

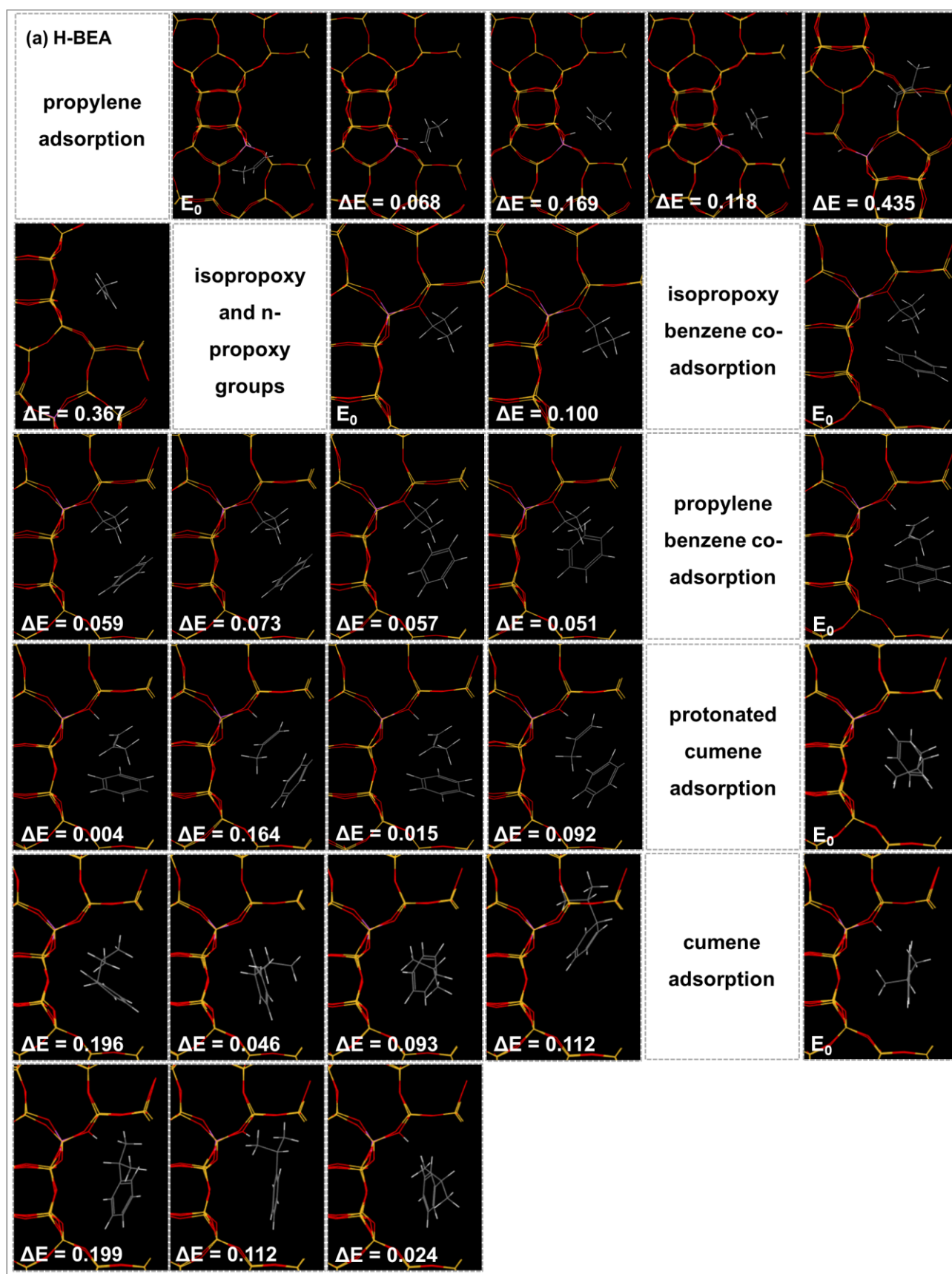
Supplementary Information for

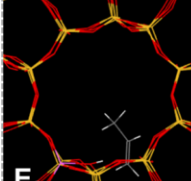
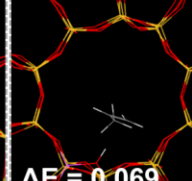
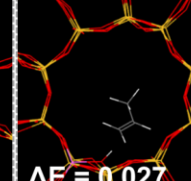
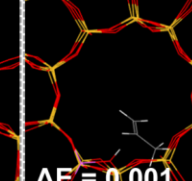
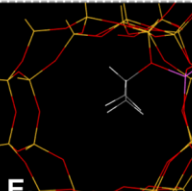
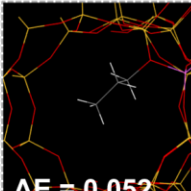
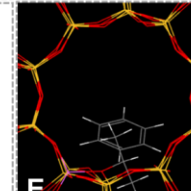
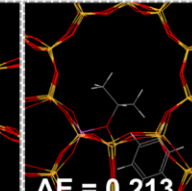
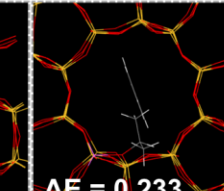
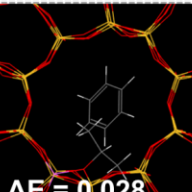
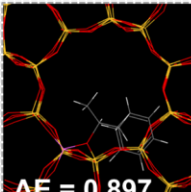
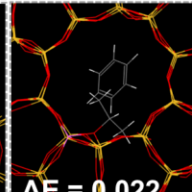
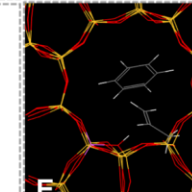
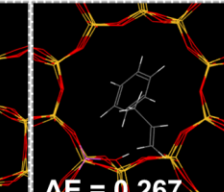
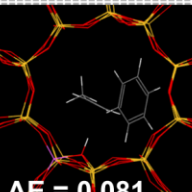
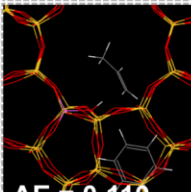
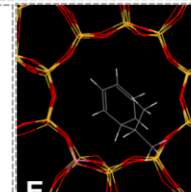
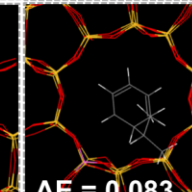
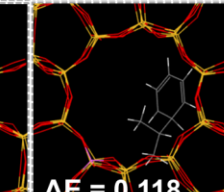
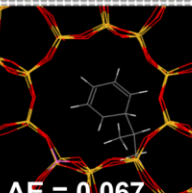
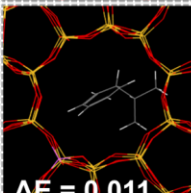
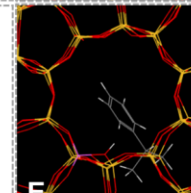
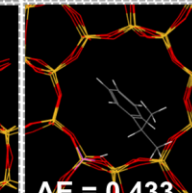
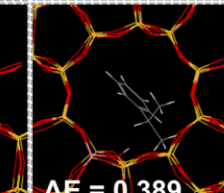
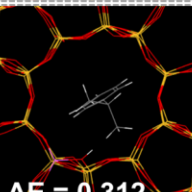
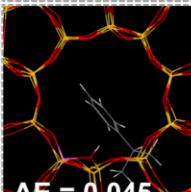
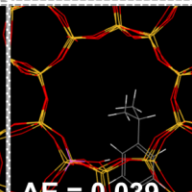
Elucidation of the Mechanism and Structure-Reactivity Relationship in Zeolite Catalyzed Alkylation of Benzene with Propylene

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(b) H-ZSM-5 propylene adsorption	 E_0	 $\Delta E = 0.069$	 $\Delta E = 0.027$	 $\Delta E = 0.001$	isopropoxy and n- propoxy groups
 E_0	 $\Delta E = 0.052$	isopropoxy benzene co- adsorption	 E_0	 $\Delta E = 0.213$	 $\Delta E = 0.233$
 $\Delta E = 0.028$	 $\Delta E = 0.897$	 $\Delta E = 0.022$	propylene benzene co- adsorption	 E_0	 $\Delta E = 0.267$
 $\Delta E = 0.081$	 $\Delta E = 0.110$	protonated cumene adsorption	 E_0	 $\Delta E = 0.083$	 $\Delta E = 0.118$
 $\Delta E = 0.067$	 $\Delta E = 0.011$	cumene adsorption	 E_0	 $\Delta E = 0.433$	 $\Delta E = 0.389$
 $\Delta E = 0.312$	 $\Delta E = 0.045$	 $\Delta E = 0.039$			

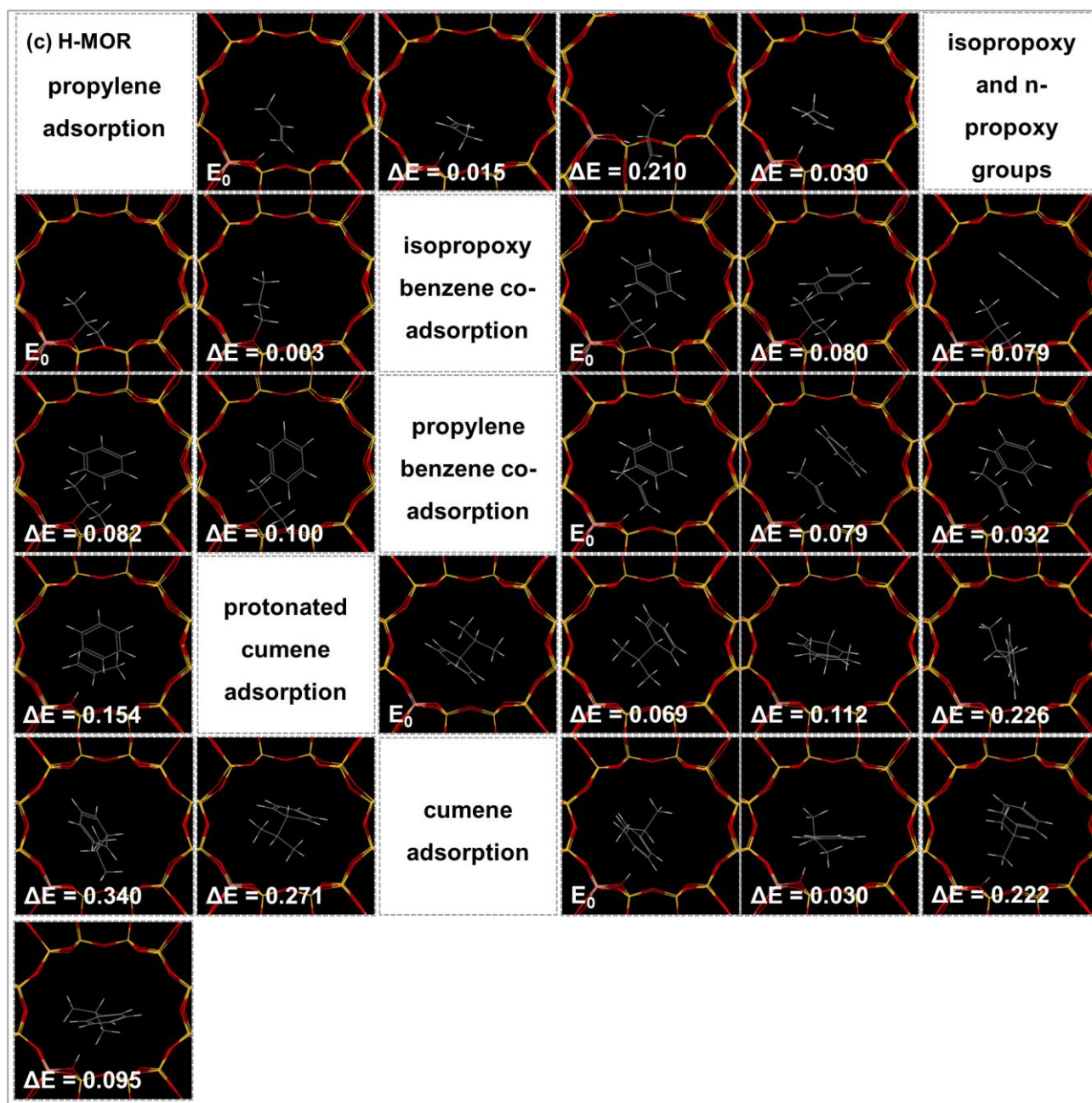


Fig. S1. All the considered orientations for each intermediate state along the reaction coordinate over (a) H-BEA, (b) H-ZSM-5, (c) H-MOR. The most thermodynamically favored orientation is labelled with E_0 , to which the relative electronic energies of other candidates are also listed.

Different orientations for each intermediate state along the reaction coordinate has been considered. At least four orientations around the BAS were constructed and the most stable orientations were determined by DFT

calculations as shown in Fig. S1. As can be seen, the structure orientation has a significant effect on the thermostability. Therefore, it's essential to do multi-geometries searching in the zeolite catalyzed systems before analyzing the reaction process.

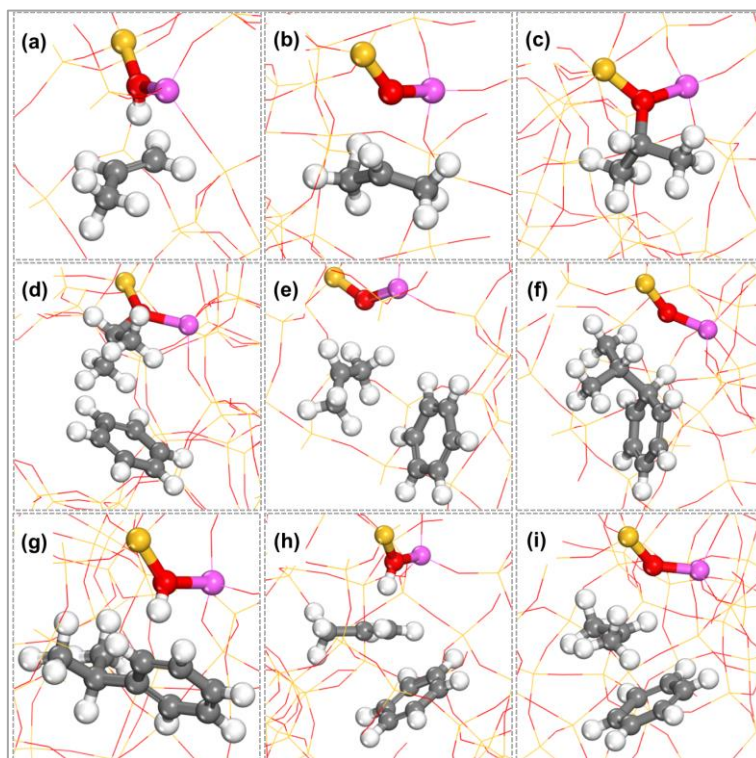


Fig. S2. Local geometry structures of all intermediates along the reaction coordinate over H-ZSM-5. **(a-i)**, corresponding to **(a)** adsorbed propylene, **(b)** TS1, **(c)** isopropoxy, **(d)** co-adsorption of isopropoxy and benzene, **(e)** TS2, **(f)** protonated cumene, **(g)** adsorbed cumene, **(h)** co-adsorption of propylene and benzene, **(i)** TS3.

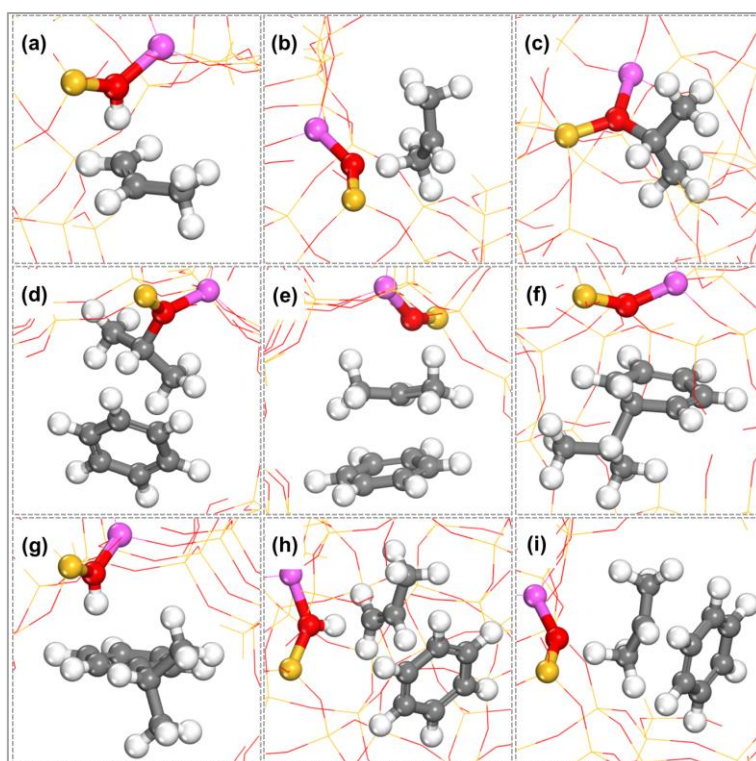


Fig. S3. Local geometry structures of all intermediates along the reaction coordinate over H-MOR. **(a-i)**, corresponding to **(a)** adsorbed propylene, **(b)** TS1, **(c)** isopropoxy, **(d)** co-adsorption of isopropoxy and benzene, **(e)** TS2, **(f)** protonated cumene, **(g)** adsorbed cumene, **(h)** co-adsorption of propylene and benzene, **(i)** TS3.

On the basis of the multi-geometries searching shown in Fig. S1, all the intermediates along the reaction coordinate could be determined as shown in Fig. S2 (H-ZSM-5) and Fig. S3 (H-MOR). For the clear understand of the reaction process, local geometry structures were intercepted from the most stable structures in Fig. S1.

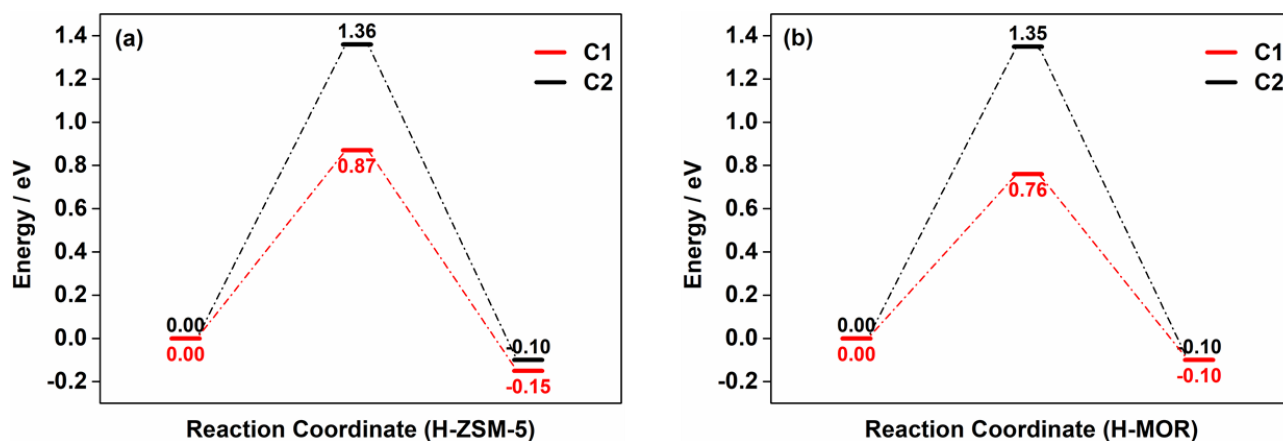


Fig. S4. Comparison of propylene protonation from C_1 and C_2 over (a) H-ZSM-5 and (b) H-MOR (electronic energy).

For the protonation of propylene, DFT calculation of two different processes were conducted. It's shown that the acidic proton prefers to bond with the C_1 atom mainly for the lower barrier. Additionally, isopropoxy is also more stable than n-propoxy. Therefore, the following work was conducted based on the protonation of propylene from C_1 atom.

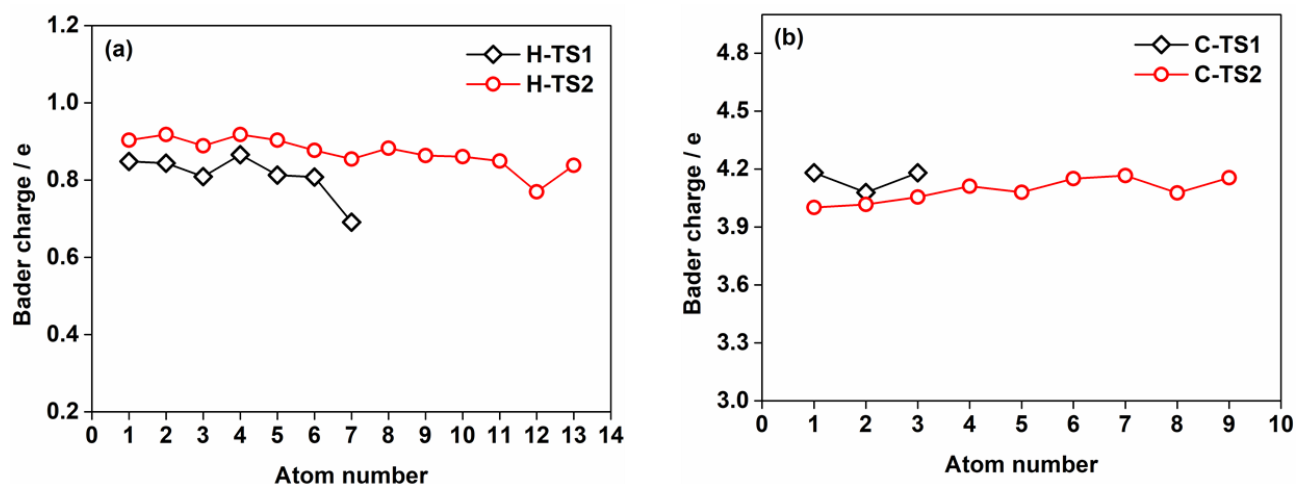


Fig. S5. Charge distribution of TS1 and TS2 structures over H-BEA. (a) Charge distribution of H atoms. (b) Charge distribution of C atoms. Atom number denotes all the C or H atoms in TS1 and TS2 structures.

TS1 and TS2 are the two transition states of the stepwise mechanism. Their thermostability difference could

be interpreted from their relative structure sizes to the corresponding channel intersection architecture as illustrated in the main text. On the other hand, these two geometries are all positively charged and the thermostability could also be reflected in the charge distribution of the structure. The charge distribution of different atoms of the structure is shown in Fig. S5. As can be seen, a larger charge variation of H atoms occurs in the TS1 structure, especially for the number 7 hydrogen atom. And the charge variation of C atoms of TS1 is also more significant. For the TS2 structure, the charge distribution looks more homogeneous, wherein the positive charge can be shared with more atoms of TS2 structure thus decreasing its instability.

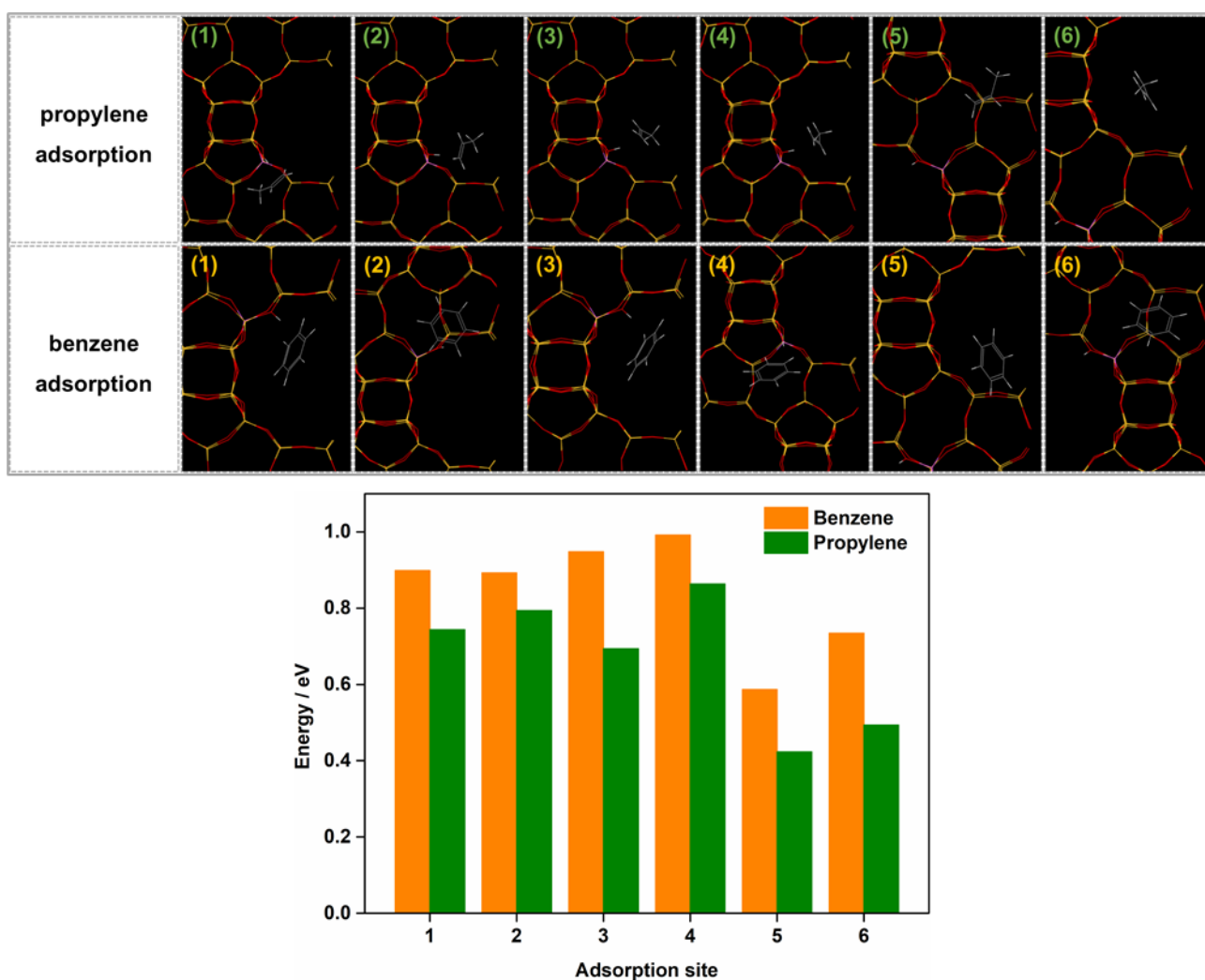


Fig. S6. Comparison of the adsorption energy (electronic energy) of propylene and benzene at different sites of H-

BEA. **(1-4)** denotes the adsorption around the BAS, **(5-6)** denotes the adsorption away from the BAS.

