-1.164133
H	-2.610599	4.071508	3.638143	H	2.001217	-3.807021	0.438344
H	-0.726517	2.741913	-1.250356	C	2.333655	-3.540775	3.149287
H	1.223186	3.052956	0.092687	C	3.136555	-3.293766	4.280166
H	-2.821107	1.656936	3.596649	C	1.793590	-4.836230	3.013863
H	1.369775	3.887509	2.293632	C	3.375740	-4.284108	5.227835
H	-0.574932	5.165375	2.975581	H	3.605710	-2.320382	4.398671
C	-2.022764	2.021482	0.199550	C	2.043521	-5.829947	3.956083
H	-2.660607	1.823800	-0.663521	H	1.156082	-5.060554	2.160789
C	-2.850320	1.938293	1.461209	C	2.832073	-5.560628	5.075099
H	-3.635016	2.709817	1.400431	H	4.007478	-4.061921	6.084929
H	-3.378659	0.978893	1.415404	H	1.610946	-6.818649	3.819583
Si	-1.884270	-1.060975	-0.791765	H	3.025512	-6.334511	5.813092
C	-1.444629	-1.052438	-2.663826	66			
C	-1.791097	-2.934770	-0.270154	TSI/M, E(ωB97XD/BSII) = -2172.55481			
C	-3.801754	-0.782970	-0.773861	au			
H	-2.153592	-1.707328	-3.191394	H	3.494334	-0.327939	3.006991
H	-0.449951	-1.499537	-2.797705	H	1.681990	-0.128360	-1.582321
C	-1.463021	0.344375	-3.293617	H	3.379106	1.806345	1.929363
H	-0.755683	-3.214576	-0.037119	Ni	0.270001	0.993616	0.029804

C	1.851270	-0.101043	-0.505171	H	0.637250	1.681470	-2.691290
C	2.403468	1.155827	0.056701	H	0.730468	3.033561	-3.830011
C	2.947896	0.950722	1.419943	H	2.186787	2.463318	-2.986450
C	3.032619	-0.279905	2.019609	C	0.762900	3.743450	1.514534
F	3.504492	1.555519	-0.872081	H	-0.278068	3.408472	1.489762
C	-3.864656	1.541241	-2.053098	H	1.235932	3.205127	2.351947
C	-1.413712	0.125774	-0.014814	C	0.824216	5.254512	1.772681
C	-1.610474	1.493644	0.369725	H	0.406161	5.820092	0.930509
C	-4.033144	0.216075	-1.968848	H	0.251953	5.534715	2.667282
H	-4.770176	2.120347	-2.241907	H	1.852475	5.601565	1.920836
C	-2.631569	2.386644	-1.847664	C	3.248862	4.177842	-0.147239
C	-1.605744	-0.512658	-1.378001	H	3.687475	4.009373	-1.136922
H	-1.573623	-0.628241	0.775295	H	2.870211	5.212262	-0.158060
C	-2.326271	2.615932	-0.358688	C	4.330461	4.041232	0.922389
H	-1.772900	1.613881	1.452982	H	5.104854	4.811684	0.812177
H	-5.052269	-0.146328	-2.121058	H	3.922169	4.138189	1.937863
C	-3.051014	-0.892156	-1.718020	H	4.820934	3.066390	0.844559
H	-2.807221	3.362091	-2.318000	Si	1.650266	3.135518	-0.072841
H	-1.749139	1.974356	-2.343708	66			
H	-1.190954	0.110083	-2.175293	TSG/J, E(ωB97XD/BSII) = -2172.565736
H	-1.000745	-1.428982	-1.385359	au			
H	-1.743731	3.540212	-0.244482	Ni	-0.409160	0.271978	0.039184
H	-3.283797	2.812358	0.149926	K	1.054911	1.054351	3.002663
H	-3.449326	-1.524042	-0.907136	H	1.034000	-4.383569	1.216624
H	-3.044001	-1.545376	-2.606089	C	1.007222	-3.477735	0.614024
K	0.192702	-0.171178	2.835644	C	0.929182	-1.161090	-0.903108
C	1.923757	-1.321875	0.175999	C	0.761458	-1.073118	0.504301
H	1.555703	-2.201814	-0.349414	C	0.919837	-2.258781	1.257734
C	2.462419	-1.466396	1.462620	H	1.212750	-0.288459	-1.480765
C	2.322389	-2.698030	2.247328	H	0.895678	-2.232370	2.342343
C	1.242080	-3.584982	2.029156	C	-0.843029	1.465321	-1.596036
C	3.208135	-3.022649	3.297748	C	0.318326	1.794593	-2.520816
C	1.066669	-4.727079	2.806357	C	0.629552	3.505162	0.582503
H	0.527758	-3.369575	1.236215	C	1.678490	2.223683	-1.924910
C	3.021787	-4.157223	4.081396	C	1.288232	4.268781	-0.528849
H	4.076557	-2.393554	3.475185	C	1.747170	3.696752	-1.643925
C	1.950121	-5.020643	3.845628	H	-0.021901	2.578589	-3.216428
H	0.226817	-5.387929	2.602322	H	1.888995	1.641874	-1.017847
H	3.732634	-4.379236	4.874337	H	1.115638	2.525945	0.698522
H	1.811375	-5.909248	4.455349	H	1.321315	5.353785	-0.429914
C	0.820915	3.621030	-1.721669	H	-1.591707	0.869586	-2.125575
H	1.194205	4.623906	-1.977349	H	0.478386	0.905352	-3.144606
H	-0.259494	3.717563	-1.589696	H	0.756834	4.063458	1.522417
C	1.113831	2.652587	-2.874891	H	2.461428	1.961208	-2.646815

H	2.150703	4.330754	-2.433718
C	-1.325000	2.066043	-0.433984
H	-2.387473	1.879966	-0.266662
C	-0.877986	3.285437	0.345375
H	-1.287908	4.179293	-0.151541
H	-1.385607	3.231656	1.313900
F	2.017653	0.241744	0.988915
C	0.988778	-3.595003	-0.796605
C	0.976958	-2.411604	-1.535077
H	1.110660	-2.450685	-2.614203
C	1.039608	-4.912782	-1.457823
C	0.322959	-5.148180	-2.643198
C	1.799309	-5.969917	-0.929692
C	0.368322	-6.386467	-3.277562
H	-0.297068	-4.354238	-3.052641
C	1.837998	-7.211493	-1.558492
H	2.388601	-5.805216	-0.030950
C	1.124342	-7.427006	-2.737462
H	-0.200863	-6.543798	-4.190810
H	2.439030	-8.011254	-1.131957
H	1.156383	-8.395714	-3.229611
Si	-1.874621	-0.190936	1.712583
C	-3.140391	-1.263976	0.748761
C	-1.497595	-1.331167	3.240374
C	-2.916569	1.223958	2.518583
H	-3.876911	-1.653772	1.467173
H	-2.587727	-2.134102	0.367675
C	-3.869788	-0.570808	-0.403649
H	-1.210839	-2.302460	2.820470
H	-0.617822	-1.009436	3.825957
C	-2.668672	-1.540135	4.208926
H	-3.260732	1.928295	1.750952
H	-3.828154	0.749949	2.911070
C	-2.239673	2.000636	3.652602
H	-3.163121	-0.262788	-1.182338
H	-4.610598	-1.228540	-0.876884
H	-4.401691	0.328097	-0.065361
H	-3.558874	-1.903709	3.683750
H	-2.426855	-2.280724	4.983271
H	-2.956197	-0.615084	4.721947
H	-2.911630	2.726842	4.128707
H	-1.884950	1.330829	4.448816
H	-1.377961	2.580971	3.288507
66			

TSH/J, E(ωB97XD/BSII) = -2172.577222 au

C	2.059453	1.956253	-0.186138
C	1.200311	3.229123	-0.175684
H	1.406668	3.800101	-1.095403
H	0.141173	2.939144	-0.253036
C	3.107034	2.027344	2.954027
C	3.455852	3.324156	2.208216
H	4.183188	3.873221	2.819138
H	3.976740	3.087414	1.279527
C	2.151894	1.080652	2.270119
H	1.587888	0.453358	2.966827
C	1.735276	1.028258	0.956364
H	0.865250	0.391197	0.769148
C	2.255833	4.207558	1.975138
H	2.106910	4.977379	2.733763
C	1.335423	4.153656	1.004142
H	0.542407	4.902527	1.052778
Ni	3.155459	-0.566298	1.309654
H	4.034409	1.484425	3.191602
H	2.664629	2.290236	3.925683
H	1.876655	1.417964	-1.123382
H	3.115621	2.214270	-0.200919
K	3.328870	-5.398680	1.535577
H	0.290321	-3.521270	2.736603
C	1.362329	-3.327067	2.720454
C	4.082709	-2.692494	2.711904
C	3.324467	-2.373025	1.522148
C	1.902925	-2.664447	1.621825
H	5.135990	-2.430095	2.736071
H	1.256128	-2.405574	0.785295
F	3.902268	-3.393735	0.279773
C	3.510866	-3.332429	3.800457
H	4.141836	-3.560247	4.658879
C	2.143373	-3.707817	3.832917
C	1.569742	-4.454266	4.965836
C	0.534451	-5.389117	4.771853
C	2.043418	-4.282302	6.280017
C	-0.002128	-6.111478	5.834295
H	0.149435	-5.558189	3.767796
C	1.516038	-5.012711	7.340697
H	2.815023	-3.541905	6.474493
C	0.489013	-5.933240	7.127439
H	-0.801949	-6.825033	5.648803

