Alkali Metal-Hydroxide-Catalyzed Mechanisms of Csp-H Silylation of Alkyne: A DFT investigation

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Contents

1 R1+R2+OH^-/NaOH/NaH→P

1.1path a R1+R2+OH^-→P

Based on the referenc, it was observed that the reaction can still proceed even when crown ether is added. Therefore, it is hypothesized that the anion (OH^-) may have played a catalytic role in the reaction. As a result, the mechanism of OH^- catalyzing the reaction was predicted and calculated below.

In Scheme S1,firstly, R1 binds with OH^- to form the intermediate IM1a, accompanied by OH^- and C2 generation, with an energy absorption of 1.8 Kcal/mol. Secondly, the intermediate IM2a is formed by the approachment of IM1a and R2. The H (Si) of R2 is captured by binding with IM2a, finally generating IM3a. However, this process is highly challenging and requires an absorption of 68.2 Kcal/mol energy. After that, the Anion and cation of IM3a combine to form IM4a, releasing 70.9 Kcal/mol energy. Ultimately, the product P is obtained through different dissociation processes (path a1 and path a2 of Figure S1), which involves adding H (R2) to C2 (R1) and $SiEt3^+$ to C1 (R1).

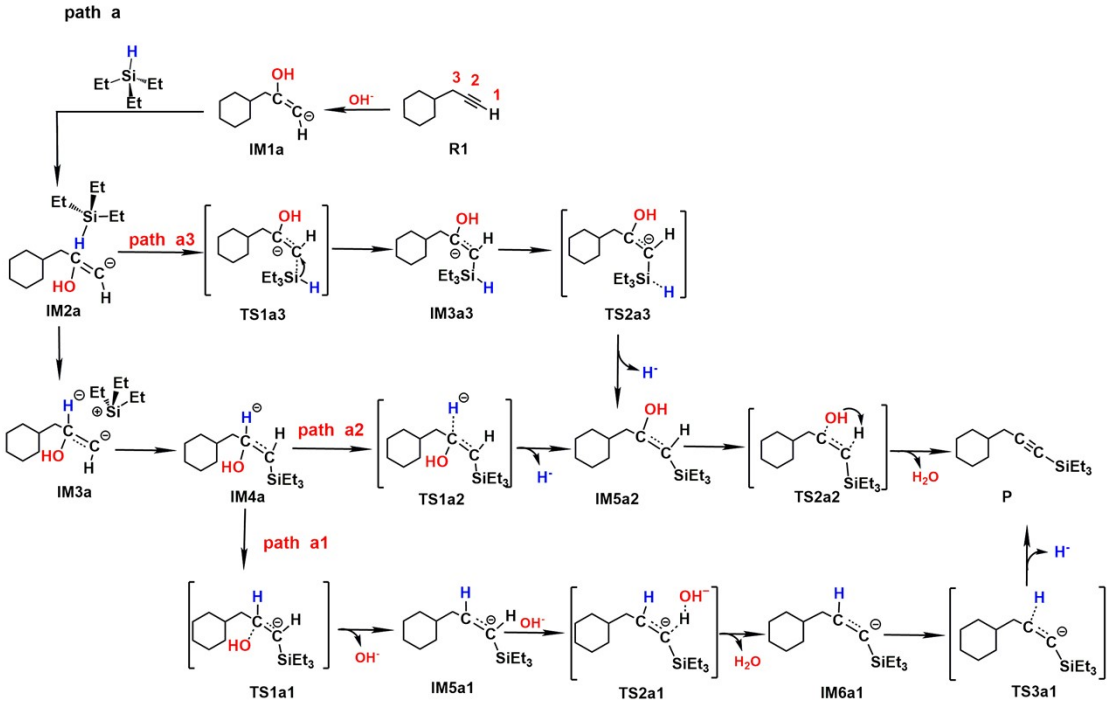
In path a1 (black line in Figure S1), IM4a removes OH^- to form IM5a1 through the transition state TS1a1, which requires overcoming a Gibbs free energy barrier of 3.7 Kcal/mol. This process releases -17.9Kcal/mol of energy, indicating that it is easily achievable. Next, the dissociated OH^- captures the H (C1) of TS2a1 to form IM6a1 and H_2O. The Gibbs free energy barrier for overcoming TS2a1 in the process of IM5a1+OH^-→IM6a1+H_2O is 16.2 kcal/mol. Finally, IM6a1 dissociates H^- to yield the product P, which requires an energy barrier of 24.1Kcal/mol to overcome.

In path a2 (red line in Figure S1), IM4a undergoes the transition state TS1a2 to eliminate H^- and form neutral IM5a2. The Gibbs free energy barrier for this process is 22.7 Kcal/mol. Finally, the OH (C2) and H (C1) of IM5a2 combine to form H_2O, which is eliminated along with the formation of product P. The Gibbs free energy barrier for the process of IM5a2→TS2a2→P+H_2O is 62.7 Kcal/mol.

In path a3 (green line in Figure S1), the Si and C1 of intermediate IM2a coordinate to form intermediate IM3a3 through the transition state TS1a3, which

requires overcoming a Gibbs free energy barrier of 14.6 Kcal/mol. Next, H(Si) of IM3a3 moves away from Si to form H^- and IM5a2 through the transition state TS2a3. The Gibbs free energy barrier for the process of IM3a3→TS2a3→H^-+IM5a2 is 3.4 Kcal/mol, releasing 17.5 Kcal/mol of energy. Subsequently, the process of IM5a2→P is the same as that in path a2 (IM5a2→P).

Based on the above data, it can be concluded that the Gibbs free energy barrier that OH^- needs to overcome as a catalyst is very high. Therefore, the catalysis in MOH (M=K/Na) still relies on M. In the references, the low yield of LiOH also indicates that the possibility of OH^- alone playing a catalytic role is very small.



Scheme S1. The detailed mechanism for R2+R1+OH^-→P via path a

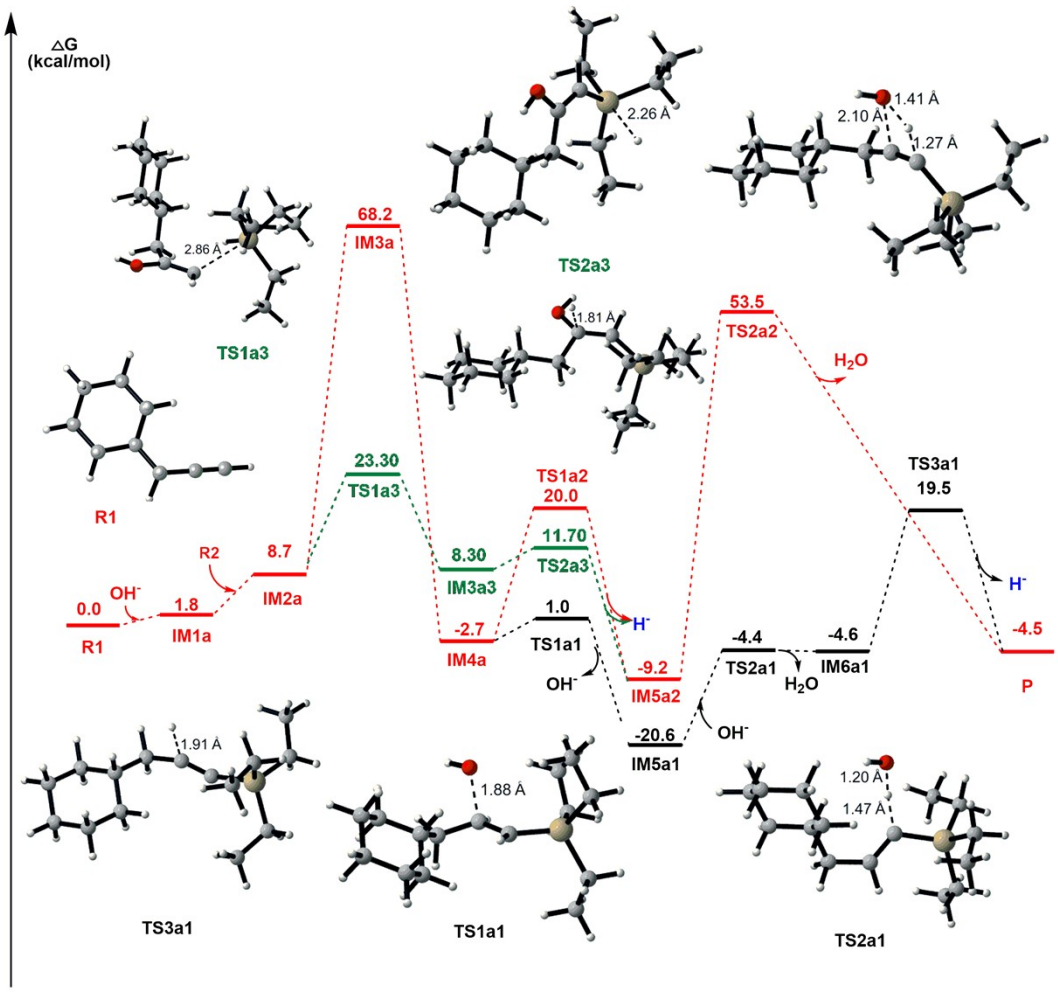


Figure S1. The Gibbs free energy surface for R2+R1+OH^-⟶P via path a with M06-L-D3/ma-def2-TZVP level.

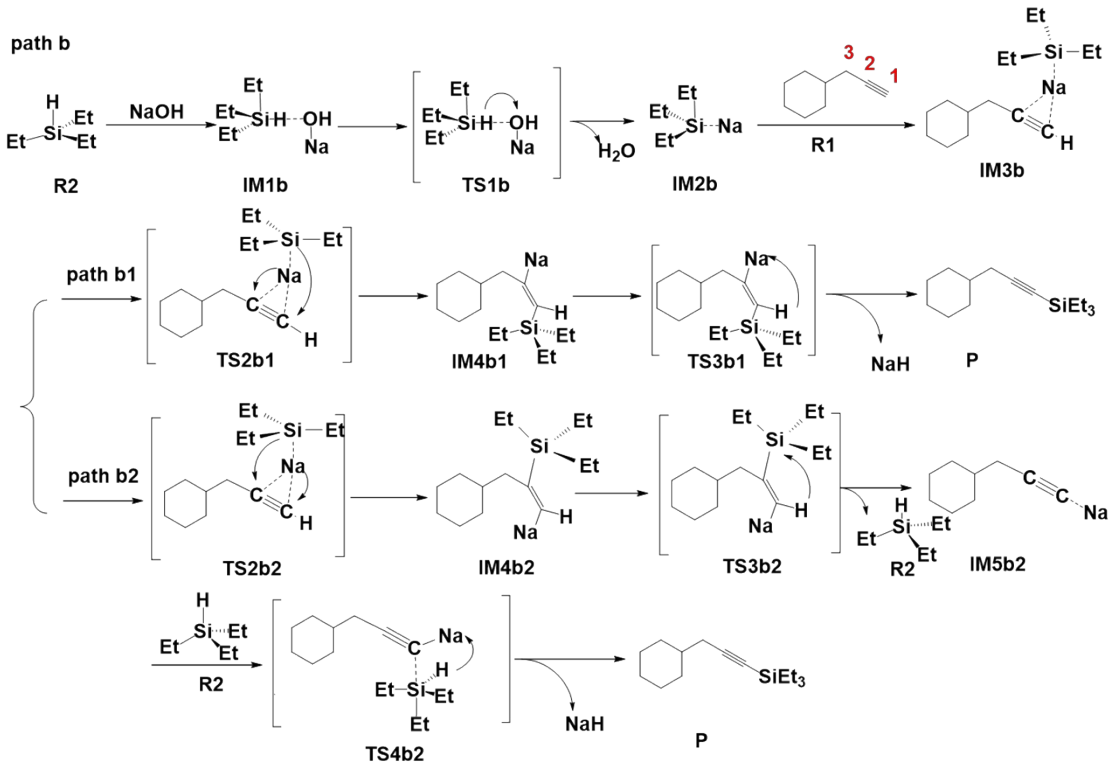
1.2 Path b R2+NaOH+R1→P

Investigating the process of NaOH-s interacting with reactant R2-s to generate P-s in pathway b (Scheme S2) . R2-s interacts with NaOH-s to form intermediate IM1b-s. According to figure S2, it then undergoes transition state TS1b-s, where the H atom on Si migrates to O(OH^-) and eliminates a molecule of H_2O to form intermediate IM2b-s. The energy barrier required for this process is 23.24 kcal/mol. Then, IM2b-s interacts with R1-s to form intermediate IM3b-s, which undergoes addition reaction of the alkyne to yield an alkene. The addition reaction of the alkyne can proceed in two ways.

In pathway b1, IM3b-s undergoes transition state TS2b1-s to form intermediate IM4b1-s, with Si adding to C1 and Na adding to C2. The energy barrier that needs to

be overcome for the process IM3b-s→TS2b1-s→IM4b1-s (black line in Figure S2) is 14.47 kcal/mol. Subsequently, IM4b1-s undergoes transition state TS3b1-s, where the H atom (C1) migrates towards the Na atom to eliminate NaH-s and obtain product P-s, with the energy barrier that needs to be overcome for the process IM4b1-s→TS3b1-s→P-s+NaH-s being 29.80 kcal/mol. This process is the rate-determining step of pathway b1 and the energy barrier that needs to be overcome without considering the influence of the solvent is 28.92 kcal/mol (red line in Figure S2), indicating that the addition of solvent is unfavorable for this reaction.

In pathway b2, IM3b-s undergoes transition state TS2b2-s to form IM4b2-s. The energy barrier that needs to be overcome for the process IM3b-s+R1-s→TS2b2-s→IM4b2-s (orange line in Figure S2) is 15.89 kcal/mol. Subsequently, it undergoes the process IM4b2-s→TS3b2-s→IM5b2-s, requiring an energy barrier of 54.98 kcal/mol. This process is the rate-determining step of pathway b2, and the energy barrier that needs to be overcome without considering the influence of the solvent (blue line in Figure S2) is 67.17 kcal/mol. Although the addition of solvent is favorable for this reaction, the overall potential energy surface indicates that this reaction is not easy to proceed. Finally, IM5b2-s reacts with R2-s and goes through a transition state TS4b2-s with an energy barrier of 25.04 kcal/mol to obtain NaH-s and product P-s.



Scheme S2. The detailed mechanism for NaOH+R2+R1→P via path b .

