

## **Supplementary Information**

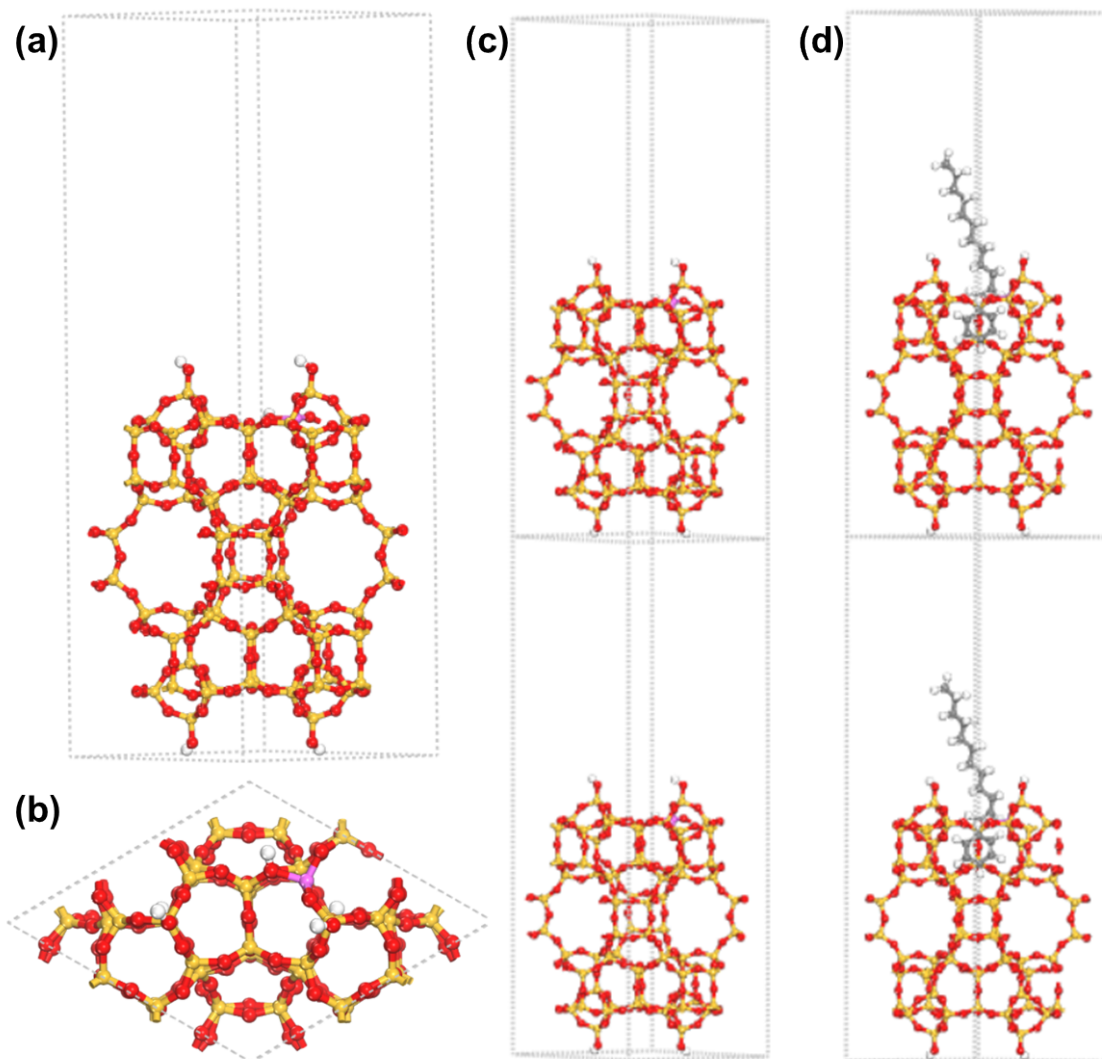
### **Insights into the alkylation of benzene with olefins: effect of chain length of the olefins**

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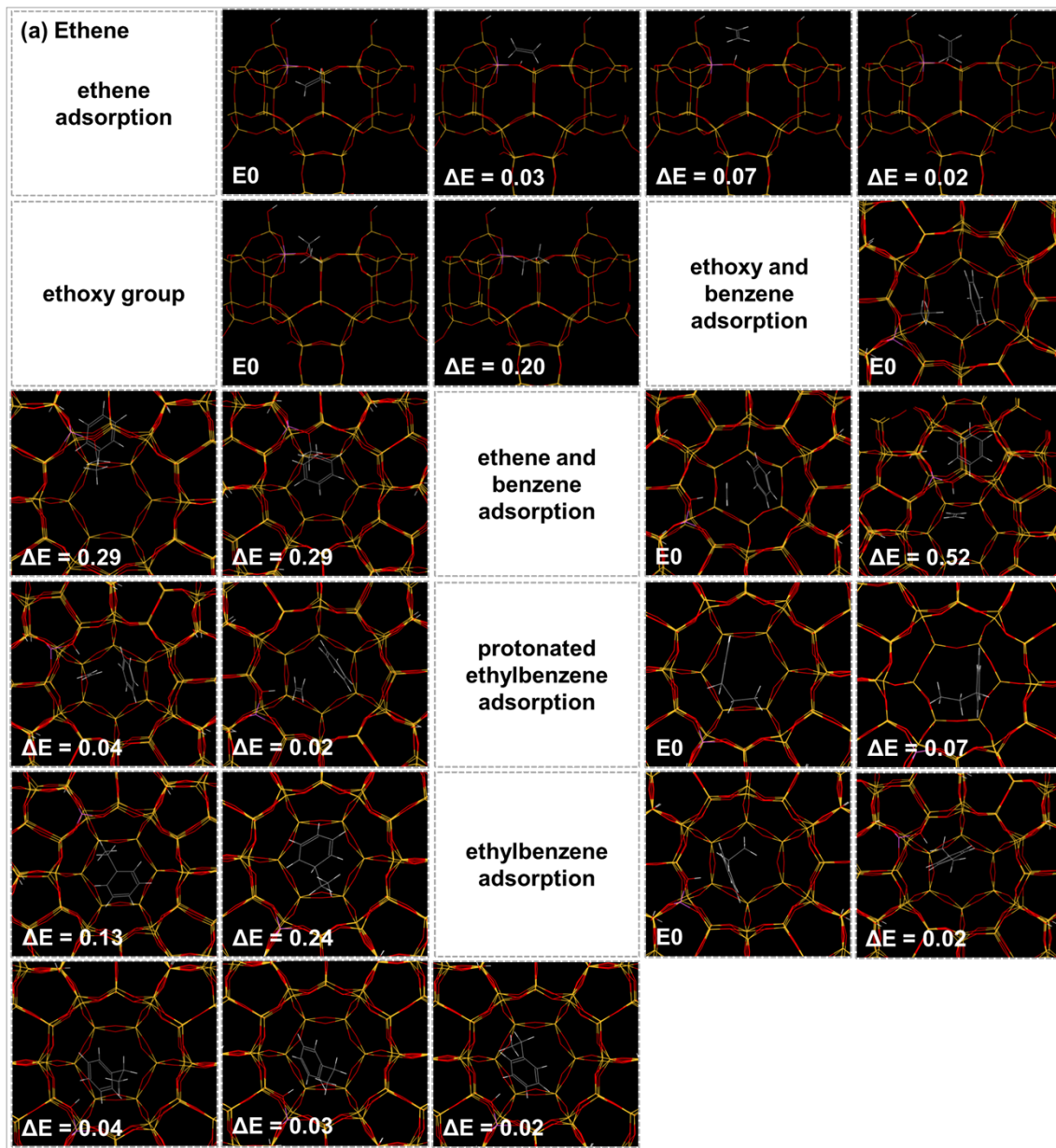
Beijing Key Laboratory of Green Chemical Reaction Engineering and Technology, Department of

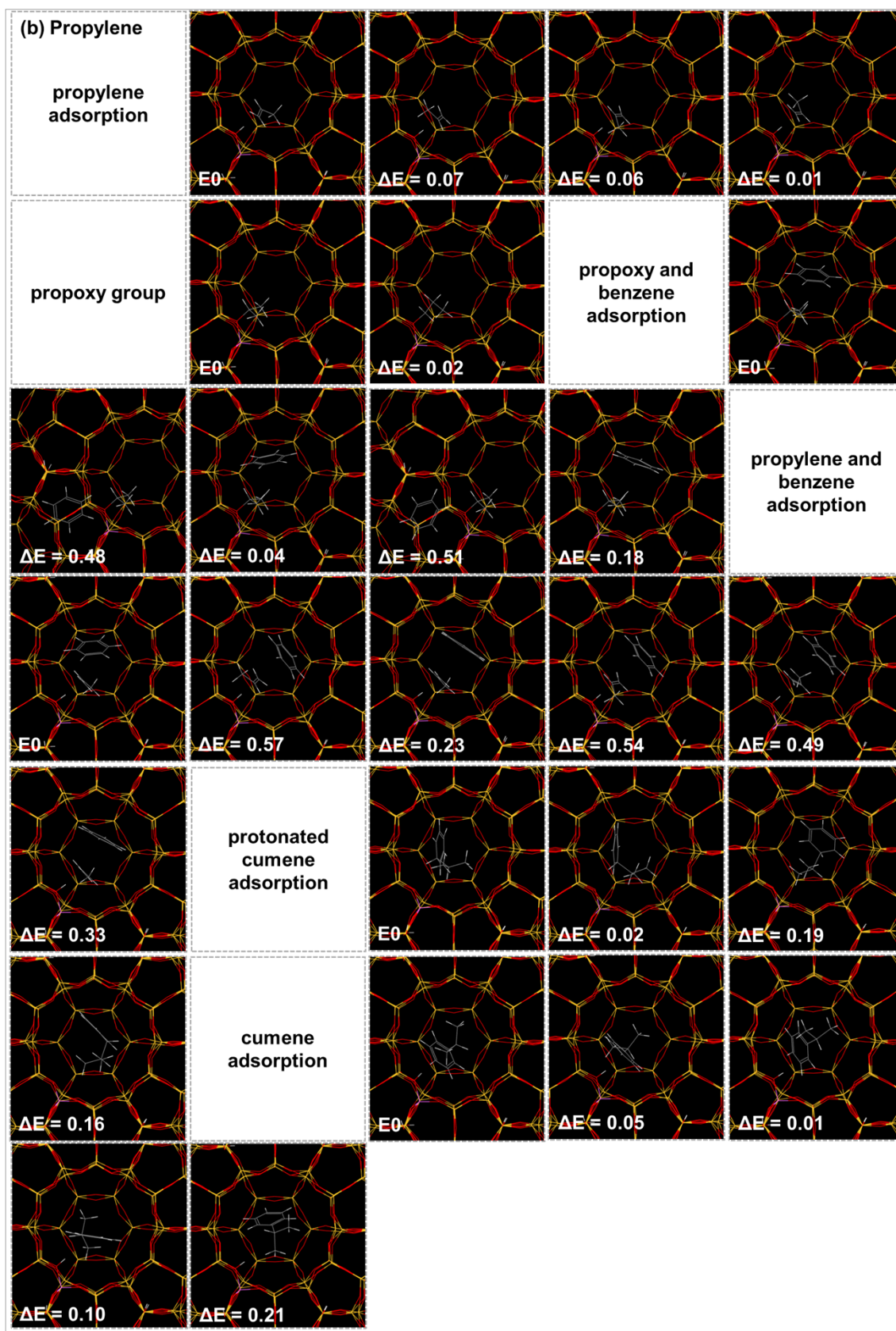
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**Fig. S1.** (a, c) Side view and (b) top view of zeolite model with a vacuum slab of 25 Å along the c axis and (d) co-adsorption of 1-dodecene and benzene at the acid site.







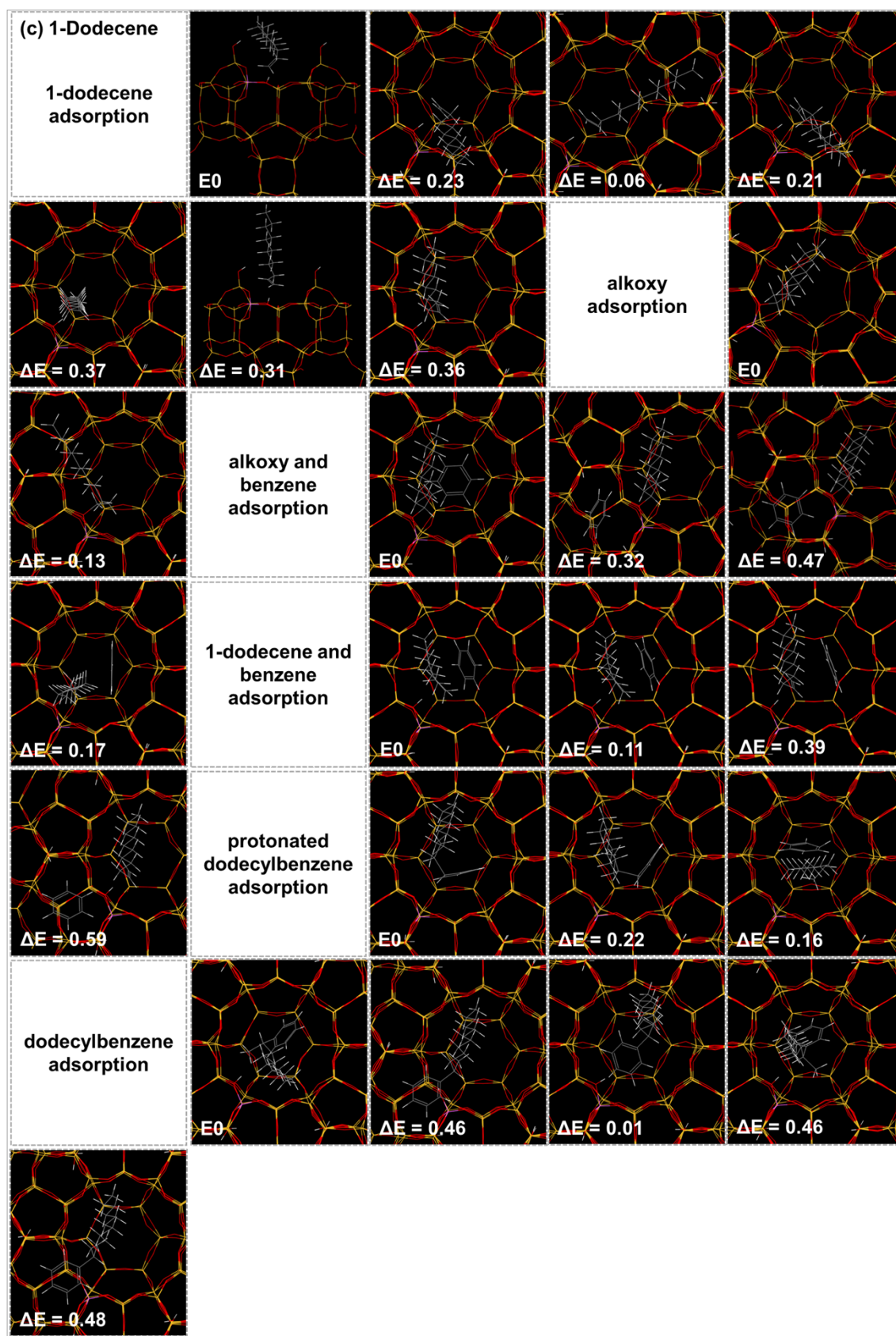
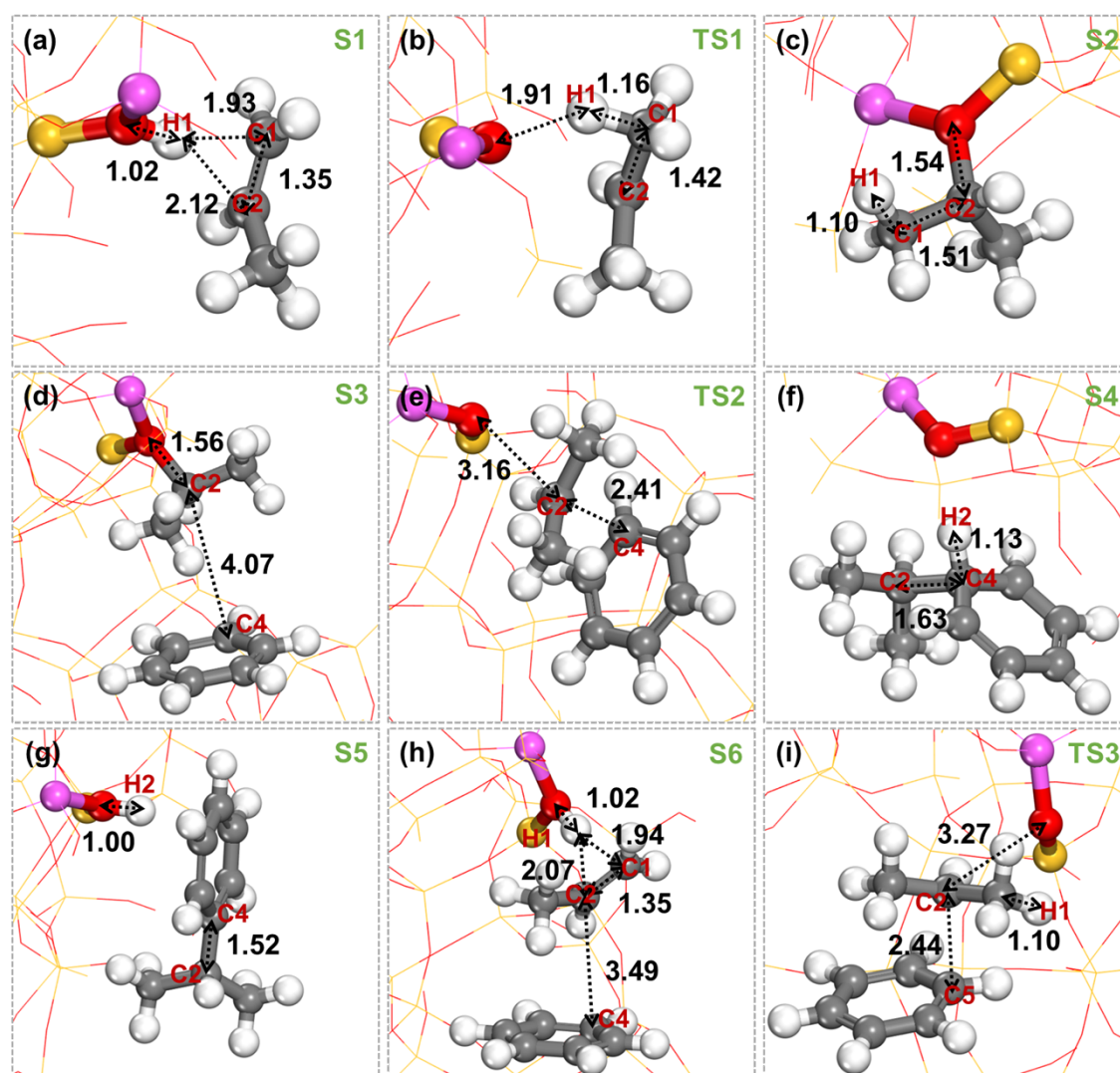


Fig. S2. All the considered orientations for each intermediate state along the reaction coordinate of

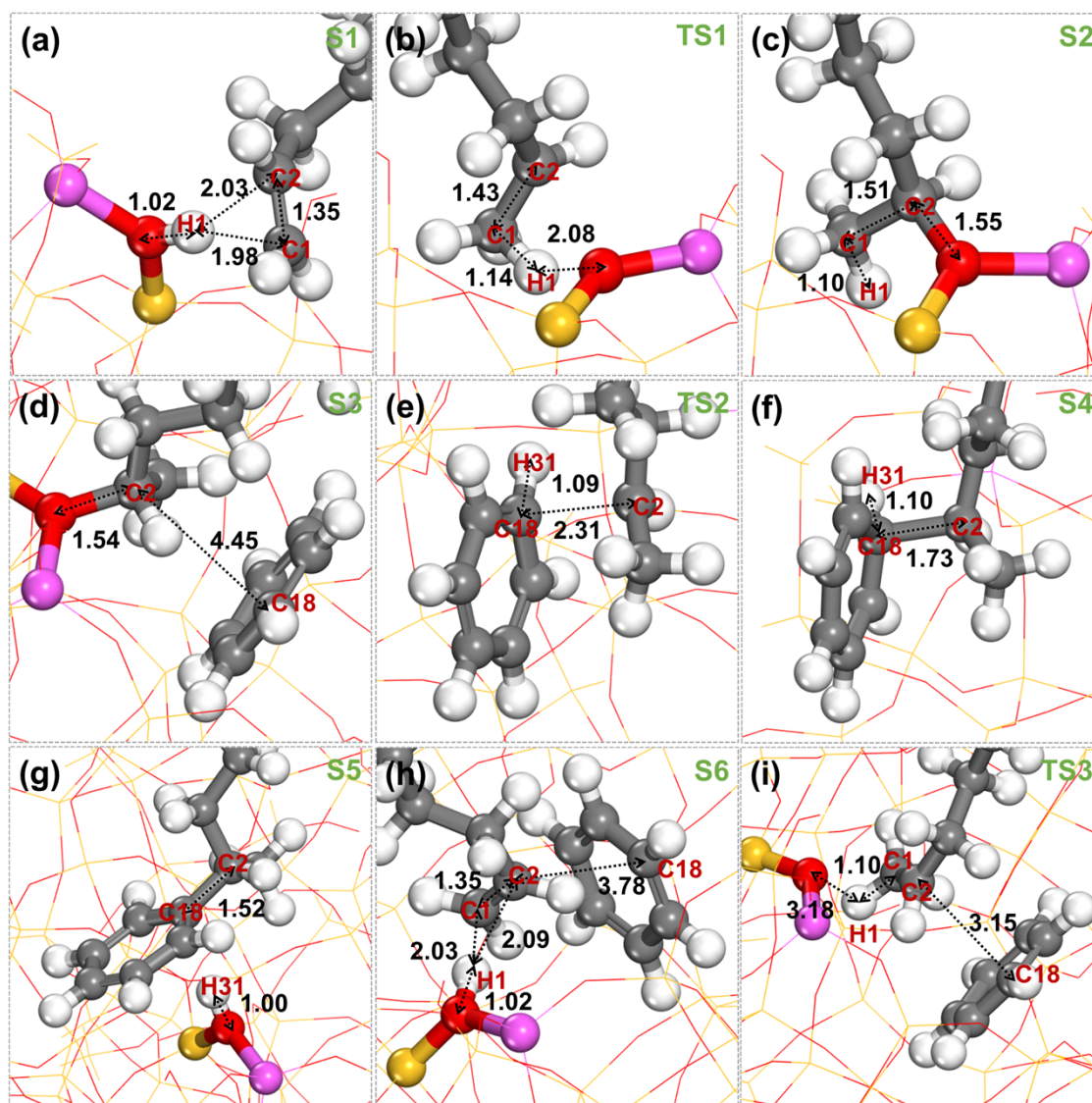
the alkylation of benzene with (a) ethene, (b) propylene, (c) 1-dodecene. The most thermodynamically favored orientation is labelled with  $E_0$ , to which the relative electronic energies of other candidates are also listed.

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. S2. 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.

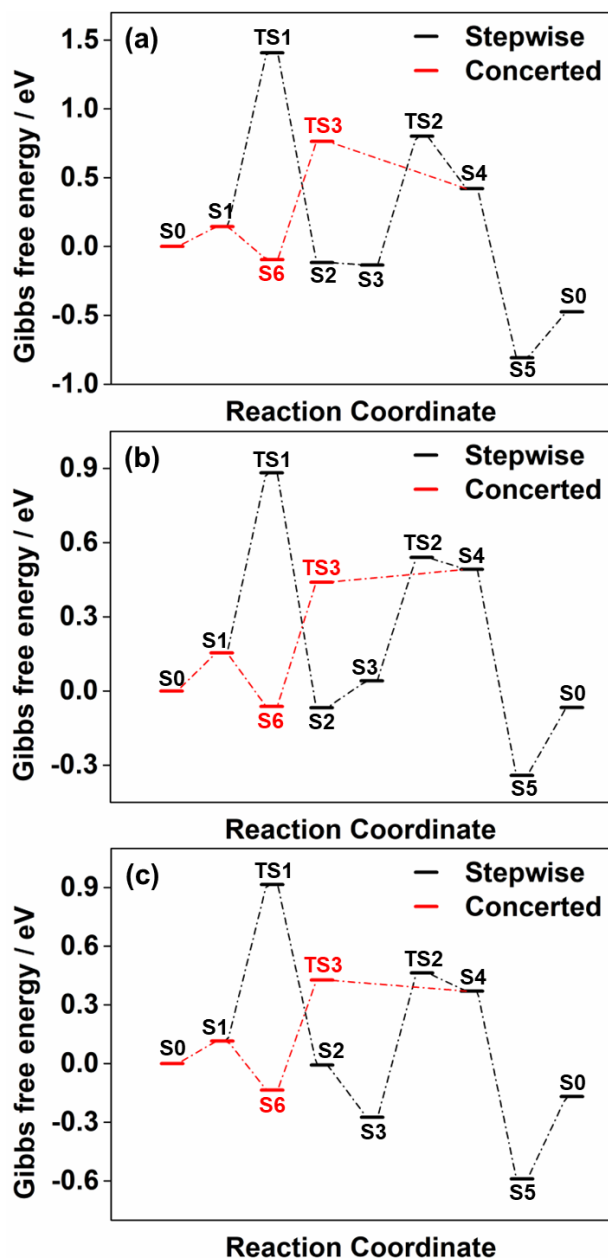


**Fig. S3.** Local geometry structures of all intermediates for the alkylation of benzene with propylene.

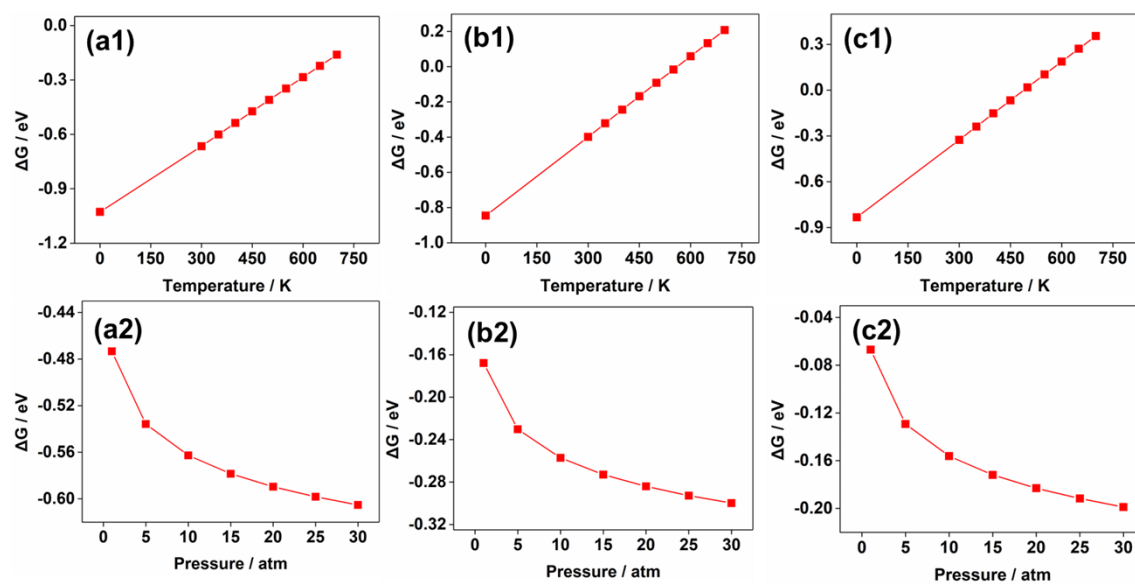
(a-i), corresponding to (a) adsorbed propylene, (b) TS1, (c) propoxy, (d) co-adsorption of propoxy and benzene, (e) TS2, (f) protonated cumene, (g) adsorbed cumene, (h) co-adsorption of propylene and benzene, (i) TS3.