Different adsorption sites of propylene and benzene were considered in this part, indicating that the adsorption site in deed has a significant effect on the adsorption energy. For the adsorption away from the BAS, the corresponding adsorption energy decreases largely compared with that around the BAS, indicative of the stronger interaction of guest species with the BAS. Therefore, for the co-adsorption of at least two molecular, it's difficult to guarantee every molecular could interact with the BAS as closely as the isolated adsorption, for which the co-adsorption energy decreases as compared with the summation of the isolated adsorption.

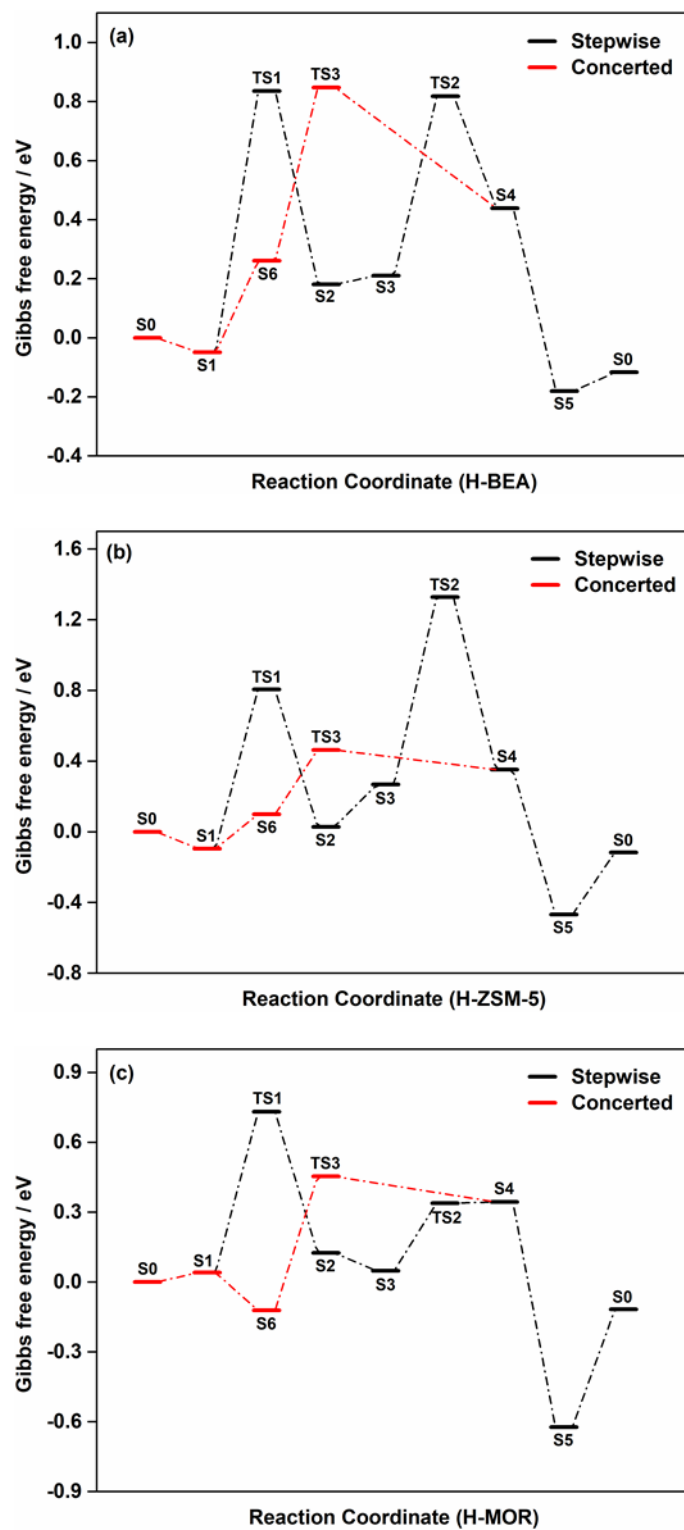


Fig. S7. Gibbs free energy diagrams of the complete reaction coordinate over (a) H-BEA, (b) H-ZSM-5 and (c) H-MOR at 600 K. The cycle consists of the stepwise and concerted mechanisms. The pressure of the gaseous molecular

is 30 atm. Two S0 states in the initial and final states denote (H-zeolite + propylene (g) + benzene (g)) and (H-zeolite + cumene (g)) respectively.

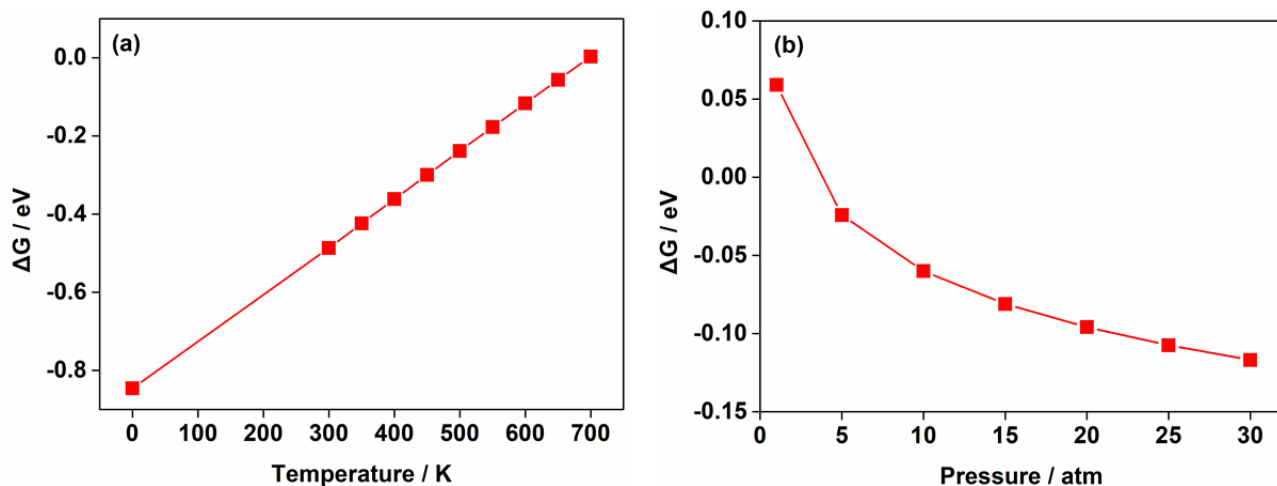
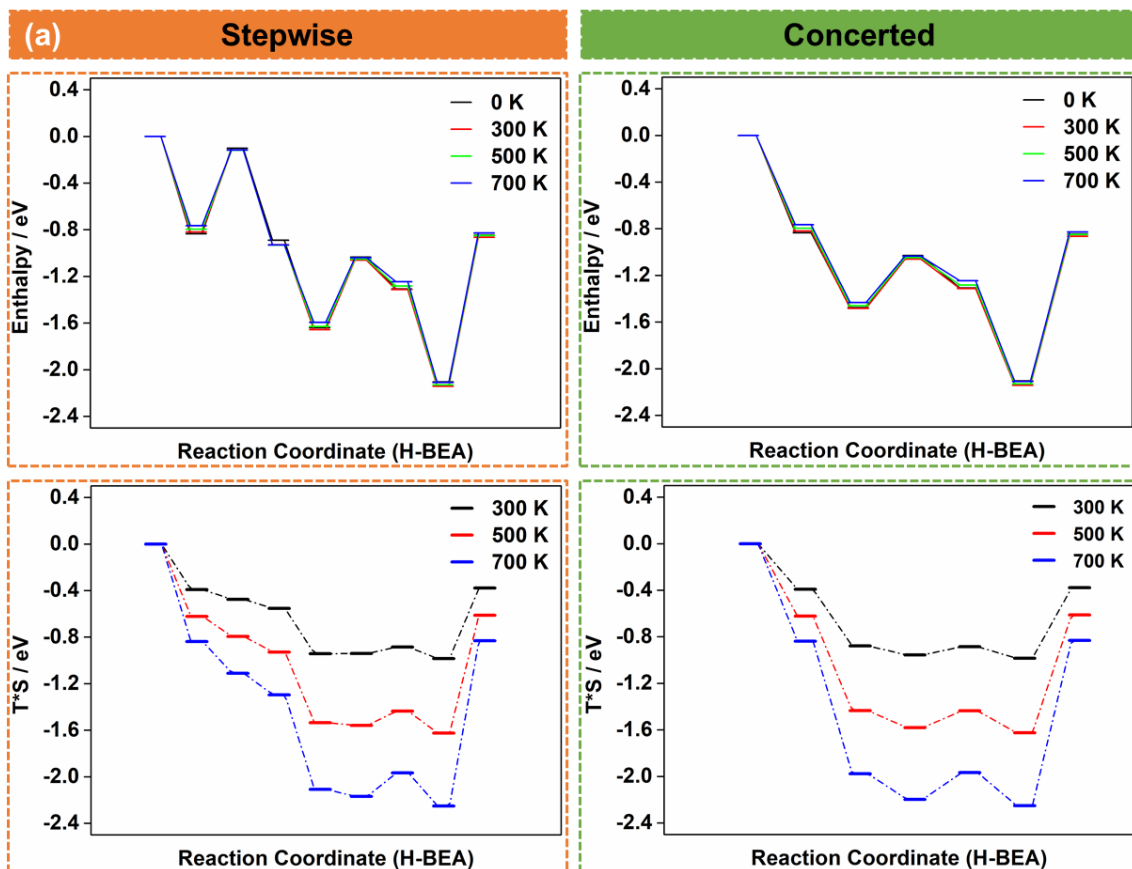
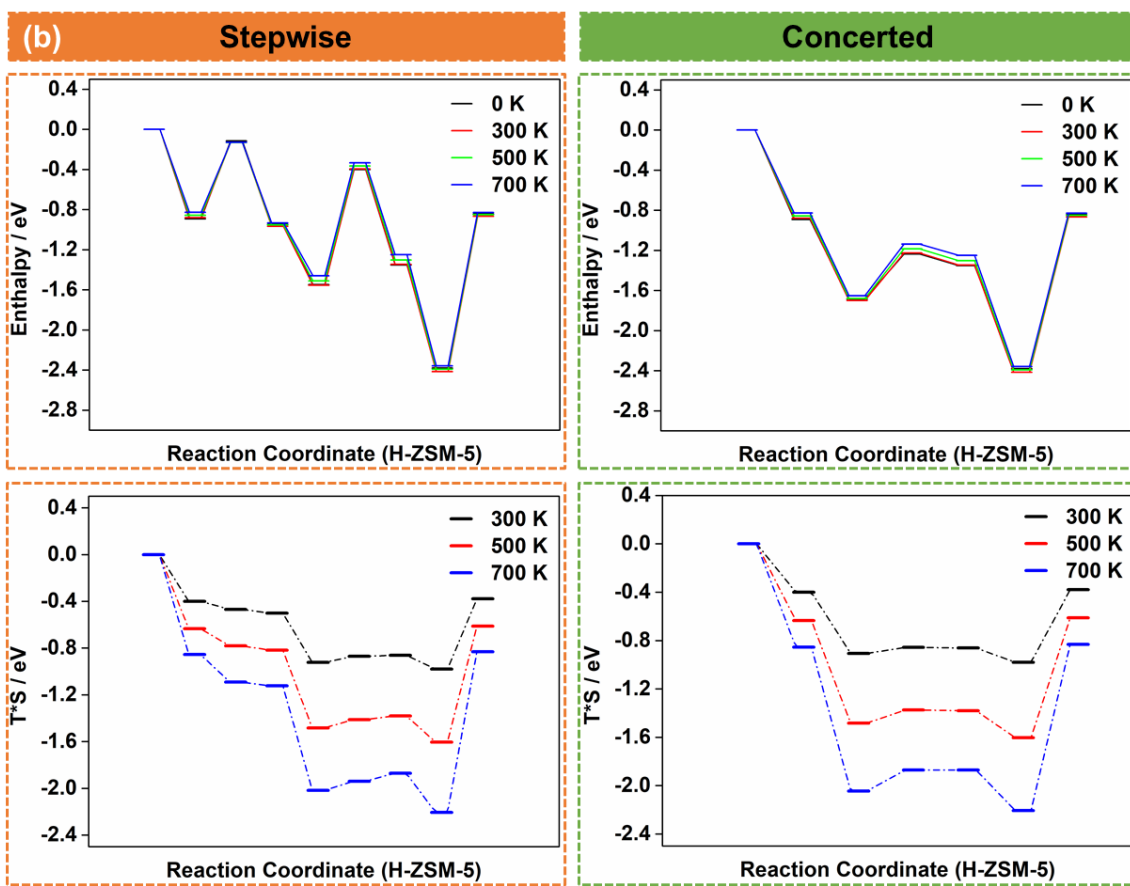


Fig. S8. Influence of **(a)** temperature (calculated at 30 atm) and **(b)** pressure (calculated at 600 K) on the reaction Gibbs free energy (thermal driving force). The reaction Gibbs free energy was calculated according to Eq. (S1) ¹ as follows and the reactants and products were all in gas phase.

$$\Delta G = G_{cumene(g)} - G_{benzene(g)} - G_{propylene(g)} \quad (S1)$$

As can be seen, the reaction Gibbs free energy increases with temperature rising, indicating the decreased thermal driving force. As for pressure, the reaction Gibbs free energy decreases as pressure increases. However, the variation contributed by pressure is less than temperature, indicating temperature has a more significant effect on the activity.





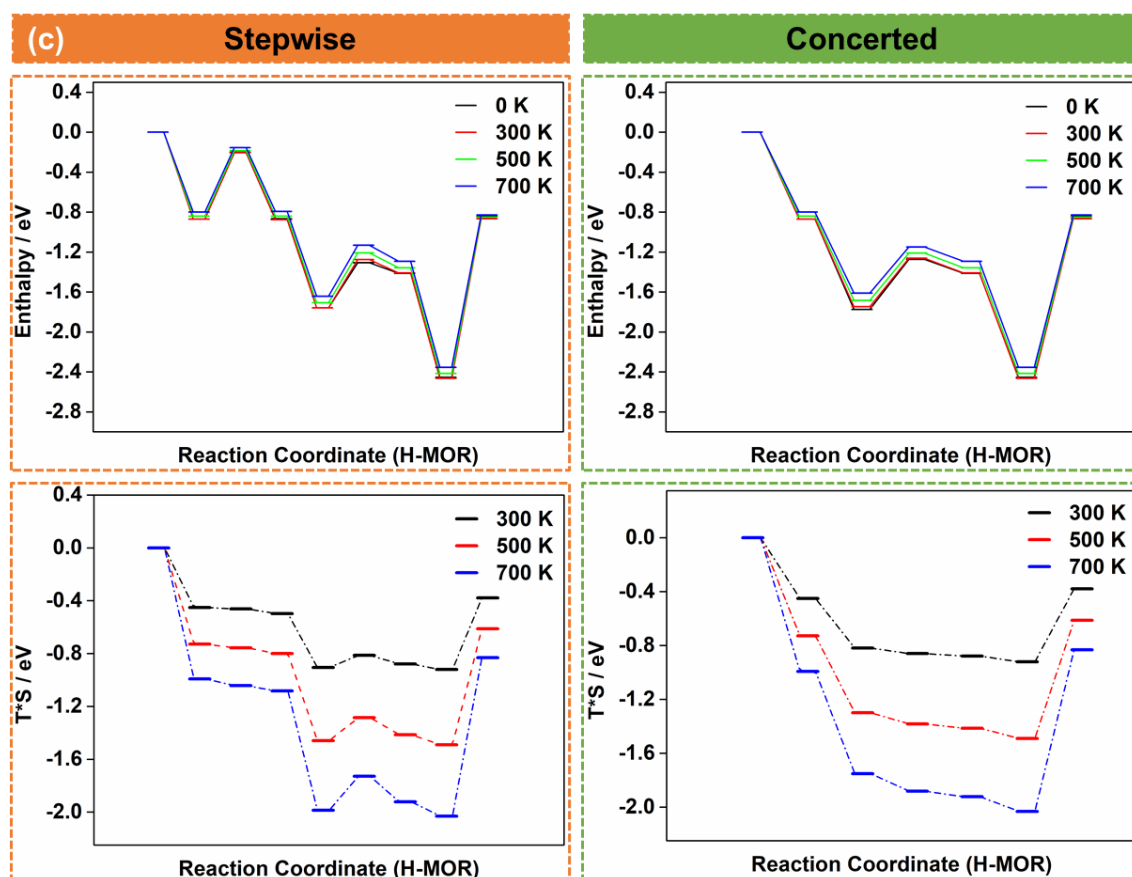
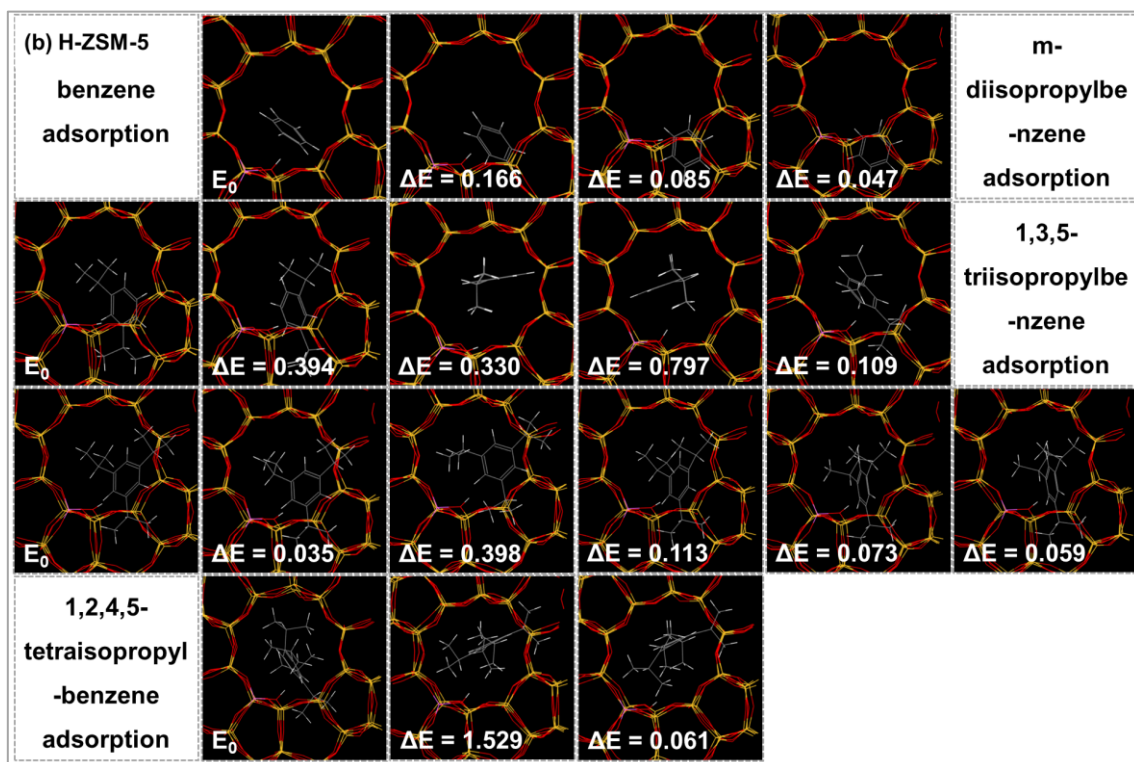
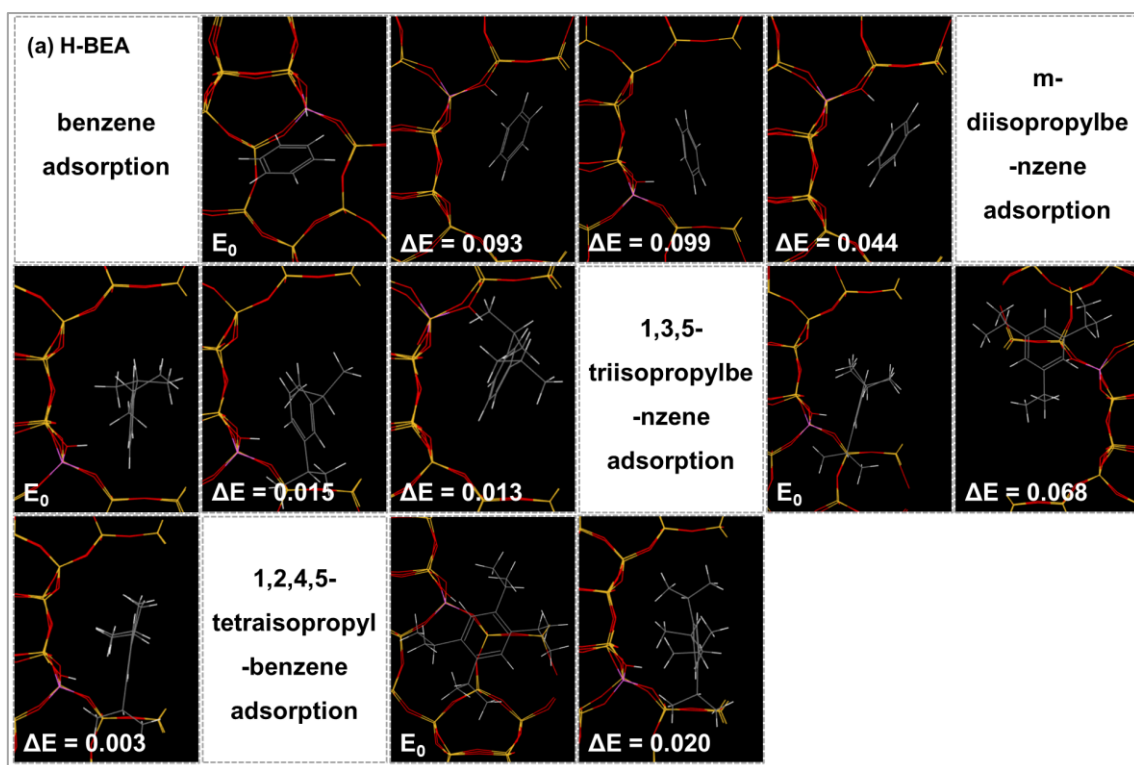


Fig. S9. The enthalpy part H (first row) and entropy part T^*S (second row) of the Gibbs free energy along the reaction coordinate over (a) H-BEA, (b) H-ZSM-5 and (c) H-MOR. Obviously, it's the entropy part that mainly accounts for the variation of reaction Gibbs free energy at different temperature.

The enthalpy part and entropy part were calculated along the reaction coordinate over these three zeolites. As can be seen, the enthalpy diagrams show a similar trend as the Gibbs free energy diagrams (see Fig. 4 and Fig. S7) and a slight variation of enthalpy with different temperature is observed, indicating that the enthalpy part represents the intrinsic qualities of the reaction. However, the entropy part varies more largely with temperature variation as compared with enthalpy, indicating it's the entropy part that mainly accounts for the variation of reaction Gibbs free energy at different temperature, further the activity.