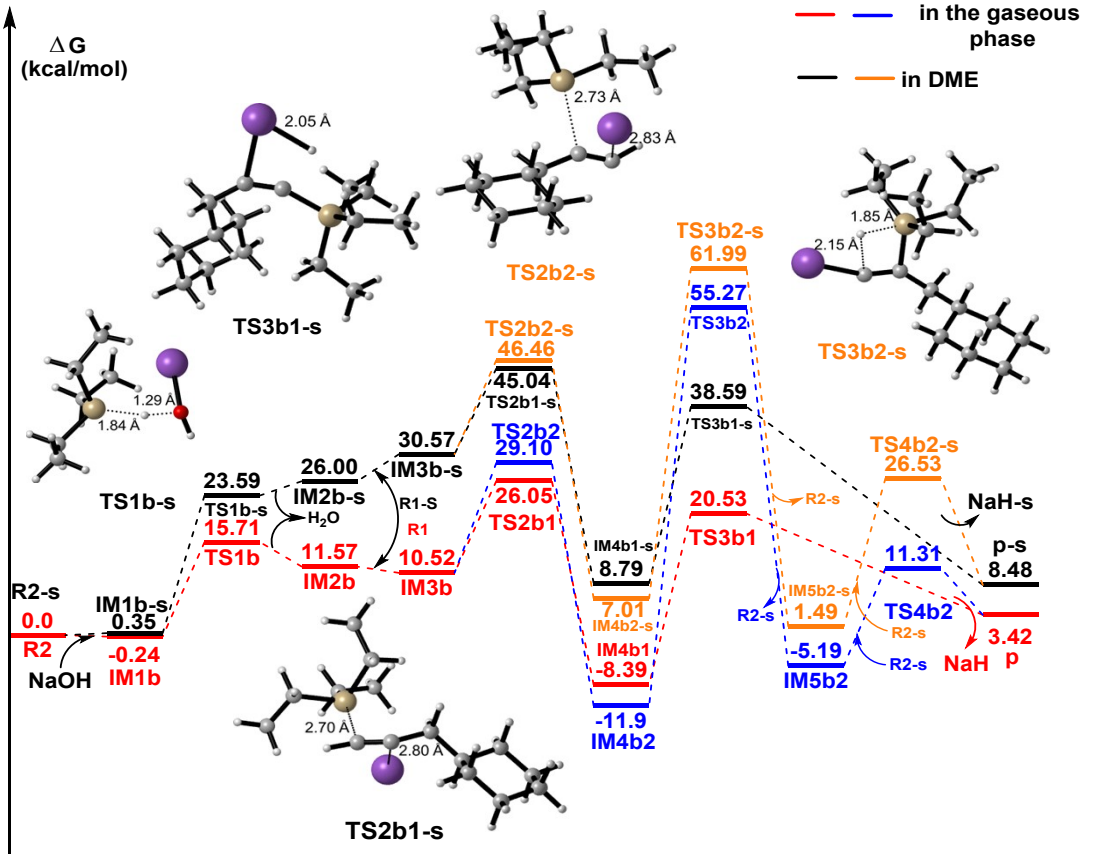
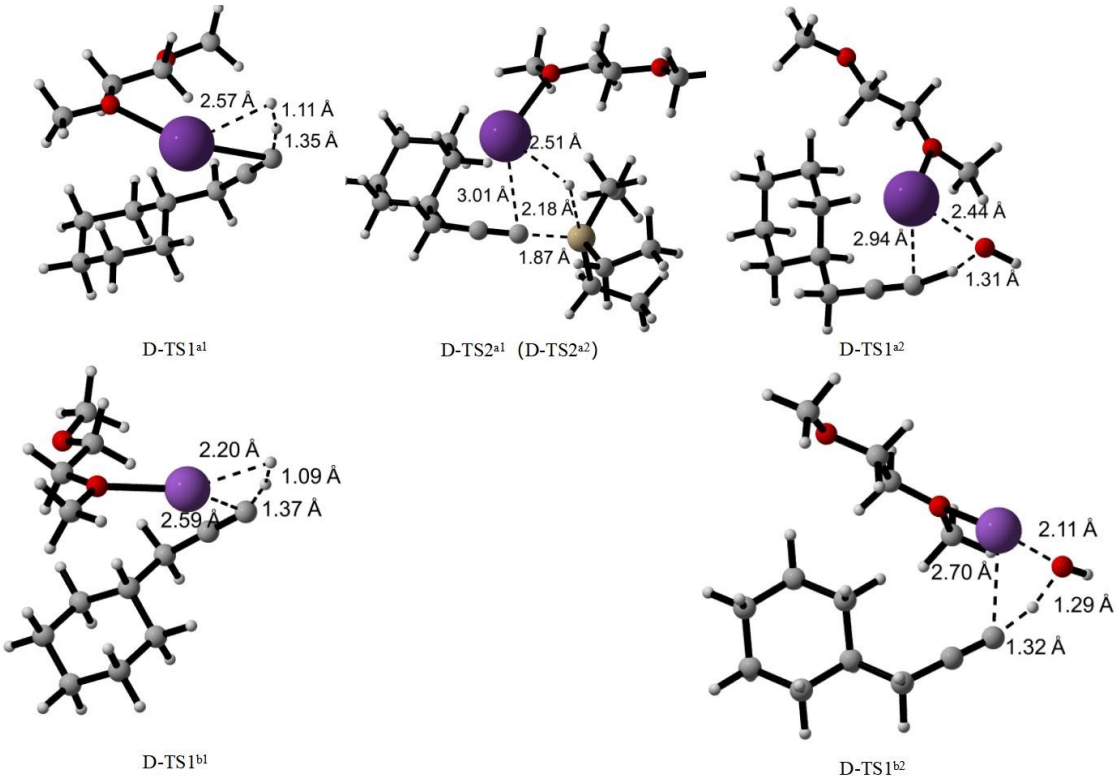


Figure S2. The Gibbs free energy surface for NaOH+R2+R1→P via path b with M06-L-D3/def2-

SVP level.

1.3 Path c R1+R2+DME+MOH/MH→P (M=K or Na)

We have considered the situation where 1,2-dimethoxyethane (DME) acts as an explicit solvent participating in the reaction, and calculated the influence on the reaction energy barrier after the O atom of 1,2-dimethoxyethane (DME) coordinates with M (K/Na). As depicted in Figure S3, when DME coordinates with the metal center (K/Na) to participate in the reaction, the energy barrier of the transition state increases, which is unfavorable for the reaction. Furthermore, the structure of the transition state is illustrated in Scheme S3.



Scheme S3. The structures of the transition state of the R1+R2+DME+MOH/MH→P (M=K or Na) .

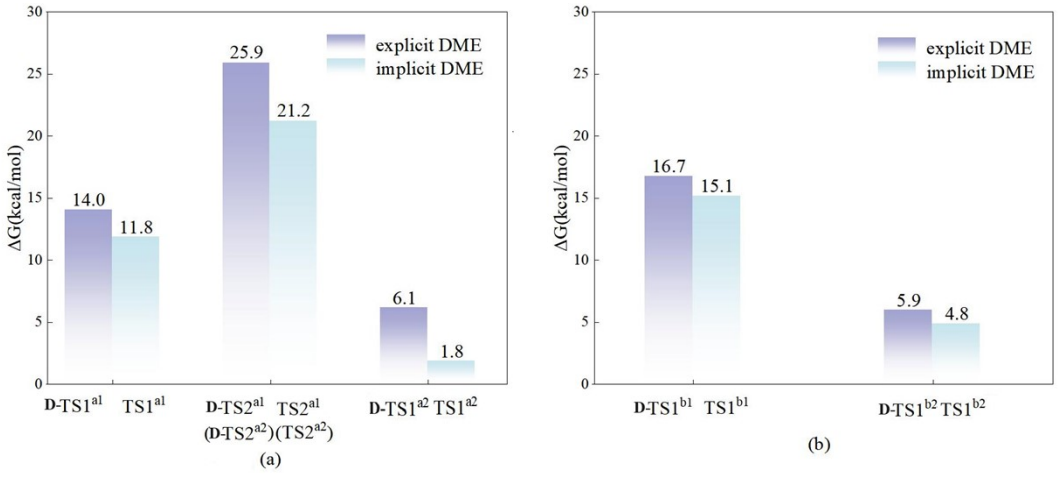


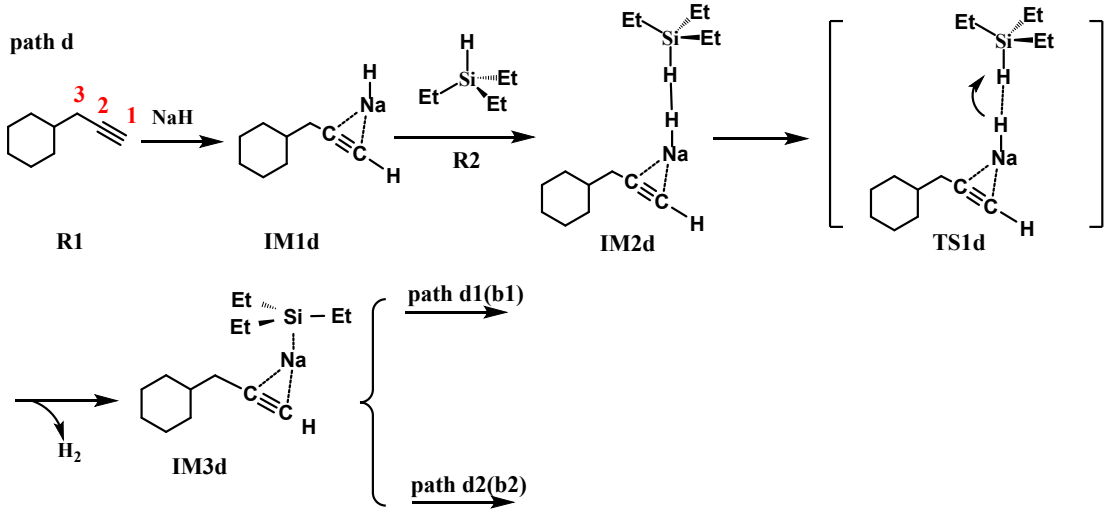
Figure S3. Comparison of Gibbs free energy barriers for KOH / KH under explicit DME or implicit DME M06-L-D3/ma-def2-TZVP level.

1.4 Path d R1+KH+R2→P

In pathway d, the process of interaction between NaH-s and reactant R1-s is investigated (Scheme S4) . The interaction between NaH-s and the electron-rich terminal alkynyl group in R1-s easily forms the intermediate IM1d-s by coordinating with the electron-deficient Na. When considering the solvent DME, the heat absorbed during this process is 4.41 kcal/mol. Subsequently, IM1d-s combines with R2-s to absorb 4.79 kcal/mol of energy and generate intermediate IM2d-s. Then, in the transition state TS1d-s, the H (Na) atom and H (Si) atom combine to produce H_2, forming the intermediate IM3d-s. The structure of TS1d-s indicates that the distance between the H (Na) atom and H (Si) atom is shortened from 1.14 Å to 1.06 Å. The Gibbs free energy barrier that needs to be overcome for the process IM2d-s → TS1d-s → IM3d-s + H2-s is 32.15 kcal/mol. IM3d-s has the same structure as IM3b-s, and the process after IM3d-s is the same as the process IM3b-s → P-s in pathway b.

Comparison of the total potential energy surfaces of pathways d1 and d2 in Figure S4 reveals that, without the solvent DME, the highest energy barrier that needs to be overcome in pathway d1 is 28.91 kcal/mol, while the highest energy barrier that needs to be overcome in pathway d2 is 67.19 kcal/mol. The addition of solvent causes an increase in the highest energy barrier that needs to be overcome for the reaction in

both pathways, indicating that the addition of solvent is unfavorable for the reaction. Therefore, in the two pathways of pathway d, pathway d1 is the preferred pathway, but completing pathway d1 still presents some challenges.



Scheme S4. The detailed mechanism for NaOH+R2+R1→P via path d.

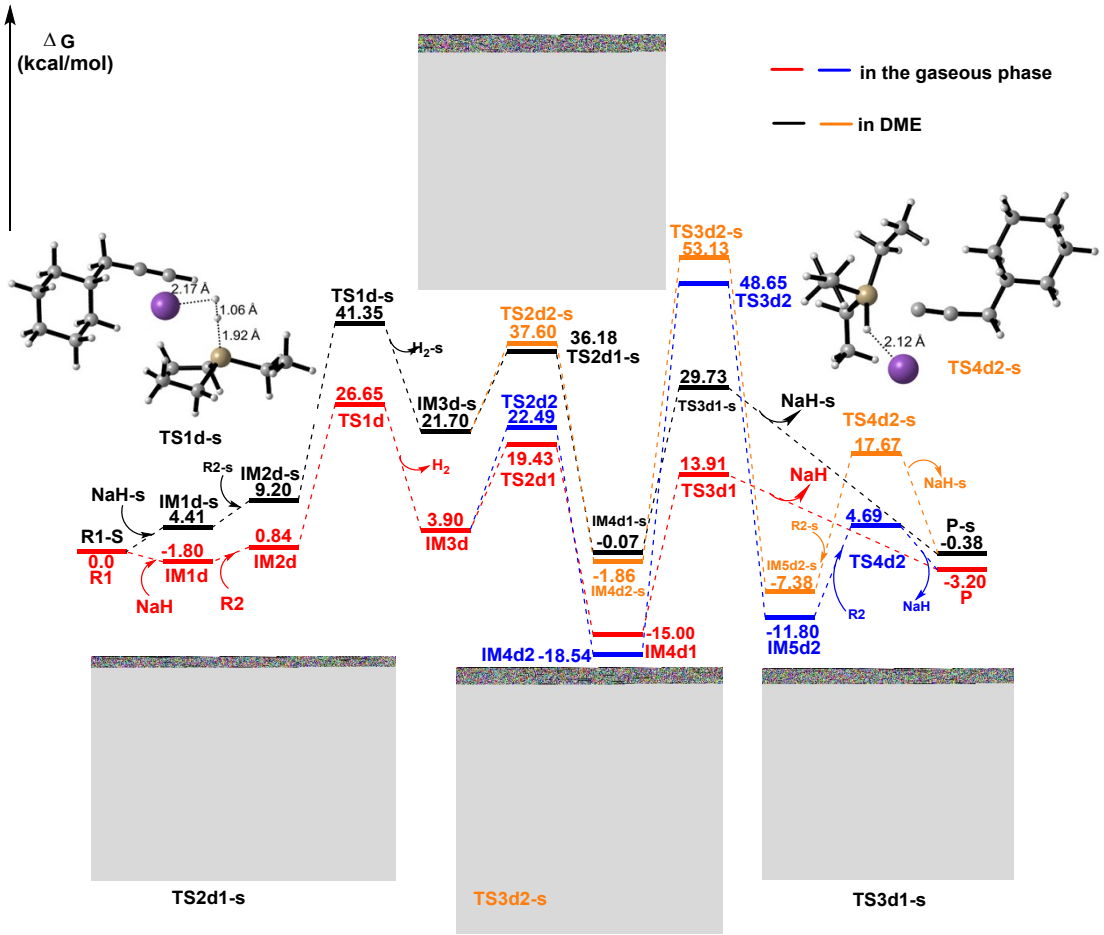
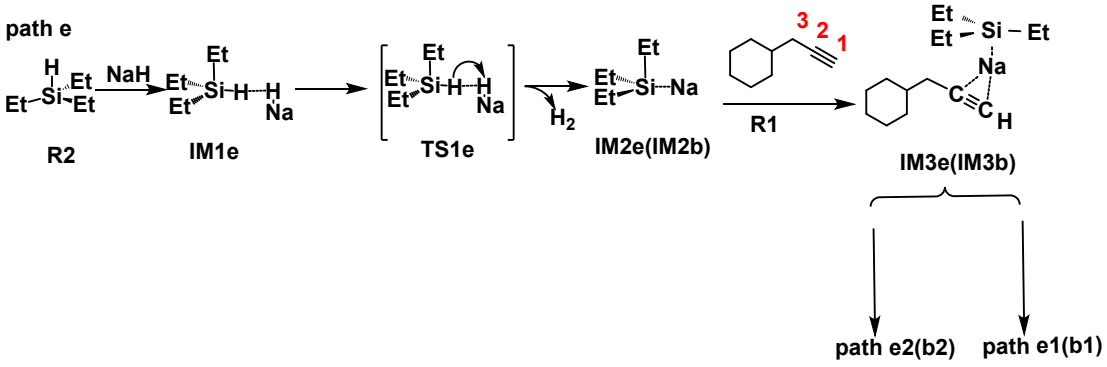


Figure S4. The Gibbs free energy surface for NaOH+R2+R1→P via path d with M06-L-D3/def2-SVP level.