**Fig. S4.** Local geometry structures of all intermediates for the alkylation of benzene with 1-dodecene. (a-i), corresponding to (a) adsorbed 1-dodecene, (b) TS1, (c) dodecoxy, (d) co-adsorption of dodecoxy and benzene, (e) TS2, (f) protonated dodecylbenzene, (g) adsorbed dodecylbenzene, (h) co-adsorption of 1-dodecene and benzene, (i) TS3.



**Fig. S5.** Gibbs free energy diagrams of the complete reaction coordinate for the alkylation of benzene with (a) ethene, (b) propylene and (c) 1-dodecene at 450 K. The cycle consists of the stepwise and concerted mechanisms. The pressure of the gaseous molecular is 1 atm. Two S0 states in the initial and final states denote (H-zeolite + olefin (g) + benzene (g)) and (H-zeolite + alkylbenzene (g)), respectively.

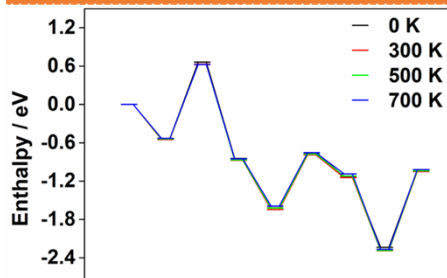


**Fig. S6.** Influence of **(a1-c1)** temperature (calculated at 1 atm) and **(a2-c2)** pressure (calculated at 450 K) on the reaction Gibbs free energy (thermal driving force). **(a)** ethene, **(b)** propylene, **(c)** 1-dodecene. The reaction Gibbs free energy was calculated according to Eq. (S1)<sup>1</sup> as follows and the reactants and products were all in gas phase.

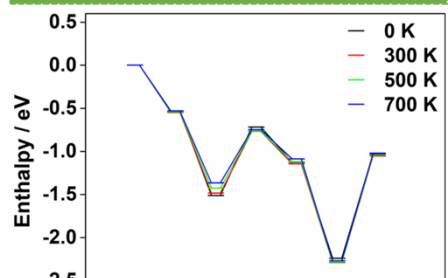
$$\Delta G = G_{\text{ethylbenzene}(g)} - G_{\text{benzene}(g)} - G_{\text{ethene}(g)}$$

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.

(a) Stepwise

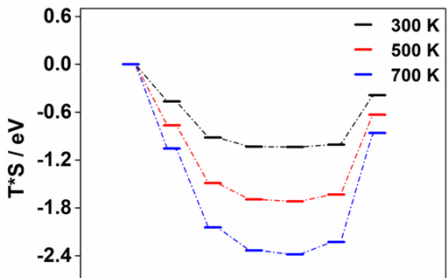
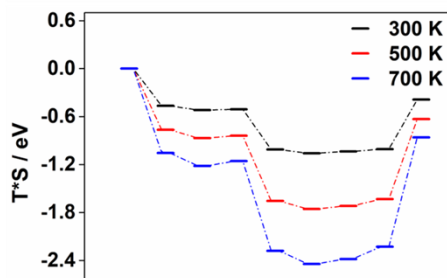


Concerted



Reaction Coordinate

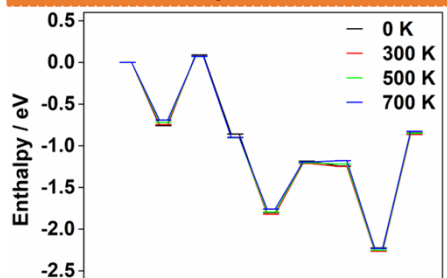
Reaction Coordinate



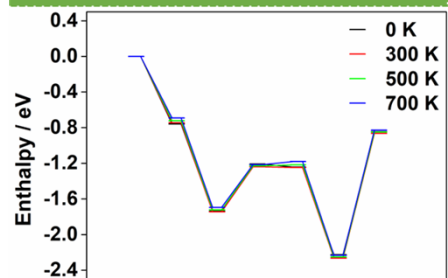
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Reaction Coordinate

(b) Stepwise

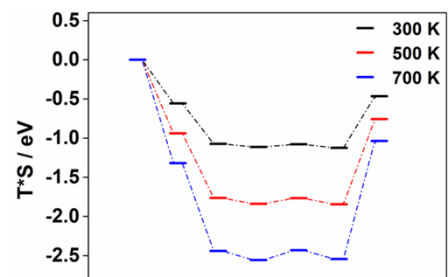
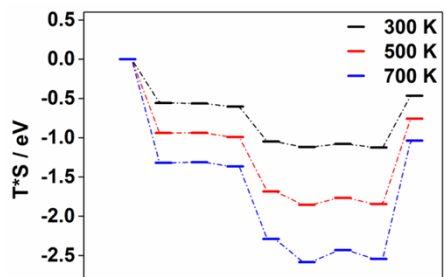


Concerted



Reaction Coordinate

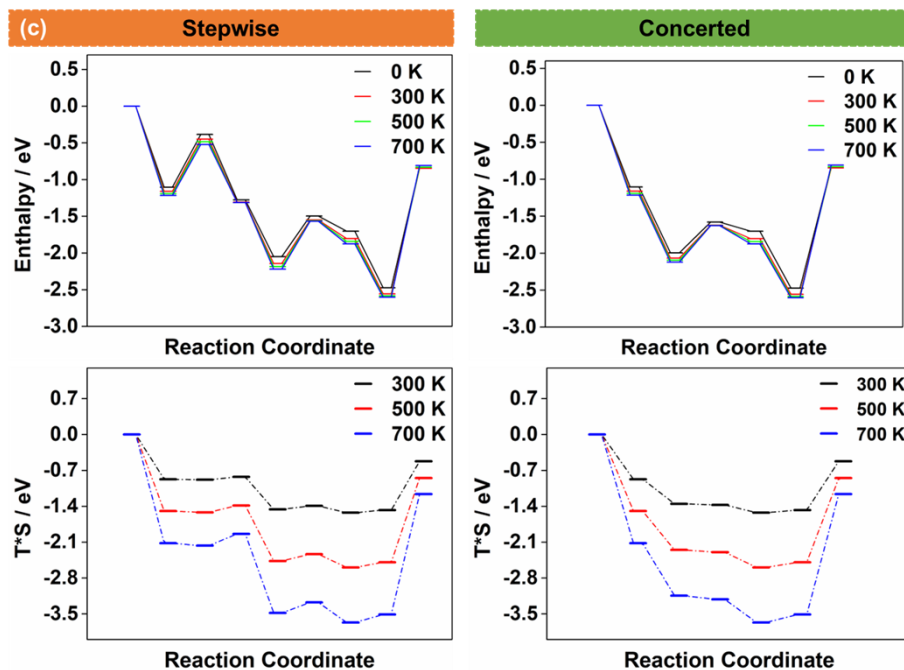
Reaction Coordinate



Reaction Coordinate

Reaction Coordinate





**Fig. S7.** The enthalpy part  $H$  (first row) and entropy part  $T^*S$  (second row) of the Gibbs free energy along the reaction coordinate for the alkylation of benzene with (a) ethene, (b) propylene and (c) 1-dodecene. 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 for these three olefins. As can be seen, the enthalpy diagrams show a similar trend as the Gibbs free energy diagrams (see Fig. 3 and Fig. S5) 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.

Regarding the alkylation of benzene with olefins in the present work, there is no release of water during the reaction process. Therefore, no obvious difference of the contribution from entropy

was observed between the stepwise and concerted mechanisms for all the three olefines. Additionally, it can also be observed that the difference among the three olefines is also limited. In fact, these limited differences are all attributed to the different interactions between intermediates and framework for the similar reaction process and identical number of reactants and products. Differently, for the MTO process, water can be released during the reaction process. For example, Brogaard et al <sup>2</sup> investigated the mechanism of the zeolite catalyzed methanol to hydrocarbon (MTH) between methanol and olefins theoretically and found that the stepwise pathway prevails at typical MTH reaction temperatures, mainly due to a higher entropy loss in the concerted as compared to the stepwise pathway. The entropy difference results from intermediate release of water in the stepwise pathway. Additionally, Wang et al <sup>1</sup> compared the alkylation of benzene with ethene and ethanol by DFT calculations, and found that the reaction Gibbs free energy  $\Delta G$  of the ethanol-involved reaction slightly decreased with temperature rising, which is different from the alkylation of benzene with ethene and the results in the present work (see Fig. S6 and S7). Such variation should be mainly attributed to the additional formation of H<sub>2</sub>O product in the ethanol process, considering that one obvious difference between the two processes lies in the intermediate release of water molecule (or not), which provides extra entropy gain for the whole reaction.

## **S1. Charge transfer analysis**

On the basis of the detailed reaction processes discussed above, a further study on the charge transfer was investigated through Bader charge analysis. Herein, the alkylation of benzene with ethene is taken as an example to illustrate the charge transfer along the reaction coordination.

### **S1.1. Stepwise mechanism**

Initially, the charge enriched ethene is adsorbed around the acidic proton with the charge transferred from ethene to zeolite (see Fig. S8a). As the reaction proceeds, the proton is detached from the framework and is bonded with C1 atom of ethene forming the ethoxy group, through which the charge of ethene further decreases and the charge of the acidic proton and framework increases concurrently. Subsequently, benzene is adsorbed near the ethoxy group leading to the charge further transferred from hydrocarbon to zeolite. Then, C2-O bond is broken and C2 atom is approaching C3 atom. As the distance of C2 and C3 reduces to covalent bond forming the protonated ethylbenzene, the charge of hydrocarbon further decreases. Due to the instability of H2 atom of benzene, it detaches and approaches the O atom originally bonded with the acidic proton to form the BAS and ethylbenzene eventually. The charge of hydrocarbon increases in this step. As the ethylbenzene desorbs, the charge of the framework restores to the original state.

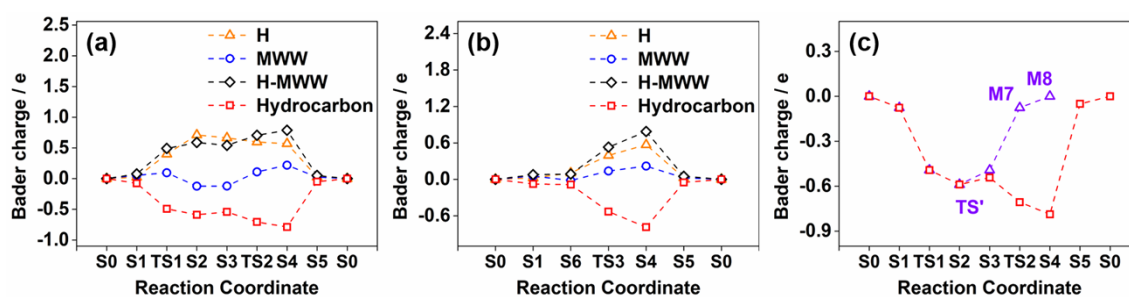
### **S1.2. Concerted mechanism**

As for the concerted pathway, co-adsorption of benzene and ethene provides more charge for zeolite compared with the stepwise pathway. As the reaction proceeds, O-H bond is broken and the distance of C2 and C3 decreases, through which the charge of hydrocarbon decreases sharply. Subsequently, the charge of hydrocarbon decreases further as C2 is covalent bonded with C3. Finally, H2 is detached and back to the framework, from this process, the charge of hydrocarbon increases to a large extent. The overall charge transfer information is shown in Fig. S8b.

It's worth noting that the charge of hydrocarbon increases slightly when forming the ethoxy group in the stepwise mechanism. This can be explained as follows. Ethene is transformed into the protonated form after bonded with the acidic proton. As the protonated ethene (positively charged)

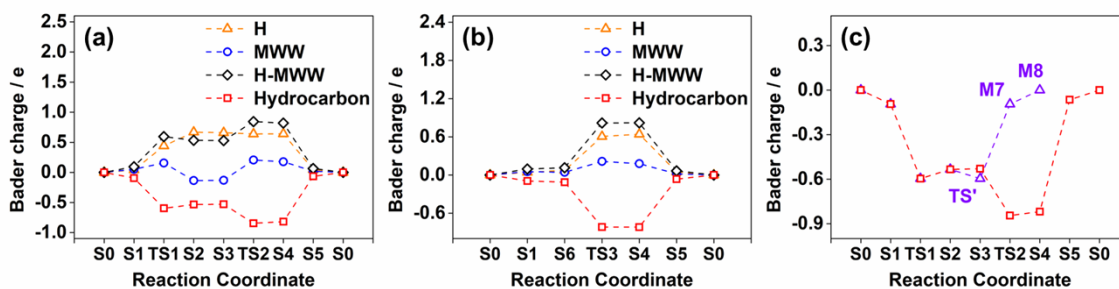
approaches the negative framework, electron will be attracted from the framework to ethene thus increasing its charge. It's worth noting that there is only ethene as the reactant in the channels before the introduction of benzene. Assuming benzene is not involved in the reaction, next step after the formation of the ethoxy group is the breaking of C2-O bond and then the H1 atom will be back to the framework again completing the reaction route (see Fig. S8c, S2-TS'-M7). In fact, this reaction without benzene involved always occurs at higher olefin concentration. And polymerization of olefin dominates in this case. This process is considered to be carbonium ions reaction mechanism of ethene itself<sup>3</sup>. However, if benzene is introduced after the formation of ethoxy group, next step is the breaking of C2-O bond and the electrophilic attacking of benzene. Therefore, it can be proposed that the overall stepwise pathway of benzene alkylation with ethene can be regarded as a coupling of two reaction routes with or without benzene involved (see Fig. S8c). Similar conclusions could also be reached for the alkylation of benzene with propylene and 1-dodecene.

The charge transfer results for the alkylation of benzene with propylene and 1-dodecene are shown in Fig. S9 and S10. Overall, the zeolite acts as a charge acceptor firstly and then turns to be a donor along the reaction coordinate. It's worth noting that the charge variations of both the acidic proton and framework are comparable, indicating charge transfer between hydrocarbon and zeolite mainly occurs via the acidic proton of the framework.

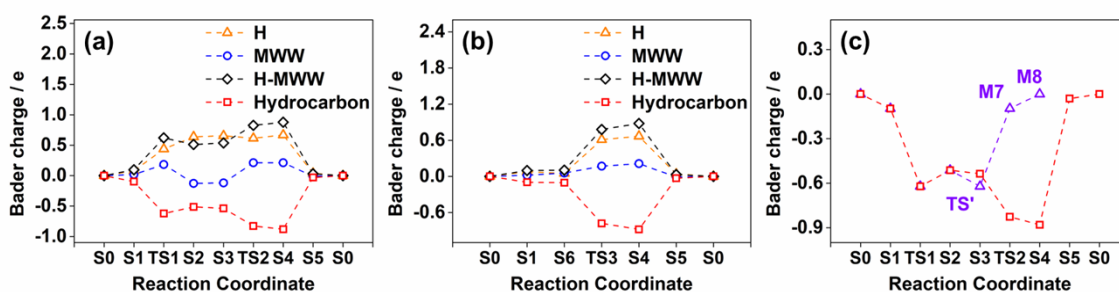


**Fig. S8.** Charge transfer information along the reaction coordinate for the alkylation of benzene

with ethene, including the (a) stepwise mechanism, (b) concerted mechanism, and (c) comparison of the reaction coordinate with or without benzene involved, of which TS', M7, and M8 correspond to the deprotonation transition state, adsorbed and desorbed ethene, respectively.



**Fig. S9.** Charge transfer information along the reaction coordinate for the alkylation of benzene with propylene, including the (a) stepwise mechanism, (b) concerted mechanism, and (c) comparison of the reaction coordinate with or without benzene involved, of which TS', M7, and M8 correspond to the deprotonation transition state, adsorbed and desorbed propylene, respectively.



**Fig. S10.** Charge transfer information along the reaction coordinate for the alkylation of benzene with 1-dodecene, including the (a) stepwise mechanism, (b) concerted mechanism, and (c) comparison of the reaction coordinate with or without benzene involved, of which TS', M7, and M8 correspond to the deprotonation transition state, adsorbed and desorbed 1-dodecene, respectively.

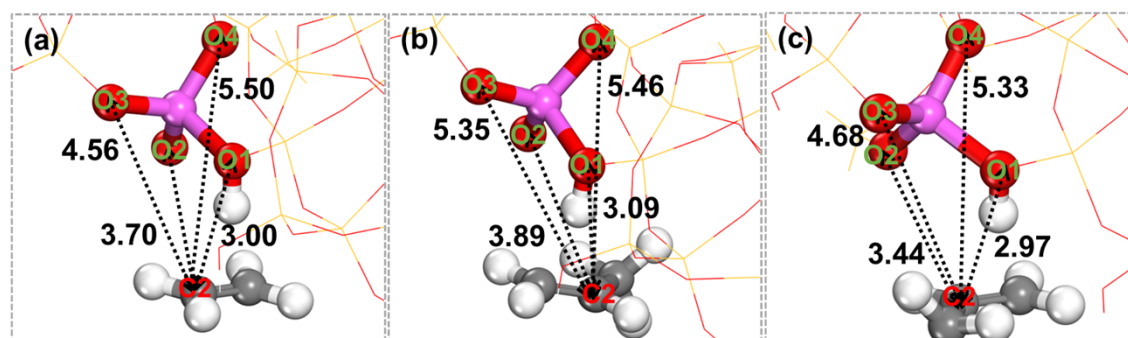
## S2. Discussion of the alkoxy formation

After the adsorption of olefins, four different oxygen sites adjacent to Al are all possible to

form the alkoxy. The distance from C2 atom of olefins to these four oxygen atoms possible forming the alkoxy are shown in Table S1 and Fig. S11. It's reasonable to assume that the protonated olefins prefer to bond with the nearest oxygen. Therefore, the oxygen with the shortest C2-O distance was chosen in the present work to form the alkoxy.

**Table S1.** The distance from C2 atom to the four oxygen atoms possible forming the alkoxy (Å).

	Ethene	Propylene	1-Dodecene
C2-O1	3.00	3.09	2.97
C2-O2	3.70	3.89	3.44
C2-O3	4.56	5.35	4.68
C2-O4	5.50	5.46	5.33



**Fig. S11.** Comparison of the distance from C2 atom to the four oxygen atoms possible forming the alkoxy over (a) ethene, (b) propylene, (c) 1-dodecene (Å).

### S3. Determination of TDTS and TDI

Herein, we take the Gibbs free energy diagrams shown in Fig. S5 as an example to illustrate this process.

For the stepwise mechanism (Fig. S5a), 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 S0 state will be determined as the TDI and the energetic span ( $\delta E$ ) 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 ( $\delta E$ ) can be calculated according Eq. (3b). The results of these two cases are shown in Table S2a. Therefore, for the maximization the energetic span ( $\delta E$ ), 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 S6 state will be determined as the TDI and the energetic span ( $\delta E$ ) 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 ( $\delta E$ ) can be calculated according Eq. (3b). The results of these two cases are shown in Table S2b. Therefore, for the maximization the energetic span ( $\delta E$ ), TS3 and S5 are determined as TDTS and TDI, respectively.

**Table S2.** 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	$\delta E$	
									Eq. (3a)	Eq. (3b)
0.00	0.15	1.41	-0.12	-0.13	0.80	0.42	-0.81	-0.47	1.41	1.74

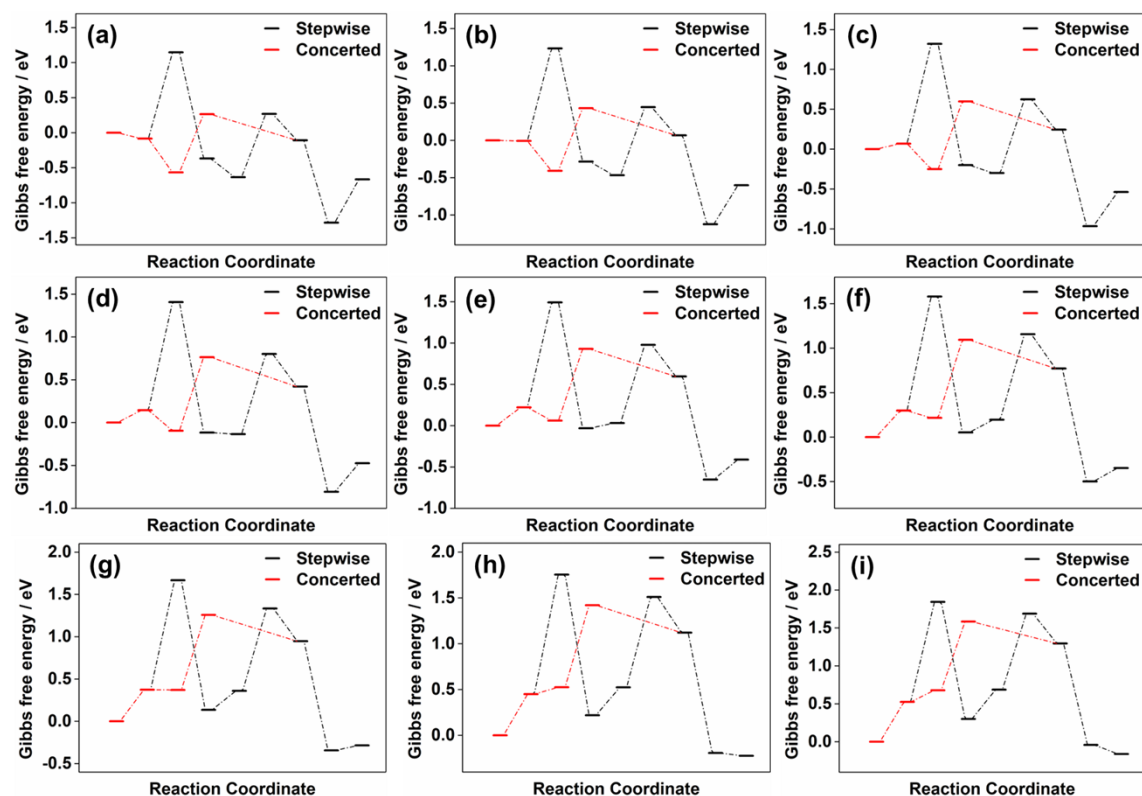
**(b) Concerted**

S0	S1	S6	TS3	S4	S5	S0	$\delta E$	
							Eq. (3a)	Eq. (3b)
0.00	0.15	-0.09	0.76	0.42	-0.81	-0.47	0.86	1.10

**S3a. 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 1 atm.

### (1) Ethene



**Fig. S12.** Gibbs free energy diagrams of the complete reaction coordinate for the alkylation of benzene with ethene 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 S3.** The TDTS and TDI of the ethene reaction cycle including **(a)** stepwise and **(b)** concerted mechanisms.

#### (a) Stepwise

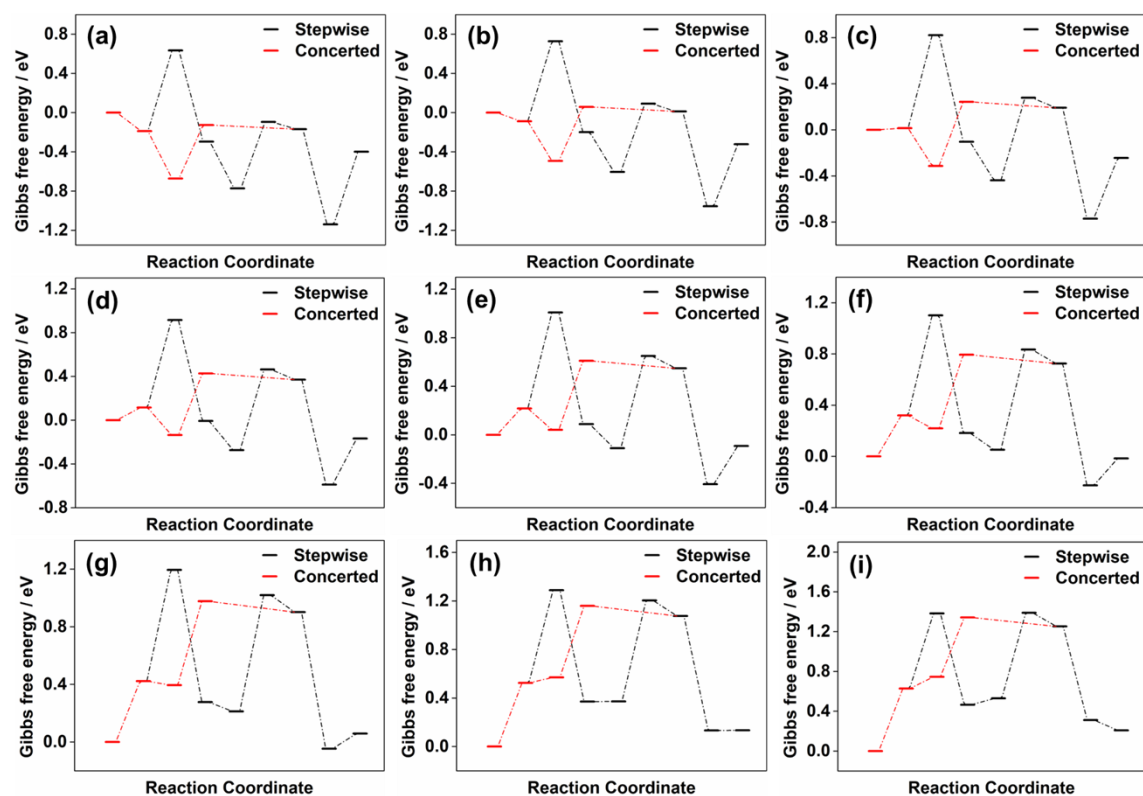
Temperature /										
K	0	300	350	400	450	500	550	600	650	700

TDS	TS1	TS1	TS1	TS1	TS1	TS1	TS1	TS1	TS1	TS1
TDI	S5	S5	S5	S5	S5	S5	S5	S5	S0	S0

**(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	S0	S0

**(2) Propylene**



**Fig. S13.** Gibbs free energy diagrams of the complete reaction coordinate for the alkylation of benzene with propylene 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 S4.** The TDTS and TDI of the propylene reaction cycle including (a) stepwise and (b) concerted mechanisms.