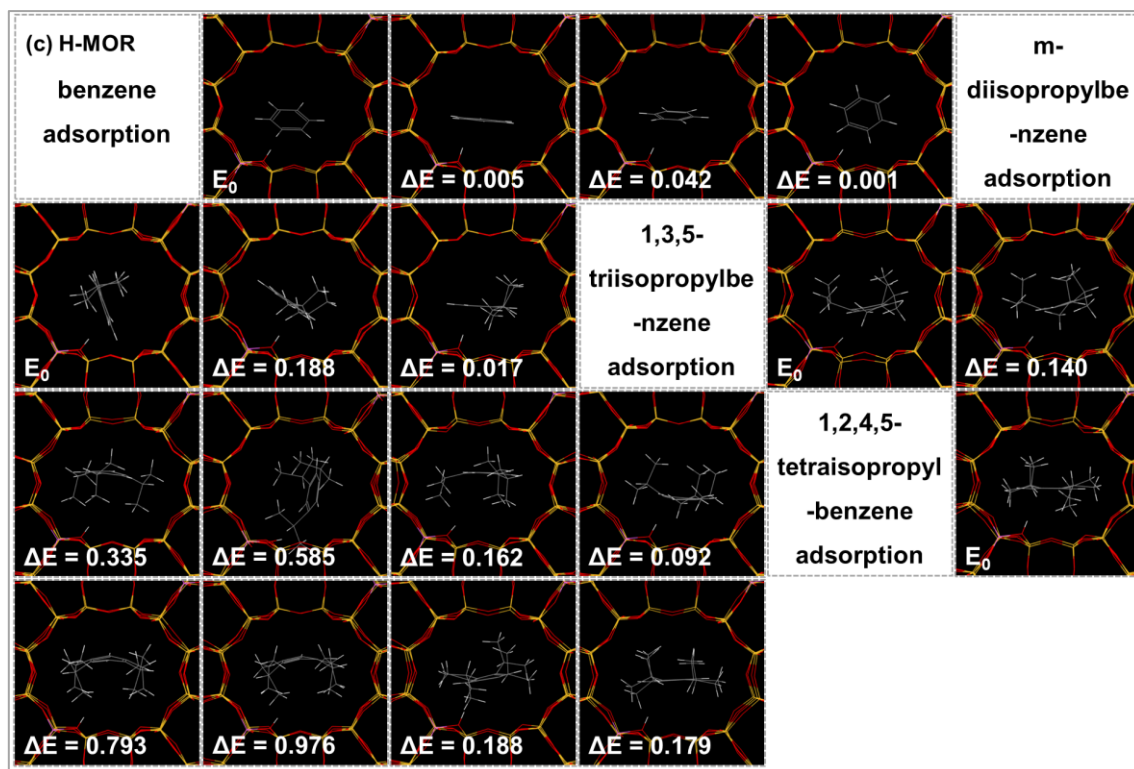


Fig. S10. All the considered orientations of each MPB around the BAS of (a) H-BEA, (b) H-ZSM-5 and (c) H-MOR. The most thermodynamically favored orientation is labelled with E_0 , to which the relative electronic energies of other candidates are also listed.

The multi-geometries searching of MPBs has also been conducted to determine the relative more stable state. As can be seen, the orientation has a significant effect the thermostability, especially for the larger size MPBs, which is assigned to the increased dispersion interaction (destabilization) of MPBs with channels. For the 1,2,4,5-tetraisopropylbenzene adsorption in H-BEA, it's difficult to construct different orientations in the channel intersection, therefore, two possible orientations were considered in the present work.

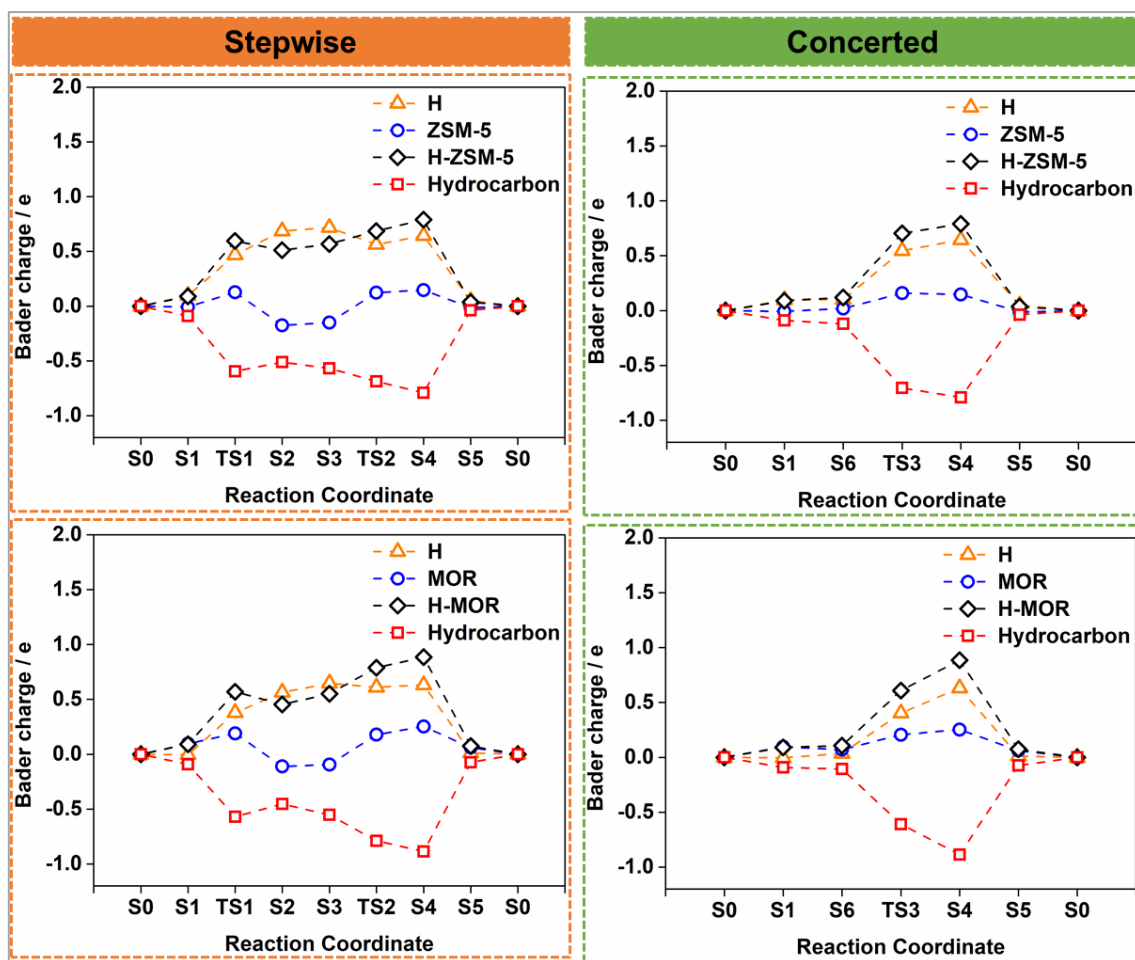


Fig. S11. Charge transfer information along the reaction coordinate over H-ZSM-5 (first row) and H-MOR (second row).

The charge transfer analysis was conducted along the reaction process. Overall, the hydrocarbon acts as a charge donor firstly and then becomes an acceptor along the reaction coordinate. The charge variation of the acidic proton is comparable with the zeolite framework, indicating charge transfer between hydrocarbon and zeolite mainly occurs via the acidic proton.

Table S1. Imaginary frequencies for all transition states.

TS1	TS2	TS3
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H-BEA	647.54i	230.45i	242.92i
H-ZSM-5	657.85i	259.46i	243.67i
H-MOR	639.65i	241.88i	251.32i

S1. Discussion of the BAS

In the present work, we consider the T9, T12, T2 sites for Al substitution of the BEA, ZSM-5, MOR unit cell according to the previously work, respectively. For the BAS, in contrast to the siting of the Al atom, the position of the acidic proton is likely determined by thermodynamics because proton jumps between oxygen atoms bonded to the same aluminum are facial, in particular when adsorbates are present.² Additionally, the accessibility should also be considered when determining the BAS. In the present work we computed the total energies of the four possible H-zeolite forms of H-BEA, H-ZSM-5, H-MOR, respectively. The results are summarized in Fig. S12.

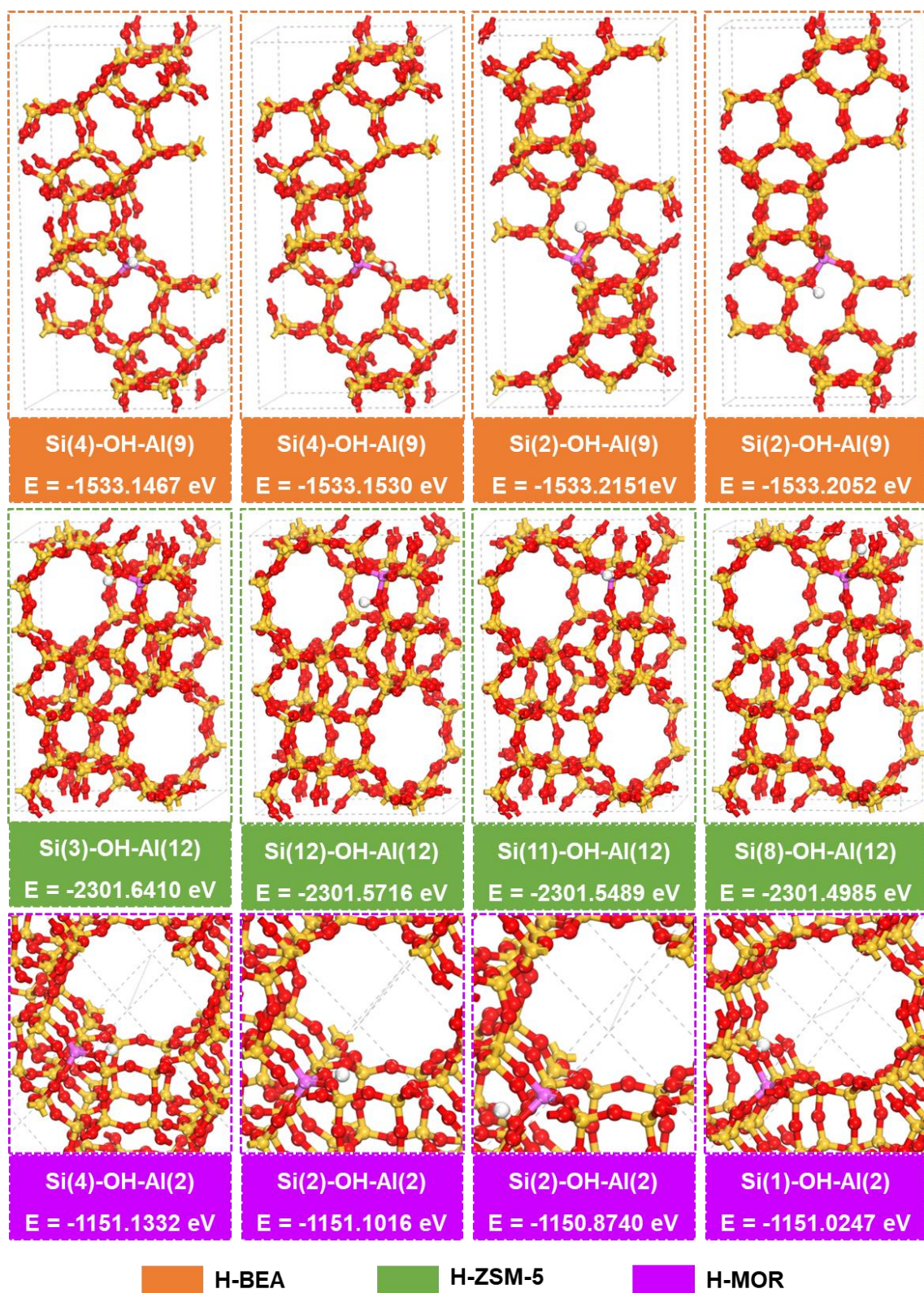


Fig. S12. Comparison of the electronic energies of the four possible H-zeolite forms.

As can be seen, the acidic protons of both H-ZSM-5 and H-MOR chosen in the present work are all the most

energetically stable, and the reaction space near the BAS is enough, which is in accordance with the previous research.^{1, 3-9} For H-BEA, the acidic proton chosen in the present work (Si(4)-OH-Al(9), E = -1533.1467 eV) seems some unstable than other acidic sites. However, the choice of BAS is not only determined by the thermostability, the accessibility is more significant to some extent. Generally, reactants are more likely to be activated by the most accessible BAS. Therefore, the structure (Si(4)-OH-Al(9), E = -1533.1467 eV) of H-BEA was chosen in the present work mainly for its better accessibility, which is also accordance with other researches.^{6, 10-12}

S2. Discussion of the isopropoxy formation

After the adsorption of propylene, four different oxygen sites adjacent to Al are all possible to form the isopropoxy. The distance of C₂ atom of the protonated propylene and these four oxygen atoms possible forming the isopropoxy are shown in Table S2 and Fig S13. It's reasonable to assume that the protonated propylene prefers to bond with the nearest oxygen. Therefore, the oxygen with the shortest C₂-O distance was chosen in the present work to form the isopropoxy.

Table S2. The distance of C₂ atom to the four oxygen atoms possible forming the isopropoxy (Å).

	H-BEA	H-ZSM-5	H-MOR
C ₂ -O ₁	3.10	3.11	3.09
C ₂ -O ₂	3.72	4.80	4.32
C ₂ -O ₃	5.52	3.93	5.71
C ₂ -O ₄	4.00	5.69	4.22

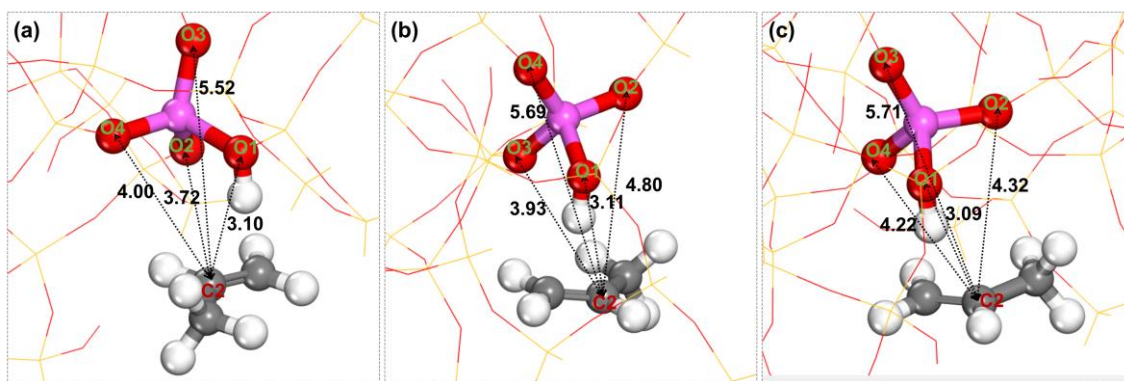


Fig. S13. Comparison of the distance of C₂ atom to the four oxygen atoms possible forming the isopropoxy over (a) H-BEA, (b) H-ZSM-5, (c) H-MOR (Å).

S3. Comparison to literature reports

There are little kinetical research reporting the reaction rates of zeolite catalyzed alkylation of benzene with propylene over zeolites. However, a similar reaction of the alkylation of benzene with isopropanol can be chosen to compare with the present results approximately. Assuming the acidities reported in Table 1 of reference¹³ are all assigned to Brønsted acid site, the TOF (based on per acid site) of the five zeolites reported could be estimated as shown in Table S3.

Table S3. Comparison of the present results with the literature experimental reports.

	TOF (site ⁻¹ *s ⁻¹)		
	Experimental results ^[a]	The present work ^[b]	
		Stepwise	Concerted
H-BEA	-	1.67	577.65
SAPO-5/4	0.00081	-	
SAPO-5/3	0.00033	-	
SAPO-5/2	0.00032	-	

SAPO-5/1	-	-	
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[a] Reaction condition: 393 K, 1 atm.

[b] Reaction condition in present work: 393 K, 1 atm.

As can be seen, reaction rates estimated of the present work are higher than the literature experimental results, the reason for which can be explained as follows: (i) zeolite models constructed in the present work are perfect without any defects, and the acid sites are fixed at the specific site. However, there are no perfect zeolite crystals in reality, and defects are inevitable. On the other hand, the acid sites are distributed all around zeolite, which is difficult to determined and the position of acidic sites even change during the reaction.² Additionally, some acid sites are unreactive for the narrow space around them. And for the reactive sites, different acid sites and even defects could have a significant effect on the reactivity; (ii) the TOF estimated from the experimental results is based on the assumption that each NH₃ molecular is corresponded to a validated Brønsted acid site. In fact, in addition to Brønsted acid site, Lewis sites and even some other inactive sites could also adsorb NH₃ molecular. Further, not all Brønsted acid sites in the framework are active or validated, especially in the narrow space, where reactants are unable to access. Therefore, the number of validated acid sites of the experiment work is overestimated, causing TOF underestimated; (iii) in the present work, the reactant position around the acid site is unchanged under various conditions. In fact, diffusion in the zeolite channels has a significant effect on the reactant concentration around the BAS. The diffusion at lower temperature is usually limited, causing the concentration of reactant around the acid sites lower, thus lowering the reaction rate at lower temperature; (iv) results in our work mainly focus on the intrinsic kinetics around the acid sites and the internal and external diffusion are out of the range of our consideration. In fact, the diffusion limitation is significant for zeolite catalyzed reactions. Therefore, a further investigation combining the intrinsic mechanism and diffusion process is significant to understand the reaction process and worth studying.

A similar theoretical work about the alkylation of benzene with ethene could be selected to compare with our present results. By comparing with the alkylation of benzene with ethene, we could find that our calculation is approximately at the same magnitude with the results in reference,¹ especially at higher temperature. Additionally, the similar kinetic trends of two mechanisms (stepwise and concerted) can be observed.

Another theoretical work conducted by Hansen *et al.*¹⁴ compared different methodologies for the theory calculation of the alkylation of benzene with ethene. Regarding the hybrid MP2:DFT method, the calculated results deviate significantly from that by PBE+D method, indicating strong methodological influence on calculation results.

Generally, there are largely two different directions in computational research.¹ One is to address the variation trends in reactivity and/or selectivity for complex reactions, and the other is to obtain absolute accuracy for relatively simple systems in order to compare with experimental measurements. In the case of the present work, understanding the kinetic trends clearly takes priority over the absolute accuracy, and we mainly focused on the varied kinetic properties with the two mechanisms (stepwise and concerted) over different zeolite frameworks. Additionally, for our research system with complicated reaction network (including side reactions) and the large zeolite periodic models, the QM:QM methodology or the hybrid MP2:DFT+D approach are technically too much expensive. Further considering that the DFT-D3 method has been widely used for theoretical simulation on zeolite catalysis and here all elementary steps/species have been modeled using a unified approach, additionally, the kinetic trends obtained in the present work agree well with the previous work, therefore, we believe that our simulation results on the kinetic trends are reasonably reliable.

S4. Determination of TDTS and TDI

Herein, we take the Gibbs free energy diagrams shown in Fig. S7a as an example to illustrate this process.

For the stepwise mechanism (Fig. S7a), the energy of TS1 is higher than TS2, therefore, TS1 is determined as

the TOF-determining transition state (TDTS). Then, two intermediates may be determined as the TOF-determining intermediate (TDI) depending on its location relative to TS1. If the TDI appears before TS1, the S1 state will be determined as the TDI and the energetic span (δE) can be calculated according Eq. (3a). However, if the TDI appears after TS1, the S5 state will be determined as the TDI and the energetic span (δE) can be calculated according Eq. (3b). The results of these two cases are shown in Table S4a. Therefore, for the maximization the energetic span (δE), TS1 and S5 are determined as TDTS and TDI, respectively.

For the concerted mechanism, only one transition state appears in the catalytic cycle, therefore, TS3 is determined as the TDTS directly. Then, two intermediates may be determined as the TOF-determining intermediate (TDI) depending on its location relative to TS3. If the TDI appears before the TS3, the S1 state will be determined as the TDI and the energetic span (δE) can be calculated according Eq. (3a). However, if the TDI appears after TS3, the S5 state will be determined as the TDI and the energetic span (δE) can be calculated according Eq. (3b). The results of these two cases are shown in Table S4b. Therefore, for the maximization the energetic span (δE), TS3 and S5 are determined as TDTS and TDI, respectively.

Table S4. Relative Gibbs free energies (referred to S0 state) of the intermediates along the reaction coordinate (eV).

(a) Stepwise

S0	S1	TS1	S2	S3	TS2	S4	S5	S0	δE	
									Eq. (3a)	Eq. (3b)
0.00	-0.05	0.84	0.18	0.21	0.82	0.44	-0.18	-0.12	0.89	0.90

(b) Concerted

S0	S1	S6	TS3	S4	S5	S0	δE	
							Eq. (3a)	Eq. (3b)
0.00	-0.05	0.26	0.85	0.44	-0.18	-0.12	0.90	0.91

S4a. Effect of temperature

The Gibbs free energy diagrams and the TDTS and TDI under different temperature are as follows. The TDTS

and TDI were determined according to Eq. (3) in the main text. The Gibbs free energies of gaseous molecular are calculated at 30 atm.

(1) H-BEA

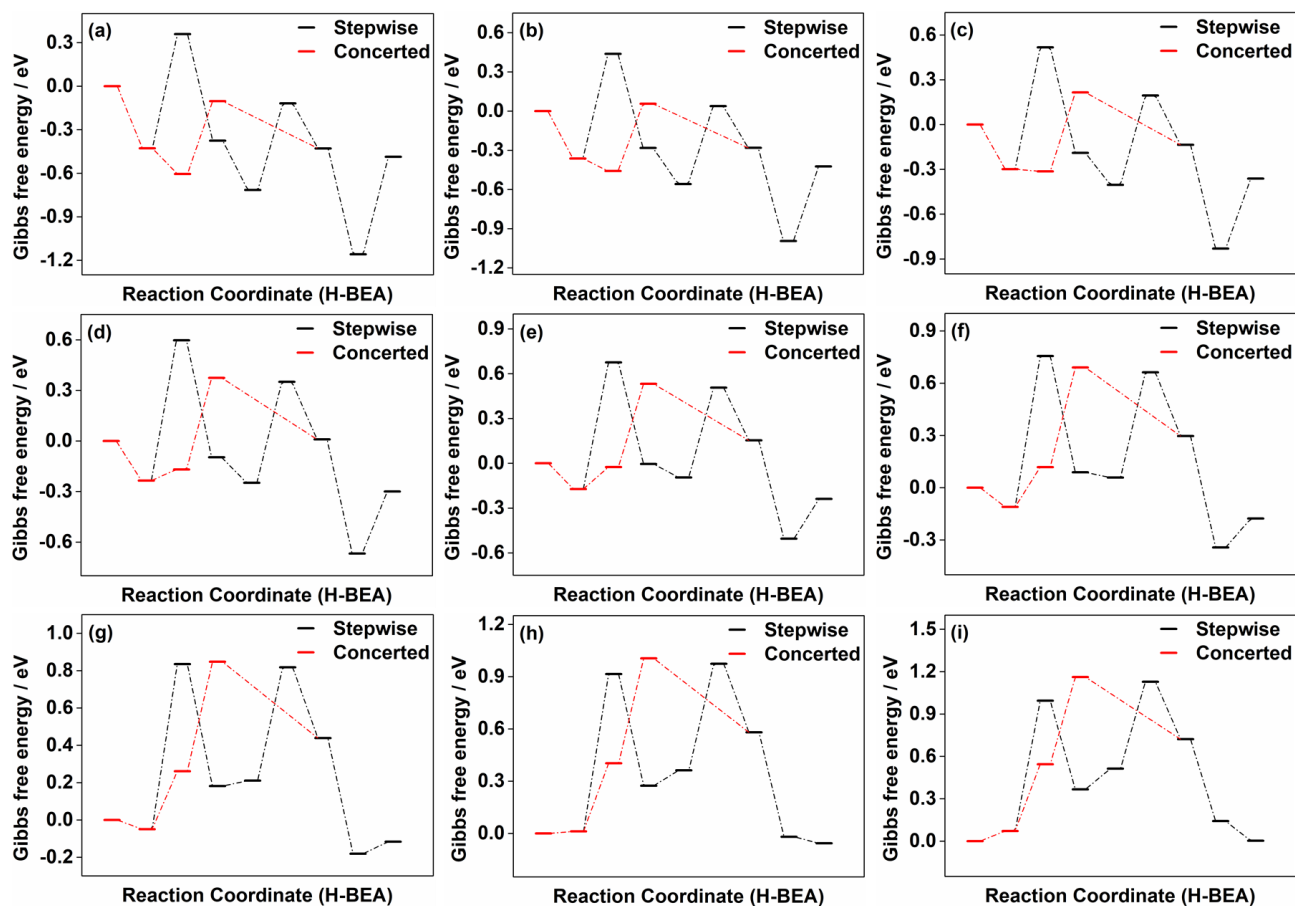


Fig. S14. Gibbs free energy diagrams of the complete reaction coordinate over H-BEA at different temperature ((a) 300 K, (b) 350 K, (c) 400 K, (d) 450 K, (e) 500 K, (f) 550 K, (g) 600 K, (h) 650 K, (i) 700 K). The cycle consists of the stepwise and concerted mechanisms.

Table S5. The TDTS and TDI of H-BEA including (a) stepwise and (b) concerted mechanisms.