H	1.899698	-4.849814	8.345247	H	-1.975455	-0.542718	1.419272
H	0.074899	-6.499498	7.957429	H	-1.070628	3.443804	1.308528
Si	4.890614	-0.468368	-0.109585	Ni	0.711558	-0.033039	1.387985
C	5.759304	1.252105	-0.106780	C	0.496730	-1.707063	2.224217
C	6.355155	-1.668170	0.186962	C	-0.276459	-1.828339	3.393070
C	4.215661	-0.667763	-1.897268	C	0.818579	-2.905941	1.558323
H	5.033510	2.049315	-0.309821	C	-0.704571	-3.066884	3.867310
H	6.437561	1.258308	-0.974483	H	-0.555491	-0.932991	3.945303
C	6.547873	1.571425	1.164851	C	0.390482	-4.144734	2.023572
H	6.695785	-1.536194	1.224967	H	1.441050	-2.867501	0.665628
H	5.950306	-2.681194	0.124009	C	-0.378075	-4.252246	3.193683
C	7.544204	-1.491756	-0.763476	H	-1.322712	-3.114518	4.761711
H	4.067013	0.347445	-2.294358	H	0.686349	-5.048864	1.495180
H	4.998525	-1.123858	-2.521224	C	-0.821822	-5.568819	3.700321
C	2.915956	-1.468585	-2.021807	C	-1.250714	-6.574522	2.820151
H	7.353789	0.845008	1.325542	C	-0.825794	-5.848843	5.075735
H	7.007658	2.568546	1.134463	C	-1.667040	-7.814813	3.296815
H	5.904240	1.533335	2.051968	H	-1.280257	-6.369032	1.752903
H	8.006449	-0.502042	-0.663835	C	-1.245702	-7.087300	5.553970
H	8.332101	-2.235041	-0.576150	H	-0.469683	-5.093823	5.772235
H	7.241197	-1.601295	-1.812558	C	-1.667753	-8.077268	4.666692
H	2.579054	-1.556688	-3.064655	H	-2.001721	-8.576019	2.596106
H	3.039573	-2.469798	-1.600555	H	-1.232655	-7.283704	6.623389
H	2.112930	-0.986063	-1.447689	H	-1.993671	-9.044962	5.039442
64				Si	2.541333	-0.216488	2.736648
J, E(ωB97XD/BSII) = -1472.774876 au				C	2.099826	0.279782	4.528921
C	-0.898097	2.370838	1.486496	C	3.497512	-1.864242	2.894852
C	-1.897576	1.537605	0.658795	C	3.867129	1.029381	2.109380
H	-1.102968	2.206578	2.551598	H	3.047685	0.454046	5.058527
H	-2.893097	1.649860	1.103648	H	1.646720	-0.602075	5.000471
H	-1.974748	1.927534	-0.359080	C	1.181595	1.490053	4.702803
C	0.489473	1.443690	-1.257799	H	2.833610	-2.593815	3.372941
H	1.228342	1.652558	-2.039892	H	3.694640	-2.263717	1.890135
H	-0.302065	2.186749	-1.387983	C	4.806828	-1.760610	3.686859
C	-0.060848	0.021390	-1.478179	H	3.421090	2.020048	1.947678
H	-0.713957	0.004507	-2.363927	H	4.592263	1.166008	2.925277
H	0.780406	-0.644499	-1.709517	C	4.601419	0.565074	0.845952
C	1.154080	1.618609	0.092141	H	0.228823	1.336949	4.180356
H	2.240615	1.628253	0.072292	H	0.952175	1.689247	5.757896
C	0.556851	2.046588	1.257064	H	1.633200	2.402744	4.293273
H	1.214381	2.402338	2.049310	H	4.629730	-1.404841	4.709198
C	-0.770925	-0.564990	-0.286694	H	5.305246	-2.735770	3.766455
H	-0.715255	-1.649034	-0.202873	H	5.520752	-1.069486	3.223213
C	-1.532597	0.076013	0.639391	H	5.298802	1.323406	0.466423

H	5.180802	-0.345464	1.036485
H	3.902430	0.323427	0.033821

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TSJ/K, E(ωB97XD/BSII)=

-1472.760923 au

C	-1.953305	-1.458524	-0.637892
C	-0.927947	-0.956195	-1.678975
H	-1.753426	-2.518801	-0.435689
H	-0.823518	-1.722970	-2.455862
H	-1.306469	-0.065863	-2.189207
C	-1.393483	1.634356	-0.131412
H	-1.781779	2.585279	0.252692
H	-1.987282	1.406861	-1.020619
C	0.092171	1.832808	-0.509707
H	0.156373	2.417197	-1.441303
H	0.569247	2.444950	0.265896
C	-1.599678	0.565042	0.914874
H	-1.632004	0.904123	1.950798
C	-1.896155	-0.746941	0.689289
H	-2.170117	-1.349604	1.554129
C	0.895306	0.558980	-0.625276
H	1.975523	0.704969	-0.576470
C	0.440597	-0.670619	-1.085368
H	1.202850	-1.422567	-1.302784
H	-2.966593	-1.415597	-1.066189
Ni	0.337715	-0.627286	0.944678
Si	2.314370	-0.656977	2.198960
C	3.593763	-1.205368	0.869460
H	3.959022	-2.202777	1.152470
H	3.098038	-1.330893	-0.099437
C	4.776589	-0.239575	0.716128
H	5.499382	-0.599178	-0.028521
H	4.441016	0.752761	0.390482
H	5.317746	-0.103064	1.658944
C	2.289173	1.243561	2.452976
H	2.445347	1.710739	1.473140
H	1.261703	1.515203	2.737178
C	3.275850	1.833459	3.466690
H	4.313825	1.666762	3.157688
H	3.138636	2.917479	3.576966
H	3.152737	1.384400	4.458620
C	2.956920	-1.480818	3.811130
H	2.412469	-1.034570	4.654833
H	2.622352	-2.527083	3.781761

C	4.466700	-1.441089	4.072498
H	5.031001	-1.926099	3.267204
H	4.846482	-0.418290	4.167086
H	4.719645	-1.966881	5.002864
C	0.355972	-1.471085	2.646425
C	-0.285355	-0.942869	3.788568
C	0.213879	-2.863065	2.425585
C	-1.073942	-1.733596	4.612028
H	-0.186723	0.118427	4.008926
C	-0.599192	-3.648656	3.235363
H	0.750092	-3.334092	1.602591
C	-1.263987	-3.101268	4.344204
H	-1.589564	-1.281340	5.456668
H	-0.686404	-4.714399	3.035089
C	-2.122970	-3.936473	5.208980
C	-2.942821	-4.935194	4.659709
C	-2.146824	-3.753107	6.600678
C	-3.755184	-5.722360	5.471116
H	-2.960913	-5.075036	3.581629
C	-2.961757	-4.537521	7.412509
H	-1.497619	-3.006297	7.050799
C	-3.769589	-5.526784	6.852135
H	-4.387475	-6.484389	5.021987
H	-2.957574	-4.382445	8.488676
H	-4.404739	-6.140022	7.486124

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K, E(ωB97XD/BSII) = -1472.793604 au

C	-2.048425	0.272894	0.911986
C	-1.411655	0.057277	-0.483035
H	-2.267928	-0.709417	1.347804
H	-1.960209	-0.744957	-0.989560
H	-1.536753	0.949745	-1.102929
C	-0.076286	2.706599	0.294407
H	0.169188	3.763049	0.455966
H	-1.005861	2.701195	-0.282130
C	1.066695	2.055971	-0.518551
H	1.000208	2.370916	-1.571916
H	2.023343	2.440657	-0.145216
C	-0.290417	2.034601	1.633733
H	0.139426	2.545061	2.493903
C	-1.169862	1.003663	1.900571
H	-1.387341	0.784071	2.946557
C	1.120616	0.550170	-0.416414
H	2.110695	0.112861	-0.564215

