Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Kinetic *vs* Thermodynamic Control on β-functionalized Cyclic Ketones: A Theoretical Investigation on Regioselective Formation of Enolates

Manuel Petroselli*, Corrado Bacchiocchi

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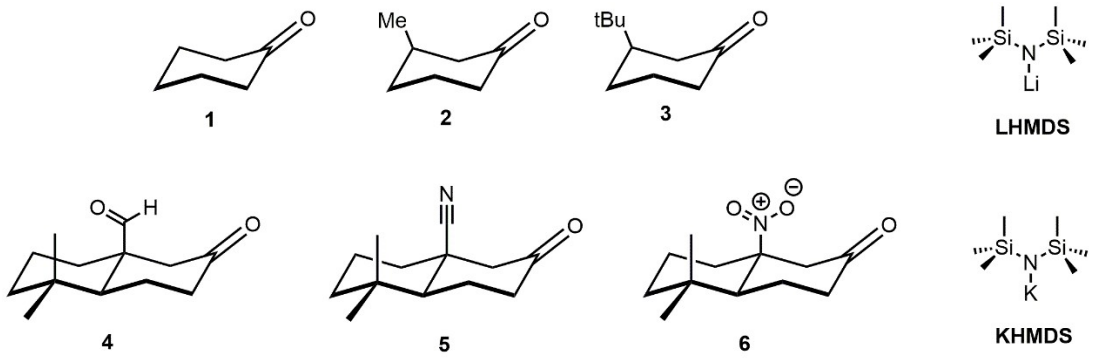
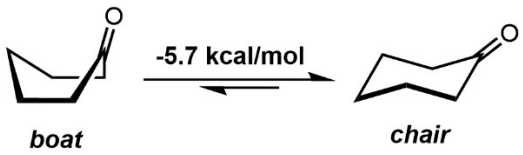
1. General Information & Computational Details

Ab initio and density functional calculations were performed using the Gaussian09 program package. [1] Optimization of all the cyclohexanone derivatives has been performed at B3LYP/6-31G(d,p) level of theory in gas phase. All structures were subjected to a full conformational search, wherein sp^2 and sp^3 hybridized groups were rotated by 180 and 120°, respectively. Moreover, chair conformation showed higher stability with respect to the boat conformation as largely reported in literature for cyclohexanone derivatives. Therefore, all the systems have been studied assuming the chair conformation. Conformational study on enolates has been performed at B3LYP/6-311+G(d,p) level of theory. Frequencies were calculated and checked out to make sure that all of them were positive and no imaginary frequencies were present. TS calculations for the deprotonation of cyclohexanone derivatives have been performed at the B3LYP/6-31G(d,p) level of theory in gas phase as previously described for theoretical optimizations. Unlike what we have previously mentioned, frequencies were calculated and checked out to make sure that one and only one was negative for each TS calculation, confirming a saddle point. Activation energy (Ea) from TS study with $(Me_3Si)_2N^-$ (LHMDS with no counter cation) are shown as averaged value considering the two hydrogens from thermodynamic and kinetic position (see Section 3.7 for details). Also, flipping geometry has been considered in ketone **2** and **3** and the relative averaged Ea was calculated taking in account the Boltzmann distribution derived by the relative stability between the initial ground state structures (see Section 3.5 for details). Zero-point energy (ZPE) was included in each result.

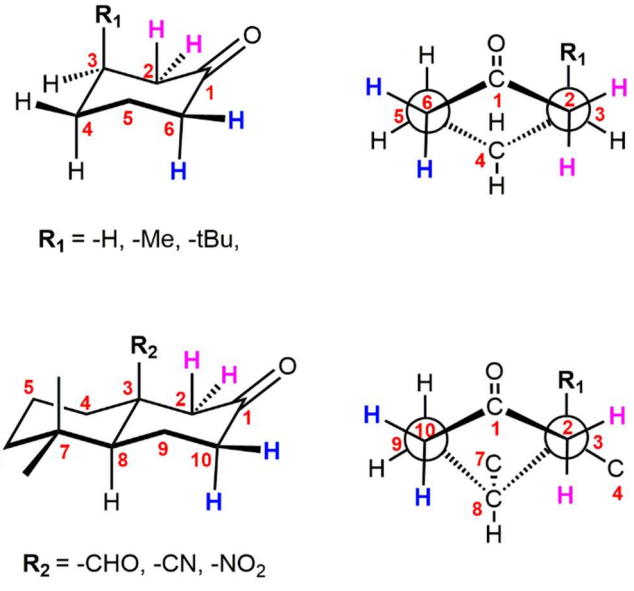
2. Schemes & Mechanisms



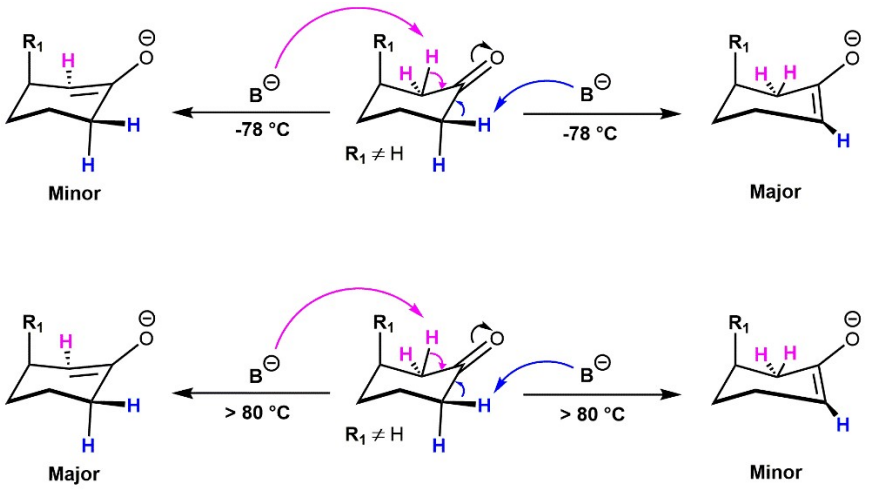
Scheme S1: β-substituted cyclic ketones **1**-**6** (left) and hindered bases (right) involved in this study.



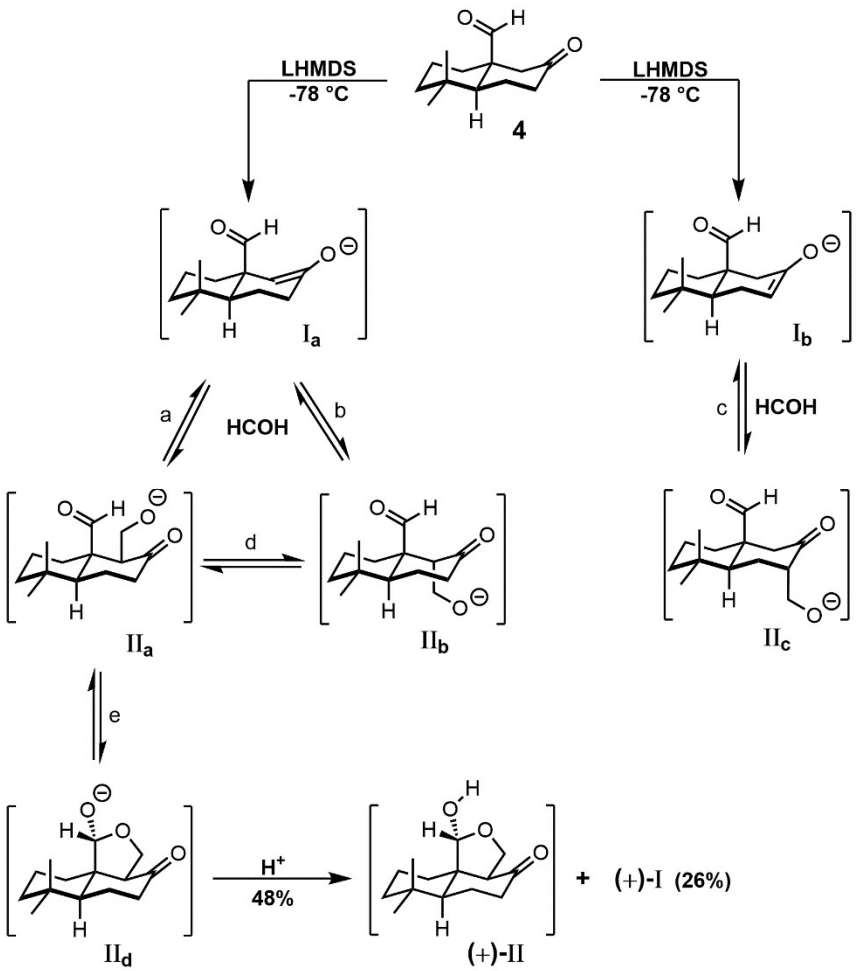
Scheme S2: Relative stabilization energy (ΔE) in the cyclohexanone between *boat* and *chair* conformation.[2]



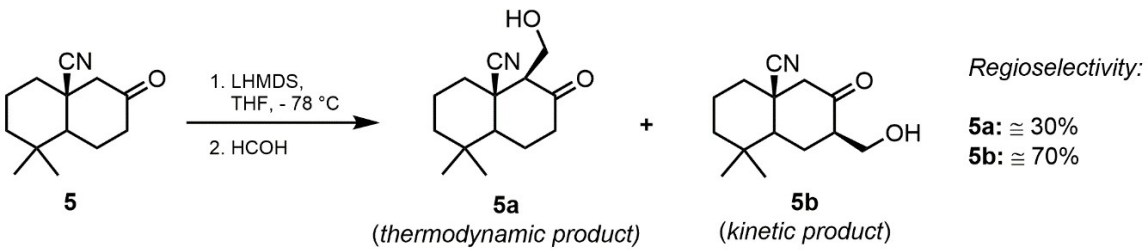
Scheme S3: Structures (in perspective) and Newman projections of model β-functionalized cyclohexanone (top) and bicyclic ketone (botton). Hydrogens from "thermodynamic" and "kinetic position" are marked in pink and blue, respectively.



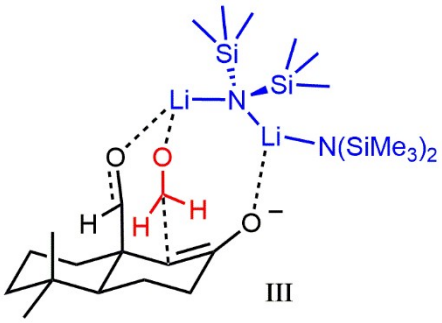
Scheme S4: Enolate formation mechanism on β-functionalized cyclohexanones under kinetic (top) and thermodynamic condition (botton) using a generic hindered base (B^-).



Scheme S5: Kinetic-controlled aldol addition on **4** with monomeric formaldehyde as reported by Angamuthu *et al.* [3]



Scheme S6: Kinetic-controlled aldol addition on **5** with monomeric formaldehyde as reported by Angamuthu *et al.* [3]



Key Points:

1. TS **III** requires formaldehyde in solution to be formed.
2. Formation of the "thermodynamic enolate" must be observed after LHMDS addition and before the addition of HCOH. Authors added HCOH after 5h from LHMDS addition.
3. LHMDS dimerization (blue structure), proposed by the authors, is not plausible due to steric hindrance (see Figure S3 and Table S1).
4. TS **III** does not explain the regio-control towards $\mathbf{I_a}$ with respect to $\mathbf{I_b}$ (see Scheme S5)
5. TS **III** could explain the stereo-control towards $\mathbf{II_a}$ with respect to $\mathbf{II_b}$, although the equilibrium between them, reported by the authors, cannot exist because they are epimers (see Scheme S5).

Scheme S7. Chelating TS structure **III** as reported by Angamuthu *et al.* to explain the unusual reactivity observed in ketone **4** (top). [3] Key points related to TS **III** (bottom) Ketone **4** is marked in black while formaldehyde (HCOH) and LHMDS (dimer) in red and blue, respectively.

3. Computational Studies

3.1 Steric Hindrance on **1**-**3**

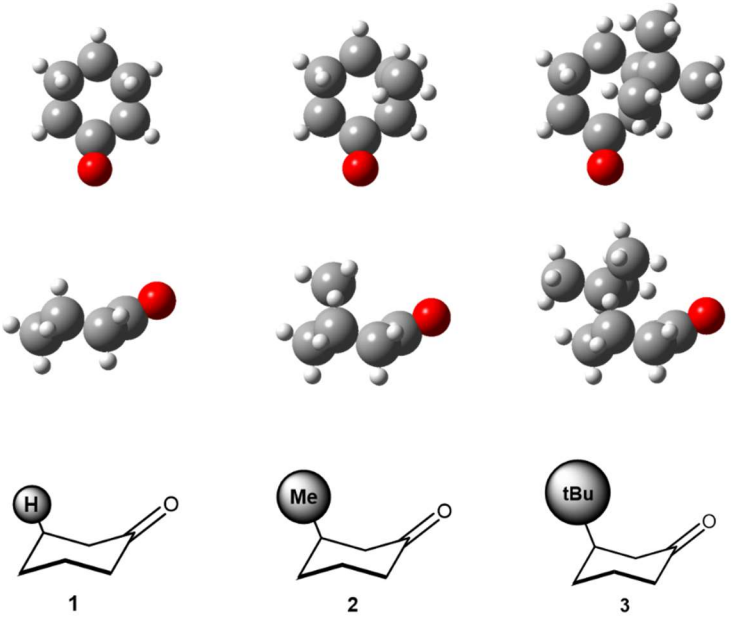


Figure S1. Size comparison of the substituent in β-position in **1**-**3**.
Top (top) and side view (middle) of optimized **1**-**3** are shown considering van der Waals radii for each atom.

3.2 Steric Hindrance on **4**-**6**

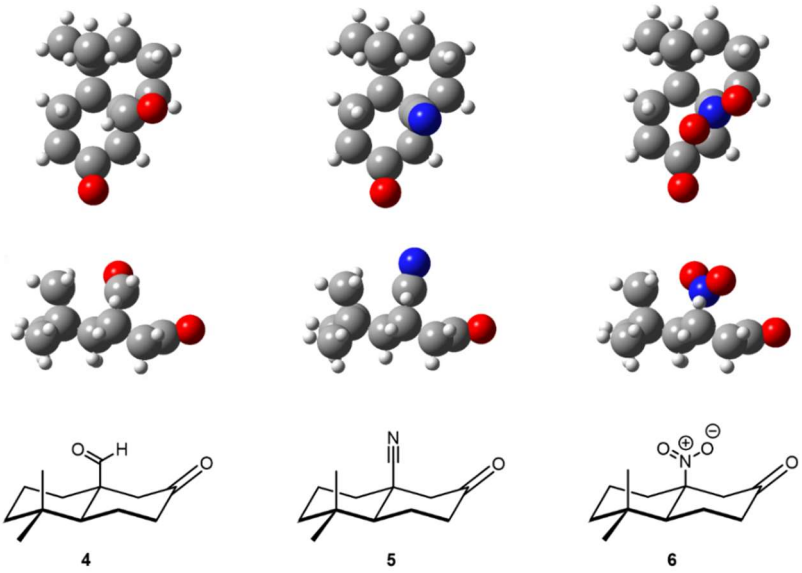


Figure S2. Size comparison of the substituent in β-position in **4**-**6**.
Top view (top) and side view (middle) of **1**-**3** are shown considering van der Waals radii for each atom.

3.3 Steric Hindrance on **LHMSD** and **KHMSD**

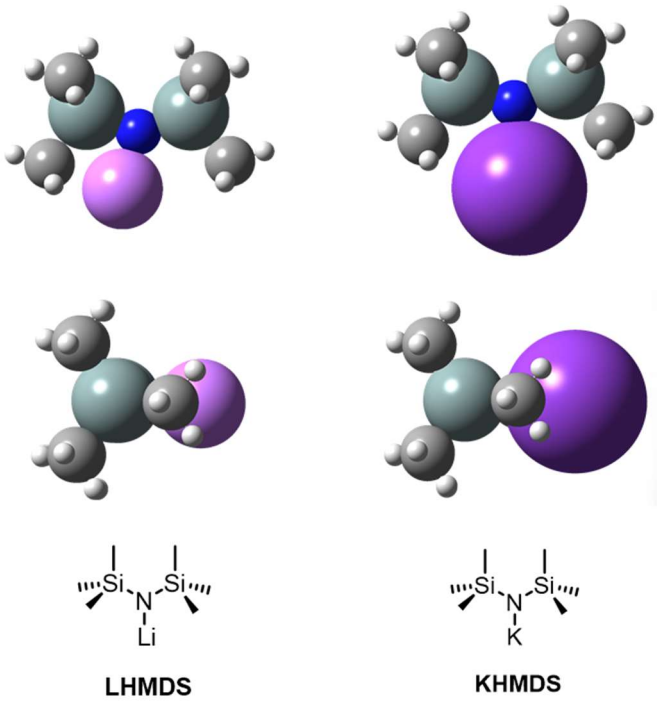


Figure S3. Size comparison in bases **LHMDS** (left) and **KHMDS** (right).
Top view (top) and side view (middle) of **LHMDS** and **KHMDS** are shown considering van der Waals radii for each atom.

Bond	Length (Å)	
	LHMDS	**KHMDS**
N-M^{+1}	1.80687	2.53653
N-Si[a]	1.70240	1.68617
Si-C[a]	1.90965	1.91450
C-H[a]	1.09727	1.09758

Table S1. Bond length (Å) in **LHMDS** and **KHMDS** calculated at B3LYP/6-31G(d,p) level of theory. M^{+1} corresponds to Li^+ and K^+. [a]Averaged value.

3.4 Electrostatic Potential Surface (ESP) Map on **4-6**

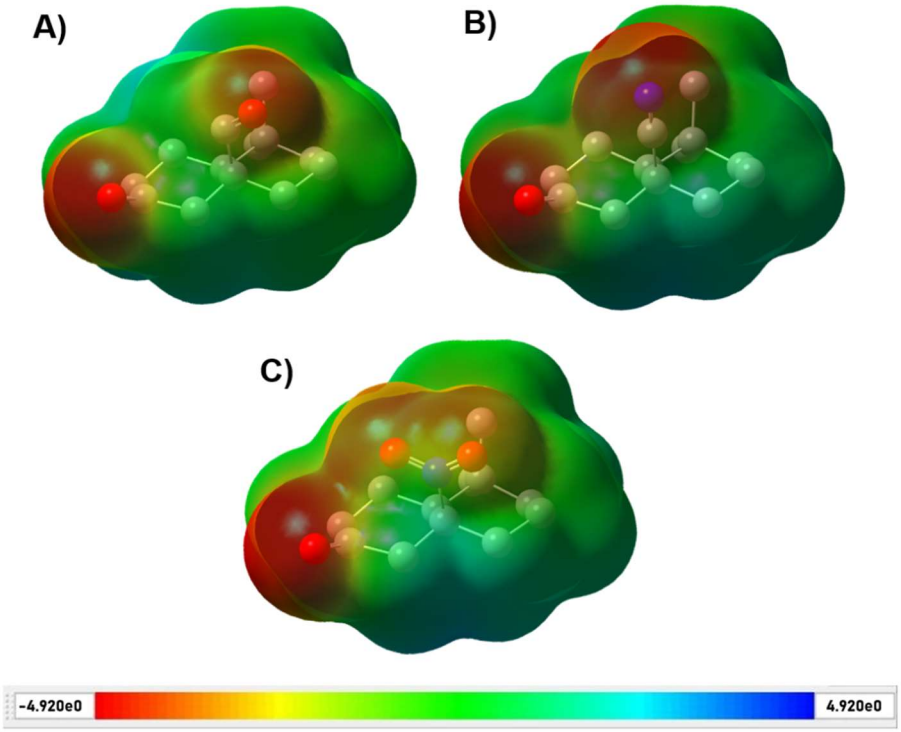
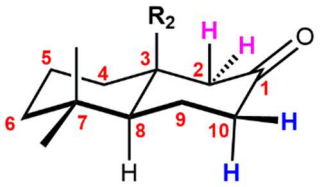


Figure S4. Electrostatic Potential Surface (ESP) Map calculated at B3LYP/6-31G(d,p) for A) **4**, B) **5** and C) **6**. Hydrogens have been hidden for better clarity.



R_2 = -CHO, -CN, $-NO_2$

Compound	Mulliken Atom Charges (MAC)	
	T-Hydrogens[a]	K-Hydrogens[a]
4	0.128579	0.121466
5	0.129280	0.122175
6	0.137776	0.119956

Table S2. Mulliken atom charges for T- and K-hydrogens in ketones **4-6** (marked in pink and blue, respectively) calculated at B3LYP/6-31G(d,p) level of theory. [a]Averaged value is reported.

3.5 TS Conformational Study on Ketone **2** and **3**

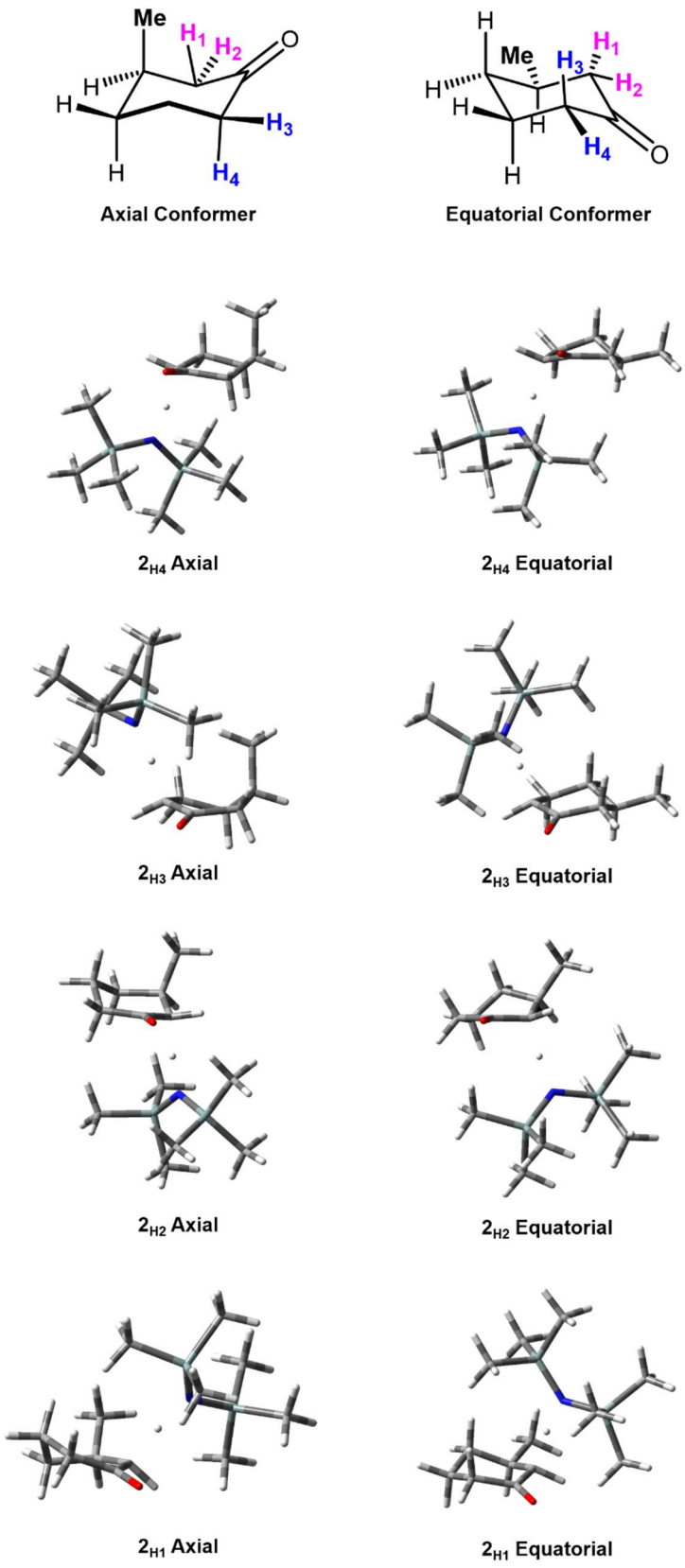
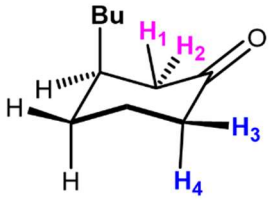
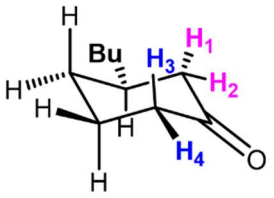


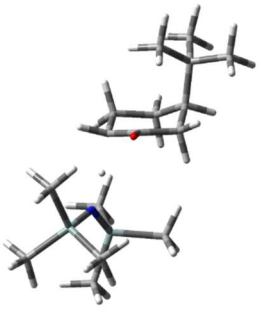
Figure S5. TS Conformational search for **2** with the Me group in axial (left) and equatorial position (right).



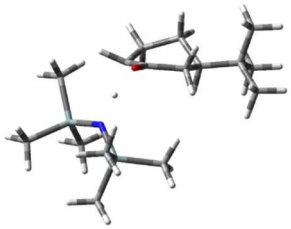
Axial Conformer



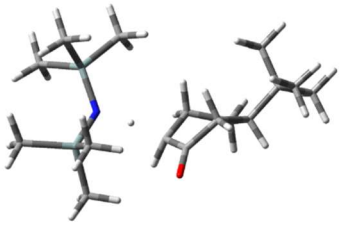
Equatorial Conformer



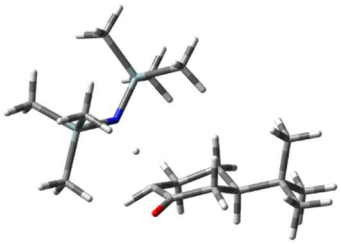
3_{H4} Axial



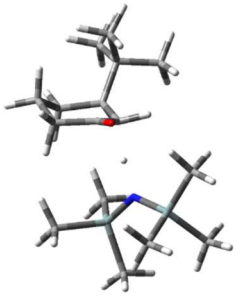
3_{H4} Equatorial



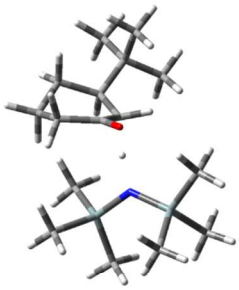
3_{H3} Axial



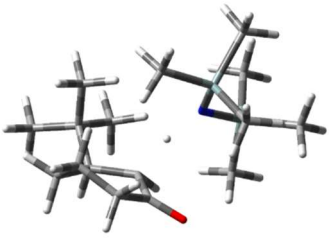
3_{H3} Equatorial



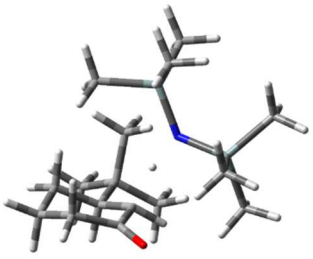
3_{H2} Axial



3_{H2} Equatorial



3_{H1} Axial



3_{H1} Equatorial

Figure S6. TS conformational search for **3** with the *t*Bu group in axial (left) and equatorial position (right).