(a) Stepwise

Temperature / K	0	300	350	400	450	500	550	600	650	700
TDTS	TS1	TS1	TS1	TS1	TS1	TS1	TS1	TS1	TS2	TS2

TDI	S5	S5	S5	S5	S5	S5	S5	S5	S0	S0
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(b) Concerted

Temperature / K	0	300	350	400	450	500	550	600	650	700
TDTs	TS3	TS3	TS3	TS3	TS3	TS3	TS3	TS3	TS3	TS3
TDI	S6	S5	S5	S5	S5	S5	S5	S5	S0	S0

(2) H-ZSM-5

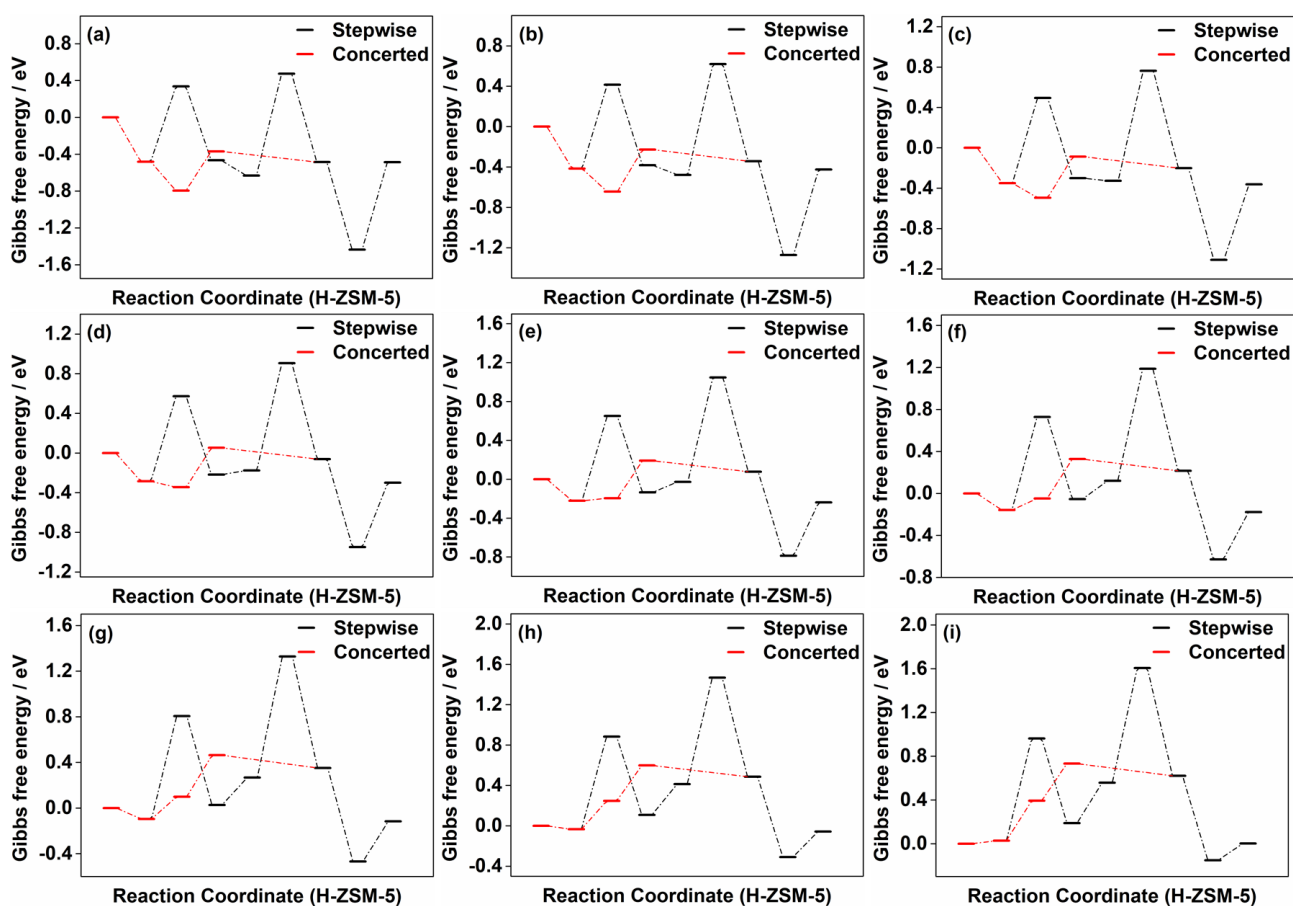


Fig. S15. Gibbs free energy diagrams of the complete reaction coordinate over H-ZSM-5 at different temperature ((a) 300 K, (b) 350 K, (c) 400 K, (d) 450 K, (e) 500 K, (f) 550 K, (g) 600 K, (h) 650 K, (i) 700 K). The cycle consists of the stepwise and concerted mechanisms.

Table S6. The TDTs and TDI of H-ZSM-5 including (a) stepwise and (b) concerted mechanisms.

(a) Stepwise

Temperature / K	0	300	350	400	450	500	550	600	650	700
TDS	TS1	TS2	TS2	TS2	TS2	TS2	TS2	TS2	TS2	TS2
TDI	S5	S5	S5	S5	S5	S5	S5	S5	S5	S5

(b) Concerted

Temperature / K	0	300	350	400	450	500	550	600	650	700
TDS	TS3	TS3	TS3	TS3	TS3	TS3	TS3	TS3	TS3	TS3
TDI	S6	S5	S5	S5	S5	S5	S5	S5	S5	S5

(3) H-MOR

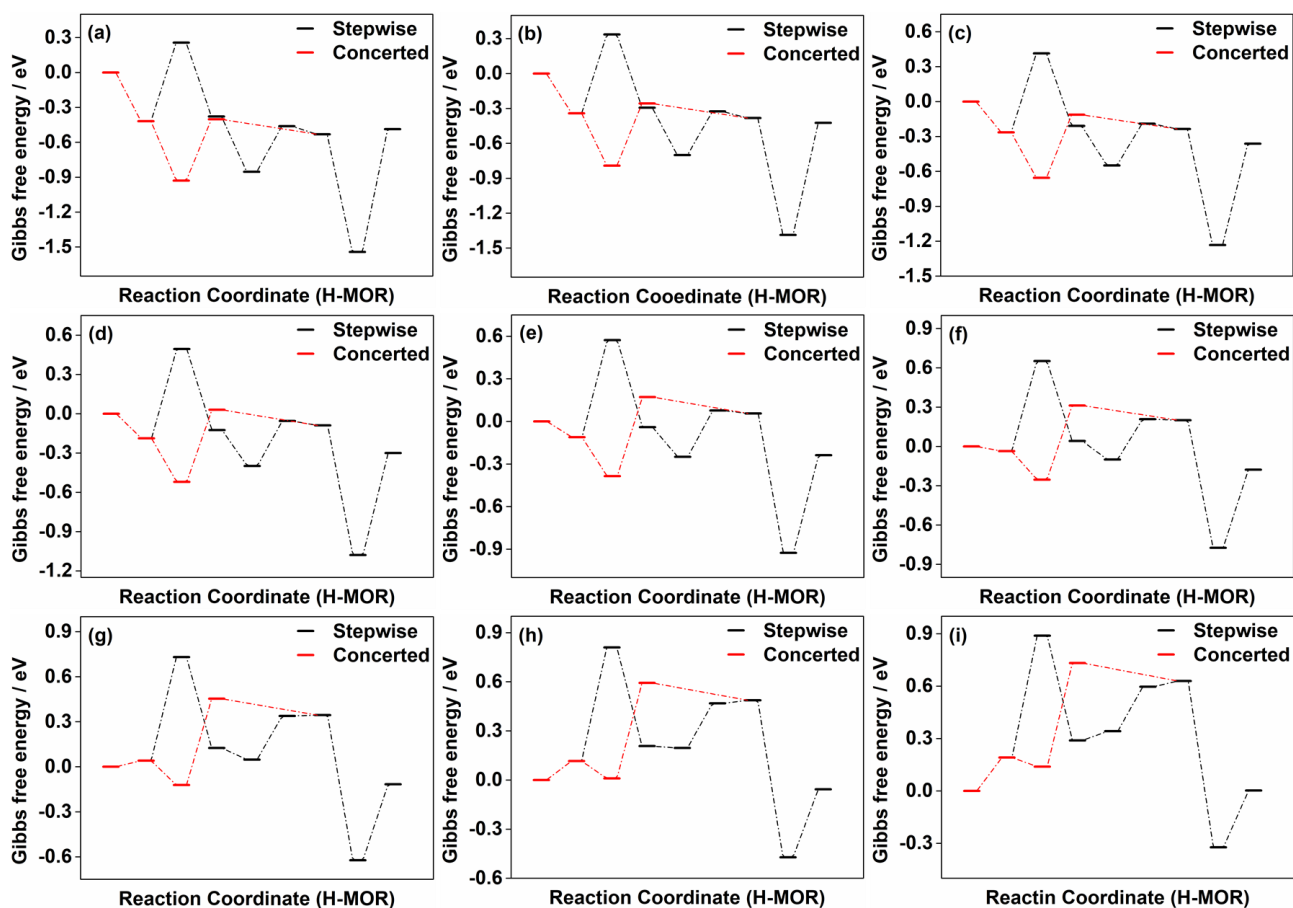


Fig. S16. Gibbs free energy diagrams of the complete reaction coordinate over H-MOR at different temperature ((a)

300 K, (b) 350 K, (c) 400 K, (d) 450 K, (e) 500 K, (f) 550 K, (g) 600 K, (h) 650 K, (i) 700 K). The cycle consists of the stepwise and concerted mechanisms.

Table S7. The TDTS and TDI of H-MOR including **(a)** stepwise and **(b)** concerted mechanisms.

(a) Stepwise

Temperature / K	0	300	350	400	450	500	550	600	650	700
TDTS	TS1	TS1	TS1	TS1	TS1	TS1	TS1	TS1	TS1	TS1
TDI	S5	S5	S5	S5	S5	S5	S5	S5	S5	S5

(b) Concerted

Temperature / K	0	300	350	400	450	500	550	600	650	700
TDTS	TS3	TS3	TS3	TS3	TS3	TS3	TS3	TS3	TS3	TS3
TDI	S6	S5	S5	S5	S5	S5	S5	S5	S5	S5

S4b. Effect of pressure

The Gibbs free energy diagrams and the TDTS and TDI under different pressure at 600 K are as follows. The TDTS and TDI were determined according to Eq. (3) in the main text.

(1) H-BEA

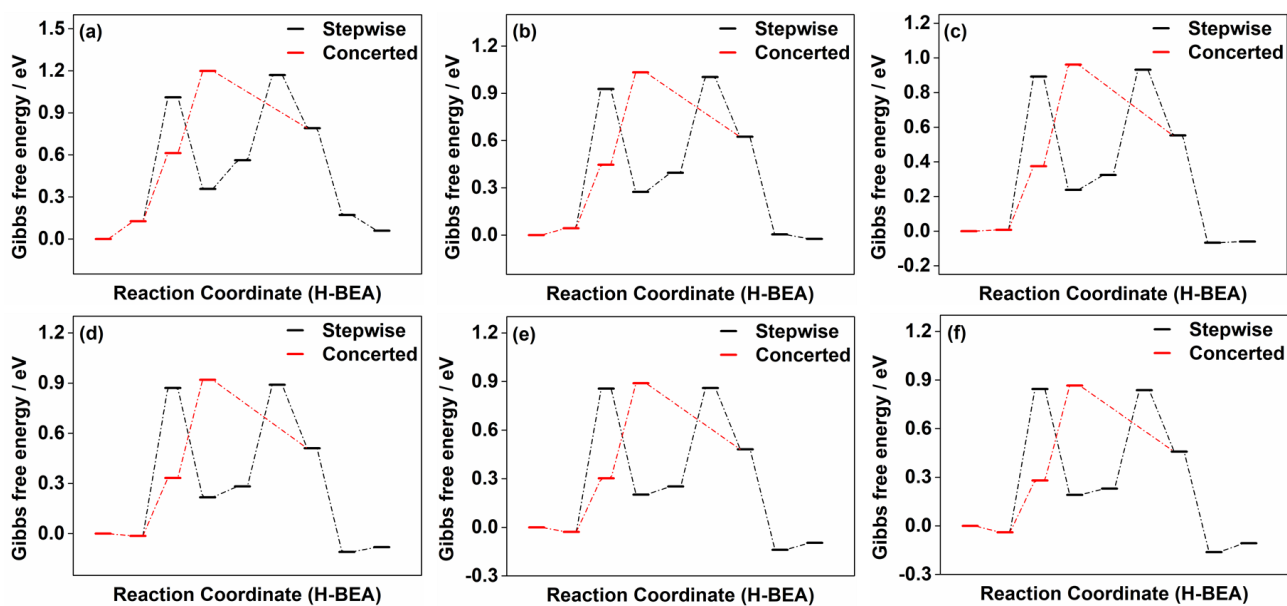


Fig. S17. Gibbs free energy diagrams of the complete reaction coordinate over H-BEA at different pressure ((a) 1 atm, (b) 5 atm, (c) 10 atm, (d) 15 atm, (e) 20 atm, (f) 25 atm). The cycle consists of the stepwise and concerted mechanisms.

Table S8. The TDTS and TDI of H-BEA including (a) stepwise and (b) concerted mechanisms.

(a) Stepwise

Pressure / atm	1	5	10	15	20	25	30
TDTS	TS2	TS2	TS2	TS2	TS2	TS1	TS1
TDI	S0	S0	S5	S5	S5	S5	S5

(b) Concerted

Pressure / atm	1	5	10	15	20	25	30
TDTS	TS3	TS3	TS3	TS3	TS3	TS3	TS3
TDI	S0	S0	S5	S5	S5	S5	S5

(2) H-ZSM-5

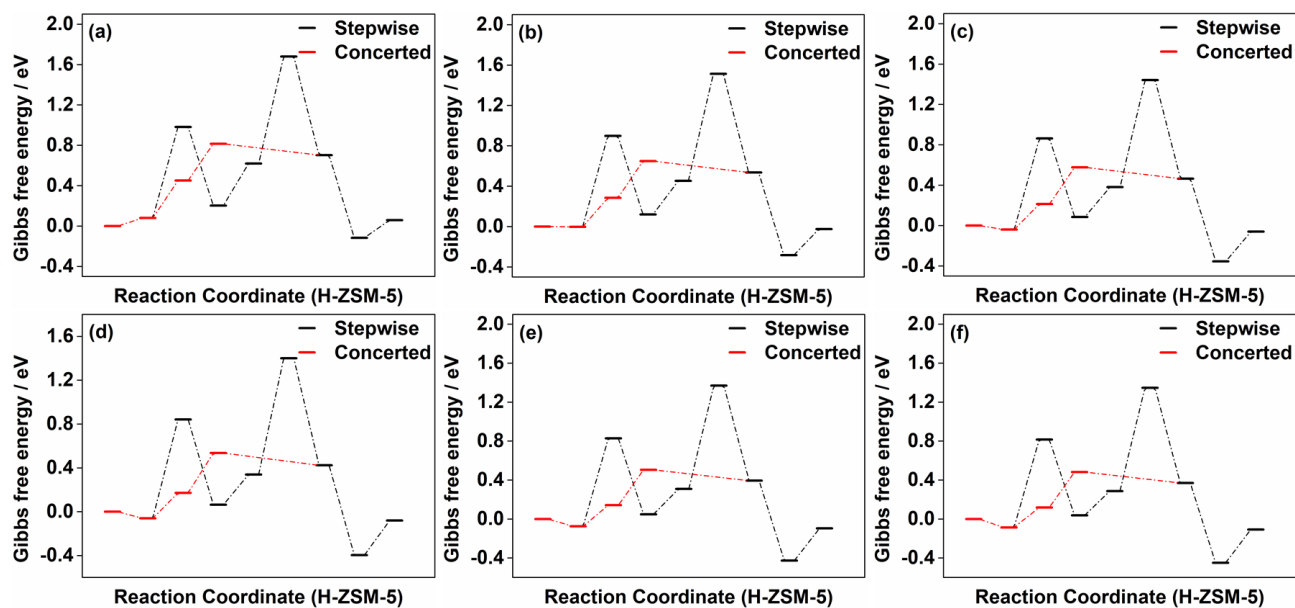


Fig. S18. Gibbs free energy diagrams of the complete reaction coordinate over H-ZSM-5 at different pressure ((a) 1 atm, (b) 5 atm, (c) 10 atm, (d) 15 atm, (e) 20 atm, (f) 25 atm). The cycle consists of the stepwise and concerted mechanisms.

Table S9. The TDTS and TDI of H-ZSM-5 including (a) stepwise and (b) concerted mechanisms.

(a) Stepwise

Pressure / atm	1	5	10	15	20	25	30
TDTS	TS2	TS2	TS2	TS2	TS2	TS2	TS2
TDI	S5	S5	S5	S5	S5	S5	S5

(b) Concerted

Pressure / atm	1	5	10	15	20	25	30
TDTS	TS3	TS3	TS3	TS3	TS3	TS3	TS3
TDI	S5	S5	S5	S5	S5	S5	S5

(3) H-MOR

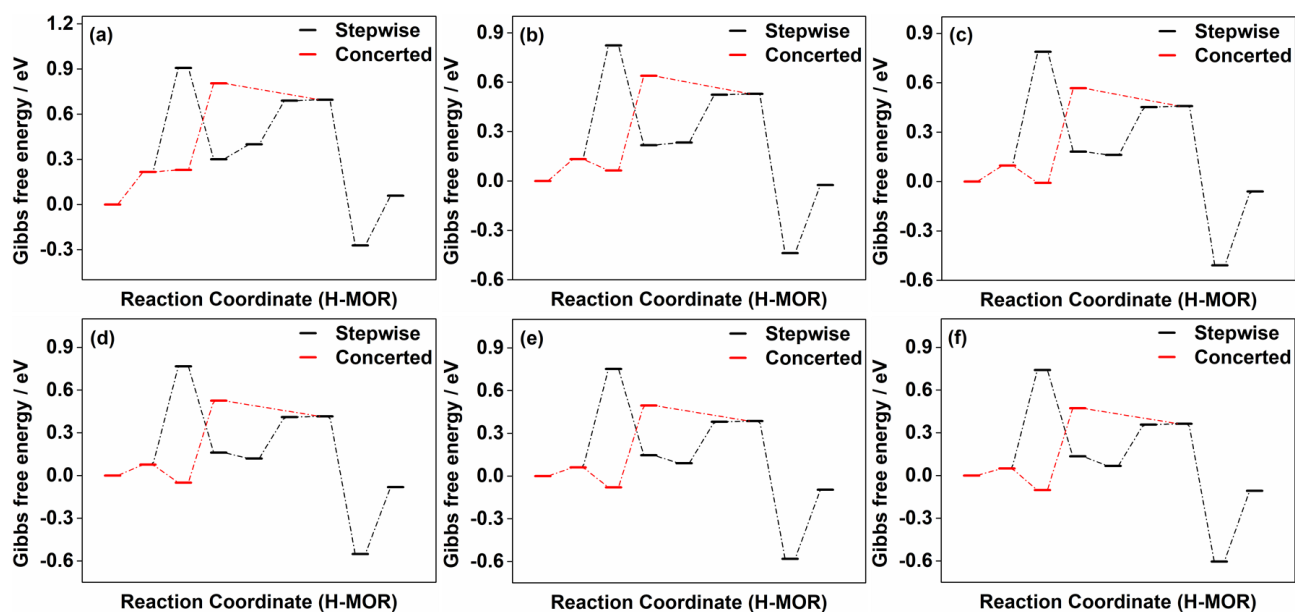


Fig. S19. Gibbs free energy diagrams of the complete reaction coordinate over H-MOR at different pressure ((a) 1 atm, (b) 5 atm, (c) 10 atm, (d) 15 atm, (e) 20 atm, (f) 25 atm). The cycle consists of the stepwise and concerted mechanisms.

Table S10. The TDTS and TDI of H-MOR including (a) stepwise and (b) concerted mechanisms.

(a) Stepwise

Pressure / atm	1	5	10	15	20	25	30
TDTS	TS1	TS1	TS1	TS1	TS1	TS1	TS1
TDI	S5	S5	S5	S5	S5	S5	S5

(b) Concerted

Pressure / atm	1	5	10	15	20	25	30
TDTS	TS3	TS3	TS3	TS3	TS3	TS3	TS3
TDI	S5	S5	S5	S5	S5	S5	S5

S5. Discussion of the carbocation

The carbocation or ion pair structure in the zeolite catalyzed system has been investigated extensively.¹⁵⁻¹⁸ For

the alkylation of benzene with olefins, this specie (protonated alkylbenzene) has always been regarded as an intermediate along the reaction coordinate. For example, Rozanska *et al.*¹⁹ started from the transition state structure for the TS2 structure of the stepwise mechanism and performed a dynamic annealing simulation without putting any constraint on the system. The transition state quickly evolved toward a carbocationic species. Then, the back-donation of the proton occurred directly completing the reaction coordinate. Similarly, for the alkylation of benzene with ethene conducted by Wang *et al.*,¹ the carbocation (protonated ethylbenzene) was formed after the co-adsorption of benzene and the ethoxy group. Subsequently, it will soon donate a proton to the zeolite and generate the ethylbenzene product. However, the carbocation was not considered by Lei *et al.* when investigating the alkylation of benzene with propylene.²⁰ The authors utilized a cluster model to investigate the reaction mechanism, wherein the carbocation can't be stabilized. The neglecting of the carbocation intermediate along the reaction coordinate may be attributed to the cluster models.

For the instability of this carbocationic specie, it's difficult to detect it experimentally.^{17, 21} Fortunately, Chowdhury *et al.* recently have identified this carbocation in the zeolite catalyzed alkylation of benzene with ethene in experiments using operando UV-Vis diffuse reflectance spectroscopy,¹⁶ evidencing the existence of the carbocation along the reaction coordinated of the alkylation of benzene with olefines.

After the formation of carbocation, next step is protonation. However, the transition state of this step was always neglected. For example, Rozanska *et al.* proposed that the cumene was obtained directly by proton back-donation from the carbocation completing the catalytic reaction.¹⁹ Also, Wang *et al.*¹ reported that the carbocation will soon donate a proton to the zeolite and generate the ethylbenzene product and this is an exothermic step and easy to occur. However, there were no evidences proving that the proton back-donation is easy to occur. Herein, we conduct a further research to attempt to elucidate this process more clearly.

For the carbocation in the present work or in the previous work, a rotation is needed firstly for the next deprotonation. Specifically, the carbocation (see Fig. 2f) needs to be rotated to make H₈ atom close to O atom initially coordinated H₁, based on which the corresponding structures were constructed as shown in Fig. S20a and Fig. S20b. And then an optimization process of the rotated carbocation (see Fig. S20a and Fig. S20c) was conducted using VASP. Interestingly, the final optimized structures were the adsorbed cumene (see Fig. S20b and Fig. S20d) rather than the more stable carbocation. Two rotated carbocation were constructed and these two initial structures adjacent to different O atoms (see Fig. S20a and Fig. S20b) were all optimized to be the adsorbed cumene state, indicating that the thermostability of the carbocation can be alerted by rotation. More importantly, the deprotonation process will occur directly and easily after rotation.

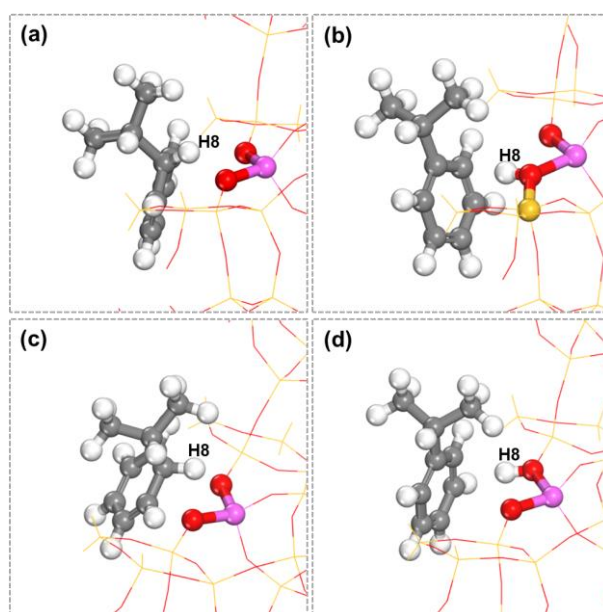


Fig. S20. Structures of the initial carbocation after rotated and the optimized structures after rotated. Both (a) and (c) denotes the rotated carbocation. (b) and (d) denotes the optimized structures corresponding to (a) and (c), respectively.

Generally, transition state exists at the chemical bond breaking and reforming process. However, no chemical

bond breaking and reforming occurs along the carbocation rotation process and the spontaneous deprotonation occurs directly only when a certain rotation degree is reached. Therefore, it seems improper to determine a transition state along the rotation process.

As discussed above, the transition state can be stabilized only by a certain degree rotation. Therefore, the carbocation can be regarded as a temporary reservoir of the transition state. That's to say, there are two directions after the formation of transition state. One way is to deprotonate to form the most stable cumene molecular, and the other way is rotating to form the relatively more stable carbocation. In the real catalytic system, the transformation between the transition state and the carbocation may be reversible, but the formation of the most stable cumene molecular will be the ultimate direction of the transition state.

Although the carbocation is unstable and difficult to capture in experiment, it's still reasonable to be included in the reaction coordinate. To say the least, neglecting the carbocation in the reaction process also has no effect on the final conclusion of the present or previous researches.

Table S11. Absolute energy of all the optimized intermediates over H-BEA.