1.5 Path e R2+KH+R1→P

Pathway e (Scheme S5)investigates the process of interaction between reactant R2-s and NaH-s. R2-s first interacts with NaH-s to form intermediate IM1e-s, which then undergoes transition state TS1e-s. The H (Na) atom and H (Si) atom combine to produce H_2, forming intermediate IM2e-s. The distance between the H (Na) atom and H (Si) atom is shortened from 1.09 Å to 1.04 Å. The Gibbs free energy barrier that needs to be overcome at this point is 39.90 kcal/mol (black line in Figure S5) . IM2e-s has the same structure as IM2b-s, and the process after IM2e-s is the same as the process after IM2b-s, which is the process of IM2b-s → P-s.

Comparison of the total potential energy surfaces in Figure S5 reveals that, without considering the influence of the solvent DME, the highest energy barrier that needs to be overcome in pathway e1 is 28.91 kcal/mol (red line in Figure S5), while the highest energy barrier that needs to be overcome in pathway e2 is 67.81 kcal/mol (blue line in Figure S5) . When considering the influence of the solvent, the highest energy barrier that needs to be overcome for the reaction increases in both pathways, indicating that the solvent has an unfavorable effect on the reaction. Therefore, among the two pathways of pathway e, pathway e1 is the preferred pathway, but completing pathway e1 still presents some difficulties.



Scheme S5. The detailed mechanism for NaH+R2+R1⟶P via path e.

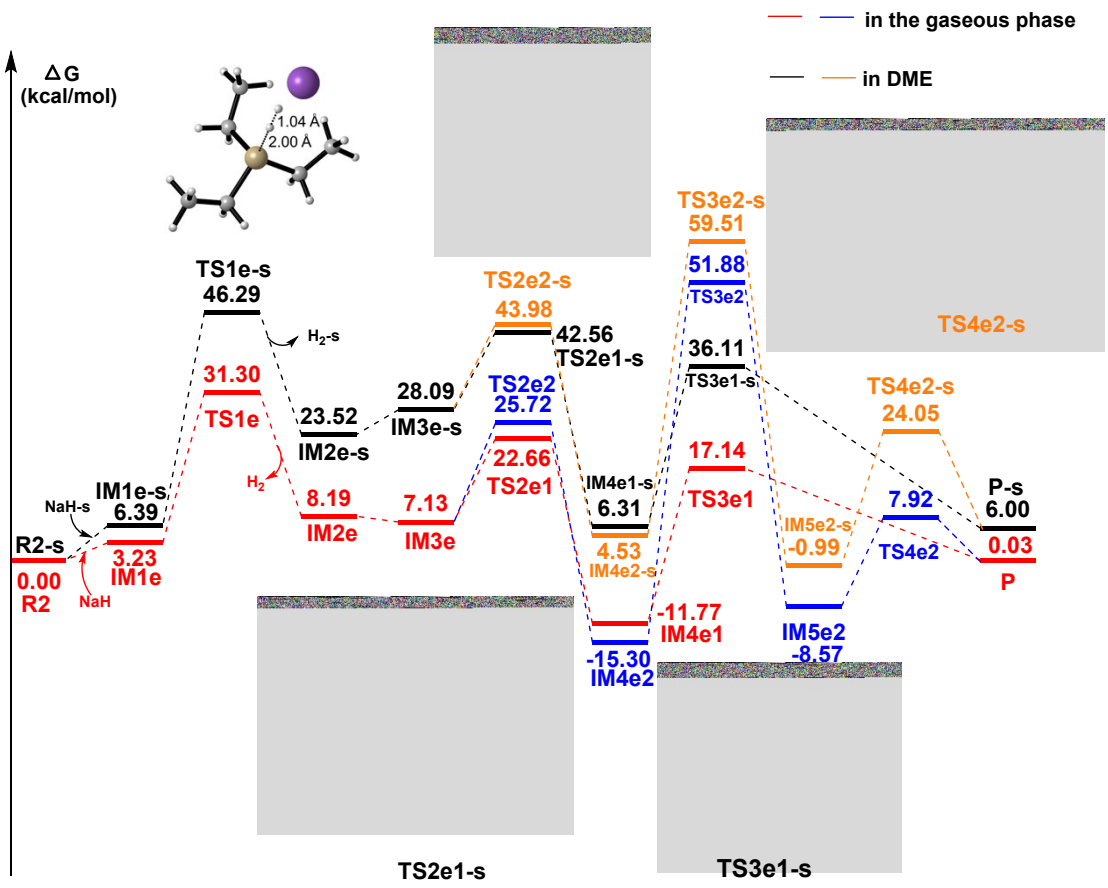


Figure S5. The Gibbs free energy surface for NaH+R2+R1→P via path e with M06-L-D3/def2-SVP level.

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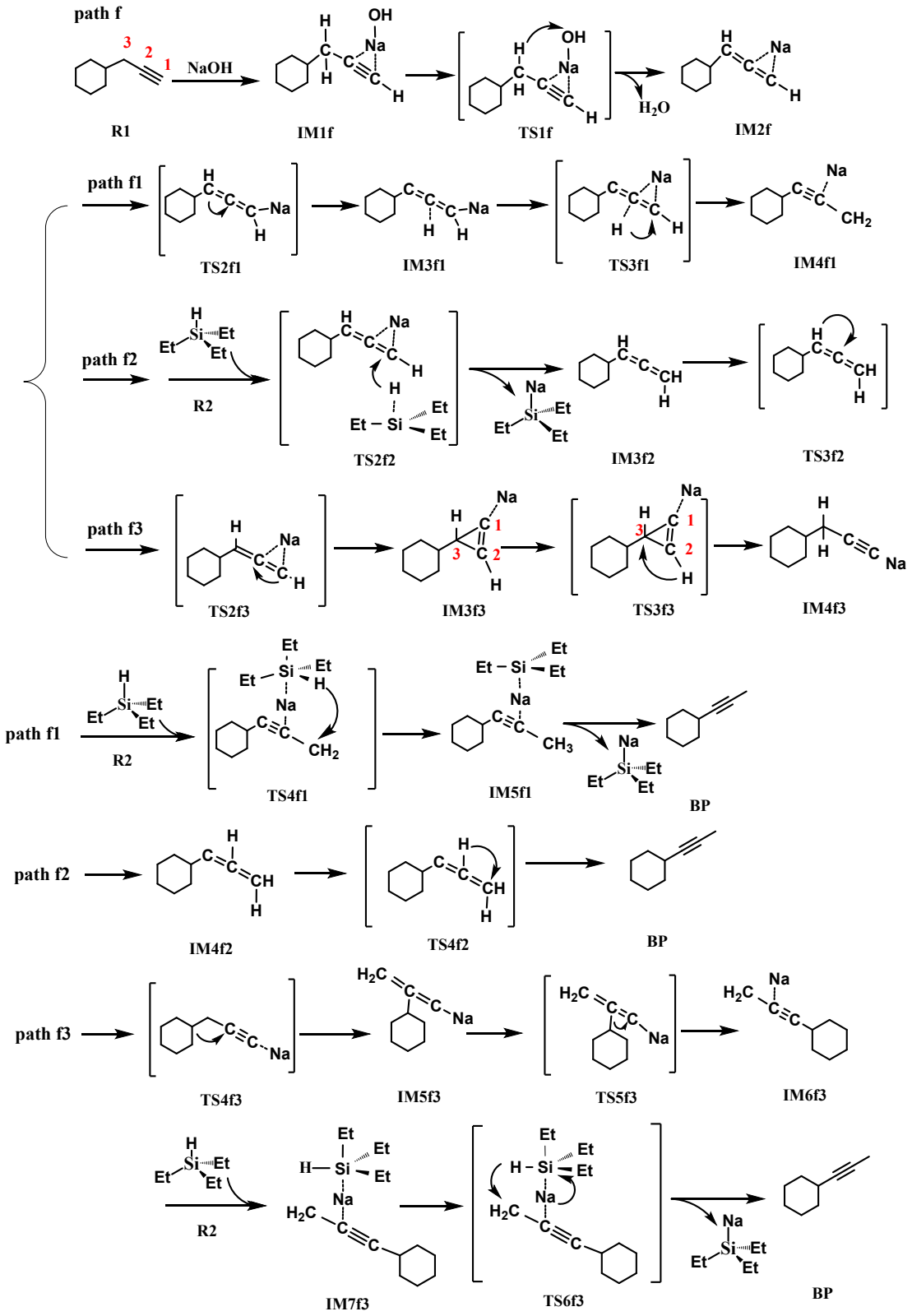
2 R1+NaOH+R2→BP

2.1 Path f R1+NaOH+R2→BP

According to the literature, Often accompanied by the formation of a small amount of byproduct 1-cyclohexyl proparyne (BP) during the reaction, the possible path of which will be elaborated here.

In pathway f (Scheme S6), the catalyst NaOH-s reacts with R1-s to form intermediate IM1f-s, where the H atom (C1 or C3) tends to approach OH^- and lose H_2O. In transition state TS1f-s, the H (C3) atom combines with OH- to lose H_2O-s and form intermediate IM2f-s. The Gibbs free energy barrier that needs to be overcome for the process IM1f-s→TS1f-s→IM2f-s is 5.22 kcal/mol. In this process, the energy of intermediate IM2f-s is higher than that of transition state TS1f-s. After a

series of optimization calculations, it was found that transition state TS1f-s does not exist in the process. Based on the analysis of the structure of IM2f-s and byproduct BP-s, it is known that the production of BP-s may be due to a triple bond rearrangement process caused by H migration or a ring migration process.



Scheme S6. The detailed mechanism for NaOH+R2+R1→BP via path f.

Therefore, in pathway f1 and pathway f2, we first investigate the triple bond rearrangement process caused by H migration. In pathway f1 (Figure S6), the process IM2f-s → IM4f1-s is undergone, where the H atom on C3 in IM2f structure finally migrates to C1. Since the distance between C3 and C1 is too long, the migration process is difficult to complete in one step, and a stepwise migration process is considered here. In this process, the energy barrier that needs to be overcome for the process IM2f-s → TS2f1-s → IM3f1-s is 65.58 kcal/mol, which is very high, and the reaction is quite difficult. From the perspective of the total potential energy surface, the highest energy barrier that needs to be overcome for this process is 82.07 kcal/mol, and the reaction cannot be completed almost.

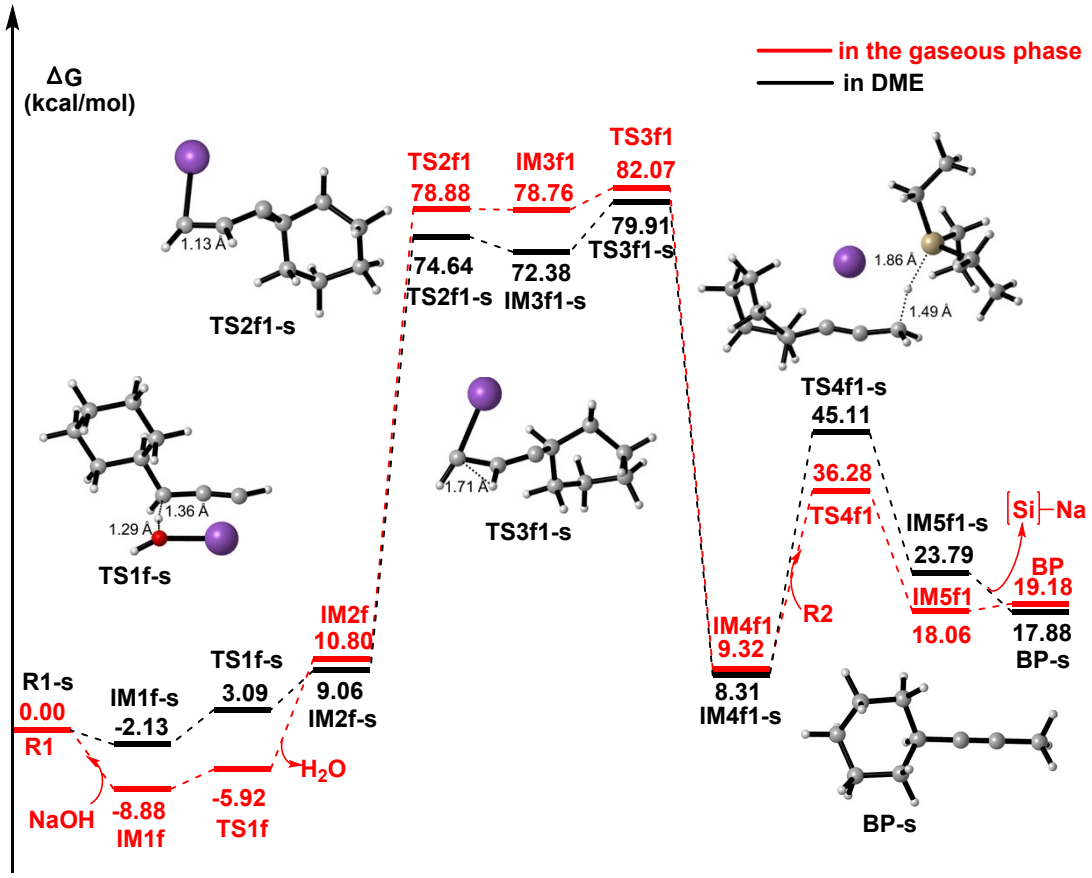


Figure S6. The Gibbs free energy surface for NaOH+R2+R1→BP via path f1 with M06-L-D3/def2-SVP level.