Atom	x	y	z	Atom	x	y	z
C	0.051171	-0.319723	-0.399975	H	0.907769	3.129897	6.003854
H	0.271828	-1.380455	-0.504705	H	1.482753	3.263088	4.338832
H	-3.015663	0.787203	0.796384	H	0.257849	2.059577	4.754261
Ni	0.656357	0.128344	1.584395	66			
C	-0.495222	-2.757496	2.840722	L, E(ωB97XD/BSII) = -2172.608488 au			
C	0.599311	-2.565362	2.017397	K	-4.935076	-0.131021	-4.595457
C	1.547648	-1.521404	2.241708	C	-1.374513	2.771546	-0.463628
C	1.343470	-0.618354	3.356870	C	0.112572	3.042141	-0.451891
C	0.274455	-0.939264	4.264466	C	-1.386420	3.261984	2.831537
C	-0.618610	-1.948292	4.013854	C	0.846189	3.349891	0.855026
H	2.523074	-1.605708	1.756084	C	-0.690091	4.529807	2.432035
H	-1.410882	-2.166715	4.725533	C	0.310621	4.569118	1.547039
H	0.165954	-0.357109	5.177499	H	0.265219	3.874666	-1.159236
H	0.727761	-3.200948	1.143839	H	0.762410	2.457257	1.478798
C	-1.524316	-3.768026	2.518933	H	-0.716907	2.400097	2.790871
C	-1.186856	-5.014190	1.967097	H	-1.062562	5.462772	2.858326
C	-2.883222	-3.491805	2.742043	H	-1.720502	2.769883	-1.500443
C	-2.170443	-5.943186	1.639837	H	0.591093	2.166677	-0.917380
H	-0.139051	-5.263292	1.818816	H	-1.761334	3.348543	3.860485
C	-3.867987	-4.421300	2.416543	H	1.908002	3.492428	0.612148
H	-3.167605	-2.526857	3.154851	H	0.737582	5.533377	1.266298
C	-3.516778	-5.651600	1.861998	C	-2.402593	2.732670	0.445896
H	-1.883790	-6.904666	1.220559	H	-3.387114	2.704483	-0.026438
H	-4.913961	-4.180530	2.590914	C	-2.580688	2.932480	1.933200
H	-4.284253	-6.378488	1.608846	H	-3.340718	3.725425	2.034456
Si	2.785063	0.458811	3.917680	H	-3.055711	2.015612	2.314453
C	4.201092	-0.692924	4.436278	Si	-3.154980	0.152357	-1.643730
C	3.369794	1.564736	2.491309	C	-2.172595	-0.571921	-3.152132
C	2.277452	1.527023	5.398368	C	-4.512655	-1.142982	-1.166693
H	5.043480	-0.087865	4.800951	C	-4.130350	1.713856	-2.384642
H	4.566022	-1.206491	3.534796	H	-2.732555	-1.008619	-4.003623
C	3.789083	-1.725910	5.492166	H	-1.642894	-1.436236	-2.734735
H	3.541213	0.927271	1.611555	C	-1.147867	0.441151	-3.676502
H	2.535209	2.222921	2.214614	H	-3.934270	-1.898815	-0.623769
C	4.620454	2.396577	2.799458	H	-5.148241	-0.673073	-0.403016
H	1.973597	0.863233	6.219734	C	-5.404920	-1.886592	-2.166993
H	3.179427	2.042417	5.758482	H	-3.580971	2.595387	-2.036178
C	1.172065	2.548794	5.111306	H	-4.058937	1.848932	-3.482361
H	2.949475	-2.336747	5.139581	C	-5.581508	1.868744	-1.909018
H	4.613692	-2.404871	5.743545	H	-0.509159	0.776838	-2.850553
H	3.470632	-1.241985	6.423835	H	-0.496312	0.025558	-4.456590
H	5.479388	1.757920	3.037584	H	-1.624966	1.344083	-4.086083
H	4.909329	3.029886	1.951105	H	-4.816429	-2.352152	-2.974827
H	4.458166	3.058553	3.659266	H	-5.951020	-2.711373	-1.691531

Atom	X	Y	Z	Atom	X	Y	Z
H	-6.190893	-1.245823	-2.603644	C	-3.402905	0.904517	-1.358738
H	-6.041808	2.811474	-2.234763	C	-2.169639	-1.943917	-1.375859
H	-6.241811	1.049037	-2.233716	H	-1.800900	-2.316604	0.731799
H	-5.620584	1.850196	-0.813902	C	-2.912705	0.995770	0.093994
Ni	-1.740611	0.675026	0.024973	H	-2.282796	-0.265041	1.744204
C	-1.441652	-1.175107	0.076873	H	-5.693656	-1.742639	-1.655233
F	-0.543742	0.795605	1.425572	C	-3.617124	-2.384211	-1.625990
C	-0.372339	-1.758880	-0.622947	H	-3.684700	1.913427	-1.684434
C	-2.114545	-2.001554	0.992866	H	-2.571606	0.607547	-2.004387
C	-0.019531	-3.095956	-0.451850	H	-1.877571	-1.199167	-2.120947
H	0.217721	-1.144791	-1.301898	H	-1.513098	-2.805687	-1.557491
C	-1.768010	-3.338510	1.172527	H	-2.254473	1.872173	0.187140
C	-0.718818	-3.919008	0.443368	H	-3.781622	1.211438	0.735196
H	0.834557	-3.500875	-0.992488	H	-3.881362	-3.160828	-0.890794
H	-2.930674	-1.586101	1.581759	H	-3.669523	-2.889655	-2.604140
H	-2.334933	-3.951347	1.871571	K	0.500761	-1.158189	2.757978
C	-0.360083	-5.342699	0.616216	C	2.331816	-1.770110	0.534921
C	0.024135	-6.131470	-0.480401	C	1.554193	-1.314564	-0.557982
C	-0.392958	-5.951606	1.881355	H	1.155727	-2.052924	-1.253880
C	0.363420	-7.472530	-0.320145	C	2.265102	-3.151354	1.008712
H	0.034460	-5.686965	-1.472763	C	3.263488	-3.716445	1.836273
C	-0.060601	-7.294132	2.042654	C	1.136137	-3.962887	0.731480
H	-0.656209	-5.352730	2.749525	C	3.137749	-5.002062	2.353770
C	0.320626	-8.062972	0.942832	H	4.168693	-3.150046	2.040125
H	0.653404	-8.061958	-1.187237	C	1.022825	-5.253221	1.241490
H	-0.086789	-7.738791	3.034923	H	0.332426	-3.556659	0.121163
H	0.583744	-9.110290	1.069148	C	2.017904	-5.784906	2.063765
H	-5.237108	-4.652191	-3.438433	H	3.934361	-5.405222	2.975581
66				H	0.141853	-5.845167	1.001252
M, E(ωB97XD/BSII) = -2172.587599 au				H	1.927376	-6.791179	2.463638
H	3.588039	-1.046456	2.153260	Si	1.286513	2.785099	-0.008808
H	1.067941	0.301371	-1.888464	C	0.086458	2.984687	-1.461180
H	3.371095	1.296898	1.676041	C	0.305125	2.718164	1.621720
Ni	-0.359535	-0.312229	0.005189	C	2.499116	4.237758	0.027995
C	1.397982	0.055116	-0.875844	H	-0.588834	3.829349	-1.264340
C	2.204496	1.114986	-0.195536	H	-0.552291	2.088473	-1.477936
C	2.842968	0.589479	1.040650	C	0.777692	3.162279	-2.819701
C	2.992331	-0.754071	1.285231	H	-0.326263	1.814672	1.583770
F	3.309413	1.488944	-1.131806	H	1.028175	2.548596	2.434827
C	-4.605600	0.005625	-1.506229	C	-0.558854	3.947080	1.920636
C	-1.896029	-1.469242	0.038334	H	2.866723	4.380913	-0.995880
C	-2.194484	-0.222958	0.648625	H	1.937720	5.149140	0.281911
C	-4.685469	-1.328145	-1.588437	C	3.693443	4.061847	0.972406
H	-5.558775	0.536604	-1.489162	H	1.522064	2.377716	-2.996052

H	0.058212	3.141437	-3.648185	C	2.845746	-6.327684	3.120943
H	1.308249	4.120369	-2.870899	H	3.060240	-4.603961	4.385858
H	-1.311308	4.104152	1.138391	C	1.347998	-6.090219	1.253423
H	-1.096672	3.854631	2.873530	H	0.470674	-4.146660	0.995682
H	0.047655	4.859231	1.975805	C	2.224473	-6.878758	2.001347
H	4.340455	4.948384	0.981299	H	3.524157	-6.931365	3.719342
H	3.374317	3.883472	2.008121	H	0.863198	-6.501038	0.370523
H	4.299946	3.208013	0.653035	H	2.420738	-7.908336	1.713480

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N, E(ωB97XD/BSII) = -2172.589391 au

C	2.948390	-0.047043	-2.235775	F	0.301415	-0.418959	5.597846
C	1.973287	0.135295	-1.046829	K	-0.546529	0.366275	0.485585
H	3.978667	0.012704	-1.857350	Si	0.847522	1.780731	4.324234
H	1.634792	1.185970	-1.046664	C	2.311352	2.412692	5.344204
H	1.095712	-0.484325	-1.284054	C	0.925725	2.532487	2.570344
C	2.131980	-2.981415	-1.145182	C	-0.766500	2.368148	5.126313
H	1.970558	-4.064873	-1.166266	H	2.269806	3.511208	5.361391
H	1.205577	-2.562671	-0.720542	H	3.240035	2.161566	4.811664
C	3.278962	-2.685519	-0.161333	C	2.355324	1.866766	6.778411
H	3.335813	-3.519935	0.548610	H	1.533172	1.858756	1.950010
H	4.227115	-2.700733	-0.723205	H	-0.105537	2.516565	2.172993
C	2.364325	-2.524145	-2.566247	C	1.458947	3.967255	2.497808
H	2.253645	-3.302233	-3.322720	H	-0.681702	2.199800	6.206556
C	2.747524	-1.321232	-3.015973	H	-0.832428	3.457835	4.986270
H	2.925750	-1.233687	-4.088674	C	-2.039392	1.686666	4.614908
C	3.195854	-1.417040	0.659525	H	2.315950	0.772921	6.793808
H	4.078023	-1.317214	1.303191	H	3.263306	2.187380	7.304658
C	2.560967	-0.174086	0.327175	H	1.496360	2.220687	7.360314
H	3.089626	0.706057	0.712551	H	2.497156	4.015207	2.844384
H	2.838889	0.793261	-2.934332	H	1.437652	4.367136	1.475202
Ni	1.690269	-1.138259	1.813345	H	0.874202	4.649201	3.127798
C	0.080390	-0.772697	3.187812	H	-2.943578	2.100626	5.079458
C	2.266079	-0.712584	4.209157	H	-2.160434	1.805259	3.526852
H	3.095152	-0.167921	4.650109	H	-2.003895	0.615764	4.838630