Intermediate	H-BEA	Adsorbed propylene	TS1	Isopropoxy	Co-adsorption of isopropoxy and benzene		TS2
Energy / eV	-1533.15	-1582.68	-1581.86	-1582.83	-1659.66		-1658.94

Intermediate	Protonated cumene adsorption	Adsorbed cumene	Co-adsorption of propylene and benzene	TS3	Benzene	Propylene	Cumene
Energy / eV	-1659.27	-1660.10	-1659.38	-1658.91	-76.03	-48.67	-125.67

Table S12. Absolute energy of all the optimized intermediates over H-ZSM-5.

Intermediate	H-ZSM-5	Adsorbed propylene	TS1	Isopropoxy	Co-adsorption of isopropoxy and benzene		TS2
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Energy / eV	-2301.64	-2351.23	-2350.36	-2351.38	-2428.08	-2426.76	
Intermediate	Protonated cumene adsorption	Adsorbed cumene	Co-adsorption of propylene and benzene	TS3	Benzene	Propylene	Cumene
Energy / eV	-2427.84	-2428.90	-2428.09	-2427.64	-76.03	-48.67	-125.67

Table S13. Absolute energy of all the optimized intermediates over H-MOR.

Intermediate	H-MOR	Adsorbed propylene	TS1	Isopropoxy	Co-adsorption of isopropoxy and benzene		TS2
Energy / eV	-1151.13	-1200.70	-1199.94	-1200.80	-1277.75		-1277.16
Intermediate	Protonated cumene adsorption	Adsorbed cumene	Co-adsorption of propylene and benzene	TS3	Benzene	Propylene	Cumene
Energy / eV	-1277.37	-1278.44	-1277.66	-1277.10	-76.03	-48.67	-125.67

Table S14. Cartesian coordinates of all the optimized intermediates over H-BEA.

H-BEA			
4.1980311393529925	10.0440825910463634	1.5090758828206847	Si1
4.2211216755582806	6.8255721171822987	1.4827563897563416	Si2
9.0172883126358343	10.0697792354933888	1.5114407664791196	Si3
9.0319696460521079	6.8666407862050303	1.5594898545664273	Si4
12.0953186406162256	10.0939997632971163	1.4419062658604864	Si5
12.1106723062038881	6.8604640937077281	1.4473931366548873	Si6
6.6896567698681109	10.8226040553093146	3.3374083898204439	Si7
8.4342759011302988	2.6699515372441849	14.8162354633245847	Si8
8.4151691711956040	5.8838900342076244	14.8079624873257796	Si9
3.6518656405866037	2.5559895272057744	14.8185617302619530	Si10
3.6275992720362544	5.7509057435527380	14.9237626663793126	Si11
0.5363214193616479	2.5362263284657685	14.7465186748243759	Si12
0.5405396350461298	5.7538373388523993	14.8220789136712128	Si13
5.9699201016944095	1.7953526565213163	16.6256162410814170	Si14
2.6631649927575674	4.2073519776780826	8.1496555316789703	Si15
5.8870145214290925	4.2002074151628763	8.0538242960601103	Si16
2.6406512597215808	9.0311490222397275	8.1618357860104140	Si17
5.8434314518165751	9.0826592372318817	8.1955239956404036	Si18
2.5554119954827623	12.1233785859223016	8.0833429594993440	Si19
5.7789494243273118	12.1944134848043184	8.0974951252779306	Si20
1.8920617911617237	6.7006798157876499	9.9818211510918911	Si21
10.0146752054916348	8.4319008803809066	21.4734265857143996	Si22

6.7994669495539846	8.4266370954596450	21.4229842444513885	Si23
10.0567464708072354	3.6380253304577610	21.4847583943629168	Si24
6.8574079201209903	3.6368309262593881	21.4956985473223199	Si25
10.0795389842605658	0.5477191099105998	21.3995640190215610	Si26
6.8510611938425452	0.5397626391649349	21.3945489537225697	Si27
10.8536803521311302	5.9639431749293728	23.2946152447333468	Si28
8.4279781444391340	10.0173492760950325	25.0564134873979683	Si29
8.4171704889466241	6.8002666422803193	25.1058029165071588	Si30
3.6437692639136974	10.0657603883463160	25.0500257557192647	Si31
3.6305274933049971	6.8678876377840474	25.0245285164541009	Si32
0.5507292518626792	10.0917478335008237	25.1286142293909016	Si33
0.5347137684354371	6.8657315354775186	25.1182870572519832	Si34
5.9602209303023841	10.8618563133971353	23.2283664298760399	Si35
4.1823408112103353	2.6261857131202864	11.7867548414564727	Si36
4.2530183794813903	5.8329035910139302	11.8766767084849540	Si37
9.0079560132091796	2.6515435977628008	11.7445324383478269	Si38
9.1619377194547376	5.8078098104942120	11.8120107813471691	Si39
12.1230522480359788	2.5762317907777148	11.8376736707553558	Si40
12.2537745651354406	5.8010710509836025	11.8706065318375149	Si41
6.6670420141711046	1.8233162293833645	9.9378945965746350	Si42
10.0393332929533905	4.1916441422033737	18.4363141741448331	Si43
6.8254883979776180	4.2125469015033623	18.4525416141298351	Si44
10.0646454448268656	9.0317880338774224	18.4320623839518944	Si45
6.8640302110984539	9.0369509624471114	18.3805711068220674	Si46
10.0876716374449931	12.1069121330337666	18.5034315914550618	Si47
6.8542363639953301	12.1151986551140709	18.4884862958328817	Si48
10.8371912139103674	6.6951699865312584	16.6378160355442262	Si49
2.6544220747389868	8.4452973449597533	5.1171291030373949	Si50
5.8697003820073670	8.3919322500442686	5.1636069544770358	Si51
2.5799086282304140	3.6531607597612217	5.1048607644165447	Si52
5.7706756508531294	3.6159939920364241	4.9965359151227116	Si53
2.5510508215460375	0.5437823905908914	5.1756575213513552	Si54
5.7691805557323557	0.5379594159148180	5.1615360763296030	Si55
1.7942929214998207	5.9776836219728153	3.3037759315564510	Si56
1.7563454809271393	10.8990918280690572	3.3131889250871001	Si57
6.6756389316228395	5.9854527581028920	3.3102150318929389	Si58
10.8893792179907525	1.7605338141582645	16.6088656997742383	Si59
5.9931740670773292	6.6801474681990971	16.6253441708168808	Si60
1.7617945835896760	1.7598679238571826	9.9590810607601288	Si61
10.8891463669024997	10.8840720698863809	23.2672106915172847	Si62
5.9733157380986093	5.9791395247204946	23.2617054271568051	Si63
4.0531225489233540	8.4321017506003226	1.7046961042035973	O1

4.2594332882294434	10.4161136144182773	26.5144994104896163	O2
2.9012168141541657	10.7651844143183375	2.1651602201070066	O3
5.5555470678130945	10.5899315936778091	2.1961770479372760	O4
4.2415760725046958	6.4801620023131212	26.4812765729442674	O5
2.9633410407714318	6.0635219714512330	2.1726729325445628	O6
5.6193527004097019	6.3122979860287760	2.1152729345233467	O7
8.9567894679941666	8.4716811085680632	1.7916997931116330	O8
10.5551699622619370	10.5853262742505940	1.5860705895963720	O9
8.1551022536441469	10.8495666139039120	2.6377491926202592	O10
10.5756468627608378	6.3644792951987235	1.6357093786483921	O11
8.1850395742951267	6.1340733798366349	2.7280308976596284	O12
12.1960663292393008	8.4776732149173721	1.5543905447808752	O13
0.2891287912824593	10.7664187677717127	2.6376333997358610	O14
0.3420429460171105	6.1980434168064678	2.6198075454924261	O15
8.5313110789795950	4.2813998751357314	15.0514402531384697	O16
8.4064239188857925	2.3581231257075252	13.2241512307646705	O17
9.7362535766585179	1.9662445018266332	15.4770231423829419	O18
7.0766645738661893	2.0845955449134701	15.4667476080071893	O19
8.4757609445110003	6.2128819714822017	13.2096759452643546	O20
9.6707627484467800	6.6288480086333745	15.5043468019098327	O21
7.0173485556956150	6.4578185816844789	15.3743081221099249	O22
3.8038063898738739	4.1465404370197909	15.1060331236869256	O23
2.0912438904767354	2.1162476124291016	14.9147005045329735	O24
4.4923822381031302	1.7569963429199711	15.9538228404988232	O25
2.0718761586376218	6.1689375316960051	15.1271183251418453	O26
4.4777517179338684	6.4997433288332687	16.0848936801346341	O27
0.3355507413173081	4.1440580210770577	14.8976748915940398	O28
12.3504606599552922	1.7943679974531959	15.9081892640141032	O29
12.2768788434304561	6.4627774126901816	15.9398226133505343	O30
4.2710442643001381	4.0618857617377868	8.3059833660073288	O31
2.2408239015565790	4.2479092546216224	6.5819851269839775	O32
1.9399679953847559	2.9304842425402069	8.8488697879062777	O33
2.1308378667068011	5.5740758301011111	8.8388815350029883	O34
6.2019647463328607	4.1609429427439766	6.4585355160632218	O35
6.5899349332671058	2.8883169071562831	8.7248542468132104	O36
6.4783459240442172	5.5431086267684293	8.6764119989012407	O37
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2.0466731952672843	12.6483443329778762	6.6771321868367854	O125
6.2377535046027752	0.1578542971361450	6.7271891660083041	O126
10.5969882202651373	0.0155925954291169	20.0051263327629698	O127
6.3639573673312571	0.0009760674755145	20.0112802429902708	O128
6.6988058427215966	6.6975735796017073	10.0562625938940613	Al1
9.4165466389558929	8.1869030664230316	10.0119608745223836	H1
8.6143132683721735	7.3671758250218025	7.9379828885962089	H2
9.3676652213036373	9.5035566006725212	8.8512509579159957	H3
11.0107188012001167	8.7575637060005391	9.3436612825576120	H4
10.8230112931858180	6.4565368590488141	7.0368757074363248	H5
10.0049178433239199	5.3597060263014873	8.1331224894595149	H6
11.4448774324369822	6.3449667172718804	8.7113130954352851	H7
10.5294735511150179	6.3266139829126056	8.1069494356114919	C1
9.6323594217057522	7.4399975887153484	8.3469296710950687	C2
9.9574802776579965	8.6081208097034203	9.0830759741455935	C3
Propoxy			
4.1767374004833213	10.0395519385424272	1.6048810445301513	Si1
4.1998461781203753	6.8385395100413389	1.5715509281512032	Si2
8.9984624161276798	10.0735119445343795	1.5998839538792327	Si3
9.0174006341303574	6.8704617527517566	1.6351720164151233	Si4
12.0809049997879132	10.1066837099365738	1.5229190337645713	Si5
12.0998129831725887	6.8728828922489900	1.5125087784087852	Si6
6.6699584678291037	10.8289690386000537	3.4497638433550177	Si7
8.4463238249143977	2.7118798469777059	14.8694367209696594	Si8
8.4072346531143136	5.9368497932596904	14.7869765184832112	Si9
3.6732238061186591	2.5199466992590054	14.8646553959000371	Si10

3.6393691348966275	5.7128233238918122	15.0323320496839319	Si11
0.5529156157873378	2.4914518379273680	14.8414122261461863	Si12
0.5569617045970983	5.7046678530437722	14.9709845206495196	Si13
5.9868214721341264	1.7967447794580280	16.6833487321934371	Si14
2.6587468363953146	4.2096637078290922	8.2484068881985753	Si15
5.8692141804246987	4.2396017582278258	8.1522021581155197	Si16
2.5610119301590815	9.0391031154766264	8.2158119550877746	Si17
5.7790906857887281	9.0923906640807548	8.3215416344430189	Si18
2.5169440255877729	12.1109680343673798	8.1463335935303967	Si19
5.7468913826744581	12.1872777804090227	8.1851607831844326	Si20
1.9152419597396777	6.7107969234684841	10.0882878516041465	Si21
10.0109710926710047	8.4694735084698056	21.5364004125515649	Si22
6.7979656844955123	8.4738751518136635	21.5067681236830630	Si23
10.0603006260861676	3.6736530612290359	21.5329129389511671	Si24
6.8655207953607968	3.6731943298963365	21.5416070106831832	Si25
10.0806877637915502	0.5605556681754754	21.4672237491245532	Si26
6.8542865629058936	0.5572016136776003	21.4824934895658686	Si27
10.8599113221158436	5.9915149745013530	23.3516957932158213	Si28
8.4419989033907576	10.0242659709371562	25.1347434201107873	Si29
8.4280920714908039	6.8013024626338359	25.1775486201473484	Si30
3.6504558548248696	10.0779797000224374	25.1413480443571622	Si31
3.6324544944316322	6.8874904239233192	25.1046710788251204	Si32
0.5519627327834867	10.1160813686297058	25.2178121444786534	Si33
0.5333893473889947	6.8855424576820079	25.1903800970458143	Si34
5.9653457912442356	10.8953616040034671	23.3190226308230706	Si35
4.1868085532973804	2.6522038533939458	11.8349915909662187	Si36
4.2673073593182913	5.8431819366510345	11.9827814165674571	Si37
9.0267863815616902	2.6489854954381848	11.8073547861426000	Si38
9.1795423326852745	5.8232474247426831	11.8171404884596924	Si39
12.1373036472743401	2.5541785518972890	11.9339876782123469	Si40
12.2925212432916240	5.7730193625585695	12.0164368349250790	Si41
6.6799217934008146	1.8664874039362911	9.9906416595184453	Si42
10.0305628989810440	4.1737456346349600	18.4885821146280627	Si43
6.8484927267847775	4.1903380528680740	18.4948749509736743	Si44
10.0427467970915334	9.0411516485409091	18.4817917249387378	Si45
6.8437974054463986	9.0510709839818873	18.4576374720924470	Si46
10.0711905933463743	12.1098583118178009	18.5840477864437617	Si47
6.8357276637497648	12.1190599694339696	18.5938650733729887	Si48
10.7928140229256257	6.6900176249489514	16.6708545001783826	Si49
2.6454691029575210	8.4627842601323806	5.1962827656335673	Si50
5.8761151696940628	8.4126407688279556	5.3055862247063814	Si51
2.5627051468195776	3.6716214127351221	5.1937108102183167	Si52

5.7481721423274079	3.6409039272185186	5.0913862092490421	Si53
2.5273608270762855	0.5743088910704935	5.2480978999306709	Si54
5.7521413587598529	0.5605350389804695	5.2449088264369470	Si55
1.7875522077451711	5.9856406331396554	3.3673787515569344	Si56
1.7531418462144075	10.9266775990214811	3.3830925904067204	Si57
6.6645268369694861	6.0179772568774847	3.4084360399324662	Si58
10.9040386269403538	1.7806750927618948	16.6773312685235311	Si59
6.0457520175223562	6.6895499852641791	16.6808167419749900	Si60
1.7592683597890235	1.7586059862168497	10.0197429729941110	Si61
10.9025562428858223	10.9047176248755839	23.3371715074630579	Si62
5.9755669719422206	6.0041753706867116	23.3331610553338571	Si63
3.9675367485639765	8.4350244912955379	1.8188505109897986	O1
4.2853532482369285	10.3912917610290592	0.0231087554436602	O2
2.8868454501538907	10.8067882555846193	2.2214096092241533	O3
5.5338361379824015	10.5427309898499662	2.3226399076188593	O4
4.2536416931419767	6.5220049928692587	26.5647511559468548	O5
2.9578753357840135	6.0260245228409905	2.2334553566322661	O6
5.6039983163379024	6.3660906502753658	2.2229675625395995	O7
8.9266253437884284	8.4743875715003956	1.8668532840649248	O8
10.5382533998087062	10.5838094689910402	1.6949020945486439	O9
8.1278259069714149	10.8413348973517980	2.7309358533611539	O10
10.5655033537136518	6.3830277049978488	1.7231315999578458	O11
8.1699918118354073	6.1407617223113613	2.8075826505027091	O12
12.1943629382759742	8.4896337568048388	1.6165175649406542	O13
0.2810592557634134	10.7687779728121598	2.7221355967031959	O14
0.3374645878642208	6.2095460270174643	2.6808425757562446	O15
8.4700667800916651	4.3326919601885727	15.0619071987850610	O16
8.4115272383377633	2.3600564315879922	13.2844043250480741	O17
9.7859940773881995	2.0745995940001212	15.5281875315617999	O18
7.1259082029797405	2.0814941926296524	15.5555888771250714	O19
8.4235877288781378	6.2468152451225070	13.1816588398686250	O20
9.7124937002260161	6.6395316869529521	15.4500220882969028	O21
7.0470658075879413	6.5639650364984057	15.3978547984992531	O22
3.8390227159754566	4.1067236174709976	15.1605292185844291	O23
2.1135323332195211	2.0824866877497881	14.9850450564502129	O24
4.5297696037119550	1.7031983986547969	15.9742206822505430	O25
2.0867669025414100	6.1055215398042675	15.3108326767202438	O26
4.5271158874808854	6.4292962963183307	16.1850262543565435	O27
0.3412172953465931	4.0948860190085492	15.0259834095394673	O28
12.3760154595035861	1.7225380070255272	15.9951782676201351	O29
12.2726635136821756	6.4105666552889744	16.0757813239257388	O30
4.2627466095212823	4.0340911702688320	8.4373492629646680	O31

2.2692076559072420	4.2885009787235484	6.6719932275561593	O32
1.8998568472140069	2.9282354842133955	8.9001568133401676	O33
2.1254903004115162	5.5680625588996033	8.9539409822766256	O34
6.1395424454773142	4.2390627541024370	6.5455515033851919	O35
6.6376966499932095	2.9362688703483211	8.7742139787611233	O36
6.4301881958212102	5.5910911458430164	8.7856097835231335	O37
4.1579011655909648	9.0107242218952930	8.4410087564160055	O38
2.0280446179379683	10.5711622920226205	8.3093934294790852	O39
1.8156402691914317	8.1629073206732841	9.3642988841874359	O40
6.2505871749831794	10.6551066566129009	8.3148950903310332	O41
6.4514242586807580	8.3280880336272372	9.5540637159031192	O42
4.1263573587664517	12.2614168888908583	8.2985711070381711	O43
1.7959459537650020	0.3018979624136190	9.3164727011870827	O44
6.4115753726446734	0.3779525767906557	9.3985661123735671	O45
8.4026055729818765	8.6068331548408050	21.7666082004679851	O46
10.3557766761289862	8.4150129639550872	19.9507376924749416	O47
10.7477581230226544	9.7593267865305009	22.1909144850740709	O48
10.5607601134504492	7.1048872671813772	22.2064073208065658	O49
6.4936329459817115	8.4142775669718244	19.9139930662513365	O50
6.0557344782875022	9.7729485591516063	22.1412668612513954	O51
6.2216023870552002	7.1148752894342451	22.1704011993356715	O52
8.4633432439736804	3.8342584718834711	21.7839331232129503	O53
10.5019080060793826	2.1162081737199174	21.6475675512877643	O54
10.8547404101131306	4.5191414945526045	22.6645131391530015	O55
6.4319407533134134	2.1134124391785836	21.6612922604314946	O56
6.0887194736759227	4.5210277187961614	22.6822768003275996	O57
8.4679643692851627	0.3855670435274470	21.5719066143288600	O58
10.7853722143800592	12.3704713423340760	22.6506532393657167	O59
6.1644312703183646	12.3714901031492150	22.6771967606473268	O60
8.5338851488027636	8.4098689620725455	24.9320841160944617	O61
8.3865319897072137	10.4021033026178529	0.1266744102467456	O62
9.7548080929833354	10.7133524572854579	24.4738070477788057	O63
7.0969066590068417	10.5978122059635016	24.4446704603357681	O64
8.3921145819138765	6.4797355424590455	0.1826569737204684	O65
9.7263418313374981	6.0808639748615212	24.5170923082907670	O66
7.0683958411919203	6.2155121940781388	24.5196494557709919	O67
3.7470747294175872	8.4854854047586397	24.8371404225987646	O68
2.1040261032867167	10.5688532196822838	25.0707509278329432	O69
4.4977431267830044	10.8754643622862286	24.0129013210245503	O70
2.0794408954134673	6.4186722014327913	25.0164639436147418	O71
4.4802196954611562	6.1203710938853932	23.9558028506119669	O72
0.4105995375016524	8.5022820796656866	25.0880611293195912	O73

12.3679525036393958	10.8177517089217758	24.0268659531639059	O74
12.3298803224760949	6.2111137979238995	23.9995530226921474	O75
3.9118263078020576	4.2540502680601486	11.7647332479162419	O76
4.2538078891962199	2.1683235212401466	13.3873201029550426	O77
2.9519442184049973	1.8811473738929638	11.1159680385884556	O78
5.5898933889830138	2.2555134248941897	11.1335387021323236	O79
4.1001300542530714	6.2128425892495889	13.5629672548278677	O80
3.1351325006495081	6.6909979693708168	11.1559061350566271	O81
5.7504877620940489	6.2068689586209844	11.4988671718078592	O82
8.9765167190004291	4.2559120907942329	11.4937274987495961	O83
10.5733906576316503	2.1621854506890283	11.7386041597012838	O84
8.1585675204676491	1.8694637251385289	10.6875275081946093	O85
10.7366584581997451	6.2545206465937717	11.8678034377367485	O86
8.4599399721759454	6.6609064189514209	10.5363176790768449	O87
12.3532230262112019	4.1654261232440017	11.8447284183561106	O88
0.3103288182068654	1.8541344252640870	10.7453383082681206	O89
0.4836046281912352	6.4853736371596709	10.8432671077670619	O90
8.4378561343290919	3.8519652383065766	18.3220923905186091	O91
10.4323218460391729	4.2606842210331886	20.0581040706307654	O92
10.8637865041111450	2.9643590477107651	17.7950666826491357	O93
10.3928990801831098	5.5916749951038325	17.7981892649959654	O94
6.4678473140662325	4.2573215982472234	20.0715241903576249	O95
6.0001464233723016	3.0015427428859294	17.7822976277720635	O96
6.5011542387039736	5.6241639587805565	17.8246283649250934	O97
8.4453334576283119	8.9873423076127743	18.1913652654705338	O98
10.5762934894514746	10.5758813343384741	18.3941706210159168	O99
10.8084458942628476	8.1639850976909862	17.3508651620083185	O100
6.3249166521285280	10.5905462334522866	18.3781234036558629	O101
6.0984943173835555	8.1867717541493352	17.3057566103276841	O102
8.4535558547970844	12.1715591156254419	18.5436286986281722	O103
10.6588784801252476	0.3363571073360146	17.3663472217827106	O104
6.2398912324654869	0.3690569412139318	17.4003740983577586	O105
4.2669006021408178	8.5319576096245822	5.0588034481743911	O106
2.1993654294030387	8.4058256089631787	6.7571616399236296	O107
1.9986854814619157	9.7892447864464032	4.5188524688403886	O108
2.0725743808875068	7.1313041956078296	4.4815552843922593	O109
6.2222486269762376	8.4192564237653080	6.8888083657240342	O110
6.6140511648398252	9.6763516567337433	4.5948134796451523	O111
6.4385432473928690	7.0321084142740702	4.6619783844584859	O112
4.1456533672650178	3.7691057204807259	4.8531037513851158	O113
2.0723973284484765	2.1258235730323585	5.1128965693632384	O114
1.7432669701324084	4.5323809036683000	4.0887962739773593	O115

6.2126206163285493	2.0894788351670672	4.9581022733300042	O116
6.4969830647526781	4.4912459766278978	3.9294346065950831	O117
4.1384549711609795	0.4161638298334069	5.1070754227121027	O118
1.8067495485676597	12.3973699411961640	4.0635366774754837	O119
6.4595500375728889	12.2814492059283005	4.1333686075728577	O120
-0.0166853756257950	10.6011581426820634	0.0785787879747762	O121
12.6355079078738655	6.3919877448137594	0.0517040838032776	O122
-0.0027928170083087	2.0338147887942393	13.3811724992858796	O123
0.1767580086878080	6.2305069395306010	13.4725167896956375	O124
2.0500514406666595	0.0016194829193322	6.6917302018878440	O125
6.2142927148430136	0.1297965328399001	6.7456590506314908	O126
10.5921115233757188	0.0278202885054918	20.0132757430522439	O127
6.3299228952017650	0.0142428435084088	20.0375165716451704	O128
6.6133757648521083	6.6973473850416649	10.0921722389224886	Al1
10.7675010533296174	8.3003312591132765	10.4436362283005657	H1
8.4501394525340316	7.4330086145109293	8.6190498197447489	H2
9.2378026435590161	9.1934930279064968	10.1410926761284141	H3
10.4000519716144879	8.9249804629864418	8.8226773707021096	H4
10.4799048709460667	6.4764646785991591	7.7467662991375770	H5
9.5331320168097644	5.1993119217460331	8.5352224651577711	H6
11.0025544229835965	5.8723093379589919	9.3251389915666500	H7
10.1196565205517146	6.1094044827620007	8.7196547868831864	C1
9.2598490806864273	7.1979852844266548	9.3235565453553875	C2
9.9578858640624759	8.4763956191880077	9.7251984818971327	C3
Co-adsorption of propoxy and benzene			
4.1946543393741829	10.0141655256330662	1.6090522201738204	Si1
4.1978505340840027	6.8044186259395998	1.5787310189859804	Si2
8.9810996312197382	10.0531868650720533	1.6189728244841444	Si3
8.9907317010858971	6.8539302522853243	1.6528590509645227	Si4
12.0755024959342379	10.0798750209976991	1.5334083120420532	Si5
12.0887099559881381	6.8540206704256788	1.5344468680641832	Si6
6.6629968946406679	10.8156288291570757	3.4596783239731979	Si7
8.4432428179653947	2.6683700445164162	14.8942410299365999	Si8
8.3959970904428740	5.8951784360142945	14.8108505823969558	Si9
3.6659820953492837	2.4936991308379599	14.8786946571393308	Si10
3.6256518386821219	5.6822571599629494	15.0504111429579659	Si11
0.5396599560899045	2.4536019746352626	14.8596950318924890	Si12
0.5412032323739837	5.6629935976129175	14.9873449979541107	Si13
5.9712816972663756	1.7654205259589921	16.7085501745157998	Si14
2.6482990738038432	4.1756201159096973	8.2576663568639681	Si15
5.8590235206074714	4.1832102093201184	8.1786599228057622	Si16
2.5296111040469831	9.0048918133877560	8.2431332733140916	Si17