3.6 Conformational Study on Enolates from **4**

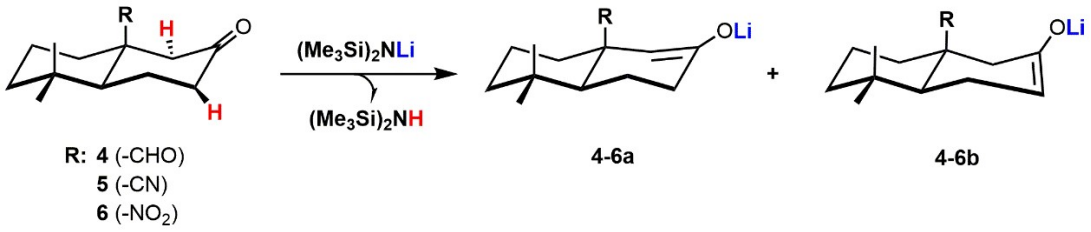


Figure S7. Thermodynamic (**4-6a**) and kinetic enolate (**4-6b**) from the deprotonation of **4-6** using **LHMDS.**

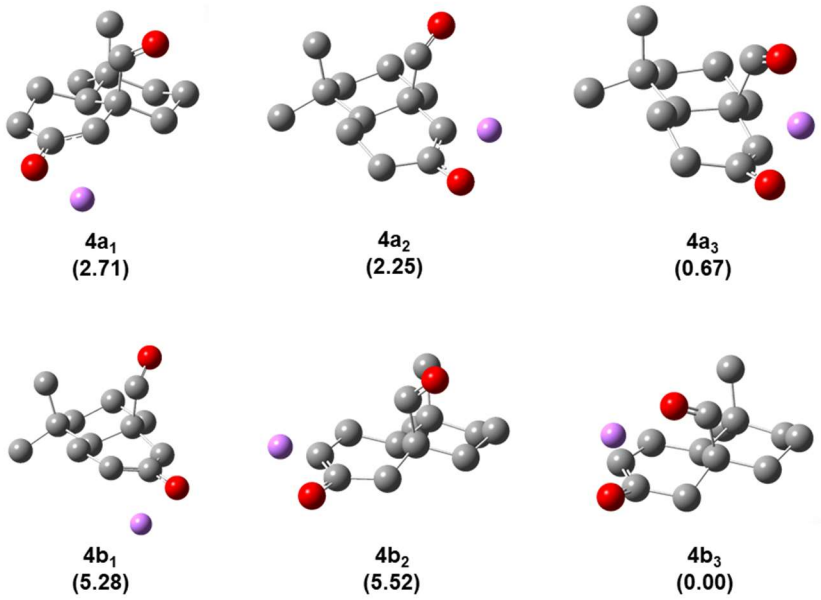


Figure S8. Enolate conformes from deprotonation of **4** are reported.
Relative stability is reported in kcal/mol in parentheses. Hydrogens have been hidden for better clarity.
Li^+ cation appears: i) under the enolate plane (Conformers $4X_1$), ii) above the enolate plane (Conformers $4X_2$) or iii) double coordinated (Conformers $4X_3$).

Conformer	Relative Stability (kcal/mol)	Relative Stability (kcal/mol)
$4a_1$	1.58	2.25
$4a_2$	2.04	2.71
$4a_3$	0.00	0.67
$4b_1$	5.52	5.52
$4b_2$	5.28	5.28
$4b_3$	0.00	0.00

Table S3. Realtive stabilities, expressed in kcal/mol, for enolates **4a** and **4b**.

3.7 Transition State (TS) Study with $(Me_3Si)_2N^-$ (No Counter Cation)

Figure S9. Hydrogens from thermodynamic (H_1 and H_2 – marked in purple) and kinetic position (H_3 and H_4 – marked in blue) with the R1 group in the axial (left) and equatorial position (right) in a general β-substituted cyclohexanone .

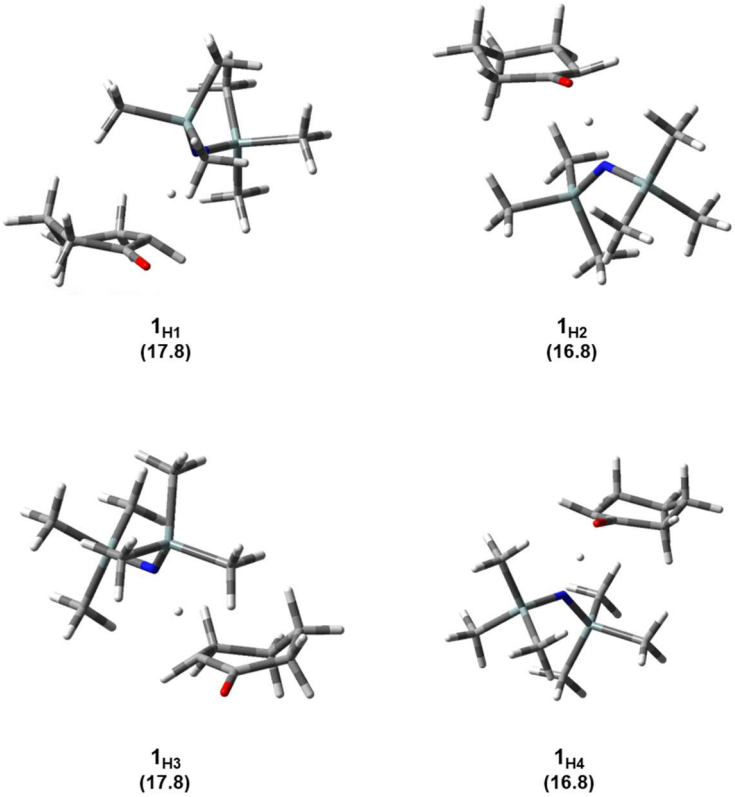


Figure S10. TS for the deprotonation of $H_{1\text{-}4}$ on **1**. Activation energy in kcal/mol is shown in parentheses.

Structure	Ea (kcal/mol)	Averaged Ea (kcal/mol)
$\mathbf{1}_{H1}$	17.8	17.3[a]
$\mathbf{1}_{H2}$	16.8	
$\mathbf{1}_{H3}$	17.8	17.3[a]
$\mathbf{1}_{H4}$	16.8	

Table S4. Activation Energies for each enolate formation on **1**.
[a]Boltzmann distribution equal to 50%.

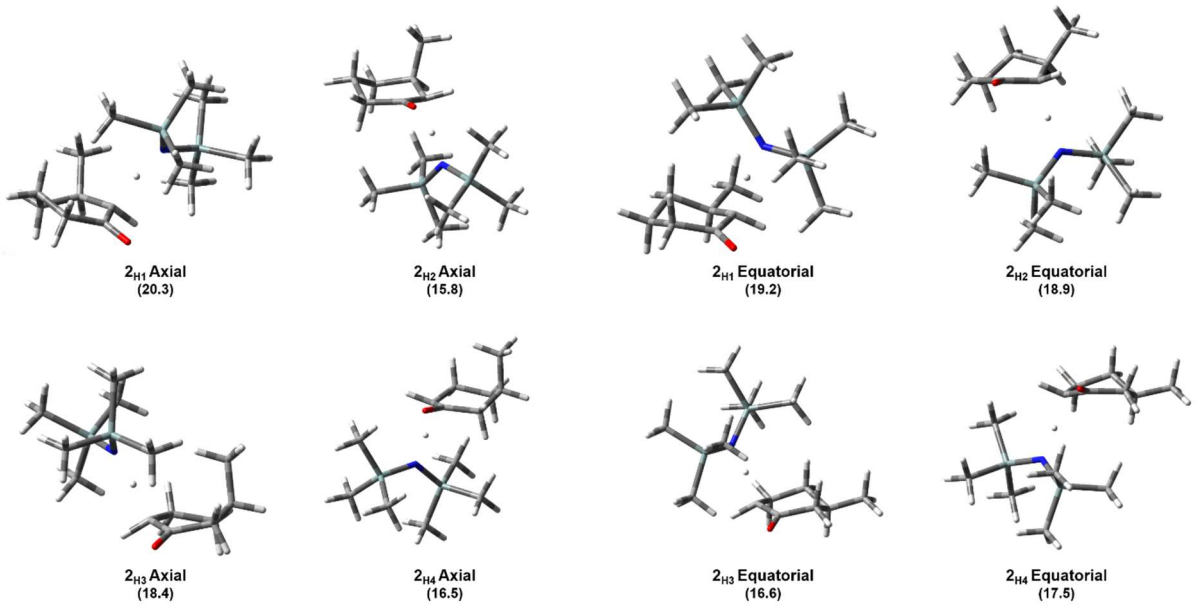


Figure S11. TS structures for the deprotonation of $H_{1\text{-}4}$ on **2**.
Activation energy in kcal/mol is shown in parentheses.

Structure	Ea_Axial (kcal/mol)	Ea_Equatorial (kcal/mol)	Averaged Ea for each H[a] (kcal/mol)	ΔE_{Ea} (kcal/mol)	Boltzmann Distribution (%)	Averaged Ea[b] (kcal/mol)
$\mathbf{2}_{H1}$	20.3	19.2	19.3	0.5	30.0	18.9
$\mathbf{2}_{H2}$	15.8	18.9	18.7		70.0	
$\mathbf{2}_{H3}$	18.4	16.6	16.7	0.8	79.5	16.8
$\mathbf{2}_{H4}$	16.5	17.5	17.5		20.5	

Table S5. Activation Energies for each enolate formation on **2**.
[a]Averaged considering relative stability (ΔE = 1.7 kcal/mol) of ketone **2** at the ground state (95.0% equatorial and 5.0% axial). [b]Averaged Ea for each position (thermodynamic vs kinetic)

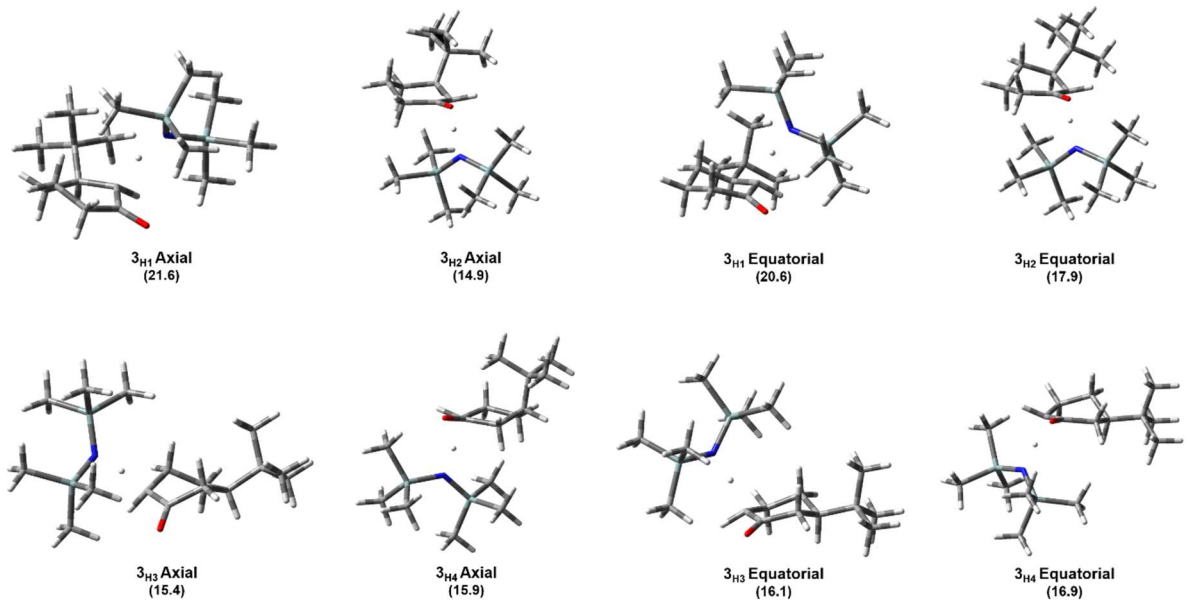


Figure S12. TS for the deprotonation of $H_{1\text{-}4}$ on **3**. Activation energy in kcal/mol is shown in parentheses.

Structure	Ea_Axial (kcal/mol)	Ea_Equatorial (kcal/mol)	Averaged Ea for each H[a] (kcal/mol)	ΔE_{Ea} (kcal/mol)	Boltzmann Distribution (%)	Averaged Ea[b] (kcal/mol)
$\mathbf{3_{H1}}$	21.6	20.6	20.8	2.9	0.7	17.9
$\mathbf{3_{H2}}$	14.9	17.9	17.9		99.3	
$\mathbf{3_{H3}}$	15.4	16.1	16.1	0.8	79.5	16.3
$\mathbf{3_{H4}}$	15.9	16.9	16.9		20.5	

Table S6. Activation Energies for each enolate formation on **3**.
[a]Averaged considering relative stability (ΔE = 4.1 kcal/mol) of ketone **3** at the ground state (99.9% equatorial and 0.1% axial). [b]Averaged Ea for each position (thermodynamic vs kinetic)

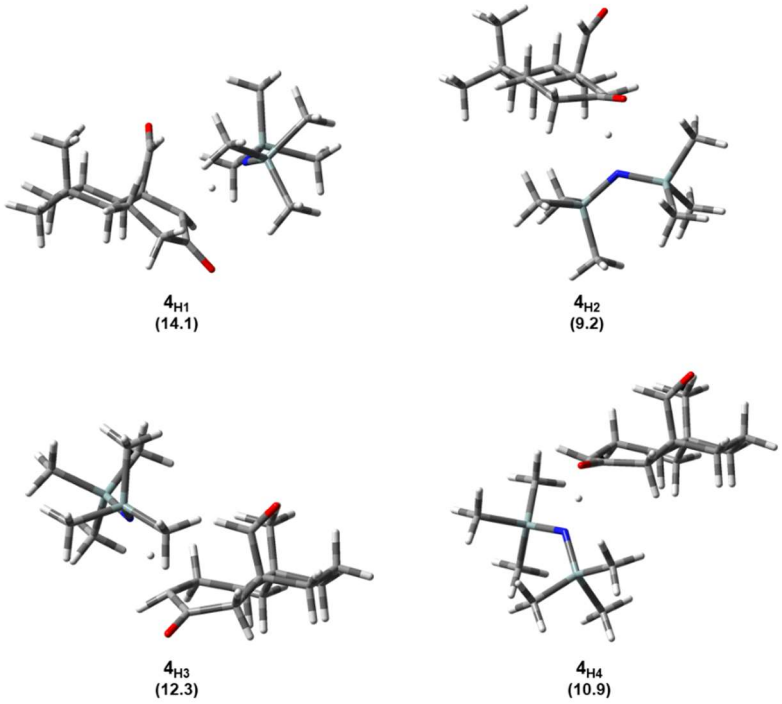


Figure S13. TS for the deprotonation of $H_{1\text{-}4}$ on **4**. Activation energy in kcal/mol is shown in parentheses.

Structure	Ea (kcal/mol)	ΔE_{Ea} (kcal/mol)	Boltzmann Distribution (%)	Averaged Ea (kcal/mol)
$\mathbf{4_{H1}}$	14.1	4.9	0.0	9.2
$\mathbf{4_{H2}}$	9.2		100.0	
$\mathbf{4_{H3}}$	12.3	1.4	8.5	11.0
$\mathbf{4_{H4}}$	10.9		91.5	

Table S7. Activation Energies for each enolate formation on **4**.

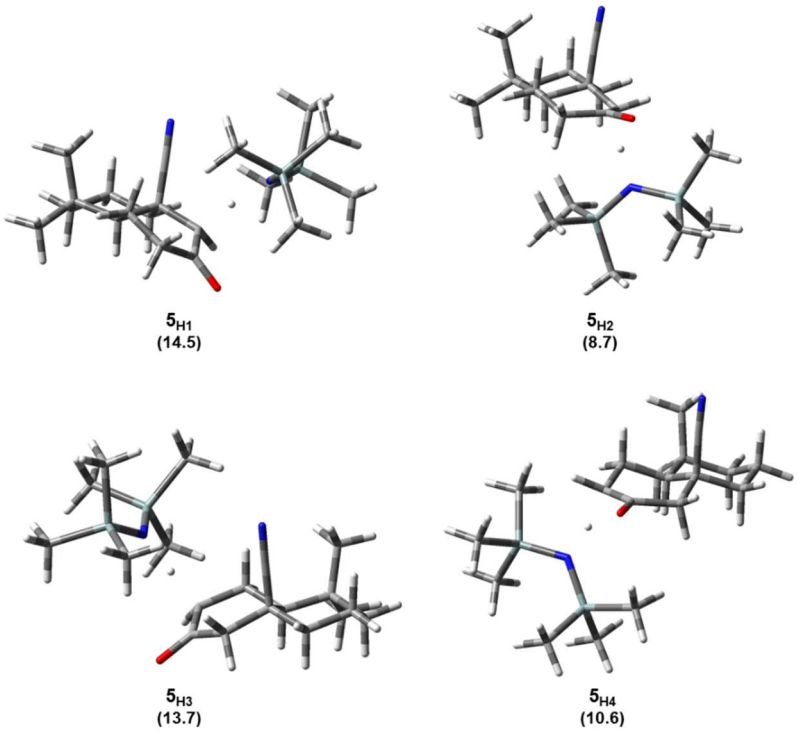


Figure S14. TS for the deprotonation of $H_{1\text{-}4}$ on **5**. Activation energy in kcal/mol is shown in parentheses.

Structure	Ea (kcal/mol)	ΔE_{Ea} (kcal/mol)	Boltzmann Distribution (%)	Averaged Ea (kcal/mol)
$\mathbf{5}_{H1}$	14.5	5.8	0.0	8.7
$\mathbf{5}_{H2}$	8.7		100.0	
$\mathbf{5}_{H3}$	13.7	3.1	0.5	10.6
$\mathbf{5}_{H4}$	10.6		99.5	

Table S8. Activation Energies for each enolate formation on **5**.

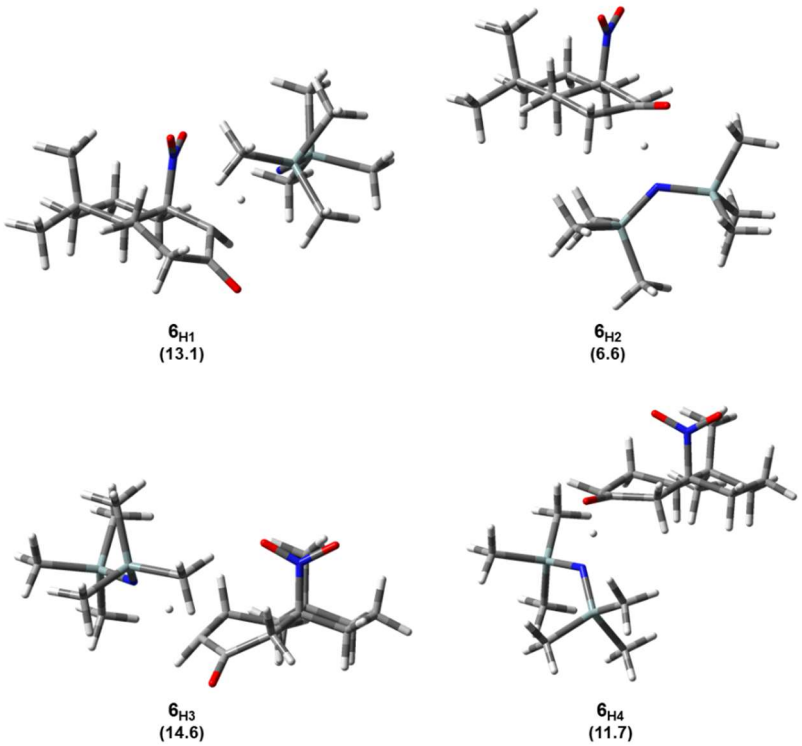


Figure S15. TS for the deprotonation of $H_{1\text{-}4}$ on **6**. Activation energy in kcal/mol is shown in parentheses.

Structure	Ea (kcal/mol)	ΔE_{Ea} (kcal/mol)	Boltzmann Distribution (%)	Averaged Ea (kcal/mol)
$\mathbf{6_{H1}}$	13.1	6.5	0.0	6.6
$\mathbf{6_{H2}}$	6.6		100.0	
$\mathbf{6_{H3}}$	14.6	2.9	0.7	11.7
$\mathbf{6_{H4}}$	11.7		99.3	

Table S9. Activation Energies for each enolate formation on **6**.

3.8 Transition State (TS) Study with **LHMDS**

Unsubstituted cyclohexanone (**1**) has been used as reference to confirm the same behaviour previously described and reported (see Figure S8 and Table S3). For practical reasons, the most stable TS structure for each set of hydrogens, from kinetic and thermodynamic positions, has been exclusively reported and shown for **4**, **5** and **6**.

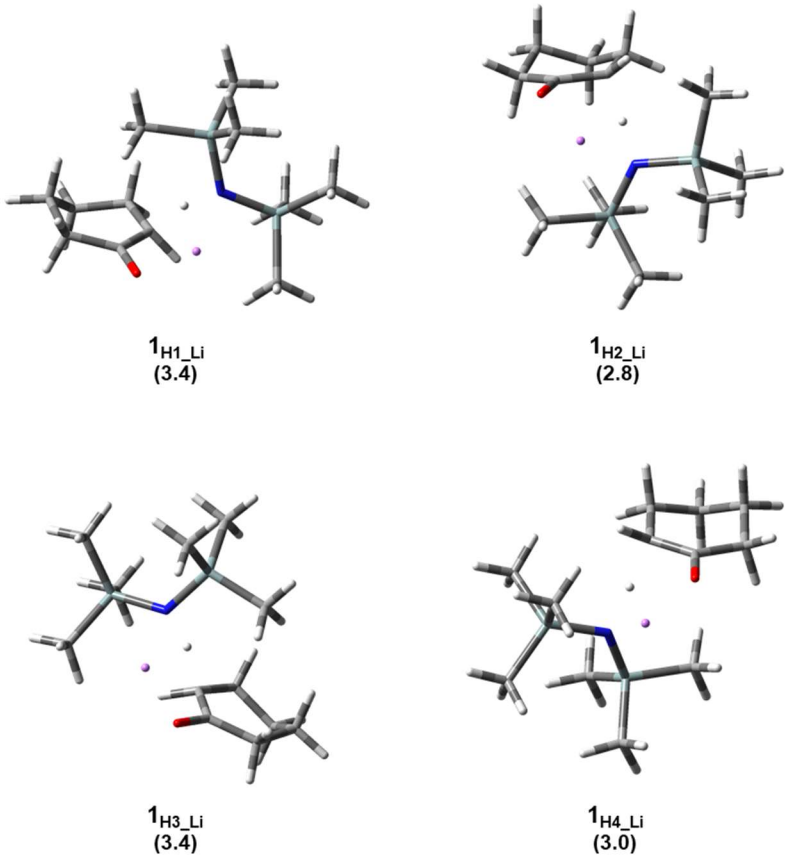


Figure S16. TS for the deprotonation of $H_{1\text{-}4}$ on **1** using **LHMDS**.
Activation energy in kcal/mol is shown in parentheses.

Structure	Ea (kcal/mol)	Averaged Ea (kcal/mol)
$\mathbf{1}_{H1\_Li}$	3.4	3.1[a]
$\mathbf{1}_{H2\_Li}$	2.8	
$\mathbf{1}_{H3\_Li}$	3.4	3.2[a]
$\mathbf{1}_{H4\_Li}$	3.0	

Table S10. Activation Energies for each enolate formation on **1** using **LHMDS** as a base.
[a]Boltzamm distribution equal to 50%.

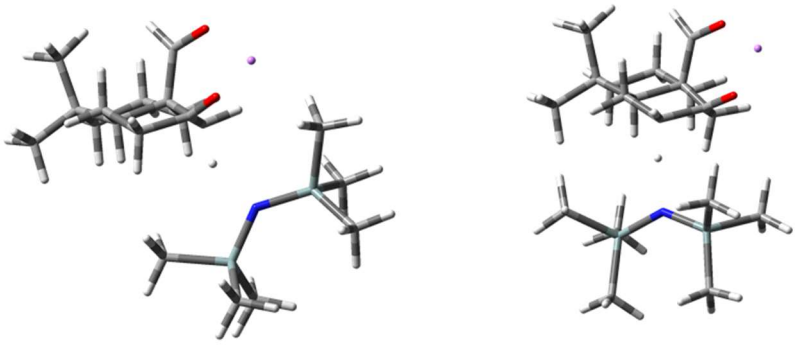


Figure S17. Most stable TS structures for the deprotonation of **4** using **LHMDS**. Activation energy in kcal/mol is shown in parentheses.

Structure	Ea (kcal/mol)	ΔE (kcal/mol)
4_{H2_Li}	24.8	5.2
4_{H4_Li}	30.0	

Table S11. Activation Energies for each enolate formation on **4** using **LHMDS** as a base.

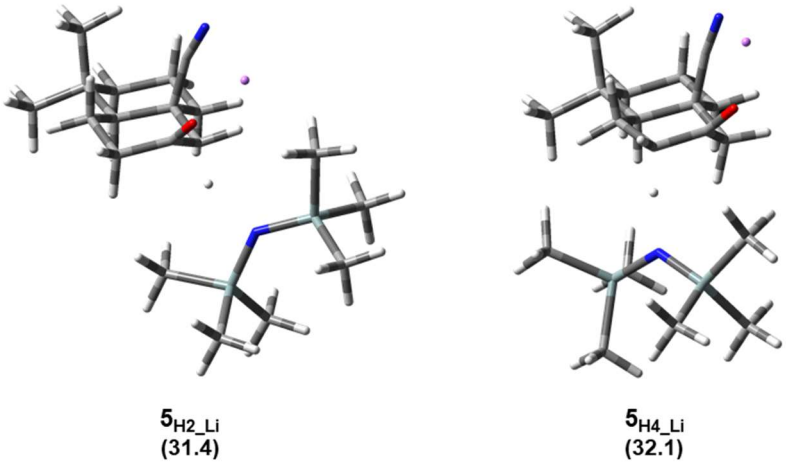


Figure S18. Most stable TS structures for the deprotonation of **5** using **LHMDS**. Activation energy in kcal/mol is shown in parentheses.

Structure	Ea (kcal/mol)	ΔE (kcal/mol)
5_{H2_Li}	31.4	0.7
5_{H4_Li}	32.1	

Table S12. Activation Energies for each enolate formation on **5** using **LHMDS** as a base.

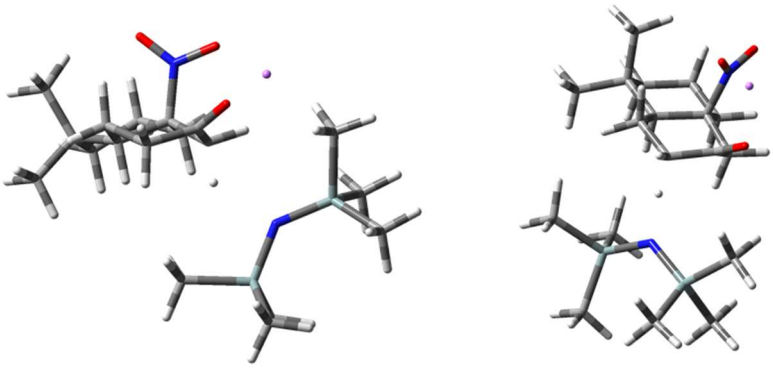


Figure S19. Most stable TS structures for the deprotonation of **6** using **LHMDS**.
Activation energy in kcal/mol is shown in parentheses.
* Only TS pre-complex could be found for $\mathbf{6}_{H2\_Li}$ after several attempts, leading to suppose an Ea slightly lower than 26.9 kcal/mol.

Structure	Ea (kcal/mol)	ΔE (kcal/mol)
$\mathbf{6}_{H2\_Li}$	26.9	5.3
$\mathbf{6}_{H4\_Li}$	32.2	

Table S13. Activation Energies for each enolate formation on **6** using **LHMDS** as a base.

3.9 Transition State (TS) Study with **KHMDS**

For practical reasons, the most stable TS structure for each set of hydrogens, from kinetic and thermodynamic position, has been exclusively reported and shown for **4**, **5** and **6**.

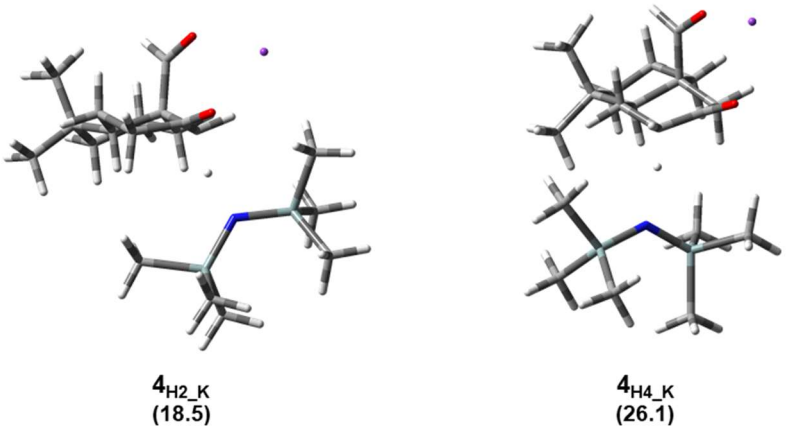


Figure S20. Most stable TS structures for the deprotonation of **4** using **KHMDS**. Activation energy in kcal/mol is shown in parentheses.

Structure	Ea (kcal/mol)	ΔE (kcal/mol)
4_{H2_K}	18.5	7.6
4_{H4_k}	26.1	

Table S14. Activation Energies for each enolate formation on **4** using **KHMDS** as a base.