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In pathway f2 (Figure S7), IM2f-s first interacts with R2-s, undergoes transition state TS2f2-s, and loses triethylsilyl sodium (Si-Na) to form intermediate IM3f2-s, where the H atom on Si in TS2f2-s structure migrates to C1. When considering the influence of the solvent, the distance between the H (Si) atom and C1 becomes smaller (1.45 Å → 1.44 Å). In the process R2-s + IM2f-s → TS2f2-s → IM3f2-s + Si-Na-s, the energy barrier that needs to be overcome is 37.03 kcal/mol. Then, IM3f2-s undergoes a process similar to the stepwise hydrogen migration in pathway f1. In the process IM3f2-s → TS3f2-s → IM4f2-s, the H atom on C3 migrates to C2. When considering the influence of the solvent DME, the distance between the H (C3) atom and the C2 atom remains at 1.18 Å, and the energy barrier that needs to be overcome in transition state TS3f2-s is 54.90 kcal/mol. The reaction difficulty is extremely high and it is difficult to complete. Then, another transition state TS4f2-s with an energy barrier of 16.69 kcal/mol is undergone, and after completing the process of H (C2) atom migrating to C1, byproduct BP-s is obtained. As shown in Figure 5, from the perspective of the total potential energy surface, when not considering the influence of the solvent, the highest energy barrier that needs to be overcome for this pathway is 96.04 kcal/mol, and the reaction difficulty is extremely high, making it difficult to complete.

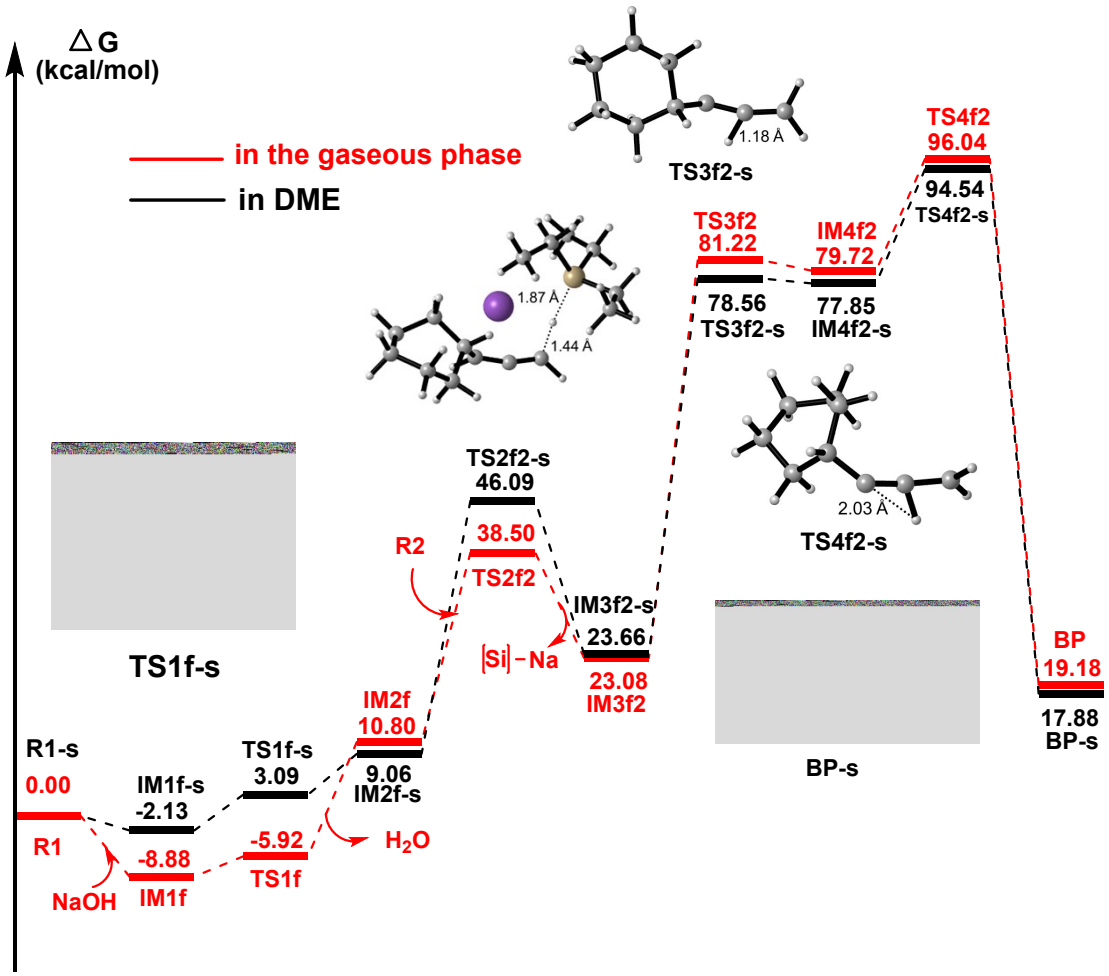

Figure S7. The Gibbs free energy surface for NaOH+R2+R1→BP via path f2 with M06-L-D3/def2-SVP level.

Pathway f3 (Figure S7) explores the process of ring migration. After undergoing the process R1-s → IM2f-s, the process IM2f-s → IM4f3-s is undergone, and the factor that the one-step hydrogen migration distance is too large to complete is still considered, so a stepwise hydrogen migration approach is chosen. The energy barrier that needs to be overcome in the process IM2f-s → TS2f3-s → IM3f3-s is 57.32 kcal/mol. The C1, C2, and C3 in the structure of intermediate IM3f3-s form a carbon ring, and then undergo transition state TS3f3-s, where the H (C2) atom on the carbon ring migrates to C3, causing the carbon ring to break and return to its original chain-like state to obtain intermediate IM4f3-s. Then, IM4f3-s undergoes the process IM4f3-s → TS4f3-s → IM5f3-s, and in transition state TS4f3-s, the cyclohexyl group on C3 migrates to C2 to obtain intermediate IM5f3-s. The energy barrier that needs to

be overcome from IM4f3-s to TS4f3-s is 97.18 kcal/mol, indicating that the difficulty of this reaction is extremely high. Then, IM5f3-s undergoes another ring migration process and undergoes transition state TS5f3-s to obtain intermediate IM6f3-s, where the cyclohexyl group ultimately migrates from C2 to C1. Then, IM6f3-s interacts with R2-s to form intermediate IM7f3-s, and then undergoes transition state TS6f3-s to lose triethylsilyl sodium (Si-Na) to obtain byproduct BP-s. As shown in Figure 6, from the perspective of the total potential energy surface, the highest energy barrier that needs to be overcome for this process is 100.45 kcal/mol, and the reaction can hardly complete.

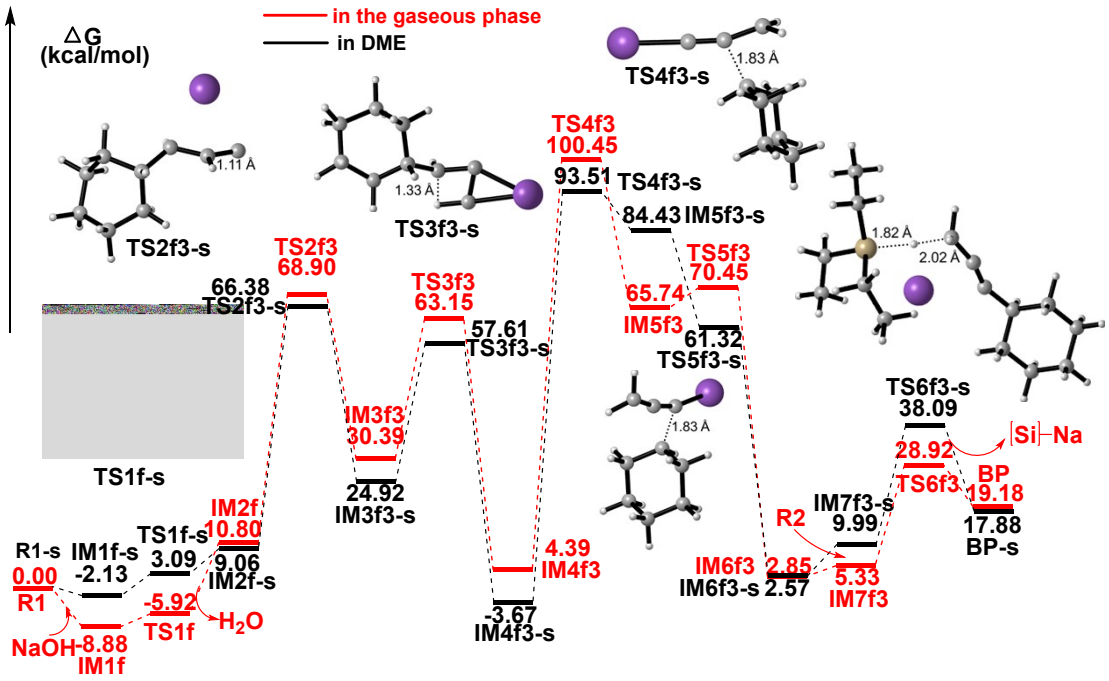

Figure S8. The Gibbs free energy surface for NaOH+R2+R1→BP via path f3 with M06-L-D3/def2-SVP level.

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3 Other Supplementary Data

To compare the effect of the implicit solvent(DME) on the reaction of R1+KOH/KH→P, the potential energy map of this reaction in the absence of the solvent is calculated below.

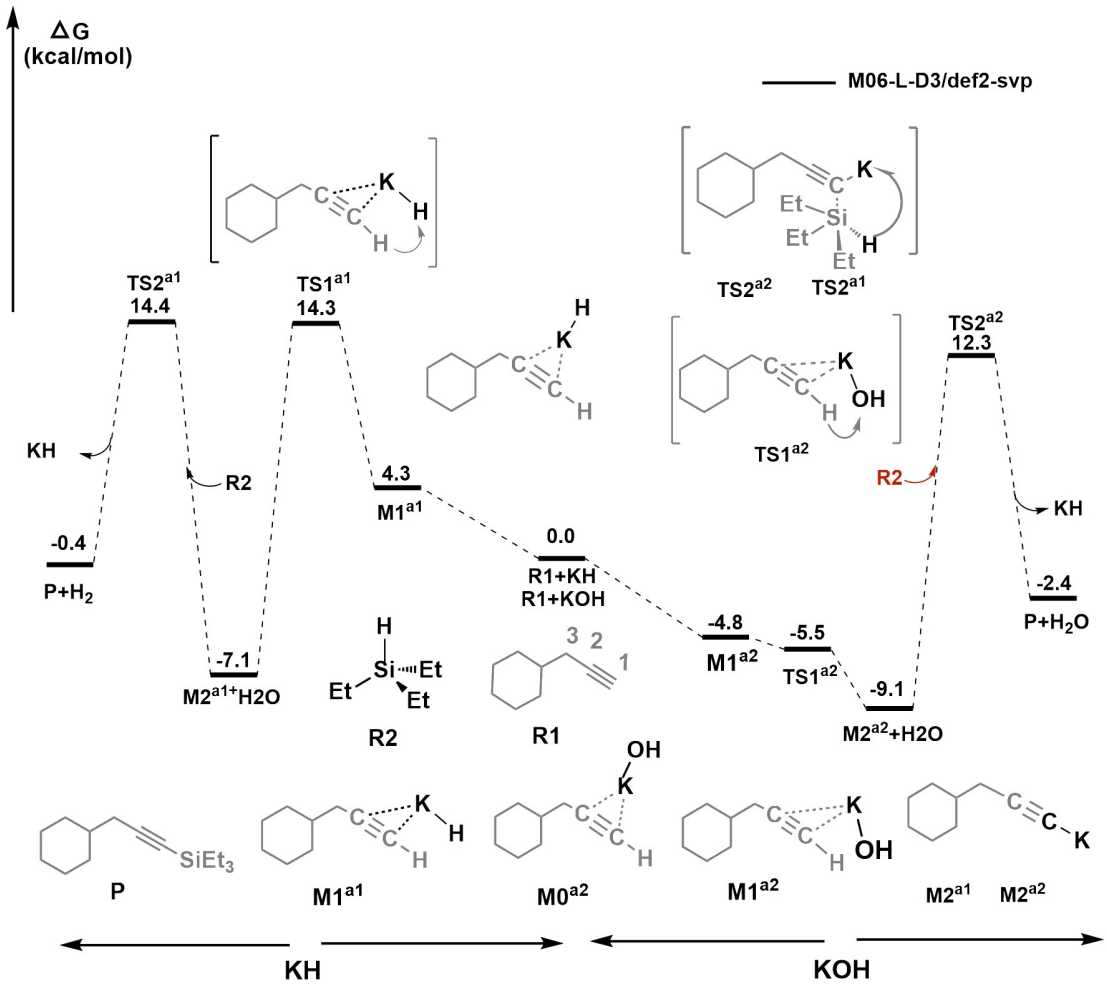

Figure S9. The Gibbs free energy surface for R1+KOH/KH→P with M06-L-D3/def2-SVP level.

4 The Cartesian coordinates

4.1 The Cartesian coordinates (Angstrom) for the optimized reactants, intermediates, transition states and product obtained at the M06-L-D3/def2-SVP level level of theory in the solvent of DME.