66

TSN/O, E(ωB97XD/BSII) = -2172.583428 au

C	0.245988	-2.149593	2.869075	H	3.842201	-1.305512	1.881371
H	-0.566869	-2.705289	2.404616	H	1.038311	0.256846	-1.876127
C	1.477858	-2.795526	3.120642	H	3.356753	1.067364	1.683006
C	0.904644	-0.125782	4.238142	Ni	-0.493708	-0.475474	-0.061597
H	-0.923206	-0.364921	3.046547	C	1.475016	-0.081715	-0.935622
C	2.486363	-1.996012	3.762840	C	2.062526	0.921660	-0.067053
H	3.494820	-2.400910	3.808150	C	2.878413	0.379984	0.989490
C	1.725139	-4.198216	2.742819	C	3.175773	-0.971753	1.083348
C	2.593829	-5.007996	3.491072	F	3.121794	1.859024	-1.230550
C	1.108140	-4.769737	1.616763				

C	-4.733922	-0.173449	-1.659479	C	-0.715810	3.810201	1.763351
C	-2.055939	-1.601684	0.007524	H	2.860329	4.474683	-0.703246
C	-2.336838	-0.305356	0.528857	H	1.948934	4.943454	0.732569
C	-4.849132	-1.507027	-1.638668	C	3.755092	3.805302	1.138597
H	-5.673302	0.380320	-1.699647	H	1.621040	2.314072	-3.063505
C	-3.512051	0.706251	-1.558344	H	0.188427	3.178074	-3.691048
C	-2.351864	-2.174318	-1.368544	H	1.493611	4.050707	-2.871983
H	-1.995113	-2.398028	0.763379	H	-1.406902	3.963710	0.925550
C	-3.037778	0.883639	-0.108568	H	-1.327729	3.701342	2.669766
H	-2.418885	-0.269436	1.624324	H	-0.134453	4.733749	1.874221
H	-5.867500	-1.898387	-1.688749	H	4.400508	4.683237	1.273561
C	-3.811730	-2.592331	-1.578674	H	3.472970	3.457702	2.142767
H	-3.767710	1.696360	-1.954886	H	4.341510	3.019595	0.652837
H	-2.679264	0.349212	-2.171294	66			
H	-2.046282	-1.494434	-2.168387	O, E(ωB97XD/BSII) = -2172.622871 au			
H	-1.719029	-3.064224	-1.488057	H	3.259491	-1.115459	1.875188
H	-2.367240	1.754236	-0.059857	H	0.852806	0.342686	-2.188267
H	-3.909346	1.147189	0.509996	H	2.943771	1.286749	1.421586
H	-4.097337	-3.292847	-0.777726	Ni	-0.517764	-0.268120	-0.186236
H	-3.880253	-3.180815	-2.508190	C	1.174079	0.033093	-1.193505
K	0.650619	-1.195422	2.641750	C	1.679448	1.032431	-0.305155
C	2.569237	-1.942864	0.254296	C	2.449328	0.562833	0.774051
C	1.754031	-1.453750	-0.785551	C	2.633015	-0.805205	1.039128
H	1.352110	-2.149671	-1.519360	F	1.946011	2.574512	-2.249157
C	2.660082	-3.381658	0.552650	C	-4.821481	0.091618	-1.580181
C	3.827128	-3.966454	1.076946	C	-2.068207	-1.388219	-0.104887
C	1.531249	-4.209364	0.382034	C	-2.352276	-0.147677	0.521422
C	3.864174	-5.316779	1.414200	C	-4.895832	-1.241605	-1.675408
H	4.721889	-3.358691	1.187872	H	-5.777865	0.616029	-1.549944
C	1.573947	-5.562450	0.711042	C	-3.623828	0.997488	-1.432767
H	0.609878	-3.772773	-0.001543	C	-2.372673	-1.844591	-1.518764
C	2.739474	-6.124028	1.233622	H	-1.936428	-2.232448	0.583207
H	4.783352	-5.746236	1.805731	C	-3.115428	1.063817	0.014298
H	0.689666	-6.178980	0.565601	H	-2.423999	-0.224095	1.617310
H	2.773591	-7.179122	1.491784	H	-5.902001	-1.661498	-1.736836
Si	1.360846	2.665442	-0.024381	C	-3.823337	-2.292137	-1.736954
C	0.219043	2.927004	-1.513891	H	-3.915250	2.010884	-1.732176
C	0.192522	2.603770	1.514647	H	-2.799399	0.725512	-2.097245
C	2.527445	4.124337	0.280550	H	-2.108235	-1.086753	-2.261117
H	-0.427563	3.788239	-1.291442	H	-1.715345	-2.699167	-1.728310
H	-0.461201	2.059340	-1.551080	H	-2.484253	1.954862	0.122221
C	0.911092	3.121771	-2.866213	H	-3.981720	1.225981	0.674483
H	-0.429129	1.694834	1.417858	H	-4.066495	-3.073428	-0.999506
H	0.836616	2.434695	2.396110	H	-3.891248	-2.793984	-2.715691

Atom	x	y	z	Atom	x	y	z
K	0.083875	0.249472	2.740518	H	-0.357326	1.553483	1.425321
C	1.972172	-1.776471	0.278354	H	-0.652838	1.468834	-3.516676
C	1.237939	-1.341430	-0.856208	Ni	-0.742301	-0.551194	0.054413
H	0.889512	-2.090118	-1.565372	F	2.751604	2.141100	-0.906974
C	2.004708	-3.206440	0.642613	C	-2.732282	-0.776194	-0.453473
C	3.155778	-3.809841	1.172244	C	-0.371385	-2.671267	0.106354
C	0.853020	-3.994186	0.480122	C	-0.312226	-2.215887	-1.189712
C	3.153112	-5.155288	1.531365	C	-2.591552	-1.009895	0.903729
H	4.068046	-3.226841	1.271418	H	-3.016449	0.231041	-0.757076
C	0.851547	-5.339617	0.838016	C	-2.826325	-1.829376	-1.539163
H	-0.048640	-3.530425	0.088280	C	-1.552373	-3.343329	0.775250
C	2.001382	-5.925884	1.367658	H	0.574146	-2.746770	0.640432
H	4.058567	-5.607545	1.928206	C	-1.453248	-2.152253	-2.174949
H	-0.051576	-5.930947	0.707673	H	-2.808119	-0.176449	1.574469
H	2.002068	-6.976455	1.645980	C	-2.437157	-2.356548	1.569466
Si	1.243166	2.893927	-0.688084	H	-3.494355	-1.466094	-2.329173
C	-0.480785	3.177751	-1.497813	H	-3.290571	-2.738523	-1.146317
C	0.398825	2.966972	1.209154	H	-2.148599	-3.877566	0.030033
C	2.446781	4.345042	-0.341254	H	-1.176373	-4.109515	1.463518
H	-1.188828	3.628295	-0.790274	H	-1.522619	-3.086021	-2.754870
H	-0.865796	2.158041	-1.681415	H	-1.211555	-1.356336	-2.889911
C	-0.497392	3.959462	-2.812896	H	-1.976778	-2.186302	2.549969
H	-0.459694	2.266894	1.142287	H	-3.418903	-2.815628	1.766553
H	1.103661	2.559563	1.960102	H	0.675051	-2.013373	-1.602467
C	-0.093515	4.327819	1.704541	K	1.094076	3.834506	-1.069340
H	2.937656	4.610487	-1.283621	C	-1.448677	2.254183	-0.297155
H	1.857322	5.221077	-0.036532	C	-1.503559	2.268215	-1.682141
C	3.509570	4.055378	0.724218	H	-2.247243	2.873446	-2.196876
H	0.173028	3.498487	-3.542874	C	-2.389801	3.045189	0.520530
H	-1.505006	4.017455	-3.249716	C	-3.730834	3.206212	0.131600
H	-0.147644	4.988698	-2.660192	C	-1.974790	3.664650	1.713250
H	-0.671202	4.848301	0.929971	C	-4.614929	3.964898	0.893559
H	-0.733185	4.281567	2.601015	H	-4.085796	2.704101	-0.764763
H	0.754627	4.977509	1.952232	C	-2.858885	4.423128	2.476386
H	4.175275	4.913311	0.892762	H	-0.944205	3.555623	2.044859
H	3.056168	3.809410	1.694296	C	-4.183981	4.579903	2.069575
H	4.145061	3.208745	0.433231	H	-5.649750	4.064384	0.574951
66				H	-2.510365	4.894101	3.392413
P, E(ωB97XD/BSII) = -2172.652862 au				H	-4.875782	5.167384	2.667351
C	-0.576724	1.493545	-2.431666	Si	2.424697	0.772438	0.460071
C	0.460822	0.824869	-1.798393	C	3.963869	-0.070735	-0.317351
C	0.652248	0.819574	-0.372973	C	2.691752	2.225270	1.715980
C	-0.461228	1.418993	0.348849	C	2.090067	-0.669071	1.757104
H	1.202692	0.326839	-2.415035	H	4.286340	-0.912281	0.310051