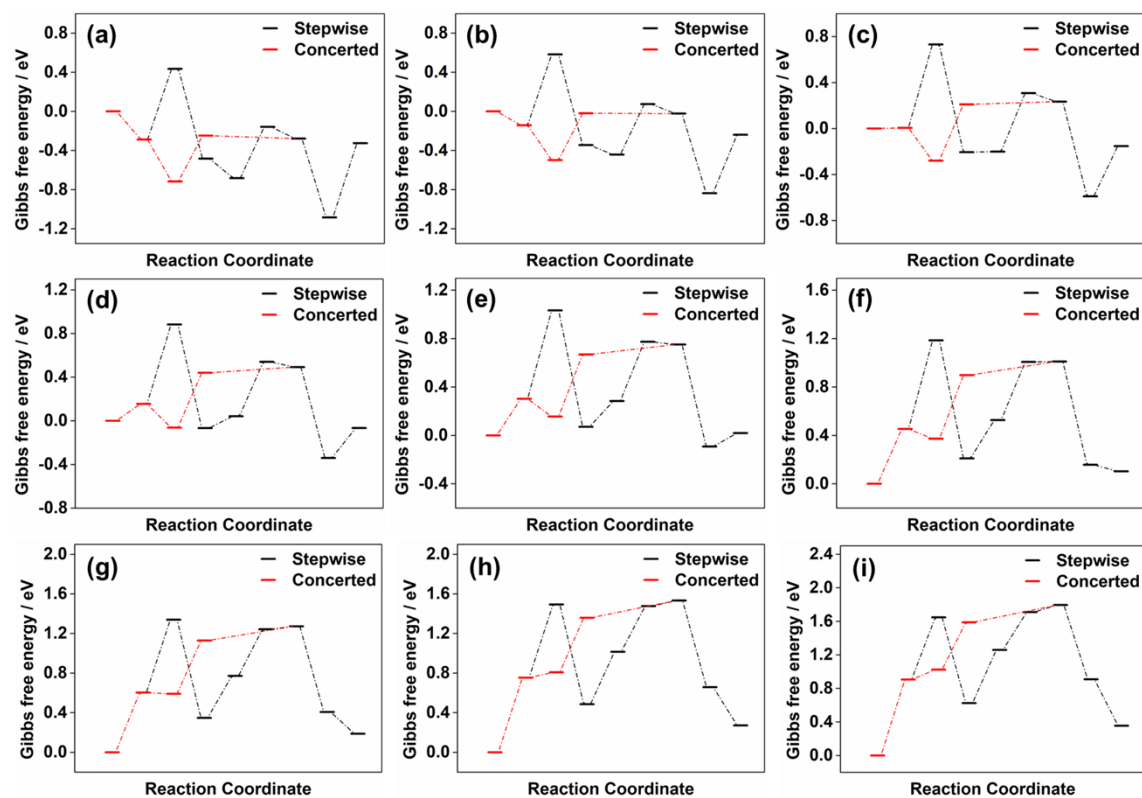
**(a) Stepwise**

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	S0

**(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	S0

**(3) 1-Dodecene**



**Fig. S14.** Gibbs free energy diagrams of the complete reaction coordinate for the alkylation of benzene with 1-dodecene 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 the 1-dodecene reaction cycle 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	TS2
TDI	S5	S5	S5	S5	S5	S5	S0	S0	S0	S0

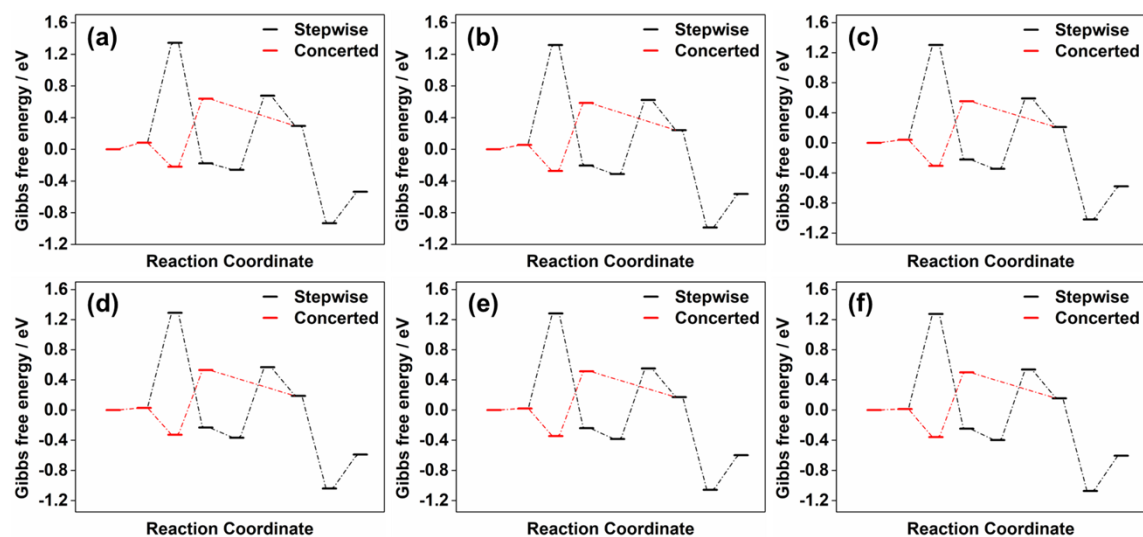
**(b) Concerted**

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	S0	S0	S0	S0

**S3b. Effect of pressure**

The Gibbs free energy diagrams and the TDTS and TDI under different pressure at 450 K are as follows. The TDTS and TDI were determined according to Eq. (3) in the main text.

**(1) Ethene**



**Fig. S15.** Gibbs free energy diagrams of the complete reaction coordinate for the alkylation of benzene with ethene at different pressure. **(a)** 5 atm, **(b)** 10 atm, **(c)** 15 atm, **(d)** 20 atm, **(e)** 25 atm, **(f)** 30 atm. The cycle consists of the stepwise and concerted mechanisms.

**Table S6.** The TDTS and TDI of the ethene reaction cycle including **(a)** stepwise and **(b)** concerted mechanisms.

**(a) Stepwise**

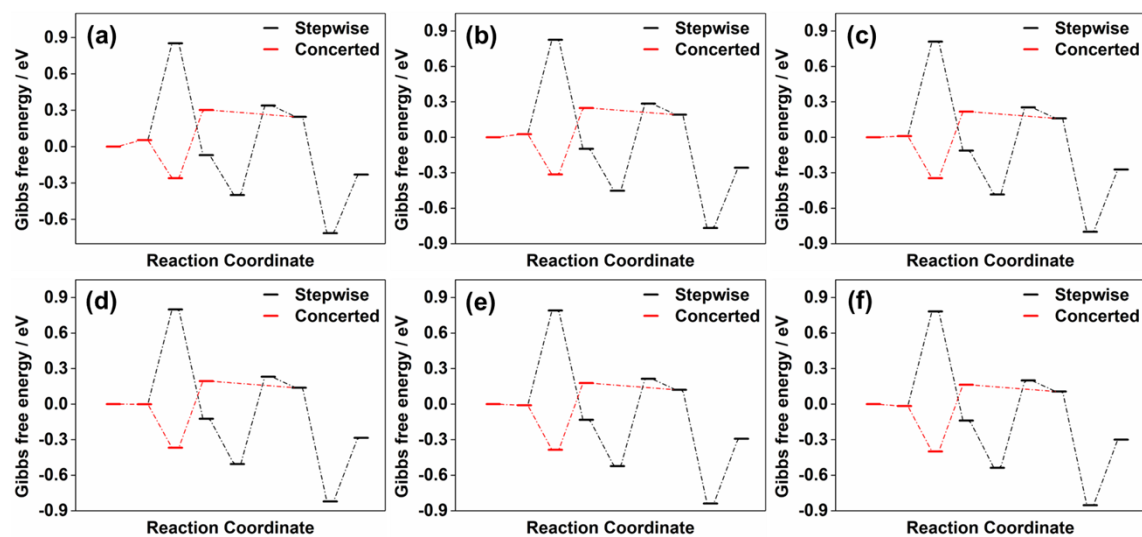
Pressure / atm	5	10	15	20	25	30
TDTS	TS1	TS1	TS1	TS1	TS1	TS1
TDI	S5	S5	S5	S5	S5	S5

**(b) Concerted**

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

**(2) Propylene**





**Fig. S16.** Gibbs free energy diagrams of the complete reaction coordinate for the alkylation of benzene with propylene at different pressure. **(a)** 5 atm, **(b)** 10 atm, **(c)** 15 atm, **(d)** 20 atm, **(e)** 25 atm, **(f)** 30 atm. The cycle consists of the stepwise and concerted mechanisms.

**Table S7.** The TDTS and TDI of the propylene reaction cycle including **(a)** stepwise and **(b)** concerted mechanisms.

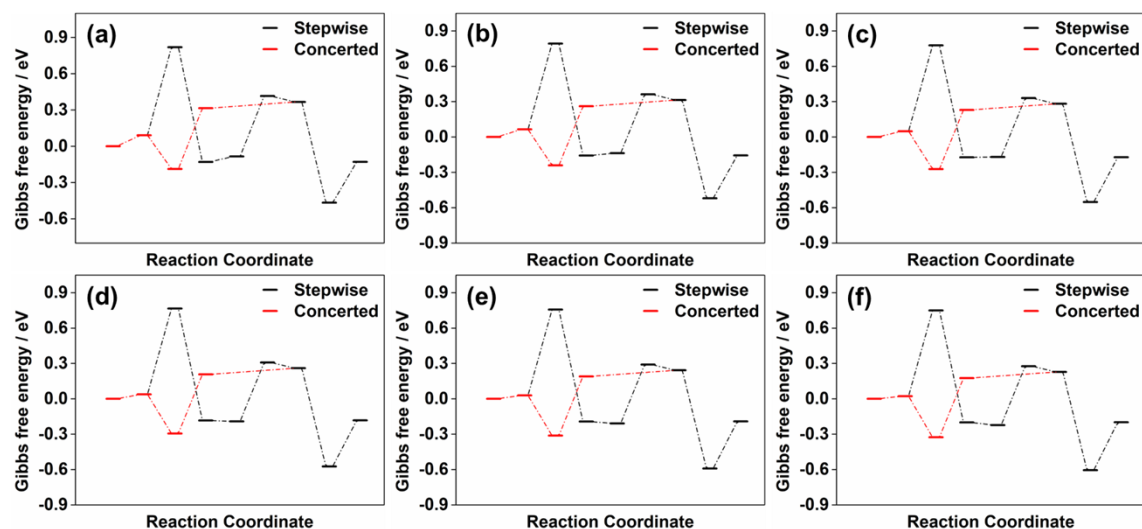
**(a) Stepwise**

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

**(b) Concerted**

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

**(3) 1-Dodecene**



**Fig. S17.** Gibbs free energy diagrams of the complete reaction coordinate for the alkylation of benzene with 1-dodecene at different pressure. **(a)** 5 atm, **(b)** 10 atm, **(c)** 15 atm, **(d)** 20 atm, **(e)** 25 atm, **(f)** 30 atm. The cycle consists of the stepwise and concerted mechanisms.

**Table S8.** The TDTS and TDI of the 1-dodecene reaction cycle including **(a)** stepwise and **(b)** concerted mechanisms.

**(a) Stepwise**

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

**(b) Concerted**

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

**Table S9.** Imaginary frequencies for all transition states.

Reactants	TS1	TS2	TS3
Ethene	686.61i	187.76i	164.80i
Propylene	377.23i	134.52i	108.87i
1-dodecene	207.28i	112.10i	113.46i

**Table S10.** Absolute energy of all the optimized intermediates for the alkylation of benzene with ethene.

Intermediate	H-MWW	Adsorbed ethene	TS1	Ethoxy	Co-adsorption of ethoxy and benzene	TS2
Energy / eV	-1752.72	-1785.26	-1783.99	-1785.69	-1862.52	-1861.56

Intermediate	Protonated ethylbenzene adsorption	Adsorbed ethylbenzene	Co-adsorption of ethene and benzene	TS3	Benzene	Ethene	Ethylbenzene
Energy / eV	-1861.98	-1863.13	-1862.29	-1861.46	-76.03	-31.97	-109.16

**Table S11.** Absolute energy of all the optimized intermediates for the alkylation of benzene with propylene.

Intermediate	H-MWW	Adsorbed propylene	TS1	Isopropoxy	Co-adsorption of isopropoxy and benzene	TS2
Energy / eV	-1752.72	-1802.17	-1801.25	-1802.38	-1879.37	-1878.65

Intermediate	Protonated cumene adsorption	Adsorbed cumene	Co-adsorption of propylene and benzene	TS3	Benzene	Propylene	Cumene
Energy / eV	-1878.79	-1879.79	-1879.22	-1878.67	-76.03	-48.67	-125.67

**Table S12.** Absolute energy of all the optimized intermediates for the alkylation of benzene with 1-dodecene.

Intermediate	H-MWW	Adsorbed 1-dodecene	TS1	Dodecoxy	Co-adsorption of dodecoxy and benzene	TS2
Energy / eV	-1752.72	-1951.23	-1950.46	-1951.495	-2028.32	-2027.68

Intermediate	Protonated dodecylbenzene adsorption	Adsorbed dodecylbenzene	Co-adsorption of 1-dodecene	TS3	Benzene	1-dodecene	Dodecylbenzene
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and							
benzene							
Energy /	-2027.72	-2028.75	-2028.18	-	-76.03	-197.37	-274.35
eV				2027.71			

**Table S13.** Cartesian coordinates of all the optimized intermediates for the alkylation of benzene with ethene.

H-MWW			
7.0511269792453612	4.2430713042060493	0.9107988091997012	O1
-0.0027996337905734	8.3426425484340481	0.9252122950255126	O2
5.7888269944769721	3.5776009877477821	3.0884051843247020	O3
1.2991199778209204	9.1868943119309137	24.0278942579153565	O4
8.4646824791010360	3.4439686457529373	3.0548313198835553	O5
-1.3482840956980606	9.2895692100277074	24.0480410264238849	O6
7.2577464218965551	5.8153550215405581	3.0869956075548957	O7
-0.0943833929769413	6.9103824998967838	24.0080999086065781	O8
1.1951135105584259	9.3664496222266180	3.1119529959325356	O9
5.9387892934369138	3.2004366241409272	24.0056691458721190	O10
-1.4473140520347831	9.0741422681952049	3.0742975355310551	O11
8.5685808243701853	3.6510988910626723	24.0659956927381273	O12
0.1348299629007714	6.9107885955026669	3.0965446804080865	O13
6.8348505790340273	5.6965556075253430	24.1876117440305620	O14
4.9518433211989930	1.3993879014452668	4.3707260591735633	O15
2.0398026889373453	11.3939295802954792	22.7206845364311505	O16
10.7776714524489989	3.7768814902915748	4.3351313438322601	O17
-3.6364848066561182	8.9502756311314293	22.7310256285147503	O18
5.7896108994655053	7.6296269120796367	4.3876639777474091	O19
1.4010407628921842	5.1538237790978769	22.6971959243988017	O20
2.3723871500796392	11.2958808712965677	4.5100927278024354	O21
4.5838794518099055	1.4122909061267281	22.5913593156697665	O22
-3.7262774458285270	9.0897785102433506	4.4544371965743492	O23
10.8530690885326351	3.6530866411738505	22.6979496188574323	O24
1.2244399561850781	4.9235394847462581	4.4966965118455251	O25
5.8488264480217076	7.9986913198091241	22.7362092872884602	O26
-1.2361346374276778	4.9077274937836890	22.6583013046153283	O27
8.4230858949799021	7.7753945902719508	4.4533638977395436	O28
-2.4608677591822872	11.2911773799535524	22.7019824119207208	O29
9.5630431327373326	1.4338863826731241	4.4189280487224414	O30
3.5745314676184039	9.2547292279997500	22.6668190208976732	O31
3.5143324019003903	3.6096381579454517	4.4727554568534140	O32
8.5923662344872085	7.5642871636349920	22.7969136120844773	O33
-1.4056736030334940	5.1189160548663635	4.3153589463837960	O34
9.3184801467181586	1.5104872536676943	22.6776857862904571	O35
-2.2529394133653664	11.2811590289891086	4.3285965400513486	O36

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3.7106316852011476	3.9057847820257665	22.7312305450296748	O37
3.5060470385455584	8.9165344757427327	4.3700790921008652	O38
5.8456408956990904	3.4919461581195006	5.7599227874270138	O39
1.2986797530658452	9.2056962642667379	21.3411078786141921	O40
8.5219338562586380	3.5059661347363744	5.7282134399245610	O41
-1.3642874091636870	9.2599764476294038	21.3698732932529616	O42
7.1711256087837238	5.8150349463022062	5.7612424949871208	O43
-0.0696281848468345	6.9110565690846837	21.3352890385557181	O44
1.2659716881167160	9.2311850877355486	5.7847095367338062	O45
5.9106489821775083	3.2875441631129174	21.3088216453493260	O46
-1.4069023868244446	9.1868820402701221	5.7490105488571501	O47
8.5448218228771751	3.7279872342524460	21.3822104728365261	O48
-0.0328151900038778	6.8936054746552671	5.7659636220027499	O49
6.8260106048718274	5.7907026298422073	21.2973224468939826	O50
7.2128367772246200	4.2521720178877169	7.8775710074469290	O51
-0.0671184299462055	8.4674242689395047	19.2124429732934026	O52
-0.0959404243819684	8.4367062639433321	7.8992185477363721	O53
7.1802178263826253	4.1958902268691878	19.1863661017711138	O54
5.5714264451625111	0.0624742030037174	6.5843012083759076	O55
8.6493008551163051	0.1681361747706613	20.4790174273661805	O56
-2.8234533875329948	4.9847437689681025	6.5610281869629956	O57
-4.4465832427367626	7.7153289825703357	20.5241454170514288	O58
4.3457930392024284	7.7752151443190138	6.6203538431027553	O59
2.8845885554832882	5.0838165223277958	20.4885616719551287	O60
8.9063699331713657	0.1870172590646109	6.6697076846379995	O61
5.3304457708123749	0.0291882804628962	20.4295225475323399	O62
-4.5316559510476537	7.8361077453670918	6.6601261361283424	O63
-2.7121873088858233	4.7785424509679766	20.4616901958239019	O64
2.7056107872137072	4.8123602969817805	6.6992399057020364	O65
4.4699542833745740	8.0635520460996997	20.4470121560431011	O66
7.2707108881750271	0.0953565510570665	4.5627722919343388	O67
6.9729612195875266	0.2385781135887961	22.5206496944778713	O68
-3.7186957451758804	6.4317456173969676	4.5416090675393130	O69
-3.4750028739110466	6.3114314787183572	22.5233973267510024	O70
3.5168136240761250	6.2632154415693151	4.6142193646505296	O71
3.6540810322088895	6.5611399881106252	22.5279696330947772	O72
7.1970450204242313	0.1010195509736544	8.6979266182428301	O73
7.0170569001645005	0.1447652889924168	18.3749581745869577	O74
-3.6330150392304348	6.3778638096983507	8.6861904331288180	O75
-3.5410551753128767	6.2952682049945379	18.4430164727616699	O76
3.5617373818154636	6.3160839620981752	8.7134091841684036	O77
3.6287038920256380	6.5642691625415370	18.4140861668178175	O78
4.7871744536014322	1.2598398410511162	8.7788388164366875	O79
2.1659952099609363	11.4180416434979879	18.3106802525546186	O80

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10.9411490260350064	3.7017158008912565	8.7358113530407469	O81
-3.6682161692663238	8.9532133152116700	18.3582097022186908	O82
5.7779715510055425	7.8103645671969923	8.8116648440143646	O83
1.3868281144992225	5.1199767360123509	18.3469839509539447	O84
2.3618513346881302	11.3927460786027357	8.8702787338563809	O85
4.6779308899588745	1.4385535580967035	18.2863866621500257	O86
-3.8652002422412206	9.0402864083657537	8.9096481269174586	O87
10.9280246545624671	3.6228264595353417	18.2262320540255196	O88
1.3440678227125131	4.8354016928623063	8.9555416394549372	O89
5.9258525336159318	7.9495649564406872	18.2598467940945355	O90
-1.2415074953321827	4.9490506239528411	18.2834860908842245	O91
8.4047790962833808	7.5418431500123528	8.8130044607054057	O92
-2.5021125429724478	11.3105781257020190	18.1888630255863859	O93
9.4493225062289259	1.5235639282111653	8.8718935110233623	O94
3.6221639578353839	9.2299528599266143	18.2611870855231793	O95
3.7018610394698075	3.6625705602787604	8.8527673101890230	O96
8.5299814100982871	7.5195240747234617	18.3652797623902302	O97
-1.2669471531110603	5.1482652868195782	8.6602600166731847	O98
9.2724151891311948	1.5704120993500492	18.3592851907329759	O99
-2.2383873042025080	11.1163593070362534	8.6783299115070243	O100
3.7523521083252813	3.9066034857948604	18.3222968637431336	O101
3.3950153750285921	8.9695976085690390	8.7483445130073285	O102
6.0559698352450315	3.2313999239236941	10.0360295315322272	O103
1.2556195061188777	9.2516247104291871	17.0450379709011095	O104
8.6390367282575937	3.7646631443189364	10.0642562582373039	O105
-1.3757752353814996	9.2034143195484788	17.0167826105163371	O106
6.8849468435510648	5.7360518514294041	10.0546662535272358	O107
-0.0173848388159934	6.9506260315594890	17.0233696967144645	O108
1.1139485172781489	9.3777289294135144	10.0700655290805035	O109
5.9755541513246984	3.3605434003797439	16.9695128565202715	O110
-1.4932077334696476	8.9916303514984168	10.0986191422472391	O111
8.5883816119936540	3.7423945567499914	16.9745618703062391	O112
0.1436830322121438	6.9245683359326069	10.0691046784719020	O113
6.9484053706399482	5.8111601132816100	17.0672242145792588	O114
3.9163851185047656	2.2071511269434358	11.0886688699864511	O115
3.2126754119476386	10.6220638688462543	16.0204236067495600	O116
10.6683349682473114	2.4698384416065688	11.0557408440395282	O117
-3.5648812177178768	10.1813994557443106	16.0191816287458835	O118
7.1039586959485721	8.1123960883082376	11.0823087498259696	O119
0.1959225381005023	4.5388080191340023	16.0643965886519595	O120
3.3509437736975185	10.2512355972883569	11.0716574605486535	O121
3.6585714230566380	2.5323393565865833	16.0711237625343557	O122
-3.3542579050065462	10.5866525617944696	11.0220067484853050	O123
10.4472844215626601	2.1281120931330353	16.0616005164628390	O124

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-0.2867131577032405	4.5438744880176740	11.0465076012345236	O125
7.4165548432180319	8.1919203823766491	16.0614425308517177	O126
2.3519958509628149	0.1488920403816746	11.7535816629850220	O127
12.0502044372248278	0.1198354583473828	15.3311904928886999	O128
-1.2192258213883349	2.1774563219934535	11.8088721410699016	O129
-6.0925218315359446	10.5801348546124654	15.2953503990077451	O130
5.9228249531465762	10.4238251704169631	11.6912544073206117	O131
1.1293768437261360	2.1583402838261607	15.3193872195633567	O132
11.6453762287868265	0.0934059421398786	11.6274092198988210	O133
2.7808946635242577	0.1154540108336954	15.4874241738001981	O134
-5.8959403302427429	10.2386141220874709	11.6529306043714094	O135
-1.4620734317438653	2.5814856214915012	15.4642561725836565	O136
1.3751229815934114	2.5852452201194565	11.6406352668404232	O137
5.7541311820384093	10.1574167139015650	15.5000765141982662	O138
3.1256448509483530	1.9489310955541559	13.5673794790203761	O139
4.0388130068260599	10.7865242064931053	13.5484671140372850	O140
11.2135106500830801	1.9139061300140687	13.5541786116054368	O141
-4.0923935929206046	10.8186607942978359	13.5347254753791262	O142
7.1506246446021020	8.9548617359662686	13.5574095066393827	O143
-0.0319221818675888	3.8013893253189490	13.5594286819875389	O144
-0.0444121069718895	8.3254485417636808	26.1963011634219036	O145
7.1947199292710771	3.9619085201942603	26.2535836691478330	O146
5.0278440639190833	3.0205980421205090	4.4152652742753995	Si1
2.0177576248655438	9.7788889764170168	22.6978703359576564	Si2
9.3292043162026683	3.0424773537086574	4.3765158652364615	Si3
-2.2037519184185479	9.6891873679023313	22.7166932914151225	Si4
7.1577444739926213	6.7552949338906156	4.4144394910349938	Si5
-0.0065248060929655	5.9692756884182883	22.6814945744713974	Si6
2.0838961553226349	9.6970437902753375	4.4379813110004251	Si7
5.0485074775570107	2.9758605451888096	22.6688243329608952	Si8
-2.2041228963712847	9.6587177991671282	4.3944018662958388	Si9
9.3050961307821325	3.1404469276016842	22.7125762053289542	Si10
-0.0216655039716560	5.9637720141231227	4.4119761408519294	Si11
4.6041178719068032	2.5987357121319539	9.6783950162217902	Si12
2.5653075571518258	10.1295066822684454	17.4171631717728062	Si13
9.9243467200923661	2.8509541255749911	9.6718025235940761	Si14
-2.7787174525948570	9.9177573663225083	17.4094700458532365	Si15
7.0538235250572034	7.3080861112170785	9.6802571032602245	Si16
0.0693025643963670	5.3840094953182680	17.4376204017001548	Si17
2.5619748417102395	10.0006201137276776	9.6805848908417467	Si18
4.5171136061421029	2.7996661602067774	17.4174104895054960	Si19
-2.7450445591840298	9.9365971076196367	9.6702926320944247	Si20
9.8162352561524084	2.7687220760028373	17.4110164996998478	Si21
-0.0149953392119628	5.3576329486337722	9.6722135954722361	Si22

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7.2098712287177662	7.3687459416405749	17.4440952205068882	Si23
2.6904604656999709	1.7163703283344909	12.0159626110130180	Si24
4.4640169311471922	11.0531987899053039	15.0957206909167940	Si25
11.6864560396917163	1.6657230277954282	12.0149419462781744	Si26
-4.5498378622796025	11.0491269534511893	15.0807430307157144	Si27
7.1743631974188133	9.4369767244272893	12.0019349847405543	Si28
-0.0397740158429454	3.2672753744324639	15.0986506619841983	Si29
4.4400633032306756	11.0139510011387944	11.9886555314131549	Si30
2.6726854193614971	1.6887484898778913	15.1093581218471957	Si31
-4.5512791075293517	11.0724707158031368	11.9931638594060477	Si32
11.6698895963157465	1.6859326809799886	15.1015119706997005	Si33
-0.0409882049773669	3.2760488239348229	12.0173707100232097	Si34
7.1689341443256778	9.4701001715012918	15.1018587306647056	Si35
5.6924719181102370	0.0845759384037610	4.9739857669609586	Si36
8.5415250872517561	0.2187326588399282	22.0887382531594803	Si37
-2.9017488932038162	5.0802698591475393	4.9505034193799196	Si38
-4.3803052816414390	7.6216774812734842	22.1450985492295693	Si39
4.2875083073380535	7.6430155541481337	5.0105419477673498	Si40
2.9085826670793913	5.1546588427598357	22.0978766440865435	Si41
8.8269270450968964	0.1281020340016939	5.0545967158888008	Si42
5.4144960067381973	0.1227042133168886	22.0436374577337837	Si43
-4.4929058024928725	7.7789072847410150	5.0430223510550762	Si44
-2.7657183913691714	4.9180166776201846	22.0760645908460518	Si45
2.7431846550499697	4.9064749024387426	5.0835067326487131	Si46
4.2939719686884672	7.9508109612883837	22.0319300505114093	Si47
5.6435747200134596	0.0131084580532875	8.1970920255152038	Si48
8.5724018908924222	0.2047984531701634	18.8667636380932393	Si49
-2.8108507343657148	5.0603800634029508	8.1743740202037927	Si50
-4.3838503014723207	7.6123170482260578	18.9197422022749606	Si51
4.2677773637804712	7.7080492832378580	8.2330726597945105	Si52
2.9129563184387668	5.1681501943216643	18.8743690389345637	Si53
8.7764263572871517	0.1737079730648523	8.2827893959716334	Si54
5.4441498057669078	0.1116051934312817	18.8190432202630298	Si55
-4.5094085523253851	7.6947934615284330	8.2725432343837948	Si56
-2.7605927394271523	4.9202587052712721	18.8530605426608240	Si57
2.8293187527642627	4.9135221043612836	8.3095898693245065	Si58
4.4099708977981775	7.9342837805565543	18.8199941477414185	Si59
7.1524394638414321	4.2767563551609058	2.5325560198587502	Si60
-0.0577373193770674	8.4365726416464568	24.5755996846563143	Si61
-0.0314398275222052	8.4366596768573388	2.5473830566264763	Si62
7.1172724772497418	4.1691422115037309	24.6353738454019755	Si63
7.1865733925838367	4.2664238574480846	6.2736464417469104	Si64
-0.0615085079390667	8.4575173163209652	20.8180587315381196	Si65
-0.0657440405743159	8.4368136648777909	6.2938669703175671	Si66