R1

C	-2.20693300	-0.86557100	-0.40924800
H	-2.18017200	-0.80417200	-1.51241100
H	-2.99871500	-1.59215500	-0.16710300
C	-0.86090200	-1.36226100	0.09417300
H	-0.91406100	-1.52954800	1.18660700
H	-0.61827800	-2.34184600	-0.34987000
C	-2.54395800	0.50562700	0.15886400
H	-3.50485200	0.86684400	-0.24130400
H	-2.68335500	0.42129700	1.25228500
C	0.25975900	-0.36643800	-0.19254800
H	0.34912200	-0.26376000	-1.29172800
C	-1.43434500	1.50708000	-0.12649900
H	-1.37164900	1.68052800	-1.21620100
H	-1.66876100	2.48593400	0.32121200
C	-0.08894500	1.00729300	0.37726300
H	0.70825000	1.73072800	0.13955800
H	-0.11342400	0.93423200	1.48130400
C	1.59622000	-0.89905100	0.33681100
H	1.75653400	-1.92360800	-0.04080000
H	1.53824300	-0.99993200	1.43561900
C	2.75259100	-0.09037900	-0.00490800
C	3.71496100	0.58886000	-0.30547900

H	4.57043400	1.18450400	-0.56774800

R2

Si	-1.15938700	-0.57833700	-0.00640800
H	-2.42940700	-1.15032600	0.56260700
C	-1.26421100	1.30623800	0.10014100
C	-2.62910800	1.92248000	-0.16683700
H	-0.51026600	1.72566900	-0.59077700
H	-0.91450200	1.59873900	1.10627800
H	-2.61341700	3.02059200	-0.08644500
H	-3.00943400	1.68443500	-1.17160100
H	-3.38500600	1.56199400	0.54773700
C	0.30151100	-1.18810400	1.01945500
C	0.57719400	-2.68172500	0.95722900
H	0.13252800	-0.87324000	2.06439900
H	1.19375600	-0.62197900	0.69553600
H	1.41356900	-2.98004100	1.60815800
H	-0.29569600	-3.27658900	1.26952100
H	0.83681800	-3.01108000	-0.06054200
C	-0.98643500	-1.18760500	-1.78586300
C	-1.98264700	-0.63247300	-2.79123700
H	-1.04375100	-2.29037700	-1.76688900
H	0.04587800	-0.96497400	-2.11271200
H	-1.85531900	-1.07472000	-3.79159900
H	-3.02538400	-0.82254100	-2.49118000
H	-1.87990900	0.45666100	-2.91357500

KOH

O	0.00000000	0.00000000	-1.48939700
H	0.00000000	0.00000000	-2.44899700
K	0.00000000	0.00000000	0.75600900

KH

H	0.00000000	0.00000000	-2.37307600
K	0.00000000	0.00000000	0.12489900

NaOH

O	0.01075100	1.02937500	0.00000000
H	-0.20426700	1.96157800	0.00000000
Na	0.01075100	-0.92696100	0.00000000

LiOH

O	0.00000000	0.00000000	0.31873300
H	0.00000000	0.00000000	1.27050400
Li	0.00000000	0.00000000	-1.27345600

NaH

Na	0.00000000	0.00000000	0.16822800
H	0.00000000	0.00000000	-1.85050900

LiH

H	0.00000000	0.00000000	-1.26984400
Li	0.00000000	0.00000000	0.42328100

H_2

H	0.00000000	0.00000000	0.37707200
H	0.00000000	0.00000000	-0.37707200.

M0[a2]

O	-5.46259600	0.86807200	-0.10992300
H	-6.13048900	1.54835600	-0.01075600
C	4.08807400	-0.77795400	0.18708400
H	4.34170600	-0.50187600	1.22654600
H	4.80839400	-1.56004400	-0.10034000
C	2.67035800	-1.32909000	0.14970000
H	2.45050200	-1.71223600	-0.86479700
H	2.57194600	-2.19355100	0.82666700
C	4.23681600	0.44470100	-0.70694000
H	5.25769900	0.85242900	-0.63717100
H	4.10302100	0.14239500	-1.76171500
C	1.63488600	-0.26513100	0.50447200
H	1.81861300	0.05554400	1.54806300
C	3.20917900	1.51138600	-0.35798600
H	3.41777000	1.90097200	0.65487500
H	3.29908400	2.37464500	-1.03598800
C	1.79282200	0.95700100	-0.39659000
H	1.06587900	1.73549900	-0.11340400
H	1.53859300	0.66624800	-1.43377500
C	0.21960600	-0.85453300	0.44109100
H	0.17049900	-1.76462700	1.06254000
H	0.01564600	-1.19184800	-0.59152300
C	-0.82859000	0.05891500	0.86125900
C	-1.68993000	0.83976800	1.22236200
H	-2.44466100	1.53718200	1.54430000
K	-3.84068700	-0.80838800	-0.36788700

M1[a2]

O	4.41784900	1.49014600	-0.63598200
H	4.54820900	2.34319000	-1.05420800
C	-4.18388800	-0.59958000	-0.46067600
H	-4.22718900	-0.27179300	-1.51517900
H	-5.02685400	-1.29621200	-0.32780000
C	-2.86365300	-1.31537500	-0.21516100
H	-2.86147800	-1.74409600	0.80505100
H	-2.75285000	-2.17115100	-0.90147900
C	-4.33988000	0.61214400	0.44693500
H	-5.28233100	1.13956100	0.22946100
H	-4.41825200	0.27240400	1.49597400
C	-1.66806000	-0.37602400	-0.35234100
H	-1.63956600	-0.01183500	-1.39779400
C	-3.15385700	1.55640300	0.31411800
H	-3.14554800	1.98986300	-0.70243300
H	-3.25746200	2.40967500	1.00302400
C	-1.83593600	0.83669100	0.55953900
H	-0.98766300	1.52828200	0.43078400
H	-1.79261200	0.49512700	1.61157300
C	-0.35816300	-1.12727700	-0.08371300
H	-0.31775400	-2.02792000	-0.72031400
H	-0.36994000	-1.50642500	0.95453700
C	0.84643500	-0.33887300	-0.29388300
C	1.84274000	0.34415100	-0.48368300
H	2.78911800	0.94997900	-0.63769500
K	4.61499700	-0.60912500	0.48566000

M1[b2]

O	4.87449900	0.13341300	-0.77293800
H	5.52595000	-0.11028800	-1.43198300
C	-3.70894200	-0.31422400	-0.29051800
H	-3.72579400	-0.43942400	-1.38848000
H	-4.68230800	-0.68357000	0.06956900
C	-2.57839500	-1.15145000	0.28851400
H	-2.62444600	-1.11819100	1.39380200
H	-2.70061900	-2.21227800	0.01404300
C	-3.53773200	1.16099200	0.04164300
H	-4.34381200	1.75728500	-0.41481300
H	-3.63804800	1.30108200	1.13370700
C	-1.20652800	-0.65108500	-0.15679100
H	-1.14705900	-0.75727700	-1.25774900
C	-2.17503500	1.67099000	-0.40444300
H	-2.11857800	1.63923900	-1.50772400
H	-2.04605800	2.72937500	-0.12708600
C	-1.04691600	0.83057300	0.17527300
H	-0.06978900	1.19447300	-0.18295200
H	-1.03123900	0.94470200	1.27655000
C	-0.09302800	-1.50874700	0.45565300
H	-0.29469700	-2.57262800	0.24079800
H	-0.14119100	-1.42565900	1.55716100
C	1.25088500	-1.18222200	0.00336700
C	2.37193700	-0.91149600	-0.40610100
H	3.43238900	-0.62229500	-0.73996400
Na	4.08653000	1.05892400	0.84627600

M1^{c2}

O	5.39467200	0.60212500	-0.45807900
H	5.36670600	0.72337000	-1.40690500
C	-3.32251000	-0.36824200	-0.53879400
H	-3.21397000	-0.24130300	-1.63139600
H	-4.28428100	-0.88447900	-0.38977500
C	-2.17624000	-1.22430300	-0.02127800
H	-2.33810700	-1.44733100	1.05058700
H	-2.15938200	-2.20096100	-0.53290600
C	-3.33982600	1.00174700	0.12385100
H	-4.15257400	1.62116300	-0.28802500
H	-3.56544600	0.88138500	1.19944500
C	-0.82576400	-0.52944500	-0.17588500
H	-0.64577500	-0.37583300	-1.25818700
C	-1.99864500	1.70467100	-0.02915700
H	-1.82633000	1.93015500	-1.09740900
H	-2.00932400	2.67854800	0.48581800
C	-0.85543900	0.84471500	0.48884300
H	0.11112600	1.35481300	0.34551500
H	-0.96615600	0.70436400	1.58133700
C	0.30446200	-1.41313400	0.36450300
H	0.22981100	-2.41548400	-0.09241700
H	0.14266600	-1.57806200	1.44589600
C	1.64473500	-0.88838500	0.15009100
C	2.76338200	-0.43963200	-0.04535200
H	3.79788500	-0.02898600	-0.21790500
Li	6.39694800	0.77789600	0.85667600

TS1[a2]

O	4.36833800	0.31756700	1.30871200
H	4.60287100	0.73364900	2.14160800
C	-4.11589000	0.34847300	0.14663400
H	-4.18756100	0.62933700	1.21320700
H	-5.06713000	0.66264700	-0.31191000
C	-2.95042500	1.09350600	-0.48703200
H	-2.94138900	0.90252600	-1.57728400
H	-3.07850600	2.18289800	-0.37392400
C	-3.93952600	-1.15929400	0.03839900
H	-4.77278500	-1.68381800	0.53287200
H	-3.98477200	-1.45419200	-1.02624500
C	-1.60612400	0.66216900	0.09409400
H	-1.60235100	0.92416000	1.17062100
C	-2.60517700	-1.60032900	0.62237900
H	-2.60492800	-1.41082400	1.71127300
H	-2.47073800	-2.68777600	0.50664600
C	-1.44265200	-0.85196400	-0.01286300
H	-0.48740100	-1.16012200	0.44278500
H	-1.37223700	-1.12321000	-1.08425300
C	-0.45454700	1.42206400	-0.57516800
H	-0.66431900	2.50541700	-0.52457300
H	-0.45632600	1.18414000	-1.65574900
C	0.86615200	1.15819800	-0.01524500
C	1.96992500	0.93383100	0.48402400
H	3.13606900	0.70550300	0.99991200
K	4.03549300	-0.81530400	-0.75821200

TS1^{b2}

O	-4.47797900	-0.51276700	-0.55200400
H	-4.85812200	-0.66629900	-1.42069200
Na	-2.97942600	-1.12179300	0.79239900
C	3.47931700	0.18664100	-0.32408900
H	3.50271500	0.26349100	-1.42633700
H	4.48169500	0.48692300	0.02057000
C	2.42545300	1.13980900	0.21934500
H	2.47119500	1.14637100	1.32510200
H	2.63658900	2.17504100	-0.09603800
C	3.18340100	-1.25332800	0.07000800
H	3.93513900	-1.93553100	-0.35781800
H	3.27096600	-1.35478200	1.16738700
C	1.01431400	0.74435200	-0.20758200
H	0.96191900	0.80972700	-1.31204800
C	1.78327000	-1.66244100	-0.36057500
H	1.73024300	-1.66873300	-1.46431000
H	1.56450600	-2.69443400	-0.04252600
C	0.73097200	-0.70585700	0.17971600
H	-0.26900900	-1.00152600	-0.18420300
H	0.69748200	-0.77761300	1.28467400
C	-0.02447300	1.71529900	0.36806200
H	0.23843200	2.74437400	0.06627300
H	0.06078500	1.71258200	1.47101100
C	-1.40114100	1.42768200	-0.01870700
C	-2.55756100	1.19216800	-0.37938800
H	-3.62833300	0.49630900	-0.61213400

TS1^{c2}

O	4.54709300	1.08706400	-0.07208400
H	4.91605200	1.45059500	-0.88192700
C	-3.12302800	-0.26107900	-0.38941100
H	-3.10277800	-0.21768800	-1.49350300
H	-4.11226900	-0.66476800	-0.12169700
C	-2.02296400	-1.19371700	0.09419400
H	-2.10867700	-1.32583600	1.18955100
H	-2.14604700	-2.19943300	-0.34014300
C	-2.94714000	1.14309400	0.16965100
H	-3.72959800	1.81602200	-0.21539300
H	-3.08188500	1.11718000	1.26653500
C	-0.62887200	-0.65802400	-0.22339900
H	-0.52919100	-0.59906000	-1.32498900
C	-1.56527400	1.69329100	-0.15173400
H	-1.47222300	1.82603700	-1.24477100
H	-1.43356900	2.69543400	0.28632700
C	-0.46678400	0.75652600	0.32877200
H	0.52101100	1.15889600	0.04074000
H	-0.47463900	0.71082500	1.43506500
C	0.44987300	-1.61738300	0.29437400
H	0.26756600	-2.62314000	-0.12266500
H	0.32566500	-1.73541700	1.38708700
C	1.82008100	-1.21616700	-0.00189800
C	2.98323700	-0.90837400	-0.28478000
H	3.98532400	-0.03705700	-0.33501500
Li	2.93457900	1.16729800	0.67895200

M2[a2]

C	-1.17260900	-0.54520800	-0.16970700
H	-0.94652600	-0.34639500	-1.23664900
C	-2.54422300	-1.21252200	-0.10185200
H	-2.52751800	-2.16746900	-0.65358700
H	-2.75648600	-1.47732400	0.95183100
C	-3.65073100	-0.31038500	-0.62853200
H	-3.49355500	-0.13937600	-1.70936100
H	-4.62927300	-0.80978100	-0.54239600
C	-3.66758100	1.03071500	0.09108800
H	-4.44930200	1.68557900	-0.32663700
H	-3.94115800	0.86976900	1.15022600
C	-2.30612500	1.70807000	0.02514600
H	-2.31928000	2.65962200	0.58091200
H	-2.08464000	1.97518300	-1.02452300
C	-1.20460800	0.79992600	0.55131200
H	-1.36536700	0.61558600	1.63131700
C	-0.07763500	-1.47218700	0.37388200
H	-0.17579500	-2.45495000	-0.12456800
H	-0.30090700	-1.67829800	1.43956300
C	1.28996100	-0.97204300	0.22891300
C	2.44938300	-0.53669600	0.08898500
H	-0.22079100	1.29048600	0.47198400
K	4.97450600	0.47575500	-0.17702700

M2[b2]

C	-0.58381100	-0.51499900	-0.17072000
H	-0.39598100	-0.33793300	-1.24875200
C	-1.90562800	-1.26893900	-0.04710300
H	-1.83790200	-2.23827600	-0.56895500
H	-2.07520600	-1.51218600	1.01937400
C	-3.08137600	-0.45912100	-0.57375900
H	-2.96106800	-0.31406200	-1.66306100
H	-4.02214300	-1.01869900	-0.44704400
C	-3.17038800	0.90104500	0.10351200
H	-4.00353200	1.48868500	-0.31465500
H	-3.40785000	0.75771200	1.17382400
C	-1.85913400	1.66403400	-0.01866300
H	-1.92258800	2.63061400	0.50676100
H	-1.68038800	1.90982800	-1.08157600
C	-0.68764300	0.84857700	0.50798700
H	-0.81059700	0.69009500	1.59698500
C	0.58221900	-1.34950600	0.37442600
H	0.54564100	-2.35043900	-0.09438200
H	0.39902000	-1.53822300	1.45043500
C	1.90635700	-0.75988200	0.18486600
C	3.02401600	-0.24434400	0.00645300
Na	5.14233300	0.68469100	-0.26536500
H	0.25927000	1.40009300	0.38806400