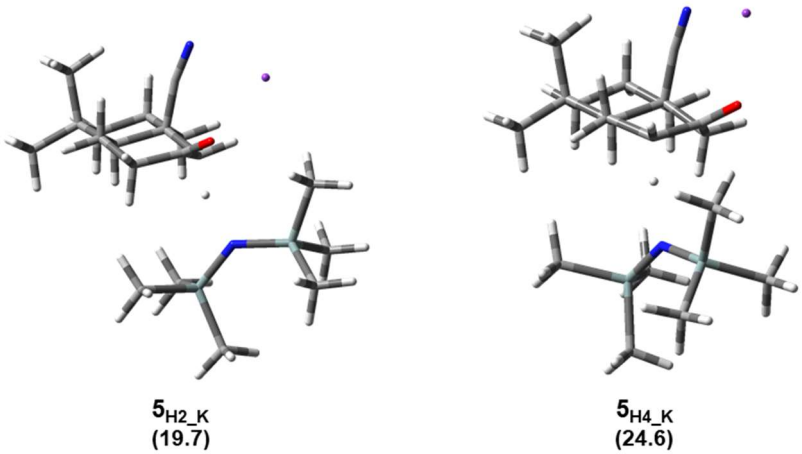


Figure S21. Most stable TS structures for the deprotonation of **5** using **KHMDS**. Activation energy in kcal/mol is shown in parentheses.

Structure	Ea (kcal/mol)	ΔE (kcal/mol)
$\mathbf{5}_{H2\_K}$	19.7	4.9
$\mathbf{5}_{H4\_k}$	24.6	

Table S15. Activation Energies for each enolate formation on **5** using **KHMDS** as a base.

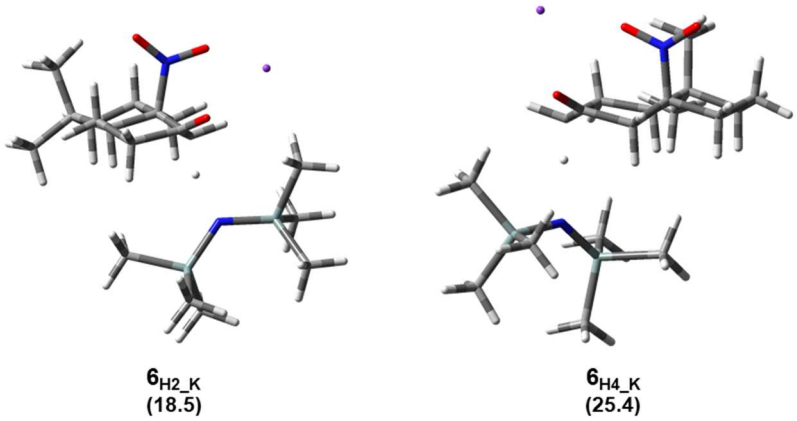


Figure S22. Most stable TS structures for the deprotonation of **6** using **KHMDS**. Activation energy in kcal/mol is shown in parentheses.

Structure	Ea (kcal/mol)	ΔE (kcal/mol)
$\mathbf{6}_{H2\_K}$	18.5	6.9
$\mathbf{6}_{H4\_k}$	25.4	

Table S16. Activation Energies for each enolate formation on **6** using **KHMDS** as a base.

3.10 Comparison Li-TS *vs* K-TS

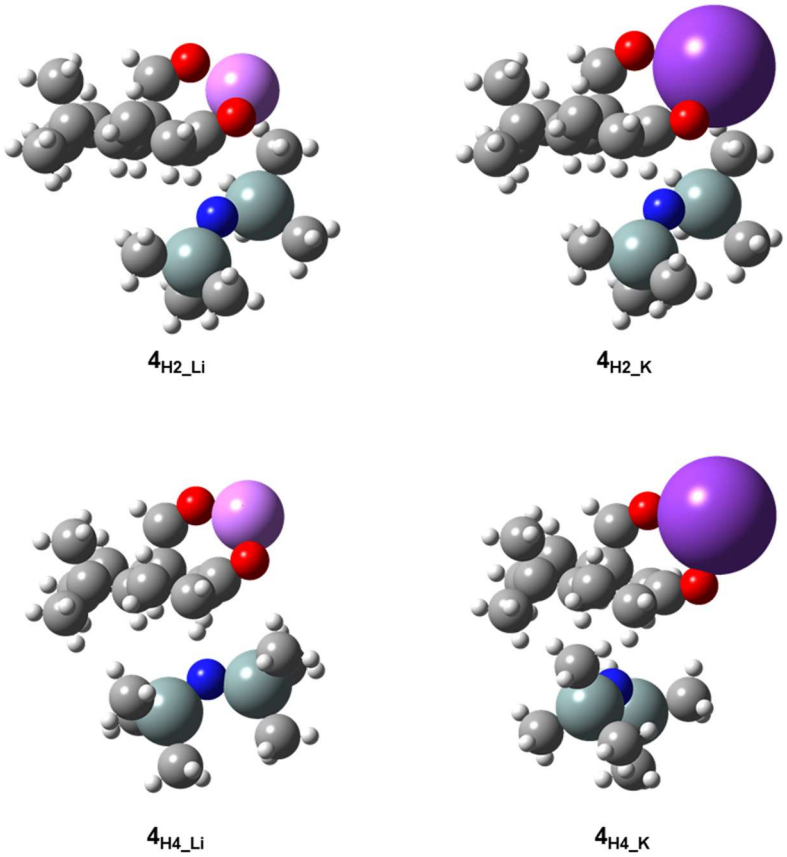


Figure S23. Most stable TS structures for the deprotonation of **4** using **LHMDS** (left) and **KHMDS** (right). In order to highlight structural differences, van der Waals radii have been considered for each atom.

TS Structure	Angle (°)		Distance (Å)
	Mol. Plane – Subst. R_1	Mol. Plane - Ketone (C=O)	Subst. R_1 (Donor) - Ketone (Donor)
4_{H2_Li}	109.467	153.091	3.108
4_{H4_Li}	107.428	150.184	3.038
4_{H2_K}	107.834	165.599	3.552
4_{H4_K}	109.149	159.266	3.320

Table S17. Structural differences in the most stable TS in **4**. Particular interest has been done to the parameters (angles and distances) where substituent R_1 (aldehyde group in this specific case) and carbonyl group of the ketone are involved, affecting the coordination of Li^+ and K^+.

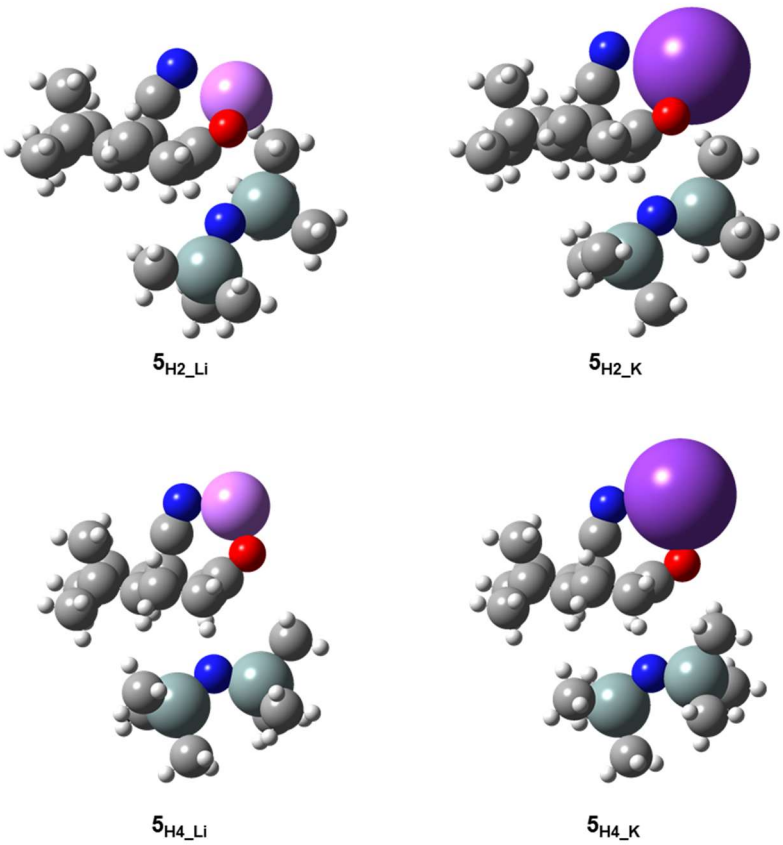


Figure S24. Most stable TS structures for the deprotonation of **5** using **LHMDS** (left) and **KHMDS** (right). In order to highlight structural differences, van der Waals radii have been considered for each atom.

TS Structure	Angle (°) Mol. Plane – Subst. R_1	Angle (°) Mol. Plane – Ketone (C=O)	Cyano Group Linearity (C-C≡N)	Distance (Å) Subst. R_1 (Donor) – Ketone (Donor)
5_{H2_Li}	110.966	142.862	162.218	3.264
5_{H4_Li}	110.197	138.470	168.465	3.157
5_{H2_K}	109.547	155.645	167.728	3.824
5_{H4_K}	109.596	147.241	172.007	3.527

Table S18. Structural differences in the most stable TS in **5**. Particular interest has been done to the parameters (angles and distances) where substituent R_1 (cyano group in this specific case) and carbonyl group of the ketone are involved, affecting the coordination of Li^+ and K^+.

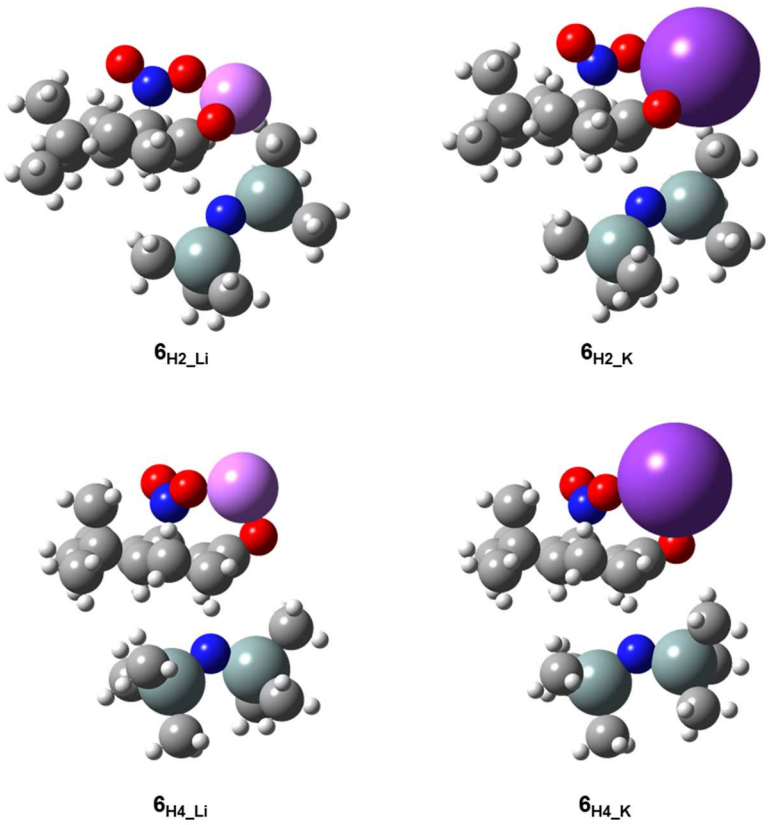
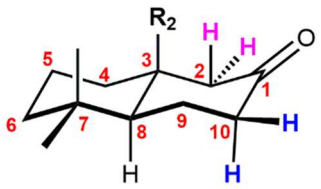


Figure S25. Most stable TS structures for the deprotonation of **6** using **LHMDS** (left) and **KHMDS** (right). In order to highlight structural differences, van der Waals radii have been considered for each atom.

TS Structure	Angle (°)		Distance (Å)
	Mol. Plane – Subst. R_1	Mol. Plane - Ketone (C=O)	Subst. R_1 (Donor) - Ketone (Donor)
$\mathbf{6}_{H2\_Li}$	112.589	149.508	3.003
$\mathbf{6}_{H4\_Li}$	107.178	145.779	2.924
$\mathbf{6}_{H2\_K}$	110.780	156.537	3.697
$\mathbf{6}_{H4\_K}$	107.823	152.680	3.101

Table S19. Structural differences in the most stable TS in **6**. Particular interest has been done to the parameters (angles and distances) where substituent R_1 (nitro group in this specific case) and carbonyl group of the ketone are involved, affecting the coordination of Li^+ and K^+.



R_2 = -CHO, -CN, -NO_2

TS Structure	Distance (Å)	
	Ketone (C=O) ▪▪▪ M^{1+}	Substituent (R_2) ▪▪▪ M^{1+}
$\mathbf{4}_{H2\_Li}$	1.88041	1.99525
$\mathbf{4}_{H4\_Li}$	1.79461	1.87819
$\mathbf{5}_{H2\_Li}$	1.88840	2.25675
$\mathbf{5}_{H4\_Li}$	1.78997	2.03557
$\mathbf{6}_{H2\_Li}$	1.91197	1.99048
$\mathbf{6}_{H4\_Li}$	1.79046	1.89527
$\mathbf{4}_{H2\_K}$	2.53397	2.71027
$\mathbf{4}_{H4\_K}$	2.47400	2.60532
$\mathbf{5}_{H2\_K}$	2.58186	2.92177
$\mathbf{5}_{H4\_K}$	2.48808	2.77399
$\mathbf{6}_{H2\_K}$	2.60430	2.74074
$\mathbf{6}_{H4\_K}$	2.49683	2.64351

Table S20. General structure and Newman projections for byciclic ketone **4**-**6** (top). Distances (Å) between donors from ligands (ketone's carbonyl and substituent R_1) with cation from the base (Li^{1+} or K^{1+}) in the TS structures of **4**, **5** and **6** (Bottom). Hydrogens from "thermodynamic" and "kinetic position" are marked in pink and blue, respectively.

3.11 Cartesian Coordinates for Optimized Systems

Cartesian coordinates for optimized ketone **1**

C	-1.79198300	0.00001800	0.10950600
C	-1.01781000	1.26646200	-0.28217400
C	0.39270400	1.28681900	0.34307900
C	0.39266200	-1.28687700	0.34297200
C	-1.01789700	-1.26642900	-0.28205800
H	0.99070900	2.13014600	-0.01191500
H	-0.92580300	1.31026300	-1.37555600
H	-1.56746700	2.16488400	0.01994700
H	-1.96927100	0.00016900	1.19446700
H	0.99061500	-2.13015300	-0.01224200
H	0.29733400	-1.38242700	1.43504400
H	0.29702100	1.38223500	1.43512600
C	1.16028800	-0.00000500	0.06519700
O	2.30641100	0.00000100	-0.34261600
H	-1.56756600	-2.16481200	0.02012500
H	-2.77867600	0.00005900	-0.36776500
H	-0.92597300	-1.31030200	-1.37542900

Cartesian coordinates for optimized ketone **2**

C	-1.30725000	1.01872600	0.42454200
C	-0.21714500	1.64968200	-0.45466500
C	1.19320200	1.19450400	-0.02466200
C	0.17893800	-0.97190100	0.91373900
C	-1.23192400	-0.52274500	0.45633200
H	1.96811100	1.53870800	-0.71446400
H	-0.37870900	1.37753700	-1.50451800
H	-0.28044500	2.74256700	-0.40901500
H	-1.20415000	1.40009100	1.45004400
H	0.29880200	-2.05757000	0.85972700
H	0.32550600	-0.66993000	1.96109100
H	1.41610400	1.61634100	0.96683000
C	1.28786800	-0.32109700	0.09612200
O	2.18582800	-0.96262800	-0.41635800
H	-1.95136300	-0.87841600	1.20537100
H	-2.29804300	1.33297800	0.07490800
C	-1.61165600	-1.16358600	-0.88788900
H	-1.62427700	-2.25533100	-0.80693700
H	-2.60699400	-0.83920500	-1.21003300
H	-0.90335200	-0.90824300	-1.68325900

Cartesian coordinates for optimized ketone **2** (Flipped)

C	-0.96449200	1.25012300	-0.08309000
C	-1.18746000	-0.21598800	0.32597800
C	-0.11233000	-1.12233100	-0.31818600
C	1.53481500	0.85204100	-0.36411500
C	0.44613100	1.73822500	0.27385800
H	-0.18373400	-2.15400900	0.03785700
H	-1.06073200	-0.27874800	1.41737600
H	-1.12622300	1.34971600	-1.16688400
H	1.50308900	0.97775100	-1.45674000
H	-0.27346700	-1.13443500	-1.40759100
C	1.30493400	-0.62394400	-0.06781100
O	2.18957200	-1.35439200	0.33735100
H	0.58455400	2.77787600	-0.04289800
H	-1.71433600	1.88665400	0.40206700
C	-2.59905000	-0.70361300	-0.01635500
H	-2.74949500	-1.74123100	0.29955900
H	-3.35994500	-0.08906800	0.47656600

H	-2.77895500	-0.65495200	-1.09707700
H	0.56825400	1.72671800	1.36498100
H	2.53912900	1.12178100	-0.02769100

Cartesian coordinates for optimized ketone **3**

C	0.28413500	1.66469000	0.61121900
C	1.36514800	1.64394300	-0.48024800
C	2.42614500	0.55971600	-0.20898300
C	0.66930500	-0.77693500	1.11271400
C	-0.41867800	0.30833100	0.87647000
H	3.12809500	0.44507100	-1.03896200
H	0.91580700	1.47299700	-1.46381100
H	1.85186300	2.62462500	-0.53438500
H	0.76372500	1.96696200	1.55332700
H	0.25706200	-1.78542400	1.18000100
H	1.14783600	-0.56204600	2.07998200
H	3.00706400	0.84608400	0.68075000
C	1.79462900	-0.79215000	0.08541500
O	2.18360600	-1.82117100	-0.43662200
H	-0.94079800	0.43416600	1.83499300
H	-0.45216600	2.44309100	0.39293800
C	-1.55716300	-0.13064800	-0.11879700
C	-2.51195100	1.05223600	-0.38219300
H	-2.04284900	1.83911700	-0.98067000
H	-3.39400200	0.70902000	-0.93339400
H	-2.86244000	1.50268900	0.55389000
C	-1.04433200	-0.66716900	-1.47192800
H	-0.51398800	0.09616100	-2.04820000
H	-0.37664300	-1.52464600	-1.35193000
H	-1.89189900	-0.99702000	-2.08331600
C	-2.38323100	-1.25046000	0.55625700
H	-2.80781500	-0.91243300	1.50853400
H	-3.21488700	-1.55212900	-0.08951400
H	-1.78687300	-2.14624700	0.75318900

Cartesian coordinates for optimized ketone **3** (Flipped)

C	-0.24712300	1.49672400	0.09541300
C	0.27891700	0.09835200	-0.29236000
C	-0.62537800	-0.98104500	0.35908900
C	-2.63396800	0.62787500	0.30694700
C	-1.71322500	1.69234100	-0.31844800
H	-0.36819900	-1.99123700	0.03675600
H	0.15116000	0.00108000	-1.38221400
H	-0.15935400	1.63891000	1.18125000
H	-2.66608700	0.77737600	1.39650800
H	-0.51100300	-0.93795100	1.45216000
C	-2.10315800	-0.77367600	0.05111500
O	-2.80672100	-1.67309700	-0.36962600
H	-2.05711500	2.69254500	-0.03216500
H	0.35986700	2.27773300	-0.37187800
C	1.81007900	-0.12266500	-0.02947800
H	-1.79189500	1.63756700	-1.41228400
H	-3.65857200	0.68915000	-0.06861300
C	2.17475800	0.01986600	1.46202400
H	1.64419200	-0.70664700	2.08614600
H	3.24697900	-0.15307100	1.60540000
H	1.95257700	1.02090300	1.84498300
C	2.22509900	-1.52968100	-0.51163700
H	1.93180200	-1.69589300	-1.55465700
H	3.31249500	-1.64557600	-0.45052900
H	1.78044000	-2.32498900	0.09316000
C	2.62610300	0.90675500	-0.84163900
H	3.69724900	0.69543800	-0.75428200
H	2.36692300	0.86883000	-1.90605700
H	2.46967600	1.93153200	-0.49283400

Cartesian coordinates for optimized ketone **4**

C	0.22973800	0.71349900	-0.32220100
C	-0.68394700	1.72675100	0.40119300
C	-2.11457400	1.74196500	-0.17353200
C	-1.80524100	-0.69940800	-0.89339000
C	-0.36236000	-0.74029300	-0.28972900
H	-2.78591000	2.37441100	0.41299900
H	-0.73079600	1.51603400	1.47498100
H	-0.26416300	2.73232400	0.31147900
H	0.20355700	0.98650200	-1.39010700
H	-2.29355200	-1.67579200	-0.82652300
H	-1.70183900	-0.45066900	-1.95921200
H	-2.08347400	2.14991900	-1.19480700
C	-2.71570700	0.34981300	-0.26756600
O	-3.84390500	0.09118300	0.10515800
C	1.74365600	0.80360600	0.07639000
C	0.51186100	-1.70254000	-1.11555100
H	0.42188700	-1.42087300	-2.17362900
H	0.12033000	-2.71958700	-1.01679900
C	1.98750700	-1.65665100	-0.70498000
H	2.57188500	-2.30431900	-1.36903000
H	2.09805800	-2.07074600	0.30204000
C	2.53535200	-0.22746400	-0.77038700
H	3.58675000	-0.20959700	-0.45669500
H	2.52273600	0.10692800	-1.81813000
C	1.99112800	0.56152100	1.58075600
H	3.05881700	0.67008200	1.80104600
H	1.45924300	1.29065300	2.20024000
H	1.69684600	-0.43725900	1.91111700
C	2.29010500	2.20421400	-0.27590500
H	3.37894100	2.22185700	-0.15744900
H	2.06662900	2.47208300	-1.31507500
H	1.88355000	2.98724000	0.37105000
C	-0.55544500	-1.28408500	1.12721700
H	-1.11225800	-0.61905200	1.82280800
O	-0.20730400	-2.38439600	1.49931900

Cartesian coordinates for optimized ketone **5**

C	0.25574600	0.62162600	-0.34653300
C	-0.64779300	1.62941500	0.38949100
C	-2.06857400	1.67785900	-0.20376900
C	-1.79357800	-0.79043300	-0.88931600
C	-0.37061400	-0.81518600	-0.25442900
H	-2.73824700	2.31044900	0.38433300
H	-0.70976900	1.36309700	1.45046700
H	-0.21347100	2.63189000	0.34447900
H	0.20256600	0.85743500	-1.42141400
H	-2.29696100	-1.75360200	-0.77505000
H	-1.66706300	-0.60360700	-1.96509600
H	-2.02087500	2.10572400	-1.21687600
C	-2.70457300	0.30366200	-0.33924800
O	-3.87062300	0.08872800	-0.07713100
C	1.77787800	0.71529500	0.01967700
C	0.50946400	-1.85464200	-0.99555900
H	0.45775700	-1.61821800	-2.06676300
H	0.07865600	-2.85358700	-0.86796700
C	1.96723300	-1.81155900	-0.53506500
H	2.55371300	-2.53793600	-1.10896800
H	2.03555700	-2.12132200	0.51453300
C	2.54791300	-0.40667200	-0.72607500
H	3.59727400	-0.38371600	-0.40812800
H	2.54818800	-0.17525000	-1.80118000
C	2.05298800	0.62958200	1.53718500
H	3.12885800	0.72975500	1.71802300
H	1.55666000	1.43893400	2.08116900
H	1.72755000	-0.31132000	1.98365400
C	2.33325200	2.06472100	-0.48656700
H	3.41955900	2.09704400	-0.35065400

H	2.12859500	2.20856600	-1.55369200
H	1.91537700	2.91706300	0.05698100
C	-0.52765800	-1.24833900	1.15020200
N	-0.67557700	-1.61474200	2.24274600

Cartesian coordinates for optimized ketone **6**

C	0.31030300	0.77391300	-0.34783800
C	-0.61317300	1.75690600	0.39992300
C	-2.03317100	1.80099900	-0.19105800
C	-1.71335400	-0.60005900	-1.07104400
C	-0.29377000	-0.66625600	-0.46285600
H	-2.71870000	2.37347700	0.43857600
H	-0.67344600	1.49653800	1.45791500
H	-0.18343900	2.76039200	0.34105000
H	0.31137700	1.09674300	-1.40191400
H	-2.20300300	-1.57751500	-1.04290500
H	-1.59448500	-0.32631400	-2.12783900
H	-2.00048800	2.30440100	-1.17022200
C	-2.64702700	0.43548500	-0.44663200
O	-3.82518000	0.19831400	-0.27811200
C	1.81765600	0.82823700	0.08373200
C	0.61271100	-1.58776200	-1.29446400
H	0.52171900	-1.24236500	-2.33226300
H	0.22008700	-2.60787700	-1.26377100
C	2.09137200	-1.55593400	-0.89028800
H	2.66936500	-2.13809000	-1.61722400
H	2.21791800	-2.05156900	0.07498000
C	2.62494900	-0.12160200	-0.83863300
H	3.67304500	-0.12349400	-0.51507300
H	2.61887200	0.29835100	-1.85526900
C	2.04464900	0.46351600	1.56700800
H	3.10297500	0.59596700	1.81687700
H	1.47076900	1.11397900	2.23358900
H	1.78535100	-0.57002500	1.80331900
C	2.36113200	2.25593100	-0.14297500
H	3.44977200	2.26139700	-0.02327200
H	2.13811200	2.61686000	-1.15386300
H	1.95431500	2.97592200	0.57253600
N	-0.51443400	-1.29551900	0.93610100
O	-1.31583700	-0.72821300	1.67687100
O	0.07442500	-2.33115000	1.22909200

Cartesian coordinates for optimized **LHMDS (No Lithium)**

N	0.00000000	0.00023200	0.00148200
Si	-1.64438700	-0.00000700	0.00029400
Si	1.64438900	0.00002700	0.00030000
C	2.44667600	0.81699800	1.54731500
H	3.54539100	0.79984100	1.51539400
H	2.13166500	1.86392200	1.63991800
H	2.13123600	0.30352300	2.46420600
C	2.44436100	0.93185500	-1.48164300
H	3.54313400	0.91275300	-1.45274200
H	2.12763100	0.48907500	-2.43425700
H	2.12900400	1.98268400	-1.49434900
C	2.44504800	-1.74897000	-0.06661300
H	3.54381200	-1.71399500	-0.06640800
H	2.13009900	-2.35241100	0.79391500
H	2.12837000	-2.28586100	-0.96956400
C	-2.44663800	0.83476300	1.53783000
H	-2.13117500	0.33194400	2.46059900
H	-2.13163600	1.88269200	1.61830300
H	-3.54535500	0.81725800	1.50614400
C	-2.44437200	0.91476700	-1.49223300
H	-2.12768500	0.46107400	-2.43971500
H	-3.54314500	0.89600000	-1.46309600
H	-2.12898800	1.96537000	-1.51700700

C	-2.44507500	-1.74961500	-0.04649700
H	-3.54383600	-1.71459500	-0.04678600
H	-2.12831800	-2.29689500	-0.94316100
H	-2.13021900	-2.34308200	0.82097600

Cartesian coordinates for optimized **LHMDS**

N	0.01265600	0.58713800	0.00000200
Si	1.62168500	0.01441600	-0.00000100
Si	-1.55998200	-0.05018400	0.00000300
C	-2.70602900	1.52458300	0.00007200
H	-3.76098200	1.23132800	0.00010700
H	-2.58951400	2.15546900	0.89881100
H	-2.58957900	2.15549000	-0.89866000
C	-2.06092800	-1.05091800	1.53359100
H	-3.11733200	-1.34390000	1.51026800
H	-1.46615600	-1.96875200	1.60482400
H	-1.88704100	-0.48192600	2.45362900
C	-2.06096400	-1.05077800	-1.53366700
H	-3.11737000	-1.34375300	-1.51035800
H	-1.88708400	-0.48170000	-2.45365400
H	-1.46620000	-1.96860900	-1.60499600
C	2.78449500	1.52812500	-0.00007000
H	2.62256400	2.15298500	-0.88879500
H	2.62254900	2.15307500	0.88859000
H	3.84231000	1.24059100	-0.00004400
C	2.05944100	-1.02564100	1.53139200
H	1.45051200	-1.93598000	1.58026100
H	3.11187000	-1.33406500	1.52841100
H	1.87868500	-0.46403700	2.45504300
C	2.05939800	-1.02575000	-1.53133200
H	3.11183400	-1.33415000	-1.52837400
H	1.45048800	-1.93610900	-1.58010300
H	1.87858700	-0.46422300	-2.45501900
Li	-0.49768300	2.32044200	0.00003300