5.7356024085703785	9.0429988975887667	8.3286216048164459	Si18
2.4951081061890341	12.0731436049938132	8.1585765459966719	Si19
5.7281629305453867	12.1414369265946949	8.2085034855867729	Si20
1.8828893462760268	6.6709843471231727	10.0987419936313394	Si21
9.9952533469972735	8.4446504234010362	21.5531841026258455	Si22
6.7837824193764842	8.4378647117821863	21.5211352675168044	Si23
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1.9401541430200142	12.4740725856709016	6.7628952779018547	O125
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11.2302122658779258	10.6277912022529115	5.7108817883088685	H2
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10.6790921181527700	11.1901053228931584	8.6845900284022619	H4
8.7537079387415186	10.2529073469644345	5.5893314666802665	H5
9.1357581484074935	11.8928487630530171	6.1742578753019144	H6
8.6114744237557925	10.6292479089155911	7.3161170642378126	H7
8.9582187223812735	6.8364956254169309	9.9488312373605723	H8
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Co-adsorption of propylene and benzene			
4.1556687578066818	10.0789731856268130	1.5455856292923282	Si1
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8.9503829046910255	6.8051506166773814	1.6055857349845748	Si4
12.0584069346529343	10.0056749219246601	1.5670129013121559	Si5
12.0459169995858471	6.7802333377296318	1.5104794582648955	Si6
6.5836861571932692	10.8217791731479007	3.3965420239504560	Si7
8.4144940849993084	2.6427212471568065	14.9100258956834484	Si8
8.3738064395304814	5.8490755009561362	14.8787799537107848	Si9
3.6321387263910099	2.4936373055318830	14.8732574230911592	Si10
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0.5044210429461022	5.6790556696489167	14.9446200297611771	Si13
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2.5377065604626630	9.0029052253141799	8.2387292600032911	Si17
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5.7003909818885257	12.1681588835725520	8.1971370138130517	Si20
1.8508558337773662	6.6812301582351026	10.0971064808872715	Si21
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6.7320529398559756	8.3788712510365464	21.5047959797055839	Si23
10.0217139870583836	3.6187790640814663	21.5443950999418483	Si24
6.8261891678569437	3.6057423084953122	21.5751692186395232	Si25
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6.8365722282916304	0.4921871193896453	21.5139280207456203	Si27
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8.3748022931088535	10.0040741118226766	25.1706603233908162	Si29
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1.6918635689290846	5.9647180922745937	3.3921732098482660	Si56
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6.3739520846706901	5.5922961342875013	17.8917735765342378	O97

8.4312800732712088	8.9124308370064771	18.1899396018247757	O98
10.5447598841977452	10.5163077248618677	18.4231196082257824	O99
10.8208416013366122	8.1048703742782902	17.3917213681820186	O100
6.3373934089242372	10.5451223633510782	18.3776591206731261	O101
6.0794842296044083	8.1479785774482174	17.2877603277610454	O102
8.4484159114246431	12.1680506709344272	18.5099585708927634	O103
10.7195843255628507	0.2534618142075096	17.3799788618548234	O104
6.1840857165258134	0.3226495464031324	17.4266003687077138	O105
4.1781412901139179	8.2057527081392188	4.9594821005471408	O106
2.2163683882438843	8.3993752169580382	6.7696207579972878	O107
2.0900119969565258	9.7951139466339505	4.5330216924592319	O108
1.7964177385972191	7.1494731036247927	4.5145414410748819	O109
6.1040718453870557	8.4482026888985882	6.8140855758383250	O110
6.3744463659852597	9.6099906394300962	4.4661109233474638	O111
6.5036297293822445	6.9774909476613756	4.6805200598264562	O112
4.1222837552080769	3.7777741553024615	4.9104482019858882	O113
2.0746191493439707	2.0936578867262696	5.1155159490158955	O114
1.7301703722493269	4.5119232871996084	4.1136572160560565	O115
6.1328287501766416	2.0363267622375747	4.8943076726225998	O116
6.4548797959242528	4.4372750400265382	3.9147272057211699	O117
4.0909289292684496	0.3161174662391451	5.0991781409575934	O118
1.7358751330807287	12.3725854952982939	4.0589216736183165	O119
6.4427597468819604	12.2273606382660205	4.1451941240679355	O120
12.6315130720362063	10.4971722792438253	0.1184963421241027	O121
12.5957299316996192	6.2909894463456109	0.0532173350525366	O122
12.6547895214186639	2.0089513989607846	13.3609566224273824	O123
0.1313199898684979	6.2096978634109821	13.3970762724820318	O124
1.9819327671918177	12.6164051352093374	6.6828301914803054	O125
6.1833436026514370	0.1341998743582047	6.7372855697428422	O126
10.5716618058998488	12.6396023392180101	20.0208485616295953	O127
6.3387116088073192	12.6077989730828790	20.0569846253070452	O128
6.6799487002386133	6.6858497920722302	10.0633374150328940	A11
9.7452269546308425	7.9914531838167289	9.7836627199470989	H1
8.6964185632347331	7.3254702252862023	7.7070422665473934	H2
10.0006853898509540	9.2422330541430249	8.5891803770507611	H3
11.3903597184424203	8.1244419043722438	9.0350955450235286	H4
11.4404694211315050	5.8776412656117794	7.8733855580761585	H5
10.0005779650813498	5.4000754625819471	6.8558624935423085	H6
9.9103669971571087	5.2993847956805329	8.6032686085897883	H7
8.3912044733465407	8.1597197245918593	5.4501557733597679	H8
10.6229003232840213	7.1560107750284425	5.1110458992425603	H9
12.6606015418387017	8.4496109120171301	5.6475295945422008	H10

12.4801271706923220	10.7961394301715821	6.4726929615774758	H11
10.2278629503155756	11.8109866689964420	6.8247531286030556	H12
8.1741833654981129	10.4947953569320340	6.3366158576852669	H13
10.3488547327592357	5.8982486086990846	7.7697621674666566	C1
9.7528435787191086	7.2163119803497073	7.9763948371123981	C2
10.3172079351232551	8.2177951469405208	8.8390143195500528	C3
9.2717407276426655	8.7410489754407728	5.7102558259706981	C4
10.5372074213244087	8.1598418075238044	5.5324297618769513	C5
11.6892680529579955	8.9062460837814257	5.8049223632087745	C6
11.5810244254473229	10.2126157075824953	6.2681011568146188	C7
10.3109379580807587	10.7846075460292106	6.4617022152176391	C8
9.1580438521122041	10.0520667671170987	6.1824588137939092	C9
Benzene			
14.8747817779742277	15.0159289811664607	14.9340037495855853	C1
14.8194535895164741	15.0460844130526290	13.5378262259756834	C2
13.5909465638813103	15.2035697628956008	12.8905707169376491	C3
12.4176895985957358	15.3309977718984332	13.6392709920262813	C4
12.4729793374717879	15.3009849661937007	15.0352484767070766	C5
13.7015495267721974	15.1433452685087673	15.6826933646248694	C6
15.8347823972974080	14.8930540806239726	15.4398503569640653	H1
15.7363220125607057	14.9465311305411479	12.9527926728653888	H2
13.5477558331395116	15.2271353540732139	11.7995227630840951	H3
11.4577874687922510	15.4541468345409090	13.1333074913551133	H4
11.5563315601882639	15.4005687215114175	15.6204594264487433	H5
13.7449209038101809	15.1199529549939022	16.7736512734254433	H6
Propylene			
7.3129069757117131	7.7163855877587837	9.0595554973855794	C1
8.2036246838803422	6.5339365652252397	8.8455803235819612	C2
9.5269169028917524	6.5181380070259713	9.0312527331009083	C3
7.7098738268751887	5.6156783149839065	8.5069396276486220	H1
10.1184105952078607	5.6192007199967140	8.8496935523410958	H2
10.0675666111147741	7.4062907031306446	9.3710956703608304	H3
6.5393688608546299	7.5020369116306069	9.8161351159089012	H4
6.7744742340085544	7.9763238443012581	8.1334034256623262	H5
7.8813563644551934	8.5987590009469095	9.3864942640098228	H6
Cumene			
8.7533491069829559	8.4915500955931549	10.3341127192483579	C1
10.1426627166391476	8.4564055132997549	10.4684018576258850	C2
10.7269553060124032	8.4103254974318524	11.7367060879893579	C3
9.9082526566577407	8.3980644350293598	12.8676293793761474	C4
8.5186389502516757	8.4303783114623645	12.7262452495180280	C5
7.9159891194557206	8.4782033503602374	11.4606699514493027	C6

6.4029683725275088	8.5472341096551077	11.3315773593127780	C7
5.8441385583646737	7.5557903283545702	10.3026109051716919	C8
5.9419844117535350	9.9799535331408258	11.0147497806321226	C9
8.3166925631087505	8.5253244679766240	9.3331182221656768	H1
10.7731910229010914	8.4606048878484916	9.5763095656028216	H2
11.8132452833379489	8.3810500383274658	11.8417217036931017	H3
10.3532070423184255	8.3581405783554139	13.8644611293227733	H4
7.8840246690310058	8.4152837159907161	13.6170477923687603	H5
6.1746074241989577	6.5276708885748089	10.5111703861355110	H6
6.1634782505072421	7.8120757212326559	9.2804796242002325	H7
4.7438839969111068	7.5722409521856209	10.3133634489999437	H8
5.9883024161365626	8.2741385937166445	12.3178978066124714	H9
4.8444107648193881	10.0275588506561597	10.9416823099758300	H10
6.2654278705949711	10.6874075338394672	11.7922356643563067	H11
6.3602194124895375	10.3208375939685979	10.0546186652427512	H12

Table S15. Cartesian coordinates of all the optimized intermediates over H-ZSM-5.

H-ZSM-5			
0.9998273611314616	8.5869431711378290	9.2266628004274018	Si1
18.9621228869762319	11.8014914883751398	4.3130382329143009	Si2
8.8143120068378131	18.7810365644360253	11.0874451413513935	Si3
11.1619926256682511	1.6321854178849000	2.4553248418728204	Si4
0.4949638286718935	6.4388549535264170	11.3691388225158914	Si5
19.4684614565356462	13.9202086173640645	2.1466466010028573	Si6
9.3370325491393782	16.6281198428801602	8.9593763496799692	Si7
10.6491802741522683	3.7736114332492163	4.5986009133880845	Si8
1.2381647454410161	5.7229121237581060	0.7628482270353959	Si9
18.7110632410458528	14.6850542503229367	12.7843312690671240	Si10
8.8346343914524823	15.9001246285334492	6.0196159571150680	Si11
11.2355794773362874	4.4880313009247592	7.5391707481058852	Si12
1.2435384041711355	2.5853709600647887	0.5071330220487396	Si13
18.7138817866410001	17.8354325253644745	13.0254285544054955	Si14
8.7502232542065528	12.7468456138877428	6.2670818339780077	Si15
11.2362343765173840	7.6451192859093267	7.2696375726958919	Si16
0.3977443954148205	1.6125779012636552	11.1850666101879384	Si17
19.5314909184634189	18.8287715848997301	2.3142604977938186	Si18
9.3824601220648720	11.8027074740141167	9.1409386054000734	Si19
10.5823916012620529	8.6005918160354238	4.3930659983892681	Si20
1.0094428449972057	4.0273499416493870	9.3355866491719244	Si21
19.0158396895869970	16.3740856668828165	4.1546980161624205	Si22
8.7819754911086818	14.2210101547241052	10.9991383519022499	Si23
11.1746724786675120	6.1744769244039794	2.5544096082010963	Si24

16.5796742268413588	8.6896169126469740	9.2018813323254331	Si25
3.3950638068914354	11.7040666804840860	4.3019047560952046	Si26
13.3868766429544603	18.8764058606174352	11.0965418433842977	Si27
6.5870154701591419	1.5248928295962716	2.4209559270661591	Si28
17.4746773804666908	6.3615090540010844	11.1922105291919181	Si29
2.4371874389410650	13.9856967756524835	2.3687230401407047	Si30
12.5151288622536168	16.5657253042138315	9.0904355699049475	Si31
7.4789822032083562	3.8432772671913167	4.4211164633577589	Si32
16.6069103003923928	5.5704872344873069	0.4839701931881648	Si33
3.3490968443691154	14.8654763332010162	13.0861008013881719	Si34
13.5852482972639628	15.7639769151673370	6.2506118289088644	Si35
6.4444256893699716	4.6378391302756601	7.2634162670559226	Si36
16.5870724051519645	2.4235288258719896	0.4432884301292161	Si37
3.3768403157194529	18.0135556335424916	13.0604400709627164	Si38
13.5515421939507412	12.6249265526272012	6.3149872645475931	Si39
6.4292614890470041	7.7846669102299400	7.2320172617159288	Si40
17.3964525507794541	1.4461412723338625	11.1682766241464027	Si41
2.5180212623324718	18.9999556140662378	2.3256788866451190	Si42
12.5458786933457134	11.6532250900681280	9.1394563785050433	Si43
7.4112370136437900	8.7626126396913140	4.3980877915953771	Si44
16.7416340728018369	3.8808158825418397	9.2939801595267824	Si45
13.2184277106184247	14.0808369839042822	11.0098720448627425	Si46
6.7497786934434565	6.3237465677946147	2.5225834658810280	Si47
8.8292924465022669	8.7695261733282166	8.9960888858086445	Si48
11.1543505811684245	11.6252586531812163	4.5508857619828307	Si49
0.9698732331482588	18.9830626829664091	11.3168564539785539	Si50
18.9907467363253097	1.4469312154928753	2.2300126415175123	Si51
9.4088335100158975	6.3954279043407771	10.9913867639863216	Si52
10.5816566608233558	14.0039382370591081	2.5527019410438418	Si53
0.3394766889220248	16.5841503353398494	9.4065271662726460	Si54
19.5807834214661085	3.8077019434490209	4.2263208249312276	Si55
8.8588325541599495	5.6417582945708906	0.3845322424580099	Si56
11.0992161214278280	14.7615190312062907	13.1617084901169719	Si57
1.0437716165750284	15.8016695863347909	6.4618801558014285	Si58
18.8521382746837745	4.5781730357485024	7.1626814179678373	Si59
8.7800535344933497	2.4838604133278666	0.4592413899492622	Si60
11.1977742806703500	17.9194654546369989	13.0784446976813111	Si61
1.1975183543806263	12.6537216766599645	6.2913656536735507	Si62
18.7665855792516894	7.7392223575042944	7.2322552086767917	Si63
9.4124945676612661	1.4500719757034226	11.1367523747216008	Si64
10.5830278292829743	18.9603238914556655	2.3961090474582196	Si65
0.4099587058293429	11.6538073492361978	9.1738504059990671	Si66

19.5818522165426963	8.7431960223983740	4.3642258322585308	Si67
8.7070238704182206	3.8145996434562033	9.2766627592632318	Si68
11.3431504667655041	16.5873506914763453	4.2610029804962002	Si69
1.1005079686602530	14.0068230022267297	11.0798766961522794	Si70
18.8746704327915396	6.3882840636515610	2.5037837399371110	Si71
13.4186840067801931	8.6313847051542556	9.2780115447351115	Si72
6.5516980526724486	11.7939356178808161	4.2515904576754995	Si73
16.5364241293903902	18.8260131015259091	10.9972996018955218	Si74
3.4277577579390162	1.6113756245263922	2.4892372758091446	Si75
12.6070910920591412	6.3830738839988390	11.2914615316926916	Si76
7.3822047040565728	14.0338985105801370	2.2418240875453619	Si77
17.3303574661531243	16.5700789442256067	9.0330633683264523	Si78
2.6270496465672903	3.8204937307449098	4.5291997775057542	Si79
13.4760684221262235	5.5601749796160522	0.6441214236996363	Si80
6.4899878346481561	14.8506903804156778	12.8978285744889547	Si81
16.7421494803420856	15.7167379831243679	6.1274631223789138	Si82
3.3100107083196169	4.6297272519639945	7.4357882017038941	Si83
13.5007462332950112	2.4133634982292462	0.5172134078811048	Si84
6.4719126294010749	18.0003022937390931	13.0158152799863558	Si85
16.6518129209056802	12.5782854306409195	6.2518501675227274	Si86
3.3347275199822399	7.7756452896055608	7.3065981081699354	Si87
12.5798586479304539	1.4794948574587186	11.1123690627213616	Si88
7.4073889643426929	18.9277880942235690	2.4203431454250914	Si89
17.3892631111490630	11.6778839368307992	9.2041225725734552	Si90
2.5948388872874300	8.6846598755553046	4.3460342949747961	Si91
13.6301944896500711	3.9819593288911062	9.5413826665115131	Si92
6.4026415291693901	16.4233846528652627	4.0181968181756726	Si93
16.3175367299271770	14.1865478564755101	10.7679549979189506	Si94
3.6404192032466685	6.2030974444798224	2.7619465675737493	Si95
3.2754353980910644	16.5067056266343108	4.1673303537086763	Al1
1.1121765921932787	7.7253147328818450	10.5957760213064311	O1
18.8095707791622111	12.6739242163819927	2.9549385151715621	O2
8.7078663539549375	17.9206664080684277	9.7143199237213480	O3
11.2743433039498804	2.4888057499704401	3.8294029278915187	O4
1.1948240662451570	6.3893446149844246	12.8305624450335163	O5
18.7162089283961599	14.0138124406470421	0.7103532594522531	O6
8.6396521701848830	16.5395249290541990	7.4995777221112450	O7
11.3518680009885600	3.8389276466750588	6.0583264806478576	O8
0.8242093201671741	4.1536582033649800	0.6171911202612550	O9
19.1070152783019260	16.2589345031440295	12.9343199480668449	O10
9.1758568979554731	14.3103834660725724	6.1425461865129591	O11
10.8661044066720098	6.0698292276359185	7.4217120291709646	O12

1.2189163278068897	2.1409036188148587	12.4897113200488139	O13
18.6763246238733203	18.2944773272302506	1.0283390278730438	O14
8.5688810347773359	12.3265621996463839	7.8280942516238783	O15
11.3849454816990221	8.0554285172598714	5.7047087194592425	O16
0.7235601348593876	2.5318850113202926	9.8904459843465649	O17
19.2335334183380446	17.8720365710321332	3.5945460564078986	O18
9.0381595985424905	12.7243729551622948	10.4301152093934153	O19
10.9194274879741791	7.6778947508468773	3.1028714336337764	O20
0.8307696460780100	5.0733022958245293	10.5603886657346777	O21
19.2134055169035811	15.3040424289594661	2.9632343346786501	O22
9.0186079136200714	15.2717503430274917	9.7886984986619687	O23
10.9700494959770865	5.1400090731139514	3.7848410065610110	O24
16.8919423995380491	7.6370430088422978	10.3894387739746374	O25
3.0660936325935770	12.6403079552022746	3.0301386734274183	O26
13.1071764848010730	17.8483827157866841	9.8773270589231448	O27
6.8922576010842658	2.5645729065439333	3.6263314964010007	O28
16.6091528925708793	6.2365343197123053	12.5552383661019249	O29
3.3333325361753041	14.2848265009035416	1.0426867648369293	O30
13.3493269994216615	16.4403494662771834	7.7066567174258696	O31
6.6149833568061114	3.9908372029773576	5.7846406551189951	O32
17.0123341372579802	3.9947479462272111	0.4006073413884561	O33
2.9384373723731114	16.4428673253312994	13.0669254450330552	O34
13.1316815220457865	14.1992061794232072	6.3141099403091321	O35
6.8607606111648423	6.2134495436488777	7.2132763746659903	O36
16.5070596039687700	1.7944934822754250	12.4847719618709299	O37
3.4163700013009310	18.6523152406872015	1.0026398396215996	O38
13.4286710934627340	12.0277623238462734	7.8237740100741879	O39
6.5483891099078360	8.3984171975379862	5.7296375933736172	O40
16.9703779755037090	2.4029195149297218	9.9284799162799420	O41
2.8916575819238255	18.0566011465124561	3.5580476040020441	O42
12.9750832143702777	12.6035481427646143	10.3824974629299653	O43
6.9678553603998798	7.7987563708731500	3.1679539173255078	O44
17.3426348691902277	5.0030341047112357	10.3090989601130367	O45
2.4533061122161395	15.2030405125708032	3.4137412054559642	O46
12.6715953643302139	15.2078368293186603	9.9709185963639193	O47
7.3549454320589565	5.1973906567533801	3.5299408527208698	O48
19.0395819135112951	6.5913837457963478	11.5505078528752971	O49
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4.8652853040537352	18.1436961165975461	5.9137060148106615	H7
4.1098249783334930	18.2958476536771535	6.6941267349998697	C1
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4.3559495133544335	15.8921121012738453	7.5743542855223458	C3
Co-adsorption of propoxy and benzene			
0.9564201967077395	8.4594930504251895	9.1842673983161465	Si1
18.9418911776494561	11.6768959795884104	4.3335143069403621	Si2
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11.1112748103206602	1.5533098325597567	2.4969020597736473	Si4
0.4870038980662379	6.3373615552590428	11.3617767915634040	Si5
19.4088832482926072	13.7971777608380819	2.1213298140200663	Si6
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10.6526967885154740	3.6471276363551333	4.6732551671951219	Si8
1.2240584588375665	5.5313372651878145	0.7261299480190442	Si9
18.6367546881273114	14.5347252106962053	12.7817726617378913	Si10
8.8138931425351696	15.8049611797758054	5.9350119544096636	Si11
11.2053312068039173	4.4326070668403883	7.6032569964944310	Si12
1.1690282630355813	2.3864858962063544	0.4759169746678134	Si13

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0.3532414330670336	1.4271282738117836	11.1597843177636022	Si17
19.5170157543580842	18.7403320614468996	2.2800022302970566	Si18
9.3066954487233460	11.7408291844839177	9.0475057826870522	Si19
10.5757017916631444	8.5253409014776409	4.4103640582266870	Si20
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13.0385238746244809	1.6281697718243540	12.5901937794175076	O141
7.0267705485193348	18.7925101593958672	0.7527319468576636	O142
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7.3581086714866313	3.8358950196349553	8.2996555171572624	O173
12.8200302965573751	16.4025902924288154	4.8828991688282759	O174
2.3168817377352986	14.0034376727083210	12.2253659525869445	O175
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19.3767302530755359	10.3154241830217170	3.9876880271042929	O188
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7.0984195557439485	0.0225408086625989	2.8208052575782729	O190
17.0956270013964904	10.0700028411823919	9.7411656155200088	O191
2.8663621897302809	10.1901009900887587	3.9293970004469276	O192
3.8857212104664245	17.2304253881690563	10.4297255038032297	H1
6.1144083984436417	17.0955354307904024	9.2373494554769273	H2
4.5696773547376539	15.5865774490339994	10.3911700526576958	H3
3.2479248042749487	16.0050482433860957	9.3064302893477233	H4
5.9363047719560180	14.7839554233416575	8.4517469807045984	H5
6.2002582992560553	15.8307416796502824	7.0339863309360648	H6
4.5869447419412017	15.1933620969930665	7.3686384866176908	H7
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2.1505507669891832	20.1775059759945101	7.3584070332969773	H13
5.5013011079845171	15.5865076618853244	7.8379923869911767	C1
5.1827937549278271	16.8065588430750346	8.7181447073874505	C2
4.1628179658160143	16.3972371177212395	9.7734272746118478	C3
4.0841790781044525	-0.0644309193383115	6.4036049501947412	C4
5.3648711326663916	-0.6221987145918423	6.3110257095088702	C5
5.7015545071659854	18.6442553378582119	7.0481161273893047	C6
4.7730438085152347	18.0280404913743872	7.9063141328098210	C7
3.4897557615406938	18.6034006171784263	7.9937557540169486	C8
3.1494240111415284	19.7477581824399309	7.2509539236731237	C9
Co-adsorption of propylene and benzene			
0.9346832167565358	8.4373647485920529	9.1975694373144776	Si1
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11.0705567290976177	1.5390281535935790	2.4368210369255459	Si4
0.4626713455504959	6.2861784252224062	11.3345885598455691	Si5
19.3811514445140105	13.7955155722559617	2.2048190180282763	Si6
9.2533419478099699	16.5032523172327288	8.9748342499009581	Si7
10.5689030667272377	3.6824136441573851	4.5728966174337131	Si8
1.1434913538527423	5.5654665399463630	0.7403609151524874	Si9
18.6339158442835071	14.5314731425776262	12.8334616013040641	Si10
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11.1612753534399296	4.4011635522493311	7.5193873873141328	Si12
1.1415278061287164	2.4259623395952508	0.4802817668524542	Si13
18.6188277024685327	17.6821599667748615	13.0779413185647631	Si14
8.6695195694472815	12.6561933825351876	6.2777464342350475	Si15
11.1356105143027815	7.5538182126466342	7.2451458963143347	Si16
0.3148277475295438	1.4423151101919476	11.1602338486493089	Si17
19.4580474366387790	18.7016036734865345	2.3645153739492493	Si18
9.2997219677392486	11.7034099708331141	9.1492499863506342	Si19
10.5027995185162819	8.4917856114295258	4.3634908277236448	Si20
0.9721264502150023	3.8643743475206036	9.3424932495428816	Si21
18.9302810797167851	16.2445620194558700	4.1916043291687988	Si22
8.6817455199113951	14.1056094250337569	11.0194377558136587	Si23
11.1137272912960778	6.0807466225314410	2.5251122454634523	Si24
16.4948606086662082	8.5356420827381907	9.1790625113469417	Si25
3.3283678633421032	11.5697357689870017	4.3266669157273840	Si26
13.3044640225692810	18.7610474501552993	11.0764262721833742	Si27
6.5086662931250290	1.4524142397060302	2.3788499445175360	Si28
17.4268196568248079	6.2079336211462746	11.1630914665456960	Si29