Atom	X	Y	Z	Atom	X	Y	Z
H	4.773856	0.670406	-0.298464	H	-2.352687	0.360788	-1.639047
C	3.775548	-0.550309	-1.759929	C	-1.997563	2.480327	-1.891346
H	3.286157	2.988339	1.198003	H	-2.473959	2.669108	-2.866252
H	1.705142	2.682074	1.916005	H	-2.791516	2.581714	-1.147431
C	3.362830	1.902689	3.054009	C	1.459133	-1.749823	-0.965073
H	2.093076	-1.604976	1.176319	C	1.728978	-0.341904	-1.116986
H	2.985363	-0.739720	2.394203	H	2.090036	0.013238	-2.077438
C	0.847424	-0.642468	2.644227	C	3.062746	0.429195	2.366174
H	3.512021	0.295457	-2.403145	H	3.236699	-0.203316	3.241120
H	4.684037	-1.015787	-2.167109	H	4.017552	0.839279	2.014546
H	2.973232	-1.298182	-1.836013	F	2.337851	1.576675	2.835821
H	4.335054	1.418248	2.899933	Si	-1.520668	0.264453	1.118934
H	3.542453	2.809074	3.649599	C	-3.245837	1.153364	1.083192
H	2.761054	1.224845	3.667581	C	-1.919128	-1.592560	0.783255
H	0.802422	-1.475736	3.361249	C	-1.308132	0.305652	3.070278
H	0.764967	0.290352	3.218428	H	-3.929785	0.587510	1.732252
H	-0.080360	-0.710783	2.045294	H	-3.677215	1.091380	0.075633
69				C	-3.241950	2.613339	1.550586
R, E(ωB97XD/BSII) = -2211.895805 au				H	-2.081226	-1.696826	-0.299434
Ni	0.005075	0.513268	-0.619358	H	-0.989854	-2.141194	0.986063
K	0.356401	2.794033	1.639956	C	-3.085072	-2.217268	1.554194
H	1.377250	-3.413355	0.371636	H	-1.172035	1.332580	3.457727
C	1.583256	-2.350690	0.273732	H	-2.302214	0.022697	3.449793
C	1.971969	0.414663	0.082966	C	-0.255661	-0.602460	3.709399
C	2.330797	-0.287626	1.290400	H	-2.566034	3.234228	0.941258
C	2.093255	-1.635494	1.387004	H	-4.231385	3.086832	1.485913
H	2.426382	1.403175	-0.048146	H	-2.923963	2.696808	2.599623
H	2.315197	-2.169000	2.308372	H	-4.035629	-1.723297	1.319910
C	-0.488371	0.456034	-2.608689	H	-3.208816	-3.284295	1.320395
C	0.414911	1.071602	-3.663054	H	-2.938107	-2.139975	2.638898
C	-0.949170	3.591035	-1.642739	H	-0.376588	-0.670710	4.800023
C	1.251605	2.320708	-3.288714	H	-0.310397	-1.619902	3.305674
C	-0.386424	4.187303	-2.899270	H	0.753836	-0.237075	3.511645
C	0.580902	3.621331	-3.626925	C	1.061347	-2.541944	-2.148561
H	-0.185050	1.307509	-4.556121	C	1.730442	-2.409765	-3.374134
H	1.475303	2.269428	-2.213787	C	-0.027166	-3.423540	-2.073943
H	-0.139048	3.139035	-1.048643	C	1.325215	-3.137433	-4.489973
H	-0.852723	5.104120	-3.260455	H	2.586420	-1.743625	-3.447054
H	-0.624916	-0.612303	-2.795721	C	-0.435378	-4.147972	-3.191321
H	1.104484	0.280104	-3.982101	H	-0.574134	-3.505778	-1.138797
H	-1.402990	4.387318	-1.036160	C	0.237882	-4.007364	-4.404731
H	2.215109	2.273206	-3.811091	H	1.861673	-3.026066	-5.429160
H	0.876959	4.097737	-4.561828	H	-1.290142	-4.815769	-3.116183
C	-1.521980	1.037820	-1.855093	H	-0.083330	-4.569140	-5.278077

S, E(ωB97XD/BSII) = -2211.898406 au

C	-1.959197	1.967570	-0.345048
C	-3.143458	2.797218	0.187159
H	-3.310429	3.650259	-0.491943
H	-4.051248	2.180391	0.089953
C	-0.134978	1.845235	2.308863
C	-0.600286	3.298454	2.068092
H	0.023721	3.954409	2.689534
H	-0.388700	3.585307	1.035218
C	-0.998921	0.734494	1.739588
H	-1.417149	0.072968	2.497949
C	-1.670491	0.744791	0.496071
H	-2.534011	0.056482	0.480998
C	-2.047917	3.529403	2.398284
H	-2.253372	3.886382	3.408618
C	-3.101895	3.304164	1.605822
H	-4.086197	3.527118	2.022293
Ni	0.037394	-0.301333	0.353429
H	0.898919	1.760502	1.942878
H	-0.063802	1.683051	3.391486
H	-2.224150	1.652381	-1.358856
H	-1.061313	2.576483	-0.460786
Si	0.653052	-0.069201	-1.901092
C	0.976339	-1.592403	-3.094844
H	0.032471	-1.815764	-3.627316
H	1.633580	-1.201062	-3.885010
C	1.573918	-2.903313	-2.579174
H	1.770610	-3.617825	-3.390765
H	2.522833	-2.738004	-2.057882
H	0.914441	-3.417549	-1.863754
C	-0.427066	0.986726	-3.132459
H	-1.470406	0.625061	-3.132824
H	-0.482441	1.999806	-2.712933
C	0.055195	1.082249	-4.585044
H	0.011665	0.113579	-5.097266
H	-0.550623	1.785941	-5.173316
H	1.094343	1.427886	-4.641806
C	2.305289	0.918914	-1.886191
H	3.149695	0.252007	-1.676928
H	2.485881	1.323653	-2.892641
C	2.297165	2.053621	-0.857814
H	1.458604	2.743489	-1.024430
H	2.184220	1.646451	0.153962
H	3.223905	2.642126	-0.874807
K	-1.801337	-2.073558	-1.115396
C	-0.239541	-2.438252	2.359961
F	-1.150961	-2.835192	1.337604
H	0.204709	-3.379131	2.709054
H	-0.841855	-2.002666	3.163618
C	0.796110	-1.472373	1.866212
C	1.490402	-0.723038	2.875120
C	1.497479	-1.734288	0.637605
C	2.732543	-0.195091	2.657219
H	0.993043	-0.553002	3.828786
C	2.841826	-1.263279	0.498872
H	1.222352	-2.610751	0.057532
C	3.443633	-0.462938	1.440870
H	3.215239	0.390408	3.435220
H	3.378959	-1.514886	-0.410118
C	4.776028	0.128048	1.202119
C	5.796140	-0.592491	0.561461
C	5.045079	1.450729	1.588130
C	7.034691	-0.010084	0.307302
H	5.618588	-1.627930	0.281047
C	6.284673	2.033361	1.337371
H	4.259125	2.035579	2.059352
C	7.286292	1.306390	0.694561
H	7.810930	-0.590490	-0.185949
H	6.465012	3.063345	1.636105
H	8.254152	1.760616	0.498017

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TSS/T, E(ωB97XD/BSII) = -2211.873337 au

C	0.919431	1.742180	0.397083
C	-0.233684	2.626197	0.903362
H	-0.481049	3.361244	0.119424
H	-1.131720	1.994567	0.992003
C	2.784278	1.777923	3.062243
C	2.455826	3.213368	2.616518
H	3.139774	3.887494	3.147998
H	2.691665	3.335435	1.557344
C	1.916375	0.664032	2.527255
H	1.639001	-0.092438	3.255960
C	1.218597	0.603165	1.336744
H	0.465961	-0.190111	1.331769
C	1.036987	3.617177	2.918113
H	0.897852	4.157511	3.855527
C	-0.066743	3.355958	2.208653

H	-1.007268	3.731651	2.616201	C	8.804234	-0.612135	1.385473
Ni	3.013776	-0.599369	1.223396	C	7.994651	1.434519	2.360055
H	3.837100	1.570684	2.823670	C	10.024071	0.000063	1.111975
H	2.730812	1.732941	4.158283	H	8.657495	-1.660055	1.135657
H	0.605733	1.335679	-0.568724	C	9.215323	2.047188	2.089017
H	1.808219	2.337434	0.189520	H	7.194449	2.009338	2.819354
Si	3.675416	-0.280732	-0.970774	C	10.236669	1.333597	1.462489
C	4.023765	-1.824690	-2.121247	H	10.816713	-0.570296	0.633474
H	3.081297	-2.055174	-2.651316	H	9.365720	3.089422	2.360389
H	4.675381	-1.427766	-2.913560	H	11.190297	1.810886	1.251872
C	4.628251	-3.133609	-1.611873	69			
H	4.821910	-3.839622	-2.431313	W, E(ωB97XD/BSII) = -2211.879847 au			
H	5.580224	-2.970780	-1.096199	C	-3.968833	0.748908	-0.900611
H	3.970981	-3.651016	-0.898903	C	-5.363816	1.311976	-0.562407
C	2.546987	0.695426	-2.222110	H	-5.883745	1.558285	-1.502354
H	1.515826	0.303722	-2.204973	H	-5.960087	0.507132	-0.107775
H	2.465282	1.722729	-1.847097	C	-2.052266	2.682513	0.802150
C	3.020644	0.748698	-3.680754	C	-3.110370	3.532827	0.063681
H	2.990585	-0.235608	-4.162245	H	-2.782603	4.579449	0.108173
H	2.396363	1.422259	-4.284172	H	-3.118187	3.274397	-0.996851
H	4.052201	1.112209	-3.757722	C	-2.416257	1.244966	1.083535
C	5.273704	0.784594	-0.985013	H	-2.114497	0.884633	2.065422
H	6.156052	0.172644	-0.769360	C	-3.194973	0.403601	0.339978
H	5.421628	1.176968	-2.001464	H	-3.465211	-0.549229	0.796120
C	5.205509	1.938360	0.018282	C	-4.497639	3.424164	0.639936
H	4.345926	2.593156	-0.178553	H	-4.762277	4.183966	1.376851
H	5.088928	1.546841	1.035239	C	-5.426393	2.498925	0.366912
H	6.109875	2.560045	0.002565	H	-6.381690	2.600832	0.885239
K	1.063424	-2.369308	-0.297147	Ni	-1.021861	-0.265495	-0.086560
C	2.805660	-2.515970	3.126641	H	-1.112615	2.710091	0.231490
F	1.096488	-2.267260	2.095584	H	-1.831655	3.159579	1.766220
H	2.720977	-3.502127	2.689091	H	-4.093544	-0.158726	-1.503215
H	2.303008	-2.373776	4.077310	H	-3.408018	1.441347	-1.523310
C	3.895234	-1.706992	2.789164	Si	-0.354454	0.444752	-2.169290
C	4.510015	-0.794775	3.728564	C	-0.309244	-0.836817	-3.612908
C	4.533058	-1.873833	1.484230	H	-1.342087	-1.161525	-3.808755
C	5.719261	-0.229105	3.472742	H	0.024468	-0.323114	-4.527421
H	4.001756	-0.606642	4.672119	C	0.573707	-2.064827	-3.380908
C	5.876651	-1.363729	1.339352	H	0.574601	-2.753723	-4.238261
H	4.324028	-2.810541	0.969094	H	1.617279	-1.775111	-3.198784
C	6.448185	-0.528012	2.258248	H	0.234238	-2.633523	-2.506628
H	6.185997	0.406261	4.220758	C	-1.273778	1.944811	-2.984813
H	6.420330	-1.610879	0.432832	H	-2.253717	1.585283	-3.333057
C	7.763752	0.094835	2.008619	H	-1.488519	2.685680	-2.202324