Cartesian coordinates for optimized **KHMDS**

N	0.00001300	0.09605600	0.00000800
Si	1.58067100	-0.49105600	0.00000500
Si	-1.58062500	-0.49109900	0.00000100
C	-2.78795900	1.01821600	-0.00007600
H	-3.83529900	0.69457500	-0.00007800
H	-2.66454800	1.64832200	0.89470000
H	-2.66452100	1.64825200	-0.89489800
C	-2.07983100	-1.51496100	1.52830800
H	-3.13680800	-1.80781700	1.50485900
H	-1.48477000	-2.43336900	1.59216300
H	-1.90714200	-0.95442500	2.45466200
C	-2.07978300	-1.51508400	-1.52823800
H	-3.13676300	-1.80793100	-1.50480200
H	-1.90705800	-0.95462700	-2.45463300
H	-1.48472700	-2.43350200	-1.59199600
C	2.78798300	1.01826800	0.00001900
H	2.66456700	1.64834700	-0.89477500
H	2.66456600	1.64833000	0.89482400
H	3.83532200	0.69461900	0.00001600
C	2.07984000	-1.51497100	1.52828700
H	1.48428300	-2.43303300	1.59247900
H	3.13664700	-1.80841500	1.50453000
H	1.90777600	-0.95420500	2.45462000
C	2.07984300	-1.51494200	-1.52829600
H	3.13664800	-1.80838800	-1.50454200
H	1.48428400	-2.43300200	-1.59250700
H	1.90778200	-0.95415800	-2.45461900
K	-0.00008000	2.63258100	-0.00000800

Cartesian coordinates for optimized **TS-1** with **$(Me_3Si)_2N^-$** (Axial Hydrogen)

C	-3.39927000	-1.65726400	-0.92082900
C	-3.51752100	-0.17545200	-1.29086600
C	-3.50224600	0.67657300	-0.01602000
C	-1.63016200	-0.89220300	0.79478600
C	-2.03661900	-1.93055700	-0.26483100
H	-3.32588900	1.73694800	-0.23552400
H	-2.67183000	0.09674200	-1.93678900
H	-4.43020200	0.01831100	-1.87272800
H	-4.21109000	-1.91418100	-0.22328700
H	-0.38814900	-0.37440700	0.37063400
H	-1.26600500	-1.32523400	1.73000100
H	-4.48686800	0.63610100	0.47181000
C	-2.48484300	0.24073200	1.06352300
O	-2.43371300	0.93767800	2.09377300
N	0.85095500	-0.01697400	-0.00280000
Si	0.98145800	1.67423000	-0.24112600
Si	2.05273900	-1.22245300	0.08620000
C	3.47871700	-0.85716300	1.31258100
H	4.18741900	-1.69433900	1.37061200
H	4.04729900	0.03572200	1.02869800
H	3.08157400	-0.68465300	2.31979300
C	2.90730600	-1.60019100	-1.58572100
H	3.63239100	-2.42094400	-1.50188100
H	2.16478400	-1.88449000	-2.34070100
H	3.44262100	-0.72362300	-1.96918600
C	1.32381400	-2.88377700	0.67072300
H	2.11076300	-3.64513100	0.74752400
H	0.85323200	-2.78796100	1.65522400
H	0.56168700	-3.25825200	-0.02014800
C	0.58383500	2.66344600	1.33389300
H	0.53173900	3.74452300	1.14701000
H	-0.37410700	2.33487800	1.75281700
H	1.35331400	2.49371900	2.09740200
C	2.70960200	2.25675500	-0.82776400
H	3.00160100	1.77668300	-1.76910300
H	2.71021000	3.34166300	-0.99733900
H	3.49074300	2.04157900	-0.09007500
C	-0.21849500	2.28165700	-1.59560700
H	-0.15634300	3.36857000	-1.73758200
H	0.00555500	1.80330400	-2.55662000
H	-1.25544400	2.04001900	-1.34156100
H	-2.04645600	-2.93938400	0.17148000
H	-3.53141900	-2.29372600	-1.80764200
H	-1.28158800	-1.96525200	-1.06767600

Cartesian coordinates for optimized **TS-1** with **$(Me_3Si)_2N^-$** (Equatorial Hydrogen)

C	3.23363600	1.20168700	-0.54205500
C	4.01498600	0.34309700	0.45894800
C	3.07735500	-0.62924100	1.18751200
C	1.68344200	-0.79359400	-0.94288500
C	2.52218900	0.31870100	-1.57745300
H	3.62943900	-1.33864300	1.81365800
H	4.78228800	-0.22878800	-0.08467300
H	4.55370600	0.97551000	1.17935200
H	2.49281000	1.80021700	0.00444300
H	1.31877400	-1.51486300	-1.67911400
H	0.40490300	-0.27927500	-0.54052300
H	2.41501200	-0.06451300	1.86033100
C	2.17923700	-1.45375100	0.24134200
O	1.84549100	-2.59331200	0.61884900
N	-0.84437000	0.09262100	-0.28395300
Si	-1.90620700	-1.24769200	-0.13037300
Si	-1.07078500	1.73066900	0.13478100
C	-0.20312700	2.22103700	1.76764000
H	-0.30804300	3.29131200	1.99047200

H	-0.62914400	1.66012000	2.60813300
H	0.86753900	1.99006600	1.73755500
C	-2.89307400	2.26242600	0.38073700
H	-2.94868100	3.32030700	0.67004700
H	-3.47797100	2.13796100	-0.53705400
H	-3.38674700	1.68077000	1.16787000
C	-0.39465000	2.91384500	-1.20281400
H	-0.52170100	3.96615700	-0.91627600
H	0.67088100	2.74607000	-1.39091800
H	-0.92123800	2.75839100	-2.15186200
C	-2.27705200	-1.72234600	1.68465400
H	-1.34351100	-1.97531000	2.19956300
H	-2.74451400	-0.89417700	2.23199800
H	-2.94707200	-2.58932000	1.75827200
C	-3.61683400	-0.98236500	-0.95350700
H	-3.49841200	-0.70188700	-2.00704600
H	-4.21066700	-1.90578400	-0.92071000
H	-4.20363900	-0.19579000	-0.46731400
C	-1.18320500	-2.79840000	-0.94946900
H	-1.86045800	-3.65245300	-0.81486900
H	-1.04410700	-2.65293900	-2.02770000
H	-0.21028700	-3.04855900	-0.51239400
H	1.88798500	0.94852500	-2.21812900
H	3.90495500	1.91375400	-1.04323200
H	3.29503300	-0.09696500	-2.25062300

Cartesian coordinates for optimized **TS-2$_{H1}$** with **(Me$_3$Si)$_2$N$^-$**

C	-3.76107000	-1.13585300	-0.59614600
C	-3.75491900	0.38829100	-0.75098800
C	-3.32669200	1.03506700	0.57093400
C	-1.56906300	-0.84954100	0.71471700
C	-2.33978200	-1.68423600	-0.33686200
H	-3.03292000	2.08371600	0.43784600
H	-3.06207800	0.67048700	-1.55350900
H	-4.74486200	0.75550200	-1.05732000
H	-4.41298300	-1.39601300	0.25107900
H	-0.32778700	-0.37566000	0.23808200
H	-1.11431800	-1.46795600	1.49275600
H	-4.17402700	1.05215700	1.27100700
C	-2.18512300	0.31313300	1.32088800
O	-1.81878600	0.81843100	2.39628400
N	0.93534800	-0.02406600	-0.09392800
Si	1.11052800	1.65051600	-0.40371300
Si	2.15395700	-1.17455600	0.22528200
C	3.47059400	-0.62562000	1.50363500
H	4.20556200	-1.41833800	1.69812100
H	4.02336100	0.26006600	1.16882600
H	2.99233700	-0.36978100	2.45617300
C	3.14252000	-1.70319300	-1.32772300
H	3.89112600	-2.47348900	-1.09811900
H	2.46945000	-2.10731800	-2.09328300
H	3.66830500	-0.85152800	-1.77459800
C	1.43131700	-2.79068200	0.93621000
H	2.22784600	-3.53076400	1.08751400
H	0.94718300	-2.61867600	1.90337900
H	0.68413900	-3.23809200	0.27201900
C	0.99518200	2.72213000	1.16651300
H	0.94739200	3.79680800	0.94482900
H	0.10317500	2.43944300	1.73680800
H	1.86433100	2.55345900	1.81438300
C	2.75788100	2.11856800	-1.26380000
H	2.86209500	1.60595100	-2.22728700
H	2.80366800	3.19887100	-1.45567200
H	3.63207900	1.85792800	-0.65607800
C	-0.24811300	2.27247400	-1.58994300
H	-0.14102900	3.34542300	-1.79584000
H	-0.20484400	1.74052900	-2.54769500

H	-1.24585200	2.11493800	-1.16917700
H	-2.46704200	-2.70184200	0.06521800
H	-4.19463600	-1.61603400	-1.48542800
C	-1.57558900	-1.84432200	-1.66698600
H	-0.57800000	-2.25824500	-1.49969300
H	-2.11432400	-2.51069800	-2.35625300
H	-1.43014200	-0.88055400	-2.16551400

Cartesian coordinates for optimized **TS-2$_{H1}$** (Flipped) with **(Me$_3$Si)$_2$N$^-$**

C	3.23378600	0.96388200	0.30686300
C	2.67741700	-0.05636700	1.31195300
C	1.63761500	-0.97023400	0.65108300
C	2.75676600	-0.62364100	-1.61488600
C	3.81280600	0.24910600	-0.92105900
H	1.29427400	-1.75379800	1.33243300
H	3.54809400	-0.65808500	1.64225700
H	2.43038100	1.64368100	-0.00864900
H	3.20492000	-1.28164400	-2.36751100
H	2.04064300	0.01708400	-2.14872400
H	0.36486400	-0.31713500	0.42063100
C	1.93207300	-1.50972800	-0.65788400
O	1.46519700	-2.56869800	-1.11589700
N	-0.88860500	0.10906800	0.25664800
Si	-2.01416700	-1.19159500	0.24601200
Si	-1.13841500	1.70778600	-0.29368900
C	-0.44621700	3.03554000	0.89480100
H	-0.67326300	4.04580600	0.52906500
H	-0.88729200	2.93465700	1.89339200
H	0.64047200	2.96453900	1.00881900
C	-2.97321700	2.20571700	-0.52504800
H	-3.04236800	3.22433400	-0.92929200
H	-3.49999000	1.54051600	-1.21836700
H	-3.51800200	2.18977500	0.42524200
C	-0.32157000	2.07253400	-1.98406400
H	-0.50550700	3.10350300	-2.31489700
H	0.76358900	1.92692500	-1.94397100
H	-0.71050000	1.39708400	-2.75493200
C	-3.59766000	-0.85096800	1.27105000
H	-3.33612500	-0.57099800	2.29862200
H	-4.20656200	-0.04184500	0.85412700
H	-4.22981400	-1.74774300	1.32163600
C	-2.61149800	-1.67356600	-1.50547800
H	-1.74928100	-1.97093300	-2.11283500
H	-3.31487900	-2.51663800	-1.48412700
H	-3.10853000	-0.84009400	-2.01677100
C	-1.27156700	-2.77574900	0.98186800
H	-0.95539900	-2.63439300	2.02212900
H	-2.01682200	-3.58229100	0.96732400
H	-0.40036400	-3.09194100	0.39885500
H	4.23767000	0.97469000	-1.62928800
H	4.00669700	1.58553500	0.78293900
C	2.11966300	0.61280700	2.57595100
H	1.80685300	-0.14494700	3.30431100
H	2.87038500	1.25269700	3.06057900
H	1.24033800	1.22040600	2.34711200
H	4.64995200	-0.38530600	-0.59289000

Cartesian coordinates for optimized **TS-2$_{H2}$** with **(Me$_3$Si)$_2$N$^-$**

C	-3.03639600	1.27039700	0.08729900
C	-3.69191200	0.48078700	-1.05292900
C	-2.68882200	-0.49461400	-1.68146900
C	-1.59371100	-0.76446900	0.60542200
C	-2.47149200	0.35019200	1.18981600
H	-3.16373300	-1.16074100	-2.40980800

H	-4.55443400	-0.08027500	-0.66678300
H	-4.09182400	1.16829700	-1.81187600
H	-2.21808300	1.87051100	-0.33070800
H	-1.33405200	-1.51839100	1.35444900
H	-0.27698300	-0.27207000	0.36453200
H	-1.91895500	0.07256000	-2.22535900
C	-1.96018900	-1.37901200	-0.65085500
O	-1.62206400	-2.52226500	-1.01048400
N	1.00798400	0.08077600	0.25527900
Si	2.05130900	-1.28122600	0.19358000
Si	1.32246600	1.72060600	-0.09398200
C	0.64744000	2.27707100	-1.79550700
H	0.81627900	3.34653000	-1.97962700
H	1.13679200	1.71681100	-2.60119300
H	-0.42876600	2.09050700	-1.88244900
C	3.17453800	2.20293300	-0.13386600
H	3.28949500	3.26375600	-0.39324600
H	3.65463500	2.04482100	0.83792100
H	3.73311300	1.62123600	-0.87626100
C	0.54348700	2.89639000	1.19373800
H	0.73468000	3.94950200	0.94873100
H	-0.54117300	2.76277000	1.26290700
H	0.95917500	2.70277400	2.18964600
C	2.61936200	-1.72725100	-1.57729900
H	1.74680000	-1.94709900	-2.20258600
H	3.16523400	-0.89986500	-2.04785700
H	3.27433200	-2.60859200	-1.59294700
C	3.66069200	-1.07584300	1.21432600
H	3.42781400	-0.80897400	2.25220200
H	4.23080000	-2.01446600	1.23288300
H	4.31969700	-0.29803100	0.81425700
C	1.20691100	-2.83241600	0.88655200
H	1.87878400	-3.69784200	0.81049400
H	0.94681900	-2.70764400	1.94478200
H	0.28658800	-3.05265400	0.33471300
H	-1.84386200	0.97775700	1.84191000
H	-3.75455100	1.98115500	0.52160400
C	-3.59874500	-0.20203900	2.08845800
H	-3.18018000	-0.82647500	2.88590400
H	-4.17833600	0.60397300	2.56235400
H	-4.29530200	-0.83122800	1.52185200

Cartesian coordinates for optimized **TS-2$_{H2}$** (Flipped) with **(Me$_3$Si)$_2$N$^-$**

C	3.32761900	0.74022600	1.12226100
C	2.34673200	1.29102600	0.06447700
C	1.73385400	0.19065900	-0.82210300
C	2.97755000	-1.63564000	0.46250700
C	2.90323000	-0.64171100	1.62436900
H	0.39105300	0.02650200	-0.39385600
H	1.53295700	1.78451300	0.62303100
H	4.33145200	0.65112700	0.67707900
H	2.53588700	-2.60460600	0.71999600
H	4.02924800	-1.83771500	0.20975000
H	1.52009600	0.52780500	-1.84124700
C	2.29563600	-1.14067500	-0.82992300
O	2.19063400	-1.95013500	-1.76893700
N	-0.91057200	0.02583000	-0.06265300
Si	-1.65904900	-1.51154700	0.07188300
Si	-1.67938900	1.55100800	0.01063900
C	-1.64539100	2.33378400	1.75634600
H	-2.08815900	3.33859400	1.77318500
H	-2.19773000	1.71256700	2.47151600
H	-0.61597100	2.41493400	2.12458000
C	-3.52385500	1.55688500	-0.50931200
H	-3.94427600	2.56842300	-0.43200100
H	-3.63691400	1.23036000	-1.54954000
H	-4.14124800	0.89728800	0.11022700

C	-0.86773500	2.82561300	-1.15257600
H	-1.42106900	3.77371600	-1.13958200
H	0.16603900	3.04141500	-0.86808700
H	-0.85490400	2.45819300	-2.18489800
C	-2.87124500	-1.64478800	1.55231700
H	-2.34826000	-1.44062000	2.49437100
H	-3.70467100	-0.93656000	1.48176200
H	-3.30229300	-2.65239600	1.62354000
C	-2.66538800	-2.01660000	-1.47391200
H	-2.01662400	-2.02254000	-2.35723300
H	-3.10038700	-3.01966300	-1.37080200
H	-3.48522000	-1.31636200	-1.67114300
C	-0.40414800	-2.90976100	0.34541700
H	-0.92370800	-3.87562600	0.39882200
H	0.33240400	-2.95897100	-0.46239400
H	0.13829300	-2.77583100	1.28871600
H	3.53935300	-0.96807400	2.45953700
H	3.42076200	1.45627100	1.95111300
C	3.04123800	2.38443200	-0.76607300
H	2.34914600	2.84280000	-1.48075500
H	3.44537600	3.18512500	-0.12975600
H	3.87221000	1.95728300	-1.34152400
H	1.87565100	-0.59084000	2.00759000

Cartesian coordinates for optimized **TS-2$_{H3}$** with **(Me$_3$Si)$_2$N$^-$**

C	-3.40357300	-1.58552700	0.24967000
C	-2.04924600	-1.77648200	-0.45393200
C	-1.54242600	-0.52309600	-1.18344000
C	-3.35160800	0.89305100	-0.02629900
C	-3.47231100	-0.24639700	1.00369500
H	-0.30858300	-0.17904800	-0.58522000
H	-1.31542000	-2.10776100	0.29857900
H	-2.14019000	-2.61921200	-1.15457700
H	-4.21003300	-1.59941900	-0.49829300
H	-3.11394200	1.84755400	0.45984500
H	-4.31947600	1.04629800	-0.52416800
H	-1.14568000	-0.71596000	-2.18344700
C	-2.33167500	0.68365100	-1.16882000
O	-2.20989800	1.61637500	-1.98503700
N	0.92564600	-0.00969900	-0.09299000
Si	1.40009200	1.61324800	0.19757900
Si	1.90688700	-1.40972300	-0.09247500
C	1.86922400	-2.35682800	1.56928400
H	2.45600900	-3.28444800	1.53537500
H	2.27058200	-1.73633000	2.37944100
H	0.84070800	-2.62037700	1.84211100
C	3.76280700	-1.10224700	-0.45565500
H	4.32202900	-2.04730300	-0.44688600
H	3.89729700	-0.64706800	-1.44365600
H	4.23143300	-0.43740500	0.27829500
C	1.36884000	-2.66144500	-1.42777600
H	2.02394800	-3.54246700	-1.42314200
H	0.34214200	-3.00851300	-1.27881600
H	1.42063900	-2.21071800	-2.42540700
C	2.49680400	1.81463200	1.75757600
H	1.97036900	1.44783800	2.64687800
H	3.43937800	1.26009800	1.68384100
H	2.74925000	2.86903900	1.93240500
C	2.38800200	2.39397000	-1.24137200
H	1.79162500	2.36648900	-2.16039600
H	2.64714700	3.44216900	-1.04111900
H	3.32051500	1.85134400	-1.43552300
C	-0.08647400	2.75935600	0.48261800
H	0.25679000	3.79058500	0.63943300
H	-0.76916100	2.74963700	-0.37289900
H	-0.65450100	2.46221300	1.37178200
H	-4.46056800	-0.17392000	1.48531800

H	-3.59695700	-2.42230300	0.93720600
C	-2.41522900	-0.14843200	2.11558100
H	-2.54072500	0.77964700	2.68636900
H	-2.50245400	-0.98618700	2.81971200
H	-1.39902400	-0.15215500	1.70993700

Cartesian coordinates for optimized **TS-2$_{H3}$** (Flipped) with **(Me$_3$Si)$_2$N$^-$**

C	3.01588100	0.79441700	-0.88670900
C	3.79955200	-0.09243300	0.09151100
C	2.81743600	-0.93473900	0.92113300
C	1.24631100	-1.04170400	-1.08390200
C	2.13778500	-0.04452000	-1.82605500
H	3.34279400	-1.66918600	1.54258300
H	4.41293200	-0.78434300	-0.50901000
H	2.38738000	1.48513500	-0.30731700
H	0.75773500	-1.74995800	-1.75812300
H	0.06149500	-0.38716400	-0.61201700
H	2.27009600	-0.27347700	1.61098700
C	1.77204800	-1.70334000	0.08591000
O	1.36707000	-2.79076400	0.53896300
N	-1.12300800	0.12010700	-0.28328500
Si	-2.30091800	-1.09719900	-0.00454200
Si	-1.15653300	1.78643100	0.08044000
C	-0.12924500	2.24466800	1.62777300
H	-0.11916200	3.32674600	1.81519300
H	-0.54070800	1.75384300	2.51785500
H	0.91075900	1.91364200	1.53065300
C	-2.89558500	2.50693700	0.42729600
H	-2.82606400	3.57300100	0.68131700
H	-3.55220600	2.41556500	-0.44475900
H	-3.38849200	2.00131800	1.26568600
C	-0.46584000	2.84877600	-1.34808100
H	-0.47172000	3.91797200	-1.09831300
H	0.56321000	2.57132600	-1.59908500
H	-1.06992200	2.71205800	-2.25280100
C	-2.60459700	-1.45506700	1.84949600
H	-1.67178600	-1.78131600	2.32288500
H	-2.95206900	-0.56103400	2.38234700
H	-3.35273000	-2.24436000	2.00216200
C	-4.02445000	-0.69279700	-0.73928500
H	-3.94415800	-0.47006100	-1.81006400
H	-4.70513000	-1.54761300	-0.62810900
H	-4.49745800	0.16992100	-0.25812800
C	-1.78781700	-2.74672900	-0.78842800
H	-2.53403000	-3.52205100	-0.56892000
H	-1.70874100	-2.66322400	-1.87923600
H	-0.81616200	-3.07430900	-0.40268200
H	1.52110900	0.62757600	-2.44004700
H	3.71055800	1.41773700	-1.46926700
C	4.74674600	0.72193400	0.98122500
H	5.30641500	0.07514900	1.66791900
H	5.47335500	1.28878400	0.38516200
H	4.18497700	1.44114500	1.59060200
H	2.80718100	-0.55912400	-2.54005500

Cartesian coordinates for optimized **TS-2$_{H4}$** with **(Me$_3$Si)$_2$N$^-$**

C	-2.92182200	1.32138500	-0.51198900
C	-2.23119600	0.42049200	-1.54758300
C	-1.43617600	-0.72334200	-0.91371600
C	-2.78217900	-0.47287600	1.23720400
C	-3.72582000	0.51361200	0.52443700
H	-1.10995000	-1.46512500	-1.64750100
H	-2.99970200	0.03722200	-2.24199000
H	-1.56918400	1.03935200	-2.17043600

H	-2.16251300	1.90677700	0.02223400
H	-3.33108700	-1.14650700	1.90528100
H	-2.07546800	0.08863300	1.86491200
H	-0.13960000	-0.25605500	-0.52649200
C	-1.94616000	-1.35116200	0.28204100
O	-1.66192400	-2.50271300	0.66344400
N	1.12646400	0.07503600	-0.28260700
Si	2.14313400	-1.30089700	-0.13941200
Si	1.41765400	1.70478700	0.12835500
C	0.78086800	2.91033900	-1.20871400
H	0.95793500	3.95717700	-0.92872700
H	1.28971800	2.72722400	-2.16247100
H	-0.29318600	2.79005600	-1.38475800
C	3.26041100	2.16644400	0.36349000
H	3.35794800	3.22001600	0.65730700
H	3.73745600	1.56260200	1.14410900
H	3.83370800	2.02482900	-0.55915100
C	0.57721900	2.23443000	1.76313700
H	0.73002700	3.29931800	1.98400200
H	-0.50285400	2.05162100	1.73600500
H	0.97997400	1.65633300	2.60340700
C	3.84483900	-1.10207600	-0.99873100
H	3.71482500	-0.82551900	-2.05193100
H	4.46771400	-0.33235300	-0.53069400
H	4.40747200	-2.04496000	-0.97014800
C	2.53410700	-1.77511300	1.67160100
H	1.60332800	-1.99134800	2.20784400
H	3.17473400	-2.66455800	1.73838000
H	3.04155800	-0.96009300	2.20280100
C	1.34937000	-2.83126100	-0.93107500
H	1.19759400	-2.69052100	-2.00821800
H	1.99727900	-3.70824100	-0.79965200
H	0.37521300	-3.04230700	-0.47647400
H	-4.12772400	1.21788300	1.26980700
H	-3.57857300	2.04633200	-1.01544700
C	-4.92359400	-0.21645200	-0.10453000
H	-5.52296000	-0.71744000	0.66501000
H	-5.57961600	0.47933900	-0.64295100
H	-4.59414200	-0.98421600	-0.81198600

Cartesian coordinates for optimized **TS-2$_{H4}$** (Flipped) with **(Me$_3$Si)$_2$N$^-$**

C	-3.19601900	-1.68809300	-0.46294700
C	-3.37710900	-0.20840700	-0.82515100
C	-3.22301400	0.62898300	0.45233700
C	-1.25448300	-0.91569600	1.05012100
C	-1.76863700	-1.95409600	0.04033700
H	-3.09536400	1.69456700	0.22154000
H	-2.56667500	0.06241600	-1.51820400
H	-3.92923100	-1.94895600	0.31666300
H	-0.07318100	-0.38852900	0.49501200
H	-0.78890300	-1.34699600	1.94002900
H	-4.14928700	0.56510500	1.04396000
C	-2.08470400	0.20979900	1.41058100
O	-1.92579100	0.91231300	2.42551900
N	1.11673800	-0.01793200	-0.01145600
Si	1.21242800	1.67690800	-0.24133000
Si	2.33436400	-1.21009700	-0.05432900
C	3.85883700	-0.85039400	1.04896300
H	4.58352900	-1.67533800	1.02206000
H	4.38473500	0.05974300	0.73858300
H	3.55081000	-0.70924800	2.09162500
C	3.04144200	-1.54461900	-1.80248500
H	3.77868300	-2.35878600	-1.79946300
H	2.23802900	-1.82244400	-2.49494900
H	3.53268200	-0.65486100	-2.21332100
C	1.67803900	-2.89213000	0.55692400
H	2.47752600	-3.64419400	0.54925600

H	1.29350200	-2.82288300	1.58025600
H	0.86339100	-3.26310900	-0.07334200
C	0.99638900	2.64572000	1.38120600
H	0.92263300	3.72893200	1.21513600
H	0.09189200	2.30988300	1.90097700
H	1.84736100	2.46805700	2.05062600
C	2.85823500	2.27509300	-1.01818300
H	3.03324600	1.81685900	-1.99857500
H	2.84005100	3.36357400	-1.16175800
H	3.72282800	2.04402800	-0.38582900
C	-0.13916600	2.29480300	-1.43910300
H	-0.09589400	3.38339000	-1.57495700
H	-0.02852200	1.82786700	-2.42513400
H	-1.13884800	2.04770700	-1.06788800
H	-1.72685600	-2.96343200	0.47305500
H	-3.41949500	-2.32632700	-1.33094900
C	-4.71130800	0.06785900	-1.52882200
H	-4.82658200	1.13272300	-1.76505200
H	-4.79682200	-0.49519300	-2.46681200
H	-5.55655900	-0.22084000	-0.89006700
H	-1.10561900	-1.98498900	-0.83987900