M2^{c2}

C	0.06305900	-0.43517800	-0.18668800
H	0.18575000	-0.29559900	-1.27938700
C	-1.14890800	-1.33697100	0.03446900
H	-0.98259400	-2.31745900	-0.44231100
H	-1.24366100	-1.54119100	1.11822800
C	-2.43634000	-0.70563000	-0.47487500
H	-2.37988000	-0.60609900	-1.57435800
H	-3.29425200	-1.36797600	-0.27646200
C	-2.66541100	0.66792900	0.13934400
H	-3.58142600	1.12660800	-0.26651600
H	-2.83873900	0.55465200	1.22538900
C	-1.46509800	1.57725100	-0.08171700
H	-1.62608300	2.55608100	0.39802300
H	-1.36135800	1.78474600	-1.16260400
C	-0.18113200	0.94017800	0.42881000
H	-0.23869100	0.82769100	1.52877400
C	1.34232400	-1.09259500	0.34646300
H	1.41656200	-2.11196500	-0.07495100
H	1.22448000	-1.24772200	1.43655700
C	2.57500500	-0.35665500	0.07814400
C	3.61724700	0.27506500	-0.15947400
H	0.68390900	1.59576400	0.23713300
Li	5.27716900	1.28070400	-0.53812400

TS2[a2,a1]

Si	-2.43882600	-0.21051900	-0.24418200
H	-2.29799000	1.65651400	-1.25383400
C	-2.47476100	-1.97824600	0.57055600
C	-3.70989600	-2.29603700	1.39712400
H	-1.56420300	-2.13334800	1.17847800
H	-2.38296400	-2.70956500	-0.25511000
H	-3.73578300	-3.33646600	1.76393500
H	-3.78977800	-1.65234500	2.28878400
H	-4.64129200	-2.14775300	0.82508700
C	-2.58218400	0.86059000	1.34006200
C	-1.55870900	0.56419300	2.42606900
H	-3.59386400	0.66061500	1.73877600
H	-2.60334700	1.93669800	1.10006900
H	-1.67112000	1.22150600	3.30293000
H	-1.63358700	-0.46942300	2.79478300
H	-0.51538300	0.67623500	2.08022700
C	-3.93507800	-0.35504000	-1.41441400
C	-5.09312700	0.56597100	-1.07331300
H	-4.28165400	-1.40475100	-1.42062100
H	-3.58059500	-0.14698400	-2.43698900
H	-5.90757200	0.51155700	-1.81336700
H	-5.54048400	0.32776900	-0.09462600
H	-4.76604600	1.61782200	-1.03037500
C	2.85587100	-0.74398500	-0.58129200
H	2.59628500	-1.64573100	0.00611900
C	4.26954800	-0.92535000	-1.12732500
H	4.30907400	-1.81423000	-1.77783800
H	4.51023000	-0.06363500	-1.77850700
C	5.30499900	-1.02403700	-0.01697200

H	5.12472300	-1.94524800	0.56600500
H	6.31431500	-1.13043300	-0.44465200
C	5.24006600	0.17769600	0.91379400
H	5.97200600	0.07647900	1.73053400
H	5.53169500	1.08634400	0.35580000
C	3.83823400	0.36205300	1.47514100
H	3.78881700	1.25440900	2.11899600
H	3.59101300	-0.49522500	2.12655500
C	2.79963500	0.45212000	0.36650300
H	2.96985200	1.37767900	-0.22093800
C	1.84246900	-0.62266100	-1.72673200
H	1.92839600	-1.50530000	-2.38356100
H	2.12498400	0.23661400	-2.36501200
C	0.46064000	-0.48522500	-1.29455100
C	-0.69914400	-0.34661000	-0.91218900
H	1.78991100	0.52644100	0.80735800
K	-0.17123400	2.48149600	-0.32343300

TS2^{b2,b1}

Si	-2.47496200	0.30387400	-0.15011000
H	-2.91816600	-0.61122800	1.09128200
C	-1.35636400	1.68534500	-0.95371300
C	-0.50918100	2.52635100	-0.01533200
H	-2.03414000	2.34609900	-1.52798600
H	-0.70433800	1.19663900	-1.70113900
H	0.15142500	3.23672200	-0.54267600
H	-1.12609000	3.12888800	0.67081800
H	0.14724100	1.90256200	0.61617700
C	-3.29983900	-0.57893500	-1.63184200
C	-3.68522100	-2.03272700	-1.42217300
H	-2.61484800	-0.50477800	-2.49448400
H	-4.19400500	0.00220500	-1.91974800
H	-4.20531800	-2.47538100	-2.28709600
H	-2.79447800	-2.66964600	-1.26904700
H	-4.35928800	-2.16860400	-0.55857200
C	-3.85312700	1.53366400	0.54430200
C	-3.70247500	1.94290900	1.99816400
H	-4.80542000	0.97648100	0.43387100
H	-3.95565500	2.43296600	-0.09297200
H	-4.56818400	2.49904500	2.39845700
H	-3.57537200	1.06058600	2.65123400
H	-2.81982500	2.58138700	2.16834300
C	2.75198100	-0.58979600	0.40046100
H	2.44894700	0.07888300	1.23075300
C	4.16093800	-1.09357400	0.70138900
H	4.16630400	-1.66675800	1.64357200
H	4.45828300	-1.80801700	-0.08977500
C	5.16905900	0.04527700	0.76223600

H	4.92813300	0.69360100	1.62439100
H	6.18028100	-0.34753400	0.95436000
C	5.15016600	0.87997200	-0.51045500
H	5.85631300	1.72193000	-0.43113600
H	5.50848900	0.26221700	-1.35436600
C	3.74726100	1.38174200	-0.82171000
H	3.73811800	1.95035800	-1.76527200
H	3.43208600	2.09435700	-0.03713300
C	2.74763600	0.23698200	-0.88277500
H	2.99915400	-0.42829700	-1.73110100
C	1.74509900	-1.74695600	0.34999700
H	1.83589300	-2.34490300	1.27405600
H	2.03124500	-2.43482000	-0.46761900
C	0.36785800	-1.30250500	0.16193800
C	-0.75434700	-0.82537100	-0.04838000
Na	-2.03333600	-2.54083400	1.17339900
H	1.73272000	0.61572600	-1.08568100

TS2^{c2,c1}

Si	-2.62078100	0.01066500	-0.08473400
H	-2.94786000	-0.74402900	1.31456400
C	-1.65149300	1.36125000	-1.08641500
C	-0.90084600	2.41530200	-0.29160100
H	-2.39351600	1.85562100	-1.74223500
H	-0.95089300	0.83775400	-1.76254200
H	-0.32139800	3.10594700	-0.92793100
H	-1.58023100	3.04272800	0.30749100
H	-0.18136400	1.96640000	0.41477100
C	-3.34062700	-1.16926700	-1.39128400
C	-3.90893000	-2.47495000	-0.86556000
H	-2.55403100	-1.37564900	-2.13781700
H	-4.12329800	-0.61238200	-1.93831900
H	-4.31800800	-3.11871900	-1.66140500
H	-3.14063100	-3.07487200	-0.34738000
H	-4.72338900	-2.31095600	-0.14163500
C	-4.13154600	1.14479400	0.45300900
C	-4.03656800	1.78186200	1.82728000
H	-5.01338900	0.47353700	0.43583900
H	-4.33196000	1.91980000	-0.31081800
H	-4.96262800	2.29033300	2.14628900
H	-3.81708800	1.02823900	2.60483300
H	-3.23291700	2.53399800	1.88988900
C	2.73175700	-0.52074200	0.52970700
H	2.41867100	0.29593500	1.21020400
C	4.14845000	-0.93391800	0.91940100
H	4.16367600	-1.30466700	1.95786300
H	4.45396200	-1.78955600	0.28771200
C	5.14023100	0.20705900	0.74379100

H	4.89262400	1.01302000	1.45848700
H	6.15711600	-0.12575200	1.00606500
C	5.10682500	0.76683900	-0.67121400
H	5.80116800	1.61677100	-0.76711400
H	5.47215100	-0.00380600	-1.37457800
C	3.69657000	1.17679600	-1.07047400
H	3.67719000	1.54198100	-2.10953300
H	3.37289200	2.02934700	-0.44517400
C	2.71263800	0.03030400	-0.89397600
H	2.97118000	-0.78928200	-1.59154300
C	1.74669200	-1.68230700	0.71686500
H	1.85097900	-2.08684500	1.73865800
H	2.03549900	-2.51310400	0.04689200
C	0.35901600	-1.31205600	0.46402500
C	-0.77854100	-0.91825200	0.17839800
H	1.69295600	0.34789600	-1.16591600
Li	-1.67943200	-1.81176000	1.80631400

H_2O

O	0.00000000	0.00000000	0.12112100
H	0.00000000	0.75071100	-0.48448300
H	0.00000000	-0.75071100	-0.48448300.

P

C	-5.33245800	-0.07619600	-0.71551800
H	-5.18496900	0.43655100	-1.68350400
H	-6.32923200	-0.54211200	-0.77090000
C	-4.25993700	-1.14126100	-0.54815900
H	-4.46556000	-1.73171300	0.36475400
H	-4.29077300	-1.85899600	-1.38450100
C	-5.28050800	0.95011700	0.40700700
H	-6.03900500	1.73380000	0.25143500
H	-5.54478600	0.45779700	1.36101000
C	-2.86434200	-0.53391300	-0.43205300
H	-2.64449300	-0.00458700	-1.37994900
C	-3.89316900	1.56331800	0.52908100
H	-3.67548800	2.15519500	-0.37863300
H	-3.85569600	2.27579100	1.36837300
C	-2.82278200	0.49549200	0.69518900
H	-1.82223500	0.95543500	0.75347600
H	-2.97117000	-0.03006100	1.65794900
C	-1.81084000	-1.63515600	-0.25754900
H	-1.92166800	-2.38036900	-1.06432600
H	-2.01605500	-2.18808700	0.67746200
C	-0.44069200	-1.15874200	-0.23692100
C	0.70726000	-0.72863300	-0.22320200
Si	2.41653900	-0.04091000	-0.15487500
C	3.60872000	-1.50458600	-0.15944500
C	5.08477400	-1.15111000	-0.07688200
H	3.40691000	-2.10154200	-1.06617500
H	3.32434300	-2.16390900	0.67956500
H	5.72428200	-2.04517700	-0.01467200
H	5.42239600	-0.58452900	-0.95803600

H	5.31633500	-0.53435200	0.80610200
C	2.66200500	1.09040600	-1.65007500
C	3.77624200	2.11963200	-1.53159300
H	1.70196800	1.60157000	-1.83859700
H	2.81934600	0.45020100	-2.53635600
H	3.88393700	2.71755800	-2.44979200
H	3.59063700	2.83093900	-0.71250900
H	4.75806500	1.66166700	-1.33595400
C	2.59075100	0.95114800	1.44225800
C	2.36987500	0.16178800	2.72157200
H	1.88810900	1.80189500	1.38732800
H	3.59517000	1.41120300	1.44617900
H	2.45803200	0.78982800	3.62161000
H	1.37045300	-0.30015700	2.75161800
H	3.10021300	-0.65492200	2.83304000

M0^{a1} (M0$^{KH)}$

H	5.98051	-2.32442	0.03312
C	-3.16032	-1.33198	-0.39761
H	-3.12088	-1.30908	-1.50179
H	-3.71832	-2.24442	-0.13497
C	-1.74301	-1.40634	0.14984
H	-1.77787	-1.54087	1.24738
H	-1.21875	-2.29134	-0.2465
C	-3.88817	-0.09295	0.10325
H	-4.89923	-0.03613	-0.33008
H	-4.0307	-0.17263	1.19648
C	-0.9453	-0.14264	-0.16059
H	-0.85085	-0.06001	-1.26076
C	-3.10081	1.17165	-0.20713
H	-3.05759	1.31398	-1.30225
H	-3.61657	2.05936	0.19159
C	-1.6837	1.09579	0.34156
H	-1.11884	2.0067	0.08359
H	-1.71735	1.06105	1.4471
C	0.4697	-0.25002	0.42292
H	0.93141	-1.19431	0.08431
H	0.40682	-0.33217	1.52272
C	1.34367	0.85871	0.08261
C	2.06796	1.79052	-0.21615
H	2.67289	2.64171	-0.4778
K	4.36712	-0.40704	-0.06654

M1^{a1} (M1^{KH})

H	-5.97195	1.39435	0.5703
C	3.45184	-1.02727	0.35576
H	3.60776	-0.79303	1.42434
H	4.09562	-1.89475	0.14107
C	1.99064	-1.38813	0.13292
H	1.85038	-1.73193	-0.90939
H	1.69859	-2.23691	0.77287
C	3.86616	0.17104	-0.48585
H	4.91467	0.44137	-0.28382
H	3.82542	-0.10454	-1.55555
C	1.06579	-0.20028	0.38498
H	1.16033	0.0852	1.45036
C	2.9499	1.36103	-0.24021
H	3.08138	1.71413	0.79858
H	3.23297	2.20901	-0.88348
C	1.48903	0.99748	-0.46155
H	0.83944	1.86225	-0.24934
H	1.32768	0.75012	-1.52815
C	-0.39555	-0.59812	0.13748
H	-0.63074	-1.51059	0.71127
H	-0.51952	-0.87562	-0.92489
C	-1.35911	0.43343	0.47961
C	-2.14713	1.31048	0.78397
H	-2.83064	2.09609	1.06066
K	-4.48159	-0.40719	-0.37654

$M0^{b1}$ ($M0^{NaH}$)

Na	4.57043600	-0.44050700	0.27054800
H	6.02263900	-1.67904600	0.98576700
C	-2.89640400	-1.07787400	-0.39631500
H	-2.98920800	-0.88920400	-1.48132000
H	-3.53822400	-1.94777400	-0.18571600
C	-1.44620900	-1.40302400	-0.07054700
H	-1.36347300	-1.69886700	0.99220900
H	-1.10207600	-2.27244700	-0.65427900
C	-3.38067700	0.14577300	0.36760200
H	-4.41951200	0.38769300	0.09253000
H	-3.39877200	-0.08456400	1.44854600
C	-0.52796100	-0.20921600	-0.31718400
H	-0.56364300	0.03128700	-1.39736300
C	-2.47065100	1.34122600	0.12679500
H	-2.54321500	1.64686300	-0.93281100
H	-2.80564600	2.21055800	0.71433200
C	-1.02094900	1.01389800	0.45236400
H	-0.37294900	1.88148500	0.24570700
H	-0.92251700	0.81068600	1.53567200
C	0.92329700	-0.56937200	0.03102000
H	1.21092600	-1.49395700	-0.49604000
H	0.99473700	-0.80679400	1.10811400
C	1.87663400	0.47664100	-0.29356300
C	2.64720300	1.37451600	-0.58272000
H	3.29043700	2.19424200	-0.85607700