C	-0.553250	2.645449	-4.141825	C	2.334773	2.443152	2.159257
H	-0.287165	1.941359	-4.939952	C	1.421640	3.568291	1.626416
H	-1.168249	3.435270	-4.597526	H	1.917210	4.523823	1.842318
H	0.378316	3.115126	-3.803810	H	1.358358	3.514319	0.536967
C	1.461833	1.083333	-2.028792	C	1.763021	1.043983	2.161962
H	2.130781	0.249061	-1.783752	H	1.959310	0.481066	3.077018
H	1.799825	1.461655	-3.004691	C	0.809037	0.510137	1.337463
C	1.612196	2.166730	-0.958612	H	0.363936	-0.427314	1.666763
H	0.991303	3.044342	-1.187568	C	0.043076	3.584128	2.234997
H	1.281071	1.783016	0.016934	H	-0.076364	4.241334	3.097692
H	2.648522	2.515658	-0.846497	C	-1.035198	2.881642	1.864324
K	1.833959	-3.130972	2.525312	H	-1.945414	3.051016	2.442626
C	-1.617491	-2.279941	2.045402	Ni	2.888123	-0.566477	1.234752
F	-2.521597	-2.683023	1.060210	H	3.277969	2.455660	1.601483
H	-1.279183	-3.231644	2.510591	H	2.607049	2.679759	3.196252
H	-2.170639	-1.722082	2.814681	H	-0.222437	0.446682	-0.526966
C	-0.510568	-1.438611	1.491854	H	0.689236	1.917855	-0.300048
C	0.219332	-0.599920	2.392594	Si	3.955386	0.242107	-0.585955
C	0.169346	-1.765835	0.214254	C	4.030415	-1.099894	-1.970963
C	1.529425	-0.210713	2.168756	H	3.030453	-1.552034	-2.040466
H	-0.280094	-0.255991	3.300543	H	4.186009	-0.567806	-2.921929
C	1.582967	-1.493575	0.109503	C	5.082634	-2.202365	-1.844152
H	-0.216622	-2.607147	-0.366755	H	5.079747	-2.880362	-2.709308
C	2.259397	-0.701788	1.019109	H	6.094323	-1.782443	-1.767641
H	2.016937	0.462016	2.868763	H	4.910732	-2.819406	-0.953978
H	2.093387	-1.842440	-0.785038	C	2.973339	1.654170	-1.461344
C	3.681966	-0.354450	0.827341	H	2.038396	1.211292	-1.829645
C	4.183232	0.895320	1.230300	H	2.681037	2.397352	-0.709907
C	4.585831	-1.258322	0.239685	C	3.685345	2.372748	-2.612849
C	5.524145	1.224796	1.052644	H	4.064557	1.670128	-3.365467
H	3.500962	1.631454	1.645025	H	3.015068	3.072009	-3.132318
C	5.925776	-0.927886	0.056041	H	4.542649	2.954020	-2.253614
H	4.229745	-2.234074	-0.087301	C	5.720563	0.995517	-0.478506
C	6.405598	0.315583	0.467439	H	6.477950	0.242170	-0.243363
H	5.879194	2.205540	1.359955	H	5.974404	1.358040	-1.485398
H	6.598661	-1.646616	-0.406010	C	5.823689	2.141697	0.529089
H	7.451602	0.575076	0.327471	H	5.143248	2.964309	0.270241
69				H	5.550881	1.794919	1.534254
TSW/X, E(ωB97XD/BSII) = -2211.850452 au				H	6.838184	2.558269	0.586583
C	0.072223	1.192852	0.222205	K	6.470049	-3.211869	3.913856
C	-1.204777	1.870053	0.758636	C	2.863375	-2.666977	3.459823
H	-1.740439	2.339158	-0.082744	F	1.637285	-1.838886	2.428583
H	-1.882384	1.087398	1.130339	H	2.678788	-3.613831	2.959699
				H	2.427943	-2.576188	4.453520

C	3.997800	-1.921495	3.135916	Si	-0.394471	0.347952	-2.803368
C	4.563893	-0.923142	3.994217	C	-1.151045	-0.790149	-4.131590
C	4.386841	-1.828004	1.692911	H	-1.953749	-1.361099	-3.647025
C	5.738290	-0.290207	3.665843	H	-1.634987	-0.158004	-4.890639
H	4.091468	-0.724909	4.958242	C	-0.162564	-1.756289	-4.791940
C	5.780423	-1.438615	1.524549	H	-0.655925	-2.391828	-5.539837
H	4.100093	-2.706575	1.099731	H	0.647005	-1.218663	-5.301252
C	6.446111	-0.665129	2.447644	H	0.290491	-2.405266	-4.037314
H	6.186086	0.419940	4.354966	C	-1.048929	2.105351	-3.201646
H	6.275697	-1.697574	0.593139	H	-2.140965	2.059790	-3.311777
C	7.836256	-0.215465	2.218583	H	-0.847681	2.798223	-2.378827
C	8.298000	1.013584	2.721329	C	-0.427610	2.662150	-4.491596
C	8.751068	-1.000822	1.491831	H	-0.558576	1.976886	-5.338666
C	9.606127	1.437965	2.503249	H	-0.880155	3.621477	-4.776401
H	7.609614	1.665022	3.251307	H	0.648997	2.830950	-4.373332
C	10.057415	-0.575397	1.268045	C	1.503599	0.437513	-2.874461
H	8.429505	-1.959416	1.088270	H	1.868997	-0.586480	-2.745214
C	10.496473	0.646721	1.777840	H	1.813510	0.765841	-3.877505
H	9.927391	2.401044	2.892739	C	2.104058	1.351124	-1.800984
H	10.736836	-1.204327	0.697385	H	1.768410	2.389997	-1.920745
H	11.517000	0.979382	1.608000	H	1.808092	1.023743	-0.797171
69				H	3.200650	1.356449	-1.822308
X, E(ωB97XD/BSII) = -2211.917183 au				K	1.456119	-3.252288	3.548911
C	-3.494653	0.892460	-0.744675	C	-1.953546	-2.722484	3.116513
C	-4.611113	1.545765	0.091646	F	0.001060	-1.783101	-1.657384
H	-5.376625	1.950730	-0.589637	H	-2.389230	-3.477718	2.467258
H	-5.121134	0.752802	0.657413	H	-2.482848	-2.489040	4.036890
C	-0.868699	2.466357	0.376040	C	-0.910226	-1.933983	2.679604
C	-2.009053	3.462881	0.081849	C	-0.321026	-0.873199	3.484485
H	-1.576059	4.471878	0.081620	C	-0.224095	-2.146651	1.414155
H	-2.393346	3.308674	-0.928415	C	0.870869	-0.263494	3.151902
C	-1.273097	1.024203	0.594493	H	-0.834504	-0.578868	4.398709
H	-0.801174	0.581776	1.470384	C	0.987065	-1.537142	1.118223
C	-2.398055	0.347125	0.130355	H	-0.645491	-2.850328	0.698217
H	-2.699059	-0.527038	0.722915	C	1.610841	-0.602263	1.982774
C	-3.128711	3.408913	1.086833	H	1.265000	0.498021	3.823672
H	-3.030016	4.091340	1.932226	H	1.439476	-1.760691	0.155631
C	-4.204084	2.611542	1.078725	C	2.864885	0.059841	1.610632
H	-4.906942	2.734469	1.904402	C	3.148120	1.384158	1.999072
Ni	-0.798776	-0.470462	-0.737601	C	3.828812	-0.595043	0.817116
H	-0.110106	2.538426	-0.411367	C	4.327388	2.015669	1.616272
H	-0.359227	2.787900	1.294063	H	2.410033	1.941403	2.570343
H	-3.929537	0.068801	-1.325317	C	5.001465	0.041065	0.423699
H	-3.092632	1.593540	-1.473739	H	3.649310	-1.619001	0.496318

C	5.264572	1.351965	0.823425
H	4.506018	3.043999	1.922645
H	5.717568	-0.493098	-0.196875
H	6.180473	1.849880	0.516726

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Y, E(ωB97XD/BSII) = -2211.904407 au