Cartesian coordinates for optimized **TS-3$_{H1}$** with **(Me$_3$Si)$_2$N$^-$**

C	-3.57874700	-0.83393400	-0.29015800
C	-2.79922200	-2.12288100	-0.01531100
C	-1.90185400	-2.45252600	-1.20907500
C	-1.28317600	0.03619000	-1.09473900
C	-2.67173600	0.41201800	-0.51234600
H	-1.18843500	-3.25382800	-0.98045200
H	-2.19341600	-2.00092500	0.88788800
H	-3.49481500	-2.95055900	0.18577100
H	-4.18045700	-0.99480800	-1.19651000
H	-0.09664900	0.03873400	-0.30969800
H	-0.92656900	0.81992000	-1.76447400
H	-2.51136900	-2.82323000	-2.04647200
C	-1.10194600	-1.25024400	-1.74376200
O	-0.26960100	-1.46835400	-2.63904700
N	1.17211700	0.13909700	0.18557700
Si	1.81108900	-1.22815100	1.00098500
Si	2.15839400	1.33328000	-0.55785200
C	3.85982300	0.71709800	-1.18911400
H	4.42272400	1.54505100	-1.64042500
H	4.48512700	0.29029600	-0.39718500
H	3.72807400	-0.05316800	-1.95705500
C	2.55964100	2.79326600	0.61532600
H	3.16380900	3.56676800	0.12253500
H	1.63902600	3.26708900	0.97576800
H	3.11302800	2.44842900	1.49691400
C	1.36011800	2.09929900	-2.10893500
H	2.07668400	2.76269100	-2.61089400
H	1.07057500	1.30913000	-2.80938900
H	0.46645700	2.69037900	-1.88339300
C	2.54677200	-2.54700900	-0.16915800
H	2.72385600	-3.50633000	0.33517100
H	1.85253000	-2.71197700	-1.00113900
H	3.49797500	-2.21764500	-0.60218600
C	3.17173700	-0.79626900	2.28076200
H	2.77577200	-0.12544000	3.05267900
H	3.54341000	-1.69933000	2.78321500
H	4.03355500	-0.29623100	1.82524200
C	0.50232700	-2.16117400	2.02782400
H	0.98509300	-2.96586600	2.59756000
H	-0.00848500	-1.50810100	2.74328500
H	-0.25943700	-2.62413100	1.39386000
H	-3.18308400	1.00868600	-1.28721400
H	-4.30035100	-0.65793100	0.51568200
C	-2.63857000	1.39273700	0.71891900

C	-1.72711000	2.59106500	0.38951000
H	-1.76843600	3.33942400	1.19167300
H	-0.69041900	2.27130700	0.27988400
H	-2.03877600	3.08289900	-0.54075500
C	-2.10874900	0.71685800	1.99570600
H	-2.74037800	-0.12415000	2.30397000
H	-1.09108500	0.35281500	1.83942300
H	-2.08802700	1.43197900	2.82883900
C	-4.05400000	1.95133600	0.98770300
H	-4.02562800	2.69607300	1.79294600
H	-4.45995200	2.44324700	0.09466800
H	-4.76453100	1.17509600	1.29083300

Cartesian coordinates for optimized **TS-3$_{H1}$** (Flipped) with **(Me$_3$Si)$_2$N$^-$**

C	2.96181900	0.15909500	-1.26909600
C	2.63717600	-0.32155200	0.15875500
C	1.27856600	-1.05272300	0.18596300
C	1.54539600	-1.69549100	-2.26882400
C	2.91800100	-1.01206300	-2.26069100
H	1.09041100	-1.51644000	1.15554100
H	3.43050100	-1.05697400	0.40504100
H	2.23803100	0.91918300	-1.58420500
H	1.55232700	-2.62442900	-2.84906800
H	0.80563400	-1.03189100	-2.73984600
H	0.04723200	-0.30130200	0.07500800
C	1.02104300	-2.02411100	-0.86064100
O	0.30243700	-3.02958000	-0.72479400
N	-1.20928000	0.16431700	0.10222700
Si	-2.30188900	-0.90065800	0.90486500
Si	-1.69334300	1.52069000	-0.82210200
C	-1.99371300	3.09864000	0.22075900
H	-2.27653000	3.95786000	-0.40213100
H	-2.79409700	2.93940600	0.95250500
H	-1.09211100	3.37365000	0.78018600
C	-3.30583200	1.27859900	-1.82992400
H	-3.54907300	2.18266100	-2.40406500
H	-3.20082300	0.45024700	-2.53995500
H	-4.16783500	1.05333200	-1.19205400
C	-0.40223600	2.02427000	-2.13289500
H	-0.78077800	2.85841000	-2.73782600
H	0.54014700	2.34738600	-1.68062700
H	-0.17833000	1.19523000	-2.81317400
C	-3.67209100	0.02855100	1.87467700
H	-3.23247700	0.68873600	2.63199800
H	-4.30083600	0.64941900	1.22571900
H	-4.33459500	-0.67744800	2.39299200
C	-3.19279400	-2.11245500	-0.26791800
H	-2.43493000	-2.68491900	-0.81346900
H	-3.82726900	-2.82177700	0.28019500
H	-3.82368600	-1.59435800	-0.99897300
C	-1.43091200	-2.00066600	2.18707800
H	-0.84395400	-1.41919900	2.90753000
H	-2.17014800	-2.58414200	2.75166700
H	-0.76212300	-2.69735000	1.67296300
H	3.18294000	-0.66698200	-3.27015700
H	3.95422900	0.62499100	-1.31158700
C	2.81126700	0.77894900	1.26723700
H	3.68690700	-1.74569200	-1.97507200
C	1.84984100	1.96592800	1.07903200
H	0.81141100	1.62644800	1.06271800
H	1.96560300	2.68686200	1.89935600
H	2.05042900	2.50240100	0.14528800
C	4.26389300	1.30517600	1.26809800
H	4.42435600	1.98891700	2.11112400
H	4.98493200	0.48354500	1.36452700
H	4.50558800	1.85616500	0.35364100
C	2.54774200	0.15434500	2.65424800

H	3.17321400	-0.73268600	2.81534700
H	2.77783300	0.87490400	3.44960400
H	1.50356600	-0.14515400	2.76818300

Cartesian coordinates for optimized **TS-3$_{H2}$** with **(Me$_3$Si)$_2$N$^-$**

C	2.30879400	1.42644600	0.78240400
C	2.65616200	0.78842400	2.13468900
C	1.57787300	-0.21473100	2.55986200
C	1.12008800	-0.70136200	0.09855300
C	2.05911800	0.42011900	-0.36958300
H	1.87686800	-0.79400900	3.43990200
H	3.62635000	0.28028400	2.07972200
H	2.76941300	1.57460800	2.89514400
H	1.38075400	1.99693800	0.91592200
H	1.03734100	-1.52347300	-0.61381700
H	-0.21586400	-0.24875000	-0.00583600
H	0.66102600	0.32819100	2.83281900
C	1.19342400	-1.20914700	1.45217400
O	0.83803700	-2.35136300	1.79735700
N	-1.50866800	0.06012400	-0.23206200
Si	-2.49837700	-1.33719000	-0.35450800
Si	-1.95961600	1.69794700	-0.07238700
C	-1.71673100	2.38122300	1.69811300
H	-1.96968200	3.44755800	1.76890600
H	-2.35396100	1.83792600	2.40612800
H	-0.68252100	2.26199000	2.03971700
C	-3.78943700	2.08281900	-0.48421200
H	-4.00442400	3.14641800	-0.31605900
H	-4.02458300	1.85870400	-1.53033800
H	-4.48099300	1.50565700	0.14037200
C	-0.95816600	2.84648600	-1.22439300
H	-1.25223000	3.89730400	-1.10212000
H	0.11840900	2.77916700	-1.03528500
H	-1.12166100	2.57245500	-2.27334400
C	-3.51621900	-1.69289900	1.22552400
H	-2.84349900	-1.83843000	2.07821100
H	-4.18672500	-0.85992500	1.47117200
H	-4.13234200	-2.59648800	1.12625500
C	-3.77370400	-1.26722600	-1.78350400
H	-3.27283900	-1.05796900	-2.73635300
H	-4.29537600	-2.22822500	-1.88667600
H	-4.53449200	-0.49377200	-1.63439400
C	-1.46668400	-2.89636900	-0.68123300
H	-2.11714200	-3.78064500	-0.71380000
H	-0.94516100	-2.83577600	-1.64439100
H	-0.71480400	-3.04290000	0.10169700
H	1.52764600	0.99754400	-1.14413400
H	3.07169300	2.16341400	0.50648300
C	3.35132400	-0.08519000	-1.13715000
C	4.19286600	-1.09099800	-0.32770900
H	4.98748000	-1.51885700	-0.95356600
H	4.67831700	-0.61913200	0.53236900
H	3.57319600	-1.91164300	0.04434300
C	4.24636100	1.10466300	-1.54476400
H	5.04490200	0.77477800	-2.22171000
H	3.66665600	1.87549500	-2.06776400
H	4.72810200	1.57622900	-0.68227300
C	2.89914700	-0.77924300	-2.44201400
H	2.29212300	-0.10463500	-3.05725500
H	3.76888000	-1.08642300	-3.03701600
H	2.30213900	-1.67225700	-2.24148000

Cartesian coordinates for optimized **TS-3$_{H2}$** (Flipped) with **(Me$_3$Si)$_2$N$^-$**

C	2.90872800	1.32245500	0.64106600

C	2.18533000	0.31571800	-0.28354600
C	1.20561000	-0.58290700	0.49839100
C	1.57255400	0.71148400	2.67421200
C	1.97691100	1.85145700	1.73658200
H	-0.10708500	-0.21761400	0.16878600
H	1.60290800	0.92522900	-0.99446800
H	3.77117800	0.84370800	1.12803700
H	0.73415400	0.99209800	3.32349700
H	2.40532900	0.45965900	3.34667500
H	1.15379000	-1.60475400	0.12247700
C	1.18176200	-0.58704400	1.94515000
O	0.77578700	-1.53329300	2.64293900
N	-1.38674400	-0.01551600	-0.24122700
Si	-2.35156500	-1.42708100	-0.08982400
Si	-1.92081600	1.59069800	-0.46177700
C	-2.15795800	2.55477000	1.17437100
H	-2.44105900	3.60232300	1.00485300
H	-2.94317900	2.08962800	1.78222900
H	-1.24203100	2.54918400	1.77619900
C	-3.59661800	1.76057700	-1.37380500
H	-3.87556500	2.81738000	-1.47944600
H	-3.54952700	1.32682500	-2.37897000
H	-4.41028100	1.25916100	-0.83728400
C	-0.70810000	2.63063100	-1.50852500
H	-1.10423500	3.63994500	-1.68153900
H	0.27008400	2.73834000	-1.02856500
H	-0.54204900	2.16370500	-2.48641100
C	-3.64010800	-1.33162500	1.32244400
H	-3.13447700	-1.17608900	2.28218600
H	-4.34053400	-0.49934900	1.18010000
H	-4.23305800	-2.25257300	1.40098300
C	-3.35135700	-1.85285500	-1.66849000
H	-2.68115700	-1.94730800	-2.53133400
H	-3.88336100	-2.80701500	-1.55437600
H	-4.09493700	-1.08674600	-1.91343400
C	-1.29866100	-2.96620500	0.26758700
H	-1.94761000	-3.83455100	0.44315600
H	-0.64584900	-3.21211900	-0.57912500
H	-0.66466400	-2.81667600	1.14818000
H	2.46414200	2.66106600	2.29810300
H	3.30781000	2.15821000	0.05296500
C	3.18152400	-0.48823100	-1.20175200
H	1.08484400	2.29013000	1.27232500
C	4.02249000	-1.50010100	-0.39923200
H	3.38416200	-2.20703700	0.13739900
H	4.68016500	-2.07090800	-1.06766000
H	4.66034100	-1.00262400	0.33977900
C	2.38002600	-1.24779200	-2.28013500
H	1.77377200	-0.55551500	-2.87541400
H	3.05628400	-1.77894600	-2.96268800
H	1.70103900	-1.98418000	-1.84335300
C	4.13319900	0.48240500	-1.93418900
H	4.74473300	-0.05586400	-2.66956000
H	3.57012200	1.25462900	-2.47264600
H	4.81804300	0.98655100	-1.24495000

Cartesian coordinates for optimized **TS-3$_{H3}$** with **(Me$_3$Si)$_2$N$^-$**

C	-2.86809000	0.03133100	-1.65796200
C	-1.39056700	-0.41400400	-1.63422800
C	-0.45188200	0.71322500	-1.19753100
C	-2.14386000	0.90198000	0.63731600
C	-3.35799100	0.58755800	-0.28062900
H	0.76319500	0.21225200	-0.65741900
H	-1.30278300	-1.28440600	-0.96939500
H	-1.10620700	-0.77963000	-2.62958500
H	-2.97262900	0.81977600	-2.41396300
H	-1.76601500	-0.02512700	1.08991600

H	-2.42057800	1.58291000	1.44551100
H	-0.03670200	1.29363200	-2.02624700
C	-0.99651300	1.55220700	-0.15585000
O	-0.60628600	2.68942000	0.16324500
N	1.97518100	-0.13277100	-0.21883300
Si	2.94834600	1.24891300	0.09836600
Si	2.35343100	-1.76957500	0.06703100
C	3.04022500	-2.13322200	1.81864900
H	3.25012400	-3.20171500	1.96209900
H	3.96968300	-1.58598100	2.01460900
H	2.31728000	-1.82816900	2.58445900
C	3.63718600	-2.50856100	-1.14724900
H	3.81472500	-3.57645900	-0.96126200
H	3.28971000	-2.40191000	-2.18184600
H	4.60129200	-1.99297600	-1.07348700
C	0.82305600	-2.89557600	-0.09820100
H	1.08730300	-3.93934900	0.11579200
H	0.03212400	-2.60269500	0.60142000
H	0.39973200	-2.85954900	-1.10729900
C	4.83020600	0.90254700	-0.03270900
H	5.16849400	0.13784700	0.67654800
H	5.09839300	0.55938800	-1.03889200
H	5.40666600	1.81477700	0.17082800
C	2.58283600	2.65392700	-1.12621800
H	1.54879500	2.98883700	-0.99232700
H	3.24842900	3.51014800	-0.95343400
H	2.71410300	2.33015200	-2.16564000
C	2.66399600	1.97862800	1.83781200
H	3.28652600	2.86400500	2.02407000
H	1.61475900	2.27953600	1.92984100
H	2.87925300	1.24457400	2.62374300
H	-3.84635800	1.55380500	-0.47334100
H	-3.50842100	-0.79508300	-1.99411200
C	-4.46224500	-0.28830500	0.41028600
C	-4.00091600	-1.74281400	0.63133000
H	-3.76506100	-2.24319800	-0.31284900
H	-3.10911000	-1.79099200	1.26355000
H	-4.78945200	-2.32357900	1.12641200
C	-4.84221800	0.32065000	1.77658700
H	-5.12919900	1.37403200	1.67365000
H	-5.69307100	-0.21638000	2.21436900
H	-4.01501400	0.26958100	2.48964900
C	-5.73527200	-0.29371700	-0.46380200
H	-6.53140200	-0.88042700	0.01158100
H	-6.11344000	0.72541400	-0.60932300
H	-5.55370200	-0.72486500	-1.45290200

Cartesian coordinates for optimized **TS-3$_{H3}$** (Flipped) with **(Me$_3$Si)$_2$N$^-$**

C	-2.21682900	0.47181800	1.24253900
C	-3.03960700	-0.47830600	0.35106900
C	-2.06757900	-1.20260500	-0.60141700
C	-0.29443100	-1.21457700	1.24104700
C	-1.18939700	-0.30495400	2.08049500
H	-2.56080800	-1.98669200	-1.18188500
H	-3.46896600	-1.24763700	1.01559300
H	-1.69055500	1.19659400	0.60847000
H	0.30414300	-1.89729100	1.84956300
H	0.78866500	-0.46359000	0.69021200
H	-1.64617500	-0.48878100	-1.32429900
C	-0.87802900	-1.88935600	0.10835600
O	-0.43472400	-2.92790400	-0.41648200
N	1.90360500	0.14256800	0.28037000
Si	3.14574500	-0.97218000	-0.12060700
Si	1.78242800	1.81245600	-0.04616300
C	0.61148100	2.21427900	-1.50439900
H	0.50267300	3.29499900	-1.66632800
H	0.99313400	1.77269400	-2.43272000

H	-0.38945500	1.80003300	-1.33956900
C	3.43109500	2.67293200	-0.49917200
H	3.26245600	3.73538700	-0.71957300
H	4.15532600	2.61485300	0.32067600
H	3.89787400	2.22454500	-1.38377400
C	1.11845900	2.79355200	1.45160900
H	1.02852000	3.86448500	1.22670600
H	0.13277100	2.43608100	1.76718100
H	1.79345900	2.68620300	2.30889200
C	3.34332800	-1.25141000	-2.00253200
H	2.40552500	-1.63110300	-2.42335100
H	3.58829100	-0.31910900	-2.52667200
H	4.13332500	-1.97867100	-2.23269200
C	4.88233300	-0.46004600	0.50816400
H	4.86195300	-0.27794900	1.58938800
H	5.61507500	-1.25616800	0.31931500
H	5.25448700	0.45116100	0.02784800
C	2.81521700	-2.67911200	0.63882200
H	3.59579400	-3.38903800	0.33414100
H	2.81778500	-2.63597200	1.73486200
H	1.84225900	-3.06717900	0.31813400
H	-0.57571000	0.41164200	2.64499100
H	-2.86642800	1.05105500	1.91065300
C	-4.27177000	0.18891400	-0.35677100
H	-1.74512000	-0.87934700	2.84457200
C	-5.28179700	0.68013900	0.70330900
H	-4.86476800	1.46841500	1.33662000
H	-6.18037000	1.08641900	0.22231000
H	-5.59696900	-0.14201200	1.35718100
C	-4.99906800	-0.84739300	-1.24018100
H	-4.38715800	-1.16303900	-2.08935000
H	-5.25851100	-1.74440000	-0.66504900
H	-5.92982600	-0.42608900	-1.64033300
C	-3.85935100	1.38559700	-1.23732400
H	-4.73522500	1.80702300	-1.74671800
H	-3.40442200	2.18583100	-0.64559700
H	-3.13924900	1.09120300	-2.00703400

Cartesian coordinates for optimized **TS-3$_{H4}$** with **(Me$_3$Si)$_2$N$^-$**

C	-2.10989000	1.38421100	-0.55074100
C	-1.41063900	0.48316800	-1.57969300
C	-0.65014400	-0.68023000	-0.94219200
C	-1.99957000	-0.38858700	1.20233700
C	-2.93683200	0.63171900	0.51877400
H	-0.33635700	-1.43082300	-1.67213700
H	-2.16010900	0.12370400	-2.30626400
H	-0.72154600	1.10371000	-2.17133200
H	-1.33849200	1.94319800	-0.00514600
H	-2.52529500	-1.04799400	1.89937300
H	-1.26589700	0.16805700	1.80238000
H	0.64367700	-0.23870000	-0.53795200
C	-1.19207100	-1.29138500	0.24611600
O	-0.96017500	-2.45634100	0.62434800
N	1.91493300	0.07513900	-0.27262900
Si	2.90919300	-1.31680000	-0.12855400
Si	2.23284600	1.69706700	0.14971500
C	1.63499900	2.92356600	-1.18638900
H	1.83499800	3.96424700	-0.89903900
H	2.14674300	2.73364600	-2.13723100
H	0.55967700	2.83088700	-1.37152200
C	4.08155300	2.12135000	0.40748500
H	4.19625900	3.17044900	0.71082100
H	4.53917300	1.50230500	1.18779200
H	4.66138400	1.97623000	-0.51052500
C	1.38497900	2.23593900	1.77780500
H	1.56303300	3.29477000	2.00851500
H	0.30066300	2.08300300	1.73569200

H	1.76111900	1.64147500	2.61895500
C	4.61202900	-1.14866400	-0.99167900
H	4.48433000	-0.87271600	-2.04530400
H	5.24781100	-0.38763900	-0.52676800
H	5.15977500	-2.10020200	-0.96166000
C	3.29684800	-1.79430600	1.68253300
H	2.36496900	-1.99490000	2.22301100
H	3.92347800	-2.69369300	1.74864600
H	3.81903400	-0.98689000	2.21099400
C	2.08902600	-2.83580400	-0.91592600
H	1.94543400	-2.69724500	-1.99446900
H	2.72026100	-3.72379700	-0.77778100
H	1.10852200	-3.02881600	-0.46715000
H	-3.21090700	1.38912300	1.27094200
H	-2.72123300	2.14039900	-1.05817400
C	-4.31883000	0.02441000	0.07037200
C	-4.19580300	-1.30877300	-0.69812700
H	-3.65132000	-1.18942300	-1.63757600
H	-3.67495900	-2.07080000	-0.11273700
H	-5.19613700	-1.69266400	-0.93905700
C	-5.09180500	1.03201300	-0.80516800
H	-6.11097900	0.67233400	-0.99458700
H	-5.17092800	2.01052800	-0.31530200
H	-4.60980600	1.18103900	-1.77596200
C	-5.16621700	-0.23399900	1.33761800
H	-5.34164300	0.69526200	1.89347600
H	-6.14427500	-0.65351900	1.07123800
H	-4.67792000	-0.94131500	2.01445600

Cartesian coordinates for optimized **TS-3$_{H4}$** (Flipped) with **(Me$_3$Si)$_2$N$^-$**

C	-2.44579600	-1.77517500	0.24018300
C	-2.68908300	-0.29933200	-0.12406300
C	-2.36157000	0.54105400	1.12390000
C	-0.30420900	-0.97835600	1.42754500
C	-0.95064300	-2.01830300	0.50137600
H	-2.22778900	1.60050600	0.87851000
H	-1.95185200	-0.03786500	-0.89886900
H	-3.02163200	-2.02162200	1.14418800
H	0.75988000	-0.41218200	0.70059800
H	0.30141800	-1.40626800	2.23048000
H	-3.19186300	0.50562700	1.84307100
C	-1.10707100	0.11269800	1.92498200
O	-0.83743500	0.79625300	2.92891900
N	1.84518300	-0.00555800	0.01558300
Si	1.85784300	1.69123500	-0.21578000
Si	3.03661500	-1.18464100	-0.29380000
C	4.77094600	-0.79391400	0.41952200
H	5.46898900	-1.62650800	0.25857800
H	5.21341000	0.09876200	-0.03645100
H	4.70877000	-0.61361700	1.49913400
C	3.32215500	-1.53709400	-2.15447100
H	4.05479000	-2.33918400	-2.31634800
H	2.38426900	-1.83696800	-2.63674400
H	3.68656600	-0.64535600	-2.67825200
C	2.56478900	-2.86308400	0.47700100
H	3.35580700	-3.60364700	0.30186200
H	2.42033900	-2.77733300	1.55951400
H	1.63624800	-3.25945900	0.05406700
C	1.79897700	2.64656600	1.42775200
H	1.65912800	3.72551000	1.27723900
H	0.98380700	2.27395000	2.05827000
H	2.73427900	2.50663900	1.98404900
C	3.38344100	2.34964900	-1.16842400
H	3.48708300	1.87597000	-2.15171400
H	3.29258300	3.43153600	-1.33251700
H	4.31582200	2.17999100	-0.61870500
C	0.35857100	2.27142700	-1.24740100

H	0.35125100	3.36115600	-1.38061000
H	0.36907000	1.81031200	-2.24230400
H	-0.58310300	1.99079400	-0.76460600
H	-0.82629800	-3.02926000	0.91419000
H	-2.79557300	-2.45106300	-0.55108200
C	-4.09063500	0.00271200	-0.76037900
H	-0.43872700	-2.03355800	-0.47500400
C	-5.24896500	-0.51147300	0.11822000
H	-5.22069400	-0.07301600	1.12102400
H	-6.21626900	-0.25064000	-0.32950000
H	-5.21826500	-1.60019000	0.22896300
C	-4.25984900	1.52271600	-0.96718000
H	-3.42269100	1.93789000	-1.54013700
H	-5.18381100	1.73654200	-1.51935800
H	-4.30977300	2.06019700	-0.01601300
C	-4.18659000	-0.66875300	-2.14732300
H	-5.14717100	-0.43822300	-2.62523400
H	-3.38960400	-0.31283300	-2.81025900
H	-4.10440500	-1.75806000	-2.08378700

Cartesian coordinates for optimized **TS-4$_{H1}$** with **(Me$_3$Si)$_2$N$^-$**

C	2.73281400	-0.61726700	0.20411000
C	2.13241200	-1.94067600	-0.30427100
C	1.28406600	-2.56253800	0.81359600
C	0.40712500	-0.16745400	1.21790300
C	1.60562900	0.44870200	0.42166300
H	0.58140700	-3.30885800	0.42413000
H	1.52342800	-1.77376600	-1.19885200
H	2.91820900	-2.64400600	-0.60187000
H	3.09246400	-0.82944300	1.22491300
H	-0.77843900	-0.10210600	0.56278000
H	0.12256600	0.47697700	2.05314500
H	1.92938200	-3.10001200	1.52077100
C	0.48112300	-1.55774400	1.65974900
O	-0.13315700	-1.99566900	2.63915200
C	4.00287100	-0.09382500	-0.54568800
C	2.21299400	1.65224100	1.17072700
H	2.49469100	1.31187500	2.17676800
H	1.45024800	2.42556300	1.29716100
C	3.43998900	2.23656800	0.45689600
H	3.87386000	3.04459000	1.06142300
H	3.11686100	2.69362200	-0.48332500
C	4.51120400	1.16942500	0.20022100
H	5.35484100	1.60078300	-0.35771500
H	4.91977500	0.84486600	1.16918000
C	3.75556600	0.21683700	-2.03670900
H	4.70009100	0.48811500	-2.52494900
H	3.35508600	-0.65738900	-2.56164600
H	3.06046000	1.04425500	-2.18912500
C	5.12686500	-1.15048100	-0.46783300
H	6.07197700	-0.72441400	-0.82650000
H	5.28438600	-1.48958400	0.56286900
H	4.91338700	-2.03070000	-1.08214200
C	0.96220000	0.91095000	-0.88198400
H	0.55034400	0.09879200	-1.51167300
O	0.81451100	2.07286500	-1.22476800
N	-2.07185200	0.06352000	-0.01121000
Si	-2.77259800	-1.37682700	-0.60279300
Si	-2.79978400	1.59376900	0.20458800
C	-4.47223900	1.56254300	1.14165200
H	-4.86292000	2.57674300	1.30043000
H	-5.24024100	0.99609500	0.60253300
H	-4.35091800	1.09347000	2.12524900
C	-3.12911900	2.52620000	-1.43201100
H	-3.54888300	3.52675700	-1.26177000
H	-2.18783700	2.64374200	-1.98089100
H	-3.82580700	1.97908300	-2.07789600

C	-1.69238400	2.76125700	1.22517700
H	-2.19677700	3.72295500	1.38517600
H	-1.45459600	2.34315300	2.20965800
H	-0.75205800	2.96048300	0.70189400
C	-3.19080900	-2.62789100	0.77419200
H	-3.48199600	-3.61038200	0.37888100
H	-2.33481300	-2.76005100	1.44487300
H	-4.02258700	-2.25513900	1.38475900
C	-4.38617700	-1.14412400	-1.61014900
H	-4.22384400	-0.49973600	-2.48191100
H	-4.75238100	-2.11198200	-1.97767700
H	-5.18881000	-0.69620500	-1.01401000
C	-1.60799800	-2.28351900	-1.82059600
H	-2.06237200	-3.21075900	-2.19353900
H	-1.38521200	-1.64950500	-2.68730300
H	-0.65429300	-2.55249800	-1.35540400

Cartesian coordinates for optimized **TS-4$_{H2}$** with **(Me$_3$Si)$_2$N$^-$**

C	2.20733000	0.21573600	0.56457800
C	2.34337400	-0.37455100	1.98466800
C	1.01437800	-0.93941800	2.51090700
C	0.29404000	-1.41295100	0.11192500
C	1.62441100	-0.83040300	-0.43856400
H	1.15990300	-1.51890800	3.42856900
H	3.10457600	-1.16363100	2.00060300
H	2.70261800	0.39705500	2.67551100
H	1.42819900	0.98901300	0.62605400
H	-0.07581400	-2.21130000	-0.53543900
H	-0.75555100	-0.52898200	0.01556600
H	0.34124300	-0.10948200	2.76620000
C	0.24358900	-1.81804000	1.51581400
O	-0.48705300	-2.71329900	1.95670000
C	3.48416200	0.96686800	0.04842600
C	1.40313400	-0.19997700	-1.82466600
H	0.57604000	0.51270700	-1.74781800
H	1.08415500	-0.98376300	-2.51879600
C	2.65675700	0.49849000	-2.36260700
H	2.42895900	0.99534200	-3.31500200
H	3.42493200	-0.25136600	-2.58253800
C	3.18509600	1.53451200	-1.36409600
H	4.09404000	2.01574900	-1.75349200
H	2.43636600	2.33309100	-1.25909800
C	4.74067600	0.07074300	0.00042600
H	5.60184300	0.65346500	-0.35009100
H	4.99351600	-0.31849300	0.99227900
H	4.62814600	-0.78176200	-0.67305900
C	3.79526200	2.16762300	0.96827200
H	4.58735400	2.78684200	0.52923900
H	2.91249400	2.80307200	1.10315400
H	4.13892300	1.85452200	1.95921500
C	2.47991200	-2.08180500	-0.56362100
H	2.75334600	-2.55122000	0.40776600
O	2.78372200	-2.64417700	-1.60449500
N	-1.95232900	0.17902900	-0.11755900
Si	-3.28369800	-0.85146300	-0.45842000
Si	-1.98899900	1.85702800	0.19889400
C	-1.11067000	2.33619100	1.82907600
H	-1.17938900	3.41645200	2.01318900
H	-1.57400900	1.82204300	2.67932300
H	-0.04775100	2.07260000	1.82831200
C	-3.73399800	2.62521300	0.38574700
H	-3.65306200	3.70651300	0.55847400
H	-4.35214700	2.48162400	-0.50703100
H	-4.27659100	2.19617700	1.23518200
C	-1.15278400	2.91271900	-1.16024900
H	-1.20366000	3.98505800	-0.92954200
H	-0.09595600	2.65256800	-1.28647900