2.3645608167878116	13.8874177593499724	2.4312676555714852	Si30
12.4437177537526686	16.4313281424805702	9.1020888493181502	Si31
7.3999419732268130	3.7525977235330941	4.3951753494363945	Si32
16.5473578331467941	5.4250401899037932	0.4637258261480260	Si33
3.2477041633907264	14.7368301027876818	13.1149080601023265	Si34
13.5048879357191858	15.6310249678428761	6.2465557178109021	Si35
6.3864964784337186	4.5431662283773058	7.2410686623820837	Si36
16.5065142412282739	2.2875693423625636	0.4553566017078083	Si37
3.2657214530028882	17.8803686201523959	13.1064853866805606	Si38
13.4674521494887447	12.5036492463097737	6.3109742830985267	Si39
6.3520168806183230	7.6764969955551772	7.2055022467230145	Si40
17.3090908187958874	1.2721184734718998	11.1840142251471377	Si41
2.4421171763097518	18.8716281575515161	2.3872068249856255	Si42
12.4636667042316436	11.5460478782004294	9.1446482847022388	Si43
7.3334683097022983	8.6466637613255681	4.3668311873899999	Si44
16.6633564479619274	3.7064842788674168	9.3138689373553376	Si45
13.1410402673785072	13.9518390632182694	11.0463700750930709	Si46
6.6681270488975617	6.2207441916735400	2.4884306763714918	Si47
8.7336125801966276	8.6723405616370748	8.9672945628587737	Si48
11.0725326959814065	11.5251912636326441	4.5624563205461577	Si49
0.8639987813188929	18.8203685137067431	11.3465763028666995	Si50
18.9039548923080467	1.3241925397382002	2.2496477237134562	Si51
9.3303394609720840	6.2872810970071313	10.9606645045915485	Si52
10.4880534204333085	13.9180687241406140	2.5773675344283560	Si53
0.2370007030295545	16.4015637083781769	9.4369068554407303	Si54
19.5220309227891171	3.6901401556884563	4.2543937173452875	Si55
8.7955987156000965	5.5599709207755792	0.3538868158780713	Si56
11.0020418624562666	14.6588911787333700	13.1757654675297253	Si57
0.9660450383926592	15.6511788188660343	6.4851837835486759	Si58
18.7942722926309109	4.4201405572382777	7.1961703907764170	Si59
8.6996020224017627	2.4075149253808226	0.4374824849762675	Si60
11.0937241033005716	17.8190667998453947	13.0885640512219510	Si61
1.1366254662488924	12.5062298587230760	6.3335566689895879	Si62
18.6893657674768399	7.5824244004654791	7.2273261536382911	Si63
9.3369261394347500	1.3409038004832849	11.1306848081301570	Si64
10.5110201427863981	18.8666781088651305	2.4070467055795404	Si65
0.3248960061033775	11.4892230374488182	9.2062445958388857	Si66
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12.5243324297388874	6.2672408934836250	11.2628806061783990	Si76
7.2894001697295021	13.9432222481514181	2.2742962653514276	Si77
17.2372393002344211	16.3889360515224496	9.0890712038949779	Si78
2.5681888170661242	3.7304374410345749	4.5167016053687750	Si79
13.3939321912859199	5.4349682414729354	0.6062395028841184	Si80
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13.5574461820449503	3.8798892182920692	9.5061848403919527	Si92
6.3199605631132503	16.3690860229898973	4.0144309787010908	Si93
16.2387148722058932	14.0129718412999456	10.8285932337011310	Si94
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3.1870085797139605	16.4116906908087081	4.2756475579067308	Al1
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16.4530372912507872	1.5909167381602445	12.5298060202118755	O37
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6.2280179517516769	19.2513531610870565	6.5430964744635185	C7
6.4228143164943354	19.4407693964355275	7.9252579962514433	C8
5.8510046098688671	0.1436563809412086	8.5753925754651199	C9
Benzene			
14.8747817779742277	15.0159289811664607	14.9340037495855853	C1
14.8194535895164741	15.0460844130526290	13.5378262259756834	C2
13.5909465638813103	15.2035697628956008	12.8905707169376491	C3
12.4176895985957358	15.3309977718984332	13.6392709920262813	C4
12.4729793374717879	15.3009849661937007	15.0352484767070766	C5
13.7015495267721974	15.1433452685087673	15.6826933646248694	C6
15.8347823972974080	14.8930540806239726	15.4398503569640653	H1
15.7363220125607057	14.9465311305411479	12.9527926728653888	H2
13.5477558331395116	15.2271353540732139	11.7995227630840951	H3
11.4577874687922510	15.4541468345409090	13.1333074913551133	H4
11.5563315601882639	15.4005687215114175	15.6204594264487433	H5
13.7449209038101809	15.1199529549939022	16.7736512734254433	H6
Propylene			
7.3129069757117131	7.7163855877587837	9.0595554973855794	C1
8.2036246838803422	6.5339365652252397	8.8455803235819612	C2
9.5269169028917524	6.5181380070259713	9.0312527331009083	C3
7.7098738268751887	5.6156783149839065	8.5069396276486220	H1
10.1184105952078607	5.6192007199967140	8.8496935523410958	H2
10.0675666111147741	7.4062907031306446	9.3710956703608304	H3
6.5393688608546299	7.5020369116306069	9.8161351159089012	H4
6.7744742340085544	7.9763238443012581	8.1334034256623262	H5
7.8813563644551934	8.5987590009469095	9.3864942640098228	H6
Cumene			
8.7533491069829559	8.4915500955931549	10.3341127192483579	C1
10.1426627166391476	8.4564055132997549	10.4684018576258850	C2
10.7269553060124032	8.4103254974318524	11.7367060879893579	C3
9.9082526566577407	8.3980644350293598	12.8676293793761474	C4
8.5186389502516757	8.4303783114623645	12.7262452495180280	C5
7.9159891194557206	8.4782033503602374	11.4606699514493027	C6
6.4029683725275088	8.5472341096551077	11.3315773593127780	C7
5.8441385583646737	7.5557903283545702	10.3026109051716919	C8
5.9419844117535350	9.9799535331408258	11.0147497806321226	C9
8.3166925631087505	8.5253244679766240	9.3331182221656768	H1
10.7731910229010914	8.4606048878484916	9.5763095656028216	H2
11.8132452833379489	8.3810500383274658	11.8417217036931017	H3
10.3532070423184255	8.3581405783554139	13.8644611293227733	H4
7.8840246690310058	8.4152837159907161	13.6170477923687603	H5

6.1746074241989577	6.5276708885748089	10.5111703861355110	H6
6.1634782505072421	7.8120757212326559	9.2804796242002325	H7
4.7438839969111068	7.5722409521856209	10.3133634489999437	H8
5.9883024161365626	8.2741385937166445	12.3178978066124714	H9
4.8444107648193881	10.0275588506561597	10.9416823099758300	H10
6.2654278705949711	10.6874075338394672	11.7922356643563067	H11
6.3602194124895375	10.3208375939685979	10.0546186652427512	H12

Table S16. Cartesian coordinates of all the optimized intermediates over H-MOR.

H-MOR			
8.9895969866576184	3.1321022253429813	4.1233609579045858	Si1
6.9324078255122332	13.5960969962866933	4.1104418494714388	Si2
6.5180595882048848	10.4782427218616281	0.3327588453181204	Si3
8.3626790868970406	0.1941357007736657	0.2692779921306275	Si4
4.1987846722218212	8.5837564461972828	7.2538237861344577	Si5
14.3234372928872968	5.2702981454263531	7.2580392638587563	Si6
11.2094610850101208	5.1707488513805764	3.4784088068487344	Si7
1.1111771580791998	8.3863097562209070	3.4555912005293408	Si8
6.4737877824281798	10.5138749375806153	3.4472288001749996	Si9
8.4544953588715845	0.0899661795130594	3.4152247675451144	Si10
8.9751052040863861	3.1911869308364240	7.2634079580379067	Si11
7.0086349694869146	13.5991041710321934	7.2214944938711261	Si12
11.2114616550113606	5.1896575466495056	0.3506760282428151	Si13
1.1796660056536963	8.3696785748342943	0.3642136253798762	Si14
4.2078848197142946	8.5414805916237242	4.1245917965638643	Si15
14.3278603383005034	5.2761069937420055	4.1623144971760473	Si16
6.8992702653437030	3.9831381795696323	1.9258942754648416	Si17
4.5043931575101590	1.8935514496356782	1.8927183857908743	Si18
8.5158542790987450	9.6889212802969151	5.7036467169814964	Si19
10.9349307108168468	11.7962209826269842	5.6115056002310766	Si20
4.8033530689133377	6.3693676959604399	1.9475542397634769	Si21
2.3999031973882547	4.2842161553260905	1.9109473221124764	Si22
10.5780852293078524	7.3080966817938062	5.6793924292600977	Si23
13.0001350937302860	9.4130133096473863	5.6647330059037975	Si24
8.9442912638833221	3.2994074625793002	11.7138255067647332	Si25
6.8575830594757319	13.5113835836747764	11.7383970847779295	Si26
6.4792261942804714	10.5253187616490411	7.9327281417175550	Si27
8.5369399036723888	0.1038082794717824	7.8402174617866303	Si28
4.2792123881734563	8.4183354803974932	14.8497993326121609	Si29
14.3261829914379710	5.2745149966719556	14.8066202136110920	Si30
11.2929630786989854	5.2256321172616031	11.0488317538428227	Si31

1.0661969397660860	8.3866741502598092	11.0437263398376704	Si32
6.4195005908107641	10.4755714817136365	11.0596207574357539	Si33
8.9126248120332612	3.2858151133844715	14.8195948307420782	Si34
6.8345020394711300	13.5735089674599756	14.8153765957417711	Si35
11.2007608788977606	5.2436732883326140	7.9306101575262389	Si36
1.1034302278174566	8.3925189694981963	7.9238597060380993	Si37
4.1566776323367902	8.4129564377590835	11.7292295487506522	Si38
14.3722511037403304	5.2482796356592836	11.6981741750090258	Si39
6.9191892026071669	4.0627894071699560	9.4737175891099739	Si40
4.5575394065410704	1.8861446402744144	9.4902341296920198	Si41
8.5684314077997161	9.6712580716173839	13.2449685955284284	Si42
11.0021577627467906	11.7718540855274849	13.3274118840704894	Si43
4.7807481226877480	6.3750562223175082	9.4168247308364776	Si44
2.4306769788076399	4.2132631208730578	9.4327581008159775	Si45
10.6548118966242598	7.3471642577668357	13.3208827572612645	Si46
13.0798156163693466	9.4628525282477103	13.3406596743122456	Si47
8.3678493295192702	0.1881506181200834	10.9721902622995824	Al1
7.8185015591451439	3.8450535893984794	3.2530591494197285	O1
4.4648040820768653	1.0035734939300698	3.2496570587444422	O2
9.0684488072213245	1.5416707085143824	3.8016470409809706	O3
7.6041576755208009	9.7534465308098959	7.0460540954928144	O4
11.0374088875561558	12.8062801894102805	6.8718382724953395	O5
6.5051566035598363	12.1185825630196007	7.6541432290512850	O6
4.9562872758361962	7.2308456599863149	0.5751775914838275	O7
1.4705245152554629	4.3272782932627099	0.5783371649435174	O8
2.7580184155974230	8.6831889740178116	0.1923332762969242	O9
10.5235957158641238	6.3401355152144285	4.3756688482282122	O10
13.9549108028740960	9.3449926112105111	4.3544182042350945	O11
12.7627189083207959	4.9607873752745908	3.8893174388741691	O12
7.6000000492371873	9.7993556976250247	4.3692361978336152	O13
10.9111132486801186	12.6187814548334973	4.2036232507158964	O14
6.4315641611240668	12.1124831090634633	3.6913448756172640	O15
7.8146298134237178	4.0529247310913874	0.5873831798745163	O16
4.3848203328499986	0.9386718439751602	0.5857612373658080	O17
8.8867692719091629	1.6867799733682249	-0.0479216771739207	O18
10.5479678780921642	6.4496742956164193	7.0568885268571160	O19
13.8892465266593046	9.2973599435130350	7.0233517782308557	O20
12.7470212119206181	5.0106531014413616	7.5086911883872922	O21
4.8499052532854883	7.3284390729244837	3.2550116482000151	O22
1.4604140250084756	4.3142727112553043	3.2356988767434585	O23
2.6589109564640570	8.7814367573009449	3.7158302446723068	O24
6.8837747579036046	0.0437530782998844	3.8165353952581755	O25

6.7993675276709009	0.0319141608308836	-0.1031525051567471	O26
0.8481408288088833	6.8405939450330342	-0.0549447377211723	O27
0.8578530108674399	6.8319682600117480	3.8343516384666478	O28
6.0463891050570258	5.3476909211108943	2.0452148709846036	O29
3.2512433784188071	2.9130403466669224	1.9101230384398338	O30
9.2751409283840811	8.2624986350474519	5.6619403036757339	O31
12.2405933087969849	10.8382096323296579	5.6381893409161830	O32
5.9202985571122717	2.6912683755751083	1.8195385888968765	O33
9.5718046705528810	10.9182309621392086	5.7281102744998149	O34
3.3787735778305752	5.5851100877847912	1.9159914785407943	O35
11.9492520643926383	8.1758388206716024	5.6211474026914772	O36
4.9762099032517941	0.1825911352585324	5.6714285787802474	O37
8.6478496963618650	3.4038245448826951	5.6846030057224395	O38
10.2659168168805177	13.5025082470976479	1.8210768660036780	O39
6.8428466703148150	10.1920651815327084	1.8967796818933591	O40
0.9024537238790928	4.9615109346239512	5.7093983319816903	O41
4.3329630788104003	8.1443972157791826	5.6947828981550748	O42
14.5193383948899264	8.6390317047947924	1.8972872324650820	O43
11.0980492779062292	5.6089898720396842	1.9160456670076205	O44
10.4381882825099943	3.7622751963278653	3.7307993830019437	O45
5.1077230048059121	9.8000357297198164	-0.1040222192249962	O46
5.0027070743314477	9.9250079698812197	3.8146927786432809	O47
10.4084125318097662	3.8065864320209593	0.0550790718696359	O48
7.8658729484557695	4.1086110171288812	10.7887722135469968	O49
4.4832034769235074	0.9200859548560161	10.7878139627723542	O50
8.9514994718526122	1.7306843578583928	11.4167288221366405	O51
7.7394737460901872	9.8318816007050760	14.6268572394520540	O52
10.8778239326971811	12.8477778595681684	14.5066086980703268	O53
6.3871087594072851	12.0669397760579642	0.0622180503845552	O54
4.8454142892874161	7.4051334367680743	8.1648851499946939	O55
1.3917918343918689	4.2493357586269864	8.1830739488330249	O56
2.6376677531865926	8.8289761188967759	7.6294870618541397	O57
10.8350532391124652	6.4974941895873624	11.9561425753515618	O58
13.8431815646102727	9.3293841773748305	11.9115333601841389	O59
12.8483957816670848	4.8463746287833906	11.3239712856339700	O60
7.6171299703668467	9.8160115417267857	11.9480777812110208	O61
11.1452047080836145	12.6483929554035370	11.8677976364710336	O62
6.2281872254008572	12.0467885696504400	11.3813370336276627	O63
7.7886495870985106	3.9131911606648262	8.1086007270650189	O64
4.5981065530824354	1.0126835643246159	8.1218219703981873	O65
9.0815145569963676	1.6187262390796060	7.6067908533025879	O66
10.5540774962648758	6.3919680303211663	14.6262917495955804	O67

14.1292344633678510	9.3862378350312756	14.5682357580994850	O68
12.7632120249918266	4.9585828834233281	15.0975868056619742	O69
4.7001461830085454	7.1768841646895591	10.8290517838315932	O70
1.6178242499704030	4.3526734238700886	10.8335534632924553	O71
2.6037955985941910	8.7626296234065482	11.3931221190160237	O72
6.8126435261344875	-0.2021208677459382	11.5677225674670652	O73
6.9710901071213449	0.0392040653646143	7.3901215929645989	O74
0.9077795774463449	6.8138491252469358	7.6057385909852533	O75
0.7989082976128276	6.8304069257820821	11.3977170086123785	O76
6.1138386255372934	5.4666814027319255	9.3946627299653791	O77
3.2237656641840888	2.8072769068975534	9.4420971688777122	O78
9.2944671055675414	8.2251546616171058	13.2171737808399872	O79
12.3842403415094360	10.9441104712908377	13.3831875777270923	O80
5.8977328924492571	2.8030569551501734	9.5916959039656806	O81
9.7040986305322114	10.8450105175165259	13.1926800421766419	O82
3.4489626775266506	5.4651185975017267	9.2658319996008558	O83
11.9433771737495817	8.3245751370726602	13.5052689488460853	O84
4.8136985127240681	0.1901244086868794	13.2764128432367752	O85
8.5604994519930369	3.6114880482405449	13.2743317868902206	O86
10.3659191545126994	13.3615092992938695	9.3716676962529295	O87
6.7978905154035978	10.2270246670788740	9.4984941356940933	O88
0.8826103486531700	4.9416622737879088	13.2606842597053056	O89
4.3003067840996820	7.9709506795116107	13.2883151995053836	O90
14.5361247581692759	8.6826730944903989	9.4831146131288868	O91
11.0923331741294184	5.6644056092048132	9.4960947323360987	O92
10.4285949723787166	3.9118110660908418	11.4163268449573039	O93
4.9970493502889664	9.9751471738452899	7.5314365686075151	O94
5.0121817743836665	9.7527696964271549	11.4235799369619748	O95
10.4103284809567764	3.8565100823042395	7.6437098232817746	O96
11.8384143910443882	12.3163238944941771	11.2647826240498450	H1
Adsorbed propylene			
8.9280806517635618	3.0868665916301121	4.1079499525175098	Si1
6.8341989640823932	13.5784779513410623	4.0758169169258398	Si2
6.5264787578838011	10.4358742776514237	0.3153489891318060	Si3
8.3344753459422183	0.1837634273655885	0.2536683060398879	Si4
4.1531741674660871	8.5938495575572933	7.2761990772447493	Si5
14.2700603391388778	5.2511927586543408	7.2592349477602500	Si6
11.1628387838674534	5.1194471406521878	3.4906896086745132	Si7
1.0835149462772655	8.3403048145299294	3.4602050039498851	Si8
6.4261435465442949	10.5152056258579041	3.4213928805644298	Si9
8.3622679010463443	0.0469458716258501	3.4083647149148035	Si10
8.9154132794927943	3.1898829802598119	7.2427261482519487	Si11

6.9727797485921119	13.5809555032486262	7.1730073726108268	Si12
11.1580186304714832	5.2142010638824896	0.3651665819730082	Si13
1.1583971220583256	8.3758757373459574	0.3529226015572335	Si14
4.1838572410316077	8.5015757802384311	4.1409693224116220	Si15
14.2857016928613838	5.2314745443454997	4.1617940010086985	Si16
6.8720844485238501	3.9678939926438632	1.8807816409771456	Si17
4.4589271264406705	1.8879530370406610	1.8597060370984200	Si18
8.4878126168399941	9.6846548311836802	5.7046468013410294	Si19
10.9167005176055802	11.7864954159653585	5.6190502474384552	Si20
4.7894278320761146	6.3643327867576946	1.9519068859705031	Si21
2.3720024910436384	4.2840350182598437	1.8982933826513508	Si22
10.5341750710974242	7.3186836604490013	5.6710599556343047	Si23
12.9730676704357002	9.4199478354299657	5.6498801007505914	Si24
8.9188144307340149	3.2297487482700351	11.6786112544406198	Si25
6.8015633719260578	13.4724427556614756	11.7267605852725989	Si26
6.4584275198976355	10.5007962832258332	7.9361289968467696	Si27
8.4652015067113080	0.1209478324927153	7.7835770303909122	Si28
4.2399688609280792	8.4392063859577711	14.8538297684028802	Si29
14.2874065078766748	5.2966189433581423	14.7923336536461054	Si30
11.2670961107648573	5.1645708480740389	11.0387195553861943	Si31
1.0112026489207027	8.3490560384779489	11.0488209737961132	Si32
6.3708046291141178	10.4356315015231242	11.0559627795457427	Si33
8.9125411388697646	3.2514873194994185	14.7996017286040722	Si34
6.8202373659768822	13.5578838139283082	14.7898182953283150	Si35
11.1365862341186670	5.2764621302658083	7.9307638650545300	Si36
1.0586554719991645	8.3694569102397161	7.9224586928969938	Si37
4.1004564276288900	8.3685064625104211	11.7352550231409687	Si38
14.3290252476548297	5.2066312764221623	11.6817834419851359	Si39
6.8765364360074432	4.0502948649376638	9.4703402743009111	Si40
4.5163798110389042	1.8613287887823793	9.4727308019549135	Si41
8.5492681478974912	9.6406073868075772	13.2278017901526379	Si42
10.9592037337991783	11.7684506326584764	13.2949840733302569	Si43
4.7454968553580299	6.3540908832280207	9.4196148974663583	Si44
2.4009059658551251	4.1842378269849245	9.4189694185394774	Si45
10.6433545951555306	7.3264987290958610	13.3190531701723671	Si46
13.0454884390316259	9.4633452998238283	13.3491618734117790	Si47
8.3049290248920151	0.1171559015305236	10.9481375782171408	Al1
7.7803486499641448	3.8111555105618202	3.2146337514840457	O1
4.4166225097149123	1.0469993312975776	3.2488329050462883	O2
8.9923544994683535	1.4950687459590906	3.7877382683784742	O3
7.5587957126297063	9.7044791384335749	7.0376985864466075	O4
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11.0192086027668648	5.6503666340065246	9.5317267228932270	O92
10.3641961216722880	3.8236677427597385	11.3896630684210134	O93
4.9505381956831318	9.9840743464941415	7.5483496415870075	O94
4.9473866408326570	9.6902632644624784	11.4341758045707262	O95
10.2895552411370339	3.9051099547703507	7.6464911667786808	O96
12.1009865964552930	12.0899797040362760	10.3833695400062780	H1
13.9585789835953058	12.3377069645335435	11.7379610209109355	H2
13.3779795990346866	10.9724783529310326	9.8059616716343392	H3
12.9210858481772384	12.4926052480422189	8.8178097872597121	H4
13.1642657631208415	0.8418460482931307	10.7646221138478797	H5
11.7319472706224222	1.0422005142651962	11.7503512447305116	H6