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7.1120936943863358	4.2847713304831156	20.8004175360737058	Si67
7.1980295086161856	4.2463742168384648	9.5036970171839812	Si68
-0.0530706395277001	8.4679836964377220	17.5833866011202993	Si69
-0.0830177602193274	8.4330156142629757	9.5267249760980661	Si70
7.1743636164217861	4.2823228005531213	17.5658090922376822	Si71
7.1555520442581715	6.6304822510787353	22.7790802487139636	Al1
7.7673800994764708	4.6412251060284850	0.3932070242299976	H1
-0.0509189252525211	9.1626249967659543	0.4107643859890184	H2
-0.2568451305991610	9.1152034803045119	26.7163126711693053	H3
6.4747416919820875	4.3336201597025799	26.7853942756796854	H4
6.1679946472153180	8.8807657830825200	23.0035374858163841	H5
Adsorbed ethene			
7.0602729034984923	4.2407807600276017	0.9123674965574762	O1
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4.3991580722355446	7.9141576104021309	18.8111069831451978	Si59
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7.1874172589595728	4.2469538721706526	9.5036484341415424	Si68
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5.7477855683013672	10.1298931295219745	15.5245395565194322	O138
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4.0628630676145345	10.7634436025608338	13.5424857510105063	O140
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5.0237542169694764	2.9958509891151017	4.4208574665327074	Si1
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-2.1843903739256425	9.6966157330628651	22.6673265442034939	Si4
7.1364944575278297	6.7472309921231020	4.4318498480989605	Si5
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2.5660418379583003	10.0692857875535644	17.3851789955107030	Si13
9.9013800674090895	2.8664461893008220	9.6930707295746164	Si14
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7.0013720257193945	7.3078875452364587	9.7031656966496556	Si16
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2.5640495614167467	10.0003507992989444	9.6947985403240811	Si18
4.4704546139720218	2.8097602137668396	17.3883807819400182	Si19
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2.6535340107698491	1.6755885038628733	12.0035416105904567	Si24
4.4687630151276263	11.0297028453669661	15.0944426544636894	Si25
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7.1757751375047185	9.4329129170956048	12.0117680309898773	Si28
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2.6306999995208500	1.6605146553617860	15.1093380821251344	Si31
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7.1644436796842941	9.4473756689882791	15.1236290565869318	Si35
5.7028312186906920	0.0647002450132402	4.9952983607806516	Si36
8.5325281960681902	0.1593362943910274	22.0733939673984665	Si37
-2.9122258553532117	5.0985198577218762	4.9970904412138877	Si38
-4.3599785704504770	7.5959633819235490	22.1113307345164536	Si39
4.2593186071097842	7.6195743089449497	5.0110937814742638	Si40
2.8845205230137192	5.1777317852089633	22.0876345495409794	Si41
8.8449511081002736	0.1252919773159251	5.0762373890691510	Si42
5.3976551785668745	0.1434780656211336	22.0371965098720075	Si43
9.9083189042574933	7.7908803843073304	5.0878378145199568	Si44
-2.7916945525160299	4.8865738368273099	22.0595692713910125	Si45
2.7331086009465988	4.8720841360442284	5.0892699219161788	Si46
4.3719080607360645	7.9332567853088642	22.0529592803506986	Si47
-1.5690434778649482	12.4891715051450820	8.2164791507182873	Si48
8.5344117909712871	0.1362315202284224	18.8547361243720886	Si49
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2.8860957961867615	5.1810317557324073	18.8632120229591571	Si53
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9.8839037322376733	7.7039979018056686	8.3146679881896102	Si56
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2.8147559275288754	4.8874154677976955	8.3147334927613681	Si58
4.4101923776533249	7.9195688863258757	18.8281717973942122	Si59
7.1528448806387939	4.2663034199191054	2.5525727982134092	Si60
-0.0665806996057583	8.4095390451324938	24.5487141205779089	Si61
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7.1382243090107336	4.1903305727820133	24.5904336661842073	Si63
7.1651932829595468	4.2578630262716359	6.2899687638679866	Si64
-0.0541939291740112	8.4422755840080317	20.7945547553005063	Si65
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7.1659901642925998	4.2456771543537437	9.5191376913901742	Si68
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7.1563159468991362	4.2336717440203326	17.5524229716276032	Si71
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6.5122074735761633	4.4123418875817926	26.7364152449695105	H4
6.8756766384774552	9.5223254396594363	22.4627980932904912	H5
7.1478948992805131	9.0901235571372219	24.5739731796147680	H6
5.5368135762135093	9.9552779171175256	24.1631229324228549	H7
8.3513952256935227	10.4988756347483960	22.9104408246519391	H8
6.7334092113220514	11.3643339813998807	22.4804930598191248	H9
6.6063426172208457	9.8284364037773972	23.9770996621942238	C1
7.2620012492708774	10.5515516885768363	22.9842521689147645	C2

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5.9199489572527311	3.1903291460892995	24.0094034500323161	O10
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4.9643415464615996	1.3672546309306213	4.3747818035687782	O15
2.0195290355026687	11.3643755325311968	22.6870311118537984	O16
10.7784799812412704	3.7767010332073316	4.3873320746131554	O17
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5.7686977191432733	7.6072813635029970	4.3890030173564742	O19
1.4255039723672538	5.1808421861675935	22.7205662145463236	O20
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3.6109900692776002	2.5472602185248290	16.0629093539568046	O122
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5.0425578847758494	2.9570418595000936	22.6651881392386017	Si8
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9.2979647348375636	3.1181349542750652	22.6694111169928050	Si10
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2.5825645581444547	10.0508832782735897	17.4057611040715265	Si13
9.9023459174883985	2.8615103349978543	9.6949434664781879	Si14
-2.7461617558528002	9.8970263673110228	17.3857212125291554	Si15
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4.4853510918724364	2.7951790947697863	17.4050952576049127	Si19
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2.6691272090030731	1.6849728912376034	12.0131042785111628	Si24
4.4689296356439892	11.0135115782885009	15.1001338610289082	Si25
11.6558536754850408	1.6458076080051798	12.0083368463212903	Si26
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7.1834555478449538	9.4467404447779444	11.9941298776255874	Si28
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4.4597856950198400	10.9996874832652125	11.9830372765869928	Si30
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5.7027500764474208	0.0601017941735258	4.9995856607132962	Si36
8.5150936497216243	0.1801367243134657	22.0378227423931534	Si37
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8.8493140163543043	0.1138870608825984	5.0781232254668520	Si42

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5.3921147274374892	0.1104220694217651	22.0264337865872726	Si43
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2.7355064024482387	4.8644914448599517	5.0834739917304210	Si46
4.3571635874117112	7.9542279542250656	22.0501119799929519	Si47
5.6513657865753659	-0.0178666892165757	8.2184980983513061	Si48
8.5139183189803767	0.1356669661464641	18.8181639475806080	Si49
-2.8179332331861007	5.0716975774863888	8.2223151020714074	Si50
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4.2288645114101673	7.6881370848424950	8.2302233967775713	Si52
2.9233841692484228	5.1932173133720170	18.8669585944059115	Si53
8.7944917412400283	0.1696392850962350	8.3025133499366017	Si54
5.3895770468181050	0.0947571127706479	18.7992276130467388	Si55
9.8867771259143602	7.6952330245673988	8.3075440033217731	Si56
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2.8166872565988963	4.8772694134744468	8.3088958723989812	Si58
4.4793143071529267	7.9445933536939792	18.8440756254164903	Si59
7.1590778673732052	4.2613896390291517	2.5485407152627571	Si60
-0.0949650017958188	8.4181104541029548	24.5484159650268872	Si61
-0.0440402782303035	8.4121911174297974	2.5691156241977740	Si62
7.1283523216873323	4.1377921073366215	24.6176861136350631	Si63
7.1701251963530259	4.2501788835243275	6.2865417673516495	Si64
-0.0661866410599075	8.4277772526235992	20.7963093979702229	Si65
-0.0503677271968579	8.4205999526430695	6.3176765643878880	Si66
7.0838162579639636	4.2764681310191550	20.7887544077265787	Si67
7.1698516749015671	4.2487632248579725	9.5154817722574467	Si68
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-0.0578371444159798	8.4172545833732961	9.5505206493698385	Si70
7.1542983062623842	4.2532768965559393	17.5544496091927016	Si71
7.1367099292382949	6.6116648733189471	22.7484197546307776	All
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-0.2175088033770791	9.1794567652424206	26.6636067183579790	H3
6.5273632426870751	4.3555479385321751	26.7736304437702195	H4
7.6240259710501928	9.9483736663175328	21.9679763408441175	H5
7.1539081385050585	8.8779220084409527	24.1911298455877777	H6
5.4919965764632961	9.5513488783777554	24.1718757423714088	H7
7.1845362034549582	11.1590982257240903	23.1941518606397388	H8
5.9838112595101691	10.6817033716105581	21.9717800366744420	H9
6.3387903268379917	9.2373425841637928	23.5502704410320440	C1
6.8048642707189897	10.3123271436502186	22.6021631248381922	C2
Co-adsorption of ethoxy and benzene			
7.1167061364986512	4.1491855658646575	0.9617090999524883	O1
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8.5284491430655702	3.3637283342272881	3.1133035743990121	O5
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-0.0108409988904095	6.7799280512174178	24.0479847753712548	O8
1.1939145312831352	9.2956248988151629	3.1726941290667585	O9
6.0385015653548830	3.0484915770283196	24.0532419548202476	O10
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8.6266257427800301	3.6426956898224638	24.0546631100592769	O12
0.1863120053722263	6.8172802853233962	3.1995937994908754	O13
6.7698922848184893	5.6060499371396864	24.1652643021304456	O14
4.9776371327222364	1.2733146765641752	4.4208626358178664	O15
2.2029143543386613	11.3046157171696606	22.7857522074032097	O16
10.8264432404164612	3.6905284398479408	4.4266295638573077	O17
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5.8076408094140870	7.5370848624683653	4.4317821242903390	O19
1.5056039660245162	5.0199314157803547	22.7760310626461866	O20
2.4167663221296802	11.2118406345714181	4.5536366584856509	O21
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1.2622797133612087	4.7998213627343578	4.5624825858817450	O25
5.9220645535699949	7.9745949481859810	22.6049729785142937	O26
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8.4441611195649351	7.6576613482883022	4.5205828761420985	O28
-2.3554607013921700	11.1394370906608717	22.6998421633626286	O29
9.6008400683186039	1.3512707756556344	4.4928386177981228	O30
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4.3363032118129690	7.7010181469870238	18.7983831018441236	Si59
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9.9940537099283908	7.6963934980752331	20.5730722368902725	O58
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3.6766776506511705	2.4150392673239822	16.1125517638404325	O122
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9.9148531491336644	2.7426968006791990	9.7807128247155219	Si14
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0.1563494247684027	5.2505918303018086	17.4955838280159099	Si17
2.5983178377767908	9.8931143868634948	9.7483350690434243	Si18
4.5684550971126008	2.5891570759308751	17.4550635402617402	Si19
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9.8715193702511179	2.6741739880344166	17.4500142086882448	Si21
0.0283881066223963	5.2662530450870664	9.7535860355802413	Si22
7.1541094478744975	7.2153160979497688	17.5163694153031386	Si23
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4.5039915279610820	10.8813874838919364	15.1494453145461883	Si25
11.6847670524925640	1.5041309718104656	12.0589287240187542	Si26
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8.6796093057049344	0.0767858579666865	22.1357482722226138	Si37
11.5537882684496260	4.9508782941683966	5.0855181352721361	Si38
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8.8618015858264449	0.0024941493555254	5.1417974677486802	Si42
5.5244216529020473	0.0165567601108699	22.0500691811748055	Si43
9.9555053210443241	7.6710217132146203	5.1569519023977914	Si44
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4.4006034199912740	7.7878382880665100	22.0757376600530257	Si47
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9.9805727957120567	7.5353001582207373	18.9739789461087511	Si51
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2.9373475705572769	4.8851208404896962	18.9572044657987462	Si53
8.8047772210659616	0.0687160276244726	8.3701291092061894	Si54

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9.9177451711099458	7.5967314117594036	8.3778965362340294	Si56
-2.7452137209323291	4.8800227762538171	18.8633002190031256	Si57
2.8503109152579809	4.7810323480030119	8.3721256532848400	Si58
4.3142223519042133	7.6992533496917392	18.8481697363061222	Si59
7.1925682340008237	4.1313291643980827	2.6068499680826629	Si60
-0.0067342493319833	8.3014898398004249	24.6118072158729184	Si61
-0.0106314603961817	8.3013392770647521	2.6383713276485632	Si62
7.1730234014709566	4.0902092328937885	24.6430596144567389	Si63
7.1993524767929546	4.1392588144002023	6.3466183593736796	Si64
-0.0054581547404657	8.3385516736840852	20.8666700534361489	Si65
-0.0200149389122002	8.3119644550589804	6.3854729302519768	Si66
7.1981730329358253	4.1576043622748609	20.8455585377544033	Si67
7.1876441558087674	4.1178671084575402	9.5745493583600805	Si68
-0.0097776500892346	8.3096487852903085	17.6381492598884009	Si69
-0.0348424352489358	8.3317643061803839	9.6161713315691735	Si70
7.1948087135706018	4.1190638692160730	17.6241755081832281	Si71
7.1477540593635700	6.6225496025271253	22.7666078797674416	All
7.8293592264899114	4.5450193636837479	0.4836818829054271	H1
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6.0028186170197726	10.4402010363263997	20.2463669530946433	H6
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5.7582409551354932	10.2833108889994591	22.7186664320604912	H8
7.5514587063709326	9.8109387409792888	22.8872044105235695	H9
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12.5483547120986270	1.5320404499350821	20.6856443321921795	H13
12.2723849932284512	0.2626415892308838	22.8059928546948747	H14
7.0773428560578591	11.9342310866952488	24.0277880025782089	H15
6.9012175943799718	10.1443881059493695	20.7968813607463581	C1
6.7268527173720383	10.1329439585806842	22.2496258051203846	C2
1.2589961625360750	0.0893251984629249	22.5048235087341126	C3
1.4037357198988798	0.8010280655254168	21.3195083351792398	C4
0.2697026977269885	1.3079782289861370	20.6619549750304579	C5
13.4207410477634479	1.1087269280982048	21.1868507199865306	C6
13.2665716260273889	0.3958946312596254	22.3729721808097324	C7
7.1844012350792941	12.3569808430235462	23.0265601094093952	C8
Protonated ethylbenzene adsorption			
7.0995685967444215	4.1104253284930401	0.9851235921702908	O1
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5.8126658345410869	3.4120476133770490	3.1355255764670202	O3
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8.4919626659405036	3.2785206039694526	3.1321772706564568	O5
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7.2893440418109599	5.6476308557367041	3.1878362289515656	O7
-0.0703759122270395	6.6898740698543619	24.0903898599308377	O8
1.2018467054917146	9.2182798926764740	3.2069486184204581	O9
5.9257176407180712	3.0542930679969649	24.0908688387047718	O10
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8.5555253804246032	3.2458466902112613	24.1086613212245702	O12
0.1288689466104551	6.7652124369936830	3.1975137235014501	O13
7.0628704566696623	5.4856696246743581	24.2328047073755037	O14
4.9729917659013694	1.2499035725693921	4.4438338152356884	O15
2.0927912610734758	11.1794212005731683	22.8111198328260585	O16
10.7931093130793574	3.6526346673261343	4.4306662135697223	O17
-3.6366614080416317	8.9114038567187706	22.7600308907163154	O18
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1.3122582042673656	4.8251875978306789	22.7453954878979054	O20
2.3987390652702514	11.1590066001544646	4.5771255310173764	O21
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10.8201955887241841	3.5699243662273448	22.7466331360292635	O24
1.2435936957419762	4.7700660608158714	4.5589005482037797	O25
5.7986007620185891	7.6593956666130030	22.8228234169315698	O26
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0.0203980025635153	5.2475011856238662	9.7657904770489239	Si22
7.1096707227416678	7.1849416785082072	17.5170172235084713	Si23
2.6494453329859846	1.5600260319820389	12.0570768929759424	Si24
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4.3109457538042664	7.4960369559271971	5.0737106665812020	Si40
2.8381419709489752	4.9186356397756050	22.1682920790577924	Si41
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9.9512834103545060	7.6544364607914543	5.1592683500489560	Si44
-2.8148755135226802	4.8372612720066401	22.1135233617498308	Si45
2.7621523309586564	4.7546753774488275	5.1455160528579960	Si46
4.3652875161835398	7.6780995006026247	22.1448971359564872	Si47
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2.8991909331460248	4.8209063221939878	18.9499501040184946	Si53
8.7970554174646374	0.0533073998672669	8.3710839329853304	Si54
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9.9089024750987367	7.5785949509275294	8.3800527824415596	Si56
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2.8369340495492477	4.7710514380610887	8.3700862066353245	Si58
4.2960705355861091	7.6475756840441038	18.9152289952977810	Si59
7.1844066301020444	4.1185212763938317	2.6078874286857503	Si60
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7.1795678454956171	3.9563129342860401	24.6850822600955055	Si63
7.1914387256496211	4.1279879632128145	6.3482689105939798	Si64
-0.0350770345652647	8.2642483142250445	20.8765709855624451	Si65
-0.0192683828442570	8.2972389767780879	6.3843913050642094	Si66
7.1754971836614452	4.1162865461844484	20.8820332483399049	Si67
7.1766466311255481	4.1055768498989496	9.5763924693062386	Si68
-0.0314856983635492	8.2533757031721873	17.6511935982908490	Si69
-0.0338613735661273	8.3096256768190599	9.6154127250460046	Si70
7.1845206409961122	4.1027528982909853	17.6556304328712130	Si71
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7.8148216043077552	4.5273381606548639	0.4810501075889107	H1
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7.0699798462594021	4.5710764499468297	26.8238377371988967	H4

7.0760914528669119	9.1785649952205102	20.7095823503204919	H5
6.3146562692367532	10.7201161599819113	20.2697962402797032	H6
8.0936244345077704	10.5946557899570450	20.3791930668188499	H7
6.1426130720419216	10.2383206218111020	22.7632781682205767	H8
7.9003672934312927	10.1075437004894386	22.8636940092882810	H9
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12.2257075093297320	0.0247968949944726	22.4447925569250089	H14
7.1269715415076123	12.1508293459974350	23.7343180677641996	H15
7.1456650169090450	10.2680773343371463	20.8318592319845273	C1
7.0807424580180918	10.5944625694892327	22.3161199579696330	C2
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1.3568488557366569	1.3312635713277994	21.4366608273212336	C4
0.1791768214028524	1.9571669163239598	20.9795244085473840	C5
13.3278052324696468	1.4966108963205016	21.3340721443201247	C6
13.2113353272189560	0.3919820125739084	22.1442327565297603	C7
7.1743612293072339	12.1653302944574087	22.6193991746631724	C8

Adsorbed ethylbenzene

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1.3388090047656327	9.1219861345336373	24.0580384875290036	O4
8.5149127099444861	3.4620133409227458	3.1474105903860536	O5
-1.2978613005685657	9.3029183545897514	24.0710158600094246	O6
7.2632157399664035	5.8098287395149883	3.1967775567398449	O7
-0.1312724582947618	6.8827920182196669	24.0526683630709499	O8
1.1773864980980546	9.4049762098449374	3.2364061865348552	O9
5.9557011811027838	3.2296016575661550	24.0613191327993050	O10
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8.5791580045590372	3.6472881888834348	24.0433958788778099	O12
0.2007909930563505	6.9125578521230642	3.1859704384309686	O13
6.8671065554830966	5.7299882390411225	24.2215736607314795	O14
4.9693735183661181	1.3816674231480248	4.4743759522729807	O15
2.0657209936576280	11.3462385567492472	22.7635096082130914	O16
10.8168555570351028	3.8094443844281156	4.4477583815998214	O17
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1.4770015303805626	5.2259736408931792	22.7546710820503435	O20
2.4086913252945203	11.3233603979090685	4.6042633082350539	O21
4.6222303637644861	1.4018805502852882	22.6813496793182985	O22
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5.9683046519971725	8.0623154044812875	22.6599859672657864	O26
-1.1566311010274029	4.8294167659990856	22.6741729295988392	O27
8.4220685095609387	7.7829170662379301	4.5545652700184958	O28
-2.4734839146673080	11.2732793546279240	22.7310259448885645	O29
9.6021717083670488	1.4655352437291127	4.5425755057967221	O30
3.6172620820943253	9.2179550732464897	22.7174586394031479	O31
3.5513248063013556	3.6064470658632408	4.5438228343512961	O32
8.6845987210365454	7.4991948699651871	22.8144495560106897	O33
-1.3821616113645936	5.1780425802547372	4.4346448896478385	O34
9.3360361433927466	1.4654080541740979	22.7061875874587855	O35
-2.1865955361713327	11.2602324585755760	4.4178040644259147	O36
3.7367581694550007	3.8890172453476937	22.7341475776890007	O37
3.4936795055034464	8.9148649030991400	4.4654898563326331	O38
5.8760797641742641	3.4801565632451590	5.8420554679839416	O39
1.3580661551709934	9.1514649130026289	21.3724691552722881	O40
8.5512904319518466	3.5533743897634569	5.8211519979122404	O41
-1.2937071860127647	9.3003889555347854	21.3887362944995054	O42
7.1524486174655948	5.8330003909853350	5.8678907939768825	O43
-0.0874030734375260	6.9013446075206302	21.3836762447232545	O44
1.2752723194281614	9.3000002990581088	5.9076488704773773	O45
5.9642322611804861	3.2442997734572110	21.3650458945764292	O46
-1.3959415515653366	9.1457904534830234	5.8503609539762609	O47
8.6047450212916381	3.6680124995325607	21.3654296474967751	O48
0.0740984568992502	6.9118971166622041	5.8572416886005856	O49
6.8927271337939064	5.7464781498892021	21.3425976285835119	O50
7.2137505728620752	4.2492177227797248	7.9681580428756256	O51
-0.0206143263715770	8.4349812795115398	19.2461928578517885	O52
-0.0629855371099737	8.4291741417484705	8.0017891251029987	O53
7.1742096332056917	4.1645292383572441	19.2190622545334087	O54
5.6006058025650329	0.0272796903808226	6.6821133831227790	O55
8.6782691706998207	0.0972026886697899	20.5148548404663700	O56
-2.7847993480048747	4.9937823847076288	6.6840300751357535	O57
-4.3390288359175422	7.6035829806916251	20.5455700275684734	O58
4.3624884193361639	7.7795925676106190	6.7080476841075383	O59
2.9169068624511540	5.1532551032683598	20.5293003226790418	O60
8.9430518266204793	0.1903018185915211	6.7777601100290825	O61
5.2931238441815225	0.0568108987523204	20.4831994734943663	O62
9.8667773576750299	7.8859950242663697	6.7784699812827647	O63
-2.6729379747148378	4.7207599853745474	20.4961226452518410	O64
2.7418254092756804	4.7752190841773707	6.7841386144076301	O65
4.4469118560560421	8.0540737311149275	20.4615565864110174	O66
7.3087367396638419	0.1273104403009832	4.6693696592871170	O67
6.9895789734410760	0.1810933478527521	22.5457533308782629	O68