K	-0.929059	-0.715756	2.155270
C	-1.862012	0.996531	-1.207157
C	-2.273845	0.795858	-2.656499
C	0.333899	3.232035	-2.463966
C	-1.226749	1.015949	-3.764853
C	-0.533115	3.420364	-3.673964
C	-1.212874	2.432078	-4.259245
H	-3.146450	1.438872	-2.856407
H	-0.245200	0.715110	-3.382345
H	0.870603	2.279086	-2.526966
H	-0.634974	4.436361	-4.056590
H	-2.633698	0.576595	-0.553406
H	-2.640637	-0.231702	-2.739064
H	1.095734	4.021925	-2.442322
H	-1.454393	0.339939	-4.598005
H	-1.858369	2.662402	-5.107660
C	-1.094822	2.013377	-0.598732
H	-1.349586	2.166761	0.459379
C	-0.446032	3.279465	-1.133845
H	-1.217497	4.063000	-1.210773
H	0.242531	3.626911	-0.351020
Si	-0.789269	-1.897054	-1.081393
C	-0.318377	-2.393866	-2.896304
C	0.005682	-3.356399	-0.062190
C	-2.678369	-2.324892	-0.907462
H	0.444285	-3.184974	-2.825253
H	0.190705	-1.538519	-3.352558
C	-1.444321	-2.871854	-3.817750
H	1.066121	-3.370553	-0.350765
H	0.028837	-3.167559	1.025749
C	-0.596962	-4.741566	-0.316439
H	-3.276332	-1.675783	-1.557601
H	-2.827713	-3.341027	-1.295314
C	-3.260226	-2.256936	0.506594
H	-2.229797	-2.113685	-3.925311
H	-1.075268	-3.098806	-4.827351
H	-1.926761	-3.779589	-3.435528
H	-0.637405	-4.961842	-1.390535

H	-0.018015	-5.545143	0.160283
H	-1.623860	-4.813244	0.062235
H	-4.295452	-2.619835	0.559575
H	-2.683170	-2.872357	1.215742
H	-3.289790	-1.218949	0.875567
Ni	-0.082794	0.252101	-0.610623
F	1.953232	0.062410	-2.634279
C	2.482485	-0.664398	-1.562625
H	3.561690	-0.452755	-1.552378
H	2.327971	-1.728842	-1.771163
C	1.829892	-0.267194	-0.263472
C	1.612773	1.146065	-0.002282
C	2.187957	-1.072671	0.887173
C	1.499989	1.589920	1.345980
H	1.872662	1.883979	-0.757003
C	2.099984	-0.602159	2.166975
H	2.543755	-2.087232	0.720568
C	1.668527	0.751359	2.435922
H	1.311880	2.648503	1.515087
H	2.360590	-1.258508	2.994995
C	1.399830	1.207473	3.813413
C	0.406369	2.175885	4.071242
C	2.075371	0.664917	4.923453
C	0.113559	2.587951	5.368894
H	-0.144994	2.607638	3.237526
C	1.776189	1.072108	6.220655
H	2.869095	-0.059948	4.764472
C	0.792953	2.034444	6.454522
H	-0.655328	3.339615	5.532093
H	2.324747	0.642400	7.055514
H	0.561994	2.350733	7.468096

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TSY/T, E(ωB97XD/BSII) = -2211.846694 au

K	-0.518401	0.937985	2.931733
C	-1.040002	2.065043	-1.119416
C	-0.521724	2.685483	-2.392036
C	-0.181803	4.882151	0.450434
C	0.226804	4.018740	-2.368048
C	-0.863025	5.539549	-0.712030
C	-0.661617	5.161405	-1.976168
H	-1.380940	2.770079	-3.075446
H	1.086175	3.924947	-1.694714
H	0.811105	4.531451	0.159771

H	-1.575010	6.334306	-0.489623	H	2.610815	-0.875653	2.068200
H	-1.699104	1.237440	-1.386514	C	2.171424	2.368261	3.125266
H	0.148881	1.928865	-2.827078	H	2.165208	4.065361	1.823785
H	-0.034824	5.613541	1.257158	H	2.495120	0.434653	4.114503
H	0.638555	4.189449	-3.370566	C	1.968452	3.134177	4.366468
H	-1.216950	5.651335	-2.776280	C	1.208235	4.323723	4.373799
C	-1.131733	2.409425	0.240039	C	2.483060	2.697133	5.604497
H	-1.903472	1.801805	0.726895	C	0.985741	5.038434	5.546547
C	-0.966868	3.701526	1.028341	H	0.778577	4.688027	3.443931
H	-1.982601	4.057010	1.268590	C	2.250457	3.407646	6.778699
Si	-0.557513	-0.958945	-0.019976	H	3.107864	1.808824	5.642467
C	-0.367614	-1.889375	-1.679100	C	1.499179	4.583246	6.761959
C	0.114532	-2.215082	1.296060	H	0.397476	5.952634	5.511549
C	-2.478916	-0.997252	0.256666	H	2.673591	3.046429	7.713245
H	-0.822161	-2.886797	-1.576475	H	1.320291	5.137447	7.679299
H	0.704712	-2.043045	-1.854882	69			
C	-0.968323	-1.159301	-2.882363	T, E(ωB97XD/BSII) = -2211.964678 au			
H	1.163285	-2.407822	1.027783	K	-0.126348	1.995884	1.426952
H	0.173340	-1.763952	2.301593	C	-1.593886	0.296130	-2.927048
C	-0.634711	-3.549477	1.390831	C	-0.682853	1.079490	-3.845916
H	-2.964550	-0.311172	-0.450369	C	-2.229919	3.160305	-1.312992
H	-2.790286	-2.003723	-0.059626	C	-0.423560	2.571173	-3.617295
C	-3.037161	-0.737872	1.659918	C	-2.487358	3.656211	-2.705997
H	-0.442597	-0.212729	-3.031744	C	-1.673953	3.392924	-3.732644
H	-0.874548	-1.746469	-3.805729	H	-1.089947	0.937310	-4.859933
H	-2.036978	-0.946954	-2.742208	H	0.046066	2.671772	-2.635848
H	-0.645368	-4.065789	0.424532	H	-1.154629	3.086250	-1.135072
H	-0.175081	-4.231654	2.119547	H	-3.411758	4.208056	-2.877278
H	-1.680734	-3.409532	1.689299	H	-1.818646	-0.666053	-3.389804
H	-4.098484	-1.005543	1.745201	H	0.285427	0.556752	-3.848507
H	-2.508980	-1.321440	2.429274	H	-2.659551	3.863842	-0.583621
H	-2.985595	0.328300	1.930221	H	0.305985	2.900128	-4.369300
Ni	0.457903	1.134467	-0.118751	H	-1.951089	3.738399	-4.729279
F	1.460436	0.674088	-1.911189	C	-2.400780	0.560323	-1.835562
C	2.653344	0.102773	-0.484850	H	-3.098119	-0.249192	-1.633414
H	3.352115	0.520545	-1.198581	C	-2.843126	1.779263	-1.055734
H	2.583006	-0.980251	-0.473344	H	-3.931513	1.853195	-1.211425
C	2.362250	0.812031	0.706370	H	-2.743022	1.527022	0.015384
C	2.259739	2.261761	0.662366	Si	-1.225435	-2.494092	-1.320939
C	2.437557	0.195579	2.012098	C	-0.200047	-3.504108	-2.589878
C	2.182685	2.979585	1.870467	C	-1.150971	-3.474121	0.333505
H	2.531931	2.779017	-0.256137	C	-3.057099	-2.761495	-1.881717
C	2.379718	0.939632	3.156728	H	-0.660928	-4.497157	-2.694502
				H	0.804477	-3.676709	-2.179900