H	-1.64213800	2.75507600	-2.12859400
C	-4.55214300	-0.98572600	0.96701900
H	-4.05240700	-1.33071100	1.87934600
H	-5.02986600	-0.02568900	1.19202700
H	-5.34819800	-1.70413600	0.73024600
C	-4.28512500	-0.32947000	-2.00712900
H	-3.63196200	-0.28723900	-2.88695200
H	-5.08901100	-1.04574200	-2.22337200
H	-4.74697400	0.65814300	-1.89512400
C	-2.74050800	-2.64060500	-0.79701500
H	-3.62415700	-3.27064900	-0.96348400
H	-2.10891200	-2.71825300	-1.68956300
H	-2.17974000	-3.04797700	0.05039000

Cartesian coordinates for optimized **TS-4$_{H3}$** with **(Me$_3$Si)$_2$N$^-$**

C	-2.46544500	0.25932400	0.74070300
C	-1.11757600	0.87473900	1.18526300
C	-0.08812000	-0.12051600	1.74143500
C	-1.55254600	-2.07054800	0.95723500
C	-2.25659900	-1.08770600	-0.02679400
H	1.00374100	-0.07113300	0.89359700
H	-0.67862700	1.42471100	0.34053100
H	-1.33312500	1.63804900	1.94325500
H	-2.99552100	-0.03974300	1.66014700
H	-1.14566000	-2.93602400	0.42034100
H	-2.31791200	-2.47516200	1.63308500
H	0.42083600	0.23354600	2.64126100
C	-0.44133000	-1.51192800	1.86720300
O	0.12434300	-2.32828800	2.61311200
C	-3.42709500	1.27620700	0.02748200
C	-3.59814400	-1.70084300	-0.47811200
H	-4.12589500	-2.05714700	0.41761500
H	-3.39685100	-2.57622400	-1.10429000
C	-4.50295600	-0.71236900	-1.21800600
H	-5.46642400	-1.18792000	-1.44611700
H	-4.05084400	-0.45277600	-2.18077600
C	-4.73325300	0.54171600	-0.36954900
H	-5.39418000	1.24614800	-0.89429000
H	-5.26225500	0.25071000	0.55081700
C	-2.80837700	1.93323200	-1.22672100
H	-3.54631000	2.59119800	-1.70280400
H	-1.93947000	2.54662800	-0.97357600
H	-2.48951300	1.20530600	-1.97603100
C	-3.80827100	2.40273100	1.01125100
H	-4.56976100	3.05636400	0.56761600
H	-4.22107200	1.99411700	1.94141000
H	-2.94910400	3.02732100	1.27177800
C	-1.31242400	-0.93877500	-1.21693700
H	-0.33789300	-0.46001800	-0.99968700
O	-1.55001600	-1.36392000	-2.33585600
N	2.09359900	0.16135900	0.10252800
Si	2.96741300	-1.23121600	-0.39100700
Si	2.58301800	1.79571500	-0.01291900
C	1.92346400	2.67290900	-1.57915000
H	2.20193600	3.73458600	-1.61106300
H	2.31605600	2.19657500	-2.48524900
H	0.82995000	2.61268500	-1.63240400
C	4.47678300	2.08137300	-0.03510300
H	4.70741800	3.15255800	-0.10630000
H	4.94052200	1.70276100	0.88301400
H	4.96694000	1.58397600	-0.87935800
C	1.97096800	2.83098600	1.46948200
H	2.32535100	3.86703400	1.39158900
H	0.87905400	2.85912700	1.53670900
H	2.34652200	2.41938300	2.41321000
C	3.68197600	-1.08850800	-2.16208800
H	2.87736500	-0.91837200	-2.88704100

H	4.39362500	-0.26075600	-2.26147300
H	4.20498900	-2.00821200	-2.45579000
C	4.44604100	-1.65363700	0.74492500
H	4.09715800	-1.80926900	1.77217600
H	4.96065500	-2.56892500	0.42371400
H	5.18608600	-0.84541900	0.76595200
C	1.88108700	-2.79038600	-0.41287500
H	2.48512300	-3.66119400	-0.69950500
H	1.44540600	-2.99094200	0.57106400
H	1.06672300	-2.70638000	-1.14178000

Cartesian coordinates for optimized **TS-4$_{H4}$** with **$(Me_3Si)_2N^-$**

C	-1.92663700	0.42595100	0.16944200
C	-0.98422000	0.87276500	-0.96728900
C	-0.05333500	-0.23782400	-1.45960800
C	-1.69537900	-1.97621400	-0.55303500
C	-2.73218000	-0.86043600	-0.22674400
H	0.46788500	0.01852400	-2.38775300
H	-1.57947700	1.29677900	-1.79241700
H	-0.37291200	1.70212400	-0.59716100
H	-1.27593900	0.09003200	0.99180100
H	-2.18784900	-2.86021400	-0.97404700
H	-1.24612300	-2.29592700	0.39560800
H	1.08792400	-0.19574500	-0.63610400
C	-0.54351500	-1.59552400	-1.50879400
O	-0.04021400	-2.51485300	-2.17487900
C	-2.79903800	1.57846100	0.78142000
C	-3.65544800	-1.32344600	0.91677200
H	-3.02034600	-1.70612400	1.72746600
H	-4.26954200	-2.16062100	0.56735900
C	-4.54333900	-0.20423700	1.46842000
H	-5.12382100	-0.57664700	2.32321400
H	-5.27107000	0.09225400	0.70589200
C	-3.69398700	0.99330900	1.90445200
H	-4.33460100	1.79238300	2.30373900
H	-3.04327100	0.67802100	2.73365900
C	-3.67964300	2.29903300	-0.26324000
H	-4.27042600	3.08433400	0.22506400
H	-3.06968300	2.77977100	-1.03362100
H	-4.38152200	1.62921400	-0.76574900
C	-1.87894200	2.63372700	1.43209900
H	-2.47680100	3.36987000	1.98422000
H	-1.18094300	2.17008600	2.13800700
H	-1.28749000	3.17806400	0.69091700
C	-3.52394900	-0.68491100	-1.51283100
H	-2.91834000	-0.37438000	-2.38998400
O	-4.71128600	-0.92100400	-1.65249100
N	2.23626500	0.03898200	0.02242800
Si	3.20670600	1.27425000	-0.65658000
Si	2.75477900	-1.18682700	1.09998300
C	3.04167700	-0.56436900	2.88721700
H	3.31613700	-1.38416200	3.56451400
H	3.83885300	0.18609200	2.93395100
H	2.13102200	-0.09698600	3.28053500
C	4.38510100	-2.04945600	0.58818200
H	4.66971400	-2.83453800	1.30111300
H	4.27658600	-2.51589100	-0.39765400
H	5.22168100	-1.34306500	0.52616800
C	1.46411500	-2.57470200	1.24534500
H	1.86049000	-3.40956900	1.83710000
H	0.55722700	-2.22068900	1.74927500
H	1.17718600	-2.95782400	0.26080200
C	4.50584000	1.99593700	0.54937900
H	4.02556400	2.41213900	1.44239900
H	5.22207000	1.23756400	0.88609500
H	5.08095900	2.80119800	0.07358100
C	4.18463000	0.72264600	-2.20331300

H	3.50398300	0.33003500	-2.96753100
H	4.75684600	1.54570700	-2.65178400
H	4.88886800	-0.08026800	-1.95672400
C	2.17013900	2.77313100	-1.21948000
H	2.81468600	3.55467800	-1.64218400
H	1.43849100	2.49760900	-1.98611000
H	1.62000600	3.21316800	-0.37970200

Cartesian coordinates for optimized **TS-5$_{H1}$** with **(Me$_3$Si)$_2$N$^-$**

C	-2.77402300	-0.52814500	-0.24969800
C	-2.22889900	-1.86456100	0.28036600
C	-1.31917600	-2.49433500	-0.78557200
C	-0.40086700	-0.10557700	-1.16244900
C	-1.58174500	0.49059300	-0.33402800
H	-0.61075000	-3.20440900	-0.34257300
H	-1.67176700	-1.68730900	1.20782000
H	-3.03870200	-2.55763100	0.53436400
H	-3.03746700	-0.68825000	-1.30717300
H	0.79027500	-0.04613600	-0.54332800
H	-0.15394800	0.54284800	-2.00704100
H	-1.91446200	-3.07149800	-1.50423100
C	-0.51322900	-1.48752900	-1.62694500
O	0.07015000	-1.91423800	-2.62911100
C	-4.09721800	-0.00858400	0.40778200
C	-2.09725800	1.80275700	-0.98670600
H	-2.35978600	1.55767000	-2.02425900
H	-1.28354400	2.53242800	-1.02916000
C	-3.31840600	2.37766200	-0.26244100
H	-3.65455300	3.29206800	-0.76818200
H	-3.03511500	2.67454200	0.75467000
C	-4.46508500	1.36026900	-0.22645000
H	-5.33218800	1.77772800	0.30391700
H	-4.79539800	1.18147900	-1.26062400
C	-4.03542800	0.10755300	1.94573500
H	-5.02335000	0.38622800	2.33386800
H	-3.76091200	-0.84918300	2.40188800
H	-3.31383700	0.84814000	2.29004000
C	-5.24071300	-0.98920600	0.06233500
H	-6.20296000	-0.58036600	0.39402300
H	-5.30634900	-1.16250900	-1.01826900
H	-5.11335900	-1.95997200	0.55118600
N	2.11536200	0.08286900	-0.03253900
Si	2.76607800	-1.37326700	0.57581500
Si	2.86825500	1.59536500	-0.23406000
C	4.38234400	1.58004500	-1.40953200
H	4.81718800	2.58059200	-1.53772600
H	5.17548500	0.92175100	-1.03499700
H	4.09440800	1.20846100	-2.40001400
C	3.48028100	2.41387900	1.38355600
H	3.86542800	3.42752200	1.20765500
H	2.65542000	2.48479100	2.10169900
H	4.28023700	1.83399300	1.85730300
C	1.66852100	2.87400200	-0.98965800
H	2.17724600	3.83195200	-1.15664900
H	1.26395100	2.54029300	-1.95144900
H	0.82679600	3.06043200	-0.31347200
C	3.08631100	-2.67339200	-0.78407900
H	3.33794700	-3.65972100	-0.37119900
H	2.21162200	-2.77964600	-1.43466400
H	3.92187700	-2.35712900	-1.42108400
C	4.43138200	-1.18714300	1.50605400
H	4.32401100	-0.56008200	2.39828200
H	4.80173500	-2.16795900	1.83266300
H	5.20837200	-0.73716800	0.87712800
C	1.59918300	-2.18725600	1.85077600
H	2.03320200	-3.10299600	2.27349800
H	1.39254300	-1.49377500	2.67338800

H	0.63484700	-2.45609500	1.40696500
C	-1.10412800	0.84206500	1.02666400
N	-0.75494500	1.16068500	2.08965500

Cartesian coordinates for optimized **TS-5$_{H2}$** with **(Me$_3$Si)$_2$N$^-$**

C	2.21823100	0.11944400	0.51550800
C	2.39530200	-0.66248900	1.83080500
C	1.06384400	-1.23939400	2.33489000
C	0.28940500	-1.43404500	-0.09243500
C	1.63569200	-0.84212600	-0.57359300
H	1.21849100	-1.94115300	3.16090400
H	3.10705400	-1.48167000	1.66946300
H	2.83284800	-0.02070500	2.60455400
H	1.40779300	0.84490200	0.67232600
H	-0.08534700	-2.16617300	-0.81051500
H	-0.76967100	-0.51339300	-0.12727900
H	0.43470800	-0.42799000	2.72705100
C	0.22477800	-1.95753400	1.26598500
O	-0.56358400	-2.83856200	1.63148400
C	3.46262300	0.97222500	0.08336700
C	1.44163300	-0.09850900	-1.92025400
H	0.62305800	0.61396300	-1.77980600
H	1.10315300	-0.81499200	-2.67725200
C	2.71099100	0.62451700	-2.37737600
H	2.51631200	1.16527700	-3.31240600
H	3.49703300	-0.10772700	-2.60263000
C	3.18907000	1.61037700	-1.30501200
H	4.09806100	2.12965400	-1.63965400
H	2.42025600	2.38636400	-1.18508100
C	4.78054100	0.16801500	0.04300500
H	5.60773300	0.83055900	-0.24134200
H	5.02032100	-0.25101700	1.02540600
H	4.75297200	-0.66111200	-0.66541900
C	3.65130600	2.13140500	1.08700800
H	4.44429300	2.80646400	0.74227600
H	2.73345000	2.72080100	1.19186900
H	3.93713100	1.77408400	2.08126800
N	-1.93327600	0.20294200	-0.21679400
Si	-3.29258800	-0.81403400	-0.49525800
Si	-1.94679500	1.83393800	0.29221800
C	-0.89275500	2.97861400	-0.81993200
H	-0.94983800	4.02307000	-0.48652300
H	0.16445900	2.69243700	-0.81777400
H	-1.23907900	2.93948400	-1.85931500
C	-1.26307100	2.08146900	2.06143900
H	-1.29572900	3.13592700	2.36588700
H	-1.85088000	1.50450000	2.78481700
H	-0.22325700	1.74725100	2.14999700
C	-3.66583400	2.67556700	0.32065400
H	-3.58118700	3.69098500	0.72948400
H	-4.09284600	2.76071200	-0.68443700
H	-4.38599700	2.13045200	0.94048900
C	-4.35373700	-1.12744000	1.06357600
H	-3.73484100	-1.59392700	1.83825600
H	-4.76614400	-0.20055300	1.47954800
H	-5.19580800	-1.80095100	0.85622300
C	-4.49089100	-0.14960000	-1.83410500
H	-3.95260700	0.04230500	-2.77005500
H	-5.28149700	-0.88070900	-2.04938500
H	-4.97937300	0.78470000	-1.53762800
C	-2.77928500	-2.54039600	-1.09892500
H	-3.67301700	-3.14862200	-1.29047200
H	-2.20258800	-2.49907900	-2.03037500
H	-2.17250400	-3.04757300	-0.34225100
C	2.56605900	-1.97281500	-0.82592600
N	3.25752000	-2.88300100	-1.05057900

Cartesian coordinates for optimized **TS-5$_{H3}$** with **(Me$_3$Si)$_2$N$^-$**

C	-2.50817500	0.32863200	0.59627000
C	-1.06955800	0.87469200	0.69034100
C	-0.10743800	-0.02268100	1.48308700
C	-1.61406000	-2.03401600	0.89595500
C	-2.47274300	-1.10924900	-0.02306100
H	1.06141300	-0.04591700	0.79081800
H	-0.68611800	1.03048100	-0.32838400
H	-1.09655200	1.86812900	1.15078400
H	-2.85881300	0.15442200	1.62600300
H	-1.16116300	-2.84143700	0.31073400
H	-2.28394100	-2.51946400	1.61509400
H	0.28562400	0.44157800	2.39096400
C	-0.50508400	-1.38378700	1.75472000
O	0.00410300	-2.12030500	2.61283500
C	-3.55333600	1.31202000	-0.04095900
C	-3.90738000	-1.69382900	-0.15086100
H	-4.27877400	-1.85498300	0.86977900
H	-3.85921900	-2.67803700	-0.63116000
C	-4.86304700	-0.75622100	-0.88963700
H	-5.86478800	-1.20301300	-0.93121600
H	-4.53539900	-0.63364700	-1.92907000
C	-4.92483500	0.59901700	-0.17785200
H	-5.62519800	1.27059800	-0.69294100
H	-5.33736500	0.43901100	0.82962500
C	-3.11632400	1.87333600	-1.41215000
H	-3.88388000	2.56014700	-1.79068500
H	-2.18216900	2.43537100	-1.32979600
H	-2.96022200	1.09711700	-2.16305100
C	-3.75898000	2.50999500	0.91190200
H	-4.56283400	3.15748800	0.54049600
H	-4.03765000	2.17545100	1.91815800
H	-2.85758900	3.12259500	0.99999700
N	2.27051200	0.12846800	0.13634500
Si	3.03151200	-1.30661600	-0.39731400
Si	2.83859900	1.73194700	0.05251200
C	2.37307900	2.63606000	-1.56846700
H	2.70738700	3.68227200	-1.57632200
H	2.81981000	2.13506600	-2.43532300
H	1.28699900	2.62943700	-1.71864300
C	4.73874000	1.92060900	0.20605000
H	5.04070800	2.97520100	0.15465800
H	5.09497500	1.51739200	1.16104900
H	5.26950100	1.38808600	-0.59171100
C	2.12643100	2.80502900	1.46305900
H	2.52170600	3.82803400	1.41607100
H	1.03425800	2.87147400	1.41715900
H	2.38834800	2.38875300	2.44238900
C	3.75900800	-1.18085900	-2.16480600
H	2.97044000	-0.93374300	-2.88495700
H	4.52828500	-0.40266000	-2.24005400
H	4.21728400	-2.12709500	-2.48208600
C	4.47877900	-1.87182800	0.71942400
H	4.12559000	-2.02278900	1.74598700
H	4.92076800	-2.81611200	0.37411200
H	5.27838200	-1.12253600	0.75318000
C	1.81615900	-2.76739500	-0.44365600
H	2.32166300	-3.67808000	-0.79031700
H	1.40076600	-2.96745800	0.54936600
H	0.98655200	-2.56554300	-1.13071100
C	-1.88579200	-1.11044600	-1.37939700
N	-1.47563000	-1.17450400	-2.46566300

Cartesian coordinates for optimized **TS-5$_{H4}$** with **(Me$_3$Si)$_2$N$^-$**

C	-1.94223600	0.37409900	0.13793000
C	-1.08602000	0.82225200	-1.05986400

C	-0.11264100	-0.26391700	-1.52245900
C	-1.74208400	-2.02905000	-0.63622800
C	-2.74938900	-0.91104300	-0.25048600
H	0.41820200	-0.00347200	-2.44372700
H	-1.75608300	1.14418900	-1.87312300
H	-0.51477500	1.71015600	-0.77088100
H	-1.24378100	0.01669500	0.90926300
H	-2.25993600	-2.87220200	-1.10388500
H	-1.29996700	-2.40758900	0.29350700
H	1.01590800	-0.19705300	-0.66728100
C	-0.57620500	-1.62910400	-1.56955600
O	-0.04192900	-2.55167000	-2.20533800
C	-2.77720900	1.51270600	0.82329400
C	-3.64178500	-1.39219300	0.92557600
H	-2.96600700	-1.74871200	1.71393200
H	-4.23799900	-2.25444900	0.60451200
C	-4.52723200	-0.27922400	1.48781800
H	-5.11275300	-0.66126300	2.33408100
H	-5.25262500	0.03876600	0.72871000
C	-3.66496000	0.90354500	1.94060200
H	-4.29616400	1.69597600	2.36551700
H	-3.01149900	0.56051600	2.75620700
C	-3.65583200	2.31235300	-0.16379600
H	-4.19958300	3.09685500	0.37769800
H	-3.04465300	2.80193500	-0.92710600
H	-4.38915100	1.69338700	-0.68392700
C	-1.80927400	2.50551000	1.50315600
H	-2.37221100	3.24385200	2.08792500
H	-1.12193900	1.98971800	2.18271700
H	-1.20508100	3.05227600	0.77438500
N	2.13840700	0.04778000	0.01735000
Si	3.10361200	1.30282600	-0.63499100
Si	2.66241300	-1.18430500	1.08576700
C	2.93477400	-0.57612800	2.88031600
H	3.21091600	-1.40068000	3.55112500
H	3.72641600	0.17918800	2.93926100
H	2.01876000	-0.11873600	3.27308300
C	4.30119900	-2.02992100	0.57429300
H	4.58786400	-2.82034700	1.28044600
H	4.20097700	-2.48658600	-0.41692900
H	5.13279500	-1.31676500	0.52408100
C	1.38249900	-2.58416400	1.21416900
H	1.78063200	-3.41582300	1.80922100
H	0.46691000	-2.23957400	1.70924000
H	1.11109700	-2.96814500	0.22560400
C	4.38330700	2.01879900	0.59465100
H	3.89078200	2.41697900	1.48919000
H	5.10439500	1.26295000	0.92659900
H	4.95434200	2.83673400	0.13593900
C	4.10154300	0.78182800	-2.17887500
H	3.43232000	0.39248400	-2.95468900
H	4.66913800	1.61679500	-2.61080100
H	4.81188400	-0.01686100	-1.93617100
C	2.05673400	2.79839700	-1.18569900
H	2.69741000	3.59813900	-1.57911200
H	1.34458900	2.52888000	-1.97253100
H	1.48440600	3.21206700	-0.34730800
C	-3.63503900	-0.67225400	-1.41074000
N	-4.36774300	-0.53080200	-2.30271400

Cartesian coordinates for optimized **TS-6$_{H1}$** with **(Me$_3$Si)$_2$N$^-$**

C	2.73036200	-0.62068400	0.28104800
C	2.21330100	-2.00016700	-0.16597800
C	1.33524100	-2.58926500	0.94700200
C	0.36259500	-0.19240500	1.22428200
C	1.56753000	0.40340500	0.47276900
H	0.68542700	-3.38680600	0.56901900
H	1.64896900	-1.90700200	-1.09316700

H	3.05118700	-2.67851500	-0.35886600
H	3.06415200	-0.76361000	1.32222900
H	-0.76160500	-0.12085400	0.57338300
H	0.07673200	0.44940400	2.06113300
H	1.96110500	-3.05656300	1.71954700
C	0.44771800	-1.58340600	1.69633100
O	-0.20914200	-1.99510800	2.65424500
C	4.01322800	-0.06910900	-0.43370500
C	2.11935800	1.64936000	1.18955400
H	2.37696700	1.31555400	2.20289600
H	1.32935200	2.39482200	1.29235800
C	3.35920700	2.25369300	0.51825700
H	3.74102200	3.07889700	1.13332000
H	3.06973700	2.69467000	-0.44030600
C	4.46512500	1.21044700	0.32118700
H	5.31843700	1.65674300	-0.20830900
H	4.84200400	0.90704600	1.30949700
C	3.83814200	0.22893400	-1.93828700
H	4.81604300	0.45934100	-2.37953900
H	3.42310200	-0.63153700	-2.47010200
H	3.18425000	1.07979800	-2.13586200
C	5.15390200	-1.10204600	-0.29635700
H	6.10642600	-0.65040200	-0.59877500
H	5.26205100	-1.44572000	0.73932900
H	4.99485900	-1.98076400	-0.92817500
N	-2.11958500	0.05719100	0.01524700
Si	-2.82798200	-1.36950300	-0.59296500
Si	-2.86070900	1.56726500	0.27572000
C	-4.54942600	1.49129900	1.18351300
H	-4.96291000	2.49442400	1.35498500
H	-5.29584900	0.92104000	0.61818600
H	-4.43842100	1.00361900	2.15931600
C	-3.17525600	2.56899400	-1.32344200
H	-3.59445800	3.56344400	-1.11818500
H	-2.23165900	2.70322800	-1.86446600
H	-3.86811700	2.04727100	-1.99391800
C	-1.78496200	2.71036900	1.36225100
H	-2.29884000	3.66259800	1.54647600
H	-1.56291300	2.25938800	2.33614200
H	-0.83648500	2.93565000	0.86439200
C	-3.45270100	-2.54148700	0.78076100
H	-3.79196800	-3.51086900	0.39099900
H	-2.65333400	-2.72158500	1.50835000
H	-4.29045800	-2.08873200	1.32535200
C	-4.32067400	-1.08968200	-1.76457900
H	-4.02416200	-0.50498200	-2.64325200
H	-4.72239000	-2.04711800	-2.12241000
H	-5.14115500	-0.55316600	-1.27447000
C	-1.60385500	-2.39333500	-1.64017800
H	-2.09352300	-3.27896800	-2.06638800
H	-1.20275500	-1.79147700	-2.46204900
H	-0.75160800	-2.74255900	-1.04887500
N	1.00594300	0.87718300	-0.91672900
O	0.78123600	0.03354500	-1.77802700
O	0.76477500	2.07600300	-1.07053800

Cartesian coordinates for optimized **TS-6_{H2}** with **$(Me_3Si)_2N^-$**

C	2.08350300	0.40377000	0.56537300
C	2.24742500	-0.14805600	1.99644800
C	0.97381400	-0.84210000	2.50616100
C	0.25967100	-1.31948200	0.10714600
C	1.50713900	-0.64261400	-0.43382500
H	1.17446000	-1.42516500	3.41030200
H	3.08000600	-0.85212200	2.03258100
H	2.49308800	0.67935900	2.67214800
H	1.25824400	1.12870800	0.61413700
H	-0.06131200	-2.12359100	-0.55817600
H	-0.85112300	-0.49133700	0.03509700

H	0.22762500	-0.08255300	2.77955800
C	0.27156100	-1.76097200	1.50120400
O	-0.37786000	-2.72386700	1.91976100
C	3.30310900	1.23542000	0.03128600
C	1.24002400	-0.00278100	-1.80422400
H	0.36955200	0.64488700	-1.66164500
H	0.93706800	-0.78007100	-2.50938400
C	2.41297400	0.81026400	-2.36293500
H	2.09368400	1.32826300	-3.27650000
H	3.22044200	0.13307600	-2.65830400
C	2.91842200	1.83869500	-1.34501300
H	3.78361700	2.38207900	-1.75065200
H	2.13266500	2.59041500	-1.18151100
C	4.61050600	0.42236100	-0.09422100
H	5.43315000	1.09374200	-0.37064800
H	4.87791900	-0.05718000	0.85162900
H	4.55919000	-0.35784900	-0.85579900
C	3.57683900	2.41665900	0.98797300
H	4.29732000	3.10827300	0.53447700
H	2.66079500	2.98073400	1.19854400
H	3.99692400	2.08702500	1.94290200
N	-2.06729800	0.14895800	-0.08824400
Si	-3.33631700	-0.94264000	-0.48041500
Si	-2.21033800	1.81655900	0.25734500
C	-1.50600200	2.94684400	-1.11759500
H	-1.62047400	4.00991500	-0.86802300
H	-0.43947300	2.76395300	-1.29205600
H	-2.02360500	2.76873400	-2.06756600
C	-1.30399900	2.33295100	1.85944400
H	-1.43974400	3.40376800	2.06023100
H	-1.70003600	1.77931000	2.71873100
H	-0.22622700	2.14333300	1.81936200
C	-3.99670200	2.45118100	0.52621700
H	-3.99178300	3.53681100	0.68969200
H	-4.64734400	2.25199600	-0.33218100
H	-4.45869500	1.98787000	1.40474200
C	-4.63501500	-1.16486800	0.90535500
H	-4.14495600	-1.49242100	1.82929200
H	-5.17479500	-0.23752800	1.12575700
H	-5.37973800	-1.92528000	0.63541100
C	-4.31824700	-0.44209900	-2.04799700
H	-3.64602300	-0.36515700	-2.91096800
H	-5.09009800	-1.18393600	-2.29244000
H	-4.81803600	0.52712700	-1.93657000
C	-2.69147100	-2.69575800	-0.82901300
H	-3.53790300	-3.37133700	-1.00909300
H	-2.04965900	-2.73164500	-1.71696000
H	-2.11563600	-3.08224500	0.01821900
N	2.54602900	-1.81807700	-0.65821100
O	3.00496600	-2.39160200	0.33074000
O	2.79810100	-2.17921600	-1.81136200