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-3.7111568704073146	6.4578997234272792	4.6901328621159477	O69
-3.3777086003221508	6.2512812311404016	22.5782346101358726	O70
3.5241389531278791	6.2605817268574784	4.7131059248071177	O71
3.8070531769428406	6.5409982572161089	22.5872203763886539	O72
7.2232540801389931	0.0974662225109136	8.7972770575504544	O73
6.9918772768345079	0.0913936047868753	18.4407855699104921	O74
-3.6544866444304080	6.3973937935416005	8.7806007742412611	O75
-3.4930813811404100	6.2031687642124842	18.4410091533978004	O76
3.5609767254347759	6.3146026750055730	8.7904786351740825	O77
3.6705622932200517	6.5565368446962804	18.4068491098533542	O78
4.8084248007901351	1.2494831127264019	8.8589788479551643	O79
2.1078384557015726	11.3157751523298042	18.3415381362614553	O80
10.9741446450345741	3.7303825878691508	8.8719426096875651	O81
-3.5935550333354360	8.8660154162059630	18.3855074122953823	O82
5.7527740247586836	7.8440289222585138	8.9259806440847598	O83
1.4053690517261859	5.1595909688823038	18.3929273118470888	O84
2.4101713982635626	11.4383206927352052	9.0024861019012548	O85
4.6724411638985499	1.4185871570808826	18.3045992959164074	O86
-3.8738956533261151	9.0540990082239823	9.0374849736631706	O87
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1.3502015356908688	4.8228516514453066	9.0230722744156768	O89
5.9863756061033602	7.9035386720652214	18.3260619967333582	O90
-1.2124557602257917	4.8165662334300174	18.3130233731182948	O91
8.3854560317990412	7.5581447829369770	8.9350794220501761	O92
-2.5517745243535632	11.2846887711381978	18.2785388254928662	O93
9.4420015333042464	1.5704335625068175	8.9585494670411752	O94
3.7049813866894894	9.2241677764413357	18.2453233865142153	O95
3.7200406931674306	3.6610199259523490	8.9592128613233672	O96
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-1.2610895374781228	5.2262460529474843	8.7925291089192381	O98
9.2672771154673494	1.4761124368116638	18.3756153974238075	O99
-2.1997829449880042	11.0990379610484204	8.7902554816642038	O100
3.7501164243528842	3.8936415137412208	18.3915759857833336	O101
3.3516328599547789	8.9697939076915194	8.8039712750519783	O102
6.0753751641394000	3.2121398757914941	10.1293332478892619	O103
1.3271363203515163	9.1048013954282432	17.0570977280057505	O104
8.6468006746033215	3.8129119535312817	10.1581094722821970	O105
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6.8390304259042809	5.7380721317542198	10.1298604693360641	O107
-0.1209325315893683	6.9033400040791344	17.0738928617423227	O108
1.1094214382126948	9.4360340257390671	10.1635292014341676	O109
5.9598763188543744	3.3553655294102316	17.0011930206705166	O110
-1.4836673899400283	8.9436218768788365	10.1852841491589530	O111
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0.2393635968423089	6.9396637614305527	10.1781332382003615	O113
6.9936343506191667	5.7778380331651098	17.0918650907434220	O114
3.9313678834898935	2.1753319971938625	11.1719941490945516	O115
3.1956985496457309	10.6187885987378969	16.0387943103277344	O116
10.6386639610113303	2.4757357581147028	11.1694715582970563	O117
-3.5457623119793360	10.1496107870108538	16.0817008083851576	O118
7.0700331079489303	8.0882904331960219	11.2051108265415298	O119
0.2587529770121724	4.5055857367754930	16.1096724273934022	O120
3.4060373830021531	10.2045736508778475	11.1491347134465286	O121
3.6246006716586443	2.5524700995462744	16.1270497428507582	O122
-3.2895713534357207	10.5779642989297678	11.1465843240443618	O123
10.4401789180152793	2.0800317121340326	16.0981250174412907	O124
-0.2459657713530445	4.5560342677775409	11.1421563880992345	O125
7.4560512696031891	8.1713840058464751	16.1201509745652487	O126
2.3543356890552718	0.1168814645252921	11.8110078028568601	O127
12.0983696799006708	0.0943429951297359	15.4412197285826363	O128
-1.2206062602231504	2.1761580595953882	11.8163859537255345	O129
-6.0928013690728111	10.5975976578913063	15.4512710788708088	O130
5.9844954652322038	10.4667608608289875	11.7362640074296625	O131
1.1063947000774434	2.0836805428349274	15.3862892580959905	O132
11.6408955442555069	0.0866301264165130	11.6410590399040519	O133
2.8269605555648010	0.0994168280037249	15.5825175142723342	O134
-5.8450858646004100	10.1806739545331819	11.6678674011902839	O135
-1.4678860009220909	2.5829128040932119	15.5612375523882189	O136
1.3801006799816673	2.5520155974361640	11.6880678586311291	O137
5.7539336842314865	10.1199032043357668	15.6145040664061536	O138
3.1077089881563271	1.9135926788174562	13.6362397909981823	O139
4.1179911902241866	10.8002666144674073	13.6049253895007745	O140
11.2714597180946541	1.8514091110339463	13.6218883183848192	O141
-4.1422147918124725	10.7952005252411674	13.6232419455452014	O142
7.1876210810567347	9.0216822152447875	13.6414626882553502	O143
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-0.0279439956979468	8.3089382550647368	26.2298283555607625	O145
7.2544986735541821	4.0023861366732092	26.2730069289416370	O146
5.0601039135744950	3.0035855495467132	4.4991166174596193	Si1
2.0617844587075034	9.7266592109171128	22.7355832863444967	Si2
9.3683672349594502	3.0740615723066451	4.4815099485068624	Si3
-2.1548764142868730	9.6802062339298818	22.7362550349114692	Si4
7.1545722809892913	6.7633881609050155	4.5136206258786435	Si5
0.0219834834401342	5.9530947457169274	22.7228557639987017	Si6
2.0909587967152889	9.7286923440867330	4.5472237681666368	Si7
5.0825736577539082	2.9688984224212569	22.7208824259808715	Si8
-2.1860244295445819	9.6377027550946863	4.4980575443448849	Si9
9.3390184448488185	3.0995026999829811	22.7183330929028102	Si10

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0.0297666415069804	5.9759123962777076	4.5084399211416102	Si11
4.6220073585623158	2.5830197088450895	9.7676148356712620	Si12
2.5800720945092790	10.0645811086603754	17.4292244794968525	Si13
9.9250419485452070	2.8839921756377782	9.7770838617063553	Si14
-2.7467340765088664	9.8943120068102655	17.4662759354286443	Si15
7.0247192057586680	7.3142003515450460	9.7848107314036934	Si16
0.0751968913817191	5.3429796928078730	17.4833442392120979	Si17
2.5756910212762465	10.0164032922934148	9.7702392517816250	Si18
4.5048287008279519	2.7971974900109013	17.4644756542337660	Si19
-2.7181347112170404	9.9212075731407143	9.7795012675677953	Si20
9.8106742442293093	2.6969502941474475	17.4583616127458363	Si21
0.0221996864163629	5.3794533651355048	9.7737852805442262	Si22
7.2597367527898573	7.3277808743502488	17.4936391141679266	Si23
2.6917124457511425	1.6841529023804289	12.0804887387510007	Si24
4.4910049212168870	11.0378960883447448	15.1676914521110238	Si25
11.6963900543031176	1.6502414040568476	12.0657132182887494	Si26
-4.5476744019906530	11.0365508776416181	15.1789539224446752	Si27
7.2021875353622518	9.4447108145426348	12.0706784846699158	Si28
-0.0325993985645276	3.2260090136434911	15.1689324278029769	Si29
4.4862590862253597	11.0163940515110887	12.0368809725703532	Si30
2.6648442824698346	1.6627973333207862	15.1815625858446133	Si31
-4.5350037448437002	11.0457278841305193	12.0653661385110471	Si32
11.6952496809358131	1.6508844358742603	15.1785139630161439	Si33
-0.0301609203936126	3.2519573651863145	12.0715920961539034	Si34
7.1867009691144137	9.4752414019002540	15.2027584478176614	Si35
5.7295007287200423	0.0743984662353935	5.0727284313543048	Si36
8.5609681835515232	0.1664026814192976	22.1243419831739345	Si37
-2.8736097875686770	5.1136361052198627	5.0760301049694396	Si38
-4.2913564208350001	7.5467277697121933	22.1690444079829021	Si39
4.2882639459499678	7.6459134651573244	5.0995280480485317	Si40
2.9800949031373301	5.1852672943097788	22.1406502108534227	Si41
8.8647528082037912	0.1526320988476119	5.1620396605705725	Si42
5.4193054040607098	0.1105519757105792	22.0954127319729245	Si43
-4.5007954584662926	7.8054782655302102	5.1630237203856417	Si44
-2.6981455780194255	4.8489859908445840	22.1118808155837527	Si45
2.7689866939499685	4.8893601297031415	5.1696557917753871	Si46
4.3814225237449724	7.9526105682177244	22.0564688851758035	Si47
-1.5453635694400942	12.4970023754891297	8.2956076303776349	Si48
8.5556925529726122	0.1258762284036757	18.9046384446454958	Si49
-2.7977642034756820	5.0938596247441419	8.2958555122918423	Si50
-4.3160915563308437	7.5243565246959809	18.9405049291675880	Si51
4.2548606984508046	7.7157548898497970	8.3187391526725829	Si52
2.9357932573161349	5.1869424475493009	18.9135009154000571	Si53
8.8026759656537585	0.1952342230894388	8.3897416468156472	Si54

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5.4158579548399723	0.0944583445232109	18.8729148755321745	Si55
9.9027009157582135	7.7192433448519022	8.3883757258298566	Si56
-2.7318533468519215	4.8265844645063902	18.8855602961342512	Si57
2.8442952859924153	4.9012128024586357	8.3942651343417527	Si58
4.4540413979184956	7.9184240942420434	18.8400891688766379	Si59
7.1873100500754123	4.2738772587758316	2.6289834118794837	Si60
-0.0370871251527047	8.4111921773518272	24.6089210944576102	Si61
-0.0116021103848798	8.4392775514237144	2.6518026676175177	Si62
7.1524513455855949	4.1986037324117476	24.6541423036485234	Si63
7.1973200607080550	4.2796486330023802	6.3652455301774316	Si64
-0.0204176594256600	8.4404160789952005	20.8511786048008467	Si65
-0.0274134902361549	8.4473300223235910	6.3978920152829257	Si66
7.1567267449929446	4.2436564715075509	20.8354674829642477	Si67
7.1935995383193045	4.2529181953732902	9.5935403325610604	Si68
-0.0322146076754706	8.4250500672063886	17.6182397755940059	Si69
-0.0483775095627283	8.4368964271211624	9.6284206215645316	Si70
7.1804676796056768	4.2469458637575110	17.6006790637224100	Si71
7.2035323237479769	6.6422481626969896	22.7979758786294937	All
7.7913588881248135	4.6818877067297802	0.4947570200933993	H1
-0.0261746947259676	9.1901109475585461	0.5252146455991171	H2
-0.0940169182674584	9.1269203087983755	26.7455834482006800	H3
6.7740227924933833	4.6433437882528779	26.8183145991671168	H4
6.3860944488341183	8.9579823295123795	22.5486058117023589	H5
4.7845092444280448	11.5055096698592099	21.5474139797378896	H6
5.5316806253384554	11.2111843786614234	19.1996721250646338	H7
7.9339047430119534	10.7725027892271275	18.6953102004064107	H8
-4.8620408411047382	10.5787642696207431	20.5661347478712813	H9
-5.6122922836805413	10.8364019059250651	22.9118803096039834	H10
7.0411736503750326	11.0561705896940232	24.5250582612672403	H11
13.0603308983958328	0.6692731868100686	25.1247081849396707	H12
12.5914746506671555	0.9197620162697352	23.4286551809834016	H13
-0.1301805859139609	1.0183132097196785	23.8964951678977719	H14
5.3440218681612226	10.9735835193770370	24.0233268747568189	H15
5.8341804585078023	11.2900369832206913	21.3335093258289099	C1
6.2566984439387703	11.1358639332223017	20.0123354720924418	C2
7.6027162599127074	10.8836856800977237	19.7299629612755965	C3
-5.9149474801030335	10.7737631696473191	20.7773404082311508	C4
8.0929178928232233	10.9186978932899645	22.1015463907565533	C5
6.7460863589337903	11.1898710253075002	22.4035867202685814	C6
6.3043537145310413	11.4768724418407704	23.8216341600390642	C7
13.3604173904117047	0.4831275363283249	24.0831492492070645	C8

Co-adsorption of ethene and benzene

7.0720937072256644	4.0788524992897459	1.0482117665103907	O1
0.0827870247431521	8.1340666178515892	1.0580669099106197	O2



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5.8820360814185388	3.3432709787792612	3.2428655849057884	O3
1.1731432246666227	9.2113900186072666	24.0569853285982802	O4
8.5616183276893967	3.2634000920122910	3.1336375901585813	O5
-1.4402726402774544	8.8085588708396010	24.2129480458608164	O6
7.3074349462394075	5.6080049186840908	3.2538490245667537	O7
0.2248435091450309	6.7100994432283905	24.0786726757674785	O8
1.2098507454110079	9.2046800356030527	3.2615577835366216	O9
5.9957131230768574	3.0382045188730578	24.1060896279578429	O10
-1.4235505469159002	8.8551109086174993	3.1689461511349091	O11
8.6268757701813588	3.3388345108703454	24.2153078085207483	O12
0.2033014942847422	6.7263884717064437	3.2465763545852275	O13
7.0186234848444453	5.5044104486322318	24.2572742175373861	O14
5.0023276844766649	1.1852097114024389	4.5303637860853074	O15
2.3589275237149749	11.2068313597777109	22.7474953386363623	O16
10.8445058573371576	3.6019684524383306	4.4723262455045161	O17
-3.6835427009696584	8.9475272897496598	22.7766488566630336	O18
5.8281179696209522	7.4440726888360924	4.5113497649490428	O19
1.4346748539295691	4.7666415627403156	22.7476879857912628	O20
2.4349863687443962	11.1191219681860627	4.6381133568449764	O21
4.8382877935280382	1.1006843629476082	22.7172217032223962	O22
-3.6891929613382084	8.9026867339484426	4.5725497346917976	O23
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10.1405121572237249	8.3892327979390267	8.1398843177451781	C2
10.7857059366416550	8.3379798129448872	9.3789178781457156	C3
10.0268346332116440	8.3913305804318075	10.5495231067824093	C4
8.6343832787724732	8.4904009838539967	10.4796496752156845	C5
7.9728071425766691	8.5340030242239884	9.2444918417731099	C6
6.4669338172402426	8.6363825208372873	9.1665215077844060	C7
5.9662974032089888	10.0231982978214091	8.7371178962777876	C8
8.2550375494972048	8.5149757546110081	7.1007072752753944	H1
10.7232989874297377	8.3449977081458986	7.2173554620836136	H2
11.8728720964927383	8.2509757021082759	9.4302157270112499	H3
10.5187920160624522	8.3489349451456203	11.5237453356515775	H4
8.0470442319274191	8.5236284188347859	11.4019904799247289	H5
6.0354314370992883	8.3785424683923946	10.1472194589766591	H6
4.8676157576991503	10.0419078337689918	8.6750212482610713	H7
6.3650826365025877	10.3010588214348289	7.7500065398984246	H8
6.2818985630565374	10.7973360183685241	9.4524046189745761	H9
6.0902658815649806	7.8825424856397586	8.4543909682447396	H10

**Table S14.** Cartesian coordinates of all the optimized intermediates for the alkylation of benzene with propylene.

H-MWW			
7.0511269792453612	4.2430713042060493	0.9107988091997012	O1
-0.0027996337905734	8.3426425484340481	0.9252122950255126	O2
5.7888269944769721	3.5776009877477821	3.0884051843247020	O3
1.2991199778209204	9.1868943119309137	24.0278942579153565	O4

8.4646824791010360	3.4439686457529373	3.0548313198835553	O5
-1.3482840956980606	9.2895692100277074	24.0480410264238849	O6
7.2577464218965551	5.8153550215405581	3.0869956075548957	O7
-0.0943833929769413	6.9103824998967838	24.0080999086065781	O8
1.1951135105584259	9.3664496222266180	3.1119529959325356	O9
5.9387892934369138	3.2004366241409272	24.0056691458721190	O10
-1.4473140520347831	9.0741422681952049	3.0742975355310551	O11
8.5685808243701853	3.6510988910626723	24.0659956927381273	O12
0.1348299629007714	6.9107885955026669	3.0965446804080865	O13
6.8348505790340273	5.6965556075253430	24.1876117440305620	O14
4.9518433211989930	1.3993879014452668	4.3707260591735633	O15
2.0398026889373453	11.3939295802954792	22.7206845364311505	O16
10.7776714524489989	3.7768814902915748	4.3351313438322601	O17
-3.6364848066561182	8.9502756311314293	22.7310256285147503	O18
5.7896108994655053	7.6296269120796367	4.3876639777474091	O19
1.4010407628921842	5.1538237790978769	22.6971959243988017	O20
2.3723871500796392	11.2958808712965677	4.5100927278024354	O21
4.5838794518099055	1.4122909061267281	22.5913593156697665	O22
-3.7262774458285270	9.0897785102433506	4.4544371965743492	O23
10.8530690885326351	3.6530866411738505	22.6979496188574323	O24
1.2244399561850781	4.9235394847462581	4.4966965118455251	O25
5.8488264480217076	7.9986913198091241	22.7362092872884602	O26
-1.2361346374276778	4.9077274937836890	22.6583013046153283	O27
8.4230858949799021	7.7753945902719508	4.4533638977395436	O28
-2.4608677591822872	11.2911773799535524	22.7019824119207208	O29
9.5630431327373326	1.4338863826731241	4.4189280487224414	O30
3.5745314676184039	9.2547292279997500	22.6668190208976732	O31
3.5143324019003903	3.6096381579454517	4.4727554568534140	O32
8.5923662344872085	7.5642871636349920	22.7969136120844773	O33
-1.4056736030334940	5.1189160548663635	4.3153589463837960	O34
9.3184801467181586	1.5104872536676943	22.6776857862904571	O35
-2.2529394133653664	11.2811590289891086	4.3285965400513486	O36
3.7106316852011476	3.9057847820257665	22.7312305450296748	O37
3.5060470385455584	8.9165344757427327	4.3700790921008652	O38
5.8456408956990904	3.4919461581195006	5.7599227874270138	O39
1.2986797530658452	9.2056962642667379	21.3411078786141921	O40
8.5219338562586380	3.5059661347363744	5.7282134399245610	O41
-1.3642874091636870	9.2599764476294038	21.3698732932529616	O42
7.1711256087837238	5.8150349463022062	5.7612424949871208	O43
-0.0696281848468345	6.9110565690846837	21.3352890385557181	O44
1.2659716881167160	9.2311850877355486	5.7847095367338062	O45
5.9106489821775083	3.2875441631129174	21.3088216453493260	O46
-1.4069023868244446	9.1868820402701221	5.7490105488571501	O47
8.5448218228771751	3.7279872342524460	21.3822104728365261	O48

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-0.0328151900038778	6.8936054746552671	5.7659636220027499	O49
6.8260106048718274	5.7907026298422073	21.2973224468939826	O50
7.2128367772246200	4.2521720178877169	7.8775710074469290	O51
-0.0671184299462055	8.4674242689395047	19.2124429732934026	O52
-0.0959404243819684	8.4367062639433321	7.8992185477363721	O53
7.1802178263826253	4.1958902268691878	19.1863661017711138	O54
5.5714264451625111	0.0624742030037174	6.5843012083759076	O55
8.6493008551163051	0.1681361747706613	20.4790174273661805	O56
-2.8234533875329948	4.9847437689681025	6.5610281869629956	O57
-4.4465832427367626	7.7153289825703357	20.5241454170514288	O58
4.3457930392024284	7.7752151443190138	6.6203538431027553	O59
2.8845885554832882	5.0838165223277958	20.4885616719551287	O60
8.9063699331713657	0.1870172590646109	6.6697076846379995	O61
5.3304457708123749	0.0291882804628962	20.4295225475323399	O62
-4.5316559510476537	7.8361077453670918	6.6601261361283424	O63
-2.7121873088858233	4.7785424509679766	20.4616901958239019	O64
2.7056107872137072	4.8123602969817805	6.6992399057020364	O65
4.4699542833745740	8.0635520460996997	20.4470121560431011	O66
7.2707108881750271	0.0953565510570665	4.5627722919343388	O67
6.9729612195875266	0.2385781135887961	22.5206496944778713	O68
-3.7186957451758804	6.4317456173969676	4.5416090675393130	O69
-3.4750028739110466	6.3114314787183572	22.5233973267510024	O70
3.5168136240761250	6.2632154415693151	4.6142193646505296	O71
3.6540810322088895	6.5611399881106252	22.5279696330947772	O72
7.1970450204242313	0.1010195509736544	8.6979266182428301	O73
7.0170569001645005	0.1447652889924168	18.3749581745869577	O74
-3.6330150392304348	6.3778638096983507	8.6861904331288180	O75
-3.5410551753128767	6.2952682049945379	18.4430164727616699	O76
3.5617373818154636	6.3160839620981752	8.7134091841684036	O77
3.6287038920256380	6.5642691625415370	18.4140861668178175	O78
4.7871744536014322	1.2598398410511162	8.7788388164366875	O79
2.1659952099609363	11.4180416434979879	18.3106802525546186	O80
10.9411490260350064	3.7017158008912565	8.7358113530407469	O81
-3.6682161692663238	8.9532133152116700	18.3582097022186908	O82
5.7779715510055425	7.8103645671969923	8.8116648440143646	O83
1.3868281144992225	5.1199767360123509	18.3469839509539447	O84
2.3618513346881302	11.3927460786027357	8.8702787338563809	O85
4.6779308899588745	1.4385535580967035	18.2863866621500257	O86
-3.8652002422412206	9.0402864083657537	8.9096481269174586	O87
10.9280246545624671	3.6228264595353417	18.2262320540255196	O88
1.3440678227125131	4.8354016928623063	8.9555416394549372	O89
5.9258525336159318	7.9495649564406872	18.2598467940945355	O90
-1.2415074953321827	4.9490506239528411	18.2834860908842245	O91
8.4047790962833808	7.5418431500123528	8.8130044607054057	O92

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-2.5021125429724478	11.3105781257020190	18.1888630255863859	O93
9.4493225062289259	1.5235639282111653	8.8718935110233623	O94
3.6221639578353839	9.2299528599266143	18.2611870855231793	O95
3.7018610394698075	3.6625705602787604	8.8527673101890230	O96
8.5299814100982871	7.5195240747234617	18.3652797623902302	O97
-1.2669471531110603	5.1482652868195782	8.6602600166731847	O98
9.2724151891311948	1.5704120993500492	18.3592851907329759	O99
-2.2383873042025080	11.1163593070362534	8.6783299115070243	O100
3.7523521083252813	3.9066034857948604	18.3222968637431336	O101
3.3950153750285921	8.9695976085690390	8.7483445130073285	O102
6.0559698352450315	3.2313999239236941	10.0360295315322272	O103
1.2556195061188777	9.2516247104291871	17.0450379709011095	O104
8.6390367282575937	3.7646631443189364	10.0642562582373039	O105
-1.3757752353814996	9.2034143195484788	17.0167826105163371	O106
6.8849468435510648	5.7360518514294041	10.0546662535272358	O107
-0.0173848388159934	6.9506260315594890	17.0233696967144645	O108
1.1139485172781489	9.3777289294135144	10.0700655290805035	O109
5.9755541513246984	3.3605434003797439	16.9695128565202715	O110
-1.4932077334696476	8.9916303514984168	10.0986191422472391	O111
8.5883816119936540	3.7423945567499914	16.9745618703062391	O112
0.1436830322121438	6.9245683359326069	10.0691046784719020	O113
6.9484053706399482	5.8111601132816100	17.0672242145792588	O114
3.9163851185047656	2.2071511269434358	11.0886688699864511	O115
3.2126754119476386	10.6220638688462543	16.0204236067495600	O116
10.6683349682473114	2.4698384416065688	11.0557408440395282	O117
-3.5648812177178768	10.1813994557443106	16.0191816287458835	O118
7.1039586959485721	8.1123960883082376	11.0823087498259696	O119
0.1959225381005023	4.5388080191340023	16.0643965886519595	O120
3.3509437736975185	10.2512355972883569	11.0716574605486535	O121
3.6585714230566380	2.5323393565865833	16.0711237625343557	O122
-3.3542579050065462	10.5866525617944696	11.0220067484853050	O123
10.4472844215626601	2.1281120931330353	16.0616005164628390	O124
-0.2867131577032405	4.5438744880176740	11.0465076012345236	O125
7.4165548432180319	8.1919203823766491	16.0614425308517177	O126
2.3519958509628149	0.1488920403816746	11.7535816629850220	O127
12.0502044372248278	0.1198354583473828	15.3311904928886999	O128
-1.2192258213883349	2.1774563219934535	11.8088721410699016	O129
-6.0925218315359446	10.5801348546124654	15.2953503990077451	O130
5.9228249531465762	10.4238251704169631	11.6912544073206117	O131
1.1293768437261360	2.1583402838261607	15.3193872195633567	O132
11.6453762287868265	0.0934059421398786	11.6274092198988210	O133
2.7808946635242577	0.1154540108336954	15.4874241738001981	O134
-5.8959403302427429	10.2386141220874709	11.6529306043714094	O135
-1.4620734317438653	2.5814856214915012	15.4642561725836565	O136

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1.3751229815934114	2.5852452201194565	11.6406352668404232	O137
5.7541311820384093	10.1574167139015650	15.5000765141982662	O138
3.1256448509483530	1.9489310955541559	13.5673794790203761	O139
4.0388130068260599	10.7865242064931053	13.5484671140372850	O140
11.2135106500830801	1.9139061300140687	13.5541786116054368	O141
-4.0923935929206046	10.8186607942978359	13.5347254753791262	O142
7.1506246446021020	8.9548617359662686	13.5574095066393827	O143
-0.0319221818675888	3.8013893253189490	13.5594286819875389	O144
-0.0444121069718895	8.3254485417636808	26.1963011634219036	O145
7.1947199292710771	3.9619085201942603	26.2535836691478330	O146
5.0278440639190833	3.0205980421205090	4.4152652742753995	Si1
2.0177576248655438	9.7788889764170168	22.6978703359576564	Si2
9.3292043162026683	3.0424773537086574	4.3765158652364615	Si3
-2.2037519184185479	9.6891873679023313	22.7166932914151225	Si4
7.1577444739926213	6.7552949338906156	4.4144394910349938	Si5
-0.0065248060929655	5.9692756884182883	22.6814945744713974	Si6
2.0838961553226349	9.6970437902753375	4.4379813110004251	Si7
5.0485074775570107	2.9758605451888096	22.6688243329608952	Si8
-2.2041228963712847	9.6587177991671282	4.3944018662958388	Si9
9.3050961307821325	3.1404469276016842	22.7125762053289542	Si10
-0.0216655039716560	5.9637720141231227	4.4119761408519294	Si11
4.6041178719068032	2.5987357121319539	9.6783950162217902	Si12
2.5653075571518258	10.1295066822684454	17.4171631717728062	Si13
9.9243467200923661	2.8509541255749911	9.6718025235940761	Si14
-2.7787174525948570	9.9177573663225083	17.4094700458532365	Si15
7.0538235250572034	7.3080861112170785	9.6802571032602245	Si16
0.0693025643963670	5.3840094953182680	17.4376204017001548	Si17
2.5619748417102395	10.0006201137276776	9.6805848908417467	Si18
4.5171136061421029	2.7996661602067774	17.4174104895054960	Si19
-2.7450445591840298	9.9365971076196367	9.6702926320944247	Si20
9.8162352561524084	2.7687220760028373	17.4110164996998478	Si21
-0.0149953392119628	5.3576329486337722	9.6722135954722361	Si22
7.2098712287177662	7.3687459416405749	17.4440952205068882	Si23
2.6904604656999709	1.7163703283344909	12.0159626110130180	Si24
4.4640169311471922	11.0531987899053039	15.0957206909167940	Si25
11.6864560396917163	1.6657230277954282	12.0149419462781744	Si26
-4.5498378622796025	11.0491269534511893	15.0807430307157144	Si27
7.1743631974188133	9.4369767244272893	12.0019349847405543	Si28
-0.0397740158429454	3.2672753744324639	15.0986506619841983	Si29
4.4400633032306756	11.0139510011387944	11.9886555314131549	Si30
2.6726854193614971	1.6887484898778913	15.1093581218471957	Si31
-4.5512791075293517	11.0724707158031368	11.9931638594060477	Si32
11.6698895963157465	1.6859326809799886	15.1015119706997005	Si33
-0.0409882049773669	3.2760488239348229	12.0173707100232097	Si34