C	-0.079324	-2.840837	-3.964679	C	-3.248014	0.664738	1.273507
H	-0.131107	-3.431841	0.735078	C	-3.025433	-0.594081	2.129898
H	-1.783501	-2.952533	1.067669	H	-3.778406	-0.638711	2.931410
C	-1.576557	-4.943995	0.226965	H	-3.199796	-1.475740	1.500492
H	-3.284957	-2.139162	-2.758956	C	-0.554748	2.379588	1.782581
H	-3.129231	-3.798251	-2.242729	C	-1.028671	1.730945	3.097561
C	-4.117580	-2.534854	-0.796771	H	-0.469785	2.183482	3.925031
H	0.402830	-1.859036	-3.879857	H	-2.080767	1.958182	3.283121
H	0.511000	-3.441952	-4.669424	C	-0.994864	1.691953	0.514882
H	-1.064700	-2.681294	-4.422519	H	-0.446082	2.020532	-0.366108
H	-0.909394	-5.499869	-0.442535	C	-2.124097	0.938576	0.297117
H	-1.554712	-5.449761	1.202188	H	-2.341338	0.677798	-0.734577
H	-2.592446	-5.051286	-0.171209	C	-0.790511	0.244780	3.103514
H	-5.139396	-2.625399	-1.189238	H	0.173660	-0.073150	3.498102
H	-4.016565	-3.261558	0.017396	C	-1.641576	-0.731084	2.705060
H	-4.033413	-1.540375	-0.337800	H	-1.313896	-1.759146	2.853691
Ni	-0.534987	-0.352437	-1.248537	Ni	-0.305593	-0.338150	0.685562
F	0.187661	1.428166	-0.892561	H	-0.869428	3.434551	1.754904
C	1.136527	-1.184971	-0.583738	H	0.543225	2.394545	1.775060
H	1.777478	-0.928857	-1.439988	H	-4.174247	0.529290	0.703346
H	1.168186	-2.269244	-0.454536	H	-3.415835	1.537563	1.910049
C	1.602045	-0.518819	0.646732	Si	0.488078	-0.561647	-1.444169
C	2.517001	0.556552	0.615016	C	0.736106	-2.350978	-2.093475
C	1.129703	-0.896411	1.923311	H	0.839924	-3.044364	-1.252742
C	2.904580	1.228997	1.769239	H	-0.200959	-2.636613	-2.594688
H	2.911728	0.869882	-0.346767	C	1.919198	-2.541795	-3.051791
C	1.511471	-0.221969	3.080286	H	1.979168	-3.575936	-3.417410
H	0.421171	-1.717645	1.994953	H	1.847733	-1.889275	-3.929421
C	2.397870	0.871710	3.034324	H	2.867627	-2.310357	-2.554606
H	3.633506	2.033687	1.695613	C	-0.777107	0.208765	-2.678673
H	1.091859	-0.529389	4.036308	H	-1.738631	-0.309325	-2.547922
C	2.751407	1.630241	4.253111	H	-0.958679	1.261215	-2.418188
C	2.927117	3.023922	4.210079	C	-0.362553	0.121858	-4.152983
C	2.902038	0.987829	5.492788	H	-0.237995	-0.918672	-4.474010
C	3.237338	3.747283	5.359079	H	-1.113751	0.577318	-4.812505
H	2.813140	3.549714	3.263940	H	0.586967	0.637533	-4.338079
C	3.206632	1.710509	6.643086	C	2.116698	0.404642	-1.713443
H	2.807270	-0.093570	5.546950	H	2.941169	-0.152414	-1.259073
C	3.374562	3.094153	6.583536	H	2.312632	0.396766	-2.795482
H	3.366434	4.825208	5.298267	C	2.132204	1.842587	-1.196077
H	3.326098	1.188144	7.589010	H	1.358559	2.460283	-1.671983
H	3.615078	3.656954	7.481490	H	1.962963	1.864840	-0.113061
67				H	3.097127	2.331606	-1.384461
U, E(ωB97XD/BSII) = -1512.076966 au				C	0.965432	-1.743813	1.190486

H	0.696826	-2.720802	0.770991	H	-0.356647	-2.136603	-0.992558
H	0.770411	-1.806156	2.271668	H	-2.647233	1.408257	-0.889467
C	2.414549	-1.452250	0.999855	Ni	0.184174	-0.608213	0.913615
C	2.970623	-0.267037	1.511654	Si	2.332841	-0.705084	2.384489
C	3.274688	-2.306933	0.295875	C	3.264179	-2.289588	1.866179
C	4.297223	0.071306	1.291390	H	3.089744	-3.072978	2.618228
H	2.322323	0.412814	2.062862	H	2.766234	-2.637123	0.950102
C	4.606479	-1.970574	0.067573	C	4.767923	-2.165295	1.597476
H	2.885303	-3.239253	-0.105113	H	5.191907	-3.120595	1.261984
C	5.143346	-0.768446	0.547579	H	4.977063	-1.427277	0.814717
H	4.693581	0.995629	1.705120	H	5.320121	-1.860838	2.492740
H	5.231837	-2.636123	-0.522985	C	3.134290	0.743868	1.422955
C	6.546536	-0.390874	0.275518	H	3.363606	0.349687	0.428242
C	7.575272	-1.344254	0.320108	H	2.407716	1.543501	1.267826
C	6.884589	0.934159	-0.040665	C	4.406777	1.335539	2.044990
C	8.894952	-0.986219	0.057017	H	5.197449	0.588286	2.166423
H	7.337109	-2.370485	0.588732	H	4.810868	2.132546	1.406605
C	8.204406	1.293963	-0.300098	H	4.216424	1.775982	3.029757
H	6.096799	1.680376	-0.110146	C	2.646294	-0.271339	4.235279
C	9.216349	0.335120	-0.253200	H	2.582813	0.821660	4.336357
H	9.676803	-1.740419	0.104233	H	1.833873	-0.667059	4.858354
H	8.441959	2.324969	-0.551070	C	3.980381	-0.761770	4.814788
H	10.246617	0.615070	-0.457541	H	4.073398	-1.851797	4.735098
67				H	4.840143	-0.323759	4.298015
TSU/V, E(ωB97XD/BSII) = -1512.062401				H	4.074612	-0.503337	5.877649
au				C	0.456814	-1.497737	2.818119
C	-2.167149	0.527820	-0.433136	H	1.046948	-2.202003	3.420446
C	-1.391725	-0.250307	-1.531510	H	-0.088352	-0.863682	3.525383
H	-2.979769	-0.102846	-0.060912	C	-0.437676	-2.302672	1.934740
H	-2.092221	-0.928687	-2.031550	C	-0.007627	-3.509604	1.325137
H	-1.045958	0.450505	-2.301013	C	-1.780361	-1.915728	1.738635
C	0.569412	1.929518	-0.657064	C	-0.839707	-4.222430	0.488009
H	1.200177	2.806358	-0.469139	H	0.999363	-3.866079	1.517563
H	-0.227747	2.278258	-1.324586	C	-2.618253	-2.648603	0.885669
C	1.418017	0.848808	-1.386462	H	-2.187528	-1.088412	2.309105
H	1.278280	0.964358	-2.473002	C	-2.160938	-3.786214	0.225281
H	2.478277	1.040083	-1.206773	H	-0.484665	-5.143205	0.032462
C	-0.067941	1.500151	0.655509	H	-3.637048	-2.307393	0.721414
H	0.336636	1.949221	1.563302	C	-3.027516	-4.524844	-0.717158
C	-1.325282	0.943347	0.748087	C	-4.390966	-4.721833	-0.449875
H	-1.836144	1.000435	1.708951	C	-2.504114	-5.037916	-1.914182
C	1.091787	-0.570629	-0.977639	C	-5.204009	-5.404984	-1.350214
H	1.918835	-1.281795	-0.975756	H	-4.808080	-4.357983	0.485818
C	-0.210206	-1.057265	-1.022236	C	-3.316634	-5.722144	-2.814364

H	-1.455735	-4.872602	-2.150293
C	-4.670693	-5.908473	-2.536734
H	-6.256029	-5.553566	-1.119509
H	-2.892418	-6.103156	-3.740042
H	-5.305319	-6.442685	-3.239033

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V, E(ωB97XD/BSII) = -1512.097075 au

C	-2.153990	-0.173456	-1.437906
C	-1.084063	-0.993087	-2.215432
H	-2.958572	-0.860349	-1.151619
H	-1.607503	-1.769773	-2.783484
H	-0.587591	-0.352416	-2.953282
C	0.511445	1.432719	-1.166271
H	0.990052	2.410175	-1.028365
H	-0.034692	1.499263	-2.113422
C	1.610056	0.350659	-1.264647
H	2.063292	0.372287	-2.268940
H	2.414225	0.611303	-0.566529
C	-0.469472	1.188039	-0.038489
H	-0.332753	1.784770	0.863974
C	-1.667263	0.511108	-0.177413
H	-2.429552	0.670967	0.588214
C	1.138459	-1.043867	-0.918239
H	1.910965	-1.706594	-0.525156
C	-0.035945	-1.649110	-1.337639
H	-0.096263	-2.731724	-1.236221
H	-2.609268	0.558603	-2.123834
Ni	-0.322945	-0.878232	0.551705
Si	2.448363	-1.268844	3.193678
C	3.430197	-2.317536	1.958449
H	3.956549	-3.099464	2.525867
H	2.688232	-2.843117	1.340970
C	4.417776	-1.574929	1.050119
H	4.951126	-2.266087	0.385250
H	3.900039	-0.849815	0.413240
H	5.171806	-1.024469	1.623825
C	1.777243	0.315395	2.423684
H	1.300363	0.007694	1.469640
H	0.942920	0.657477	3.052598
C	2.736566	1.478635	2.162893
H	3.597342	1.176166	1.557211
H	2.234591	2.297994	1.632310
H	3.128001	1.887248	3.102378
C	3.459632	-0.910090	4.760280

H	2.930152	-0.134911	5.333378
H	3.439852	-1.810687	5.391344
C	4.914924	-0.484458	4.523584
H	5.483339	-1.276731	4.022440
H	4.981362	0.410975	3.894668
H	5.430050	-0.260462	5.466346
C	0.914939	-2.274250	3.717862
H	1.265552	-3.188067	4.215603
H	0.385407	-1.685246	4.479690
C	-0.015144	-2.623322	2.591063
C	0.097174	-3.855482	1.927199
C	-1.102031	-1.768219	2.249029
C	-0.813110	-4.257288	0.953215
H	0.900679	-4.530439	2.215005
C	-2.007123	-2.181374	1.242793
H	-1.366184	-0.942573	2.910729
C	-1.874584	-3.420073	0.582049
H	-0.711965	-5.236756	0.493697
H	-2.889295	-1.578118	1.054569
C	-2.810908	-3.787125	-0.500047
C	-4.168629	-3.431793	-0.446850
C	-2.355397	-4.473531	-1.637412
C	-5.033240	-3.739715	-1.493331
H	-4.555704	-2.928334	0.435285
C	-3.219538	-4.783414	-2.684387
H	-1.304708	-4.740801	-1.713661
C	-4.562777	-4.414572	-2.619895
H	-6.081037	-3.457771	-1.425106
H	-2.838629	-5.305759	-3.558534
H	-5.237108	-4.652191	-3.438433