M0[c1]

H	5.35098000	-1.34853500	2.11617500
C	-2.46888500	-0.90674800	-0.36177100
H	-2.55412400	-0.73878800	-1.45076200
H	-3.19912900	-1.69506500	-0.12047100
C	-1.05927700	-1.38013900	-0.03969400
H	-0.99703900	-1.65447700	1.03015500
H	-0.81823400	-2.29718600	-0.60171300
C	-2.80711900	0.38275800	0.37189900
H	-3.81650100	0.72979000	0.09978800
H	-2.83672100	0.18511100	1.45899600
C	-0.01904100	-0.30088800	-0.32707600
H	-0.03974300	-0.08755900	-1.41337300
C	-1.77475100	1.46436900	0.08894900
H	-1.82529400	1.74583000	-0.97859400
H	-2.00614100	2.38139200	0.65330800
C	-0.36585600	0.98917700	0.41188600
H	0.37087800	1.77436000	0.17507900
H	-0.27781400	0.80663100	1.49971600
C	1.38656000	-0.81071200	0.01981600
H	1.57051400	-1.77343700	-0.48550300
H	1.44198100	-1.02746100	1.10169200
C	2.44820100	0.11271000	-0.33685900
C	3.32327900	0.90008000	-0.65132200
H	4.06868400	1.61332400	-0.96094000
Li	4.52967800	-0.43919200	0.94049600

TS1[a1]

H	-4.69779	-0.27246	0.52196
C	2.92953	-0.10655	-0.89649
H	2.53043	-0.68438	-1.75037
H	3.93822	0.21648	-1.19902
C	2.03662	1.1021	-0.65527
H	2.4872	1.74769	0.12184
H	1.97074	1.72405	-1.56302
C	3.0011	-1.00767	0.32803
H	3.61326	-1.89895	0.11752
H	3.51805	-0.4709	1.14397
C	0.63893	0.69616	-0.19664
H	0.18986	0.09415	-1.01596
C	1.6127	-1.41047	0.80338
H	1.13825	-2.05645	0.03989
H	1.67693	-2.02339	1.71631
C	0.73589	-0.19079	1.04267
H	-0.26801	-0.48648	1.39466
H	1.15983	0.41194	1.86743
C	-0.25963	1.91826	0.02868
H	-0.19824	2.57865	-0.85418
H	0.15322	2.51449	0.86326
C	-1.65703	1.5901	0.29637
C	-2.84291	1.32541	0.52889
H	-3.95356	0.53023	0.57792
K	-2.65419	-1.33811	-0.50842

TS1[b1]

Na	2.47753000	1.53451500	-0.73713300
H	4.55384000	1.42679800	-0.04913400
C	-2.70647600	-0.30595100	-0.76282600
H	-2.47024000	0.12980900	-1.75092400
H	-3.67123800	-0.82275300	-0.88607500
C	-1.61919100	-1.30166900	-0.38525800
H	-1.90295300	-1.82340000	0.54800500
H	-1.52484700	-2.08683000	-1.15311600
C	-2.82319800	0.81117600	0.26282300
H	-3.58627600	1.54283300	-0.04626100
H	-3.17759000	0.38912400	1.22060900
C	-0.26950400	-0.62312100	-0.16725900
H	0.02653300	-0.16132300	-1.13412800
C	-1.48420100	1.49751600	0.48836100
H	-1.18555700	2.02377900	-0.43759600
H	-1.57179500	2.27633800	1.26216200
C	-0.40674200	0.49232700	0.86675100
H	0.56086500	0.99964700	1.03723100
H	-0.65483300	0.03410800	1.84219900
C	0.81369400	-1.64079000	0.21376300
H	0.79449100	-2.47561400	-0.50827300
H	0.55043900	-2.09320000	1.18752300
C	2.16050800	-1.08152600	0.27788700
C	3.31198000	-0.62793400	0.33862000
H	4.14511000	0.44085600	0.17906000

TS1^{c1}

H	4.57895000	2.09967400	-0.09735600
C	-2.53134700	-0.69118400	-0.29705400
H	-2.56102200	-0.70785400	-1.40155200
H	-3.39946900	-1.28101700	0.03706500
C	-1.23966100	-1.33675700	0.17860900
H	-1.25509000	-1.41674300	1.28213500
H	-1.15798900	-2.37008800	-0.19653600
C	-2.64034100	0.74698700	0.18513500
H	-3.56473400	1.21470100	-0.18903100
H	-2.71996100	0.75625100	1.28759900
C	-0.00479300	-0.53803500	-0.23298100
H	0.04615300	-0.53207500	-1.33898000
C	-1.42507600	1.55952500	-0.23658400
H	-1.40778700	1.64179400	-1.33811600
H	-1.49458700	2.59144700	0.14236900
C	-0.12950600	0.91144000	0.23044300
H	0.72749300	1.50291500	-0.14228300
H	-0.07908600	0.93886500	1.33645000
C	1.26528500	-1.21574100	0.29468900
H	1.29198100	-2.26049200	-0.06012800
H	1.19709200	-1.29104700	1.39589400
C	2.51568800	-0.55956000	-0.07092000
C	3.59419700	-0.06446500	-0.43092200
H	4.32399000	1.07407500	-0.36703100
Li	3.01579600	1.72211100	0.64233500

TS1^{KH}

H	3.62405	0.49368	-1.77095
C	-2.99988	-1.20754	-0.58197
H	-3.13248	-0.87793	-1.62847
H	-3.47444	-2.19966	-0.51632
C	-1.5125	-1.31062	-0.27849
H	-1.37265	-1.74513	0.73019
H	-1.02177	-2.00735	-0.97843
C	-3.6917	-0.2185	0.345
H	-4.75933	-0.12834	0.08822
H	-3.6606	-0.6081	1.37929
C	-0.82151	0.05006	-0.32321
H	-0.91076	0.44002	-1.3562
C	-3.01226	1.14276	0.30376
H	-3.14503	1.58462	-0.70054
H	-3.49691	1.84018	1.00553
C	-1.52535	1.03441	0.60702
H	-1.03962	2.02176	0.545
H	-1.38652	0.69327	1.65124
C	0.6734	-0.08063	-0.00906
H	1.09151	-0.88133	-0.66566
H	0.75767	-0.4554	1.03155
C	1.45598	1.15214	-0.16716
C	2.47371	1.64141	-0.72221
H	3.05854	2.53165	-0.91276
K	3.82258	-0.73278	0.37138

TS1^{Na}

Na	1.88375	-1.50795	1.08208
H	2.84002	-1.62427	-0.73051
C	-2.57148	0.40983	0.72442
H	-2.37282	-0.08716	1.69201
H	-3.50774	0.97288	0.86465
C	-1.4248	1.35818	0.40782
H	-1.66396	1.93992	-0.50193
H	-1.29637	2.09816	1.21479
C	-2.74016	-0.64835	-0.35672
H	-3.54742	-1.34896	-0.0906
H	-3.06009	-0.15958	-1.29475
C	-0.1136	0.61221	0.16844
H	0.11133	0.09784	1.13135
C	-1.4401	-1.39809	-0.61004
H	-1.184	-1.99549	0.287
H	-1.56301	-2.12795	-1.42535
C	-0.29827	-0.44177	-0.9231
H	0.64242	-0.98866	-1.11211
H	-0.50876	0.08682	-1.87088
C	1.04018	1.57463	-0.14015
H	1.04162	2.37366	0.62436
H	0.79545	2.11101	-1.0766
C	2.39119	1.02016	-0.28751
C	3.20378	0.06797	-0.48518
H	4.27169	-0.08936	-0.60213

M2^{KH}

H	-2.65788	-1.2541	-1.22101
C	3.39741	0.8279	-0.46839
H	3.35438	0.65111	-1.55906
H	4.19867	1.56982	-0.31622
C	2.05783	1.38106	-0.0026
H	2.13196	1.6706	1.06423
H	1.81591	2.31025	-0.54652
C	3.73911	-0.47855	0.23365
H	4.68931	-0.88736	-0.1472
H	3.90505	-0.27893	1.30859
C	0.91841	0.37368	-0.15771
H	0.83267	0.14517	-1.23997
C	2.61562	-1.49474	0.08573
H	2.52635	-1.78594	-0.97756
H	2.8585	-2.42163	0.63093
C	1.28634	-0.92525	0.55994
H	0.48083	-1.66744	0.44407
H	1.34738	-0.71641	1.64602
C	-0.41707	0.95181	0.32529
H	-0.48793	1.99644	-0.04189
H	-0.33787	1.09515	1.42361
C	-1.73645	0.28402	0.0016
C	-1.73512	-0.72595	-0.89899
H	-0.85491	-1.15096	-1.43051
K	-4.45047	-0.02314	0.15217

M2^{NaH}

H	4.16455700	-0.93862200	-0.64986700
C	-2.86083400	-0.73988300	-0.46266500
H	-2.76445600	-0.70706500	-1.56364800
H	-3.72683800	-1.38978200	-0.25653100
C	-1.59230500	-1.33578100	0.13021700
H	-1.72699600	-1.47493100	1.22059600
H	-1.41229100	-2.34449000	-0.27852300
C	-3.11225600	0.66832700	0.05648800
H	-4.01243000	1.10083200	-0.40981200
H	-3.32508200	0.62237300	1.14058800
C	-0.36422800	-0.45506300	-0.09842100
H	-0.21170000	-0.38146900	-1.19600600
C	-1.90234200	1.56154700	-0.17555900
H	-1.76018800	1.70289200	-1.26304800
H	-2.07949700	2.56824100	0.23742400
C	-0.63920400	0.95580000	0.41902500
H	0.23155700	1.60313200	0.22579900
H	-0.73983600	0.90977700	1.52118000
C	0.89694500	-1.08088800	0.50926500
H	0.88610300	-2.17148100	0.26779000
H	0.77570300	-1.03498800	1.61211800
C	2.20044700	-0.43021800	0.12657400
C	3.15528500	-1.26866300	-0.33540000
H	3.02765200	-2.37156500	-0.44315700
Na	3.45315400	1.55055300	-0.10745900

TS2^{KH}

H	-2.88404800	1.26475200	1.43680500
C	2.78032900	-1.35564100	0.49663100
H	2.82647500	-1.18457600	1.58765400
H	3.19089300	-2.36505600	0.33379100
C	1.32935800	-1.29930300	0.04520800
H	1.26845900	-1.56767200	-1.02702000
H	0.72065400	-2.04442800	0.58095800
C	3.62872500	-0.30964900	-0.21091600
H	4.66783800	-0.33693400	0.15482400
H	3.67966100	-0.55147100	-1.28856600
C	0.71944100	0.08823400	0.22958500
H	0.74059900	0.33774100	1.30795200
C	3.03458800	1.07997700	-0.03844700
H	3.09042400	1.36806400	1.02725600
H	3.62976400	1.82930200	-0.58466700
C	1.58250700	1.13384400	-0.48988800
H	1.15802600	2.13676600	-0.32497200
H	1.52380800	0.95662900	-1.58048400
C	-0.72800900	0.14584900	-0.22394900
H	-1.45020500	-1.19554800	0.98778600
H	-0.93443600	-0.50352500	-1.09148500
C	-1.46626900	1.28944000	-0.13574300
C	-2.44810400	1.82469000	0.57569000
H	-2.85143000	2.83577900	0.43505300
K	-3.63009900	-0.87181400	-0.18125800

TS2^{NaH}

Na	3.38364200	-1.41573700	-0.45178800
H	3.55730700	2.20155100	-0.43590100
C	-2.47732800	-1.25977600	-0.20280900
H	-2.37954900	-1.45534600	-1.28663400
H	-3.11109000	-2.07011200	0.19214400
C	-1.09915800	-1.30885900	0.43905900
H	-1.20222700	-1.20825400	1.53635500
H	-0.61940100	-2.28498600	0.26889400
C	-3.14378600	0.09160500	0.00287000
H	-4.12584200	0.12231500	-0.49615900
H	-3.34542500	0.23636100	1.08019800
C	-0.18980900	-0.19196000	-0.06424100
H	-0.04551300	-0.32281200	-1.15375400
C	-2.25298000	1.21886400	-0.49473100
H	-2.14618600	1.14003800	-1.59214400
H	-2.72107500	2.19881500	-0.30745900
C	-0.87163600	1.16755200	0.14233800
H	-0.23419600	1.97102600	-0.25896800
H	-0.95823600	1.35799900	1.22902100
C	1.17506500	-0.15195000	0.60483200
H	1.54918000	-1.92025500	0.34659100
H	1.14906600	-0.38606500	1.67913900
C	2.17122800	0.68925400	0.18773600
C	2.58931300	1.93986100	0.02180900
H	2.00767600	2.82528000	0.34715500

M3

C	1.95787500	1.22940200	0.28218900
H	1.94630500	1.26367600	1.38545800
H	2.48669800	2.14152700	-0.03391000
C	0.52327500	1.23487600	-0.21947200
H	0.02095000	2.19174700	-0.00996600
H	0.52625800	1.13749800	-1.32021300
C	-0.28803100	0.07685000	0.39556800
H	-0.68320500	0.41025300	1.36949100
C	0.61867700	-1.15242000	0.63520400
H	1.04375900	-1.09591400	1.65163400
H	0.01712100	-2.07451600	0.61785300
C	1.75377700	-1.21115800	-0.37368800
H	2.30409300	-2.16077300	-0.29001900
H	1.32740600	-1.20993600	-1.39226700
C	2.70144700	-0.02087300	-0.19980200
H	3.50087900	-0.27495000	0.51535700
H	3.21339500	0.18559500	-1.15385000
C	-1.46128100	-0.26482700	-0.48648700
H	-1.21883900	-0.70534100	-1.46618100
C	-2.72432200	-0.06788100	-0.19568800
C	-3.98278500	0.13378200	0.10471100
H	-4.49173300	1.07321500	-0.14154100
H	-4.58487200	-0.62857600	0.61293800