11.5802836187108866	1.0745726609862720	9.9403559997815840	H7
12.0758751993401123	0.6068925421230326	10.7986942760169615	C1
13.6454797865836035	12.8463975916996311	10.8158447872649308	C2
13.1213040492820792	12.0378874364380479	9.7923644342980918	C3
Propoxy			
8.8474668151889393	3.0918209702295352	4.1493479654758634	Si1
6.7569735709678200	13.5401584376176896	4.0856623472845959	Si2
6.5054653119630581	10.4857310008286682	0.3298407061792545	Si3
8.2717372731510110	0.1704472910682312	0.2623182006665790	Si4
4.0947303911793007	8.6293883190875018	7.2944575218661969	Si5
14.2732539658104596	5.2823844706725964	7.2935977585268779	Si6
11.1066693454276368	5.0990814161304714	3.5142997001577512	Si7
0.9946687919161052	8.3630644994842793	3.4959705594138155	Si8
6.3653110049299517	10.4648594611795343	3.4284044534563178	Si9
8.2867893608735788	0.0461215462233499	3.4185301546923279	Si10
8.9288571792932938	3.1941358597369272	7.2880242763363894	Si11
6.9020219213829614	13.6040254791107831	7.1807474746368216	Si12
11.1028647965632032	5.2114694767814473	0.3828626748171972	Si13
1.1385060265988858	8.3861137623777520	0.3944047233721930	Si14
4.1141958793893130	8.4669814519858946	4.1673900868529170	Si15
14.2066225719717476	5.2508131597086649	4.1852398078170800	Si16
6.7943718735960701	3.9481249828423373	1.9471892429321496	Si17
4.3717114511004391	1.8772455411959561	1.8870085303920618	Si18
8.4125215627497063	9.6483422449628549	5.7200908652460107	Si19
10.8163036603261897	11.7862002231252490	5.6419169574147716	Si20
4.7168715012113047	6.3477949375190228	1.9611847603245021	Si21
2.2935424610183315	4.2791539699808929	1.9088062005962887	Si22
10.4830805477926852	7.2978368390186183	5.6958183663882043	Si23
12.8899713259539688	9.4297481208658773	5.6769900726957303	Si24
8.7798511088372528	3.2656947264482752	11.7354046927918443	Si25
6.8051177025777214	13.4466076333585267	11.7537253015874636	Si26
6.4156797743710587	10.5108662815889975	7.9544990557373438	Si27
8.3754738784953062	0.1506720146002534	7.8096239580944067	Si28
4.2214675953179119	8.4565321856352060	14.8793406747859365	Si29
14.2380722040386996	5.3067718241563906	14.8187873307397346	Si30
11.1625605360948992	5.1524406758406203	11.0837985141508746	Si31
0.9505400952119237	8.3471191141994048	11.0628530722553329	Si32
6.2962706718174948	10.4344190935454595	11.0702302237109560	Si33
8.8585815612192782	3.2379737800087200	14.8481950319528053	Si34
6.7488597237116856	13.5903129293944751	14.8119565096624992	Si35
11.1338677807109772	5.2680759940982789	7.9648200720524525	Si36
1.0169266007767672	8.4085721607645780	7.9399052685002198	Si37

4.0594519140223948	8.3658852506476435	11.7662182146308485	Si38
14.2363062303616594	5.2120533267734910	11.7018359221166204	Si39
6.8334908588947361	4.0861233827613432	9.4789107502347729	Si40
4.4876432763940750	1.8672063198895614	9.4790493433936405	Si41
8.5129281234107861	9.6931674610152001	13.2039139195338961	Si42
10.9251879566283883	11.7775347198090010	13.2545302560152507	Si43
4.6959685832014371	6.3699754129633677	9.4560067065385649	Si44
2.3543269098975435	4.1746519784930882	9.4687814122036809	Si45
10.5621855470936836	7.3160194916523222	13.3541677610597187	Si46
12.9870578062002267	9.4179384622248765	13.3871321701655894	Si47
8.2708844489631481	0.1048642679138136	11.0006539939532093	Al1
7.6691150641957595	3.8291885018538547	3.3075362106018620	O1
4.3128586797381558	0.9671433985470151	3.2298598638183158	O2
8.8862620024353500	1.5032158663837158	3.8119083909621052	O3
7.5031080049291417	9.6892710609092951	7.0650788573344245	O4
10.8978307328876483	12.8141346270324981	6.8934715348225266	O5
6.5447823217776140	12.1055008472615384	7.6994215842122591	O6
4.8837882530391639	7.2985131108790071	0.6522325393411378	O7
1.3266123460569919	4.3164110322322307	0.6018953397954511	O8
2.7077227539220106	8.7688902384089804	0.2312184496820728	O9
10.4571732660087573	6.2619567858063023	4.4456781513838433	O10
13.8673006864407320	9.3666106957167834	4.3804124302174010	O11
12.6621165462037411	4.8411299308405216	3.9023252315425405	O12
7.4961920790408536	9.8167426950189167	4.3926696533871326	O13
10.7498649975455915	12.5871032843361323	4.2223481406111780	O14
6.2516264372791088	12.0657596908060629	3.6376964731619106	O15
7.7583690849105258	3.9651465592555510	0.6434904958685101	O16
4.2645202389700225	0.9480448084842579	0.5617035593945671	O17
8.8995203381126906	1.6357415948483955	15.1297076901194547	O18
10.5039143421287751	6.5041141538277785	7.1144543637938371	O19
13.7519587671860464	9.2654220673087462	7.0500268953276874	O20
12.6996219002008033	5.0697648595092559	7.6009516266309198	O21
4.7310988622756183	7.2122619871033669	3.3371372415482705	O22
1.3992923157691404	4.3472533630667325	3.2633184615580104	O23
2.5526898068397159	8.6814163807884270	3.7963356353003528	O24
6.7143694885348042	-0.0214065525643982	3.8152015609731378	O25
6.7046896977316637	0.1371170885980185	15.0268307015769960	O26
0.8694348512154955	6.8494639626860181	15.1070372397839421	O27
14.4250438139391459	6.8252846856607841	3.8613586428732303	O28
5.9691154692553958	5.3339622424009034	2.0005962001029038	O29
3.1143031088168507	2.8908423309832334	1.9078007877102012	O30
9.1458722225623763	8.2068350558592922	5.6373657613262713	O31

12.1564781419382690	10.8715822052741071	5.6753141715363338	O32
5.7867781379667651	2.6790479339204425	1.8457778819319786	O33
9.4907436048457754	10.8566731754951000	5.7875149422253314	O34
3.2992570391405223	5.5580450844674099	1.8529800493350248	O35
11.8147377420944402	8.2179559983322203	5.5806427805004395	O36
4.7605081206299777	0.0924180611041253	5.6475404351430685	O37
8.5387239417770378	3.3614317854754430	5.7182295238018277	O38
10.1142787489826880	13.4611955770245402	1.8237670744665300	O39
6.7869490478020360	10.1347355835445541	1.8917385979892385	O40
0.7924473007504725	4.9588569053274707	5.7348957336223165	O41
4.2716625409311231	8.1440930793347537	5.7516950539954097	O42
14.4613651468039492	8.6272607546387317	1.9274210451529290	O43
10.9882502287685107	5.5725442265836742	1.9623420249701093	O44
10.3011881833088133	3.7042338093027469	3.7405226943173484	O45
5.1068409278747078	9.8138062500846441	14.9947197284834122	O46
4.9067458933889547	9.8295780465330083	3.7701486531703501	O47
10.3481027620996002	3.8083750715703975	0.0461310018558795	O48
7.6991035250780628	4.1203089241070741	10.8522365363664264	O49
4.5312171224647555	0.8875598617155748	10.7665933382396144	O50
8.7206720644112412	1.7083872077615596	11.4056384160219153	O51
7.7670384980818596	9.9069040081082562	14.6307884717239318	O52
10.7264278053808848	12.7810233364116677	14.4989763594759182	O53
6.3677582100664800	12.0833415759164797	0.1240658501230741	O54
4.6811261184064623	7.4588545653036196	8.2532163713608089	O55
1.3466177350486364	4.2385969927347187	8.1912749901867610	O56
2.5270109203767266	8.9177293019161130	7.6212319317378308	O57
10.7164659596131777	6.3992312591019909	12.0286766296034404	O58
13.7668502444898948	9.3037847117474595	11.9605938833502883	O59
12.7190056437958496	4.7542115439314321	11.3496558805827394	O60
7.4623717571455597	9.7533878472324176	11.9798512041847491	O61
11.2185265970822456	12.6973045983811623	11.8472597793068282	O62
6.1157060330456110	12.0124560823883311	11.3708685101505171	O63
7.7832474488121459	3.9338046866523415	8.1698520761953226	O64
4.4826359191693435	0.9946073326400774	8.1055537010418650	O65
9.0566288858689106	1.6262227130413263	7.6644969800528004	O66
10.3960037012635294	6.4148095324396897	14.6954232983901658	O67
14.0467969331216374	9.3742651339124734	14.6080920504399323	O68
12.6612976157903194	5.0729380249409459	-0.0435426431013729	O69
4.6322796780926616	7.1183044557188051	10.8990403222643462	O70
1.5025301367340065	4.3283157187166719	10.8466425076016879	O71
2.4971038917254083	8.6630481624609139	11.4248504989300468	O72
8.4044472579409835	13.3347777858803855	11.6879172455156368	O73

6.8593735104954341	0.1928990279760998	7.2055629158925010	O74
0.9094078180234352	6.8183479467494479	7.6257965120356692	O75
14.3975020172434665	6.7926185155408740	11.3563505059509957	O76
6.0581932818132378	5.5069782782241976	9.3529674494037316	O77
3.1193103979148602	2.7479950145051695	9.5063049458257733	O78
9.2482178868752314	8.2502217223596013	13.1963801924266182	O79
12.2447937577952111	10.8684528951287227	13.4731684875151938	O80
5.7883053783048490	2.8417337798302742	9.5122067307029017	O81
9.6277839880694920	10.8667747322857924	12.9888830877656982	O82
3.4000774869331329	5.4062763569676173	9.3222539126945634	O83
11.9027470910647093	8.2255093809460398	13.5245424598816566	O84
4.6933595228932745	0.1447933183697166	13.2698137166554666	O85
8.4603700394227008	3.5623628708516586	13.3122731916750041	O86
10.0312530311358401	13.3788164597069166	9.3380093637793031	O87
6.7011197569789882	10.1757058278895531	9.5170205358855160	O88
0.7668565560341758	4.9515746450622542	13.2699853829121679	O89
4.2058957273403372	7.9563277763632243	13.3333288483515169	O90
14.4491853212060164	8.6932090311544457	9.5030197723168914	O91
10.9649943256152689	5.6280595821618125	9.5400396743911458	O92
10.2822138774239082	3.8328525696040572	11.4044021190206983	O93
4.9112759894772928	10.0185855150172962	7.5463890066151507	O94
4.8750665369639412	9.7224203069337403	11.4157895156933371	O95
10.3743679993765596	3.8813848917805580	7.5903788504529910	O96
12.3079669495914956	10.7311128046645443	10.3410404052897107	H1
13.2579371432225450	12.2831668360456696	12.0557083526531734	H2
13.7039083012486316	11.6221425414856707	9.7237979288447178	H3
12.0649074566107686	12.1076864308731693	9.2251877870245522	H4
12.5106606837162602	0.3456246728608856	10.6317717385448702	H5
11.3725380871814323	1.0591117524786926	11.7970644591506559	H6
10.8983166072813749	0.8466680779866339	10.0871129759311291	H7
11.4513715973403443	0.3996699751748544	10.9242281961296275	C1
12.6465775576175119	12.6795674209177243	11.2379377078347833	C2
12.6626497409914212	11.7304179782978508	10.0616577106978742	C3
Co-adsorption of propoxy and benzene			
8.8055091038258055	3.0807615836915869	4.1318222158688878	Si1
6.7161021161847136	13.5007909236692125	4.0595369763764984	Si2
6.4670688817115920	10.4703423047272377	0.3216026062119440	Si3
8.2617453820706910	0.1316101352527350	0.2253449307641509	Si4
4.0647377143365162	8.5890454857455829	7.2816718861044540	Si5
14.2429004533593222	5.2540347660937563	7.2663965606742007	Si6
11.0823170713259085	5.0675763754320728	3.4966555800793087	Si7
14.7670774082621747	8.3272096112200735	3.4803236266770434	Si8

6.3392677038434728	10.4243345938347485	3.4184450782471130	Si9
8.2464922554833873	0.0241526138538651	3.3864418454723824	Si10
8.8898981844225435	3.1674176653350221	7.2714121248383776	Si11
6.8710475958172790	13.5731810514937532	7.1512191905724611	Si12
11.0653451593992589	5.1839645197430171	0.3659028697066739	Si13
1.0948220210163877	8.3643436584272255	0.3734767315517276	Si14
4.0993346565945101	8.4033207973998305	4.1606737101398767	Si15
14.1815180816397977	5.2156159826347013	4.1589608063560313	Si16
6.7710680296328771	3.9247099478752325	1.9265798585760756	Si17
4.3483147468729300	1.8491922969640937	1.8672705953226381	Si18
8.4017447713078184	9.6245656166806217	5.6990658940617802	Si19
10.7993581927289455	11.7695469242657609	5.6121728335339593	Si20
4.6875615560350408	6.3196982869280962	1.9354226455621075	Si21
2.2670319298819117	4.2454429693045164	1.8821431526829517	Si22
10.4735277799857212	7.2741701397806047	5.6809482011525789	Si23
12.8745589295700267	9.4119261122917273	5.6590579452275582	Si24
8.7350795096069760	3.2249135377186540	11.7154036166837905	Si25
6.7564962573375809	13.4106987631695045	11.7239105004160038	Si26
6.3912628089601018	10.4801159857459130	7.9271307423941417	Si27
8.3430913524539321	0.1190136524182120	7.7811596551184783	Si28
4.1787421385779986	8.4694788543684307	14.8695820931923350	Si29
14.2058782277811986	5.2840936562684213	14.8035071849623758	Si30
11.1136193429835846	5.1035095622552760	11.0658331278505138	Si31
14.7138671685000322	8.2851517431287345	11.0409470463845629	Si32
6.2520456794005117	10.3995985549209422	11.0402215716720331	Si33
8.8498663656640275	3.1879611567581430	14.8262506119982849	Si34
6.7385751775850160	13.5723079740505064	14.7836178335817543	Si35
11.1099287356714793	5.2330960781739755	7.9445832512663186	Si36
0.9869021080722532	8.3834943350178008	7.9178068395769321	Si37
4.0385291232765548	8.3330518679534560	11.7556488920215205	Si38
14.1907514431168966	5.1575198312444268	11.6844157769009840	Si39
6.7936243851930129	4.0443344428353267	9.4686817389957429	Si40
4.4528574377096186	1.8301576787710141	9.4594124809710678	Si41
8.4546608101081304	9.6586275819165550	13.1849428807184488	Si42
10.8724935646181322	11.7305141551108871	13.2184982587976361	Si43
4.6532606475795646	6.3368864850655511	9.4623773927647576	Si44
2.3106276102737144	4.1439069180174597	9.4614455943563360	Si45
10.5035805525344195	7.2646579043795008	13.3285666609008082	Si46
12.9320415078296040	9.3498902682323788	13.3568668172137066	Si47
8.2262258203705407	0.0649765227147765	10.9692557826361323	Al1
7.6431107088151746	3.8499650951416249	3.2934180916456781	O1
4.2692375981971580	0.9188096441578644	3.1947199333261795	O2

8.8183122647228309	1.4951928718775709	3.7742378278473216	O3
7.4906383722285321	9.6693075868477028	7.0430111284226786	O4
10.8800321169765652	12.7921083509859539	6.8674258005166973	O5
6.5065938408175628	12.0752526223511278	7.6681899220591943	O6
4.8255761234143106	7.3200526657350720	0.6614877228817182	O7
1.2826378294657599	4.2849581018802647	0.5873443688706389	O8
2.6495183401803919	8.7836606186020330	0.1718186112562538	O9
10.4517882754929712	6.2360171336673647	4.4328816731161433	O10
13.8673439681223947	9.3371344824296987	4.3736707390272684	O11
12.6408457014157243	4.7976082791011763	3.8648185097997212	O12
7.4867350797070475	9.7882256666181426	4.3705182214799851	O13
10.7258355825091893	12.5818381064919240	4.1985088128769004	O14
6.2017274726680132	12.0224009761193820	3.6358818189464679	O15
7.7425048968721084	3.8902987867832692	0.6297390217445830	O16
4.2661297754710841	0.9434991846846197	0.5260184300387089	O17
8.9190783516724608	1.5832561375028438	15.0865405132048096	O18
10.4951678133453168	6.4808961522064470	7.0999866811129060	O19
13.7220818516151333	9.2576595099696686	7.0426083391656586	O20
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10.2300852906853468	3.7784203435717298	11.2839718525744672	O93
4.8138181805442164	9.8701796280129876	7.4503358384145280	O94
4.8263333787572442	9.5732051651639267	11.3089823855278766	O95
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Co-adsorption of propylene and benzene			
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9.4504900876644804	10.7051215198220415	13.0133081822469503	O82
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4.5270412806248626	0.0301035325031010	13.1806673610687799	O85
8.3112346775176924	3.3943557177536450	13.1943175195294149	O86
9.9247235852766256	13.2255446763829685	9.2291564109337632	O87
6.5525935870446697	10.0501691879646859	9.4257806781909004	O88
0.6155238208131616	4.8185276624266011	13.1596912061245082	O89
4.0677451115774517	7.8159056587395392	13.2262210136956675	O90

14.3106518698213332	8.5586227737692795	9.3960929536088251	O91
10.8333145027109765	5.5210471279904798	9.4247184558916786	O92
10.1556057319555588	3.7569724077976452	11.3280723653838180	O93
4.7620740615014849	9.8703508810472389	7.4505817798873570	O94
4.7324508969395502	9.5818079228149209	11.3190303144616724	O95
10.1579761994631372	3.7553726230511040	7.5313940603490153	O96
13.1930565538776357	10.9824240605140506	10.2320595729492378	H1
14.1925718154432268	12.9338946806991935	11.2938240552617675	H2
12.4494478019785308	12.0515312505774936	8.8982946213347578	H3
11.7598967858503816	12.4376920555867425	11.2255597083819971	H4
11.2557513452073081	0.8366038235343807	8.9474419755994301	H5
12.8822382874871302	1.1411750763984791	9.6264758604230458	H6
11.4603688882867427	1.4548030964640959	10.6131579119572734	H7
3.5890223784492945	12.6645562448510400	12.0487225551102615	H8
2.3030167161052719	11.1856650414904468	13.5750697814910577	H9
14.1870013024890405	12.1007192911229478	14.8885512570780687	H10
11.9255031428697755	0.8172418619410878	14.6697564372969946	H11
13.2232398468551189	2.3002130160803409	13.1569411664809586	H12
1.3604215878729484	1.3900193929743516	11.8588370209805856	H13
11.8699947983559682	0.7683992219422064	9.8556689433160258	C1
11.9580841645656530	-0.6252882630810813	10.3825859053621912	C2
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13.4968229027515392	1.2478810922420058	13.2493849574749714	C8
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TS3			
8.7245345120070219	2.9897344595078210	4.0967755260336007	Si1
6.6428072607512814	13.4520577404437152	4.0612047620947447	Si2
6.4023024147758862	10.3190200955005249	0.2731964388413000	Si3
8.2027435248702893	0.0304098119412489	0.2077624783416267	Si4
4.0080501014514045	8.4868043999533818	7.2114945314588326	Si5
14.0857101056258927	5.1871407679242196	7.1836557287270759	Si6
10.9944902067900099	4.9852982814060898	3.4335305589813161	Si7
14.6986429256651867	8.2059323034844596	3.3876371383417232	Si8
6.2462585372531256	10.3907263900381839	3.3844579231719432	Si9
9.8068248067746744	13.6379915716217148	3.3872563239721627	Si10
8.7483988473303267	3.0589067155966925	7.2290083053625862	Si11
6.8376056371687621	13.4678210845811392	7.1544588785627026	Si12
10.9900244061765839	5.0954354587382973	0.2996462672461072	Si13

14.7869122757691827	8.3013126463275917	0.2886579888021490	Si14
4.0330064116218995	8.3332698293713143	4.0799830402709274	Si15
14.1033308620476827	5.0964009600140132	4.0764570314861057	Si16
6.6964648430509470	3.8126803801990286	1.8386377889752505	Si17
4.2698080032730008	1.7289355108834217	1.8135836147450535	Si18
8.3169610885296752	9.5603389589235768	5.6628881828697040	Si19
10.7416925960981526	11.6626795862509134	5.5586342036741136	Si20
4.6254339847875219	6.2085218265169324	1.8905554661377257	Si21
2.1962535414342672	4.1244953827145414	1.8354939056084687	Si22
10.3700915577107917	7.1906404385048797	5.6228549777479628	Si23
12.8057134117450104	9.2935133891089521	5.6058290842511811	Si24
8.7255272751728814	3.1345863164240888	11.6239808479529501	Si25
6.5962116776981592	13.4027689320562562	11.6409476798365095	Si26
6.3132735307407835	10.3849839210821830	7.9022004869241664	Si27
9.9849863116574262	13.6720144089281366	7.7563931370705053	Si28
4.0929972115608590	8.3450654748805047	14.8149116287782068	Si29
14.1239987385695684	5.2111785254788829	14.7459504870230109	Si30
11.1081008640987573	5.0701549392744072	10.9937517808608529	Si31
14.6361869366097608	8.2304546191218044	10.9956654513534424	Si32
6.1972521785916950	10.3404376931192701	11.0190999957698459	Si33
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6.6968934943754999	13.4429283522142917	14.7158671649678414	Si35
10.9647772855364991	5.1649686983596448	7.8816197607998362	Si36
14.6939522595021206	8.3015372377578274	7.8619849775112920	Si37
3.9521566471962379	8.2639954524520682	11.6987522324544155	Si38
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6.6744058142297220	3.9279242317609966	9.4626991378751697	Si40
4.3051284023799354	1.7566189262431011	9.4399569976543347	Si41
8.3879442764658805	9.5227687104369902	13.1874752890945555	Si42
10.7752511387046503	11.7002901028135984	13.2034608524732242	Si43
4.5695940457367641	6.2480055744067720	9.3770728598315589	Si44
2.2091675766268528	4.0864807020930760	9.3540158583028656	Si45
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12.8485066624018902	9.3666046126916669	13.2906102742494205	Si47
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7.4173376999774163	9.5775672636882714	7.0169864018192536	O4
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13.7895772694330319	9.1689421247011271	4.3207002886209143	O11
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6.0995948934948183	11.9901613790405630	3.6052083679812750	O15
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14.3526874997633058	6.6524744096514583	3.6930751994126254	O28
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14.3492412874203907	8.5287724330375472	1.8342253024146380	O43
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4.7996837613939078	9.7177006433050597	3.7099813911577546	O47
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1.1244717908917312	4.1721054481878843	8.1449107057028804	O56
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13.6332709401732100	9.1698637010711668	11.8665818584142677	O59
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4.4613347766406601	0.8833080287565805	8.0813938335897948	O65
8.9503741706976854	1.4858395535957687	7.5364938848305121	O66
10.3028580973150401	6.3011387960869980	14.6052640786589745	O67
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12.5579343560187411	4.9467787059669144	15.0576445073664811	O69
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1.4422565474233857	4.1954048636044190	10.7912646813215183	O71
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8.1606388374499872	13.4716929612802510	11.3708297602932511	O73
8.4453636307022961	13.6512254538392384	7.1990251151911302	O74
14.4824073067499128	6.7274902538497976	7.5233938125964146	O75
14.3277795580393672	6.6642881360978610	11.2687546105411407	O76
5.9150812275115756	5.3579913349855062	9.3265944786897492	O77
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9.1122991950074201	8.0732304795895597	13.0548421369989587	O79
12.1561755766331494	10.8226102883703881	13.2931861578194948	O80
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8.3835650228905685	3.3561131197516945	13.2071169147169449	O86
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6.6009596868335896	10.0627377325751031	9.4664701421249102	O88
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14.3723986718406884	8.5857187191875717	9.4323529617791291	O91

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13.7674982137940844	11.3272387173661180	10.5493495717771815	H1
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13.2623159886832092	12.1522935390601372	8.9726267785410556	H3
12.2258344859882886	12.1225510522422315	10.4563436978409214	H4
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3.1837951886237281	12.6842335145112060	10.7994246770009514	H8
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13.1421826833648243	0.5392193580127532	14.9953058569014051	H11
0.3303245702948104	2.1997189062436497	13.4160313591099509	H12
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Benzene			
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13.5909465638813103	15.2035697628956008	12.8905707169376491	C3
12.4176895985957358	15.3309977718984332	13.6392709920262813	C4
12.4729793374717879	15.3009849661937007	15.0352484767070766	C5
13.7015495267721974	15.1433452685087673	15.6826933646248694	C6
15.8347823972974080	14.8930540806239726	15.4398503569640653	H1
15.7363220125607057	14.9465311305411479	12.9527926728653888	H2
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11.4577874687922510	15.4541468345409090	13.1333074913551133	H4
11.5563315601882639	15.4005687215114175	15.6204594264487433	H5
13.7449209038101809	15.1199529549939022	16.7736512734254433	H6
Propylene			
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7.9159891194557206	8.4782033503602374	11.4606699514493027	C6
6.4029683725275088	8.5472341096551077	11.3315773593127780	C7
5.8441385583646737	7.5557903283545702	10.3026109051716919	C8
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6.1746074241989577	6.5276708885748089	10.5111703861355110	H6
6.1634782505072421	7.8120757212326559	9.2804796242002325	H7
4.7438839969111068	7.5722409521856209	10.3133634489999437	H8
5.9883024161365626	8.2741385937166445	12.3178978066124714	H9
4.8444107648193881	10.0275588506561597	10.9416823099758300	H10
6.2654278705949711	10.6874075338394672	11.7922356643563067	H11
6.3602194124895375	10.3208375939685979	10.0546186652427512	H12

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