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7.1689341443256778	9.4701001715012918	15.1018587306647056	Si35
5.6924719181102370	0.0845759384037610	4.9739857669609586	Si36
8.5415250872517561	0.2187326588399282	22.0887382531594803	Si37
-2.9017488932038162	5.0802698591475393	4.9505034193799196	Si38
-4.3803052816414390	7.6216774812734842	22.1450985492295693	Si39
4.2875083073380535	7.6430155541481337	5.0105419477673498	Si40
2.9085826670793913	5.1546588427598357	22.0978766440865435	Si41
8.8269270450968964	0.1281020340016939	5.0545967158888008	Si42
5.4144960067381973	0.1227042133168886	22.0436374577337837	Si43
-4.4929058024928725	7.7789072847410150	5.0430223510550762	Si44
-2.7657183913691714	4.9180166776201846	22.0760645908460518	Si45
2.7431846550499697	4.9064749024387426	5.0835067326487131	Si46
4.2939719686884672	7.9508109612883837	22.0319300505114093	Si47
5.6435747200134596	0.0131084580532875	8.1970920255152038	Si48
8.5724018908924222	0.2047984531701634	18.8667636380932393	Si49
-2.8108507343657148	5.0603800634029508	8.1743740202037927	Si50
-4.3838503014723207	7.6123170482260578	18.9197422022749606	Si51
4.2677773637804712	7.7080492832378580	8.2330726597945105	Si52
2.9129563184387668	5.1681501943216643	18.8743690389345637	Si53
8.7764263572871517	0.1737079730648523	8.2827893959716334	Si54
5.4441498057669078	0.1116051934312817	18.8190432202630298	Si55
-4.5094085523253851	7.6947934615284330	8.2725432343837948	Si56
-2.7605927394271523	4.9202587052712721	18.8530605426608240	Si57
2.8293187527642627	4.9135221043612836	8.3095898693245065	Si58
4.4099708977981775	7.9342837805565543	18.8199941477414185	Si59
7.1524394638414321	4.2767563551609058	2.5325560198587502	Si60
-0.0577373193770674	8.4365726416464568	24.5755996846563143	Si61
-0.0314398275222052	8.4366596768573388	2.5473830566264763	Si62
7.1172724772497418	4.1691422115037309	24.6353738454019755	Si63
7.1865733925838367	4.2664238574480846	6.2736464417469104	Si64
-0.0615085079390667	8.4575173163209652	20.8180587315381196	Si65
-0.0657440405743159	8.4368136648777909	6.2938669703175671	Si66
7.1120936943863358	4.2847713304831156	20.8004175360737058	Si67
7.1980295086161856	4.2463742168384648	9.5036970171839812	Si68
-0.0530706395277001	8.4679836964377220	17.5833866011202993	Si69
-0.0830177602193274	8.4330156142629757	9.5267249760980661	Si70
7.1743636164217861	4.2823228005531213	17.5658090922376822	Si71
7.1555520442581715	6.6304822510787353	22.7790802487139636	All
7.7673800994764708	4.6412251060284850	0.3932070242299976	H1
-0.0509189252525211	9.1626249967659543	0.4107643859890184	H2
-0.2568451305991610	9.1152034803045119	26.7163126711693053	H3
6.4747416919820875	4.3336201597025799	26.7853942756796854	H4
6.1679946472153180	8.8807657830825200	23.0035374858163841	H5

Adsorbed propylene

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1.3427362636604894	9.0757417911706089	24.0051661248879640	O4
8.4813917231466753	3.4372031973529831	3.0820091220371943	O5
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0.1575289962949924	6.8764163889424621	3.1117630153859444	O13
6.9050120920438562	5.648882589611134	24.1728103063390520	O14
4.9581727388552901	1.3605697016592608	4.3785332278320439	O15
2.0351880536670990	11.3088593162082205	22.7176822679076018	O16
10.7843908793489405	3.7736044731987928	4.3842143733258787	O17
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1.4214830564392051	5.1301619912363350	22.7027128561637852	O20
2.3868239505130875	11.2843288019162920	4.5030206085242215	O21
4.5978126808067419	1.3680395134574581	22.5991066844042479	O22
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1.2210473682034850	4.8759821817475535	4.5091893852168319	O25
5.8961209474993082	7.9480852408121319	22.7261961101833663	O26
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3.6155853966273686	9.2038925683879480	22.6469791507115339	O31
3.5192075148230786	3.5734377563812978	4.4671856228243403	O32
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3.4819277698053970	8.8812005529156828	4.3799148321105710	O38
5.8425102161361853	3.4569245401941457	5.7659920818192854	O39
1.3378552687799097	9.1152315004268125	21.3196496172210104	O40
8.5182449082639220	3.4875461149996503	5.7548561684518234	O41
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3.5392467697364025	6.2876427701728810	8.7142792274201479	O77
3.6696880530637084	6.5234328877589389	18.4007365582306051	O78
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2.5922567586268643	10.0396395586358977	17.3953686620372103	Si13
9.9073782265966894	2.8464734740165381	9.6962023063248992	Si14
-2.7425309686964141	9.8772635984564801	17.3982889336741486	Si15
7.0134118047518346	7.2930214623035949	9.7006136866631394	Si16
0.0662029483302837	5.3292357712842424	17.4207047812276414	Si17
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4.5055058076479906	2.7720560137023900	17.3993818129069062	Si19
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0.0041978167410006	5.3541062515842803	9.6998095202830186	Si22
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4.4890098394197455	10.9882758306291066	15.0923980684855330	Si25
11.6639694010862307	1.6264342615802643	12.0127138796855739	Si26
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7.2016897227541996	9.4353237539065589	15.1175710474492604	Si35
5.7062091832633488	0.0529586633178698	4.9908545496633279	Si36
8.5449141630066592	0.1277878913752845	22.0640976923041165	Si37
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4.2727639647487576	7.6102603181614850	5.0147436016602818	Si40
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9.9198844736153795	7.7728021338416680	5.0844837722495440	Si44
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2.7439782966961004	4.8640546984230717	5.0870558924552194	Si46
4.3601785526246450	7.8998165770173063	22.0302685805070482	Si47
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5.4332394135098765	0.0753171146422910	18.8005837802502036	Si55
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7.1637596179226346	4.2544600953085743	2.5483198230903894	Si60
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-0.0394383882898515	8.4022952152705894	2.5712002082773111	Si62
7.1488036013108989	4.1156640123374597	24.6144253029807807	Si63
7.1740512757204851	4.2419283341402698	6.2859246678521972	Si64
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-0.0480909128959137	8.4208437940216978	6.3195164055317141	Si66
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7.1752491059126022	4.2302201454544139	9.5148181671814331	Si68
-0.0320220418225592	8.4023146982724004	17.5610187061701311	Si69
-0.0551723062215377	8.4150970532504026	9.5521940601322779	Si70
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5.8225114721443196	11.3537212873224220	22.8093053035081041	H6
5.9916690165874389	10.2134178253688859	24.9510694288505377	H7
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-6.3236430653840117	12.0933233161328726	21.9417971712591893	H9
7.6300796303290239	10.6002919606610106	21.1354905659471264	H10
-5.6167357001610148	10.5401904272956894	22.4733926088597116	H11
7.8989612284415598	11.0255214734967257	22.1171251527822683	C1
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TS1

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5.7720073140541794	7.5876183362194771	4.3913885268354322	O19
1.4552612181078657	5.1472819205594211	22.7308915759145869	O20
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1.2338200320008705	4.8407457388628359	4.4927021175443000	O25
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9.5728633976012283	1.4018429877385314	4.4463474265584155	O30
3.4969997657149454	9.1462900593178169	22.6075312367694927	O31
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7.1501331200963021	5.7615848721423690	5.7518412324394239	O43
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5.9403950901790656	3.1866128843275874	21.2914558277804886	O46
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4.3192228377249693	7.7246606881370292	6.6203304338974567	O59
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7.2871544774351795	0.0535972797700642	4.6032317692198825	O67
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10.7022164559037130	6.3855260278813777	4.5916234953520911	O69
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3.7541958847261805	6.4832409982250878	22.5157439003035691	O72
7.2182720601260186	0.0544694311045460	8.7069208345478586	O73
6.9751718829337692	0.0502229999302875	18.3131592277458282	O74
-3.6870509215321454	6.3434648414663499	8.7069678491599110	O75
-3.4823832645268129	6.1574464543719838	18.3947257275710143	O76
3.5332106700305368	6.2545269641525314	8.7023038954428049	O77
3.7009830232670309	6.5123870627831533	18.4098451917903567	O78
4.8007046106286708	1.1946619041587445	8.8045680149805179	O79
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5.9946237018073569	7.9004524531967686	18.2611319659975422	O90
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3.6895187215321030	9.1839171173238476	18.2586588483482508	O95
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8.5962062052467729	7.3940070114234198	18.2693140976729005	O97
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-1.5006416240972853	8.8709124927932894	10.0937177760411476	O111
8.5723533254624638	3.6892699825034345	16.9864691133746071	O112
0.2463742694172453	6.8862240183175940	10.1002738843556763	O113
6.9265100597046905	5.7524325461839760	17.0075208070099535	O114
3.9199793712941009	2.1603211315316577	11.1020173674315981	O115
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3.3895511456810334	10.1547267786957072	11.0737148282189306	O121
3.6189625036741759	2.5087084695072304	16.0609573971474795	O122
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10.4043370335870975	2.0995981525182876	15.9961684230498768	O124
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13.2011179716302038	2.1188776341163962	11.7007479438386461	O129
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1.1076583057608687	2.0325419959777609	15.2911176240072919	O132
11.5917992472256319	0.0455819860105033	11.5940121901730091	O133
2.8245861798773002	0.0497863858406184	15.5266995620329329	O134
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12.9648624290454730	2.5008554070676889	15.5263276067762597	O136
1.3708787075377167	2.5015733817253478	11.6482970371531813	O137
5.7434293022641629	10.1044800331034299	15.5185277102967820	O138
3.1245538215104882	1.8413209216650912	13.5656906941818534	O139
4.0569939573859370	10.7429480798167809	13.5418825187824261	O140
11.2862765475985842	1.8533059441734916	13.5431735568673837	O141
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7.1522268088611911	8.9578279771936362	13.5529190033925655	O143
-0.0944064589863447	3.6693423934729390	13.5543152963077400	O144
-0.0501708561667549	8.3405847396441803	26.1425261916139071	O145
7.1893046636356797	3.9144128712305033	26.2289665115276414	O146
5.0463064746565642	2.9412692442698352	4.4188327411923130	Si1
1.9689245037840726	9.7243005161908851	22.5938785827703867	Si2
9.3527804866598334	3.0130280790045725	4.4194331808217946	Si3
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5.0551906502506920	2.8994497391076184	22.6432782733728573	Si8
-2.2036298265795122	9.5741874607992088	4.4282468164909599	Si9
9.2892049208842860	3.1169603842233609	22.6683474198244106	Si10
0.0144475893681331	5.9148301065285516	4.4259960979246458	Si11
4.6068714647077469	2.5427296194450477	9.6892512313280577	Si12
2.5748338747621791	10.0104019110557214	17.4117628493495253	Si13
9.9143762874087571	2.8322665935400995	9.6866061282143221	Si14
-2.7589650991280936	9.8438344451008177	17.3744859483602205	Si15
7.0077897641763363	7.2787551249432001	9.6970202476679717	Si16
0.0715079813928430	5.3036309519031315	17.3941784689696561	Si17
2.5594046625382463	9.9625085242487899	9.6962484548419674	Si18
4.4893976548576084	2.7508222071944504	17.4074457662661253	Si19
-2.7294279959766405	9.8581584858883957	9.6917602087735339	Si20
9.7914303899208708	2.6879992682918807	17.3774465378959668	Si21
0.0123494460197260	5.3272652828218723	9.6997246541114901	Si22
7.2380740248842352	7.2981725828505404	17.3984034945007124	Si23
2.6930489852224095	1.6384921666510748	12.0100207856780958	Si24
4.4452756305006309	10.9845543969316299	15.1020741127127494	Si25
11.6814781095721631	1.6152268181695619	11.9851065969432664	Si26
-4.5540212850471367	10.9941460433287865	15.0919736802841644	Si27
7.1730810868351433	9.4160552794535430	11.9934765804855683	Si28
-0.0495595276753733	3.1602673457359236	15.0997937275064533	Si29
4.4480251245671649	10.9738366168633519	11.9804145604335908	Si30
2.6686438362078322	1.6106215114800315	15.1105403252814483	Si31
-4.5411362666817183	11.0038878036773422	11.9821096547252228	Si32
11.6658039909116091	1.6228190960736812	15.1064656946701401	Si33
-0.0497796731938038	3.1949094900782478	11.9981483432329075	Si34
7.1656618030359676	9.4422031744353170	15.1044498725318004	Si35
5.7072015020072513	0.0130336338843939	5.0040909987920710	Si36
8.5223405254346680	0.1635933256685278	22.0293152669056340	Si37
-2.8837879766943799	5.0535465659708079	4.9996631411522765	Si38
-4.3370461773770499	7.4798357811450851	22.0695139830786395	Si39
4.2677637907029347	7.5875665971167461	5.0107806660660188	Si40
2.9449492347874369	5.1169533515672114	22.0851485711090447	Si41
8.8487226642994745	0.0867905279852478	5.0769452204481276	Si42
5.4005214465380149	0.0436656216185245	22.0079162280889555	Si43
9.9144907434305409	7.7336551292111428	5.0677683450848940	Si44
-2.6990112336197516	4.8174378532205644	22.0395417680801202	Si45
2.7551311421555846	4.8296400815724629	5.0768952731698542	Si46
4.3575670919353602	7.8994845010672101	22.0334188185903344	Si47
-1.5557365220378765	12.4480652174335447	8.2255177937108339	Si48

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8.5305052393519034	0.1050638819607582	18.8066766118607589	Si49
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4.2278736966110717	7.6558274690743779	8.2322403130063488	Si52
2.9259060674972579	5.1456770488043784	18.8615212039011269	Si53
8.7986545113120211	0.1403875732926302	8.3029954689211607	Si54
5.4082953590121159	0.0401370213369184	18.7801316703274601	Si55
9.8831699018071468	7.6681135501859554	8.2952783717222349	Si56
-2.7228690680157306	4.7759285326449055	18.8195248904405652	Si57
2.8198636110712210	4.8411984630187188	8.3018761296373142	Si58
4.4765341757449439	7.8846759724328210	18.8225204083031947	Si59
7.1725238694361675	4.2172059303109739	2.5456578277020396	Si60
-0.1192186614238944	8.3839530897103547	24.5189873271651351	Si61
-0.0323684860247431	8.3802001827573669	2.5651650564532571	Si62
7.0997863269044927	4.1265816132992761	24.6104049557521307	Si63
7.1807296621769687	4.2205652368743074	6.2827733701974484	Si64
-0.0970491357476844	8.3790422306967614	20.7725765522170747	Si65
-0.0410636375712690	8.3829115666877634	6.3147020555204314	Si66
7.0807941914099688	4.2586100800114126	20.7877263627072786	Si67
7.1804752123853053	4.2197903460645936	9.5112220477219473	Si68
-0.0707058017817124	8.3623117770752113	17.5451806233474770	Si69
-0.0549536324016238	8.3800746197926763	9.5473634067876656	Si70
7.1507969683545891	4.2368259118595333	17.5496635343500174	Si71
7.0978557675235407	6.5947569288199510	22.7682653682263592	All
7.7785578672168363	4.6086354451769322	0.4086404389416715	H1
-0.0522533948695312	9.1149317208388823	0.4319597037608456	H2
-0.2112531448285946	9.1644251773643273	26.6272633015825839	H3
6.5336888723892939	4.3815052139735204	26.7684880586017151	H4
6.5189732920548273	8.6766722524196975	25.2969328999283469	H5
5.3579404165917390	9.9307326010440882	23.4903473222386623	H6
7.2440625728986188	10.2732586917669177	24.9995712030088555	H7
8.0716617114420544	8.8153197741174765	24.4089312627903468	H8
7.2815422224583779	11.1749480751180510	22.4996403039102724	H9
6.4097416327906913	10.2377768407814624	21.2657662163854013	H10
7.9771548098389582	9.6504360083232807	21.9017089744683595	H11
7.0400189747355961	10.1560238245366570	22.1626533174769236	C1
6.3147037083887039	9.4393356509334208	23.2804319647142712	C2
7.0877337644589247	9.2723694153579572	24.5698224813383383	C3
Co-adsorption of isopropoxy and benzene			
6.9935099488725996	4.1390718054782925	1.0645861952708979	O1
-0.0776203555823747	8.2410398003532066	1.0868608958585908	O2
5.7618551163842184	3.3975026580445302	3.2323707283205243	O3
1.1787750101275920	9.0831891971985534	24.0744707180858661	O4
8.4437370067398323	3.3794178168037790	3.1984193331504458	O5

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-1.4617061555511124	9.1838911706823474	24.0969200080481478	O6
7.1387789444261820	5.6969374475598800	3.2561819599881230	O7
-0.2298146282709070	6.7982558191574158	24.0608813905283903	O8
1.0857814000985933	9.2997904213210330	3.2737371837890317	O9
5.8773636331986481	3.1010913084364971	24.1195533249271428	O10
-1.5448097876387950	8.9180116756702716	3.2409916681744493	O11
8.4792381735717886	3.6240894262069081	24.0601954084253897	O12
0.1047594134760357	6.8089967364044055	3.2561769302220194	O13
6.6605824725368450	5.6447505961782483	24.1519828426442942	O14
4.8556510716777437	1.2651811479722848	4.5502838298392660	O15
1.9948170304388393	11.2850121369527727	22.7856640850479408	O16
10.7351386286335533	3.6874629045438749	4.5301565048490211	O17
-3.7181965665821952	8.8048186437754552	22.7361211218060077	O18
5.6957094548469209	7.5445085565753605	4.5315699666149376	O19
1.4267048075596724	5.1641413085540098	22.8077114445864240	O20
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11.6490761033651893	1.6077721358588966	12.0569606978484636	Si26
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5.3890757928819877	0.0877261610608314	22.0782252125272862	Si43
9.9251171037767723	7.7723592354370137	5.1379553392063606	Si44
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4.3760353094655446	7.8927686631495426	22.0858749543638382	Si47
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7.0944401805376298	4.2292643571805275	20.8549008867337520	Si67
7.1709254830280944	4.2422917002462137	9.5654588984377238	Si68
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7.7837982139975903	4.6329894766156903	0.4597603682930099	H1
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6.6125448285851487	4.3902584829511024	26.8370884073592251	H4
6.1113747181640719	8.7890149247183569	23.3502847373099343	H5
5.0816081423986637	12.3909854528958121	22.4453098962106345	H6
4.6029755594616244	11.1800994879683877	24.5338413951869789	H7
6.3777318906612148	9.8078857158111195	25.6406840080595799	H8
8.6543837957330609	9.6776359124553331	24.5984657660059298	H9
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7.8672480711334112	10.2719817583993596	24.1321016842366163	C4
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7.1452563970034220	11.7309405930188095	22.3140428082662723	C6
-6.9755179260301610	12.3973641230640030	20.9853216573951755	C7
-0.4220588722513750	1.2689627767362055	20.8087570305625391	C8
7.0931023755523412	11.4436618832762260	19.8304909981926194	C9
Co-adsorption of propylene and benzene			
6.9346868072173784	4.0226608689835741	1.1281990350817916	O1
-0.1554177584768199	8.1433911806327810	1.1468423204651099	O2
5.6795204802862873	3.3469321778992445	3.3052385828196833	O3
1.2030384388247244	8.8701838327746891	24.2018510989449958	O4
8.3578050564675141	3.2566413897591953	3.2792751336304877	O5
-1.4333804743896104	9.1188664934939485	24.1955766797360852	O6
7.1179843650613908	5.6094047964852107	3.2948839003574335	O7
-0.3195565947157397	6.6720705870616577	24.2001651196054439	O8
1.0463432998941196	9.1692237041498394	3.3298234058159535	O9
5.7654492712769247	3.0238079072705770	24.2128912971501791	O10
-1.5909013001074475	8.8271363504350440	3.3190212692758068	O11
8.4090564856017327	3.3127467414886738	24.2202899238309861	O12
0.0257119463227160	6.6940726361708034	3.3053057334133955	O13
6.7940088707038591	5.4741010338017917	24.3624946860198115	O14
4.8272237868025494	1.1762649179198419	4.5991621277145427	O15
1.8524278960039187	11.1193507605355641	22.9225123034090430	O16
10.6580596141142507	3.5855108640317228	4.5882010926643515	O17
-3.7119320722487252	8.6954316586440310	22.8852112363204334	O18
5.6442092113876763	7.4187564152561052	4.5873123069024260	O19
1.2761613692878466	4.9965441334468039	22.8960746422971475	O20
2.2545376753345696	11.1010491627174499	4.6980234721231904	O21
4.4328604162190048	1.2071906993206289	22.8131735556723996	O22
-3.8670910452016916	8.8943753581419376	4.6999895859896901	O23
10.7182410761039080	3.3824993240707468	22.8772646917045392	O24
1.0907498689892163	4.6898895809203092	4.6966909670802730	O25
5.7779832398229063	7.7916943250294723	22.9132371453527526	O26
-1.3462723400496932	4.6202708145510165	22.8226570345595512	O27
8.2793968908070994	7.5727270291938815	4.6688318068079520	O28
-2.6253904355733999	11.0780924123734827	22.8530802179661023	O29
9.4453523772921955	1.2403088795531172	4.6389760158577920	O30
3.4779187293011224	9.0416459208928721	22.8503754606639973	O31
3.3906358005013777	3.3887081283030600	4.6684784322469834	O32
8.5147715457925166	7.3144558005257112	22.9168939226770512	O33
-1.5380665763937298	4.9492188001065154	4.5642070905815677	O34
9.2079504020862544	1.2287445767767931	22.7653408633161618	O35
-2.3469493150007068	11.0527185826533731	4.5654932814844642	O36
3.5550804175603434	3.7005162144990349	22.8875102130380661	O37



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3.3539925381821591	8.6985210939705855	4.5824362746261702	O38
5.7120125018986601	3.2811334795778899	5.9744522261356421	O39
1.2080554249459023	8.9136711123642591	21.5171768526660117	O40
8.3883487202831724	3.3028566768644794	5.9533803820563138	O41
-1.4482967010101584	9.1005195261575569	21.5169864667180413	O42
7.0300615237818880	5.6089106957243278	5.9676019811339929	O43
-0.2728543753321446	6.6891345858404891	21.5270344482655673	O44
1.1230926148917293	9.0790267930159896	6.0038676452563804	O45
5.7756050017226581	3.0550168224777607	21.5126124879193412	O46
-1.5470013522765065	8.9371083479833082	5.9946271391971120	O47
8.4168401112424043	3.4761394842008952	21.5423532439064864	O48
-0.0882493741482979	6.6960354359146166	5.9779705459312984	O49
6.7092234040102117	5.5542377705905217	21.4799423606588569	O50
7.0637675207146993	4.0597572815515042	8.0904797586802140	O51
-0.1693997844157833	8.2151270059983279	19.3818136835569490	O52
-0.1770505414689252	8.2167780562047792	8.1263397811389133	O53
7.0181494914701990	3.9502994510137204	19.3752836703555573	O54
-1.7874433361853281	12.3395443097450155	6.8206005540967558	O55
1.2564124779251173	12.2955884822860391	20.6385568268833559	O56
11.4913822076027703	4.7875767783342340	6.8143630525251568	O57
9.9903834961039131	7.4159658556504855	20.6865979419727104	O58
4.2103316635143901	7.5426648140001964	6.8223496945370385	O59
2.7102129965680453	4.9132270972871064	20.6679965124336178	O60
1.6109547645295619	12.4630663194759670	6.8863707831742680	O61
-2.0801765745697969	12.3847853679323929	20.6122538379117834	O62
9.7258931903250154	7.6634635061623246	6.8979677974933553	O63
11.5565220804604500	4.5442844979798869	20.6493540102507076	O64
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10.5711126969681821	6.2370352393668842	4.8053634343713503	O69
10.8720184486282427	6.0459540658537172	22.7530846720484163	O70
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3.5689806515870433	6.3561417931330064	22.7044654382849131	O72
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-0.4035252991857776	12.4243053133243659	18.5511530780063438	O74
10.6243704407137454	6.1871033648954965	8.9128655846701488	O75
10.7523498302010569	5.9895219345623749	18.5696664754685230	O76
3.4120453442838827	6.0939439112771261	8.9147797929202337	O77
3.5368567730918063	6.3752181352183426	18.6057367036925072	O78
4.6712906604699658	1.0274866128339812	9.0302043852560399	O79
1.9043600292932137	11.1063510118009159	18.4233118137032044	O80
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1.2375066652201321	5.0342356571020863	18.5140513414856045	O84
2.2681316190774279	11.2218422348387303	9.1206792948146695	O85
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10.7675532894842281	3.3230894829899822	18.4417960701147479	O88
1.2035047137193366	4.5951880341129643	9.1503045719439253	O89
5.8446651160580201	7.7297009838697637	18.4555848419378066	O90
-1.3797670593282265	4.6334958528550745	18.4848256618384212	O91
8.2413342273961590	7.3790571752621252	9.0521522046070153	O92
-2.7269440513154235	11.1122311930731410	18.4109250873633137	O93
9.3199671806746149	1.3579972377841860	9.0569095056100828	O94
3.5573731532364175	9.0475164569025477	18.4424627570031490	O95
3.5743353199259196	3.4361914424279343	9.0391344534579243	O96
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9.1133933663970748	1.2667726560376631	18.5694585714090579	O99
-2.3173756500949518	10.8850815963271064	8.9306532513898613	O100
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5.9169762940765755	3.0321254369844288	10.2530312832728949	O103
1.2131882531312224	8.8361524895119476	17.2000277076690509	O104
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6.7251961514470047	5.5440519225409091	10.2618952047399095	O107
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6.8971995946272235	5.5901506922918625	17.2666165272589858	O114
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3.4799329024880681	2.3686053443276176	16.2381341077144050	O122
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13.0400529764719195	1.9718386222657200	11.9825372000565675	O129
8.2126094645345056	10.3875103362520260	15.5406795430224438	O130
5.8624052350352560	10.2918366317774410	11.8847644461948061	O131
0.9613688938223623	1.9021335264358175	15.5034514273219379	O132
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1.2053670504077088	2.3300829522260904	11.8525134813121742	O137
5.6285012745186442	9.9245835206737461	15.7418556820614146	O138
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-0.2020387699451138	8.1118555212918491	26.3699841545794342	O145
7.0871449312458692	3.7483084255384429	26.4300041608049980	O146
4.9047800063700464	2.7985611730832365	4.6280895590309363	Si1
1.9064616767984450	9.5022378933542679	22.8797297320777595	Si2
9.2100151623049467	2.8492153466372372	4.6068731248004431	Si3
-2.3055952469090459	9.4861633028513204	22.8664699196860575	Si4
7.0156550657670991	6.5493734857869716	4.6220339978897922	Si5
-0.1676840280459011	5.7447157250422416	22.8687769247325470	Si6
1.9459611937749486	9.5045547371106487	4.6474579041595945	Si7
4.8961856884084698	2.7734795797726290	22.8685735119734908	Si8
-2.3326577990054020	9.4302858426135305	4.6393278755573268	Si9
9.1694242878915801	2.8593251517917939	22.8615884170902000	Si10
-0.1326293392975519	5.7591781298974389	4.6297598090560150	Si11
4.4699659396075644	2.3877453158389601	9.8934814748365270	Si12
2.4347997695896995	9.8382811561261789	17.5702030933249382	Si13
9.7824314935267758	2.6668855360534645	9.8950113122592622	Si14
-2.8774085371390425	9.7158120678207531	17.5999111416953724	Si15
6.8849137084797141	7.1201959580344134	9.9041405266364588	Si16
-0.1135975753762297	5.1596910281361126	17.6243767406364924	Si17
2.4429319019565137	9.8000521816108783	9.8854877496016087	Si18
4.3345248092593787	2.6245479589843201	17.5918491046301142	Si19
-2.8450889285347332	9.7020063319506527	9.9081283165334550	Si20
9.6575752947656852	2.4698771981813734	17.6268563190663450	Si21
-0.1214614446334195	5.1628611754636387	9.8997841344776187	Si22
7.1310966904728135	7.1507551554575333	17.6425640689973235	Si23