M4^{KH}

C	-1.66283600	1.21358700	0.66269100
H	-2.75043100	1.38842400	0.72846200
H	-1.18413100	2.13422900	1.03297000
C	-1.29667600	0.02536600	1.54333300
H	-0.19704800	-0.07971500	1.59286800
H	-1.61508500	0.21299500	2.58040800
C	-1.90606600	-1.26866300	1.02269300
H	-1.59832000	-2.12123800	1.64828800
H	-3.00664800	-1.21259100	1.10643900
C	-1.53867100	-1.51075700	-0.43401600
H	-2.01000000	-2.43228700	-0.80980900
H	-0.44842600	-1.68977800	-0.51224300
C	-1.91926800	-0.32641800	-1.30938600
H	-1.62948500	-0.50320100	-2.35799400
H	-3.01742300	-0.21926900	-1.31044800
C	-1.30883200	0.98719200	-0.80775700
H	-1.75188400	1.80617500	-1.40446500
C	0.17786800	1.03877600	-1.08662200
H	0.48641800	0.69084000	-2.08531000
C	1.10508100	1.52178100	-0.29027600
C	2.02856200	1.97336400	0.52064300
H	2.54638200	1.32493100	1.24698900
H	2.32131700	3.03000400	0.52567300
H	3.54608100	-0.86387500	2.10094500
K	2.53861600	-1.23110600	-0.15845100

M4^{NaH}

C	0.96540600	-1.41195900	0.72053300
H	1.95122500	-1.90213400	0.79534900
H	0.23838500	-2.13051100	1.13205700
C	0.98248400	-0.13104200	1.54508200
H	-0.03518300	0.29704900	1.59572900
H	1.24999500	-0.35906500	2.58852100
C	1.93643800	0.90282600	0.96420600
H	1.89259900	1.83767700	1.54455200
H	2.97413900	0.53411700	1.05793400
C	1.64759200	1.17141400	-0.50518100
H	2.36831900	1.89273400	-0.92051900
H	0.66095300	1.66616500	-0.60291700
C	1.65354800	-0.11300200	-1.31907500
H	1.42730400	0.08944800	-2.37856400
H	2.66868700	-0.54466400	-1.30058900
C	0.67975500	-1.15601200	-0.75979900
H	0.84571800	-2.09712900	-1.31647900
C	-0.75478900	-0.76750900	-1.04613200
H	-0.95145600	-0.39292000	-2.06365700
C	-1.78086700	-0.90773400	-0.23609100
C	-2.79420300	-1.03126800	0.58437000
H	-3.09473400	-0.23548400	1.27888000
H	-3.38697500	-1.95276100	0.62552800
Na	-1.96913500	1.91164400	-0.28706000
H	-2.36068000	2.93510800	1.43435100

TS3^{KH}

C	-1.38760600	0.63255500	1.33264900
H	-2.40846700	0.49954300	1.73329400
H	-0.89753300	1.37613300	1.98160400
C	-0.65141300	-0.69404200	1.41959500
H	0.42438100	-0.49046700	1.27302700
H	-0.70595100	-1.09132700	2.44540700
C	-1.18779000	-1.72785000	0.43521800
H	-0.57446600	-2.64692400	0.45329200
H	-2.18815400	-2.05179000	0.77320400
C	-1.32197100	-1.18414700	-0.98278700
H	-1.77607800	-1.94109200	-1.64135000
H	-0.32927100	-0.97731800	-1.42952400
C	-2.12817000	0.10398400	-1.00471400
H	-2.21597500	0.48902300	-2.03380300
H	-3.15791300	-0.11275600	-0.66873400
C	-1.51549800	1.17339700	-0.08946800
H	-2.23905900	2.00884400	-0.05336200
C	-0.26481500	1.78879900	-0.70821800
H	-0.55647300	2.38341300	-1.59835400
C	1.01872300	1.80274300	-0.37382300
C	2.15199300	1.61458800	0.37151000
H	3.05931800	1.24770600	-0.12623100
H	2.42225400	2.44089800	1.04217700
H	2.33016300	0.43461000	1.61108500
K	2.13329000	-1.19098200	-0.32429000

TS3^{NaH}

H	4.16455700	-0.93862200	-0.64986700
C	-2.86083400	-0.73988300	-0.46266500
H	-2.76445600	-0.70706500	-1.56364800
H	-3.72683800	-1.38978200	-0.25653100
C	-1.59230500	-1.33578100	0.13021700
H	-1.72699600	-1.47493100	1.22059600
H	-1.41229100	-2.34449000	-0.27852300
C	-3.11225600	0.66832700	0.05648800
H	-4.01243000	1.10083200	-0.40981200
H	-3.32508200	0.62237300	1.14058800
C	-0.36422800	-0.45506300	-0.09842100
H	-0.21170000	-0.38146900	-1.19600600
C	-1.90234200	1.56154700	-0.17555900
H	-1.76018800	1.70289200	-1.26304800
H	-2.07949700	2.56824100	0.23742400
C	-0.63920400	0.95580000	0.41902500
H	0.23155700	1.60313200	0.22579900
H	-0.73983600	0.90977700	1.52118000
C	0.89694500	-1.08088800	0.50926500
H	0.88610300	-2.17148100	0.26779000
H	0.77570300	-1.03498800	1.61211800
C	2.20044700	-0.43021800	0.12657400
C	3.15528500	-1.26866300	-0.33540000
H	3.02765200	-2.37156500	-0.44315700
Na	3.45315400	1.55055300	-0.10745900

M5^{KH}

C	-2.70001800	-1.46592500	-0.27880000
H	-2.78290700	-1.89730000	0.73476200
H	-3.18140600	-2.19694100	-0.94751500
C	-1.22575600	-1.28308900	-0.65171500
H	-1.08918400	-1.41064700	-1.73948100
H	-0.62555600	-2.08699800	-0.18664700
C	-0.65444400	0.08018900	-0.22594900
H	-0.90109500	0.81229600	-1.01895100
C	-1.38607500	0.56043900	1.03326500
H	-0.90665600	1.47075500	1.42761200
H	-1.25988500	-0.20268800	1.82393800
C	-2.87397000	0.81173500	0.76544100
H	-3.44311400	0.70435900	1.70411500
H	-3.02621800	1.85671700	0.44783400
C	-3.43580900	-0.13563200	-0.30010800
H	-4.51894800	-0.27763100	-0.16028000
H	-3.32425900	0.31343800	-1.30268000
C	0.85671700	0.04630200	-0.06441600
H	1.17018700	-0.97075200	0.27974800
C	1.78737200	1.02113300	-0.22698500
C	1.30086800	2.38397900	-0.64262800
H	0.24109700	2.47622200	-0.97201300
H	1.41501100	3.10183900	0.19160600
H	1.91560800	2.82048600	-1.45108200
K	3.70021100	-0.87515500	0.24844200

M5^{NaH}

C	-2.52664600	-1.23419600	-0.34237900
H	-2.70319700	-1.68347300	0.65132700
H	-3.08514400	-1.86521100	-1.05173600
C	-1.03030100	-1.25271100	-0.66753500
H	-0.87782700	-1.35884200	-1.75524300
H	-0.56659200	-2.15029900	-0.21898500
C	-0.28365700	0.00002000	-0.17295700
H	-0.38732800	0.78439800	-0.94557200
C	-0.98047200	0.54152000	1.08067800
H	-0.39029500	1.36405800	1.51617500
H	-0.98699800	-0.25363400	1.84943500
C	-2.40959200	1.00815800	0.78291100
H	-3.01753000	0.94772500	1.70114400
H	-2.40524800	2.07482100	0.50381700
C	-3.06339800	0.18799100	-0.33363800
H	-4.15985200	0.19932500	-0.23068300
H	-2.85560700	0.65045700	-1.31473300
C	1.19404100	-0.27200400	0.04064100
H	1.33114000	-1.28187400	0.49580900
C	2.28457200	0.50064000	-0.20075800
Na	3.84620400	-1.12762300	0.46815000
C	2.08414400	1.87422900	-0.77881300
H	1.05584300	2.14726700	-1.10082100
H	2.38645100	2.64964300	-0.05060400
H	2.74179100	2.05761000	-1.64788700

TS4^{KH}

C	-2.85129	0.61126	-0.91475
H	-2.72209	-0.11505	-1.73652
H	-3.59778	1.3351	-1.27607
C	-1.52623	1.31889	-0.63229
H	-1.7081	2.32878	-0.22965
H	-0.96438	1.45964	-1.56933
C	-0.64232	0.54185	0.3661
H	-0.91553	0.86674	1.38819
C	-0.94994	-0.95731	0.29156
H	-0.25681	-1.52273	0.93862
H	-0.75774	-1.29319	-0.74335
C	-2.3947	-1.25872	0.69873
H	-2.71417	-2.20004	0.22288
H	-2.44942	-1.44279	1.78385
C	-3.35174	-0.12451	0.31724
H	-4.36903	-0.51622	0.16385
H	-3.43459	0.59574	1.15016
C	0.79373	0.85934	0.2313
H	1.09035	0.22665	-1.59059
C	1.86028	1.32137	0.72533
C	3.23642	1.55201	0.28105
H	3.37617	1.21772	-0.77711
H	3.5085	2.61906	0.29813
H	3.99524	1.05669	0.91096
K	2.46706	-1.46322	-0.37472

TS4^{NaH}

C	-2.49131100	-0.62241300	-1.04712100
H	-2.64756200	-1.60939400	-0.57724500
H	-3.01629100	-0.66987900	-2.01384700
C	-0.99679400	-0.38147200	-1.26758000
H	-0.83469400	0.25601300	-2.15268700
H	-0.48710200	-1.33698800	-1.47658800
C	-0.31970200	0.27399300	-0.05044700
H	-0.44103100	1.37336800	-0.14588800
C	-1.04013200	-0.13283100	1.23418800
H	-0.48473700	0.22145400	2.11668400
H	-1.02441500	-1.23433500	1.29488600
C	-2.47934400	0.38916600	1.25259700
H	-3.08969900	-0.25776300	1.90393200
H	-2.51477500	1.38913800	1.71551300
C	-3.09241100	0.44788000	-0.15047100
H	-4.18812500	0.35319700	-0.09679200
H	-2.90443900	1.43702700	-0.60472300
C	1.15191200	0.10476600	-0.02497200
H	0.99874900	-1.74940300	0.23486900
C	2.31559900	0.58031000	-0.09313400
Na	3.03125600	-1.74890000	0.30644400
C	3.13959500	1.78874200	-0.27892500
H	2.55499200	2.72734300	-0.31591600
H	3.89181000	1.91057900	0.51688100
H	3.71903000	1.73869600	-1.21477100

BP

C	-2.68707300	0.05055600	-0.38641700
H	-2.54336500	0.22640500	-1.46686900
H	-3.77682600	0.04106500	-0.23312700
C	-2.03641600	1.18647800	0.38621400
H	-2.55575800	2.13971400	0.20493200
H	-2.14914000	0.98952000	1.46641900
C	-0.55300300	1.32005700	0.03295400
H	0.00198700	1.73943600	0.88709600
H	-0.41197500	2.03231200	-0.79562600
C	0.07306700	-0.03629900	-0.36547700
H	-0.14678000	-0.21081800	-1.43659200
C	-0.60634500	-1.17073300	0.41401400
H	-0.07456900	-2.12046100	0.25484600
H	-0.51138900	-0.95076500	1.49124400
C	-2.07824400	-1.29722500	0.01274900
H	-2.18141800	-2.01229200	-0.81934000
H	-2.64422900	-1.73483900	0.85075400
C	1.52391500	-0.03197800	-0.21970800
C	2.73365500	-0.02324700	-0.08040900
C	4.17355600	-0.01463300	0.07763600
H	4.51182800	-0.80221500	0.76705200
H	4.68965900	-0.17888500	-0.87984000
H	4.53329900	0.94395300	0.47970900

5 The energy of all structures

5.1 The number of imaginary frequencies and Electronic Energy + Thermal Free Energy Correction for the optimized reactants, product and transition states obtained at the M06-L-D3/def2-SVP level of theory in the solvent of DME in the processes.

Table 1. The number of imaginary frequencies and the relative Gibbs free energy of transition states in the reaction of R1+R2 to P.

Transition states	Imaginary frequency (cm^{-1})	Electronic Energy + Thermal Free Energy Correction (a.u)
$TS1^{a2}$	-1446.26	-1026.508655
$TS1^{b2}$	-1523.14	-588.891977
$TS1^{c2}$	-1477.92	-434.193078
$TS1^{a1}$	-1871.65	-951.291060
$TS1^{b1}$	-1890.22	-513.672109
$TS1^{c1}$	-1865.95	-358.969983
$TS2^{a1}$($TS2^{a2}$)	-315.57	-1477.451072
$TS2^{b1}$($TS2^{b2}$)	-106.72	-1039.832346
$TS2^{c1}$($TS2^{c2}$)	-108.41	-885.130771

Table 2.The relative Gibbs free energy of reactants, intermediates and product in the reaction of R1+R2 to P.

Names	Electronic Energy + Thermal Free Energy Correction (a.u)
R1	-350.872846
R2	-527.329192
KOH	-675.627026
NaH	-238.016933
LiOH	-83.328579
KH	-600.440947
NaH	-162.827500
LiH	-8.126903
$M0^{a2}$	-1026.522106
$M1^{a2}$	-1026.526271
$M1^{b2}$	-588.894790
$M1^{c2}$	-434.202964
$M2^{a1}(M2^{a2})$	-950.156019
$M2^{b1}(M2^{b2})$	-512.543065
$M2^{c1}(M2^{c2})$	-357.845054
$M0^{a1}$	-951.308926
$M0^{b1}$	-513.695750
$M0^{c1}$	-358.995461
$M1^{a1}$	-951.312154

Table 3. The number of imaginary frequencies and the relative Gibbs free energy of transition states in the reaction of R1+R2 to BP.

Transition states	Imaginary frequency (cm^{-1})	Electronic Energy + Thermal Free Energy Correction (a.u)
$TS1^{KH}$	-830.00	-951.279121
$TS1^{NaH}$	-980.04	-513.659301
$TS2^{KH}$	-812.30	-951.281241
$TS2^{NaH}$	-999.61	-513.653894
$TS3^{KH}$	-826.16	-951.284791
$TS3^{NaH}$	-920.83	-513.649063
$TS4^{KH}$	-796.70	-951.278691
$TS4^{NaH}$	-869.64	-513.655410

Table 4.The relative Gibbs free energy of reactants, intermediates and product in the reaction of R1+R2 to BP.

Names	Electronic Energy + Thermal Free Energy Correction (a.u)
R1	-350.872846
R2	-527.329192
KH	-600.440947
NaH	-238.016933
$M0^{KH}$	-951.308926
$M0^{NaH}$	-513.695750
$M1^{KH}$	-951.312154
$M2^{KH}$	-951.331215
$M2^{NaH}$	-513.722228
M3	-350.868358
$M4^{KH}$	-951.308961
$M4^{NaH}$	-513.697630
$M5^{KH}$	-951.325005
$M5^{NaH}$	-513.712661
BP	-350.877562