Cartesian coordinates for optimized **TS-6$_{H3}$** with **(Me$_3$Si)$_2$N$^-$**

C	-2.34838400	0.52830500	0.60482700
C	-0.88402700	1.01295500	0.59506200
C	0.04873800	0.14086500	1.44780200
C	-1.49547200	-1.86709800	0.96630700
C	-2.50415300	-0.96852600	0.19054800
H	1.22688000	0.03102600	0.77400700
H	-0.51871300	1.08023200	-0.43493900
H	-0.86806700	2.03218200	0.99394900
H	-2.62859000	0.48615600	1.66980400
H	-0.97994200	-2.53999000	0.27376400
H	-2.04950400	-2.51072300	1.65599900
H	0.45098800	0.65475400	2.32491500
C	-0.40274800	-1.17813000	1.81819100
O	0.06715700	-1.86864200	2.73521600
C	-3.40294300	1.49379100	-0.04203700

C	-3.94965700	-1.43706800	0.43493400
H	-4.07170600	-1.45461600	1.52542400
H	-4.06539500	-2.46601100	0.08362600
C	-5.02129500	-0.52580300	-0.17506900
H	-6.01336700	-0.86920200	0.14613100
H	-4.99851600	-0.62049900	-1.26396100
C	-4.82170500	0.93442800	0.24438700
H	-5.56718200	1.57294400	-0.24963600
H	-5.01055900	1.02157200	1.32480200
C	-3.20537800	1.70701900	-1.55913300
H	-3.89200900	2.48605400	-1.91302000
H	-2.18654400	2.03330600	-1.78417800
H	-3.40413200	0.81055100	-2.14982700
C	-3.31538100	2.87679200	0.63924000
H	-4.16748800	3.49809500	0.33740300
H	-3.33772800	2.78674600	1.73168900
H	-2.40330400	3.41339200	0.36539500
N	2.45785600	0.12283200	0.15036900
Si	3.16942000	-1.36553700	-0.29375000
Si	3.07588000	1.70012500	-0.02466200
C	2.65395200	2.51548900	-1.70364700
H	3.01999300	3.54872800	-1.77283000
H	3.09296900	1.94839500	-2.53297200
H	1.56944400	2.53157300	-1.86371600
C	4.97952900	1.83805200	0.13938900
H	5.31525400	2.87798500	0.03064300
H	5.31335800	1.48044400	1.12033400
H	5.50147800	1.24399500	-0.61988000
C	2.38324800	2.87887400	1.30855100
H	2.80911400	3.88509900	1.20300600
H	1.29401800	2.97354200	1.24588200
H	2.62325900	2.51672400	2.31463000
C	3.92754500	-1.36604500	-2.05344100
H	3.16137300	-1.12744200	-2.80029900
H	4.72814200	-0.62356900	-2.15683800
H	4.35276000	-2.34523700	-2.31119600
C	4.57629600	-1.92807900	0.87412400
H	4.20294100	-2.00948100	1.90138200
H	4.98498700	-2.90609100	0.58653100
H	5.40463300	-1.20988400	0.88104000
C	1.89324100	-2.77450900	-0.28392700
H	2.35506800	-3.72302400	-0.58673800
H	1.46362000	-2.90897900	0.71418000
H	1.07786600	-2.55866500	-0.98351700
N	-2.16725500	-1.18569700	-1.30418900
O	-1.07075500	-0.80898300	-1.70387200
O	-2.98668300	-1.76889200	-2.02173600

Cartesian coordinates for optimized **TS-6$_{H4}$** with **(Me$_3$Si)$_2$N$^-$**

C	-1.75668200	0.49545900	0.19186100
C	-0.88936600	0.88546900	-1.01912700
C	0.03392100	-0.24365400	-1.47279600
C	-1.60670800	-1.94907700	-0.49553600
C	-2.55815000	-0.82588800	-0.02588200
H	0.55709300	-0.01929400	-2.40767500
H	-1.53170500	1.23582800	-1.83759100
H	-0.27424500	1.73929000	-0.71896900
H	-1.04171000	0.19327000	0.97289000
H	-2.17640700	-2.77686700	-0.93040900
H	-1.12113800	-2.35070900	0.40058200
H	1.18550300	-0.19617100	-0.63518400
C	-0.47743300	-1.58963900	-1.48841000
O	-0.00101900	-2.54103100	-2.12777300
C	-2.58529000	1.66398700	0.83268100
C	-3.29839400	-1.23917500	1.25890900
H	-2.51614900	-1.55211700	1.96165600
H	-3.91821300	-2.11781200	1.05941800
C	-4.12230600	-0.12106800	1.90747600

H	-4.50916400	-0.47176300	2.87329200
H	-4.99383500	0.09771900	1.28470800
C	-3.27586200	1.13825600	2.11808200
H	-3.89269500	1.93972100	2.54781600
H	-2.49429700	0.92009700	2.86070900
C	-3.63471600	2.27218700	-0.12393600
H	-4.10994800	3.13858000	0.35288900
H	-3.17030700	2.61801900	-1.05154000
H	-4.43040600	1.57344900	-0.39110700
C	-1.62682800	2.79563300	1.26246300
H	-2.16370700	3.52884000	1.87720100
H	-0.79026000	2.40708600	1.85377300
H	-1.20799500	3.32789600	0.40453700
N	2.32076800	0.03243900	0.02132900
Si	3.30830700	1.24866000	-0.67267500
Si	2.83688600	-1.19206400	1.10293900
C	3.13943600	-0.56145000	2.88457100
H	3.41118500	-1.37983300	3.56462900
H	3.94321100	0.18232100	2.92218900
H	2.23551900	-0.08396600	3.28138400
C	4.45505800	-2.07361300	0.58687900
H	4.73588100	-2.85656300	1.30359300
H	4.33567700	-2.54568700	-0.39495100
H	5.29832000	-1.37632000	0.51493700
C	1.53545800	-2.56847700	1.26553500
H	1.93112300	-3.40463700	1.85576400
H	0.63761700	-2.20518600	1.77956100
H	1.23594200	-2.95165500	0.28472100
C	4.61355300	1.96573700	0.52910600
H	4.13698800	2.39713800	1.41689000
H	5.32047500	1.20270700	0.87477900
H	5.19884200	2.75908700	0.04584000
C	4.28101400	0.66411800	-2.20974200
H	3.59606300	0.27074400	-2.96961200
H	4.86372800	1.47433700	-2.66783900
H	4.97505200	-0.14420700	-1.95233100
C	2.29213900	2.75300700	-1.25444700
H	2.94906600	3.52400500	-1.67737400
H	1.56493500	2.47903400	-2.02569500
H	1.73940500	3.20558800	-0.42319400
N	-3.59511100	-0.68525700	-1.16659400
O	-3.18200200	-0.37841300	-2.27983200
O	-4.78383100	-0.92749000	-0.93030200

Cartesian coordinates for optimized **TS-1$_{H1}$** with **LHMDS**

C	-3.87586300	-0.51357200	-1.33233500
C	-4.05046400	0.61183500	-0.30652000
C	-3.48553400	0.20406900	1.06223000
C	-1.63075400	-1.03778800	-0.22178000
C	-2.38517100	-0.81910100	-1.53914800
H	-3.32983900	1.06962700	1.71660200
H	-3.53159500	1.50874700	-0.66900500
H	-5.10587100	0.88810900	-0.20136800
H	-4.39178600	-1.41582400	-0.97493800
H	-0.39471000	-0.39139600	-0.13468100
H	-1.17799800	-2.02867900	-0.12257700
H	-4.20387300	-0.43860000	1.59147100
C	-2.20046600	-0.60434800	1.01697700
O	-1.61902500	-0.82704800	2.12929100
N	0.87975200	0.02230700	0.22504100
Si	1.10741200	1.73337000	-0.04454800
Si	2.03030600	-1.24406400	-0.11277200
C	3.84685500	-0.71362000	-0.00332600
H	4.50227200	-1.57239900	-0.19101300
H	4.09756200	0.05504700	-0.74167300
H	4.09821700	-0.31748000	0.98628600
C	1.74788200	-2.06205700	-1.79717400
H	2.43223700	-2.90324700	-1.95699500

H	0.72496400	-2.44010900	-1.89635700
H	1.90998800	-1.34287100	-2.60762000
C	1.77962400	-2.58025400	1.23866600
H	2.43330300	-3.44127800	1.05921900
H	2.04386400	-2.21240200	2.24273700
H	0.75520200	-2.97448300	1.27508600
C	2.33691200	2.48451700	1.19420000
H	2.41653400	3.56969400	1.05836000
H	2.01665300	2.31000900	2.22901500
H	3.34224100	2.06533900	1.08477800
C	1.71145300	2.14024400	-1.79806800
H	1.02123800	1.74670500	-2.55275500
H	1.78435300	3.22365100	-1.94947300
H	2.70039900	1.71568100	-2.00345000
C	-0.55161600	2.61557200	0.20836500
H	-0.43170600	3.69947400	0.09914200
H	-1.29511200	2.29224200	-0.52758900
H	-0.96752200	2.43122200	1.20569700
H	-2.27169500	-1.70093100	-2.17998900
H	-4.34357100	-0.23673700	-2.28474400
H	-1.93662300	0.01366800	-2.10122200
Li	0.17053400	-0.63860400	1.93580000

Cartesian coordinates for optimized **TS-1$_{H2}$** with **LHMDS**

C	3.31585700	-0.62189100	-1.55361600
C	4.25356200	-0.10035200	-0.45890600
C	3.45826700	0.59523800	0.65421500
C	1.63044400	-1.16274100	0.28664000
C	2.33187100	-1.65208200	-0.98061400
H	4.07648900	0.81550700	1.53099300
H	4.81538100	-0.94308000	-0.03386400
H	4.99577100	0.59088700	-0.87432300
H	2.76335300	0.22115200	-1.99016500
H	1.16207300	-1.96229200	0.86572400
H	0.40501700	-0.51196200	0.09425400
H	3.08575200	1.56839900	0.29962300
C	2.25334300	-0.19715900	1.13356400
O	1.73569600	0.14391200	2.24828400
N	-0.87000400	0.01437900	0.29362600
Si	-2.07573900	-1.23244600	0.05028200
Si	-1.01049700	1.66833400	-0.26313600
C	-0.30805400	2.79817200	1.10993500
H	-0.33073200	3.84731000	0.79393900
H	-0.91173000	2.74620100	2.02879300
H	0.73242000	2.57005500	1.37207300
C	-2.78343200	2.26883100	-0.57199400
H	-2.76292000	3.30741700	-0.92315800
H	-3.30070500	1.67777100	-1.33449900
H	-3.39051600	2.24313800	0.33874700
C	-0.00894000	1.97593300	-1.84080200
H	-0.07713400	3.02185000	-2.16141000
H	1.05052100	1.74105500	-1.69560500
H	-0.37342200	1.35045000	-2.66303900
C	-3.67323200	-0.87843500	1.01654000
H	-3.47296400	-0.75773500	2.08860400
H	-4.18170500	0.02679400	0.67227400
H	-4.37858700	-1.71145100	0.91127200
C	-2.52518200	-1.48335000	-1.77709100
H	-1.63519600	-1.72544600	-2.36897000
H	-3.23761700	-2.30760800	-1.89956800
H	-2.98027700	-0.59020300	-2.21881600
C	-1.42757500	-2.89604200	0.69810300
H	-2.22987900	-3.64212900	0.65917600
H	-0.59535000	-3.28263200	0.10156700
H	-1.09137800	-2.83951600	1.74067800
H	1.58773700	-1.91641400	-1.74349600
H	3.89303700	-1.07165600	-2.36982600
H	2.88404800	-2.58017700	-0.76899200

Li	-0.06376600	0.29440300	2.06349500

Cartesian coordinates for optimized **TS-1$_{H3}$** with **LHMDS**

C	-3.87585900	-0.51356900	1.33234100
C	-2.38516600	-0.81909200	1.53915400
C	-1.63074700	-1.03779000	0.22178900
C	-3.48553700	0.20404000	-1.06223300
C	-4.05046500	0.61182400	0.30651200
H	-0.39469300	-0.39139900	0.13467700
H	-1.93662000	0.01368300	2.10122100
H	-2.27168800	-1.70091600	2.18000400
H	-4.39178000	-1.41582700	0.97495600
H	-3.32985200	1.06958700	-1.71662100
H	-4.20387400	-0.43864400	-1.59145900
H	-1.17798800	-2.02868100	0.12259600
C	-2.20046400	-0.60436800	-1.01697100
O	-1.61902600	-0.82707900	-2.12928500
N	0.87975400	0.02230300	-0.22504500
Si	1.10739300	1.73337000	0.04454100
Si	2.03032300	-1.24405300	0.11277500
C	1.74791200	-2.06203400	1.79718500
H	2.43228000	-2.90321200	1.95701400
H	1.91000600	-1.34283700	2.60762400
H	0.72500000	-2.44010000	1.89637100
C	3.84686400	-0.71358600	0.00332200
H	4.50229300	-1.57235500	0.19100700
H	4.09821700	-0.31744200	-0.98629100
H	4.09756500	0.05508500	0.74166700
C	1.77965400	-2.58025500	-1.23865100
H	2.43334300	-3.44127000	-1.05919700
H	0.75523700	-2.97449400	-1.27506700
H	2.04388900	-2.21240800	-2.24272500
C	1.71144100	2.14025300	1.79805600
H	1.02121500	1.74674100	2.55274600
H	2.70037600	1.71566800	2.00344600
H	1.78436700	3.22366000	1.94944600
C	2.33687500	2.48452800	-1.19421900
H	2.01661100	2.31001100	-2.22903100
H	2.41648200	3.56970700	-1.05838400
H	3.34221100	2.06536500	-1.08480300
C	-0.55164600	2.61555300	-0.20836200
H	-0.43174500	3.69945700	-0.09915800
H	-0.96756500	2.43118100	-1.20568400
H	-1.29512800	2.29222700	0.52760900
H	-5.10587200	0.88809600	0.20135900
H	-4.34356600	-0.23672300	2.28474700
H	-3.53159500	1.50874100	0.66898300
Li	0.17053400	-0.63861600	-1.93580600

Cartesian coordinates for optimized **TS-1$_{H4}$** with **LHMDS**

C	-3.41538400	0.20542700	-1.50668700
C	-2.39980500	-0.94573600	-1.52965000
C	-1.63676900	-1.08808000	-0.21238100
C	-3.46127800	0.22752700	1.01902200
C	-4.30300600	0.11836100	-0.25994100
H	-1.14125000	-2.05779400	-0.10090400
H	-2.93806700	-1.87866200	-1.75576300
H	-1.69332600	-0.80155600	-2.35752400
H	-2.88954300	1.16987000	-1.51127100
H	-4.03685800	-0.02505500	1.91602800
H	-3.12246900	1.26366800	1.16194400
H	-0.42517700	-0.38811900	-0.13047000
C	-2.22137300	-0.64974000	1.01669300
O	-1.64790500	-0.85460900	2.13699500
N	0.85184500	0.02086400	0.23826700

Si	1.99081000	-1.24967900	-0.13172500
Si	1.10984600	1.73336000	0.00107200
C	-0.50161400	2.65972600	0.37644600
H	-0.34987100	3.74177700	0.29054600
H	-1.30098200	2.38450200	-0.31880100
H	-0.85983300	2.45988900	1.39328400
C	1.62510800	2.16667000	-1.77404800
H	1.72942700	3.25025400	-1.90406900
H	2.58416300	1.71195100	-2.04641600
H	0.87888800	1.81694200	-2.49627900
C	2.42364100	2.42641200	1.18642400
H	2.50521000	3.51481400	1.08055300
H	2.16469400	2.22132900	2.23267700
H	3.41617900	2.00371600	1.00314100
C	1.67734000	-2.04519500	-1.82174300
H	2.35967300	-2.88354200	-2.00381700
H	0.65359100	-2.42299900	-1.91051100
H	1.82713900	-1.31494800	-2.62475300
C	3.81301100	-0.73294000	-0.05385800
H	4.09159800	-0.35834100	0.93664800
H	4.45531600	-1.59408100	-0.27340800
H	4.05343400	0.04701200	-0.78378700
C	1.76127200	-2.59900400	1.20940300
H	0.73733800	-2.99231100	1.26137100
H	2.41046500	-3.45903400	1.00975000
H	2.04397500	-2.23964200	2.21131800
H	-5.06947800	0.90171200	-0.26861700
H	-4.02764900	0.18032300	-2.41561200
H	-4.83760600	-0.84121200	-0.26609600
Li	0.14177000	-0.65058500	1.94602500

Cartesian coordinates for optimized **TS-4$_{H2}$** with **LHMDS**

C	-2.46679300	0.38088900	-0.43893300
C	-2.74482800	-0.20366900	-1.83969700
C	-1.43575900	-0.57650400	-2.57790600
C	-1.64156500	-0.64668400	0.41677300
H	-1.63384600	-1.07655700	-3.52898900
H	-3.38072600	-1.09663200	-1.76970200
H	-3.29403400	0.51557300	-2.45259500
H	-1.74552200	1.19718000	-0.58193700
H	-0.86347400	0.33856800	-2.78034400
C	-0.59670500	-1.47248600	-1.70628100
O	-0.18651000	-2.57926100	-2.11397700
C	-3.69099100	1.07119100	0.25424600
C	-1.31531100	-0.04127800	1.81980400
H	-0.55239000	0.72675900	1.65046100
H	-0.83715300	-0.80127800	2.45010000
C	-2.53740100	0.56214500	2.52118200
H	-2.21222900	1.03379000	3.45526200
H	-3.24540900	-0.22287500	2.81694400
C	-3.23169200	1.60339500	1.63685900
H	-4.09801400	2.02602600	2.16061300
H	-2.53435800	2.43591100	1.47209500
C	-4.93646600	0.17121100	0.41124700
H	-5.78824900	0.77769700	0.73698100
H	-5.22115200	-0.30285900	-0.53341400
H	-4.81418900	-0.61738500	1.15857300
C	-4.11098700	2.29492000	-0.59264400
H	-4.84219700	2.89602400	-0.04177000
H	-3.25427300	2.93841500	-0.81905800
H	-4.57929700	2.00640700	-1.53859100
C	-2.34648200	-1.96896600	0.68385900
H	-3.34078700	-1.94529000	1.15441400
O	-1.85048900	-3.07552500	0.46361600
C	-0.34000600	-0.99290100	-0.32931100
Li	-0.12158200	-3.46134200	-0.45456600
H	0.49324000	-0.18319700	-0.32063900
H	0.20881000	-1.72463700	0.26386600

N	2.14338500	0.28986500	0.02639000
Si	2.44498600	1.90614800	-0.40003500
Si	3.17549900	-0.91810100	0.60059200
C	2.45128300	-2.71339100	0.32636400
H	3.23081300	-3.46420700	0.49868000
H	1.64404800	-2.93306900	1.04566900
H	2.10231600	-2.82722400	-0.70936900
C	3.50133400	-0.87720600	2.48115700
H	4.12355500	-1.71551700	2.81926500
H	4.01287000	0.05018900	2.76287700
H	2.56159100	-0.90808000	3.04621900
C	4.88416700	-1.01949900	-0.24190500
H	5.49098400	-1.84452800	0.15155100
H	4.78303500	-1.16131000	-1.32383400
H	5.45104800	-0.09388300	-0.08841600
C	3.37085300	2.92954100	0.92038400
H	2.83723300	2.91452400	1.87792400
H	4.37461300	2.52702700	1.10276300
H	3.48918800	3.97820000	0.61981000
C	3.42554300	2.12878100	-2.02358700
H	2.92036600	1.63028900	-2.85960000
H	3.54734700	3.18633500	-2.29004500
H	4.42683600	1.69026100	-1.94522700
C	0.79069500	2.82742200	-0.69168800
H	0.95864200	3.87433700	-0.97122400
H	0.21323900	2.36692700	-1.50420300
H	0.16445100	2.82723300	0.20942200

Cartesian coordinates for optimized **TS-4$_{H4}$** with **LHMDS**

C	1.87120600	-0.42072800	-0.29806200
C	1.21892800	-0.00541800	-1.63874200
C	0.02015700	0.97072100	-1.48169100
C	0.85230300	1.61515500	0.77383100
C	2.17887900	0.84328900	0.60150400
H	1.97073200	0.45490500	-2.29907200
H	0.86343800	-0.90380200	-2.15735300
H	1.07508700	-0.92006800	0.27140700
H	0.96968000	2.46933100	1.44578100
H	0.10745400	0.94208300	1.21613700
C	0.30578600	2.04737600	-0.56768700
O	0.10891600	3.26822200	-0.80493600
C	3.00589100	-1.50507000	-0.40861100
C	2.72116400	0.36539700	1.98369500
H	1.87412900	-0.10663400	2.49261700
H	3.00677700	1.22718500	2.59332900
C	3.87145400	-0.64170900	1.88138800
H	4.13756600	-0.98014200	2.88834600
H	4.77607200	-0.16605100	1.48368100
C	3.48346600	-1.85297100	1.02557800
H	4.32562400	-2.55304000	0.95835600
H	2.67295800	-2.39315300	1.53312200
C	4.20877100	-1.10538400	-1.29563400
H	4.82698300	-1.98876700	-1.48647300
H	3.88702100	-0.71982000	-2.26959800
H	4.86578900	-0.36129600	-0.83713700
C	2.40260000	-2.79349500	-1.01837300
H	3.12158300	-3.61498700	-0.92953000
H	1.48311600	-3.09068300	-0.50257800
H	2.17174000	-2.67511700	-2.08295800
C	3.22391700	1.76536500	0.03465400
H	4.22481600	1.35406000	-0.14832100
O	3.06713100	2.96914400	-0.18368900
Li	1.60139300	4.14179200	-0.33477700
H	-0.32367500	1.33517100	-2.45353700
H	-0.89888800	0.38110900	-0.93997400
N	-2.15112400	-0.25648900	-0.01430600
Si	-3.27470100	1.01018300	0.19702800
Si	-2.24590200	-1.95473000	0.03417900

C	-1.66183800	-2.76096200	-1.60302400
H	-1.88286800	-3.83668100	-1.61823300
H	-2.17543100	-2.30273600	-2.45685700
H	-0.58300000	-2.65170900	-1.77527700
C	-3.96548900	-2.72841300	0.33961300
H	-3.87354800	-3.81720200	0.44509200
H	-4.43755800	-2.34643500	1.25024400
H	-4.65208600	-2.53446500	-0.49232200
C	-1.15078400	-2.70631600	1.41863500
H	-1.09329300	-3.79974700	1.35243100
H	-0.12201700	-2.32160300	1.39940400
H	-1.56371700	-2.45562400	2.40305800
C	-5.06162700	0.50515700	0.63604200
H	-5.51147400	-0.12368400	-0.14052900
H	-5.11528000	-0.04872400	1.57861200
H	-5.68715700	1.40018500	0.74239400
C	-2.75434300	2.21081800	1.59700500
H	-2.59325400	1.67060100	2.53654800
H	-1.83089700	2.74829300	1.35750200
H	-3.52640400	2.96901400	1.77893400
C	-3.42952900	2.10542700	-1.36251400
H	-4.19998500	2.87511100	-1.22808700
H	-2.49341300	2.62432000	-1.60083100
H	-3.70835400	1.50615000	-2.23738400

Cartesian coordinates for optimized **TS-5$_{H2}$** with **LHMDS**

C	2.56840900	0.48712100	0.44358900
C	2.70659400	-0.01276000	1.89608700
C	1.33196400	-0.26778200	2.57135100
C	1.68188900	-0.47499100	-0.40816700
H	1.45367000	-0.69201900	3.57042500
H	3.29039000	-0.94043400	1.92937000
H	3.25222500	0.72152100	2.49363900
H	1.96525600	1.40585800	0.47925400
H	0.77964500	0.67661000	2.64719000
C	0.56505000	-1.21911400	1.70062100
O	0.26218600	-2.36596000	2.08231600
C	3.91668200	0.88782900	-0.24659000
C	1.45108000	0.08568100	-1.83016100
H	0.83281200	0.98256700	-1.71405200
H	0.85971100	-0.62477100	-2.41738900
C	2.76897700	0.42862800	-2.52817000
H	2.55617100	0.87987600	-3.50340900
H	3.33364200	-0.48971400	-2.73515700
C	3.60350600	1.39497100	-1.67996200
H	4.54871900	1.62204300	-2.18755400
H	3.05990300	2.34650000	-1.60020300
C	4.93363100	-0.27193600	-0.30262200
H	5.85445400	0.06959800	-0.78736200
H	5.20560900	-0.62193200	0.69771200
H	4.57566100	-1.13670600	-0.86817600
C	4.56129100	2.05706700	0.52771200
H	5.42102200	2.44522700	-0.02860100
H	3.85519400	2.88343500	0.66559700
H	4.92612100	1.75308900	1.51327900
C	0.32123600	-0.76861700	0.30680500
Li	0.21366200	-3.42622900	0.52041300
H	-0.51441800	0.02441100	0.24530900
H	-0.18747100	-1.54093700	-0.27049800
N	-2.25083500	0.25903200	-0.03202800
Si	-2.62721100	1.88368500	0.28716400
Si	-3.19010600	-1.04297300	-0.54847600
C	-2.30415800	-2.76848100	-0.25813900
H	-3.01555400	-3.58633100	-0.41801000
H	-1.48364300	-2.92138800	-0.98047400
H	-1.94800900	-2.82903800	0.77956100
C	-3.57779900	-1.08423100	-2.41634900
H	-4.13683200	-1.98111600	-2.71158500

H	-4.17547700	-0.21156500	-2.70313600
H	-2.65778200	-1.05064200	-3.01261900
C	-4.85103400	-1.27822000	0.35872600
H	-5.39401000	-2.16536600	0.00974400
H	-4.69995600	-1.37743200	1.43959000
H	-5.50392100	-0.41167100	0.20238100
C	-3.56588900	2.78530400	-1.10956600
H	-3.01483000	2.72878000	-2.05557200
H	-4.55090500	2.33462700	-1.28122300
H	-3.72746500	3.84590200	-0.87934000
C	-3.64579400	2.16197300	1.87752100
H	-3.13469100	1.74031500	2.75125900
H	-3.81982000	3.22737900	2.07439900
H	-4.62489600	1.67391000	1.81102200
C	-1.01242300	2.88261300	0.54592900
H	-1.22299700	3.93733700	0.75901200
H	-0.42911100	2.49506500	1.39188500
H	-0.37187100	2.85295100	-0.34483500
C	2.17327500	-1.87911400	-0.48647100
N	2.22062200	-3.04548600	-0.43878500

Cartesian coordinates for optimized **TS-5$_{H4}$** with **LHMDS**

C	1.83857000	-0.44312800	-0.25794700
C	1.21813300	0.02427200	-1.59151600
C	0.09588000	1.09693900	-1.46184600
C	0.82381300	1.59965100	0.85461100
C	2.14009200	0.75768100	0.70655600
H	2.00381700	0.42571700	-2.24536800
H	0.79913900	-0.84241900	-2.10658300
H	1.04894700	-0.98005400	0.28167000
H	0.95945100	2.41569700	1.56986600
H	0.02352200	0.92608800	1.18911100
C	0.47151400	2.12740900	-0.52039600
O	0.58991300	3.35792700	-0.77216900
C	3.02815100	-1.45568400	-0.39780100
C	2.64711400	0.26224800	2.08205600
H	1.80208800	-0.25491600	2.55173400
H	2.89156200	1.11908400	2.72000500
C	3.83380400	-0.69562000	1.94884900
H	4.10850000	-1.06936600	2.94142600
H	4.71214000	-0.15338200	1.57526300
C	3.48974500	-1.86989400	1.02537900
H	4.35306000	-2.54019200	0.93633000
H	2.68892000	-2.45867800	1.49300200
C	4.22637100	-0.89667400	-1.19556200
H	5.00182000	-1.66616000	-1.27478500
H	3.94222300	-0.61906700	-2.21459900
H	4.69208200	-0.02235500	-0.73259000
C	2.53303000	-2.72982400	-1.11354200
H	3.31317300	-3.49846900	-1.08876700
H	1.64170100	-3.14146700	-0.62994800
H	2.29171400	-2.54463000	-2.16393700
Li	2.24090600	4.04236600	-0.87101900
H	-0.15327200	1.51553200	-2.44053200
H	-0.87245700	0.55624500	-0.97100800
N	-2.09895100	-0.14182700	-0.13329900
Si	-3.32138900	1.00228100	0.21390200
Si	-2.23158400	-1.84291700	-0.07004000
C	-1.56278300	-2.69119200	-1.64665900
H	-1.70908600	-3.77763900	-1.60226700
H	-2.09101000	-2.32274000	-2.53358100
H	-0.49329700	-2.51776600	-1.80849100
C	-4.00080400	-2.53971800	0.11715500
H	-3.97411800	-3.63317800	0.20386000
H	-4.51042800	-2.15422800	1.00690500
H	-4.62243700	-2.29444200	-0.75075600
C	-1.26439700	-2.61188900	1.39548300
H	-1.33839000	-3.70670600	1.40190800