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11.5208934760639288	1.4495138598830042	12.2248304805394028	Si26
-4.6777374874610613	10.8529152281222814	15.3126920167995308	Si27
7.0650230193381951	9.2466126382572931	12.2078320836761982	Si28
-0.2007928414363054	3.0256671332846001	15.3066255905364468	Si29
4.3451479283894408	10.7956976859603753	12.1766898461030237	Si30
2.5163193850029417	1.4633764387794637	15.3105816007564517	Si31
-4.6555581783490334	10.8517124357117840	12.1920833617854463	Si32
11.5234572564685323	1.4375027614655504	15.3122106472921757	Si33
-0.1996893288764203	3.0477562356018795	12.2201615625488298	Si34
7.0539815024207266	9.2656733805147322	15.3241897589295171	Si35
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1.1636914447370232	12.4347790639265785	22.2455621063678386	Si37
11.4035884491780006	4.8933868033859360	5.2048826854371004	Si38
9.9894710614430977	7.3511069747348969	22.3115483479429031	Si39
4.1424966124612173	7.4237293506840860	5.2119692282332402	Si40
2.7785049651504958	4.9782468129594326	22.2791702726200178	Si41
1.5027564430507088	12.4275100283460436	5.2722372336559031	Si42
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9.7880893579575421	7.5873091750241413	5.2824369451308106	Si44
11.5442062640867817	4.6479872390049017	22.2647200308025255	Si45
2.6116693161109152	4.6805737368387330	5.2803964092856148	Si46
4.2359015040294565	7.7469430355047670	22.2298114279995573	Si47
-1.6838470360087001	12.2907850914007799	8.4325427148565364	Si48
1.1549698945784694	12.4070987724914783	19.0301406781729803	Si49
11.4890983452869690	4.8891326051042778	8.4265519013332728	Si50
9.9860665892649667	7.3393855977214608	19.0800432985525816	Si51
4.1067290911571721	7.4923864202538493	8.4340590722020305	Si52
2.7602216734374880	5.0100925951867721	19.0550322503423111	Si53
1.4575823261474143	12.4818993558102811	8.4968718219902009	Si54
-1.9746030643628938	12.4221700212181059	19.0013724346082995	Si55
9.7620321031818253	7.5150999298857375	8.5091791612358971	Si56
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4.3266399300057854	7.7402928526578956	19.0161695028466795	Si59
7.0336880595972122	4.0658172285965319	2.7495720720097094	Si60
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-0.1691554382823037	8.2220821701389806	2.7697780204104028	Si62
7.0037583371046548	3.9373715023922067	24.8091323682136426	Si63
7.0483668867738416	4.0632978956960830	6.4870265504854228	Si64
-0.1799660423367087	8.2258468436636960	20.9879212225268823	Si65
-0.1724137979940785	8.2319648658499727	6.5209101157059255	Si66
6.9764357383742306	4.0463006443021179	20.9900295045437062	Si67

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7.0502475004724934	4.0554478659812006	9.7156293851996747	Si68
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-0.1729996653971417	8.2183322724895955	9.7542598284687525	Si70
7.0366788200027530	4.0483769964766108	17.7586065264972817	Si71
7.0493852784552526	6.4236710580134488	22.9475907460105901	All
7.6293555142793341	4.4551731334726581	0.6089615672502422	H1
-0.1932479190225598	8.9702987269296415	0.6427318256768466	H2
-0.2666406855699455	8.9347811794689918	26.8780879634492571	H3
6.6011837758136291	4.3921753000629797	26.9669557938847859	H4
6.1978767018175285	8.7239116045292580	22.9857767825787818	H5
5.8032436659693323	10.8684710505391244	21.8904506513223645	H6
6.2858031376940469	10.6144160667402314	24.2608823762152177	H7
8.0345026842951270	10.0781676798719619	23.8719868057596294	H8
7.8646003639981510	11.2499443566468642	20.4970113253701065	H9
7.4430332206997036	9.5432850516413747	20.4040039550020182	H10
-5.6537688197178646	10.0646566295140900	21.4775060625846557	H11
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11.7281414888209756	0.8865110830940347	21.6678700950185998	H13
4.1724988663789242	11.8983082158883295	19.6952918074604035	H14
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7.7851753653600078	10.3297174259397941	21.0974645050451599	C1
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7.0484740903834089	10.3843561278275160	23.5128522541229188	C3
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-0.1498536670915582	2.4076592500807799	20.6754786046287862	H17
-6.0869416551717572	10.9850147687811095	21.0425085875477897	C1
7.2574280225134729	10.5159539801993560	21.8982052453088016	C2
7.3056107665478374	10.6532910940933316	23.3528248062145636	C3
13.2411808112382072	0.7846595215335646	21.6379491431537900	C4
5.3926842105932797	12.0325009672298577	21.4609170997722352	C5
5.2600634470709817	11.4910558106109217	20.1629019598282930	C6
5.8244479744795807	12.1485221149494187	19.0716783104101282	C7
13.7049380975928710	0.8652738132827816	19.2649081707979377	C8
-0.6378689159195637	1.4396715012052095	20.5451950518592099	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 for the alkylation of benzene with 1-dodecene.

H-MWW			
7.0511269792453612	4.2430713042060493	0.9107988091997012	O1
-0.0027996337905734	8.3426425484340481	0.9252122950255126	O2
5.7888269944769721	3.5776009877477821	3.0884051843247020	O3
1.2991199778209204	9.1868943119309137	24.0278942579153565	O4
8.4646824791010360	3.4439686457529373	3.0548313198835553	O5
-1.3482840956980606	9.2895692100277074	24.0480410264238849	O6
7.2577464218965551	5.8153550215405581	3.0869956075548957	O7
-0.0943833929769413	6.9103824998967838	24.0080999086065781	O8
1.1951135105584259	9.3664496222266180	3.1119529959325356	O9
5.9387892934369138	3.2004366241409272	24.0056691458721190	O10
-1.4473140520347831	9.0741422681952049	3.0742975355310551	O11
8.5685808243701853	3.6510988910626723	24.0659956927381273	O12
0.1348299629007714	6.9107885955026669	3.0965446804080865	O13
6.8348505790340273	5.6965556075253430	24.1876117440305620	O14
4.9518433211989930	1.3993879014452668	4.3707260591735633	O15
2.0398026889373453	11.3939295802954792	22.7206845364311505	O16
10.7776714524489989	3.7768814902915748	4.3351313438322601	O17
-3.6364848066561182	8.9502756311314293	22.7310256285147503	O18
5.7896108994655053	7.6296269120796367	4.3876639777474091	O19
1.4010407628921842	5.1538237790978769	22.6971959243988017	O20
2.3723871500796392	11.2958808712965677	4.5100927278024354	O21
4.5838794518099055	1.4122909061267281	22.5913593156697665	O22
-3.7262774458285270	9.0897785102433506	4.4544371965743492	O23
10.8530690885326351	3.6530866411738505	22.6979496188574323	O24
1.2244399561850781	4.9235394847462581	4.4966965118455251	O25
5.8488264480217076	7.9986913198091241	22.7362092872884602	O26
-1.2361346374276778	4.9077274937836890	22.6583013046153283	O27

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8.4230858949799021	7.7753945902719508	4.4533638977395436	O28
-2.4608677591822872	11.2911773799535524	22.7019824119207208	O29
9.5630431327373326	1.4338863826731241	4.4189280487224414	O30
3.5745314676184039	9.2547292279997500	22.6668190208976732	O31
3.5143324019003903	3.6096381579454517	4.4727554568534140	O32
8.5923662344872085	7.5642871636349920	22.7969136120844773	O33
-1.4056736030334940	5.1189160548663635	4.3153589463837960	O34
9.3184801467181586	1.5104872536676943	22.6776857862904571	O35
-2.2529394133653664	11.2811590289891086	4.3285965400513486	O36
3.7106316852011476	3.9057847820257665	22.7312305450296748	O37
3.5060470385455584	8.9165344757427327	4.3700790921008652	O38
5.8456408956990904	3.4919461581195006	5.7599227874270138	O39
1.2986797530658452	9.2056962642667379	21.3411078786141921	O40
8.5219338562586380	3.5059661347363744	5.7282134399245610	O41
-1.3642874091636870	9.2599764476294038	21.3698732932529616	O42
7.1711256087837238	5.8150349463022062	5.7612424949871208	O43
-0.0696281848468345	6.9110565690846837	21.3352890385557181	O44
1.2659716881167160	9.2311850877355486	5.7847095367338062	O45
5.9106489821775083	3.2875441631129174	21.3088216453493260	O46
-1.4069023868244446	9.1868820402701221	5.7490105488571501	O47
8.5448218228771751	3.7279872342524460	21.3822104728365261	O48
-0.0328151900038778	6.8936054746552671	5.7659636220027499	O49
6.8260106048718274	5.7907026298422073	21.2973224468939826	O50
7.2128367772246200	4.2521720178877169	7.8775710074469290	O51
-0.0671184299462055	8.4674242689395047	19.2124429732934026	O52
-0.0959404243819684	8.4367062639433321	7.8992185477363721	O53
7.1802178263826253	4.1958902268691878	19.1863661017711138	O54
5.5714264451625111	0.0624742030037174	6.5843012083759076	O55
8.6493008551163051	0.1681361747706613	20.4790174273661805	O56
-2.8234533875329948	4.9847437689681025	6.5610281869629956	O57
-4.4465832427367626	7.7153289825703357	20.5241454170514288	O58
4.3457930392024284	7.7752151443190138	6.6203538431027553	O59
2.8845885554832882	5.0838165223277958	20.4885616719551287	O60
8.9063699331713657	0.1870172590646109	6.6697076846379995	O61
5.3304457708123749	0.0291882804628962	20.4295225475323399	O62
-4.5316559510476537	7.8361077453670918	6.6601261361283424	O63
-2.7121873088858233	4.7785424509679766	20.4616901958239019	O64
2.7056107872137072	4.8123602969817805	6.6992399057020364	O65
4.4699542833745740	8.0635520460996997	20.4470121560431011	O66
7.2707108881750271	0.0953565510570665	4.5627722919343388	O67
6.9729612195875266	0.2385781135887961	22.5206496944778713	O68
-3.7186957451758804	6.4317456173969676	4.5416090675393130	O69
-3.4750028739110466	6.3114314787183572	22.5233973267510024	O70
3.5168136240761250	6.2632154415693151	4.6142193646505296	O71

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3.6540810322088895	6.5611399881106252	22.5279696330947772	O72
7.1970450204242313	0.1010195509736544	8.6979266182428301	O73
7.0170569001645005	0.1447652889924168	18.3749581745869577	O74
-3.6330150392304348	6.3778638096983507	8.6861904331288180	O75
-3.5410551753128767	6.2952682049945379	18.4430164727616699	O76
3.5617373818154636	6.3160839620981752	8.7134091841684036	O77
3.6287038920256380	6.5642691625415370	18.4140861668178175	O78
4.7871744536014322	1.2598398410511162	8.7788388164366875	O79
2.1659952099609363	11.4180416434979879	18.3106802525546186	O80
10.9411490260350064	3.7017158008912565	8.7358113530407469	O81
-3.6682161692663238	8.9532133152116700	18.3582097022186908	O82
5.7779715510055425	7.8103645671969923	8.8116648440143646	O83
1.3868281144992225	5.1199767360123509	18.3469839509539447	O84
2.3618513346881302	11.3927460786027357	8.8702787338563809	O85
4.6779308899588745	1.4385535580967035	18.2863866621500257	O86
-3.8652002422412206	9.0402864083657537	8.9096481269174586	O87
10.9280246545624671	3.6228264595353417	18.2262320540255196	O88
1.3440678227125131	4.8354016928623063	8.9555416394549372	O89
5.9258525336159318	7.9495649564406872	18.2598467940945355	O90
-1.2415074953321827	4.9490506239528411	18.2834860908842245	O91
8.4047790962833808	7.5418431500123528	8.8130044607054057	O92
-2.5021125429724478	11.3105781257020190	18.1888630255863859	O93
9.4493225062289259	1.5235639282111653	8.8718935110233623	O94
3.6221639578353839	9.2299528599266143	18.2611870855231793	O95
3.7018610394698075	3.6625705602787604	8.8527673101890230	O96
8.5299814100982871	7.5195240747234617	18.3652797623902302	O97
-1.2669471531110603	5.1482652868195782	8.6602600166731847	O98
9.2724151891311948	1.5704120993500492	18.3592851907329759	O99
-2.2383873042025080	11.1163593070362534	8.6783299115070243	O100
3.7523521083252813	3.9066034857948604	18.3222968637431336	O101
3.3950153750285921	8.9695976085690390	8.7483445130073285	O102
6.0559698352450315	3.2313999239236941	10.0360295315322272	O103
1.2556195061188777	9.2516247104291871	17.0450379709011095	O104
8.6390367282575937	3.7646631443189364	10.0642562582373039	O105
-1.3757752353814996	9.2034143195484788	17.0167826105163371	O106
6.8849468435510648	5.7360518514294041	10.0546662535272358	O107
-0.0173848388159934	6.9506260315594890	17.0233696967144645	O108
1.1139485172781489	9.3777289294135144	10.0700655290805035	O109
5.9755541513246984	3.3605434003797439	16.9695128565202715	O110
-1.4932077334696476	8.9916303514984168	10.0986191422472391	O111
8.5883816119936540	3.7423945567499914	16.9745618703062391	O112
0.1436830322121438	6.9245683359326069	10.0691046784719020	O113
6.9484053706399482	5.8111601132816100	17.0672242145792588	O114
3.9163851185047656	2.2071511269434358	11.0886688699864511	O115

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3.2126754119476386	10.6220638688462543	16.0204236067495600	O116
10.6683349682473114	2.4698384416065688	11.0557408440395282	O117
-3.5648812177178768	10.1813994557443106	16.0191816287458835	O118
7.1039586959485721	8.1123960883082376	11.0823087498259696	O119
0.1959225381005023	4.5388080191340023	16.0643965886519595	O120
3.3509437736975185	10.2512355972883569	11.0716574605486535	O121
3.6585714230566380	2.5323393565865833	16.0711237625343557	O122
-3.3542579050065462	10.5866525617944696	11.0220067484853050	O123
10.4472844215626601	2.1281120931330353	16.0616005164628390	O124
-0.2867131577032405	4.5438744880176740	11.0465076012345236	O125
7.4165548432180319	8.1919203823766491	16.0614425308517177	O126
2.3519958509628149	0.1488920403816746	11.7535816629850220	O127
12.0502044372248278	0.1198354583473828	15.3311904928886999	O128
-1.2192258213883349	2.1774563219934535	11.8088721410699016	O129
-6.0925218315359446	10.5801348546124654	15.2953503990077451	O130
5.9228249531465762	10.4238251704169631	11.6912544073206117	O131
1.1293768437261360	2.1583402838261607	15.3193872195633567	O132
11.6453762287868265	0.0934059421398786	11.6274092198988210	O133
2.7808946635242577	0.1154540108336954	15.4874241738001981	O134
-5.8959403302427429	10.2386141220874709	11.6529306043714094	O135
-1.4620734317438653	2.5814856214915012	15.4642561725836565	O136
1.3751229815934114	2.5852452201194565	11.6406352668404232	O137
5.7541311820384093	10.1574167139015650	15.5000765141982662	O138
3.1256448509483530	1.9489310955541559	13.5673794790203761	O139
4.0388130068260599	10.7865242064931053	13.5484671140372850	O140
11.2135106500830801	1.9139061300140687	13.5541786116054368	O141
-4.0923935929206046	10.8186607942978359	13.5347254753791262	O142
7.1506246446021020	8.9548617359662686	13.5574095066393827	O143
-0.0319221818675888	3.8013893253189490	13.5594286819875389	O144
-0.0444121069718895	8.3254485417636808	26.1963011634219036	O145
7.1947199292710771	3.9619085201942603	26.2535836691478330	O146
5.0278440639190833	3.0205980421205090	4.4152652742753995	Si1
2.0177576248655438	9.7788889764170168	22.6978703359576564	Si2
9.3292043162026683	3.0424773537086574	4.3765158652364615	Si3
-2.2037519184185479	9.6891873679023313	22.7166932914151225	Si4
7.1577444739926213	6.7552949338906156	4.4144394910349938	Si5
-0.0065248060929655	5.9692756884182883	22.6814945744713974	Si6
2.0838961553226349	9.6970437902753375	4.4379813110004251	Si7
5.0485074775570107	2.9758605451888096	22.6688243329608952	Si8
-2.2041228963712847	9.6587177991671282	4.3944018662958388	Si9
9.3050961307821325	3.1404469276016842	22.7125762053289542	Si10
-0.0216655039716560	5.9637720141231227	4.4119761408519294	Si11
4.6041178719068032	2.5987357121319539	9.6783950162217902	Si12
2.5653075571518258	10.1295066822684454	17.4171631717728062	Si13

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9.9243467200923661	2.8509541255749911	9.6718025235940761	Si14
-2.7787174525948570	9.9177573663225083	17.4094700458532365	Si15
7.0538235250572034	7.3080861112170785	9.6802571032602245	Si16
0.0693025643963670	5.3840094953182680	17.4376204017001548	Si17
2.5619748417102395	10.0006201137276776	9.6805848908417467	Si18
4.5171136061421029	2.7996661602067774	17.4174104895054960	Si19
-2.7450445591840298	9.9365971076196367	9.6702926320944247	Si20
9.8162352561524084	2.7687220760028373	17.4110164996998478	Si21
-0.0149953392119628	5.3576329486337722	9.6722135954722361	Si22
7.2098712287177662	7.3687459416405749	17.4440952205068882	Si23
2.6904604656999709	1.7163703283344909	12.0159626110130180	Si24
4.4640169311471922	11.0531987899053039	15.0957206909167940	Si25
11.6864560396917163	1.6657230277954282	12.0149419462781744	Si26
-4.5498378622796025	11.0491269534511893	15.0807430307157144	Si27
7.1743631974188133	9.4369767244272893	12.0019349847405543	Si28
-0.0397740158429454	3.2672753744324639	15.0986506619841983	Si29
4.4400633032306756	11.0139510011387944	11.9886555314131549	Si30
2.6726854193614971	1.6887484898778913	15.1093581218471957	Si31
-4.5512791075293517	11.0724707158031368	11.9931638594060477	Si32
11.6698895963157465	1.6859326809799886	15.1015119706997005	Si33
-0.0409882049773669	3.2760488239348229	12.0173707100232097	Si34
7.1689341443256778	9.4701001715012918	15.1018587306647056	Si35
5.6924719181102370	0.0845759384037610	4.9739857669609586	Si36
8.5415250872517561	0.2187326588399282	22.0887382531594803	Si37
-2.9017488932038162	5.0802698591475393	4.9505034193799196	Si38
-4.3803052816414390	7.6216774812734842	22.1450985492295693	Si39
4.2875083073380535	7.6430155541481337	5.0105419477673498	Si40
2.9085826670793913	5.1546588427598357	22.0978766440865435	Si41
8.8269270450968964	0.1281020340016939	5.0545967158888008	Si42
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2.9129563184387668	5.1681501943216643	18.8743690389345637	Si53
8.7764263572871517	0.1737079730648523	8.2827893959716334	Si54
5.4441498057669078	0.1116051934312817	18.8190432202630298	Si55
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7.1865733925838367	4.2664238574480846	6.2736464417469104	Si64
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7.1980295086161856	4.2463742168384648	9.5036970171839812	Si68
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6.1679946472153180	8.8807657830825200	23.0035374858163841	H5
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9.8188366241402889	2.7655029657663115	9.6857097184654943	Si14
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11.4560039225401979	4.9735650702146188	4.9909185682709181	Si38
9.9287720212833825	7.4503784621690441	22.0745892919780289	Si39
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7.0860724368695873	7.2246769906375574	17.3769362684233819	Si23
2.5975519928540911	1.5816095236941254	11.9888547787269566	Si24
4.3781492316977042	10.8761460263097423	15.0777110631240063	Si25
11.5802233972862076	1.5296235653550407	11.9780506106317262	Si26
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7.1215636555767254	9.3478351481190938	11.9704069769433978	Si28
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11.4603294049334927	4.9735590835141457	4.9988165828823945	Si38
9.9797499460645227	7.4563523847579916	22.0900565645093536	Si39
4.1919487656525352	7.5189972012924349	4.9777508884798145	Si40
2.8707979466189055	4.9994984422934392	22.0926813981756283	Si41
8.7696587533181969	0.0164332388416708	5.0657524850521147	Si42
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11.6435401004653194	4.7925297806291294	21.9816961051016300	Si45
2.6690290605928557	4.7698593888159113	5.0458616903579561	Si46
4.2743042447722939	7.8074996987541301	21.9979848880501443	Si47
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2.8541162604029955	4.9451781405679025	18.8731434015123369	Si53
8.7285616883474564	0.0792236491143913	8.2916492099694139	Si54
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11.6183012518449278	4.8449826782408989	18.7632912412500517	Si57
2.7444202258387764	4.7739992201372470	8.2714702339447257	Si58
4.2974324434030571	7.7556743165791078	18.7881786466887739	Si59
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7.0141650861511593	4.1740843594713288	20.7551137773937313	Si67
7.0948975832742951	4.1560591461425940	9.4936561739764294	Si68
-0.1384475961489473	8.2972072602419082	17.5443229010935156	Si69
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7.0150108322205273	6.5097884802668435	22.7533278768085090	All
7.6894756036492291	4.5403772287599509	0.3931587981710987	H1
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6.4403224913831068	4.2583866531888548	26.7258256372172980	H4
6.5844604155303426	10.1394499223991801	21.5050379723741010	H5
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5.7602909706608552	8.3980172138842608	25.3318268345287443	H7
4.5342456425420545	9.4741367619212262	24.6392864481131539	H8
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7.2194398101025197	10.4389276044057535	25.7956916253738626	H10
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6.8433948111564007	11.6846828349237661	28.1634922085181074	H13
12.6992726696942810	0.0927014133967271	27.4973454508809958	H14
5.3107658649577631	10.5576096144466156	29.7989369744280630	H15
3.9293505835235898	11.4052775490390470	29.1077814062652429	H16
12.1242367540339178	1.1065583933262593	29.8253263630586787	H17
13.5120029611744350	0.2673746655343155	30.5225224592321176	H18
4.7670833380509450	11.5176481480781003	32.0795772207466356	H19
3.3710900845123728	12.3248941081463279	31.3681201031821253	H20
12.8746309038037055	1.2473336765539353	32.8532291657547475	H21
11.4759187152272517	2.0504693814833637	32.1385402142041912	H22
4.1361711569230071	12.4420569997139694	34.3715955552407308	H23
9.9519028630985691	0.7318861557460684	33.6516492800626708	H24
10.5745703890650304	1.8428409596086297	35.8166702166597517	H25
10.7887011589625263	2.9785408175308228	34.4663403117567384	H26
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6.8492997428932076	11.2171982013934599	22.8833978727987493	H28
12.2020093070886073	2.1851916978421015	35.1909163610806672	H29
6.2066373816041285	10.4107356621849423	22.5008549847987709	C1
6.3100897776304858	9.2337980498804253	23.4469437991629377	C2
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6.1244168193513415	10.5052441863623542	25.6688686050557102	C4

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5.4328796030244133	10.4745760962492955	27.0365661630713241	C5
5.7550759583110311	11.6366534659682550	27.9796499288411304	C6
5.0112540426671099	11.5044726152941763	29.3129890734239673	C7
12.4356223366605185	0.1574033825868814	30.2977679090739720	C8
4.4427388353894077	12.4612840191771816	31.6034660636625802	C9
11.8062065369699702	1.1057334166184314	32.6076805349642456	C10
11.0173067953860784	0.8831084654042199	33.9004251335009315	C11
11.1510082292328221	2.0323766309946785	34.8986675654083243	C12
Co-adsorption of dodecoxy and benzene			
7.0939543555700979	3.9834178251760792	0.9547573546523378	O1
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1.1588687423473552	9.0382231483117543	24.0056961845608683	O4
8.4983123537720093	3.1946359442009964	3.1094856457753877	O5
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5.9842141909952247	2.8914266369472745	24.0361603466955813	O10
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6.8216001870154326	5.4337362135174203	24.1636169932065172	O14
4.9847505112020398	1.1348161985539811	4.4161102749612775	O15
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5.7971697580304395	7.3746387160873157	4.4081460611437402	O19
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3.4193049820909955	8.8466566145452887	22.6685230396337438	O31
3.5395307684394610	3.3453560717863757	4.4956050234658527	O32
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1.1639823347171969	9.1334152686514916	21.3162782093012240	O40
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3.4429766795300187	8.8336535957053215	18.3204304347868820	O95
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8.6546447279361640	3.5617045368666327	10.0934051995947289	O105
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1.1343253179316157	9.1731393587870915	10.1257134324652363	O109
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3.2537484736694067	10.1769914711325669	16.0210391188848007	O116
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5.9911265161265677	10.2354477930585102	11.7752009725535203	O131
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6.8990552274178309	5.5565823976480626	17.1374566867858071	O114
3.8796930120700903	2.0426309041355979	11.1323075481685905	O115