H	-0.19604500	-2.36048500	1.38163200
H	-1.66590400	-2.24817400	2.34878200
C	-4.84989200	0.92534500	-0.92802300
H	-4.55435000	1.01739800	-1.97986800
H	-5.38983700	-0.02142700	-0.82279400
H	-5.55792800	1.73481000	-0.70946300
C	-3.98159700	0.91413800	2.00578600
H	-4.45448700	-0.05098000	2.21906200
H	-3.16865600	1.04397300	2.73038600
H	-4.72759200	1.69516100	2.20011100
C	-2.68742400	2.79775400	0.02915600
H	-3.51922100	3.48877000	0.21314400
H	-1.90141200	3.05358000	0.74943300
H	-2.30528300	3.01534400	-0.97415300
C	3.07942800	1.74853200	0.13899800
N	3.63587300	2.67437400	-0.29987500

Cartesian coordinates for optimized **TS-6$_{H2}$** with **LHMDS**

C	2.42590100	0.52874400	0.48007700
C	2.76463300	-0.04682000	1.87119700
C	1.48671500	-0.43368900	2.66610100
C	1.56543200	-0.48796600	-0.32896600
H	1.72806200	-0.95586300	3.59473100
H	3.41444100	-0.92376900	1.77621000
H	3.32210200	0.68837700	2.45608400
H	1.67069000	1.30914700	0.65180800
H	0.92929500	0.47964100	2.91402300
C	0.59908500	-1.30083900	1.81663200
O	0.21550100	-2.42249300	2.18034500
C	3.58144300	1.31314100	-0.24304400
C	1.27070900	-0.02626400	-1.77118100
H	0.48946700	0.73777300	-1.68475500
H	0.82294200	-0.85273500	-2.33373900
C	2.50411000	0.54487200	-2.47509400
H	2.20822900	0.89986700	-3.46827500
H	3.24982800	-0.24170200	-2.63877700
C	3.10258100	1.70149000	-1.66748400
H	3.94636300	2.14393500	-2.20988200
H	2.34312500	2.49113100	-1.58304200
C	4.94074000	0.58666300	-0.31652700
H	4.94131000	-0.25122700	-1.01107100
H	5.70649400	1.29779100	-0.64465400
H	5.25183700	0.20647100	0.66172200
C	3.80726700	2.62834900	0.54123800
H	4.50131000	3.27280000	-0.00797400
H	2.87389900	3.18524200	0.67779100
H	4.24673300	2.45234500	1.52824700
C	0.28138200	-0.77733800	0.44942100
Li	-0.15828800	-3.28513300	0.51548600
H	-0.41059200	0.09503100	0.49195600
H	-0.35516600	-1.44380700	-0.12229600
N	-2.38573900	0.28766200	-0.04010100
Si	-2.68870300	1.91626500	0.29940000
Si	-3.34585700	-0.99378300	-0.53688800
C	-2.46123400	-2.72179700	-0.22697100
H	-3.15101500	-3.55324300	-0.40671800
H	-1.62238900	-2.84921500	-0.93316000
H	-2.14579100	-2.77018600	0.82611700
C	-3.73379000	-1.06969800	-2.40426300
H	-4.30045200	-1.96715600	-2.68283600
H	-4.32561700	-0.19787900	-2.70576200
H	-2.81464400	-1.05288100	-3.00247400
C	-5.00782400	-1.22591100	0.37076200
H	-4.85916000	-1.30748300	1.45352300
H	-5.66293300	-0.36370500	0.20012600
H	-5.54768000	-2.11994800	0.03446600
C	-1.04098500	2.82484300	0.68621500
H	-1.20823200	3.88475000	0.91182400

H	-0.53595100	2.38882000	1.55930400
H	-0.34704000	2.78129200	-0.16382900
C	-3.47951900	2.90913900	-1.12815700
H	-3.59298200	3.97213700	-0.88064200
H	-2.87473300	2.84075400	-2.04005400
H	-4.47601400	2.52135700	-1.37200800
C	-3.78644900	2.22999600	1.83067200
H	-4.78792000	1.80645500	1.69224400
H	-3.35968300	1.76044300	2.72506100
H	-3.90633700	3.30038600	2.04067200
N	2.25518100	-1.89871800	-0.48939900
O	3.45208100	-1.96830700	-0.67294800
O	1.53112000	-2.92277400	-0.47275400

Cartesian coordinates for optimized **TS-6$_{H4}$** with **LHMDS**

C	-1.65192000	0.55114500	-0.33324200
C	-1.05667100	0.04774700	-1.66266800
C	0.02228600	-1.05349400	-1.49808200
C	-0.79009800	-1.56031600	0.79698700
C	-1.98474100	-0.57331300	0.69712800
H	-1.85074500	-0.32534200	-2.32033100
H	-0.59908200	0.89686700	-2.17374400
H	-0.81690200	1.04453200	0.18065800
H	-1.01182900	-2.38171300	1.48468500
H	0.06409000	-0.97971400	1.17575900
C	-0.39861400	-2.07935300	-0.56843700
O	-0.45985000	-3.31591900	-0.81346700
C	-2.76453700	1.65070200	-0.45969600
C	-2.34052800	0.02501300	2.06420700
H	-1.40817500	0.46097700	2.44092700
H	-2.62382200	-0.76925300	2.76011200
C	-3.41956200	1.11396500	1.99396400
H	-3.52262900	1.57071800	2.98441900
H	-4.38924200	0.66096200	1.76615200
C	-3.06780900	2.19289700	0.96277600
H	-3.88336800	2.92346700	0.89823800
H	-2.18629700	2.74569300	1.31435300
C	-4.06260900	1.14911500	-1.12962200
H	-4.73901400	1.99578400	-1.28773000
H	-3.86843200	0.70211400	-2.10891200
H	-4.61106600	0.41895600	-0.52955100
C	-2.22572400	2.82904200	-1.29812000
H	-2.92678800	3.66907700	-1.24714100
H	-1.25761200	3.17913400	-0.92689000
H	-2.10955100	2.56603600	-2.35342900
Li	-2.12608900	-3.57909600	-1.41358000
H	0.30776100	-1.47861000	-2.46457800
H	0.99472900	-0.54928800	-0.97340600
N	2.22531000	0.09381900	-0.09201900
Si	3.41363200	-1.08974600	0.26407700
Si	2.44064100	1.79148100	-0.07376000
C	1.89570500	2.61631200	-1.70848300
H	2.05849800	3.70076700	-1.67605200
H	2.47863200	2.22019200	-2.54793300
H	0.83813200	2.45560200	-1.94367900
C	4.22726600	2.41505700	0.18452600
H	4.23989000	3.51048000	0.24520400
H	4.67719700	2.03226000	1.10676000
H	4.87959800	2.12578500	-0.64621400
C	1.44226100	2.64201200	1.32238700
H	1.57265800	3.73128500	1.30592000
H	0.36462800	2.44552700	1.26232100
H	1.78003000	2.28349400	2.30191100
C	4.95292100	-1.05782700	-0.86498100
H	4.66377300	-1.13386300	-1.91987400
H	5.52810200	-0.13349000	-0.74961700
H	5.62725000	-1.89500800	-0.64476200
C	4.05385500	-1.00625400	2.06270300

H	4.55189900	-0.05436800	2.27671100
H	3.22853100	-1.10970900	2.77718100
H	4.77413300	-1.80802700	2.26852100
C	2.73302000	-2.86497100	0.08083700
H	3.54453300	-3.57552800	0.28021000
H	1.93074000	-3.09609800	0.79064800
H	2.35807100	-3.07923500	-0.92551800
N	-3.16322900	-1.48763600	0.24945000
O	-4.08658700	-1.71698500	1.00370400
O	-3.08624500	-2.03279700	-0.88525600

Cartesian coordinates for optimized **TS-4$_{H2}$** with **KHMDS**

C	2.33570600	-0.69715800	-0.39380500
C	2.72070000	-0.05360900	-1.73808000
C	1.47974100	0.45964100	-2.48898800
C	1.60149300	0.36552500	0.50038300
H	1.75038500	1.03315600	-3.37808500
H	3.41816200	0.77826600	-1.58046700
H	3.24336400	-0.77266700	-2.37249500
H	1.53772700	-1.41534500	-0.61049100
H	0.88095300	-0.39510200	-2.82876600
C	0.57674800	1.31804600	-1.62317400
O	0.01101900	2.30917300	-2.12627200
C	3.45303900	-1.56583000	0.27833200
C	1.18084200	-0.28428900	1.85532600
H	0.34329600	-0.95049100	1.62830800
H	0.77638400	0.48444800	2.52435800
C	2.30524200	-1.06328600	2.54689300
H	1.90082400	-1.55159100	3.43935500
H	3.08839500	-0.38790400	2.91000200
C	2.90386700	-2.12161300	1.61639400
H	3.70361000	-2.66777300	2.12953200
H	2.12490100	-2.85923100	1.38789200
C	4.79321700	-0.83484600	0.50847400
H	5.55764600	-1.55792000	0.80901000
H	5.15044700	-0.34657900	-0.40216100
H	4.74878100	-0.08096800	1.29619600
C	3.74669100	-2.77882700	-0.63413500
H	4.39316000	-3.49023400	-0.11120900
H	2.82732100	-3.30292000	-0.90948700
H	4.26179900	-2.49048600	-1.55378800
C	2.48383700	1.55173600	0.86567800
H	3.39344600	1.33884100	1.45012800
O	2.23118900	2.72103800	0.61774600
C	0.36522200	0.89234000	-0.24717000
H	-0.64028300	0.10403300	-0.22163800
H	-0.10657300	1.67890800	0.34070400
N	-1.98700400	-0.52102900	0.02394300
Si	-2.33133500	-2.01855300	-0.72944900
Si	-3.07176900	0.45830300	0.90144900
C	-2.60168000	2.32681500	0.80886600
H	-3.43022900	2.93738100	1.18297100
H	-1.72557000	2.55274400	1.42959300
H	-2.40811600	2.60863900	-0.23232600
C	-3.12450500	0.07612700	2.76692200
H	-3.79020400	0.75575300	3.31169800
H	-3.47620000	-0.94562400	2.94236100
H	-2.12654600	0.15505300	3.21191700
C	-4.87636400	0.42027300	0.29330600
H	-5.50930500	1.07389600	0.90447900
H	-4.95098100	0.75655000	-0.74568500
H	-5.30326300	-0.58595600	0.34356700
C	-3.34726600	-1.85984600	-2.33278700
H	-4.33658200	-1.43470600	-2.13799500
H	-2.84376500	-1.19923500	-3.04674900
H	-3.49366200	-2.83110800	-2.81943900
C	-0.73614300	-2.92904800	-1.23496800
H	-0.09700100	-3.13575200	-0.37064400

H	-0.98414900	-3.89092700	-1.69675900
H	-0.15088200	-2.36183200	-1.96551300
C	-3.26847200	-3.24808000	0.38712800
H	-3.43845000	-4.20178800	-0.12561200
H	-2.70167300	-3.45668300	1.30071600
H	-4.24728200	-2.86268000	0.69035400
K	0.12228700	4.12223300	-0.37046300

Cartesian coordinates for optimized **TS-4$_{H4}$** with **KHMDS**

C	-1.32111500	-1.18037100	0.22389900
C	-0.97114900	-0.33457500	1.45784400
C	-0.29772400	1.00161700	1.07729200
C	-1.50412600	0.92992100	-1.15162200
C	-2.26505000	-0.35686800	-0.74606100
H	-1.86500700	-0.15334400	2.06833900
H	-0.27396700	-0.88648500	2.08858700
H	-0.39369400	-1.26724200	-0.35609000
H	-2.11250700	1.56644700	-1.79958100
H	-0.61947800	0.62999100	-1.72190200
C	-1.01260900	1.74143800	0.03065700
O	-1.19880300	2.96699500	0.05865300
C	-1.74716900	-2.65505900	0.52396600
C	-2.60234200	-1.19675100	-2.00947800
H	-1.68699400	-1.25661200	-2.60685900
H	-3.33546000	-0.66419000	-2.62765400
C	-3.08286100	-2.61788900	-1.69580000
H	-3.22013000	-3.16037700	-2.63650200
H	-4.06914000	-2.60328900	-1.21827900
C	-2.07331300	-3.35991900	-0.81664300
H	-2.43187100	-4.37366900	-0.60723000
H	-1.13959900	-3.47308100	-1.38059600
C	-2.93298500	-2.78340400	1.50268400
H	-3.10454300	-3.83855900	1.73603300
H	-2.73120500	-2.27213700	2.44706700
H	-3.87252500	-2.39203900	1.10585900
C	-0.54553800	-3.39833100	1.14958700
H	-0.76194100	-4.46936800	1.20936500
H	0.35930900	-3.26924400	0.55055100
H	-0.32785700	-3.05341400	2.16248800
C	-3.56973800	0.02671600	-0.08917800
H	-4.35063000	-0.75014700	-0.05288100
O	-3.83850800	1.12972600	0.36500200
H	-0.13538000	1.64172300	1.94706600
H	0.74980400	0.73516700	0.66900200
N	2.42643600	0.30868400	0.01549600
Si	3.41959500	-0.10530500	1.32088100
Si	2.72182500	0.50388100	-1.63434800
C	1.88213200	-0.84307000	-2.71497900
H	2.04259700	-0.66988100	-3.78577600
H	2.29064700	-1.82989200	-2.47109500
H	0.79950000	-0.89664200	-2.55097900
C	4.55030400	0.45286300	-2.18671700
H	4.63221400	0.55252800	-3.27556600
H	5.12711500	1.26556700	-1.73481800
H	5.03156100	-0.48962400	-1.90483000
C	2.07242600	2.17370700	-2.30675800
H	2.22272800	2.25953200	-3.38961600
H	1.00774400	2.33371500	-2.10752600
H	2.60980600	2.99958500	-1.82841800
C	3.89145300	-1.95805100	1.39693600
H	2.99533800	-2.58803900	1.42776000
H	4.46446100	-2.25214400	0.51064600
H	4.49880900	-2.19682000	2.27827100
C	5.07495000	0.84301700	1.43149800
H	5.72907100	0.61676600	0.58423400
H	4.90350500	1.92498800	1.43493000
H	5.62042200	0.58739000	2.34782600
C	2.56668800	0.25093500	2.99672700

H	3.24203700	0.01691400	3.82738500
H	2.28995600	1.30723900	3.08364600
H	1.65998100	-0.34671200	3.13994200
K	-3.43076500	3.67290700	0.83604700

Cartesian coordinates for optimized **TS-5$_{H2}$** with **KHMDS**

C	-2.29270400	-0.76656200	0.48359200
C	-2.57433300	-0.12130600	1.85426100
C	-1.29657700	0.45209200	2.50583200
C	-1.60299200	0.25881700	-0.47145500
H	-1.52272600	0.98921200	3.43070100
H	-3.31325900	0.68275200	1.74735700
H	-3.01321100	-0.85710800	2.53319100
H	-1.51053900	-1.52268200	0.63879500
H	-0.61000100	-0.37038800	2.74805500
C	-0.57380900	1.38314600	1.55951400
O	-0.20610400	2.51353300	1.91902700
C	-3.50234000	-1.53657800	-0.14716100
C	-1.24655600	-0.38975500	-1.83159400
H	-0.44264500	-1.10666200	-1.63613200
H	-0.82482900	0.36974600	-2.49988700
C	-2.44952600	-1.08369600	-2.47363000
H	-2.13243200	-1.57889900	-3.39820900
H	-3.20102200	-0.33944100	-2.76831700
C	-3.06003800	-2.11451000	-1.51783100
H	-3.92153200	-2.60357400	-1.98906500
H	-2.31702100	-2.90382400	-1.33859300
C	-4.76006300	-0.65832500	-0.32015200
H	-5.57038900	-1.25753800	-0.74971100
H	-5.11694200	-0.27139500	0.63929400
H	-4.60334800	0.19701400	-0.98198600
C	-3.87317500	-2.73065800	0.75841000
H	-4.61794000	-3.36118200	0.26078500
H	-2.99954400	-3.35574800	0.97365700
H	-4.30548400	-2.41184200	1.71157700
C	-0.32894500	0.85642100	0.19787500
H	0.60361300	0.11352100	0.21137600
H	0.07488100	1.63240700	-0.45446500
N	2.14335000	-0.49053500	0.00386900
Si	2.32202200	-2.13857800	0.38590600
Si	3.28551900	0.64837400	-0.51409000
C	2.51474400	2.42016600	-0.68149400
H	3.30436100	3.14416000	-0.91473500
H	1.77498700	2.46088600	-1.49435900
H	2.04861800	2.71144100	0.26868100
C	4.04355800	0.31897200	-2.23585200
H	4.60470800	-0.62292800	-2.24210700
H	3.26131000	0.23181300	-2.99942600
H	4.73292800	1.11352000	-2.54884400
C	4.75224700	0.94376800	0.67135500
H	5.41608400	1.73977100	0.31034200
H	4.39585400	1.22974800	1.66809300
H	5.35770000	0.03916700	0.79074700
C	4.10597300	-2.71495700	0.74897400
H	4.77181000	-2.53842500	-0.10396700
H	4.52927000	-2.18727800	1.61079900
H	4.13672600	-3.78912000	0.97020000
C	1.31790500	-2.60405700	1.94724900
H	0.24042800	-2.44889600	1.80721000
H	1.45535800	-3.65828400	2.21736500
H	1.63060300	-1.99810300	2.80601500
C	1.68417500	-3.30889100	-0.98675800
H	2.22316600	-3.13911300	-1.92605400
H	1.81085000	-4.36493500	-0.71673000
H	0.61763800	-3.15326200	-1.19415600
C	-2.40889200	1.48376800	-0.71389700
N	-2.82474600	2.56306000	-0.86726800
K	-0.51299600	4.15290800	-0.05183000

Cartesian coordinates for optimized **TS-5$_{H4}$** with **KHMDS**

C	1.68680800	-1.01132300	-0.34308300
C	1.07562600	-0.17009800	-1.48273200
C	0.07142800	0.91798400	-1.02867700
C	0.92551400	0.75376100	1.32069400
C	2.14678300	-0.10427200	0.85359200
H	1.88324400	0.30766200	-2.05377500
H	0.56079600	-0.83840200	-2.17796000
H	0.86785900	-1.59443000	0.09681400
H	1.18505800	1.36171200	2.19200100
H	0.10459600	0.07572600	1.58271400
C	0.47720700	1.64136200	0.17547500
O	0.46894400	2.87987300	0.31377000
C	2.75567100	-2.06576100	-0.80061200
C	2.69654200	-0.95191000	2.02701900
H	1.84122000	-1.50089100	2.43905500
H	3.06229400	-0.29065000	2.82094500
C	3.77561300	-1.93993500	1.57942600
H	4.08047300	-2.55457400	2.43387900
H	4.67353400	-1.39539500	1.26010500
C	3.25653000	-2.83639100	0.44987500
H	4.03754500	-3.54202500	0.14157600
H	2.42818900	-3.44381400	0.83957400
C	3.95807700	-1.45120900	-1.55082400
H	4.64530100	-2.24989700	-1.85077500
H	3.64494900	-0.93593400	-2.46353900
H	4.53125800	-0.74050000	-0.95062800
C	2.08819700	-3.09209200	-1.74020700
H	2.78587400	-3.90863400	-1.95698800
H	1.19158200	-3.52816600	-1.28887000
H	1.79969600	-2.64782800	-2.69702200
H	-0.15236500	1.61162300	-1.84356300
H	-0.95330500	0.41707000	-0.71267500
N	-2.47746100	-0.16330500	-0.13517500
Si	-3.58227400	1.12735100	-0.10823300
Si	-2.66128800	-1.81814000	0.17235700
C	-2.03880000	-2.89491300	-1.28140000
H	-2.05893500	-3.96671300	-1.04570600
H	-2.66549800	-2.73781900	-2.16711400
H	-1.01239200	-2.63765200	-1.56882800
C	-4.43627400	-2.43675000	0.51952800
H	-4.44062600	-3.51033300	0.74713800
H	-4.88670700	-1.91833000	1.37409600
H	-5.09229000	-2.27896900	-0.34311200
C	-1.66758900	-2.41356300	1.70645900
H	-1.79996400	-3.48820800	1.88546100
H	-0.58783800	-2.23703700	1.61155000
H	-2.00248200	-1.88487500	2.60715300
C	-5.28351300	0.78851300	-0.91306300
H	-5.16559500	0.43491200	-1.94422700
H	-5.85228600	0.02724900	-0.36900500
H	-5.89612200	1.69888600	-0.94224400
C	-3.96902200	1.77995800	1.64954400
H	-4.43601400	1.00102100	2.26435400
H	-3.05132100	2.09079800	2.16436300
H	-4.64989400	2.64087600	1.63451300
C	-2.91292100	2.64734000	-1.06257400
H	-3.65710900	3.45370800	-1.05331000
H	-1.98972400	3.04541900	-0.62736400
H	-2.71148800	2.39885300	-2.11192200
C	3.14925300	0.90426300	0.44346800
N	3.82525900	1.80845300	0.15804700
K	2.49639200	4.21009600	-0.24348000

Cartesian coordinates for optimized **TS-6$_{H2}$** with **KHMDS**

C	2.14187000	-0.95291700	-0.40882100

C	2.44522600	-0.56087600	-1.87214900
C	1.22881200	0.08656700	-2.57580400
C	1.53456900	0.22501400	0.39760600
H	1.50363500	0.51050000	-3.54533500
H	3.29462100	0.12415700	-1.91554100
H	2.73031400	-1.45367900	-2.43474900
H	1.26579500	-1.61363000	-0.45697200
H	0.46050300	-0.67991400	-2.75240100
C	0.57377000	1.15865400	-1.73262200
O	0.24617800	2.25725100	-2.21154900
C	3.22755300	-1.84520400	0.29908100
C	1.20203500	-0.15637000	1.84718600
H	0.31304000	-0.79527200	1.79261000
H	0.90645800	0.74323400	2.39489400
C	2.35060800	-0.89133600	2.54240400
H	2.03631500	-1.17872600	3.55196400
H	3.20989000	-0.21981200	2.67144100
C	2.75608100	-2.13752000	1.74875200
H	3.55189500	-2.68016400	2.27362500
H	1.89310200	-2.81661400	1.70991200
C	4.65508600	-1.26048700	0.32356500
H	4.74892000	-0.38119800	0.96157200
H	5.34694900	-2.02277400	0.69961300
H	4.99336200	-0.97388500	-0.67616400
C	3.29627900	-3.20012000	-0.44327500
H	3.90875700	-3.90632800	0.12767500
H	2.30254200	-3.64395500	-0.56693900
H	3.75303400	-3.10638800	-1.43330700
C	0.31199300	0.79429000	-0.32473500
H	-0.65274700	0.07062500	-0.25391100
H	-0.06961100	1.63509300	0.24722300
N	-2.15067000	-0.47810900	0.05754400
Si	-2.57544900	-2.03542200	-0.50278400
Si	-3.20113600	0.66824700	0.74302500
C	-2.52398800	2.47478900	0.54305400
H	-3.31098100	3.20015900	0.77963900
H	-1.68945300	2.65201300	1.23691600
H	-2.20346500	2.63204800	-0.49495600
C	-3.45771300	0.48965000	2.62481600
H	-4.09102300	1.28455800	3.03890100
H	-3.93253700	-0.46913700	2.86145300
H	-2.49852500	0.51284000	3.15629100
C	-4.94121700	0.76648000	-0.03446100
H	-4.88278700	1.00414400	-1.10287700
H	-5.47800300	-0.18438000	0.05704700
H	-5.55627600	1.53635100	0.44825700
C	-1.03004000	-3.13103400	-0.75451800
H	-1.31994700	-4.14333700	-1.06074300
H	-0.36974300	-2.73832500	-1.53749500
H	-0.44603100	-3.22380900	0.16904200
C	-3.69215900	-3.02372000	0.69057000
H	-3.90954400	-4.02675100	0.30277300
H	-3.21287300	-3.14176500	1.66938400
H	-4.65353300	-2.52390900	0.85733500
C	-3.46056600	-2.03981700	-2.19460900
H	-4.41676300	-1.50706800	-2.14544400
H	-2.85125000	-1.53957300	-2.95721900
H	-3.66620300	-3.05791300	-2.54855200
N	2.50101200	1.48834900	0.48508100
O	3.61366900	1.46861800	-0.01579400
O	2.03168500	2.51548900	1.01482400
K	0.24055300	4.07811800	-0.34962000

Cartesian coordinates for optimized **TS-6$_{H4}$** with **KHMDS**

C	1.58636300	-0.93016300	-0.41782700
C	1.00702700	-0.01208900	-1.51348200
C	-0.03664900	1.00243700	-1.00102000
C	0.74960300	0.68845400	1.36395300

C	1.93797700	-0.19695100	0.91407800
H	1.81845100	0.51846500	-2.02413300
H	0.52359400	-0.64293500	-2.26389200
H	0.74627500	-1.55800300	-0.09180400
H	0.98996500	1.23716000	2.27919400
H	-0.10271400	0.02414700	1.56181900
C	0.30758600	1.64432800	0.27694000
O	0.18876300	2.85684400	0.52230600
C	2.68374900	-1.94173300	-0.90475400
C	2.33661500	-1.19244000	2.01103400
H	1.41486200	-1.72614700	2.27003000
H	2.65217700	-0.65069600	2.90664900
C	3.40118800	-2.20516500	1.57125900
H	3.52995700	-2.94882700	2.36558200
H	4.36795000	-1.70369100	1.46363600
C	3.00394700	-2.90638200	0.26735300
H	3.80079900	-3.59293900	-0.04424000
H	2.11703900	-3.52717900	0.45350000
C	3.97952700	-1.26469700	-1.40396300
H	4.65027600	-2.02654200	-1.81557100
H	3.77923900	-0.54418900	-2.20254500
H	4.53405200	-0.74874900	-0.61661400
C	2.11840200	-2.78983100	-2.06357000
H	2.80879600	-3.60846000	-2.29440800
H	1.15035300	-3.23133300	-1.80638100
H	1.98979000	-2.20492400	-2.97893500
H	-0.28213200	1.74874200	-1.76398000
H	-1.03456700	0.45575600	-0.74099300
N	-2.57074700	-0.21893800	-0.09465300
Si	-3.66086200	1.06960500	0.08614800
Si	-2.73361700	-1.90067300	-0.01756500
C	-2.10845000	-2.75802100	-1.61111400
H	-2.11365600	-3.85215200	-1.52506000
H	-2.74149500	-2.48912600	-2.46487600
H	-1.08643800	-2.45032700	-1.86427200
C	-4.49177400	-2.59681000	0.25855400
H	-4.47462000	-3.69302600	0.30807000
H	-4.92814300	-2.23293000	1.19608200
H	-5.17142400	-2.31201100	-0.55144100
C	-1.70957700	-2.68549800	1.40725800
H	-1.82869800	-3.77579800	1.44334100
H	-0.63372000	-2.48562000	1.31537800
H	-2.03084000	-2.28521600	2.37643700
C	-5.46114600	0.74172500	-0.46701800
H	-5.49802800	0.40166200	-1.50871500
H	-5.94797600	-0.02491500	0.14449000
H	-6.06597200	1.65474800	-0.39468300
C	-3.78514200	1.71646700	1.88311600
H	-4.15320900	0.93352800	2.55698200
H	-2.80245900	2.03102500	2.25633900
H	-4.46300000	2.57526000	1.97146800
C	-3.12942100	2.59759600	-0.94491700
H	-3.88629500	3.38842400	-0.86825500
H	-2.17873000	3.01816400	-0.59842800
H	-3.02444900	2.34187900	-2.00660800
N	3.09778500	0.82843800	0.73047100
O	4.04787900	0.82149500	1.49481900
O	2.97273300	1.67958000	-0.17190700
K	1.96813100	4.05392300	-0.75637200

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