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3.2606104768607080	10.1354212186776227	15.9898623186712179	O116
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13.1501449116557048	1.9635924560226503	11.7788605003477862	O129
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-0.1102643576113442	3.5354563338546754	13.5772600628059230	O144
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2.0548698718338505	9.4664334550099145	22.7305467955254770	Si2
9.3397980960324958	2.8192364989731962	4.4359404959617921	Si3
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4.5320619126749673	2.4852929994759561	17.4151842225775084	Si19
-2.7025635543619515	9.7046260268253732	9.7154842939928834	Si20
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7.2335897022049904	9.2127976980598376	12.0401706971370537	Si28
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1.4540911090142448	12.4156794573219695	22.0770708298885410	Si37
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10.0214321874569716	7.4712014369856359	22.1600865814019841	Si39
4.2946135049432801	7.4052442205868676	5.0220321696893615	Si40
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4.3395954779769799	7.5964810950368911	22.0909300781557718	Si47
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4.2518576675584185	7.4914461267544503	8.2424334475997600	Si52
2.8701781431247158	4.7637857475340253	18.9203608691292899	Si53
1.5913024024735947	12.4660877550320546	8.3314220645185273	Si54
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7.1784104035876704	4.0461647934191527	6.3084011242324269	Si64
-0.0385234394938170	8.1756387739345548	20.8362429956341302	Si65
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7.1650542687071219	4.0175904973240719	20.8271652355137995	Si67
7.1824072590670891	4.0426515283418283	9.5365719466534333	Si68
-0.0405019877702983	8.1903188789714783	17.6090676875837495	Si69
-0.0284814437203043	8.2138439690801430	9.5781856102734082	Si70
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7.1499927498630971	6.4879914543866395	22.7846728186709235	All
7.8002074504477044	4.4297680919365199	0.4371594702588337	H1
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5.9932813133947853	11.8506326980868320	21.4755095050272793	H5
6.9299615536311725	9.7413034484392487	22.3987548820436224	H6
7.4915972088752394	9.5637770291377890	24.7377499465952440	H7
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5.3126911137751138	11.7145717765750685	25.2650560492764633	H9
7.0162829387849603	11.8918722035736941	25.6850303389893995	H10
6.7866027512362592	9.8156984980199358	27.1796956110948713	H11
5.0555394791172343	9.8287811605911575	26.8399180036401148	H12
6.6460477223518852	12.1268743432416688	28.1254490591006068	H13
4.9214106117421483	12.1905814185281116	27.7677727353586938	H14
6.2213971080182269	10.1615775134437580	29.6801903314486921	H15
4.4920512481031496	10.3164490242044344	29.3648714599646681	H16
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13.5008582291446544	0.0045816850345510	30.5752281959448275	H18
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4.0374374351417321	10.8457843148579602	31.8626161189355415	H20
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3.5964739924813562	11.4099927071929717	34.3259761342180099	H24
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4.7457550107939666	11.0538525364216191	22.4432690174033169	H27
5.5924261393303976	12.4569343359627780	23.1284140067801367	H28
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0.9927591498201946	2.1771410270475262	23.0817622490290688	H33
1.4622237653047894	0.1262169835913113	24.4242474668811553	H34
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6.5946536751146567	10.1517035040379220	24.4824126057211480	C3
6.2088808429568259	11.1490731264796832	25.5672632632980203	C4
5.9430442764887266	10.4811239010980657	26.9222852307459242	C5
5.7385808510041656	11.5007204785904626	28.0452719167683355	C6
5.4344187492296481	10.8913097293545000	29.4165827284789820	C7
5.3308778186211372	11.9471491322647534	30.5211311068870046	C8
4.9992627916144263	11.3885297374081613	31.9064207779025999	C9
4.9220209868910079	12.4686881055510828	32.9882071680376470	C10
4.5654134157718280	11.9370878735197472	34.3775994534779272	C11
11.7129386572601977	0.5339602491394912	35.4402254343625032	C12
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1.1174353038104741	1.1351576289897582	21.1943771115817654	C15
1.1375643864688638	1.2142024793846442	22.5909747741679112	C16
1.3872529733789560	0.0669810050640233	23.3379977240804237	C17
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Protonated dodecylbenzene adsorption			
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1.3738526842434506	8.8614693781454275	24.0544040426146495	O4
8.4653075839297021	3.2174970170947663	3.0988738964393212	O5
-1.2529326397980487	9.1121552566540842	24.0040430167928598	O6
7.2921535903479091	5.6032414885692585	3.1099619298488714	O7
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1.2005612654391760	9.1365092798029544	3.1240065231996565	O9
5.9091476938740453	3.0671572694926721	24.0510024617157043	O10
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0.1142141504890795	6.6861835509246328	3.1260369212779326	O13
7.0959050169076381	5.4830760319532450	24.1668115293589167	O14
4.9726257127184113	1.1913304148852557	4.3742670342989491	O15
2.0553750605926009	11.1017025980541408	22.7995471309320230	O16
10.7696827663260812	3.5848866513357276	4.3927626247584435	O17
-3.5843253260078676	8.8206825692203701	22.7645921099120621	O18
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4.6909458527098282	1.2423901381164331	22.5648704458113762	O22
-3.7221012325605143	8.8963521320692003	4.5130512487570948	O23
10.8018985691439919	3.4850904387980353	22.6578235746759056	O24
1.2197875349177716	4.6993578766115407	4.5108095720210715	O25
5.8115471999693069	7.6073427581623880	22.7197327302484524	O26
-1.3221090693707245	4.7109857447143160	22.6393392692060829	O27
8.4268389793371234	7.5745249586616472	4.4932617210301542	O28
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9.5842801928893593	1.2278833541889229	4.4711325232445196	O30
3.6063251142464230	8.9818169855581402	22.6365661566214307	O31
3.5103947374211568	3.3908187873679245	4.4744852256001906	O32
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5.8343482933944646	3.2940343303250343	5.7646189030452453	O39
1.2832949101241145	8.9925902990170936	21.3654697966461526	O40
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7.1732871019344611	5.6087345479056703	5.7816860655541795	O43
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5.8287781424461400	3.2955941233867230	21.3528473034698756	O46
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8.4927462008070105	3.2242026170204268	21.3397723721073653	O48
0.0202595383083484	6.6909428898081709	5.8002352353612689	O49
7.2249029523611732	5.5906003269176008	21.2949989443810956	O50
7.1666044500525752	4.0468901483422046	7.8986729852981084	O51
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7.1598122100371206	3.9316342525252144	19.2065630041121196	O54
-1.6600544617931128	12.4092612411968588	6.6278591218268073	O55
1.6375776192600329	12.2954431892097915	20.4673801827117430	O56
11.5762802265401596	4.7688459968911809	6.6352524956725834	O57
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4.3708471877040358	7.5403071527967809	6.6202669015807905	O59
2.7497621936483050	4.6861728968832921	20.5290748433238157	O60
1.7463255716121724	12.4200434515022451	6.7026094282695921	O61
-1.8377602570022198	12.3842973142395323	20.3858760157615428	O62
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7.0946224075448550	0.0960611048932485	22.4254699655751892	O68
10.7207647573608043	6.2381025172734432	4.6085145975393926	O69
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3.5115741204436004	6.0445759042880898	4.6163869190189111	O71
3.4575917417402247	6.3309239558846553	22.5010322137194763	O72
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4.8012506125194561	1.0333827532159576	8.8702018932543467	O79
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6.7595591051969643	5.6357879588531237	21.2340750052010279	O50
7.1105776754277255	4.1592255780040928	7.7200215608764591	O51
0.0671222217122986	8.3122794516170870	19.0179326925433223	O52
-0.0916309157149771	8.3381734569470485	7.7523805925682838	O53
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9.7814886474955394	7.7669652572757535	20.1663851239614225	O58
4.2539075624028371	7.7120989648651026	6.4558078376100898	O59
2.7726126130423503	4.8686119003659467	20.2661602315455838	O60
8.8922794166648718	0.0645626846940177	6.5264228614626179	O61
-1.8156117642040988	12.4596012072703353	20.3591594372730924	O62
9.7789181054428749	7.7279696650891907	6.5153877163031853	O63
-2.8012674889897609	4.8791566268147673	20.2983166711121612	O64
2.6902515381599374	4.6733772085515044	6.5286005651857897	O65
4.2695171597176751	7.7664107414295112	20.4805625443915069	O66
0.0170307456780963	12.4959414423121249	4.4332129169644388	O67
7.2145906033811222	0.1596049648630850	22.2849938184692462	O68
10.6691377692127674	6.3293892082762850	4.4235518053057632	O69
-3.7009458950609626	6.4342094278504307	22.2555981961065008	O70
3.4782586139943850	6.1513568678253288	4.4574681910519640	O71
3.5172750193033901	6.1427785533844226	22.4618419936113085	O72
7.1700892541742238	0.0116820772637487	8.5458107997571915	O73
7.0613734080240791	0.0133889899175264	18.2732640474745232	O74
10.7242078962714515	6.2913905947051356	8.5395432867577679	O75
10.7439406686728134	6.2633428201097026	18.1934641188853945	O76
3.5016861991212740	6.2205722663963581	8.5318493013939172	O77
3.6097334573791038	6.4298393633256605	18.2861328312942035	O78
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2.2295210662455274	11.3677991824518543	17.8785856896619819	O80
10.9321448367413208	3.6256317902577915	8.6388593297937959	O81
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1.3030874398403727	5.1416183087810667	18.0916177916363168	O84
2.3514907369474667	11.3390050943109575	8.7691948885961075	O85
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-3.9161422416385170	8.9530132234335777	8.7294891218331827	O87
10.8565366938265981	3.5954293874589083	18.1402769326673940	O88
1.2991596615138929	4.7223294707514691	8.7679857567745234	O89
5.8821584333174339	7.8382516686720134	18.3850895622472557	O90
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3.5457254691471665	9.1135797683551178	18.3772093988695175	O95
3.6719310450608735	3.5661038037933301	8.7000248952721631	O96
8.4799815923101995	7.6373792416194544	17.8912544323088696	O97
-1.3116727382722229	5.1274151845864919	8.5462973263007882	O98
9.2683703536298214	1.4909418005253727	18.1180959926549754	O99

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1.3806832004826086	9.0685796145658788	16.8366832162382565	O104
8.5842065287938940	3.7160026809908095	9.8831085765698514	O105
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5.8834294403191638	3.3239892945675056	16.7596605443843991	O110
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6.8035760617129197	5.7812059403181033	16.9589026058432530	O114
3.8406235484164477	2.1166451862942353	10.9326635798360314	O115
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10.5487535091550839	2.3710715444904285	10.9306408385479905	O117
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2.3058616413205812	0.0206787502445558	11.5535007498525353	O127
11.5986512997400641	0.0755317537137738	15.3636634490426420	O128
13.1301193267572636	2.1013094337789346	11.5694920011180287	O129
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1.1715673800180901	2.2439378080867569	15.1665607569504690	O132
11.5740264029828879	0.0048822198015148	11.4538667334635775	O133
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12.9830609536892769	2.3260843700102884	15.3129749202370480	O136
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4.9953877180466417	2.8838571536549669	4.2378732676815352	Si1
1.8986011108229386	9.6696537779845428	22.6088602521851705	Si2
9.2997185138396041	2.9618964668818242	4.2552784451520038	Si3
-2.2657156011887007	9.5104774779535859	22.4232470675635760	Si4
7.0809813727301547	6.6486488961469687	4.2483017003267802	Si5
-0.0449109146216058	5.8627739988868450	22.5029391677586119	Si6
2.0207254027079093	9.6163573918790348	4.2651727739401872	Si7
4.9678953089263418	2.8254664648602006	22.5510785697974363	Si8
-2.2591363627158083	9.5208659672859355	4.2691522322578050	Si9
9.2589211584938482	2.9985675746210281	22.4468992064863926	Si10
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4.5571297767873391	2.4936531746382609	9.5337609299503878	Si12
2.6797140871438598	9.9359570442459972	17.2698550743424093	Si13
9.8643387020627298	2.7820916967419427	9.5246507701252465	Si14
-2.6877539271489761	9.9633841480419161	17.2313448481752545	Si15
6.9635203773660370	7.2191625319980739	9.5312748736253887	Si16
-0.0517296670365281	5.3756476738767258	17.2256276027139954	Si17
2.5174786171572459	9.9255292198055045	9.5547570399278516	Si18
4.4809690102987147	2.6619389273231411	17.2544879431734159	Si19
-2.7776649437379595	9.8126225483519924	9.5048642251212740	Si20
9.7523041826536385	2.7874431751927462	17.2682698358432809	Si21
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7.0036896575917140	7.3523561844971077	17.2991599476385609	Si23
2.6363645473497779	1.5817494967303938	11.8629012451197529	Si24
4.4967692366101231	11.0156834155180441	14.9505627971242738	Si25
11.6169039409200323	1.5776562091531696	11.8440884205260950	Si26
-4.5363980392350367	10.8766822013625450	14.9153419459037782	Si27
7.1235801788510944	9.3450142497743780	11.8396950290965730	Si28
-0.1273550970868904	3.1820072035801550	14.9369972821690595	Si29
4.3900289021880914	10.9353197044991166	11.8572806064329743	Si30
2.5998664251073089	1.5218557069032883	14.9359397475369740	Si31
-4.6076768336857787	10.9428942299899248	11.7959763091126710	Si32
11.5497189351638987	1.6480619235104954	14.9728332726209317	Si33
-0.1146616211676565	3.1712316688254871	11.8541809404487317	Si34
7.1526968138089124	9.4027674144592766	14.9381011594941171	Si35
-1.5625317017162743	12.4638454657389932	4.8368552787208010	Si36
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11.5033645317970983	4.9894358935627405	4.8334311120462328	Si38
9.8479995025272995	7.7396814846166269	21.7908789018187754	Si39
4.2194457984367615	7.5490472313662398	4.8476056129475458	Si40
2.7374287356785381	4.8088264546180479	21.8810463501338894	Si41

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11.4925401791177659	5.0401839793673631	21.9014315196424114	Si45
2.7161666303477712	4.7834170507498373	4.9144166110794556	Si46
4.0932761654318419	7.5902689512596639	22.0592619449377096	Si47
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8.6566558244595253	0.0777466874764267	18.6159978472395160	Si49
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9.9527186779007408	7.6424344017537233	18.5679899344522887	Si51
4.1928989461734787	7.6253451876444736	8.0689528434819877	Si52
2.8172917998006515	5.0490771765309219	18.6552609664645317	Si53
8.7509151225371475	0.0926601799600885	8.1389229483609640	Si54
5.4964585017854679	0.0595741894743345	18.7497400243833461	Si55
9.8444588396311197	7.6046815932062284	8.1278770429969498	Si56
11.5722187843478341	4.9435650858147637	18.6843719837169893	Si57
2.7920532581250219	4.8041986837555459	8.1376500490988022	Si58
4.3297015338786924	7.7765175285988972	18.8532940866907133	Si59
7.1152280232275373	4.1617861734722839	2.3755325410540227	Si60
-0.1928738641265966	8.3020497240876150	24.3753977345195594	Si61
-0.0890504046685408	8.3290116229517182	2.4014277989279647	Si62
7.1149081343999425	4.0622305956405498	24.4579241814131905	Si63
7.1287054163381001	4.1629203787324869	6.1163373285976235	Si64
-0.0780208256031516	8.3400039434714710	20.6143911173115093	Si65
-0.0913424321663650	8.3311614236080445	6.1479115618165334	Si66
6.9936191098761205	4.1498958443571583	20.6636768903582713	Si67
7.1231252583680229	4.1598052703757347	9.3459752766438253	Si68
0.0136921204002523	8.4075067497429554	17.3927401006162654	Si69
-0.1002620686407489	8.3388033311615377	9.3794668149133571	Si70
7.0372701332583123	4.2498906667070724	17.4362444471061195	Si71
7.1274117980395069	6.5651508643634537	22.6474788050221782	All
7.7523625664254325	4.5546816959217109	0.2485661199291101	H1
-0.1067988979628156	9.0529593072171792	0.2662442733518752	H2
-0.8179818840951461	7.7623338493905685	26.4734752831222302	H3
7.1000863973425385	3.0163332509489837	26.4533748745605557	H4
4.6515614756092205	10.9824394353588648	20.2245426034102280	H5
12.5528527590335983	0.1420547327043195	22.0360139845515555	H6
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7.8802282975879336	10.9353550910339568	22.1315778399004195	H8
6.1367838004548423	10.1454690131100822	23.7869825192319979	H9
5.8500670450756544	11.7978079069827650	24.2826743806033178	H10
-6.1697558389173386	11.9699207617857599	25.0248024413520938	H11
-5.9259830455373672	10.2769410708506630	24.6023374437620745	H12
6.4157208967388213	11.2530709942143297	26.6390612788877412	H13

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6.8541818282096720	9.5702186701294991	26.3308835615423789	H14
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-5.2294403766362407	10.0517535099412125	27.1178169388175121	H16
7.5870556590789082	9.3213644181735802	28.8768902178350402	H17
7.0334249878943655	10.9841640473424302	29.0869678012928681	H18
-5.1076911543892551	11.6805013216968128	29.8112020724333604	H19
-4.5170566114839419	10.0360726077073448	29.5787876867909425	H20
7.7129658597156929	10.8339897002524790	31.5702893579539712	H21
8.3557818170341918	9.2052452408800338	31.3556630481393626	H22
-4.4563965296771819	11.6532153907728553	32.2631779908671987	H23
-3.7850550797732985	10.0425671410597328	32.0180036907485572	H24
-4.2718924100485962	10.4411286131795258	34.4524449707712961	H25
9.1422508596347534	9.1250777445435407	33.8304568418283012	H26
6.0649306238455818	9.9935865510039203	20.6617123620878722	H27
4.7750495149732251	10.3167509706058542	21.8516123902672526	H28
-5.9824013489097920	10.7423987145734383	34.0746575208109590	H29
6.9724640433980714	11.1735636387438522	19.0262526432595251	H30
5.8650811118514614	8.6242720830662414	23.0696296173905218	H31
-0.6823883279388187	2.1457519580138822	21.5478575360095306	H32
0.3947550268410183	3.5368148480957959	19.8135377800249017	H33
1.1859445846077330	2.4964926063583937	17.6879086237987622	H34
0.8287751659973875	0.0691639144153998	17.2908843544217810	H35
5.3581016619565300	10.7515395793162050	21.0346616036663043	C1
6.0800218500722112	11.9958167225082928	21.5329128375316223	C2
7.1671365438576338	11.6543002938033364	22.5734955076764798	C3
6.6449465331790920	11.1274421005446769	23.9081069342967574	C4
7.7472454405442450	10.9954596857389966	24.9558657385275922	C5
7.2582916574561800	10.5988883171514985	26.3486801113761047	C6
-6.0725631919578094	10.7071516591007754	27.4021194319819159	C7
7.9180015395654664	10.3743614744785653	28.8266282842963584	C8
-5.4136766179797782	10.6190500921608084	29.8587763589754722	C9
-5.8070648271439884	10.2752558040789754	31.2949846061234958	C10
-4.7051131188414281	10.5782531409748444	32.3124647013318693	C11
-5.0803534377304187	10.2028304079986274	33.7451481645016500	C12
7.1166156382213392	12.2402248245606415	19.2112675898736747	C13
13.9055315567782571	0.3114397162838851	20.4172416251893019	C14
-0.3403366451016138	1.6857713865565371	20.6159723090761489	C15
0.2713934289947753	2.4687235723394809	19.6437073780248568	C16
0.7039604348038691	1.8873414250802172	18.4498159118511147	C17
0.5105150202268569	0.5238749429611129	18.2303479317644914	C18
Co-adsorption of 1-dodecene and benzene			
7.1359752138800800	3.9618247829791424	1.0069189426899658	O1
0.0308477091463386	8.0754600583052039	1.0234505753813650	O2
5.8545490168081145	3.2849025432051944	3.1666965012007418	O3

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1.1283963068119505	9.1599369681528398	24.0713050266317623	O4
8.5343535072016650	3.1875145477821660	3.1711795220013870	O5
-1.4774918121589082	8.6893031197388151	24.1071898234597057	O6
7.3009026822991991	5.5433800487388929	3.1790008137961334	O7
0.2260980959822829	6.6304638083612817	24.0972678013204842	O8
1.2195232121336010	9.1212830195961931	3.2018818354768381	O9
5.9461304166200399	3.0306475151029839	24.1501920458564179	O10
-1.4143672778286507	8.7558028787413669	3.1912091699271410	O11
8.5973182768154430	3.2821446928780706	24.1143950587252078	O12
0.2204603523724198	6.6351741389696395	3.1887541414775802	O13
7.0680363016176599	5.4669471887565697	24.3265268559148566	O14
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6.6184276251820719	9.0642197808985348	24.7927159005740378	H8
5.0062305355599515	11.0227823315440254	25.2268987183475701	H9
6.3995447658557785	12.0998185329011854	25.3647353851113344	H10
7.2734334895602455	10.6412659402343710	27.2731450110032547	H11
5.8237878429464027	9.6451064943461002	27.1349906001105623	H12
13.1131864261903601	0.1376243019523442	27.8461116202687151	H13
4.4121193192469095	11.7110407738857472	27.6304433400910767	H14
6.5700512567381999	11.0298454677595892	29.7157738887898297	H15
5.0149497271850514	10.2183027173542929	29.5300519218934596	H16
3.8480115774866768	12.4240141122358168	30.0423663665172391	H17
12.6423399663387563	0.6710159610121958	30.2888690093533448	H18
5.8833016566661422	11.4961393705434727	32.1541092161406397	H19
4.2568381088354643	10.8499759434289142	31.9341388000298920	H20
12.1581475901425389	1.2451308617086083	32.7172793605756098	H21
10.5210082183206577	0.6467422535352233	32.4521999998567665	H22
5.2360980202477112	12.0572307044849723	34.5800015470363036	H23
3.5796815530142716	11.5100252208679361	34.3281448666185511	H24
10.8964594141079374	0.6414283588692631	36.2319612374326923	H25
9.9433293880275677	1.3321037443827513	34.9008697748751118	H26
4.8615896567451777	11.1883641383456123	22.9838413741970697	H27
6.2782166668084338	11.8831334992005822	22.1771467457440004	H28
11.6142796309522929	1.8694525294200697	35.1673786134577853	H29
-5.0885402608641366	10.7121187904390247	20.3150098089034934	H30
-6.5233529070445391	12.1953893557184525	18.9099727492948837	H31
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0.1059665899981312	2.3205126033020429	22.2899683681116692	H33
1.5787983235090954	0.8647215826592363	23.6757244420798045	H34
-4.6578182115841109	11.2931594132428774	22.6907249040680803	H35
5.7597146002849398	10.9153047047552061	22.4177439893988861	C1
6.7437052937211126	10.1683059164185181	23.1617279669146718	C2
6.8852777205045790	10.1379761976007270	24.6088317527585652	C3
6.0699859551529638	11.0572804276278678	25.5144901455653468	C4
6.2042416439432175	10.6733736844409961	26.9955460619444381	C5
5.4675993458950556	11.6238447900427886	27.9448390198764187	C6

5.5189376143249405	11.1953710424152391	29.4167220085223420	C7
4.8818496113114680	12.2119471480583393	30.3703997140392623	C8
4.8604990103419130	11.7709258376667076	31.8374374389720991	C9
11.5284762575367346	0.3390521528826110	32.7879620843512285	C10
4.2371519230989731	12.3939165457730720	34.2507985535605428	C11
10.9501083380762534	0.9907148404536422	35.1899661925886846	C12
-5.5472100399652557	11.6040315560406917	20.7480193755382096	C13
0.8655549346669098	-0.0666507591268338	19.9623290700712914	C14
0.2889471369355063	1.0803047056428954	20.5241022908352910	C15
0.5337123011869300	1.4106940893567819	21.8651332797591671	C16
1.3545851321917133	0.5904186937527237	22.6431144296193665	C17
-5.3091520280717281	11.9294637820358655	22.0917934077088738	C18
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
1-dodecene			
15.9245796150000984	23.6550311900000310	17.3806152449999018	C1
17.0721950700000491	23.0067253150000184	17.6036014699999299	C2
17.4409904549999339	21.6716842650000885	17.0320854199998806	C3
17.7337646499999124	20.6149635299999190	18.1095962599999183	C4
18.1454696499999812	19.2602901400000448	17.5323390900000931	C5
18.5236091599999497	18.2258300700000575	18.5946235650000347	C6
18.9664993350000088	16.8847007699999772	18.0067996850000611	C7
19.4626960850000330	15.8788700000000205	19.0475597550000586	C8
19.8872108399999448	14.5407848250000171	18.4403801049998961	C9
20.4403152449999581	13.5393991599999097	19.4547844049999696	C10
20.8796005250000505	12.2152452449999060	18.8260440900000958	C11
21.4327392650000448	11.2166595450000628	19.8406944399998864	C12
17.8170299649999819	23.4636154200000391	18.2679004549999391	H1
18.3424835300001021	21.7826347199999049	16.3994254900001124	H2
16.6350803499999991	21.3171348599998822	16.3671550699999848	H3
16.8409137750000646	20.4942150000000112	18.7475051749999011	H4
18.5337962949999024	20.9883098599999585	18.7740688450001159	H5
19.0019893700000608	19.4024944400000621	16.8481254549999093	H6



17.3249301749999809	18.8629360150000025	16.9076252099999991	H7
19.3362045449999442	18.6344203849999346	19.2230491599999809	H8
17.6685237750000468	18.0657043350000279	19.2761802799999771	H9
19.7699604199999968	17.0609951050000994	17.2679157349999848	H10
18.1291599299999007	16.4410400350000749	17.4372787400000782	H11
18.6733741600000869	15.7083148950000133	19.8023357349999785	H12
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20.6499652799999822	14.7240447900000149	17.6611385299998958	H14
19.0248451400001173	14.0892505599999751	17.9164295100000359	H15
21.2981300350000069	13.9920196499999268	19.9859790900001144	H16
19.6789264699998867	13.3395843349999410	20.2312603150000569	H17
21.6421089150001222	12.4181051399999021	18.0535583550000212	H18
20.0236740199999375	11.7655305950000866	18.2924346850001029	H19
21.7538299649999090	10.2816343349999446	19.3580093350000837	H20
20.6757946149999938	10.9583597200000309	20.5974998600001058	H21
15.1530399299999612	23.2375145100000680	16.7274455949999670	H22
15.7140197899999023	24.6237583200000998	17.8367004550000985	H23
22.3023510150000703	11.6326351050000909	20.3729400700000696	H24

Dodecylbenzene

16.5688796570304291	14.2891095590263486	8.8098622024054443	H1
16.6585693788390792	13.0954534799040818	11.0220742179623681	H2
14.9300263640409749	13.6134797045932938	12.7539697751358734	H3
14.5165965026900405	15.0985541616921441	11.9037317013352446	H4
16.8184491558747347	16.0024482431549302	12.3199332182228130	H5
17.3082115805278463	14.4642798758483604	13.0357380855877469	H6
15.5576922253152876	14.7476320422669112	14.8236318757955470	H7
15.0802202974948703	16.2887135541040244	14.1181112334347674	H8
16.0843939894579755	15.7937541232498528	17.0023961395167049	H9
16.5498523470954346	16.7573267315637757	19.2696048721498805	H10
15.4938418739628112	15.5160241936385450	9.5157951143292188	H11
17.1554736146117293	15.3404200025335715	10.1179394503458209	H12
13.3912709844214834	14.4773895031743489	9.6343695206324309	H13
15.7237958858238027	11.0305376987496402	10.7470939833582211	H14
13.8988616953004964	9.5428979124191393	9.9699000043719330	H15
11.8018807879368630	10.5208603944194667	9.0286289339759715	H16
11.5646819110858914	12.9975822256009259	8.8756804429740139	H17
17.8789301548723891	15.6784426046373433	15.2396972487133890	H18
17.3503886001814784	17.2359375053025019	14.6001683453719320	H19
15.5700182298850951	17.3599811964488921	16.3805661322182274	H20
17.8080940786283293	18.3399102045123072	16.9519473296941854	H21
15.9956186957540893	18.3330568307494204	18.7072983313845604	H22
18.2085009784726459	19.3455092687650101	19.3188371172984859	H23
17.0014254447617787	17.6653800690763170	21.5925067139043492	H24
16.4042869427013258	19.2416280712307426	21.0770586814638428	H25

17.8915125498509084	19.4638649726834494	23.0992333891303296	H26
18.6181412228581493	20.2954022924099178	21.7071486746461488	H27
19.2292476890185036	18.7063283924140897	22.2088019521912337	H28
18.3619941172334258	16.7643681283644668	17.5239273130064461	H29
18.7987282891206817	17.7674662087495605	19.8397533118668434	H30
16.2816365494922692	14.7824886577389414	9.7501689091765638	C1
15.8027576243314858	13.7542496376403260	10.7853429635698763	C2
15.3523853368150007	14.4059258260825960	12.1117575768573715	C3
16.4435544901089372	15.1393988427007944	12.8963145434260174	C4
15.9463426258377332	15.6172621806026228	14.2629568608469803	C5
13.5135329049794510	13.3942468547245888	9.7132607231809001	C6
14.6963097231099589	12.8609647922155705	10.2499963487462225	C7
14.8109292154921626	11.4658357119441234	10.3307769649489174	C8
13.7825408979052586	10.6264008976670752	9.8953756411533451	C9
12.6098297662819565	11.1718945032100940	9.3696348535932366	C10
12.4801934569651092	12.5605987006278070	9.2804482416129623	C11
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16.4546468866653086	16.7085183700633308	16.5036391153692463	C13
17.4635678820613442	17.3998467234191168	17.4209402060305756	C14
16.8970463515262246	17.7012158073797536	18.8102283841200872	C15
17.8847079826326976	18.3837614016363666	19.7567139692387812	C16
17.3198451070088275	18.6293942399774188	21.1574249106638028	C17
18.3147227063164557	19.3102925225018183	22.0956214051056250	C18

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